



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:27 PM UTC

PDB ID : 2J8S / pdb_00002j8s
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

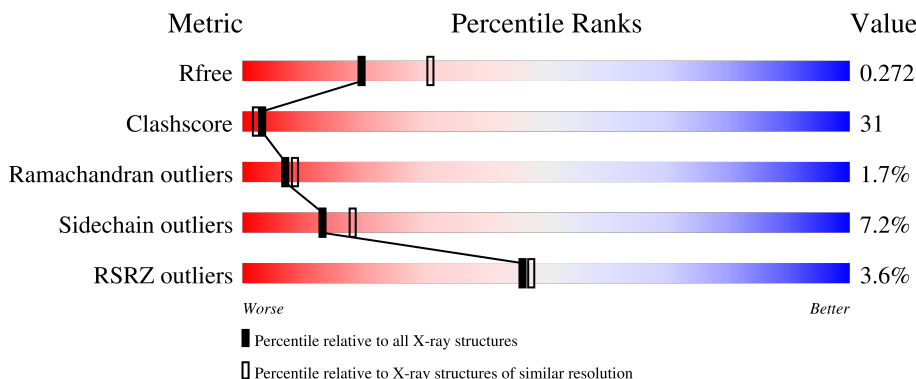
1 Overall quality at a glance

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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	1055	
1	C	1055	
2	D	169	
2	E	169	

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	-
3	LMT	A	3048	-	-	X	-
3	LMT	B	3037	-	-	X	-
4	LMU	A	3049	-	-	X	-

2 Entry composition [i](#)

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.

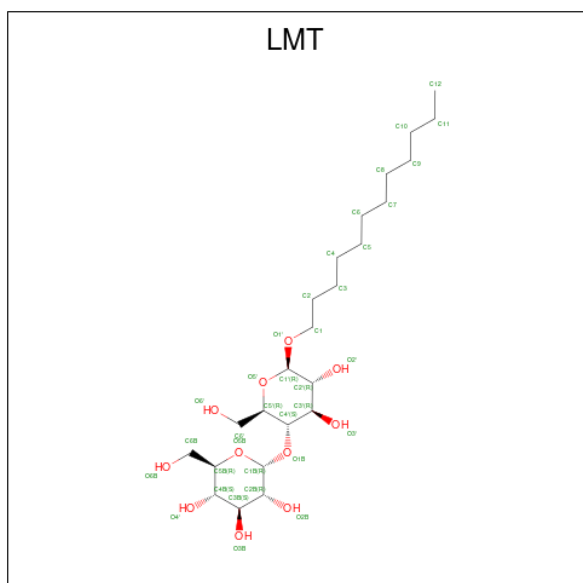
- Molecule 1 is a protein called ACRIFLAVINE RESISTANCE PROTEIN B.

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.

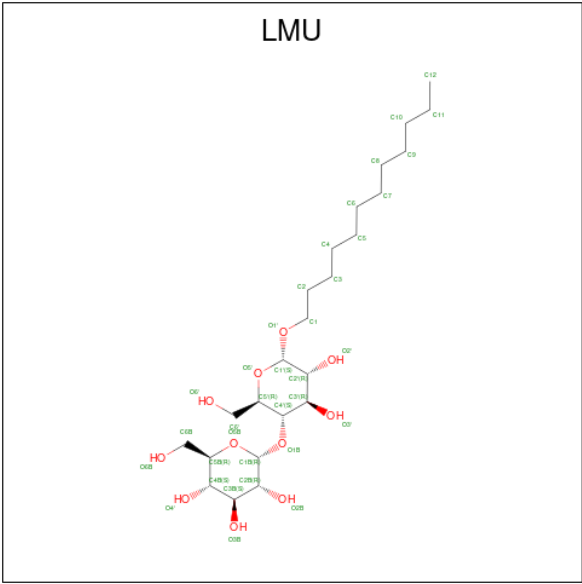
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	156	Total	C	N	O	S	0	0	0
			1177	741	206	229	1			
2	E	153	Total	C	N	O	S	0	0	0
			1159	732	203	223	1			

- Molecule 3 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 4 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



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

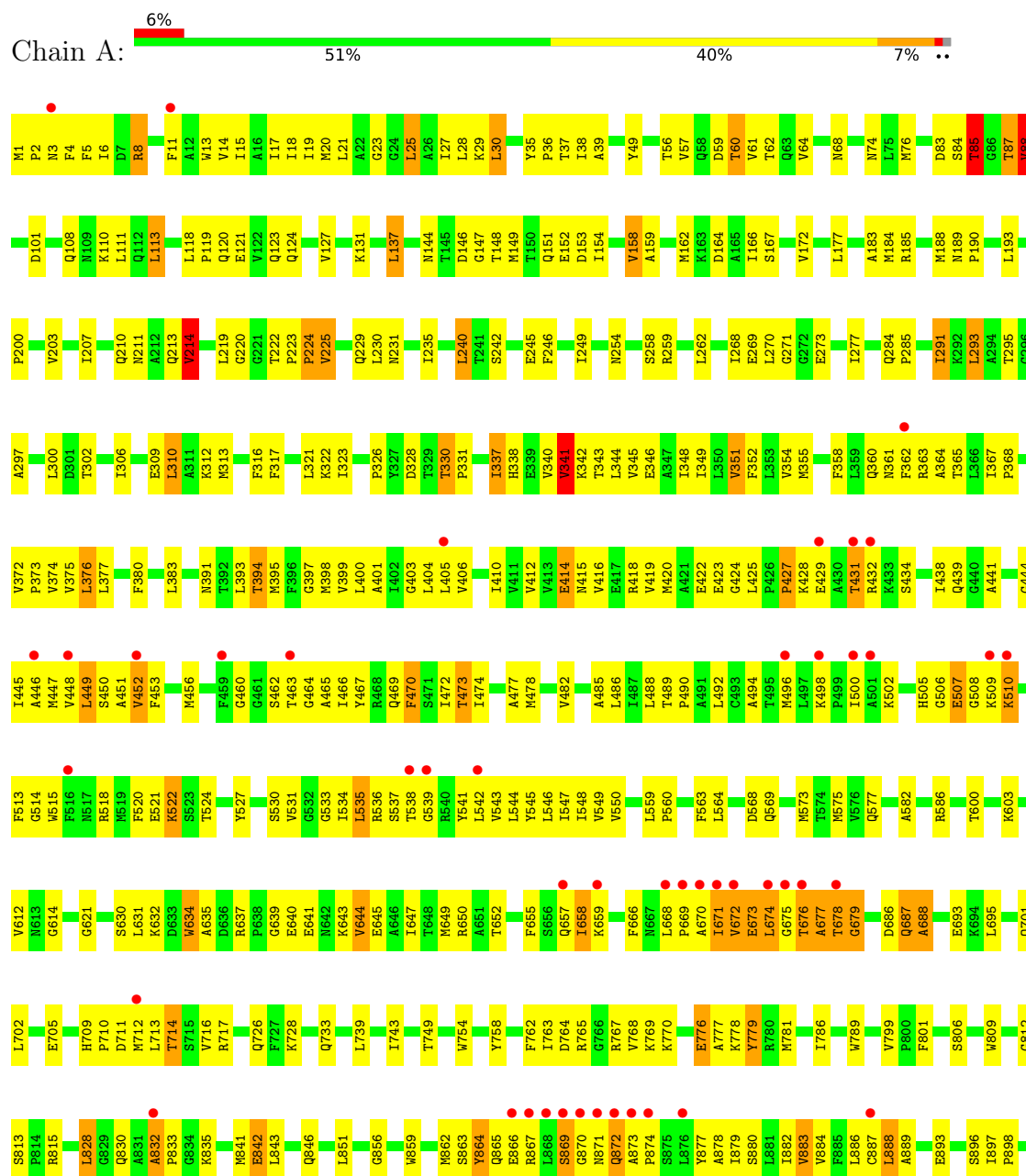
- Molecule 5 is water.

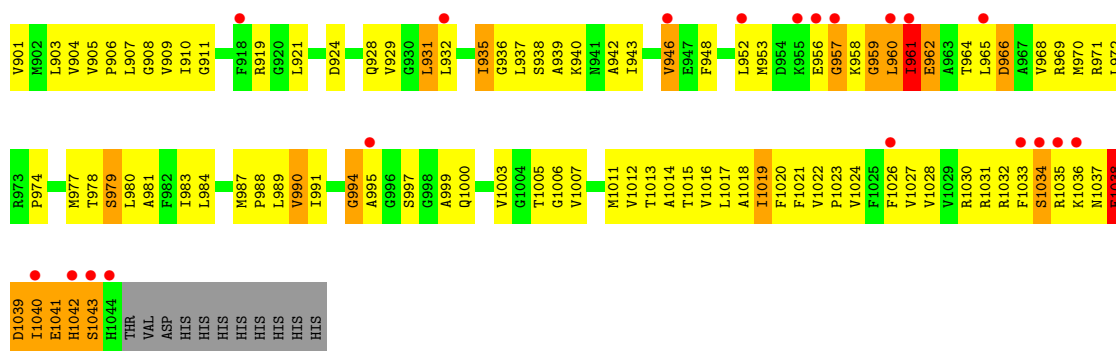
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	118	Total 118	O 118	0	0
5	B	99	Total 99	O 99	0	0
5	C	117	Total 117	O 117	0	0
5	D	10	Total 10	O 10	0	0
5	E	6	Total 6	O 6	0	0

3 Residue-property plots

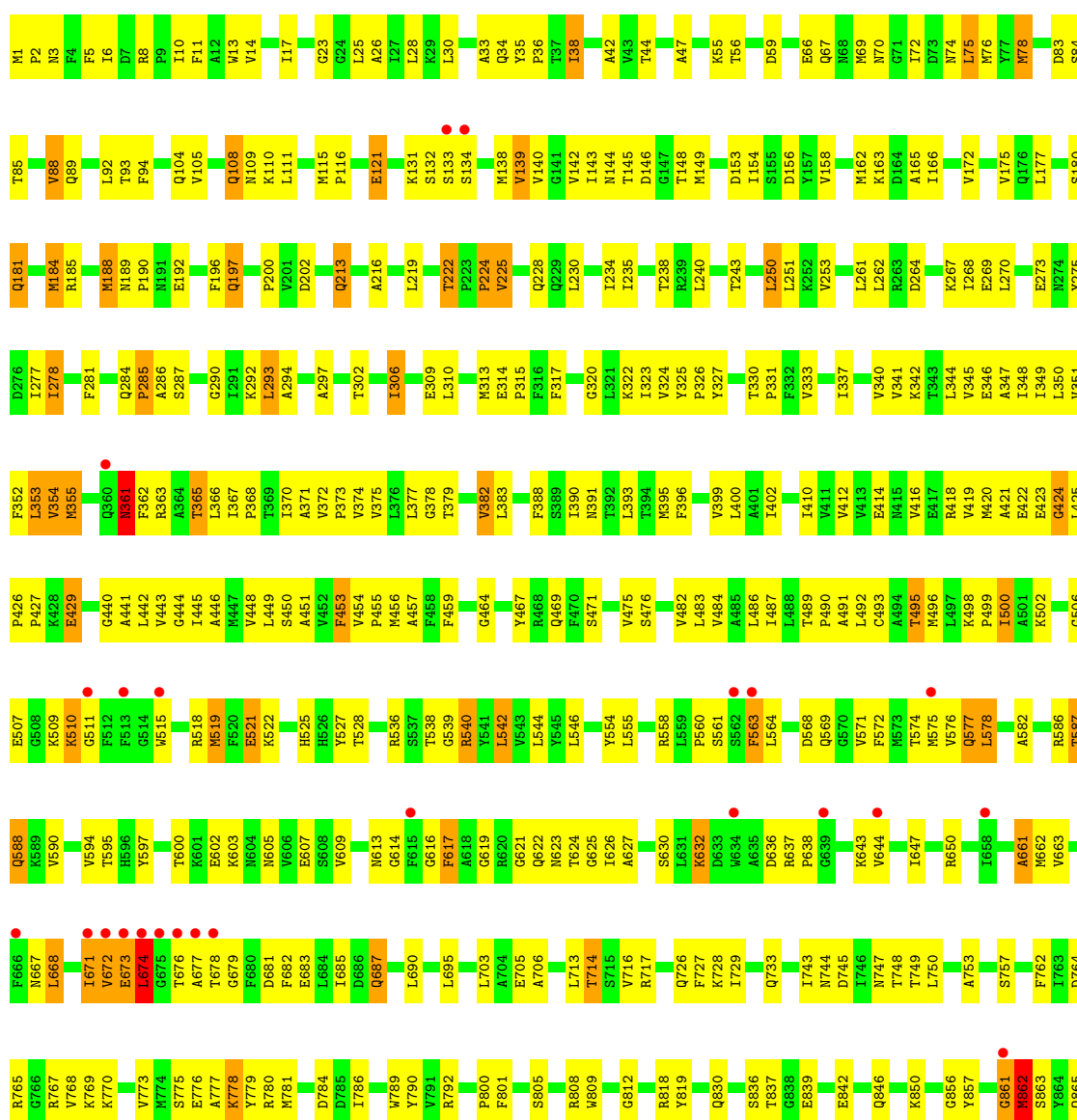
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

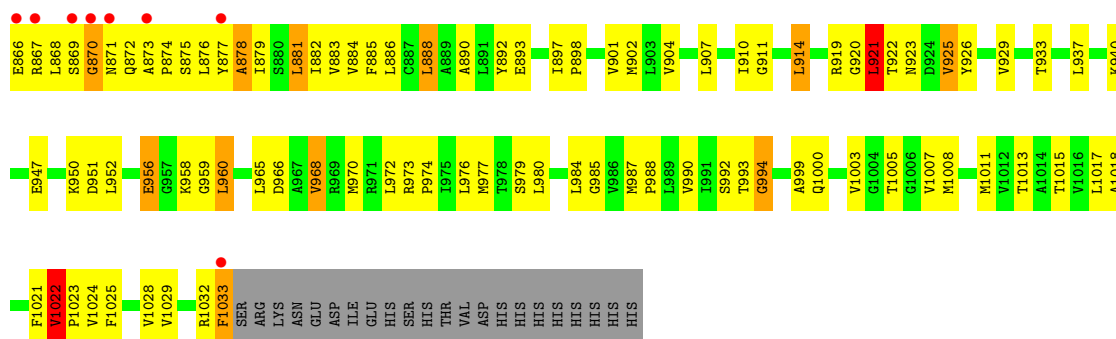
• Molecule 1: ACRIFLAVINE RESISTANCE PROTEIN B



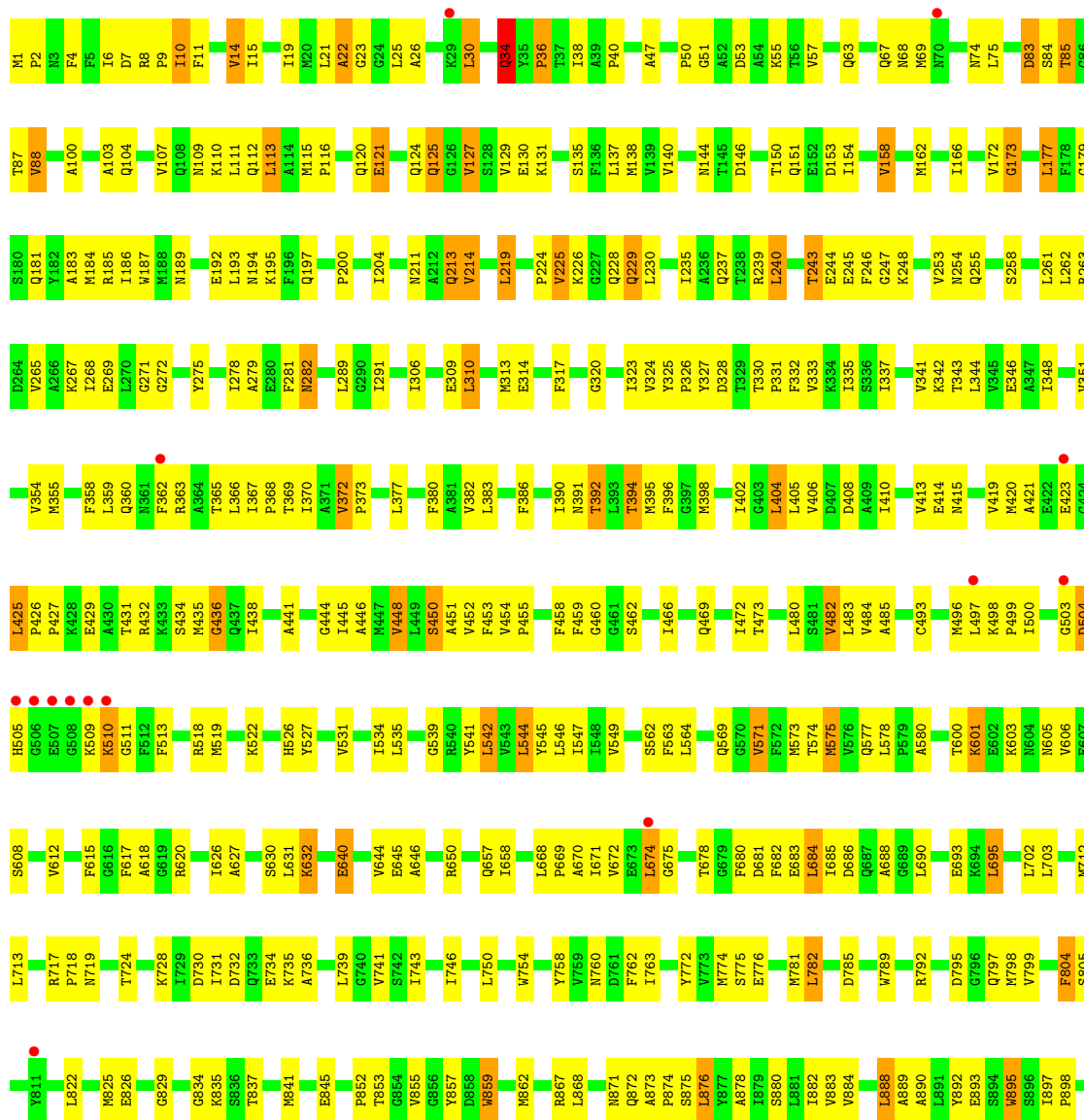


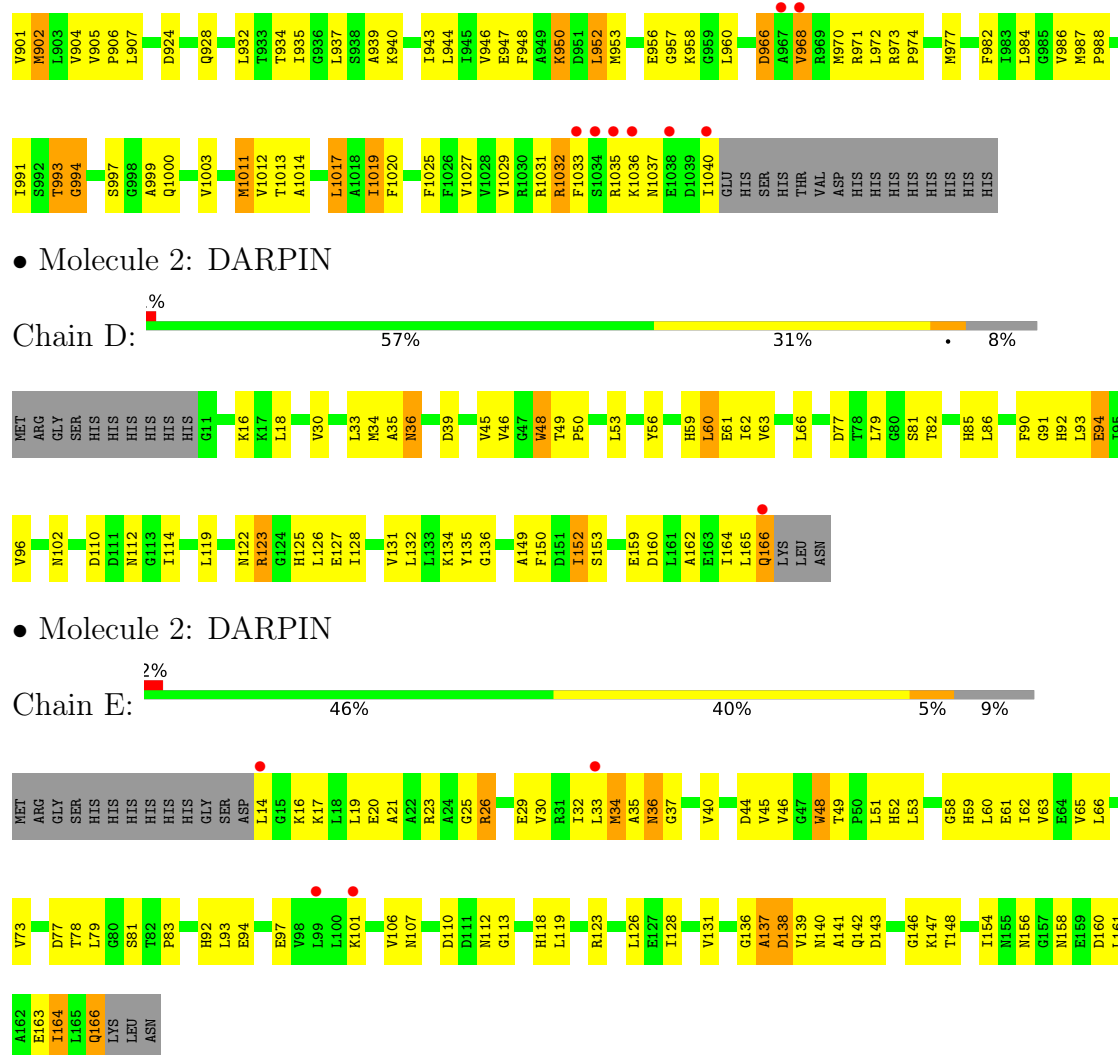
● Molecule 1: ACRIFLAVINE RESISTANCE PROTEIN B





● Molecule 1: ACRIFLAVINE RESISTANCE PROTEIN B





4 Data and refinement statistics

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) 95.8 (34.36-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	0/8095	0.97	37/10991 (0.3%)
1	B	0.47	1/7999 (0.0%)	0.96	22/10863 (0.2%)
1	C	0.48	0/8058	0.97	35/10941 (0.3%)
2	D	0.42	0/1196	0.89	3/1626 (0.2%)
2	E	0.37	0/1178	0.84	2/1602 (0.1%)
All	All	0.47	1/26526 (0.0%)	0.96	99/36023 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1022	VAL	CA-CB	6.02	1.57	1.53

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	SER	N-CA-C	-11.20	99.86	113.19
1	A	85	THR	N-CA-C	-9.35	101.88	113.28
1	B	862	MET	N-CA-C	-8.74	102.53	113.01
1	B	878	ALA	N-CA-C	-8.25	102.36	111.36
1	B	85	THR	N-CA-C	-8.08	103.33	113.02
1	A	84	SER	N-CA-C	-8.01	103.96	112.93
1	B	685	ILE	N-CA-C	7.87	119.81	108.48
1	C	255	GLN	N-CA-C	-7.87	102.65	111.07
1	A	888	LEU	N-CA-C	-7.63	102.61	112.23
1	A	676	THR	N-CA-C	-7.54	103.82	112.87
1	A	341	VAL	N-CA-C	-7.21	103.75	110.53
1	B	867	ARG	N-CA-C	-7.15	104.37	113.23
1	A	966	ASP	N-CA-C	-7.14	104.44	113.01
1	C	229	GLN	N-CA-C	-6.95	104.79	113.55
1	A	137	LEU	N-CA-C	-6.93	102.94	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	LEU	N-CA-C	-6.79	98.63	109.76
1	B	225	VAL	N-CA-C	-6.68	98.71	108.87
1	C	542	LEU	N-CA-C	-6.67	104.01	111.28
1	A	535	LEU	N-CA-C	-6.66	104.10	111.36
1	C	782	LEU	CA-C-N	6.57	126.07	119.24
1	C	782	LEU	C-N-CA	6.57	126.07	119.24
1	C	137	LEU	N-CA-C	-6.51	104.10	111.14
1	C	632	LYS	N-CA-C	-6.48	102.44	110.41
1	A	273	GLU	N-CA-C	-6.41	104.72	112.54
1	C	225	VAL	N-CA-C	-6.37	98.48	108.23
1	C	618	ALA	N-CA-C	-6.28	104.18	113.61
1	C	74	ASN	N-CA-C	6.22	120.21	112.24
1	C	685	ILE	N-CA-C	6.18	117.49	108.53
1	B	361	ASN	N-CA-C	6.18	118.88	110.35
2	E	126	LEU	N-CA-C	6.15	118.77	111.33
1	A	776	GLU	N-CA-C	-6.08	101.93	110.50
1	C	219	LEU	N-CA-C	-6.07	99.30	109.07
1	C	325	TYR	CA-C-N	6.04	126.56	120.04
1	C	325	TYR	C-N-CA	6.04	126.56	120.04
1	B	453	PHE	N-CA-C	5.93	120.69	112.45
1	C	719	ASN	N-CA-C	-5.90	101.39	109.71
1	B	188	MET	N-CA-C	5.88	118.79	110.50
1	A	472	ILE	N-CA-C	5.88	116.06	110.42
1	B	184	MET	N-CA-C	-5.83	101.65	110.28
1	C	876	LEU	N-CA-C	-5.83	104.84	111.14
1	A	688	ALA	N-CA-C	-5.81	100.93	109.18
1	C	214	VAL	N-CA-C	5.81	116.56	108.89
1	C	85	THR	N-CA-C	-5.80	105.78	112.92
1	B	672	VAL	N-CA-C	5.80	116.23	108.11
1	A	8	ARG	CA-C-N	5.76	125.45	119.05
1	A	8	ARG	C-N-CA	5.76	125.45	119.05
1	A	1039	ASP	N-CA-C	-5.75	104.98	113.72
1	A	225	VAL	N-CA-C	-5.74	103.80	110.05
1	A	640	GLU	N-CA-C	-5.74	106.12	113.23
1	C	83	ASP	N-CA-C	5.73	118.90	110.59
1	A	714	THR	N-CA-C	5.72	118.22	108.90
1	B	521	GLU	N-CA-C	-5.71	105.58	112.54
1	A	397	GLY	N-CA-C	-5.70	105.59	112.49
1	C	34	GLN	N-CA-C	-5.69	104.71	111.03
1	A	87	THR	N-CA-C	5.68	119.31	110.17
1	C	606	VAL	N-CA-C	5.63	116.42	108.36
1	A	291	ILE	N-CA-C	5.59	116.00	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	837	THR	N-CA-C	-5.54	104.62	111.33
1	A	464	GLY	N-CA-C	5.54	118.92	112.50
1	A	644	VAL	N-CA-C	5.53	116.92	110.62
2	D	91	GLY	N-CA-C	5.52	122.43	114.10
1	B	189	ASN	CA-C-N	5.51	125.34	119.28
1	B	189	ASN	C-N-CA	5.51	125.34	119.28
1	A	931	LEU	N-CA-C	-5.49	104.69	111.33
1	A	779	TYR	N-CA-C	5.48	119.96	113.16
1	B	181	GLN	N-CA-C	-5.48	103.25	110.43
1	B	667	ASN	N-CA-C	-5.47	103.68	110.41
1	B	690	LEU	N-CA-C	5.46	117.67	111.11
2	D	60	LEU	N-CA-C	5.45	117.64	111.11
1	C	754	TRP	N-CA-C	5.44	119.09	112.23
1	A	1021	PHE	N-CA-C	5.42	117.27	111.36
1	C	462	SER	N-CA-C	-5.42	105.53	111.82
1	B	661	ALA	N-CA-C	5.38	115.47	107.88
1	C	230	LEU	N-CA-C	5.31	118.27	109.46
1	C	22	ALA	N-CA-C	-5.29	105.42	111.14
1	C	776	GLU	N-CA-C	-5.29	102.45	110.28
2	D	160	ASP	N-CA-C	-5.28	105.42	111.07
1	C	173	GLY	N-CA-C	-5.25	103.64	112.77
1	C	84	SER	N-CA-C	-5.25	106.83	113.18
1	A	277	ILE	N-CA-C	5.23	116.01	108.48
1	C	30	LEU	N-CA-C	5.20	115.97	109.57
1	A	219	LEU	N-CA-C	-5.19	100.77	109.24
1	C	466	ILE	N-CA-C	-5.18	105.49	110.72
2	E	45	VAL	N-CA-C	5.16	118.29	111.17
1	B	74	ASN	N-CA-C	5.14	118.34	111.24
1	A	864	TYR	N-CA-C	-5.13	104.95	111.11
1	C	888	LEU	N-CA-C	-5.12	105.62	111.14
1	A	214	VAL	N-CA-C	5.09	116.61	108.87
1	A	460	GLY	N-CA-C	5.09	120.63	111.62
1	A	88	VAL	CB-CA-C	-5.09	103.04	110.62
1	C	895	TRP	N-CA-C	-5.07	107.22	113.41
1	B	542	LEU	N-CA-C	-5.05	105.77	111.28
1	A	813	SER	N-CA-C	5.04	117.25	110.29
1	C	240	LEU	N-CA-C	-5.03	103.76	110.55
1	B	588	GLN	N-CA-C	-5.02	105.52	111.69
1	A	832	ALA	CA-C-N	5.01	126.11	119.84
1	A	832	ALA	C-N-CA	5.01	126.11	119.84
1	C	130	GLU	N-CA-C	5.01	117.42	109.50
1	A	295	THR	N-CA-C	5.00	117.81	110.30

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	636	0
1	B	7849	0	8001	471	0
1	C	7908	0	8059	418	0
2	D	1177	0	1159	53	0
2	E	1159	0	1147	62	0
3	A	105	0	136	84	0
3	B	105	0	138	50	0
3	C	140	0	184	57	0
4	A	35	0	46	51	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	1642	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 31.

All (1642) 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:C2	3:C:3043:LMT:C1	1.78	1.61
3:C:3046:LMT:O3'	3:C:3046:LMT:H11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:937:LEU:HB3	1:C:1011:MET:HE3	1.43	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
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:C:573:MET:HE3	1:C:626:ILE:HD11	1.45	0.96
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:448:VAL:HA	3:A:3047:LMT:H61	1.49	0.94
1:A:887:CYS:HB3	3:A:3047:LMT:H51	1.49	0.94
1:A:447:MET:HB2	3:A:3047:LMT:C4	1.98	0.94
1:A:451:ALA:HA	3:A:3047:LMT:H102	1.47	0.93
1:A:932:LEU:O	3:A:3048:LMT:H102	1.68	0.93
2:E:34:MET:HA	2:E:34:MET:HE3	1.51	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
1:B:184:MET:HE3	1:B:185:ARG:H	1.34	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:3049:LMU:H12	4:A:3049:LMU:O2'	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: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
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:A:953:MET:HE1	1:A:1026:PHE:HE2	1.40	0.87
1:B:361:ASN:HD22	1:B:361:ASN:N	1.71	0.87
1:A:510:LYS:HD3	1:A:513:PHE:HB2	1.57	0.86
1:C:575:MET:HE3	1:C:617:PHE:HB2	1.57	0.86
1:A:309:GLU:HG3	1:A:313:MET:HE3	1.56	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:C:69:MET:HE1	1:C:107:VAL:HG13	1.57	0.86
1:A:188:MET:HE1	1:A:200:PRO:HA	1.58	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
1:B:973:ARG:HG2	1:B:977:MET:HE2	1.58	0.86
1:C:741:VAL:HG11	1:C:799:VAL:HG11	1.56	0.85
1:A:188:MET:HE2	1:A:193:LEU:HD11	1.55	0.85
1:C:366:LEU:HD23	1:C:496:MET:HE1	1.57	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:449:LEU:C	1:A:451:ALA:H	1.85	0.84
1:A:18:ILE:CG1	3:B:3037:LMT:H112	2.07	0.84
1:A:887:CYS:HB3	3:A:3047:LMT:C5	2.07	0.84
1:C:522:LYS:HG2	1:C:526:HIS:HE1	1.41	0.84
1:C:640:GLU:CD	1:C:640:GLU:H	1.83	0.84
1:A:669:PRO:HB3	1:A:675:GLY:HA3	1.59	0.84
1:B:885:PHE:HD1	1:B:902:MET:HE1	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:1011:MET:HE2	1:C:1011:MET:HA	1.59	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:HE	1:A:867:ARG:HA	1.42	0.81
1:A:21:LEU:O	1:A:25:LEU:HD22	1.81	0.81
1:A:355:MET:HE2	1:A:368:PRO:HG3	1.61	0.81
1:A:635:ALA:HB2	4:A:3049:LMU:O4'	1.81	0.81
1:B:69:MET:HG3	1:B:78:MET:HE1	1.63	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:B:361:ASN:H	1:B:361:ASN:ND2	1.73	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
3:C:3042:LMT:O1'	3:C:3042:LMT:C6'	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: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:B:879:ILE:HG21	3:B:3037:LMT:H31	1.63	0.79
1:C:162:MET:HA	1:C:313:MET:HE1	1.64	0.79
1:A:38:ILE:HG13	1:A:39:ALA:N	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O2'	4:A:3049:LMU:C1	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:O2B	3:C:3042:LMT:C5B	2.30	0.78
1:A:200:PRO:HD2	1:A:749:THR:HG22	1.65	0.78
1:A:348:ILE:O	1:A:351:VAL:HG12	1.83	0.78
1:A:669:PRO:O	1:A:671:ILE:HG22	1.83	0.77
1:C:953:MET:HE2	1:C:960:LEU:HA	1.64	0.77
1:B:76:MET:HE3	1:B:93:THR:HG22	1.67	0.77
1:B:987:MET:HG3	1:B:1008:MET:HE1	1.67	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:63:GLN:HE22	1:C:67:GLN:HE21	1.29	0.77
1:C:359:LEU:HD12	1:C:365:THR:HA	1.66	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:A:932:LEU:C	3:A:3048:LMT:H102	2.10	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
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:449:LEU:C	1:A:451:ALA:N	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:62:ILE:O	2:E:66:LEU:HG	1.86	0.75
1:A:144:ASN:OD1	1:A:149:MET:HG2	1.85	0.74
1:B:367:ILE:HG12	1:B:496:MET:HE3	1.68	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:B:868:LEU:C	1:B:870:GLY:H	1.92	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
1:A:447:MET:C	3:A:3047:LMT:H61	2.12	0.73
1:C:154:ILE:O	1:C:158:VAL:HG12	1.88	0.73
1:B:250:LEU:HD12	1:C:734:GLU:HG2	1.70	0.73
1:C:458:PHE:HZ	3:C:3046:LMT:H51	1.53	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:196:PHE:C	1:B:197:GLN:HE21	1.97	0.73
1:B:703:LEU:HD23	1:B:716:VAL:HG22	1.69	0.73
1:C:7:ASP:C	1:C:9:PRO:HD3	2.14	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:956:GLU:HB2	1:B:958:LYS:HG3	1.70	0.72
1:B:1022:VAL:HG22	1:B:1023:PRO:HD3	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
1:A:911:GLY:HA3	1:A:1013:THR:OG1	1.89	0.72
1:A:188:MET:HE1	1:A:200:PRO:CA	2.19	0.72
1:A:445:ILE:HA	1:A:448:VAL:HG22	1.71	0.72
1:A:568:ASP:CG	1:A:637:ARG:HH22	1.96	0.72
1:B:714:THR:HG23	1:B:830:GLN:HG3	1.72	0.72
2:D:36:ASN:N	2:D:36:ASN:HD22	1.86	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:3043:LMT:C2	3:C:3043:LMT:O1'	2.37	0.72
1:B:26:ALA:O	1:B:30:LEU:HB2	1.90	0.71
1:A:634:TRP:H	1:A:634:TRP:CD1	2.06	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: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:214:VAL:HG11	1:B:747:ASN:HB3	1.71	0.71
1:A:425:LEU:HD23	1:A:429:GLU:HG3	1.72	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:184:MET:HE3	1:B:185:ARG:N	2.06	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:A:687:GLN:NE2	1:A:856:GLY:HA3	2.05	0.70
1:A:712:MET:HA	1:A:832:ALA:HB3	1.74	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:492:LEU:HD22	1:B:496:MET:HE2	1.73	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
1:C:902:MET:HE3	1:C:902:MET:HA	1.74	0.69
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:A:534:ILE:O	1:A:537:SER:HB3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:897:ILE:N	1:A:898:PRO:HD2	2.08	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
1:C:138:MET:HE2	1:C:140:VAL:HG22	1.76	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: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:674:LEU:C	1:B:676:THR:H	2.01	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:960:LEU:HD12	1:A:961:ILE:N	2.09	0.67
1:A:1007:VAL:O	1:A:1011:MET:HB2	1.94	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:28:LEU:C	1:A:29:LYS:HD2	2.20	0.66
1:A:341:VAL:C	4:A:3049:LMU:H62	2.21	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
1:B:350:LEU:O	1:B:354:VAL:HG13	1.96	0.66
3:B:3037:LMT:C3'	3:B:3037:LMT:O2B	2.44	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
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
3:C:3042:LMT:O3'	3:C:3042:LMT:H1B	1.95	0.66
1:A:345:VAL:HG23	4:A:3049:LMU:H72	1.78	0.65
1:A:537:SER:C	1:A:539:GLY:H	2.03	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:H5B	3:B:3035:LMT:H6E	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
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
1:C:875:SER:CB	3:C:3044:LMT:H3B	2.27	0.64
3:C:3042:LMT:O1'	3:C:3042:LMT:H6E	1.97	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:B:420:MET:HE1	1:B:427:PRO:HG3	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:VAL:HB	4:A:3049:LMU:C4	2.28	0.64
1:A:726:GLN:OE1	1:A:812:GLY:HA3	1.98	0.64
1:A:781:MET:HG3	1:C:228:GLN:OE1	1.97	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: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:485:ALA:C	1:A:486:LEU:HD12	2.23	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:162:MET:HA	1:C:313:MET:CE	2.28	0.63
1:A:1037:ASN:CG	1:A:1038:GLU:H	2.04	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:11:PHE:CE1	3:B:3036:LMT:O6'	2.50	0.63
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.81	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:681:ASP:HB3	1:B:861:GLY:H	1.64	0.62
2:D:152:ILE:C	2:D:152:ILE:HD13	2.24	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:A:1038:GLU:HG2	1:A:1040:ILE:N	2.13	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:HZ2	1:C:601:LYS:HB3	1.65	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:C:151:GLN:OE1	1:C:278:ILE:HG23	1.99	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:B:492:LEU:HB3	1:B:496:MET:HE2	1.81	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:A:1038:GLU:C	1:A:1040:ILE:H	2.06	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
2:E:34:MET:HA	2:E:34:MET:CE	2.27	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:63:GLN:HE22	1:C:67:GLN:NE2	1.97	0.61
1:C:425:LEU:HB3	1:C:429:GLU:HG2	1.81	0.61
1:A:717:ARG:HH12	1:A:828:LEU:HD23	1.65	0.61
1:A:960:LEU:HD22	1:A:1030:ARG:HB3	1.80	0.61
1:B:177:LEU:HD23	1:B:177:LEU:H	1.65	0.61
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:C:420:MET:HE3	1:C:500:ILE:HG13	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:83:ASP:OD2	1:A:815:ARG:HD3	2.01	0.61
1:A:533:GLY:HA2	1:A:536:ARG:HD3	1.82	0.61
2:E:77:ASP:OD1	2:E:81:SER:HB3	2.00	0.61
1:A:447:MET:C	3:A:3047:LMT:C6	2.74	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:A:358:PHE:HB2	1:A:977:MET:HE3	1.83	0.60
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:H82	3:C:3042:LMT:H122	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:A:958:LYS:O	1:A:959:GLY:C	2.44	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:C:110:LYS:NZ	1:C:113:LEU:HD23	2.17	0.60
1:C:332:PHE:CD1	1:C:569:GLN:HA	2.36	0.60
3:C:3042:LMT:H6E	3:C:3042:LMT:C2'	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NZ	1:A:522:LYS:HB3	2.18	0.59
1:B:165:ALA:HB3	1:B:313:MET:HE1	1.82	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
1:B:492:LEU:HD22	1:B:496:MET:CE	2.32	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
3:C:3042:LMT:O3'	3:C:3042:LMT:C1B	2.50	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:872:GLN:O	1:B:876:LEU:N	2.35	0.59
1:B:987:MET:CG	1:B:1008:MET:HE1	2.32	0.59
1:B:1011:MET:O	1:B:1015:THR:HG23	2.02	0.59
1:C:547:ILE:HG12	3:C:3043:LMT:C12	2.33	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:1022:VAL:HB	1:A:1023:PRO:HD3	1.83	0.59
1:B:355:MET:HE1	1:B:410:ILE:HG23	1.85	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:A:675:GLY:C	1:A:677:ALA:H	2.11	0.59
1:B:420:MET:HE2	5:B:2045:HOH:O	2.02	0.59
3:C:3042:LMT:H2B	3:C:3042:LMT:H3'	1.83	0.59
2:D:35:ALA:C	2:D:36:ASN:HD22	2.10	0.59
1:B:674:LEU:C	1:B:676:THR:N	2.58	0.59
1:C:892:TYR:O	1:C:893:GLU:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:868:LEU:C	1:B:870:GLY:N	2.61	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
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:C:1013:THR:O	1:C:1017:LEU:HB2	2.03	0.58
1:B:351:VAL:O	1:B:355:MET:HB2	2.03	0.58
1:B:1013:THR:HG22	1:B:1017:LEU:HD12	1.84	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:C:1031:ARG:C	1:C:1033:PHE:H	2.11	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:412:VAL:O	1:A:416:VAL:HG23	2.03	0.58
1:A:675:GLY:C	1:A:677:ALA:N	2.61	0.58
1:B:222:THR:HG23	1:C:275:TYR:CB	2.30	0.58
2:E:35:ALA:C	2:E:37:GLY:H	2.12	0.58
1:A:146:ASP:O	1:A:148:THR:HG23	2.04	0.57
1:A:341:VAL:C	4:A:3049:LMU:C6	2.77	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:A:354:VAL:CG2	1:A:984:LEU:HD12	2.34	0.57
1:A:893:GLU:CD	1:C:10:ILE:HG23	2.29	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: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
1:B:885:PHE:CD1	1:B:902:MET:HE1	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3037:LMT:C3'	3:B:3037:LMT:H2O1	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:O	1:B:893:GLU:HG3	2.03	0.57
1:A:542:LEU:HD21	1:A:1028:VAL:CG2	2.34	0.57
1:A:677:ALA:O	1:A:678:THR:C	2.47	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:36:PRO:HG3	1:C:469:GLN:CD	2.30	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:582:ALA:HB3	1:B:623:ASN:CB	2.35	0.57
1:B:590:VAL:O	1:B:594:VAL:HG23	2.03	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:30:LEU:HD23	1:B:390:ILE:HG13	1.87	0.57
1:B:302:THR:O	1:B:306:ILE:CG2	2.53	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:A:575:MET:HE3	1:A:666:PHE:CE1	2.40	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: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:443:VAL:C	3:B:3036:LMT:O2'	2.48	0.56
1:B:767:ARG:HA	5:B:2072:HOH:O	2.04	0.56
1:C:901:VAL:HG23	1:C:902:MET:N	2.21	0.56
1:B:907:LEU:O	1:B:1013:THR:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:57:VAL:HG13	1:A:88:VAL:HG22	1.88	0.56
1:A:345:VAL:HG23	4:A:3049:LMU:C6	2.36	0.56
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
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:A:361:ASN:C	1:A:363:ARG:H	2.14	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:C:953:MET:HE1	1:C:960:LEU:CD2	2.36	0.56
1:A:344:LEU:C	4:A:3049:LMU:H112	2.31	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: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:HD12	1:C:497:LEU:O	2.06	0.55
3:B:3037:LMT:O2B	3:B:3037:LMT:H3'	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: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:A:427:PRO:O	1:A:431:THR:HG22	2.07	0.55
1:B:84:SER:HB3	5:B:2017:HOH:O	2.06	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:MET:C	1:A:449:LEU:H	2.15	0.55
1:A:712:MET:CB	1:A:835:LYS:HG3	2.36	0.55
1:A:896:SER:C	1:A:898:PRO:HD2	2.32	0.55
3:A:3047:LMT:C3B	1:C:8:ARG:HH21	2.14	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:7:ASP:O	1:C:9:PRO:HD3	2.07	0.55
1:C:75:LEU:HD13	1:C:75:LEU:C	2.32	0.55
1:C:686:ASP:OD1	1:C:690:LEU:HB2	2.06	0.55
1:C:1011:MET:HE2	1:C:1014:ALA:HB3	1.88	0.55
1:A:432:ARG:HG2	1:A:432:ARG:NH1	2.22	0.55
1:B:563:PHE:CE2	1:B:564:LEU:HD13	2.41	0.55
1:C:575:MET:HE1	1:C:617:PHE:CD2	2.42	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: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:83:ASP:HB2	1:C:87:THR:CG2	2.37	0.55
1:C:690:LEU:H	1:C:690:LEU:HD12	1.71	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:726:GLN:CD	1:B:812:GLY:HA3	2.32	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:A:341:VAL:HG22	1:A:395:MET:HE2	1.89	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: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:776:GLU:CD	1:B:778:LYS:NZ	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:PRO:HD2	1:B:429:GLU:HG3	1.90	0.54
1:A:213:GLN:HG3	1:B:56:THR:HG23	1.89	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: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:A:300:LEU:HD23	1:A:330:THR:HG23	1.88	0.54
1:A:348:ILE:CG2	4:A:3049:LMU:H123	2.35	0.54
1:B:5:PHE:CG	1:B:487:ILE:HG23	2.42	0.54
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:A:524:THR:O	1:A:527:TYR:HB3	2.08	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:B:83:ASP:OD2	1:B:83:ASP:C	2.50	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:N	2:D:61:GLU:OE1	2.41	0.54
1:A:901:VAL:HG11	1:A:943:ILE:HG13	1.90	0.54
1:C:423:GLU:CB	1:C:425:LEU:HD13	2.38	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:A:452:VAL:C	3:A:3048:LMT:H121	2.33	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:HG22	1:C:991:ILE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:PRO:HG2	1:C:125:GLN:HE21	1.73	0.53
1:C:372:VAL:HG22	1:C:373:PRO:HD3	1.90	0.53
2:E:26:ARG:NH1	2:E:26:ARG:HB3	2.23	0.53
1:A:146:ASP:O	1:A:147:GLY:C	2.51	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:76:MET:HE2	1:B:94:PHE:O	2.07	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
1:C:50:PRO:CG	1:C:125:GLN:HE21	2.22	0.53
1:C:1037:ASN:O	1:C:1040:ILE:HG23	2.08	0.53
1:A:338:HIS:HA	1:A:341:VAL:HG23	1.91	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
1:B:222:THR:HG21	1:C:275:TYR:C	2.34	0.53
2:D:48:TRP:HD1	2:D:53:LEU:HD13	1.73	0.53
1:A:35:TYR:CZ	1:A:564:LEU:HD13	2.43	0.53
1:A:953:MET:HE1	1:A:1026:PHE:CE2	2.32	0.53
3:C:3042:LMT:H2B	3:C:3042:LMT:O3'	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:C:194:ASN:ND2	1:C:798:MET:HG3	2.24	0.53
1:C:370:ILE:C	1:C:373:PRO:HD2	2.34	0.53
1:C:1011:MET:HA	1:C:1011:MET:CE	2.35	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:85:THR:HG22	1:A:87:THR:H	1.73	0.53
1:A:537:SER:O	1:A:539:GLY:N	2.39	0.53
1:A:883:VAL:CB	3:A:3047:LMT:H111	2.38	0.53
1:A:948:PHE:O	1:A:952:LEU:HG	2.09	0.53
1:C:575:MET:HE1	1:C:617:PHE:HD2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:60:LEU:HD22	2:E:94:GLU:OE2	2.08	0.53
1:A:108:GLN:NE2	1:B:109:ASN:HB3	2.24	0.52
1:A:1037:ASN:O	1:A:1038:GLU:HB3	2.08	0.52
1:B:121:GLU:H	1:B:121:GLU:CD	2.17	0.52
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.90	0.52
1:B:414:GLU:HG3	1:B:977:MET:HE1	1.91	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
1:C:841:MET:HE3	1:C:859:TRP:CD2	2.43	0.52
1:A:883:VAL:CG1	3:A:3047:LMT:C11	2.79	0.52
1:B:650:ARG:HH11	1:B:650:ARG:HB2	1.73	0.52
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:A:447:MET:HB2	3:A:3047:LMT:H42	1.89	0.52
3:A:3047:LMT:O2'	3:A:3047:LMT:C1	2.54	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:420:MET:HE1	1:A:498:LYS:O	2.09	0.52
1:A:506:GLY:C	1:A:508:GLY:H	2.18	0.52
1:A:541:TYR:C	1:A:543:VAL:H	2.15	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:N	1:B:668:LEU:HD23	2.24	0.52
1:A:889:ALA:O	1:C:10:ILE:HD11	2.09	0.52
5:A:2018:HOH:O	1:C:104:GLN:HG3	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
1:A:448:VAL:HG21	1:A:943:ILE:HD13	1.91	0.52
1:A:712:MET:HB3	1:A:835:LYS:HG3	1.92	0.52
1:A:1038:GLU:C	1:A:1040:ILE:N	2.68	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:188:MET:HE1	1:A:200:PRO:HG3	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.90	0.52
1:C:946:VAL:O	1:C:947:GLU:C	2.53	0.52
1:C:953:MET:HE1	1:C:960:LEU:HD23	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:B:890:ALA:HB3	3:B:3036:LMT:H12	1.91	0.52
1:A:18:ILE:CD1	3:B:3036:LMT:H61	2.40	0.52
1:A:641:GLU:O	1:A:650:ARG:NH2	2.39	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:75:LEU:HD21	1:B:92:LEU:HB3	1.91	0.51
1:B:278:ILE:CG2	1:B:613:ASN:HB3	2.30	0.51
1:B:454:VAL:CG2	1:B:455:PRO:HD3	2.40	0.51
1:C:177:LEU:HD13	1:C:179:GLY:C	2.35	0.51
1:C:314:GLU:HG2	1:C:317:PHE:CE1	2.45	0.51
1:A:418:ARG:O	1:A:422:GLU:HG3	2.09	0.51
1:A:871:ASN:CG	1:A:872:GLN:N	2.67	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:B:780:ARG:O	1:B:781:MET:HE2	2.10	0.51
1:C:671:ILE:HG12	1:C:862:MET:HE1	1.91	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:220:GLY:HA2	1:B:781:MET:SD	2.50	0.51
1:B:636:ASP:C	1:B:638:PRO:HD3	2.36	0.51
1:A:83:ASP:C	1:A:85:THR:H	2.18	0.51
1:A:210:GLN:CD	1:A:249:ILE:HG23	2.36	0.51
1:A:573:MET:HE2	1:A:668:LEU:HD21	1.91	0.51
1:B:5:PHE:CD1	1:B:487:ILE:HG23	2.45	0.51
1:B:414:GLU:CG	1:B:977:MET:HE1	2.41	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:B:869:SER:O	1:B:870:GLY:C	2.53	0.51
1:C:876:LEU:HD13	1:C:932:LEU:HD21	1.93	0.51
1:A:60:THR:HG22	1:A:61:VAL:CG2	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:VAL:O	4:A:3049:LMU:C6	2.58	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:243:THR:HG23	5:B:2033:HOH:O	2.10	0.51
1:B:544:LEU:HD23	1:B:1021:PHE:HZ	1.75	0.51
1:B:717:ARG:HG2	1:B:717:ARG:HH11	1.74	0.51
1:C:21:LEU:HD12	1:C:22:ALA:N	2.26	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: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:47:ALA:HB3	1:B:88:VAL:CG1	2.40	0.51
1:B:418:ARG:O	1:B:422:GLU:HG3	2.11	0.51
1:C:291:ILE:CD1	1:C:306:ILE:HD13	2.41	0.51
1:C:434:SER:C	1:C:436:GLY:H	2.18	0.51
1:C:451:ALA:HB1	1:C:883:VAL:HG12	1.92	0.51
1:A:210:GLN:OE1	1:A:249:ILE:HG23	2.11	0.51
1:A:229:GLN:HE21	1:A:229:GLN:HA	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
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:C:541:TYR:N	1:C:541:TYR:CD2	2.79	0.51
1:C:1032:ARG:HG3	1:C:1032:ARG:O	2.11	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:645:GLU:O	1:A:649:MET:HG3	2.11	0.50
1:A:932:LEU:CA	3:A:3048:LMT:C10	2.88	0.50
1:B:162:MET:O	1:B:166:ILE:HG12	2.11	0.50
1:B:251:LEU:HD11	1:B:262:LEU:HD12	1.93	0.50
1:B:253:VAL:O	1:B:253:VAL:HG23	2.11	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
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:980:LEU:HD23	1:A:980:LEU:O	2.11	0.50
1:C:600:THR:O	1:C:603:LYS:NZ	2.42	0.50
1:A:351:VAL:HG23	1:A:981:ALA:HB1	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ALA:HB2	1:A:482:VAL:CG2	2.42	0.50
1:A:446:ALA:HA	1:A:478:MET:HE2	1.93	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:25:LEU:HG	3:B:3037:LMT:H22	1.93	0.50
1:A:1042:HIS:O	1:A:1043:SER:O	2.30	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:A:537:SER:C	1:A:539:GLY:N	2.69	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:682:PHE:CZ	1:B:857:TYR:HB2	2.47	0.50
1:B:683:GLU:HG2	1:B:819:TYR:CG	2.47	0.50
1:B:968:VAL:CG2	1:B:1023:PRO:HG3	2.42	0.50
1:B:1013:THR:CG2	1:B:1017:LEU:HD12	2.41	0.50
1:C:100:ALA:HB1	1:C:131:LYS:HD2	1.93	0.50
1:C:261:LEU:O	1:C:262:LEU:C	2.54	0.50
1:A:449:LEU:CB	1:A:478:MET:HE1	2.42	0.50
1:A:960:LEU:O	1:A:964:THR:HG23	2.11	0.50
3:A:3047:LMT:O5B	3:A:3047:LMT:O6'	2.30	0.50
1:B:363:ARG:CD	1:B:498:LYS:HE3	2.37	0.50
1:B:544:LEU:HD23	1:B:1021:PHE:CZ	2.46	0.50
1:C:405:LEU:C	1:C:405:LEU:HD12	2.37	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:A:655:PHE:C	1:A:657:GLN:N	2.69	0.49
1:A:972:LEU:HD13	1:A:972:LEU:C	2.36	0.49
1:B:23:GLY:O	1:B:26:ALA:HB3	2.12	0.49
1:B:420:MET:HE3	1:B:427:PRO:N	2.27	0.49
1:B:879:ILE:HG12	3:B:3037:LMT:C3	2.42	0.49
1:A:8:ARG:CZ	3:B:3036:LMT:H6'2	2.41	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:447:MET:C	1:A:449:LEU:N	2.69	0.49
1:A:449:LEU:HB2	1:A:478:MET:HE1	1.94	0.49
1:A:456:MET:HE3	1:A:877:TYR:OH	2.11	0.49
1:B:574:THR:HG23	1:B:627:ALA:HB3	1.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:712:MET:C	1:C:713:LEU:HD23	2.38	0.49
3:C:3042:LMT:O3'	3:C:3042:LMT:C2B	2.60	0.49
1:A:328:ASP:OD1	1:A:330:THR:HB	2.12	0.49
1:A:444:GLY:HA2	3:A:3047:LMT:H21	1.95	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:A:1037:ASN:CG	1:A:1038:GLU:N	2.70	0.49
1:B:442:LEU:HA	1:B:445:ILE:HD13	1.93	0.49
2:E:49:THR:H	2:E:52:HIS:HB2	1.78	0.49
1:A:268:ILE:HD12	1:A:268:ILE:N	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:C:327:TYR:CE1	1:C:571:VAL:HG13	2.47	0.49
2:D:94:GLU:N	2:D:94:GLU:CD	2.70	0.49
1:A:405:LEU:C	1:A:405:LEU:HD23	2.38	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:C:950:LYS:C	1:C:950:LYS:HD2	2.38	0.49
1:B:574:THR:HG22	1:B:627:ALA:O	2.13	0.49
1:B:577:GLN:HE21	1:B:577:GLN:C	2.20	0.49
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:244:GLU:H	1:C:244:GLU:CD	2.19	0.49
1:C:657:GLN:O	1:C:658:ILE:C	2.55	0.49
1:C:688:ALA:HB3	1:C:690:LEU:CD1	2.40	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
1:C:398:MET:O	1:C:402:ILE:HG12	2.13	0.49
3:C:3046:LMT:O6'	3:C:3046:LMT:O5B	2.30	0.49
1:A:673:GLU:OE1	1:A:673:GLU:HA	2.12	0.49
1:A:1031:ARG:NH1	1:A:1039:ASP:OD2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:50:PRO:HG2	1:C:125:GLN:NE2	2.28	0.49
1:C:181:GLN:O	1:C:272:GLY:HA2	2.13	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:C:4:PHE:O	1:C:8:ARG:HG2	2.13	0.48
1:A:575:MET:HE3	1:A:666:PHE:HE1	1.78	0.48
1:A:1020:PHE:O	1:A:1023:PRO:HD2	2.14	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
1:C:446:ALA:CB	1:C:482:VAL:HG13	2.41	0.48
1:C:605:ASN:C	1:C:632:LYS:HG2	2.38	0.48
3:C:3046:LMT:O6'	3:C:3046:LMT:O1B	2.30	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
1:B:344:LEU:O	1:B:348:ILE:HG13	2.13	0.48
3:B:3037:LMT:O2B	3:B:3037:LMT:O3'	2.30	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:70:ASN:O	1:B:110:LYS:HE3	2.13	0.48
1:B:625:GLY:O	1:B:626:ILE:HD13	2.14	0.48
1:C:380:PHE:CZ	1:C:395:MET:HE1	2.48	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:A:919:ARG:HH21	1:A:1005:THR:CG2	2.26	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:B:778:LYS:HZ2	1:B:779:TYR:HE1	1.62	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:4:PHE:O	1:A:8:ARG:HG3	2.13	0.48
1:A:110:LYS:O	1:A:113:LEU:HB2	2.13	0.48
1:A:309:GLU:HG3	1:A:313:MET:CE	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:94:GLU:CD	2:D:94:GLU:H	2.22	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:N	1:A:743:ILE:HD12	2.29	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:B:230:LEU:HD23	1:B:230:LEU:H	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:732:ASP:CG	1:C:735:LYS:HG3	2.39	0.48
1:C:947:GLU:HG3	1:C:948:PHE:N	2.29	0.48
1:A:781:MET:HG3	1:C:228:GLN:CD	2.39	0.47
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:HG2	1:C:432:ARG:HH11	1.79	0.47
2:E:14:LEU:N	5:E:2001:HOH:O	2.46	0.47
2:E:34:MET:HE1	2:E:40:VAL:HG12	1.96	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: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
1:C:498:LYS:HG2	1:C:499:PRO:HD2	1.96	0.47
1:C:503:GLY:C	1:C:505:HIS:H	2.22	0.47
1:C:888:LEU:O	1:C:889:ALA:C	2.56	0.47
1:C:973:ARG:N	1:C:974:PRO:HD2	2.29	0.47
1:C:1019:ILE:HG22	1:C:1020:PHE:CD1	2.48	0.47
1:A:453:PHE:HE2	1:A:932:LEU:HD23	1.79	0.47
1:A:919:ARG:HB3	1:A:921:LEU:CD2	2.43	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:20:MET:HE2	1:A:374:VAL:HG22	1.95	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:A:956:GLU:O	1:A:957:GLY:C	2.56	0.47
1:B:687:GLN:NE2	1:B:856:GLY:HA3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:LYS:HZ1	1:C:113:LEU:HD23	1.78	0.47
1:C:225:VAL:O	1:C:226:LYS:C	2.58	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: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:A:886:LEU:O	1:C:14:VAL:HB	2.15	0.47
1:A:959:GLY:O	1:A:960:LEU:C	2.58	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:B:278:ILE:HD13	1:B:588:GLN:OE1	2.15	0.47
1:B:451:ALA:O	1:B:455:PRO:HG2	2.14	0.47
1:B:733:GLN:NE2	1:B:743:ILE:HD11	2.29	0.47
1:C:63:GLN:NE2	1:C:67:GLN:HE21	2.05	0.47
1:C:186:ILE:HD13	1:C:268:ILE:HG23	1.96	0.47
1:C:332:PHE:HA	1:C:335:ILE:CG2	2.44	0.47
1:C:408:ASP:OD1	1:C:482:VAL:HG12	2.15	0.47
1:C:872:GLN:HA	3:C:3044:LMT:H2B	1.96	0.47
3:C:3042:LMT:H6D	3:C:3042:LMT:C1	2.44	0.47
2:D:61:GLU:HB2	5:D:2002:HOH:O	2.14	0.47
2:E:138:ASP:HB3	2:E:141:ALA:HB2	1.96	0.47
1:A:763:ILE:HD11	1:B:59:ASP:HB3	1.97	0.47
1:A:948:PHE:HD2	1:A:970:MET:HE3	1.80	0.47
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:C:253:VAL:HG23	1:C:253:VAL:O	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:352:PHE:CD1	1:A:352:PHE:C	2.93	0.47
1:A:372:VAL:HG22	1:A:405:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1031:ARG:C	1:C:1033:PHE:N	2.73	0.47
3:C:3046:LMT:H12	3:C:3046:LMT:H2'	1.39	0.47
1:A:36:PRO:O	1:A:38:ILE:HG23	2.15	0.47
1:A:338:HIS:HA	1:A:341:VAL:CG2	2.45	0.47
1:A:671:ILE:CG2	1:A:675:GLY:HA2	2.43	0.47
1:B:144:ASN:HA	1:B:320:GLY:O	2.15	0.47
1:B:441:ALA:C	1:B:445:ILE:HD12	2.40	0.47
1:C:162:MET:HE1	1:C:323:ILE:HD11	1.96	0.47
1:A:62:THR:OG1	1:A:88:VAL:HG13	2.16	0.46
1:A:428:LYS:HE2	1:A:432:ARG:HH21	1.71	0.46
1:B:363:ARG:HH11	1:B:498:LYS:CE	2.28	0.46
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.96	0.46
1:B:420:MET:CB	1:B:500:ILE:HG23	2.45	0.46
1:B:586:ARG:HH11	1:B:586:ARG:HG2	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:426:PRO:HG2	1:C:429:GLU:HB3	1.96	0.46
1:C:541:TYR:CZ	3:C:3043:LMT:H41	2.50	0.46
1:A:68:ASN:O	1:A:110:LYS:HB3	2.16	0.46
1:A:448:VAL:HG21	1:A:943:ILE:CD1	2.45	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:355:MET:HE3	1:B:355:MET:HA	1.98	0.46
1:C:671:ILE:HD11	1:C:674:LEU:HD11	1.95	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:69:MET:CG	1:B:78:MET:HE1	2.39	0.46
1:B:184:MET:HE2	1:B:268:ILE:HG22	1.96	0.46
1:B:650:ARG:HB2	1:B:650:ARG:NH1	2.31	0.46
1:C:775:SER:HB2	1:C:789:TRP:CZ2	2.51	0.46
1:A:474:ILE:O	1:A:477:ALA:HB3	2.15	0.46
1:A:953:MET:CE	1:A:1026:PHE:HE2	2.22	0.46
3:A:3046:LMT:C11	4:A:3049:LMU:C9	2.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:423:GLU:HB2	1:A:425:LEU:HD13	1.96	0.46
1:A:1038:GLU:HG2	1:A:1040:ILE:O	2.15	0.46
1:B:575:MET:HA	1:B:626:ILE:CD1	2.45	0.46
1:B:595:THR:HG23	1:B:609:VAL:HB	1.97	0.46
1:C:615:PHE:CD1	1:C:615:PHE:C	2.93	0.46
1:C:631:LEU:HD11	1:C:644:VAL:HG12	1.96	0.46
1:A:56:THR:OG1	1:C:213:GLN:NE2	2.48	0.46
1:B:145:THR:HG21	1:B:322:LYS:HE2	1.97	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:578:LEU:HD22	1:B:661:ALA:HB2	1.98	0.46
1:C:472:ILE:HG23	1:C:473:THR:N	2.31	0.46
1:C:578:LEU:HD12	1:C:578:LEU:N	2.30	0.46
1:C:888:LEU:CD2	1:C:943:ILE:HD11	2.46	0.46
1:A:59:ASP:HB3	1:C:763:ILE:HD11	1.98	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:B:577:GLN:NE2	1:B:577:GLN:C	2.74	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:668:LEU:C	1:A:670:ALA:N	2.72	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:A:1033:PHE:O	1:A:1034:SER:HB3	2.16	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:C:971:ARG:C	1:C:974:PRO:HD2	2.40	0.46
2:E:44:ASP:C	2:E:44:ASP:OD2	2.58	0.46
1:A:162:MET:HE3	1:A:317:PHE:HZ	1.81	0.46
1:A:188:MET:HE1	1:A:200:PRO:CB	2.46	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: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:B:1022:VAL:N	1:B:1023:PRO:CD	2.79	0.46
1:C:545:TYR:CD2	1:C:1025:PHE:HZ	2.33	0.46
2:D:59:HIS:O	2:D:63:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:LEU:HD11	1:A:644:VAL:HG12	1.98	0.45
1:A:678:THR:C	1:A:679:GLY:O	2.60	0.45
1:B:600:THR:C	1:B:602:GLU:H	2.24	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:NZ	1:C:601:LYS:CB	2.78	0.45
1:A:404:LEU:HD22	1:A:449:LEU:CD2	2.47	0.45
1:A:448:VAL:C	1:A:451:ALA:HB2	2.41	0.45
1:B:309:GLU:HG3	1:B:313:MET:HE3	1.97	0.45
1:B:475:VAL:HG23	1:B:476:SER:N	2.31	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:B:1033:PHE:CD2	1:B:1033:PHE:N	2.82	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:C:972:LEU:C	1:C:972:LEU:HD13	2.41	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:36:PRO:HG3	1:B:469:GLN:HG3	1.98	0.45
1:B:175:VAL:HA	1:B:290:GLY:O	2.16	0.45
1:B:190:PRO:HB3	1:B:789:TRP:CD2	2.50	0.45
1:B:632:LYS:HA	1:B:632:LYS:HE2	1.99	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:453:PHE:CE1	3:A:3048:LMT:H122	2.52	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:A:1:MET:O	1:A:4:PHE:HB3	2.16	0.45
1:A:11:PHE:CZ	1:A:15:ILE:HD11	2.52	0.45
1:B:607:GLU:HB3	1:B:630:SER:O	2.17	0.45
1:B:974:PRO:HA	1:B:977:MET:HE3	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:ALA:HB2	4:A:3049:LMU:H4O1	1.77	0.45
1:A:693:GLU:H	1:A:693:GLU:CD	2.23	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
1:B:872:GLN:O	1:B:873:ALA:C	2.60	0.45
2:D:16:LYS:HD3	2:D:16:LYS:C	2.42	0.45
2:D:165:LEU:O	2:D:166:GLN:OE1	2.35	0.45
1:A:425:LEU:N	1:A:425:LEU:HD12	2.32	0.45
1:B:492:LEU:CD2	1:B:496:MET:HE2	2.44	0.45
1:B:538:THR:O	1:B:539:GLY:C	2.59	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:281:PHE:O	1:C:282:ASN:C	2.60	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:188:MET:HE1	1:A:200:PRO:CG	2.47	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:678:THR:O	1:A:679:GLY:C	2.60	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:7:ASP:OD2	1:C:432:ARG:NH2	2.49	0.45
1:C:999:ALA:O	1:C:1003:VAL:HG23	2.17	0.45
1:B:10:ILE:HD12	1:C:895:TRP:NE1	2.31	0.45
1:B:33:ALA:O	1:B:391:ASN:HA	2.17	0.45
1:B:190:PRO:HB3	1:B:789:TRP:CE3	2.52	0.45
1:C:413:VAL:HG22	1:C:493:CYS:SG	2.57	0.45
3:C:3044:LMT:H6E	3:C:3044:LMT:C5B	2.45	0.45
3:C:3046:LMT:O6'	3:C:3046:LMT:O6B	2.30	0.45
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:A:1032:ARG:HG3	1:A:1032:ARG:HH11	1.83	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:B:968:VAL:HG21	1:B:1023:PRO:CG	2.46	0.44
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.98	0.44
1:C:121:GLU:CD	1:C:121:GLU:H	2.25	0.44
1:C:404:LEU:HD11	1:C:937:LEU:CD2	2.41	0.44
2:D:56:TYR:CE1	2:D:90:PHE:CE2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:328:ASP:OD2	1:C:330:THR:HB	2.17	0.44
1:C:730:ASP:O	1:C:805:SER:HA	2.16	0.44
2:D:134:LYS:C	2:D:136:GLY:H	2.26	0.44
1:A:883:VAL:HB	3:A:3047:LMT:H112	1.99	0.44
1:A:1016:VAL:HG23	1:A:1017:LEU:CD1	2.48	0.44
1:B:139:VAL:O	1:B:326:PRO:HD2	2.17	0.44
1:B:143:ILE:HG22	1:B:286:ALA:HB2	2.00	0.44
1:B:605:ASN:OD1	1:B:637:ARG:HG2	2.16	0.44
1:C:542:LEU:N	1:C:542:LEU:HD22	2.33	0.44
2:E:14:LEU:HA	2:E:17:LYS:HD3	2.00	0.44
1:A:29:LYS:HE3	1:A:29:LYS:HA	2.00	0.44
1:A:36:PRO:HG3	1:A:469:GLN:HG3	1.99	0.44
1:A:166:ILE:HD12	1:A:306:ILE:HG23	2.00	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:A:188:MET:CE	1:A:200:PRO:HG3	2.47	0.44
1:A:505:HIS:C	1:A:507:GLU:N	2.75	0.44
1:A:506:GLY:C	1:A:508:GLY:N	2.75	0.44
1:A:887:CYS:SG	3:A:3047:LMT:H72	2.51	0.44
1:A:1018:ALA:O	1:A:1022:VAL:HG23	2.18	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
1:A:872:GLN:HE21	1:A:872:GLN:CA	2.30	0.44
1:B:674:LEU:HD12	1:B:674:LEU:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:857:TYR:CD1	1:B:857:TYR:C	2.95	0.44
1:B:959:GLY:O	1:B:960:LEU:C	2.60	0.44
1:B:1007:VAL:O	1:B:1011:MET:HB2	2.18	0.44
1:C:213:GLN:HG2	1:C:239:ARG:CD	2.47	0.44
1:C:432:ARG:HG2	1:C:432:ARG:NH1	2.33	0.44
1:C:880:SER:O	1:C:884:VAL:HG23	2.18	0.44
2:D:36:ASN:N	2:D:36:ASN:ND2	2.58	0.44
1:A:343:THR:HA	1:A:346:GLU:OE2	2.17	0.44
1:A:453:PHE:CD2	3:A:3048:LMT:C12	3.01	0.44
1:A:964:THR:HG22	1:A:1026:PHE:HD2	1.83	0.44
1:B:293:LEU:HD23	1:B:294:ALA:N	2.33	0.44
1:B:400:LEU:O	1:B:933:THR:HG21	2.18	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:980:LEU:HD13	1:B:980:LEU:C	2.43	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:6:ILE:HD11	1:C:431:THR:HG22	2.00	0.44
1:C:146:ASP:C	1:C:146:ASP:OD2	2.61	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: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:A:49:TYR:HE1	1:A:60:THR:HG21	1.83	0.43
1:A:341:VAL:CA	4:A:3049:LMU:H62	2.48	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:34:GLN:HG2	1:B:35:TYR:CE1	2.53	0.43
1:B:138:MET:HE2	1:B:140:VAL:CG2	2.47	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:420:MET:HE1	1:B:499:PRO:HA	2.00	0.43
1:B:673:GLU:O	1:B:674:LEU:C	2.61	0.43
1:B:885:PHE:HD1	1:B:902:MET:CE	2.20	0.43
1:C:213:GLN:HG2	1:C:239:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:35:ALA:C	2:E:37:GLY:N	2.76	0.43
1:A:3:ASN:HA	1:A:6:ILE:CD1	2.43	0.43
1:A:380:PHE:CE1	1:A:398:MET:HE3	2.54	0.43
1:A:398:MET:O	1:A:401:ALA:HB3	2.18	0.43
1:C:291:ILE:HG21	1:C:306:ILE:CD1	2.47	0.43
1:C:351:VAL:HG12	1:C:355:MET:HE2	2.00	0.43
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:188:MET:HE3	1:A:203:VAL:HG21	1.99	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: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:B:1032:ARG:HG2	1:B:1032:ARG:HH11	1.83	0.43
1:C:362:PHE:O	1:C:365:THR:HG22	2.18	0.43
2:D:49:THR:O	2:D:50:PRO:C	2.61	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:C:1011:MET:O	1:C:1012:VAL:C	2.60	0.43
1:A:399:VAL:HG11	1:A:989:LEU:HD11	2.00	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:C:333:VAL:O	1:C:337:ILE:HD13	2.19	0.43
2:E:49:THR:O	2:E:52:HIS:N	2.50	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:887:CYS:CB	3:A:3047:LMT:C5	2.90	0.43
1:A:969:ARG:CG	1:A:970:MET:N	2.81	0.43
1:B:603:LYS:O	1:B:603:LYS:HG2	2.17	0.43
1:B:911:GLY:HA3	1:B:1013:THR:OG1	2.18	0.43
1:C:504:ASP:O	1:C:504:ASP:CG	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:743:ILE:HD12	1:C:743:ILE:C	2.44	0.43
1:C:993:THR:O	1:C:994:GLY:O	2.36	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:A:1026:PHE:O	1:A:1030:ARG:HB2	2.19	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:63:GLN:NE2	1:C:67:GLN:NE2	2.63	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
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: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:B:992:SER:OG	1:B:1000:GLN:NE2	2.51	0.43
3:B:3036:LMT:O3'	3:B:3036:LMT:H1B	2.18	0.43
1:C:1035:ARG:HG2	1:C:1035:ARG:O	2.18	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:A:948:PHE:CD2	1:A:970:MET:HE3	2.54	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:B:373:PRO:O	1:B:377:LEU:HD13	2.19	0.43
1:B:420:MET:CE	1:B:499:PRO:HA	2.48	0.43
1:C:669:PRO:HG2	1:C:675:GLY:O	2.18	0.43
1:A:980:LEU:HD23	1:A:980:LEU:C	2.44	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:11:PHE:O	1:C:14:VAL:HG22	2.19	0.43
1:C:68:ASN:O	1:C:110:LYS:HB3	2.19	0.43
1:C:127:VAL:CG2	1:C:127:VAL:O	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:449:LEU:HD11	1:A:936:GLY:O	2.19	0.42
1:A:531:VAL:O	1:A:535:LEU:HG	2.19	0.42
1:A:687:GLN:HE21	1:A:687:GLN:HB2	1.56	0.42
1:A:762:PHE:CE1	1:A:764:ASP:HB2	2.54	0.42
1:C:448:VAL:HG22	1:C:884:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:LYS:HE3	1:A:510:LYS:HB2	1.81	0.42
1:A:712:MET:HB2	1:A:835:LYS:HG3	2.00	0.42
1:A:865:GLN:O	1:A:866:GLU:C	2.62	0.42
1:B:674:LEU:HD22	1:B:862:MET:HE2	2.02	0.42
1:B:892:TYR:O	1:B:893:GLU:C	2.62	0.42
1:B:904:VAL:O	1:B:907:LEU:HB2	2.19	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:49:THR:O	2:E:52:HIS:HB2	2.19	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
1:A:108:GLN:CD	1:B:109:ASN:HB3	2.44	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:HG2	1:B:717:ARG:NH1	2.33	0.42
1:C:426:PRO:HG2	1:C:429:GLU:CB	2.50	0.42
1:A:462:SER:O	1:A:463:THR:C	2.62	0.42
1:B:457:ALA:HB2	1:B:471:SER:OG	2.19	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
2:E:23:ARG:C	2:E:25:GLY:H	2.26	0.42
1:A:341:VAL:HG13	3:A:3046:LMT:H62	2.01	0.42
1:A:960:LEU:C	1:A:962:GLU:H	2.27	0.42
1:A:999:ALA:O	1:A:1003:VAL:HG23	2.20	0.42
1:B:188:MET:HE2	1:B:773:VAL:HG22	2.02	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:671:ILE:HG12	1:C:862:MET:CE	2.48	0.42
1:C:686:ASP:OD2	1:C:690:LEU:O	2.38	0.42
1:A:30:LEU:HD12	1:A:30:LEU:HA	1.82	0.42
1:A:159:ALA:HB2	1:A:177:LEU:CD2	2.50	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:764:ASP:OD2	1:A:769:LYS:NZ	2.45	0.42
1:A:901:VAL:HG11	1:A:943:ILE:CG1	2.50	0.42
1:A:990:VAL:HG22	1:A:990:VAL:O	2.18	0.42
1:A:1016:VAL:HG23	1:A:1017:LEU:HD12	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:420:MET:HE3	1:A:500:ILE:HB	2.02	0.42
1:A:686:ASP:OD1	1:A:688:ALA:O	2.37	0.42
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
1:C:563:PHE:CD2	1:C:862:MET:HE3	2.55	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
2:D:48:TRP:HZ3	2:D:77:ASP:CG	2.28	0.42
1:A:83:ASP:HB2	1:A:85:THR:HG22	2.02	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:B:284:GLN:O	1:B:285:PRO:C	2.62	0.42
1:B:421:ALA:HB2	1:B:500:ILE:CD1	2.49	0.42
1:B:979:SER:CB	1:B:1015:THR:HG21	2.50	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:HB3	1:A:522:LYS:HZ2	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:30:VAL:HG21	2:D:62:ILE:HD13	2.01	0.42
2:D:114:ILE:HG21	2:D:119:LEU:HD21	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:A:358:PHE:CB	1:A:977:MET:HE3	2.48	0.42
1:A:841:MET:HE3	1:A:859:TRP:CD2	2.54	0.42
1:A:960:LEU:C	1:A:962:GLU:N	2.78	0.42
1:B:768:VAL:N	5:B:2072:HOH:O	2.49	0.42
1:C:414:GLU:OE2	1:C:414:GLU:C	2.63	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:8:ARG:HG3	1:B:8:ARG:HH11	1.85	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
1:C:115:MET:N	1:C:116:PRO:HD2	2.34	0.41
1:C:244:GLU:CD	1:C:244:GLU:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:VAL:O	1:C:386:PHE:HD1	2.03	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: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
1:A:666:PHE:CD1	1:A:666:PHE:N	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:681:ASP:OD2	1:C:826:GLU:OE2	2.38	0.41
1:C:804:PHE:HD2	1:C:804:PHE:O	2.03	0.41
2:D:92:HIS:HB3	2:D:94:GLU:OE2	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:A:676:THR:HG21	1:A:862:MET:HE1	2.02	0.41
1:A:863:SER:O	1:A:864:TYR:C	2.63	0.41
1:A:1012:VAL:O	1:A:1016:VAL:HG13	2.20	0.41
1:C:348:ILE:HG12	1:C:402:ILE:HD12	2.01	0.41
1:C:640:GLU:CD	1:C:640:GLU:N	2.62	0.41
1:C:670:ALA:HB3	1:C:862:MET:CE	2.49	0.41
1:C:682:PHE:HE2	1:C:684:LEU:HD23	1.86	0.41
2:E:23:ARG:C	2:E:25:GLY:N	2.78	0.41
1:A:189:ASN:ND2	1:A:779:TYR:OH	2.53	0.41
1:A:328:ASP:CG	1:A:331:PRO:HD3	2.45	0.41
1:A:404:LEU:HD22	1:A:449:LEU:HD21	2.03	0.41
1:A:449:LEU:HB3	1:A:478:MET:SD	2.61	0.41
1:A:768:VAL:HG12	1:B:67:GLN:HE22	1.84	0.41
1:B:861:GLY:C	1:B:863:SER:N	2.76	0.41
1:B:952:LEU:HD13	1:B:966:ASP:HB3	2.03	0.41
1:C:354:VAL:HG22	1:C:984:LEU:HD12	2.02	0.41
1:C:441:ALA:HB2	1:C:947:GLU:HG2	2.01	0.41
1:C:535:LEU:HD12	1:C:535:LEU:HA	1.88	0.41
1:C:646:ALA:HB1	1:C:650:ARG:NH1	2.35	0.41
1:A:76:MET:HE3	1:A:864:TYR:CE2	2.55	0.41
1:A:452:VAL:CG1	1:A:880:SER:OG	2.69	0.41
1:A:643:LYS:O	1:A:647:ILE:HG13	2.21	0.41
1:A:869:SER:O	1:A:870:GLY:C	2.62	0.41
1:A:1005:THR:OG1	1:A:1006:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:ARG:HE	1:B:540:ARG:HB2	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:C:11:PHE:O	1:C:11:PHE:HD1	2.03	0.41
1:C:26:ALA:O	1:C:30:LEU:HG	2.21	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:328:ASP:CG	1:C:330:THR:HB	2.45	0.41
1:C:544:LEU:HD13	3:C:3043:LMT:H92	2.02	0.41
1:C:774:MET:HB3	5:C:2032:HOH:O	2.20	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:HD13	1:A:972:LEU:O	2.21	0.41
1:B:776:GLU:O	1:B:777:ALA:C	2.63	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
1:C:1029:VAL:O	1:C:1033:PHE:HD1	2.04	0.41
2:E:118:HIS:NE2	2:E:147:LYS:O	2.54	0.41
2:E:141:ALA:O	2:E:148:THR:HG22	2.21	0.41
1:A:5:PHE:HE2	1:A:11:PHE:CD1	2.38	0.41
1:A:19:ILE:CG1	3:B:3036:LMT:H101	2.51	0.41
1:A:60:THR:HG23	1:A:119:PRO:CG	2.51	0.41
1:A:87:THR:HG22	1:A:88:VAL:N	2.35	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:393:LEU:HD23	1:A:470:PHE:CD1	2.52	0.41
1:A:893:GLU:OE2	1:C:10:ILE:HG23	2.21	0.41
1:A:958:LYS:O	1:A:959:GLY:O	2.39	0.41
1:B:366:LEU:C	1:B:366:LEU:HD13	2.46	0.41
1:B:493:CYS:C	1:B:495:THR:H	2.29	0.41
1:B:568:ASP:OD2	1:B:644:VAL:HG12	2.21	0.41
1:B:1024:VAL:O	1:B:1028:VAL:HG22	2.21	0.41
1:C:125:GLN:OE1	1:C:125:GLN:HA	2.20	0.41
1:C:326:PRO:O	1:C:630:SER:HB2	2.20	0.41
1:C:445:ILE:HD11	1:C:944:LEU:HD21	2.01	0.41
1:C:510:LYS:HG2	1:C:511:GLY:N	2.34	0.41
1:C:841:MET:HE3	1:C:859:TRP:CE2	2.55	0.41
1:C:952:LEU:HD13	1:C:956:GLU:HB3	2.03	0.41
2:D:48:TRP:HZ3	2:D:77:ASP:OD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:166:GLN:OE1	2:D:166:GLN:HA	2.20	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:53:ASP:O	1:C:57:VAL:HG12	2.21	0.41
1:C:211:ASN:ND2	1:C:760:ASN:HD21	2.19	0.41
1:C:898:PRO:O	1:C:901:VAL:HG22	2.21	0.41
2:D:102:ASN:N	2:D:102:ASN:HD22	2.19	0.41
2:E:110:ASP:OD1	2:E:110:ASP:C	2.63	0.41
1:A:222:THR:HA	1:A:224:PRO:HD3	2.01	0.40
1:A:486:LEU:HD12	1:A:486:LEU:N	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:332:PHE:CA	1:C:335:ILE:HG22	2.48	0.40
1:C:852:PRO:O	1:C:853:THR:C	2.64	0.40
1:C:1031:ARG:O	1:C:1033:PHE:N	2.54	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:806:SER:HB2	2:E:112:ASN:CG	2.45	0.40
1:A:871:ASN:CG	1:A:872:GLN:H	2.28	0.40
1:A:1038:GLU:O	1:A:1039:ASP:HB3	2.22	0.40
1:B:144:ASN:ND2	1:B:148:THR:CG2	2.84	0.40
1:B:597:TYR:CD2	1:B:597:TYR:C	2.99	0.40
1:B:999:ALA:O	1:B:1003:VAL:HG13	2.21	0.40
1:C:192:GLU:CD	1:C:195:LYS:HD3	2.46	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:960:LEU:HD13	1:A:1027:VAL:HA	2.03	0.40
4:A:3049:LMU:H12	4:A:3049:LMU:H2O2	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:LEU:HD13	1:B:929:VAL:HG12	2.04	0.40
1:B:539:GLY:O	1:B:540:ARG:C	2.63	0.40
1:B:578:LEU:HD23	1:B:578:LEU:N	2.36	0.40
1:B:616:GLY:O	1:B:617:PHE:C	2.63	0.40
1:B:892:TYR:O	1:B:950:LYS:HE3	2.22	0.40
1:C:546:LEU:HD12	1:C:546:LEU:HA	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:242:SER:OG	1:A:245:GLU:HG3	2.22	0.40
1:A:345:VAL:H	4:A:3049:LMU:H81	1.83	0.40
1:A:348:ILE:CD1	4:A:3049:LMU:H123	2.50	0.40
1:A:657:GLN:O	1:A:658:ILE:C	2.64	0.40
1:A:901:VAL:CG2	1:A:946:VAL:HG11	2.52	0.40
1:B:11:PHE:HD2	1:B:11:PHE:O	2.03	0.40
1:B:44:THR:CG2	1:B:89:GLN:HG3	2.52	0.40
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.92	0.40
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:C:867:ARG:HG2	1:C:871:ASN:HD21	1.86	0.40
1:C:934:THR:O	1:C:935:ILE:C	2.64	0.40
1:C:953:MET:HE1	1:C:960:LEU:HD22	2.04	0.40
3:C:3042:LMT:C3'	3:C:3042:LMT:C2B	2.86	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:777:ALA:O	1:A:781:MET:HE3	2.21	0.40
1:A:877:TYR:O	1:A:880:SER:HB3	2.22	0.40
1:B:225:VAL:HG22	1:C:781:MET:HG3	2.03	0.40
1:B:877:TYR:O	1:B:881:LEU:HB2	2.22	0.40
1:C:127:VAL:HG23	1:C:127:VAL:O	2.22	0.40
1:C:360:GLN:NE2	1:C:513:PHE:HB3	2.36	0.40
1:C:372:VAL:N	1:C:373:PRO:CD	2.85	0.40
2:E:34:MET:HE2	2:E:40:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	4	3
1	B	1031/1055 (98%)	945 (92%)	73 (7%)	13 (1%)	9	12
1	C	1038/1055 (98%)	947 (91%)	80 (8%)	11 (1%)	11	15
2	D	154/169 (91%)	146 (95%)	6 (4%)	2 (1%)	9	12
2	E	151/169 (89%)	130 (86%)	17 (11%)	4 (3%)	4	3
All	All	3416/3503 (98%)	3109 (91%)	250 (7%)	57 (2%)	7	8

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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	791 (93%)	59 (7%)	14	20
1	B	839/861 (97%)	773 (92%)	66 (8%)	11	16
1	C	846/861 (98%)	787 (93%)	59 (7%)	14	19
2	D	120/132 (91%)	113 (94%)	7 (6%)	18	27
2	E	118/132 (89%)	110 (93%)	8 (7%)	14	20
All	All	2773/2847 (97%)	2574 (93%)	199 (7%)	13	18

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	30	LEU
1	A	60	THR
1	A	64	VAL
1	A	74	ASN
1	A	85	THR
1	A	88	VAL
1	A	111	LEU
1	A	113	LEU
1	A	121	GLU
1	A	127	VAL
1	A	158	VAL
1	A	214	VAL
1	A	224	PRO
1	A	240	LEU
1	A	262	LEU
1	A	270	LEU
1	A	293	LEU
1	A	310	LEU
1	A	330	THR
1	A	337	ILE
1	A	341	VAL
1	A	351	VAL
1	A	376	LEU
1	A	394	THR
1	A	414	GLU
1	A	431	THR
1	A	449	LEU

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Mol	Chain	Res	Type
1	A	452	VAL
1	A	470	PHE
1	A	473	THR
1	A	522	LYS
1	A	577	GLN
1	A	612	VAL
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	801	PHE
1	A	828	LEU
1	A	833	PRO
1	A	842	GLU
1	A	872	GLN
1	A	883	VAL
1	A	935	ILE
1	A	946	VAL
1	A	961	ILE
1	A	962	GLU
1	A	971	ARG
1	A	990	VAL
1	A	1019	ILE
1	A	1038	GLU
1	A	1040	ILE
1	A	1041	GLU
1	A	1042	HIS
1	B	3	ASN
1	B	38	ILE
1	B	55	LYS
1	B	75	LEU
1	B	78	MET
1	B	88	VAL
1	B	105	VAL
1	B	108	GLN
1	B	111	LEU
1	B	121	GLU
1	B	139	VAL

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Mol	Chain	Res	Type
1	B	163	LYS
1	B	172	VAL
1	B	192	GLU
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	285	PRO
1	B	293	LEU
1	B	306	ILE
1	B	354	VAL
1	B	355	MET
1	B	361	ASN
1	B	365	THR
1	B	382	VAL
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
1	B	578	LEU
1	B	587	THR
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	713	LEU
1	B	714	THR
1	B	778	LYS
1	B	784	ASP
1	B	850	LYS

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Mol	Chain	Res	Type
1	B	862	MET
1	B	881	LEU
1	B	888	LEU
1	B	914	LEU
1	B	921	LEU
1	B	925	VAL
1	B	937	LEU
1	B	956	GLU
1	B	960	LEU
1	B	965	LEU
1	B	968	VAL
1	B	1022	VAL
1	B	1033	PHE
1	C	10	ILE
1	C	14	VAL
1	C	34	GLN
1	C	55	LYS
1	C	88	VAL
1	C	113	LEU
1	C	121	GLU
1	C	125	GLN
1	C	127	VAL
1	C	153	ASP
1	C	158	VAL
1	C	177	LEU
1	C	213	GLN
1	C	224	PRO
1	C	229	GLN
1	C	243	THR
1	C	289	LEU
1	C	310	LEU
1	C	324	VAL
1	C	344	LEU
1	C	372	VAL
1	C	383	LEU
1	C	392	THR
1	C	394	THR
1	C	404	LEU
1	C	425	LEU
1	C	448	VAL
1	C	450	SER
1	C	482	VAL

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Mol	Chain	Res	Type
1	C	483	LEU
1	C	518	ARG
1	C	519	MET
1	C	544	LEU
1	C	571	VAL
1	C	575	MET
1	C	601	LYS
1	C	640	GLU
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	822	LEU
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	993	THR
1	C	1011	MET
1	C	1017	LEU
1	C	1019	ILE
1	C	1036	LYS
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	D	166	GLN
2	E	26	ARG
2	E	34	MET
2	E	48	TRP
2	E	119	LEU
2	E	123	ARG

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Mol	Chain	Res	Type
2	E	154	ILE
2	E	164	ILE
2	E	166	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) 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	237	GLN
1	A	254	ASN
1	A	338	HIS
1	A	361	ASN
1	A	505	HIS
1	A	526	HIS
1	A	569	GLN
1	A	577	GLN
1	A	687	GLN
1	A	701	GLN
1	A	865	GLN
1	A	872	GLN
1	A	928	GLN
1	A	941	ASN
1	A	1000	GLN
1	A	1001	ASN
1	A	1037	ASN
1	A	1042	HIS
1	B	3	ASN
1	B	58	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	254	ASN
1	B	360	GLN
1	B	361	ASN
1	B	469	GLN

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Mol	Chain	Res	Type
1	B	505	HIS
1	B	584	GLN
1	B	592	ASN
1	B	687	GLN
1	B	701	GLN
1	B	733	GLN
1	B	747	ASN
1	B	846	GLN
1	B	871	ASN
1	B	941	ASN
1	B	1000	GLN
1	B	1001	ASN
1	C	3	ASN
1	C	67	GLN
1	C	81	ASN
1	C	125	GLN
1	C	194	ASN
1	C	197	GLN
1	C	211	ASN
1	C	213	GLN
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	737	GLN
1	C	747	ASN
1	C	846	GLN
1	C	871	ASN
1	C	1037	ASN
2	D	36	ASN
2	D	59	HIS
2	D	102	ASN
2	D	122	ASN
2	E	92	HIS
2	E	125	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 oligosaccharides 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	C	3043	-	36,36,36	1.72	5 (13%)	47,47,47	1.76	10 (21%)
3	LMT	C	3046	-	36,36,36	0.64	1 (2%)	47,47,47	1.32	7 (14%)
3	LMT	A	3048	-	36,36,36	1.48	4 (11%)	47,47,47	1.33	6 (12%)
3	LMT	C	3042	-	36,36,36	0.51	0	47,47,47	1.51	6 (12%)
3	LMT	B	3036	-	36,36,36	0.52	0	47,47,47	1.60	8 (17%)
3	LMT	B	3037	-	36,36,36	0.72	1 (2%)	47,47,47	1.99	9 (19%)
3	LMT	C	3044	-	36,36,36	0.43	0	47,47,47	1.54	6 (12%)
3	LMT	A	3046	-	36,36,36	1.16	4 (11%)	47,47,47	1.39	5 (10%)
4	LMU	A	3049	-	36,36,36	0.54	0	47,47,47	1.23	4 (8%)
3	LMT	B	3035	-	36,36,36	0.47	0	47,47,47	1.20	6 (12%)
3	LMT	A	3047	-	36,36,36	0.64	1 (2%)	47,47,47	1.67	9 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	C	3043	-	-	9/21/61/61	0/2/2/2
3	LMT	C	3046	-	-	9/21/61/61	0/2/2/2
3	LMT	A	3048	-	-	11/21/61/61	0/2/2/2
3	LMT	C	3042	-	-	14/21/61/61	0/2/2/2
3	LMT	B	3036	-	-	13/21/61/61	0/2/2/2
3	LMT	B	3037	-	-	17/21/61/61	0/2/2/2
3	LMT	C	3044	-	-	11/21/61/61	0/2/2/2
3	LMT	A	3046	-	-	13/21/61/61	0/2/2/2
4	LMU	A	3049	-	-	12/21/61/61	0/2/2/2
3	LMT	B	3035	-	-	12/21/61/61	0/2/2/2
3	LMT	A	3047	-	-	11/21/61/61	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3043	LMT	C2-C1	6.72	1.78	1.51
3	A	3048	LMT	C2-C1	-5.43	1.28	1.51
3	A	3048	LMT	O1'-C1'	3.73	1.46	1.40
3	C	3043	LMT	O1'-C1'	3.45	1.45	1.40
3	A	3046	LMT	O5B-C5B	3.37	1.52	1.44
3	C	3043	LMT	O5B-C5B	3.15	1.52	1.44
3	C	3043	LMT	O5B-C1B	3.11	1.49	1.41
3	C	3043	LMT	O1B-C1B	3.11	1.50	1.41
3	B	3037	LMT	O1'-C1'	2.76	1.44	1.40
3	C	3046	LMT	O1'-C1'	2.60	1.44	1.40
3	A	3048	LMT	O5B-C1B	2.50	1.48	1.41
3	A	3048	LMT	O5B-C5B	2.40	1.50	1.44
3	A	3046	LMT	O5B-C1B	2.38	1.48	1.41
3	A	3046	LMT	O1'-C1'	2.32	1.44	1.40
3	A	3047	LMT	O1'-C1'	2.31	1.44	1.40
3	A	3046	LMT	C6B-C5B	2.11	1.58	1.51

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3037	LMT	O1'-C1'-C2'	5.82	117.11	108.27
3	B	3036	LMT	C1-O1'-C1'	-5.48	104.33	113.68
3	B	3037	LMT	O5B-C5B-C4B	-5.40	99.97	109.70
3	C	3044	LMT	O1'-C1'-C2'	5.31	116.33	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3047	LMT	O1'-C1'-C2'	5.14	116.07	108.27
3	C	3043	LMT	O1'-C1-C2	-4.87	92.85	109.37
3	C	3042	LMT	C1B-O1B-C4'	-4.86	106.46	117.98
4	A	3049	LMU	C3'-C4'-C5'	-4.81	100.28	110.93
3	B	3037	LMT	O5'-C1'-C2'	-4.77	100.56	110.37
3	C	3044	LMT	C1-O1'-C1'	-4.69	105.68	113.68
3	B	3037	LMT	C1'-O5'-C5'	-4.61	104.72	113.72
3	C	3043	LMT	O5B-C5B-C6B	4.59	117.82	106.44
3	A	3048	LMT	O1'-C1-C2	4.44	124.44	109.37
3	A	3046	LMT	O5B-C5B-C4B	4.40	117.63	109.70
3	B	3037	LMT	C1B-O1B-C4'	-4.33	107.70	117.98
3	C	3046	LMT	C3'-C4'-C5'	-4.33	101.33	110.93
3	A	3047	LMT	O5B-C1B-C2B	4.25	119.09	110.37
3	C	3043	LMT	O5'-C5'-C4'	4.11	118.22	109.72
3	C	3044	LMT	C1'-O5'-C5'	-4.09	105.73	113.72
3	A	3047	LMT	O5B-C5B-C4B	3.97	116.85	109.70
3	B	3037	LMT	C1B-O5B-C5B	-3.91	106.08	113.72
3	C	3043	LMT	C3'-C4'-C5'	-3.86	102.37	110.93
3	B	3036	LMT	O5B-C1B-C2B	3.84	118.27	110.37
3	C	3042	LMT	O1B-C4'-C3'	3.75	116.77	107.23
3	C	3043	LMT	O1B-C4'-C3'	3.75	116.76	107.23
3	B	3036	LMT	C6B-C5B-C4B	-3.66	104.04	113.02
3	A	3047	LMT	C3'-C4'-C5'	-3.43	103.34	110.93
3	A	3046	LMT	C3'-C4'-C5'	-3.34	103.53	110.93
3	C	3042	LMT	C4B-C3B-C2B	-3.27	105.09	110.83
3	B	3037	LMT	O1B-C4'-C5'	-3.26	100.94	109.48
4	A	3049	LMU	O5'-C1'-C2'	3.25	117.06	110.37
3	B	3036	LMT	C1B-C2B-C3B	3.17	116.69	110.01
3	A	3047	LMT	O5'-C1'-C2'	-3.16	103.88	110.37
3	C	3042	LMT	C1-O1'-C1'	-3.06	108.45	113.68
3	A	3047	LMT	C1B-O5B-C5B	3.06	119.70	113.72
3	C	3044	LMT	O5B-C5B-C6B	3.01	113.90	106.44
3	A	3047	LMT	C1B-O1B-C4'	-2.89	111.12	117.98
3	C	3042	LMT	C6'-C5'-C4'	-2.86	105.32	113.38
3	C	3043	LMT	O5'-C5'-C6'	-2.81	99.47	106.44
3	B	3037	LMT	O1B-C1B-O5B	-2.81	103.31	110.69
3	B	3035	LMT	O5'-C1'-C2'	-2.72	104.78	110.37
3	A	3046	LMT	C1B-O5B-C5B	2.71	119.02	113.72
3	C	3043	LMT	C6B-C5B-C4B	-2.70	106.38	113.02
3	A	3048	LMT	C3B-C4B-C5B	-2.66	105.41	110.23
3	C	3046	LMT	O5B-C5B-C4B	-2.63	104.96	109.70
3	A	3048	LMT	C1B-O5B-C5B	2.61	118.81	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3035	LMT	C1B-O1B-C4'	-2.60	111.81	117.98
3	C	3046	LMT	C1B-C2B-C3B	2.59	115.45	110.01
3	B	3035	LMT	O1B-C1B-C2B	2.58	114.44	108.09
3	B	3037	LMT	O5'-C5'-C6'	2.57	112.81	106.44
3	C	3046	LMT	C1'-O5'-C5'	-2.51	108.81	113.72
3	B	3036	LMT	O1B-C4'-C3'	2.48	113.53	107.23
3	C	3044	LMT	O5'-C1'-C2'	-2.43	105.37	110.37
3	A	3047	LMT	C6B-C5B-C4B	-2.43	107.06	113.02
3	A	3046	LMT	O5B-C5B-C6B	2.41	112.42	106.44
3	C	3043	LMT	O1B-C1B-O5B	2.39	116.98	110.69
3	A	3047	LMT	O1'-C1-C2	2.33	117.29	109.37
3	C	3046	LMT	C1B-O1B-C4'	-2.33	112.47	117.98
4	A	3049	LMU	C1'-C2'-C3'	2.30	114.84	110.01
3	B	3036	LMT	O5'-C5'-C6'	2.24	111.98	106.44
3	C	3043	LMT	O1'-C1'-C2'	2.22	111.65	108.27
3	B	3036	LMT	C1'-O5'-C5'	-2.22	109.39	113.72
3	C	3044	LMT	C1B-O1B-C4'	-2.20	112.76	117.98
3	B	3035	LMT	C1'-O5'-C5'	-2.19	109.45	113.72
4	A	3049	LMU	C1B-O1B-C4'	-2.16	112.85	117.98
3	C	3046	LMT	C1B-O5B-C5B	-2.15	109.52	113.72
3	A	3048	LMT	O1'-C1'-C2'	2.15	111.54	108.27
3	C	3046	LMT	C1-O1'-C1'	-2.15	110.01	113.68
3	C	3043	LMT	C1B-O5B-C5B	2.13	117.88	113.72
3	C	3042	LMT	C6B-C5B-C4B	-2.12	107.83	113.02
3	A	3048	LMT	C2'-C3'-C4'	2.11	114.47	109.68
3	A	3048	LMT	C1'-C2'-C3'	2.08	114.39	110.01
3	B	3035	LMT	O5'-C1'-O1'	-2.07	105.16	110.04
3	B	3036	LMT	O1B-C1B-O5B	2.06	116.12	110.69
3	A	3046	LMT	O3B-C3B-C4B	2.06	115.23	110.38
3	B	3035	LMT	C6B-C5B-C4B	-2.02	108.05	113.02

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3047	LMT	C2'-C1'-O1'-C1
3	A	3047	LMT	O5'-C1'-O1'-C1
3	B	3036	LMT	O5'-C1'-O1'-C1
3	B	3036	LMT	C2-C1-O1'-C1'
3	C	3046	LMT	C2'-C1'-O1'-C1
4	A	3049	LMU	C2'-C1'-O1'-C1
4	A	3049	LMU	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
3	C	3044	LMT	O5B-C1B-O1B-C4'
3	A	3048	LMT	O5B-C1B-O1B-C4'
3	B	3036	LMT	C4B-C5B-C6B-O6B
3	C	3042	LMT	C3'-C4'-O1B-C1B
4	A	3049	LMU	C4B-C5B-C6B-O6B
3	A	3048	LMT	O5B-C5B-C6B-O6B
3	C	3043	LMT	O5'-C5'-C6'-O6'
3	B	3037	LMT	O5B-C5B-C6B-O6B
3	B	3037	LMT	O5'-C5'-C6'-O6'
3	A	3047	LMT	C4'-C5'-C6'-O6'
3	C	3043	LMT	O5B-C5B-C6B-O6B
3	A	3047	LMT	C4B-C5B-C6B-O6B
3	B	3037	LMT	O5B-C1B-O1B-C4'
3	B	3036	LMT	O5B-C5B-C6B-O6B
3	B	3037	LMT	C4B-C5B-C6B-O6B
3	C	3043	LMT	C4'-C5'-C6'-O6'
3	C	3044	LMT	C4B-C5B-C6B-O6B
3	A	3046	LMT	O5B-C5B-C6B-O6B
3	A	3047	LMT	O5B-C5B-C6B-O6B
3	C	3046	LMT	O5'-C5'-C6'-O6'
3	A	3048	LMT	C4B-C5B-C6B-O6B
3	B	3037	LMT	C4'-C5'-C6'-O6'
3	A	3048	LMT	O5'-C1'-O1'-C1
3	C	3046	LMT	O5'-C1'-O1'-C1
3	C	3046	LMT	C4'-C5'-C6'-O6'
4	A	3049	LMU	O5B-C5B-C6B-O6B
3	A	3046	LMT	C4'-C5'-C6'-O6'
3	A	3046	LMT	C4B-C5B-C6B-O6B
3	A	3048	LMT	C2'-C1'-O1'-C1
3	A	3046	LMT	O5'-C5'-C6'-O6'
3	C	3044	LMT	O5B-C5B-C6B-O6B
3	A	3048	LMT	O5'-C5'-C6'-O6'
3	C	3043	LMT	C4B-C5B-C6B-O6B
3	C	3042	LMT	O5B-C1B-O1B-C4'
3	B	3037	LMT	O5'-C1'-O1'-C1
3	A	3047	LMT	O5'-C5'-C6'-O6'
3	C	3046	LMT	O5B-C5B-C6B-O6B
3	A	3048	LMT	O1'-C1-C2-C3
3	C	3044	LMT	O1'-C1-C2-C3
4	A	3049	LMU	O5'-C5'-C6'-O6'
3	C	3042	LMT	C5'-C4'-O1B-C1B
3	B	3037	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
3	B	3037	LMT	O1'-C1-C2-C3
3	A	3046	LMT	O1'-C1-C2-C3
3	B	3036	LMT	O1'-C1-C2-C3
3	B	3035	LMT	O5'-C1'-O1'-C1
3	C	3046	LMT	C4B-C5B-C6B-O6B
3	B	3036	LMT	C9-C10-C11-C12
3	B	3037	LMT	C2B-C1B-O1B-C4'
3	C	3042	LMT	C2B-C1B-O1B-C4'
3	B	3037	LMT	C1-C2-C3-C4
3	B	3035	LMT	O1'-C1-C2-C3
3	A	3046	LMT	C1-C2-C3-C4
3	A	3046	LMT	C2-C1-O1'-C1'
3	C	3042	LMT	C2-C1-O1'-C1'
3	B	3035	LMT	C3-C4-C5-C6
3	C	3044	LMT	C11-C10-C9-C8
3	C	3043	LMT	O1'-C1-C2-C3
3	A	3047	LMT	C11-C10-C9-C8
3	B	3036	LMT	C4-C5-C6-C7
4	A	3049	LMU	C2-C3-C4-C5
4	A	3049	LMU	C1-C2-C3-C4
3	B	3035	LMT	C2-C3-C4-C5
3	A	3046	LMT	C7-C8-C9-C10
3	B	3036	LMT	C7-C8-C9-C10
3	B	3037	LMT	C11-C10-C9-C8
3	B	3036	LMT	C11-C10-C9-C8
3	C	3042	LMT	C3-C4-C5-C6
3	A	3046	LMT	C6-C7-C8-C9
3	A	3048	LMT	C5-C6-C7-C8
3	B	3036	LMT	C2-C3-C4-C5
3	C	3042	LMT	O5'-C5'-C6'-O6'
3	B	3037	LMT	C5-C6-C7-C8
3	C	3042	LMT	C2-C3-C4-C5
3	A	3047	LMT	C9-C10-C11-C12
3	C	3043	LMT	C9-C10-C11-C12
3	C	3046	LMT	C11-C10-C9-C8
3	B	3035	LMT	C9-C10-C11-C12
3	C	3044	LMT	C9-C10-C11-C12
3	B	3037	LMT	C4-C5-C6-C7
3	B	3035	LMT	C2-C1-O1'-C1'
3	B	3036	LMT	C5'-C4'-O1B-C1B
3	A	3048	LMT	C9-C10-C11-C12
4	A	3049	LMU	C9-C10-C11-C12

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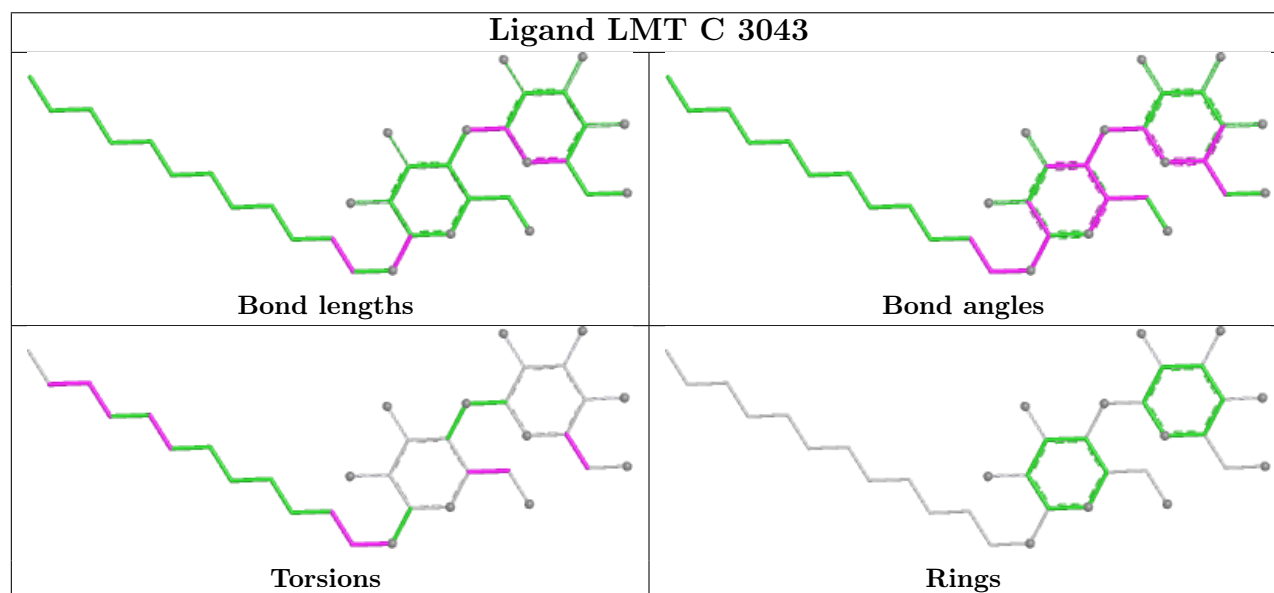
Mol	Chain	Res	Type	Atoms
3	A	3047	LMT	C7-C8-C9-C10
3	C	3044	LMT	C3-C4-C5-C6
3	A	3046	LMT	C9-C10-C11-C12
3	B	3037	LMT	C6-C7-C8-C9
3	C	3046	LMT	C6-C7-C8-C9
4	A	3049	LMU	C3-C4-C5-C6
3	A	3048	LMT	C4'-C5'-C6'-O6'
3	B	3036	LMT	C3'-C4'-O1B-C1B
3	A	3046	LMT	C4-C5-C6-C7
3	C	3042	LMT	C6-C7-C8-C9
3	C	3042	LMT	C11-C10-C9-C8
3	C	3043	LMT	C11-C10-C9-C8
3	A	3047	LMT	O5B-C1B-O1B-C4'
3	B	3037	LMT	C2-C1-O1'-C1'
3	A	3046	LMT	C5-C6-C7-C8
4	A	3049	LMU	C4'-C5'-C6'-O6'
3	C	3044	LMT	C7-C8-C9-C10
3	C	3042	LMT	C5-C6-C7-C8
4	A	3049	LMU	C11-C10-C9-C8
3	A	3048	LMT	C1-C2-C3-C4
3	C	3046	LMT	C9-C10-C11-C12
3	A	3046	LMT	C11-C10-C9-C8
3	B	3035	LMT	C11-C10-C9-C8
3	A	3047	LMT	C2-C1-O1'-C1'
3	C	3043	LMT	C2-C1-O1'-C1'
3	C	3044	LMT	C2-C1-O1'-C1'
3	B	3035	LMT	C4B-C5B-C6B-O6B
4	A	3049	LMU	O1'-C1-C2-C3
3	B	3035	LMT	C7-C8-C9-C10
3	B	3037	LMT	C9-C10-C11-C12
3	B	3035	LMT	C2'-C1'-O1'-C1
3	B	3035	LMT	C6-C7-C8-C9
3	C	3042	LMT	C1-C2-C3-C4
3	B	3035	LMT	C5-C6-C7-C8
3	C	3043	LMT	C6-C7-C8-C9
3	C	3042	LMT	C9-C10-C11-C12
3	B	3036	LMT	O5B-C1B-O1B-C4'
3	C	3044	LMT	C5-C6-C7-C8
3	C	3044	LMT	C5'-C4'-O1B-C1B
3	C	3042	LMT	O5B-C5B-C6B-O6B
3	B	3037	LMT	C3-C4-C5-C6

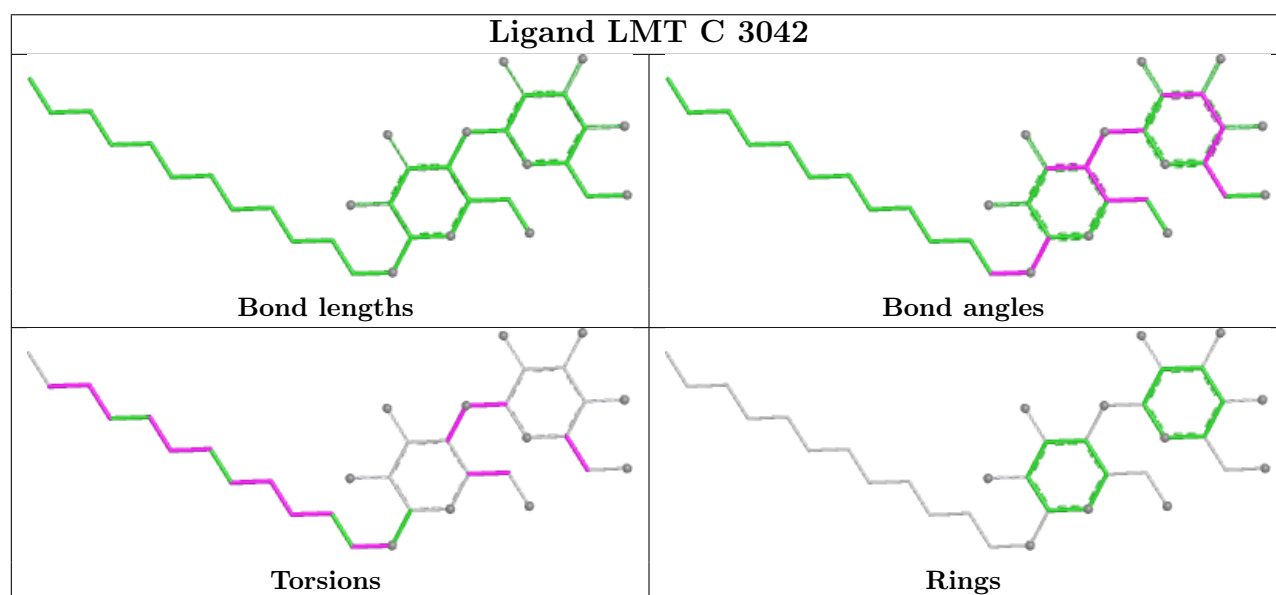
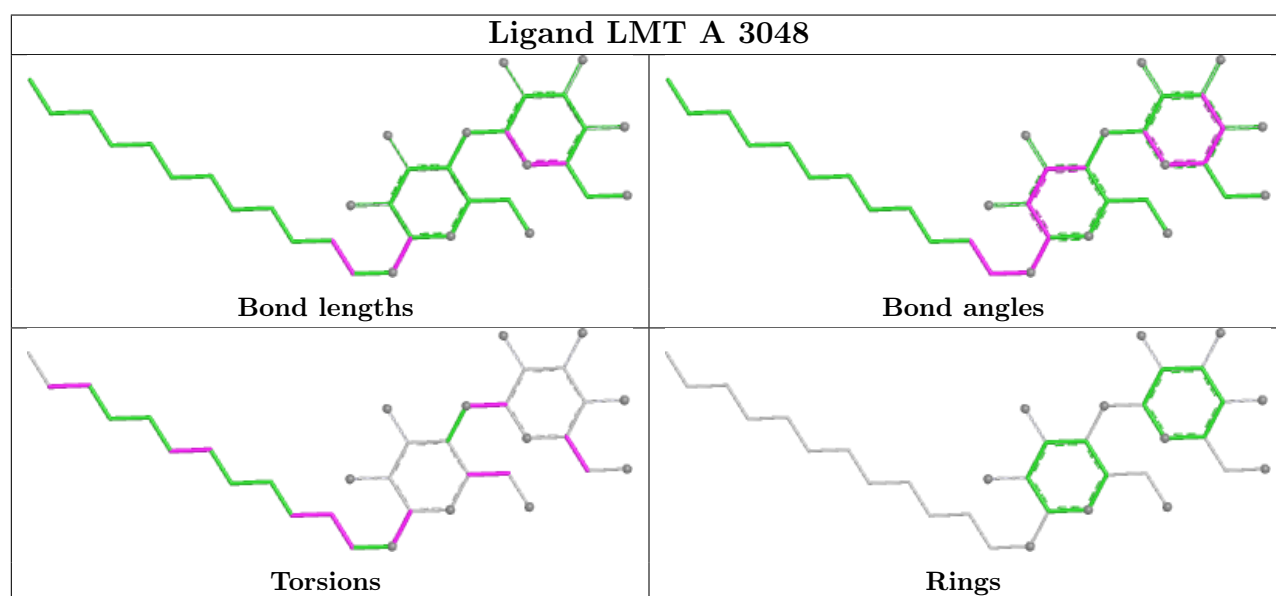
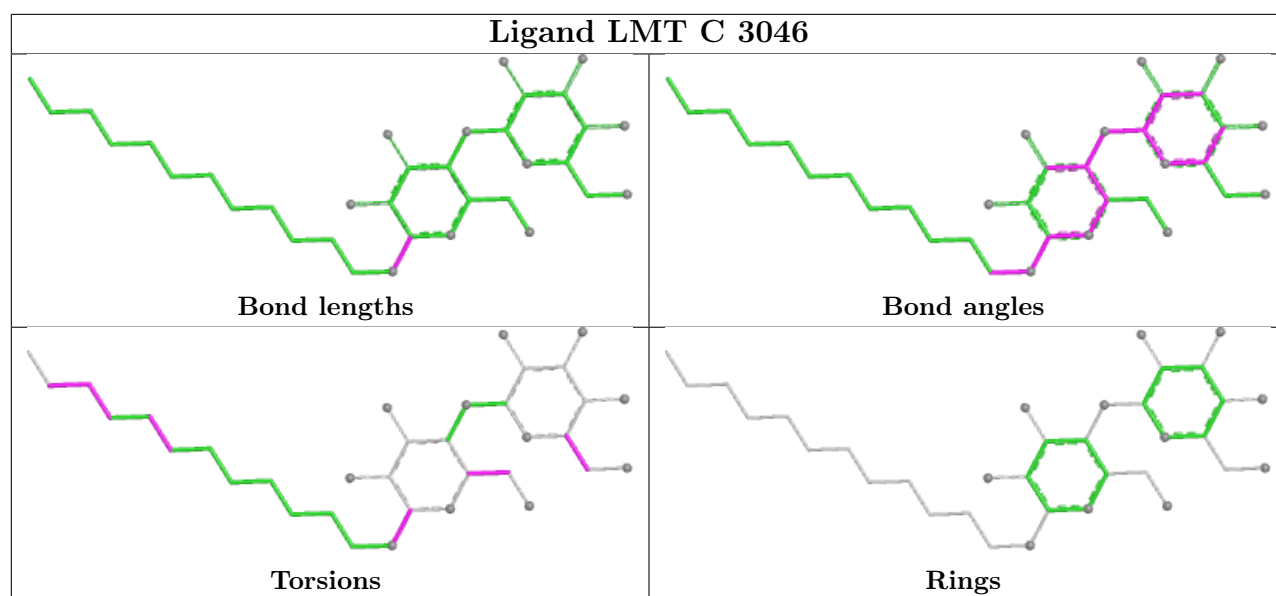
There are no ring outliers.

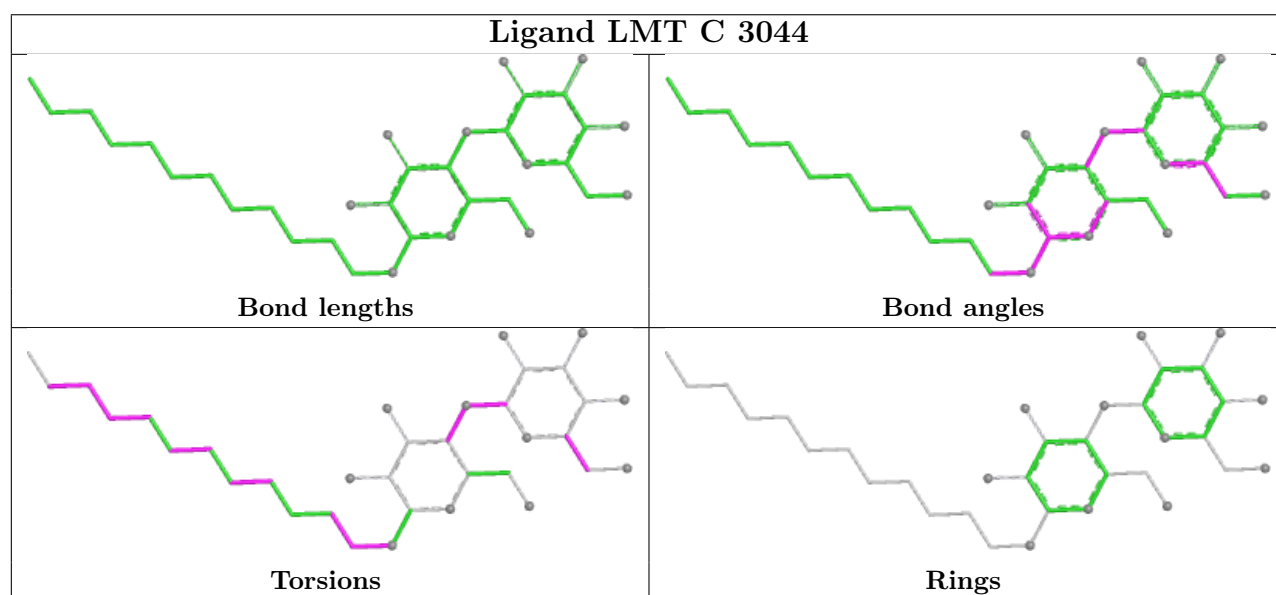
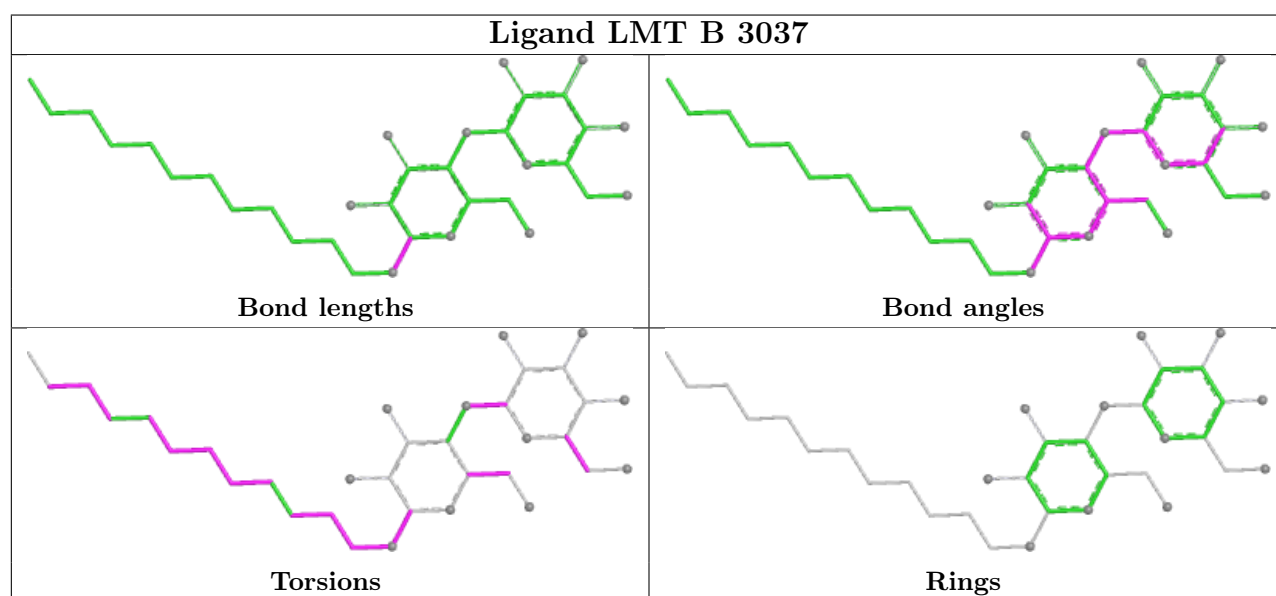
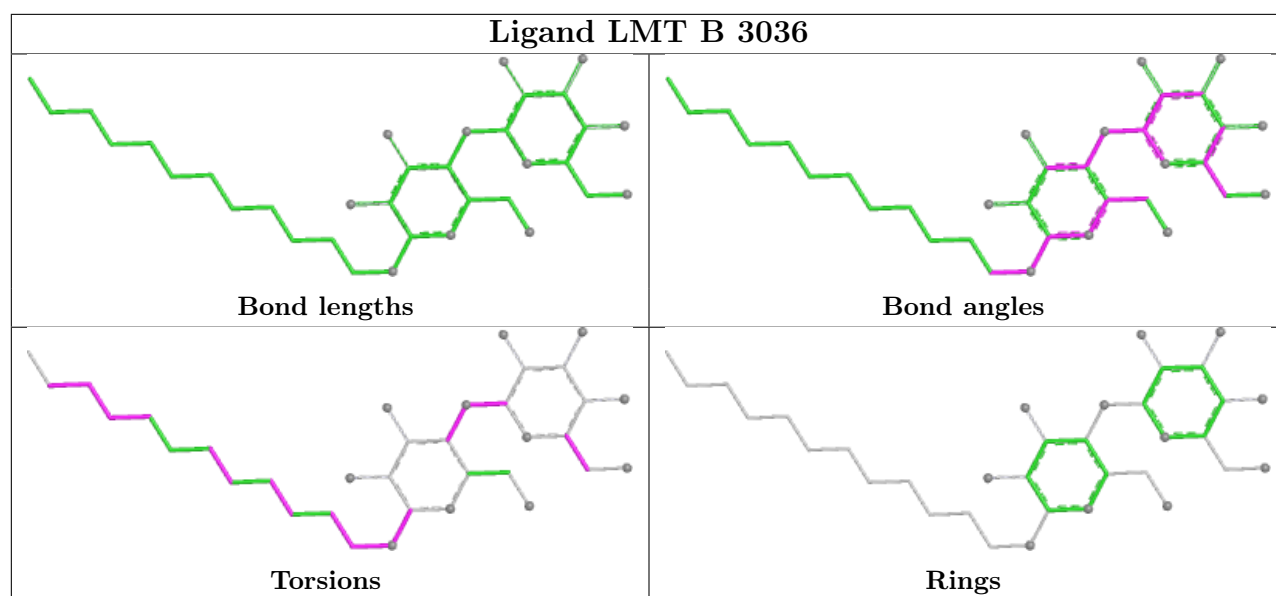
11 monomers are involved in 236 short contacts:

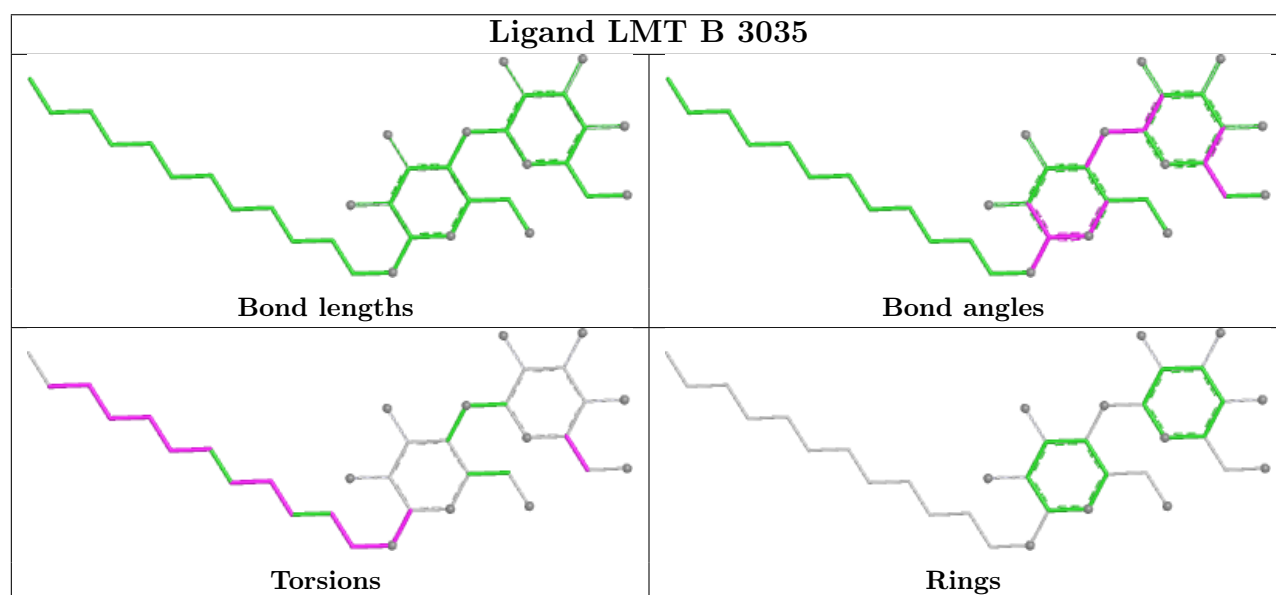
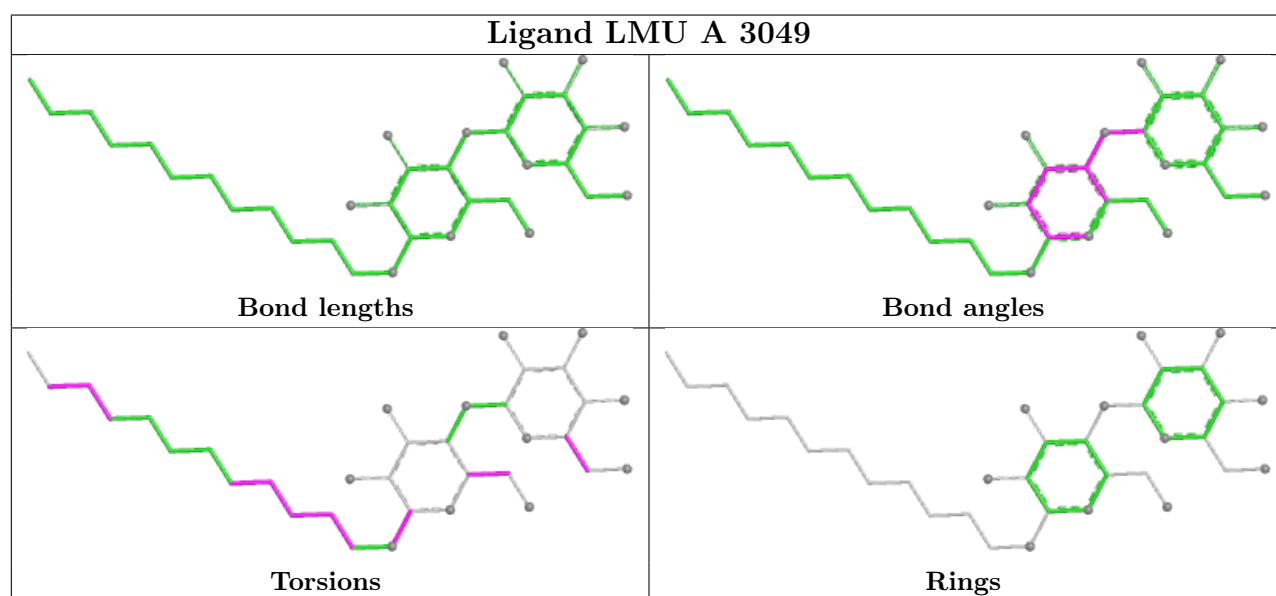
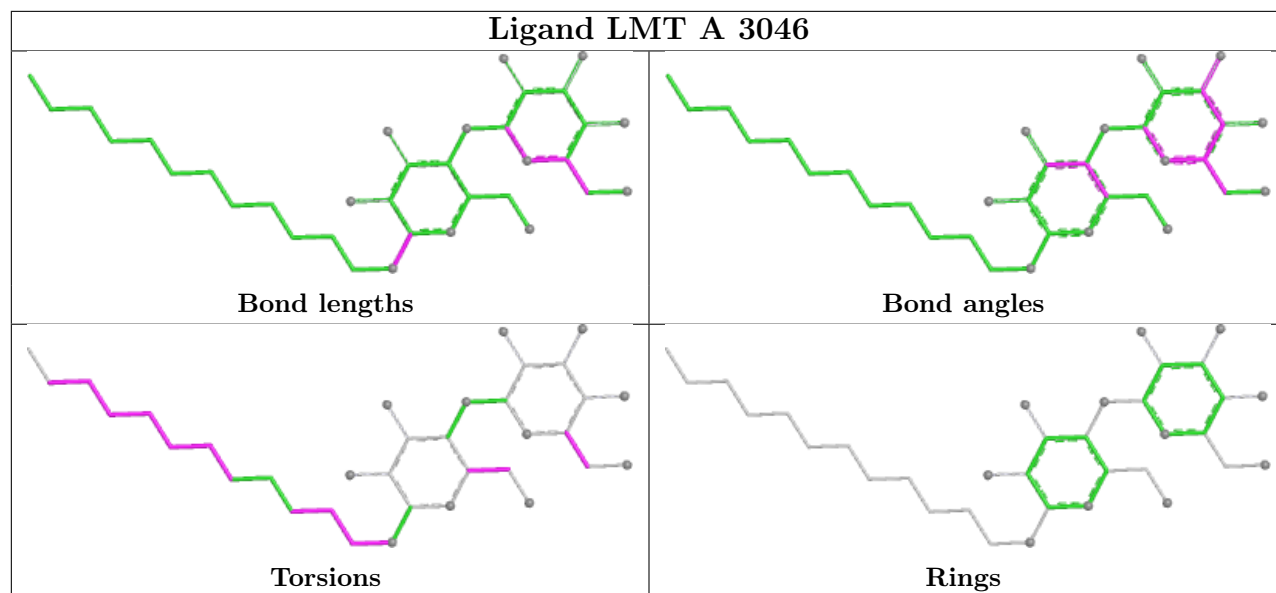
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3043	LMT	15	0
3	C	3046	LMT	14	0
3	A	3048	LMT	26	0
3	C	3042	LMT	17	0
3	B	3036	LMT	18	0
3	B	3037	LMT	29	0
3	C	3044	LMT	11	0
3	A	3046	LMT	10	0
4	A	3049	LMU	51	0
3	B	3035	LMT	3	0
3	A	3047	LMT	48	0

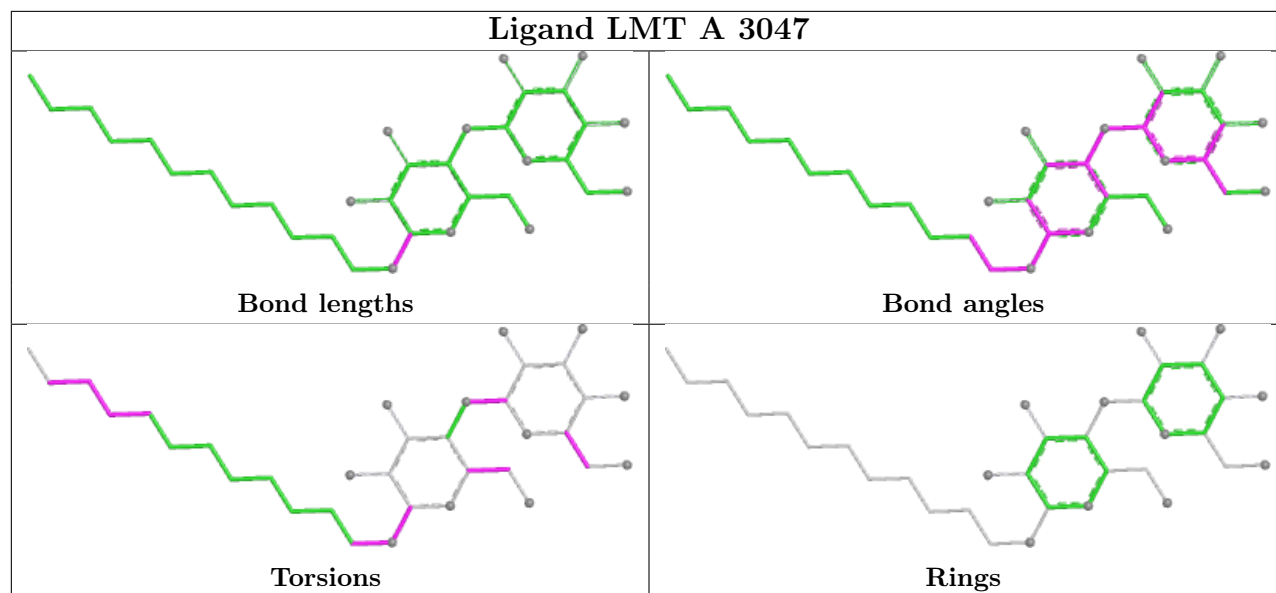
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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%)	0.26	66 (6%)	26	25	13, 43, 87, 106	0
1	B	1033/1055 (97%)	0.13	32 (3%)	51	52	14, 40, 66, 89	0
1	C	1040/1055 (98%)	0.01	22 (2%)	63	64	16, 36, 62, 94	0
2	D	156/169 (92%)	0.01	1 (0%)	85	88	25, 39, 63, 75	0
2	E	153/169 (90%)	0.55	4 (2%)	57	58	28, 54, 76, 81	0
All	All	3426/3503 (97%)	0.15	125 (3%)	46	47	13, 40, 73, 106	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	873	ALA	6.4
1	C	1040	ILE	6.3
1	A	674	LEU	5.5
1	B	563	PHE	5.1
1	B	672	VAL	5.0
1	C	1034	SER	4.9
1	A	1044	HIS	4.9
1	A	918	PHE	4.8
1	C	506	GLY	4.7
1	A	1040	ILE	4.6
1	A	868	LEU	4.3
1	A	459	PHE	4.2
1	A	675	GLY	4.2
1	A	961	ILE	4.2
1	B	873	ALA	4.2
1	B	674	LEU	4.1
1	A	538	THR	4.0
1	B	513	PHE	3.9
1	A	670	ALA	3.9
1	A	870	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	510	LYS	3.6
1	B	666	PHE	3.6
1	B	515	TRP	3.6
1	B	134	SER	3.6
1	A	869	SER	3.5
1	A	362	PHE	3.5
1	A	539	GLY	3.5
1	A	872	GLN	3.5
1	A	874	PRO	3.5
1	C	508	GLY	3.5
1	A	448	VAL	3.4
2	E	14	LEU	3.4
1	A	678	THR	3.4
1	A	671	ILE	3.4
2	D	166	GLN	3.3
1	C	1038	GLU	3.3
1	C	1033	PHE	3.3
1	A	876	LEU	3.3
1	B	678	THR	3.2
1	A	1035	ARG	3.1
1	B	676	THR	3.1
1	C	967	ALA	3.1
1	A	676	THR	3.0
1	A	1043	SER	3.0
1	B	871	ASN	3.0
1	A	932	LEU	3.0
1	A	866	GLU	2.9
1	A	510	LYS	2.9
1	A	1042	HIS	2.9
1	B	575	MET	2.9
1	A	672	VAL	2.8
1	A	516	PHE	2.8
1	B	644	VAL	2.8
1	B	866	GLU	2.8
1	A	431	THR	2.8
1	C	1035	ARG	2.8
1	B	877	TYR	2.7
1	B	673	GLU	2.7
1	C	70	ASN	2.7
1	B	867	ARG	2.7
1	B	639	GLY	2.6
1	A	712	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	957	GLY	2.6
1	C	497	LEU	2.6
1	B	1033	PHE	2.6
2	E	99	LEU	2.6
1	A	11	PHE	2.6
1	A	952	LEU	2.5
1	C	423	GLU	2.5
1	A	960	LEU	2.5
1	A	452	VAL	2.5
1	A	1033	PHE	2.5
1	B	658	ILE	2.5
1	A	496	MET	2.5
1	C	503	GLY	2.4
1	C	1036	LYS	2.4
2	E	33	LEU	2.4
1	B	615	PHE	2.4
1	A	498	LYS	2.4
1	A	887	CYS	2.4
1	A	668	LEU	2.4
1	A	946	VAL	2.4
1	A	446	ALA	2.4
1	A	659	LYS	2.4
1	A	956	GLU	2.4
1	C	811	TYR	2.4
1	A	965	LEU	2.3
1	A	429	GLU	2.3
1	A	501	ALA	2.3
1	A	955	LYS	2.3
1	A	1034	SER	2.3
1	A	3	ASN	2.3
1	B	675	GLY	2.3
1	B	562	SER	2.3
1	A	657	GLN	2.2
1	B	870	GLY	2.2
1	A	509	LYS	2.2
1	A	432	ARG	2.2
1	A	871	ASN	2.2
1	A	1036	LYS	2.2
1	B	360	GLN	2.2
1	A	542	LEU	2.2
1	B	133	SER	2.2
1	B	869	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	867	ARG	2.2
1	B	634	TRP	2.2
1	B	861	GLY	2.2
1	C	362	PHE	2.2
1	C	29	LYS	2.1
1	A	995	ALA	2.1
1	C	507	GLU	2.1
2	E	101	LYS	2.1
1	C	674	LEU	2.1
1	A	463	THR	2.1
1	A	500	ILE	2.1
1	B	671	ILE	2.1
1	C	505	HIS	2.1
1	A	1026	PHE	2.1
1	A	832	ALA	2.1
1	A	669	PRO	2.1
1	C	968	VAL	2.0
1	B	677	ALA	2.0
1	A	405	LEU	2.0
1	B	511	GLY	2.0
1	C	509	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LMT	C	3042	35/35	0.69	0.25	94,97,104,105	0
3	LMT	A	3047	35/35	0.75	0.24	75,83,117,118	0

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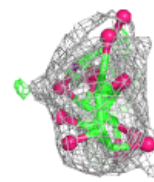
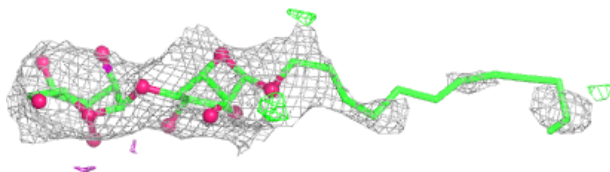
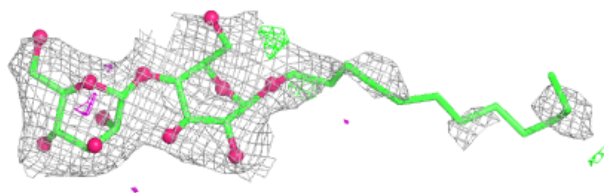
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LMT	C	3044	35/35	0.75	0.19	57,84,94,95	0
3	LMT	C	3046	35/35	0.76	0.24	103,106,110,111	0
3	LMT	B	3036	35/35	0.79	0.17	65,78,86,87	0
3	LMT	A	3048	35/35	0.80	0.22	90,92,116,117	0
4	LMU	A	3049	35/35	0.81	0.22	90,98,121,121	0
3	LMT	B	3035	35/35	0.83	0.15	56,67,69,71	0
3	LMT	B	3037	35/35	0.83	0.31	124,128,147,149	0
3	LMT	C	3043	35/35	0.84	0.19	64,70,112,113	0
3	LMT	A	3046	35/35	0.86	0.13	48,59,69,70	0

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

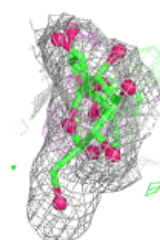
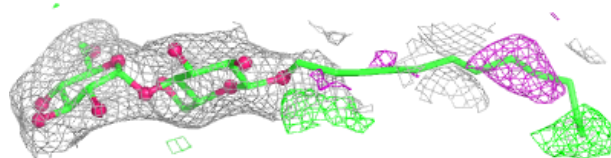
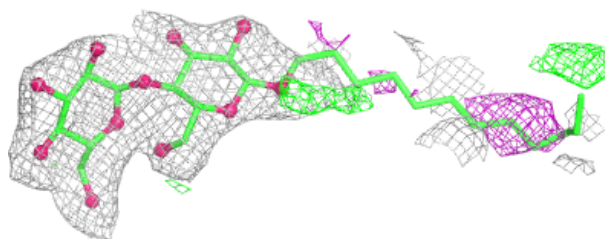
Electron density around LMT C 3042:

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

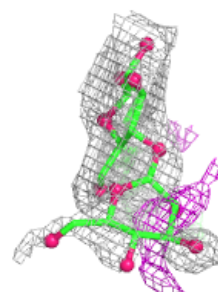
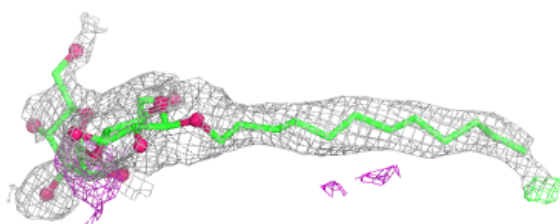
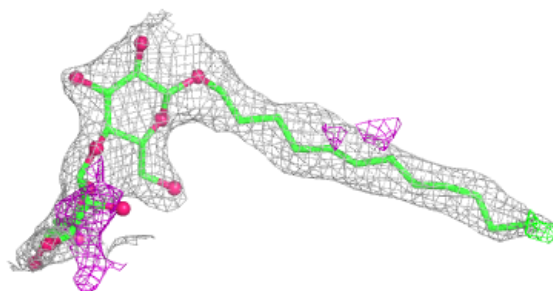


Electron density around LMT A 3047:

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

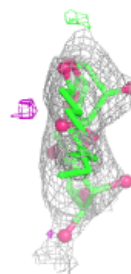
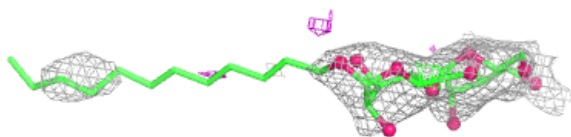
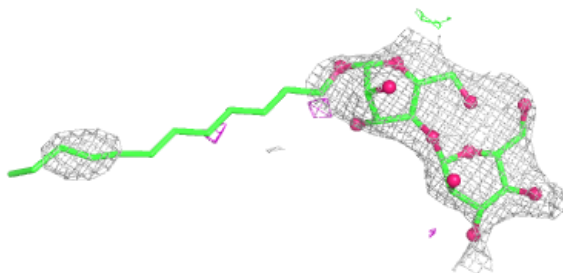
**Electron density around LMT C 3044:**

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

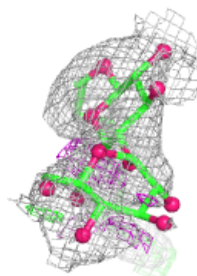
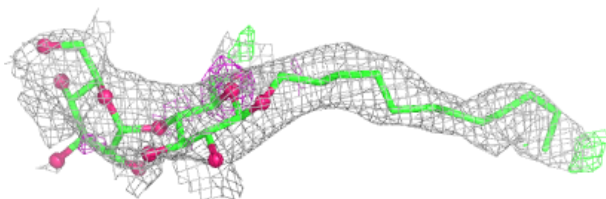
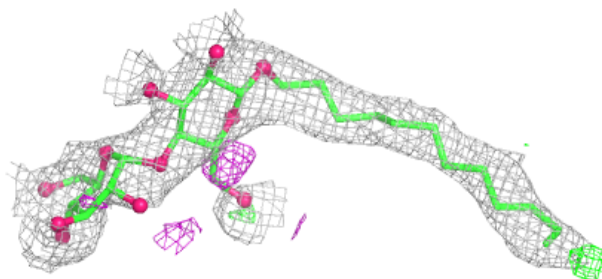


Electron density around LMT C 3046:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

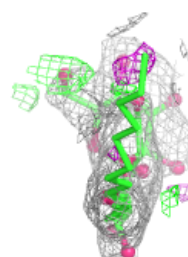
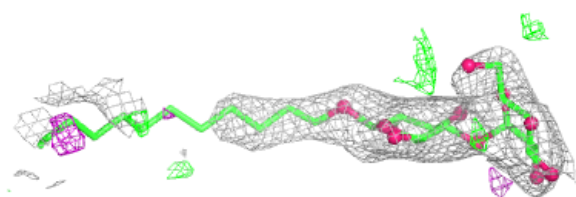
**Electron density around LMT B 3036:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

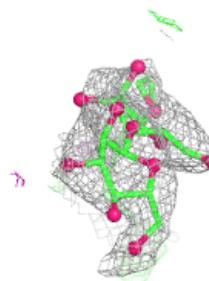
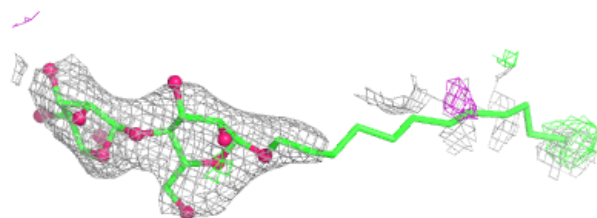
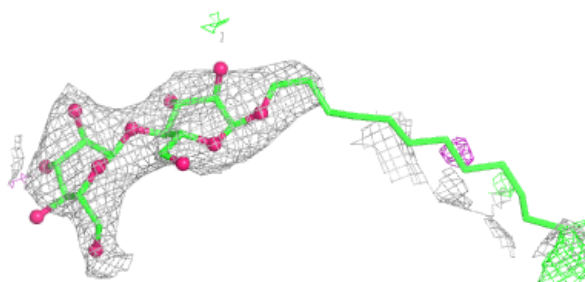


Electron density around LMT A 3048:

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

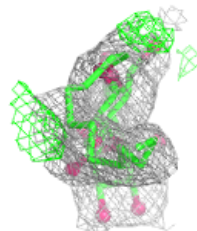
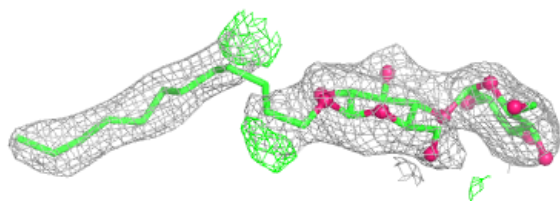
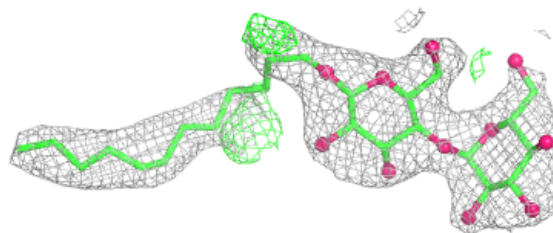
**Electron density around LMU A 3049:**

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

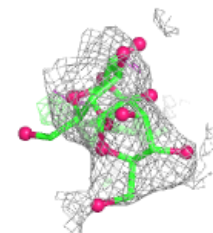
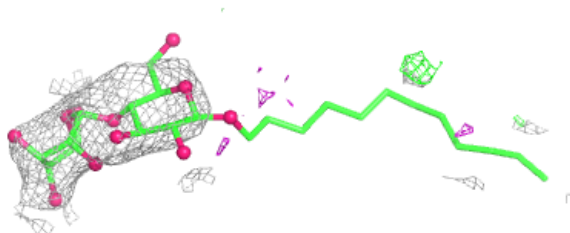
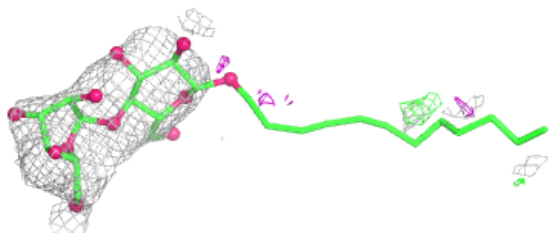


Electron density around LMT B 3035:

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

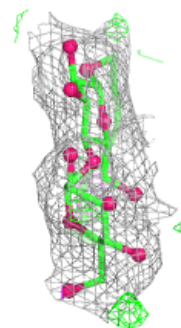
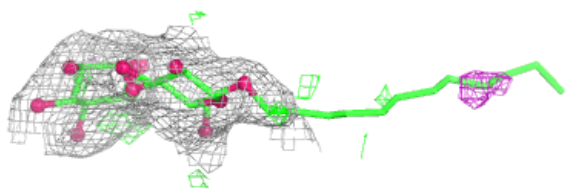
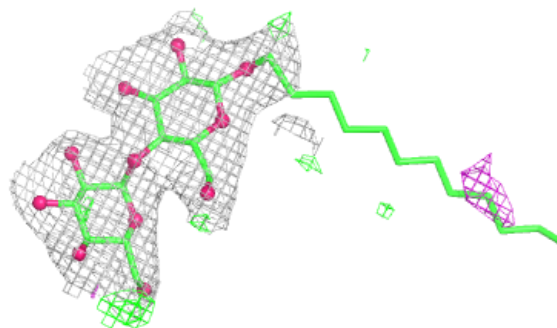
**Electron density around LMT B 3037:**

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

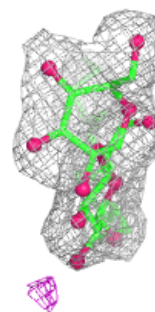
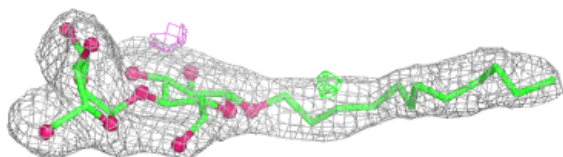
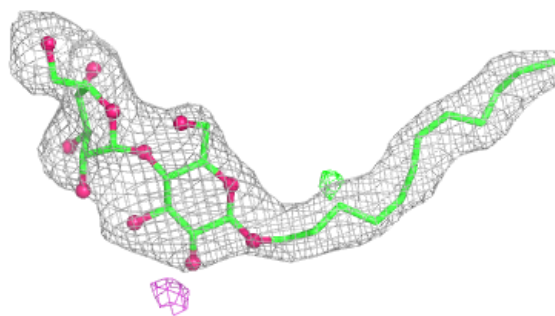


Electron density around LMT C 3043:

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

**Electron density around LMT A 3046:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.