



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:44 PM UTC

PDB ID : 4U95 / pdb_00004u95
Title : Coupling of remote alternating-access transport mechanisms for protons and substrates in the multidrug efflux pump AcrB
Authors : Pos, K.M.
Deposited on : 2014-08-05
Resolution : 2.00 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

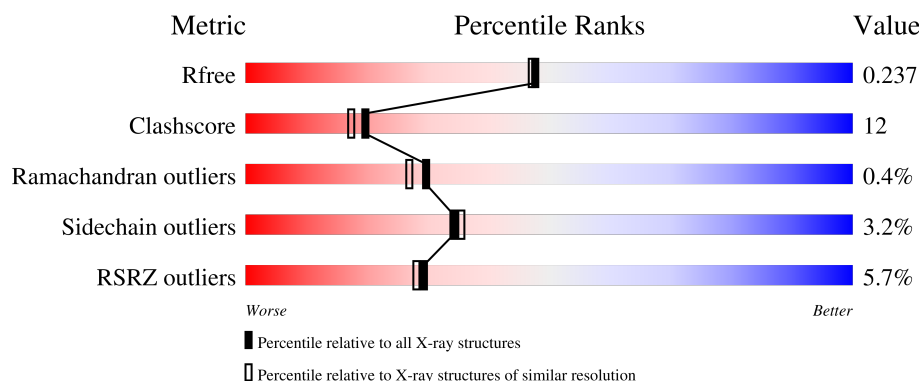
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	1057	11% 74% 22% ..
1	B	1057	4% 79% 17% ..
1	C	1057	3% 77% 19% ..
2	D	169	3% 83% 8% 8%
2	E	169	5% 69% 20% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28451 atoms, of which 27 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1044	Total	C	N	O	S	0	0	0
			7911	5088	1305	1474	44			
1	B	1033	Total	C	N	O	S	0	0	0
			7845	5049	1294	1458	44			
1	C	1033	Total	C	N	O	S	0	0	0
			7845	5049	1294	1458	44			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	940	ALA	LYS	engineered mutation	UNP P31224
A	1050	LEU	-	expression tag	UNP P31224
A	1051	GLU	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
A	1054	HIS	-	expression tag	UNP P31224
A	1055	HIS	-	expression tag	UNP P31224
A	1056	HIS	-	expression tag	UNP P31224
A	1057	HIS	-	expression tag	UNP P31224
B	940	ALA	LYS	engineered mutation	UNP P31224
B	1050	LEU	-	expression tag	UNP P31224
B	1051	GLU	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
B	1054	HIS	-	expression tag	UNP P31224
B	1055	HIS	-	expression tag	UNP P31224
B	1056	HIS	-	expression tag	UNP P31224
B	1057	HIS	-	expression tag	UNP P31224
C	940	ALA	LYS	engineered mutation	UNP P31224
C	1050	LEU	-	expression tag	UNP P31224
C	1051	GLU	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224

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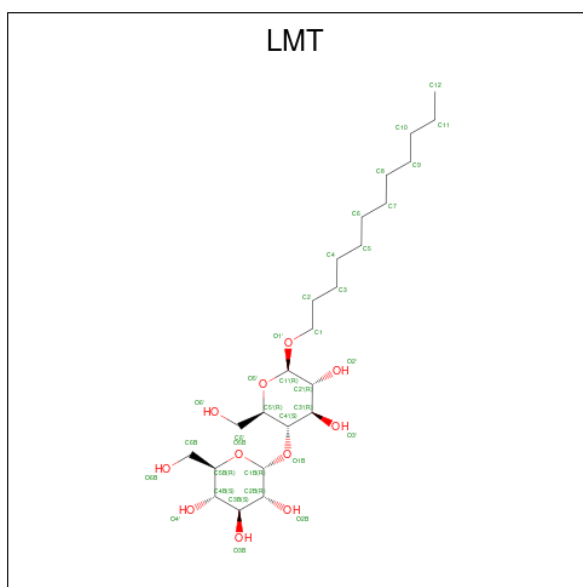
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPin.

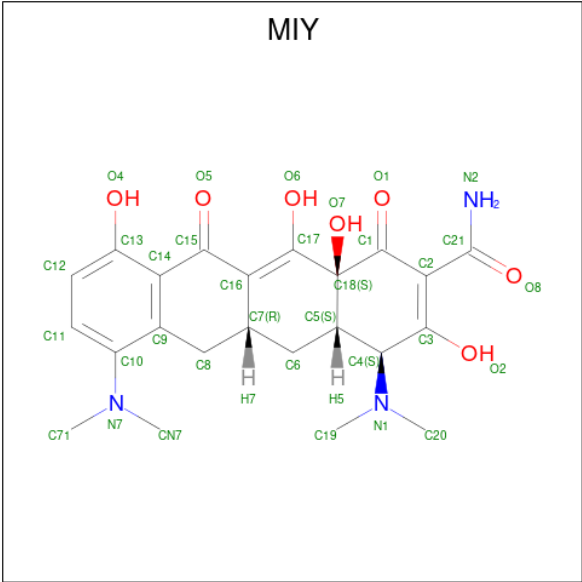
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	156	Total	C	N	O	S	0	0	0
			1177	741	206	229	1			
2	E	152	Total	C	N	O	S	0	0	0
			1151	726	202	222	1			

- 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	B	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		

- Molecule 4 is (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (CCD ID: MIY) (formula: $C_{23}H_{27}N_3O_7$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	0
			60	23	27	3	7		

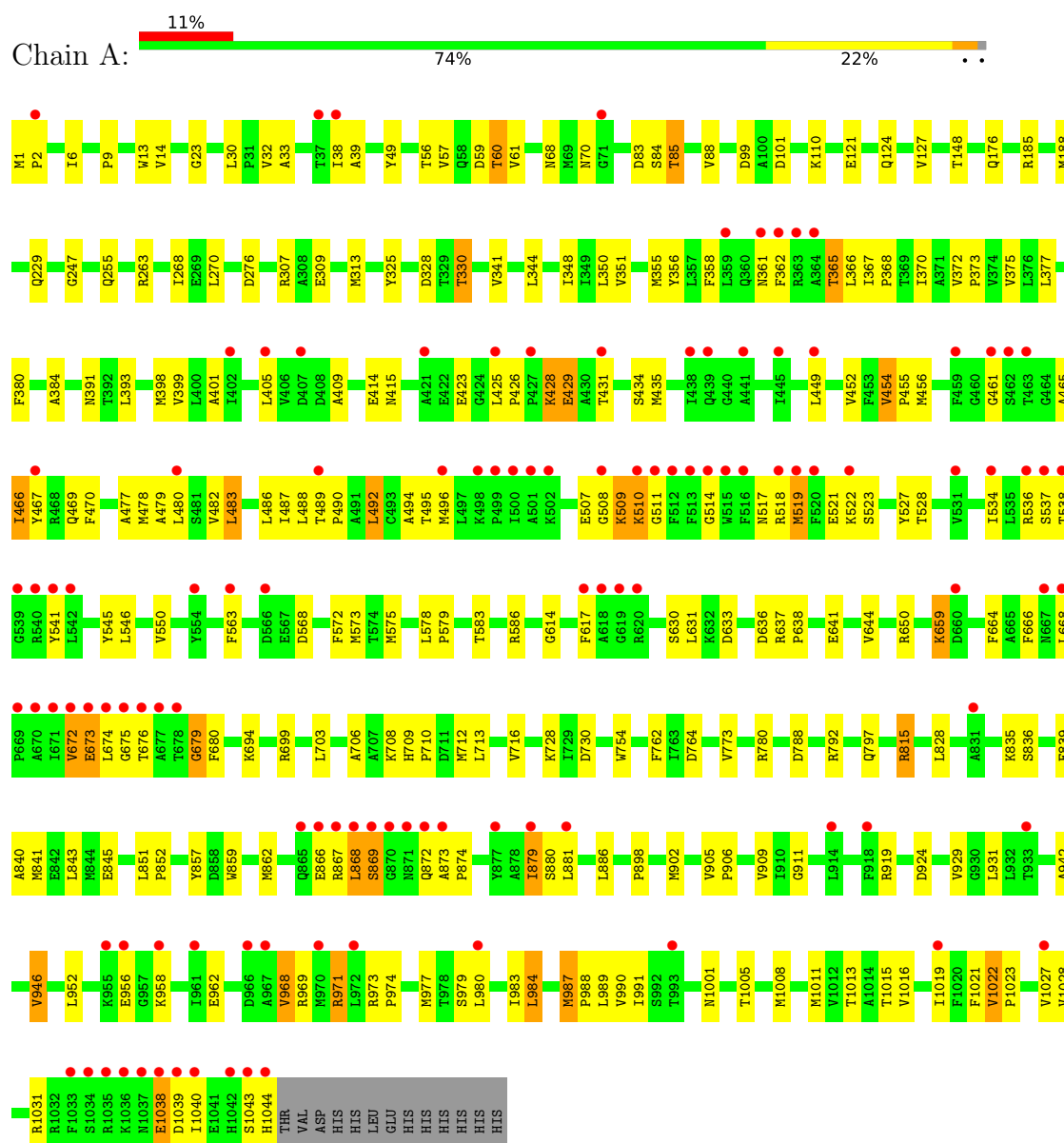
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	693	Total	O	0	0
			693	693		
5	B	723	Total	O	0	0
			723	723		
5	C	749	Total	O	0	0
			749	749		
5	D	112	Total	O	0	0
			112	112		
5	E	80	Total	O	0	0
			80	80		

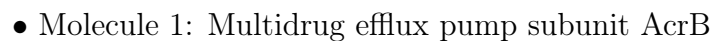
3 Residue-property plots

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: Multidrug efflux pump subunit AcrB



- Molecule 1: Multidrug efflux pump subunit AcrB



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	145.91Å 162.32Å 245.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.99 – 2.00 48.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.4 (48.99-2.00) 89.4 (48.99-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.194 , 0.237 0.197 , 0.237	Depositor DCC
R_{free} test set	17472 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28451	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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

5.1 Standard geometry

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

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	0.49	0/8061	0.81	5/10950 (0.0%)
1	B	0.50	0/7995	0.80	3/10859 (0.0%)
1	C	0.53	0/7995	0.80	1/10859 (0.0%)
2	D	0.50	0/1196	0.73	0/1626
2	E	0.38	0/1170	0.72	0/1591
All	All	0.50	0/26417	0.79	9/35885 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	TYR	CA-C-N	5.97	125.59	119.56
1	A	325	TYR	C-N-CA	5.97	125.59	119.56
1	A	454	VAL	CB-CA-C	-5.37	108.66	114.35
1	A	679	GLY	N-CA-C	5.12	119.10	112.54
1	C	125	GLN	N-CA-C	-5.11	107.10	113.38
1	A	1022	VAL	CB-CA-C	-5.07	108.97	114.35
1	B	905	VAL	CB-CA-C	-5.06	108.89	113.70
1	B	189	ASN	CA-C-N	5.04	124.82	119.28
1	B	189	ASN	C-N-CA	5.04	124.82	119.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	689	GLY	Peptide

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	7911	0	8033	228	0
1	B	7845	0	7993	173	0
1	C	7845	0	7993	179	0
2	D	1177	0	1159	10	0
2	E	1151	0	1136	29	0
3	A	35	0	46	3	0
3	B	35	0	46	3	0
3	C	35	0	46	2	0
4	B	33	27	25	0	0
5	A	693	0	0	22	0
5	B	723	0	0	27	0
5	C	749	0	0	33	0
5	D	112	0	0	3	0
5	E	80	0	0	5	0
All	All	28424	27	26477	606	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 12.

All (606) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:THR:HG23	1:B:837:THR:HG22	1.28	1.14
1:C:979:SER:HA	1:C:1011:MET:HE3	1.25	1.11
1:B:108:GLN:HG3	1:C:112:GLN:HG3	1.38	1.05
1:B:414:GLU:HG3	1:B:977:MET:HE1	1.40	1.01
1:A:83:ASP:OD1	1:A:85:THR:HG22	1.65	0.96
1:C:671:ILE:HG13	1:C:862:MET:HE1	1.49	0.95
1:C:493:CYS:SG	5:C:1864:HOH:O	2.27	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.52	0.91
1:C:575:MET:HE1	1:C:617:PHE:HD2	1.37	0.89
1:B:678:THR:HG21	1:B:831:ALA:H	1.39	0.88
1:B:514:GLY:O	5:B:1697:HOH:O	1.93	0.86
1:A:509:LYS:HE3	1:A:518:ARG:HH22	1.39	0.85
1:C:70:ASN:O	1:C:110:LYS:NZ	2.09	0.85
1:C:510:LYS:HG3	1:C:511:GLY:H	1.40	0.85
1:B:420:MET:HE1	1:B:499:PRO:HA	1.58	0.84
1:A:919:ARG:HH11	1:A:1005:THR:HG21	1.42	0.83
1:B:968:VAL:HG21	1:B:1023:PRO:HG3	1.58	0.83
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.09	0.82
1:B:1:MET:N	5:B:1399:HOH:O	2.11	0.82
1:C:447:MET:HE1	1:C:891:LEU:HD13	1.60	0.82
1:A:509:LYS:HB2	1:A:514:GLY:HA3	1.60	0.81
2:E:34:MET:HE1	2:E:40:VAL:CG1	2.11	0.81
1:A:983:ILE:HG23	1:A:1008:MET:HG3	1.61	0.80
1:C:391:ASN:H	1:C:394:THR:HG22	1.45	0.80
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.65	0.79
1:B:414:GLU:CG	1:B:977:MET:HE1	2.12	0.79
1:A:968:VAL:HG21	1:A:1023:PRO:HG3	1.64	0.79
1:B:420:MET:CE	1:B:499:PRO:HA	2.12	0.79
2:E:30:VAL:O	2:E:34:MET:HG2	1.83	0.79
1:A:355:MET:HE2	1:A:355:MET:HA	1.63	0.78
1:B:518:ARG:N	5:B:1697:HOH:O	2.04	0.78
1:C:507:GLU:HG2	1:C:518:ARG:HG2	1.67	0.77
1:B:414:GLU:HG3	1:B:977:MET:CE	2.14	0.76
3:B:1101:LMT:H5B	3:B:1101:LMT:H6E	1.66	0.76
1:A:509:LYS:HG3	1:A:514:GLY:CA	2.16	0.76
1:A:527:TYR:CE2	1:A:968:VAL:HG13	2.21	0.76
1:A:987:MET:HE3	1:A:987:MET:HA	1.67	0.76
1:A:509:LYS:CB	1:A:514:GLY:HA3	2.16	0.76
1:B:744:ASN:O	1:B:748:THR:HG23	1.86	0.75
1:C:1:MET:N	5:C:1352:HOH:O	2.19	0.75
2:E:34:MET:HE1	2:E:40:VAL:HG12	1.69	0.75
1:A:32:VAL:HG21	3:A:1101:LMT:H11	1.68	0.74
1:A:509:LYS:CE	1:A:518:ARG:HH22	2.01	0.74
1:A:659:LYS:NZ	5:A:1201:HOH:O	2.20	0.73
1:B:1011:MET:SD	5:B:1385:HOH:O	2.44	0.73
1:C:372:VAL:HG22	1:C:373:PRO:HD3	1.69	0.73
1:C:168:ARG:NH1	5:C:1937:HOH:O	2.20	0.73
1:C:578:LEU:HD22	1:C:587:THR:HG22	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:987:MET:HB3	1:A:988:PRO:HD3	1.70	0.73
1:C:587:THR:HG21	1:C:623:ASN:HA	1.70	0.73
1:A:866:GLU:O	1:A:869:SER:N	2.18	0.72
1:B:420:MET:HE1	1:B:427:PRO:HG3	1.71	0.72
1:A:414:GLU:CD	1:A:974:PRO:HG3	2.13	0.72
1:C:367:ILE:HD13	5:C:1864:HOH:O	1.89	0.72
1:C:1033:PHE:O	5:C:1786:HOH:O	2.08	0.72
1:C:29:LYS:NZ	5:C:1928:HOH:O	2.23	0.72
2:D:34:MET:HE2	2:D:34:MET:HA	1.72	0.72
1:C:376:LEU:HD11	1:C:402:ILE:HD11	1.72	0.71
1:B:974:PRO:HA	1:B:977:MET:CE	2.20	0.71
1:C:324:VAL:HG12	1:C:326:PRO:HD3	1.73	0.71
1:A:586:ARG:HB3	5:A:1371:HOH:O	1.90	0.70
1:C:259:ARG:NH2	2:E:155:ASN:OD1	2.25	0.70
1:C:70:ASN:HB3	5:C:1559:HOH:O	1.92	0.70
1:A:358:PHE:HB2	1:A:977:MET:HE3	1.74	0.69
1:B:527:TYR:CE2	1:B:968:VAL:HG13	2.26	0.69
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.24	0.69
1:A:1038:GLU:HG2	1:A:1039:ASP:H	1.57	0.69
1:C:937:LEU:HD13	1:C:1011:MET:SD	2.33	0.69
1:C:448:VAL:CG2	1:C:884:VAL:HG13	2.23	0.69
1:A:461:GLY:HA3	1:A:868:LEU:HD21	1.73	0.68
1:C:391:ASN:H	1:C:394:THR:CG2	2.07	0.68
1:A:568:ASP:OD2	1:A:637:ARG:NH2	2.25	0.68
1:A:509:LYS:HD3	1:A:511:GLY:O	1.94	0.68
1:B:510:LYS:HG3	1:B:511:GLY:N	2.09	0.68
2:E:15:GLY:N	5:E:221:HOH:O	2.25	0.68
1:C:423:GLU:HB2	1:C:425:LEU:HD13	1.76	0.68
1:B:468:ARG:NH1	5:B:1809:HOH:O	2.22	0.67
1:C:34:GLN:O	1:C:392:THR:HB	1.94	0.67
1:A:509:LYS:HG3	1:A:514:GLY:HA3	1.74	0.67
1:C:32:VAL:HG12	1:C:337:ILE:HD13	1.76	0.67
1:B:575:MET:CE	1:B:626:ILE:HD11	2.23	0.67
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.76	0.67
1:A:563:PHE:O	1:A:924:ASP:HB2	1.94	0.67
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.77	0.67
1:A:469:GLN:OE1	5:A:1739:HOH:O	2.12	0.67
1:C:104:GLN:HG3	5:C:1834:HOH:O	1.95	0.66
1:B:225:VAL:HG13	1:C:781:MET:HG3	1.78	0.66
1:B:919:ARG:HG2	1:B:919:ARG:HH11	1.61	0.66
1:C:111:LEU:HD21	1:C:127:VAL:CG2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HB3	1:A:2:PRO:HD3	1.76	0.66
1:B:447:MET:HE2	1:B:447:MET:HA	1.78	0.65
1:C:674:LEU:HD11	1:C:862:MET:SD	2.36	0.65
1:A:536:ARG:NH2	5:A:1465:HOH:O	2.30	0.65
1:A:815:ARG:NH1	5:A:1448:HOH:O	2.29	0.65
1:B:467:TYR:OH	1:B:928:GLN:OE1	2.12	0.65
1:B:108:GLN:CG	1:C:112:GLN:HG3	2.24	0.65
1:A:545:TYR:HB2	1:A:1021:PHE:CE1	2.31	0.64
1:C:575:MET:HE1	1:C:617:PHE:CD2	2.26	0.64
1:A:509:LYS:CG	1:A:514:GLY:HA3	2.27	0.64
1:A:528:THR:CG2	1:A:969:ARG:HB3	2.27	0.64
1:A:307:ARG:NE	5:A:1496:HOH:O	2.22	0.64
1:A:546:LEU:O	1:A:550:VAL:HG23	1.98	0.64
1:C:336:SER:O	1:C:340:VAL:HG23	1.98	0.64
1:A:990:VAL:HG23	1:A:991:ILE:HG23	1.80	0.64
1:B:324:VAL:HG12	1:B:326:PRO:HD3	1.80	0.64
2:E:45:VAL:HG22	5:E:209:HOH:O	1.98	0.64
1:A:527:TYR:HE2	1:A:968:VAL:HG13	1.61	0.63
1:B:573:MET:HB3	1:B:666:PHE:CE1	2.33	0.63
1:C:151:GLN:NE2	1:C:279:ALA:O	2.31	0.63
2:E:34:MET:HE2	2:E:69:ASN:CB	2.28	0.63
1:B:456:MET:HE3	1:B:471:SER:HB2	1.81	0.63
1:A:401:ALA:O	1:A:405:LEU:HG	1.99	0.63
2:D:25:GLY:HA2	2:D:62:ILE:HD12	1.80	0.63
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.81	0.63
1:A:568:ASP:CG	1:A:644:VAL:HG23	2.24	0.62
1:B:919:ARG:NE	5:B:1488:HOH:O	2.22	0.62
1:C:448:VAL:HG23	1:C:884:VAL:HG13	1.81	0.62
1:A:568:ASP:OD2	1:A:644:VAL:HG23	1.98	0.62
1:B:778:LYS:HE2	1:B:779:TYR:OH	1.99	0.62
1:C:395:MET:HE2	1:C:395:MET:HA	1.81	0.62
1:C:32:VAL:CG1	1:C:337:ILE:HD13	2.29	0.62
1:B:987:MET:HG3	1:B:1008:MET:HE1	1.82	0.62
1:A:431:THR:HG21	1:A:494:ALA:HB2	1.82	0.62
1:A:361:ASN:O	1:A:365:THR:HG22	1.99	0.61
1:C:939:ALA:O	1:C:943:ILE:HG12	1.99	0.61
1:C:369:THR:O	1:C:372:VAL:HG13	2.00	0.61
1:A:528:THR:HG21	1:A:969:ARG:HB3	1.82	0.61
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.82	0.61
1:B:536:ARG:NH2	5:B:1202:HOH:O	2.29	0.61
1:A:1038:GLU:C	1:A:1040:ILE:H	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ARG:NH2	5:A:1878:HOH:O	2.33	0.61
1:B:331:PRO:O	1:B:335:ILE:HG12	2.01	0.61
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.82	0.61
1:B:671:ILE:HG22	1:B:673:GLU:OE1	2.01	0.61
1:B:522:LYS:HG3	5:B:1789:HOH:O	2.00	0.60
1:C:376:LEU:HD11	1:C:402:ILE:CD1	2.30	0.60
1:B:778:LYS:HE2	1:B:779:TYR:CZ	2.37	0.60
2:E:15:GLY:N	5:E:216:HOH:O	2.33	0.60
1:A:509:LYS:HG3	1:A:514:GLY:N	2.16	0.60
1:A:857:TYR:OH	5:A:1829:HOH:O	2.16	0.60
1:C:1032:ARG:NH2	5:C:1935:HOH:O	2.33	0.60
2:E:44:ASP:HB2	5:E:209:HOH:O	2.01	0.60
1:C:875:SER:O	1:C:879:ILE:HG22	2.01	0.60
1:A:489:THR:HB	1:A:490:PRO:HD3	1.84	0.60
1:B:841:MET:O	1:B:845:GLU:HG3	2.01	0.60
1:A:973:ARG:O	1:A:977:MET:HG3	2.02	0.59
1:B:974:PRO:HA	1:B:977:MET:HE2	1.83	0.59
1:C:34:GLN:OE1	5:C:1837:HOH:O	2.17	0.59
1:C:452:VAL:HG13	1:C:884:VAL:HG21	1.82	0.59
1:A:461:GLY:CA	1:A:868:LEU:HD21	2.32	0.59
1:B:589:LYS:NZ	5:B:1433:HOH:O	2.36	0.59
1:A:979:SER:OG	1:A:1015:THR:HG21	2.03	0.59
1:B:340:VAL:HG21	1:B:395:MET:HB3	1.85	0.59
1:A:188:MET:HE2	1:A:773:VAL:HG12	1.84	0.59
1:B:678:THR:HG23	1:B:837:THR:CG2	2.20	0.58
1:A:13:TRP:CZ2	1:A:492:LEU:HD11	2.38	0.58
1:A:573:MET:CE	1:A:668:LEU:HD13	2.33	0.58
1:A:14:VAL:HG13	1:B:886:LEU:HB3	1.86	0.58
1:B:314:GLU:OE2	5:B:1308:HOH:O	2.16	0.58
1:C:226:LYS:NZ	5:C:1204:HOH:O	2.35	0.58
1:C:423:GLU:CB	1:C:425:LEU:HD13	2.33	0.58
1:A:509:LYS:HG3	1:A:514:GLY:H	1.69	0.58
1:B:734:GLU:OE1	5:B:1696:HOH:O	2.17	0.58
2:E:26:ARG:O	2:E:30:VAL:HG23	2.03	0.58
2:E:34:MET:HE2	2:E:69:ASN:CG	2.29	0.58
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.84	0.58
1:C:389:SER:O	1:C:394:THR:HG21	2.04	0.58
1:B:202:ASP:CG	1:B:792:ARG:HH22	2.11	0.58
2:E:91:GLY:HA2	2:E:128:ILE:HD12	1.85	0.58
1:C:162:MET:HE1	1:C:323:ILE:HD11	1.86	0.57
1:C:367:ILE:HG21	5:C:1864:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:ALA:O	1:C:482:VAL:HG23	2.04	0.57
1:A:56:THR:O	1:A:60:THR:HB	2.04	0.57
1:C:40:PRO:HB2	1:C:94:PHE:O	2.05	0.57
1:C:971:ARG:C	1:C:974:PRO:HD2	2.29	0.57
1:A:709:HIS:N	1:A:710:PRO:HD3	2.19	0.57
1:B:527:TYR:HE2	1:B:968:VAL:HG13	1.68	0.57
1:A:1038:GLU:HA	5:A:1556:HOH:O	2.03	0.57
1:A:328:ASP:OD1	1:A:330:THR:HB	2.04	0.57
1:A:351:VAL:O	1:A:355:MET:HG2	2.05	0.57
1:C:671:ILE:CG1	1:C:862:MET:HE1	2.30	0.57
1:A:39:ALA:HB2	1:A:673:GLU:HG3	1.87	0.57
1:B:342:LYS:HD2	5:B:1901:HOH:O	2.03	0.57
1:B:875:SER:O	1:B:879:ILE:HG13	2.04	0.57
1:B:974:PRO:HA	1:B:977:MET:HE3	1.87	0.57
1:C:392:THR:HG21	5:C:1506:HOH:O	2.04	0.57
1:B:412:VAL:O	5:B:1380:HOH:O	2.17	0.56
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.87	0.56
1:A:841:MET:O	1:A:845:GLU:HG3	2.06	0.56
1:C:195:LYS:HE3	1:C:196:PHE:CE2	2.40	0.56
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.05	0.56
1:B:281:PHE:CE2	1:B:324:VAL:HG11	2.40	0.56
1:C:364:ALA:HA	1:C:367:ILE:HD12	1.87	0.56
1:A:952:LEU:HA	1:A:956:GLU:OE1	2.06	0.56
1:A:380:PHE:CZ	1:A:398:MET:HE3	2.41	0.56
1:B:869:SER:N	5:B:1618:HOH:O	2.38	0.56
1:B:919:ARG:HG2	1:B:919:ARG:NH1	2.20	0.56
2:D:166:GLN:NE2	5:D:285:HOH:O	2.38	0.55
1:B:355:MET:HE3	1:B:359:LEU:HD12	1.87	0.55
1:B:586:ARG:HD3	5:B:1329:HOH:O	2.05	0.55
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.87	0.55
1:A:482:VAL:O	1:A:486:LEU:HG	2.06	0.55
1:B:352:PHE:CE2	1:B:365:THR:HG21	2.41	0.55
1:C:765:ARG:NE	5:C:1518:HOH:O	2.39	0.55
1:A:968:VAL:CG2	1:A:1023:PRO:HG3	2.36	0.55
1:C:676:THR:OG1	5:C:1334:HOH:O	2.18	0.55
1:C:872:GLN:HG3	5:C:1346:HOH:O	2.06	0.55
1:A:708:LYS:C	1:A:710:PRO:HD3	2.32	0.55
1:A:1038:GLU:CG	1:A:1039:ASP:H	2.20	0.55
1:B:678:THR:CG2	1:B:831:ALA:H	2.16	0.55
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.88	0.54
1:C:372:VAL:HG22	1:C:373:PRO:CD	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:LEU:O	1:A:984:LEU:HB2	2.06	0.54
1:B:885:PHE:HD1	1:B:902:MET:HE1	1.72	0.54
1:C:587:THR:CG2	1:C:623:ASN:HA	2.35	0.54
1:C:714:THR:HG22	5:C:1378:HOH:O	2.08	0.54
1:B:247:GLY:HA2	1:B:268:ILE:HD12	1.90	0.54
1:C:452:VAL:HG13	1:C:884:VAL:CG2	2.38	0.54
1:B:659:LYS:HD3	1:B:659:LYS:N	2.21	0.54
1:A:537:SER:O	1:A:538:THR:HB	2.08	0.54
1:C:971:ARG:O	1:C:974:PRO:HD2	2.07	0.54
1:B:678:THR:HB	1:B:830:GLN:HB2	1.90	0.54
1:A:57:VAL:HG12	1:A:88:VAL:HG22	1.89	0.54
1:A:676:THR:HG22	1:A:679:GLY:H	1.71	0.54
1:C:307:ARG:NH1	5:C:1377:HOH:O	2.31	0.54
1:C:370:ILE:O	1:C:373:PRO:HD2	2.08	0.54
1:C:689:GLY:N	5:C:1414:HOH:O	2.20	0.54
1:A:575:MET:HB2	1:A:617:PHE:CE1	2.43	0.54
1:A:641:GLU:O	1:A:650:ARG:NH2	2.27	0.54
1:A:672:VAL:O	1:A:675:GLY:N	2.31	0.53
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.90	0.53
1:B:678:THR:HG22	1:B:679:GLY:N	2.21	0.53
1:C:743:ILE:HD12	5:C:1920:HOH:O	2.07	0.53
1:C:999:ALA:O	1:C:1003:VAL:HG23	2.08	0.53
1:C:901:VAL:O	1:C:904:VAL:HG12	2.09	0.53
1:C:943:ILE:O	1:C:947:GLU:HB3	2.07	0.53
1:C:897:ILE:HD11	1:C:950:LYS:HD3	1.89	0.53
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.73	0.53
1:B:673:GLU:C	1:B:675:GLY:H	2.16	0.53
1:A:699:ARG:O	1:A:703:LEU:HG	2.09	0.53
1:C:111:LEU:HD21	1:C:127:VAL:HG21	1.88	0.53
1:A:919:ARG:HH11	1:A:1005:THR:CG2	2.17	0.53
1:B:281:PHE:CZ	1:B:324:VAL:HG11	2.44	0.53
1:A:33:ALA:O	1:A:391:ASN:HA	2.09	0.52
1:A:617:PHE:CE2	1:A:666:PHE:HZ	2.27	0.52
1:B:352:PHE:CE2	1:B:365:THR:CG2	2.93	0.52
1:B:659:LYS:CD	1:B:659:LYS:H	2.22	0.52
1:C:96:SER:O	5:C:1640:HOH:O	2.19	0.52
1:C:987:MET:SD	1:C:1008:MET:HE1	2.49	0.52
1:A:1:MET:N	5:A:1440:HOH:O	2.42	0.52
1:A:49:TYR:HE2	1:A:60:THR:HG21	1.75	0.52
1:C:897:ILE:HB	1:C:898:PRO:HD3	1.89	0.52
1:B:418:ARG:HD2	1:B:970:MET:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:944:LEU:HB3	1:B:971:ARG:HD2	1.92	0.52
1:C:48:SER:HB3	1:C:125:GLN:HG2	1.92	0.52
1:A:431:THR:O	1:A:435:MET:HG2	2.10	0.52
1:A:1027:VAL:O	1:A:1031:ARG:HG3	2.10	0.52
1:A:365:THR:O	1:A:368:PRO:HD2	2.10	0.51
1:A:380:PHE:CE2	1:A:398:MET:HE3	2.45	0.51
1:A:263:ARG:NH2	2:D:155:ASN:O	2.41	0.51
1:C:362:PHE:CE2	1:C:366:LEU:HD22	2.45	0.51
1:C:510:LYS:CG	1:C:511:GLY:H	2.15	0.51
1:A:70:ASN:O	1:A:110:LYS:HE3	2.10	0.51
1:B:38:ILE:HD13	1:B:466:ILE:CG1	2.40	0.51
1:B:673:GLU:CD	1:B:673:GLU:H	2.16	0.51
1:B:987:MET:CG	1:B:1008:MET:HE1	2.40	0.51
1:C:631:LEU:HD11	1:C:644:VAL:HG22	1.91	0.51
1:C:351:VAL:O	1:C:355:MET:HG3	2.11	0.51
1:C:725:PRO:HD2	5:C:1353:HOH:O	2.09	0.51
1:B:2:PRO:O	1:B:6:ILE:HG13	2.09	0.51
1:A:2:PRO:O	1:A:6:ILE:HG13	2.10	0.51
1:A:488:LEU:O	1:A:492:LEU:HB2	2.11	0.51
1:C:688:ALA:O	5:C:1376:HOH:O	2.19	0.51
1:B:762:PHE:CE2	1:B:764:ASP:HB2	2.46	0.51
1:C:446:ALA:HB2	1:C:482:VAL:HG13	1.93	0.51
1:A:426:PRO:HB2	1:A:429:GLU:OE1	2.12	0.51
1:C:85:THR:OG1	1:C:87:THR:HG23	2.11	0.51
1:A:509:LYS:CG	1:A:510:LYS:N	2.73	0.50
1:A:792:ARG:NH1	5:A:1808:HOH:O	2.44	0.50
1:B:344:LEU:HD23	1:B:402:ILE:HD11	1.92	0.50
1:B:678:THR:HG21	1:B:831:ALA:N	2.19	0.50
1:B:138:MET:HE2	1:B:140:VAL:CG2	2.41	0.50
1:B:492:LEU:O	1:B:496:MET:HB2	2.11	0.50
1:A:712:MET:SD	1:A:835:LYS:HE2	2.51	0.50
1:A:971:ARG:HD2	5:A:1314:HOH:O	2.10	0.50
1:B:575:MET:HE2	1:B:626:ILE:HD11	1.92	0.50
1:C:575:MET:HE2	1:C:666:PHE:HZ	1.77	0.50
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.94	0.50
1:C:13:TRP:O	1:C:17:ILE:HG13	2.12	0.50
2:E:25:GLY:HA2	2:E:62:ILE:HD12	1.94	0.50
1:A:32:VAL:CG2	3:A:1101:LMT:H11	2.40	0.50
1:A:942:ALA:O	1:A:946:VAL:HG13	2.12	0.50
1:A:987:MET:HE2	1:A:990:VAL:HG21	1.93	0.50
1:C:587:THR:HG21	1:C:622:GLN:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:618:ALA:N	5:C:1451:HOH:O	2.37	0.50
1:A:428:LYS:HB2	1:A:428:LYS:NZ	2.27	0.50
1:A:836:SER:OG	1:A:839:GLU:HG3	2.12	0.50
3:B:1101:LMT:H6E	3:B:1101:LMT:C5B	2.39	0.50
1:C:808:ARG:NH1	1:C:810:GLU:OE2	2.45	0.50
1:B:355:MET:CE	1:B:359:LEU:HD12	2.42	0.49
1:C:70:ASN:HB2	5:C:1824:HOH:O	2.11	0.49
1:B:873:ALA:N	1:B:874:PRO:HD2	2.27	0.49
1:A:124:GLN:O	1:B:117:LEU:HD21	2.13	0.49
1:C:392:THR:HG23	1:C:396:PHE:CE2	2.47	0.49
1:C:509:LYS:HG2	1:C:510:LYS:HE3	1.93	0.49
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.93	0.49
1:B:420:MET:HE2	5:B:1532:HOH:O	2.12	0.49
1:A:987:MET:HE2	1:A:990:VAL:CG2	2.43	0.49
1:A:59:ASP:HB3	1:C:763:ILE:HD11	1.94	0.49
1:B:676:THR:HG22	1:B:677:ALA:H	1.78	0.49
1:B:696:THR:OG1	1:B:825:MET:HE1	2.12	0.49
1:C:281:PHE:CE1	1:C:324:VAL:HG11	2.47	0.49
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.94	0.49
1:A:792:ARG:NH1	5:A:1725:HOH:O	2.43	0.49
1:B:510:LYS:HG3	1:B:511:GLY:H	1.75	0.49
1:C:534:ILE:HG12	1:C:541:TYR:CZ	2.48	0.49
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.94	0.49
1:C:898:PRO:O	1:C:902:MET:HG2	2.12	0.49
1:B:673:GLU:O	1:B:674:LEU:CB	2.60	0.49
1:C:256:ASP:OD1	1:C:256:ASP:N	2.45	0.49
1:C:904:VAL:HG13	1:C:938:SER:HB3	1.94	0.49
1:A:534:ILE:HB	1:A:541:TYR:CE1	2.48	0.48
1:B:420:MET:HE1	1:B:427:PRO:CG	2.41	0.48
1:B:558:ARG:HG3	1:B:558:ARG:NH1	2.28	0.48
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.48	0.48
1:A:1022:VAL:HB	1:A:1023:PRO:HD3	1.94	0.48
2:E:16:LYS:NZ	2:E:20:GLU:OE1	2.45	0.48
1:B:671:ILE:O	1:B:672:VAL:HB	2.13	0.48
1:C:57:VAL:HG13	1:C:82:SER:HB3	1.95	0.48
1:C:370:ILE:C	1:C:373:PRO:HD2	2.39	0.48
2:E:34:MET:C	2:E:36:ASN:H	2.20	0.48
1:A:23:GLY:HA3	1:A:377:LEU:O	2.12	0.48
1:A:344:LEU:O	1:A:348:ILE:HG13	2.12	0.48
1:B:990:VAL:O	5:B:1488:HOH:O	2.20	0.48
1:C:575:MET:CE	1:C:666:PHE:HZ	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:897:ILE:O	1:C:901:VAL:HG13	2.14	0.48
1:A:39:ALA:HB2	1:A:673:GLU:CG	2.42	0.48
1:B:897:ILE:N	1:B:898:PRO:CD	2.77	0.48
2:E:34:MET:HE2	2:E:69:ASN:HB3	1.94	0.48
1:C:392:THR:HG22	1:C:393:LEU:HD23	1.94	0.48
1:B:555:LEU:HD11	1:B:914:LEU:HD23	1.96	0.48
1:B:600:THR:HG22	1:B:601:LYS:HD3	1.94	0.48
1:C:835:LYS:NZ	5:C:1918:HOH:O	2.45	0.48
1:C:543:VAL:O	1:C:547:ILE:HG13	2.14	0.48
1:B:714:THR:HG22	5:B:1273:HOH:O	2.13	0.48
2:E:91:GLY:HA2	2:E:128:ILE:CD1	2.44	0.48
1:C:124:GLN:HB3	5:C:1564:HOH:O	2.14	0.48
1:A:309:GLU:HG3	1:A:313:MET:HE3	1.95	0.47
1:A:414:GLU:OE2	1:A:974:PRO:HG3	2.14	0.47
1:A:1001:ASN:O	1:A:1005:THR:HG23	2.13	0.47
1:B:873:ALA:N	1:B:874:PRO:CD	2.77	0.47
1:A:9:PRO:HG3	1:A:495:THR:HG21	1.96	0.47
1:A:428:LYS:O	1:A:431:THR:HG22	2.13	0.47
1:A:898:PRO:O	1:A:902:MET:HG3	2.14	0.47
1:C:365:THR:O	1:C:368:PRO:HD2	2.14	0.47
1:A:483:LEU:HD23	1:A:487:ILE:HD12	1.96	0.47
1:A:568:ASP:CG	1:A:637:ARG:HH22	2.21	0.47
1:B:672:VAL:C	1:B:673:GLU:O	2.56	0.47
1:C:23:GLY:HA3	1:C:377:LEU:O	2.15	0.47
1:A:509:LYS:HD2	1:A:510:LYS:H	1.79	0.47
1:A:987:MET:HA	1:A:987:MET:CE	2.40	0.47
1:A:517:ASN:O	1:A:521:GLU:HG2	2.14	0.47
1:B:574:THR:HB	1:B:627:ALA:HB3	1.96	0.47
1:B:892:TYR:O	1:B:950:LYS:HE3	2.14	0.47
1:C:453:PHE:HD1	1:C:456:MET:SD	2.38	0.47
1:C:568:ASP:CG	1:C:644:VAL:HG23	2.40	0.47
1:A:350:LEU:HD13	1:A:984:LEU:O	2.15	0.47
1:A:415:ASN:ND2	1:A:434:SER:OG	2.23	0.47
1:A:575:MET:HE3	1:A:664:PHE:CZ	2.49	0.47
1:B:673:GLU:O	1:B:674:LEU:HB2	2.14	0.47
1:A:393:LEU:HD11	1:A:466:ILE:HG13	1.96	0.47
1:A:792:ARG:NE	5:A:1349:HOH:O	2.23	0.47
1:B:186:ILE:HB	1:B:773:VAL:HG12	1.96	0.47
1:B:575:MET:HE1	1:B:626:ILE:HD11	1.94	0.47
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.96	0.47
2:D:115:THR:HB	2:D:116:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:MET:HE3	1:B:427:PRO:N	2.30	0.47
1:C:416:VAL:HG22	1:C:431:THR:HA	1.97	0.47
1:B:38:ILE:HD13	1:B:466:ILE:HG12	1.96	0.47
1:B:588:GLN:NE2	5:B:1627:HOH:O	2.47	0.47
1:A:492:LEU:O	1:A:496:MET:HB2	2.15	0.47
1:B:575:MET:HA	1:B:626:ILE:HD13	1.96	0.47
2:E:28:ASP:O	2:E:32:ILE:HG12	2.14	0.47
1:A:987:MET:CE	1:A:990:VAL:HG21	2.45	0.46
1:B:400:LEU:HD13	1:B:929:VAL:CG1	2.45	0.46
1:B:489:THR:HG21	5:B:1259:HOH:O	2.15	0.46
1:A:1016:VAL:O	1:A:1019:ILE:HG22	2.14	0.46
1:A:694:LYS:HD3	5:A:1680:HOH:O	2.15	0.46
1:A:968:VAL:HG21	1:A:1023:PRO:CG	2.40	0.46
1:A:987:MET:HE1	1:A:1008:MET:SD	2.55	0.46
1:B:673:GLU:OE1	1:B:673:GLU:N	2.39	0.46
1:A:631:LEU:HD11	1:A:644:VAL:HG22	1.98	0.46
1:A:716:VAL:HA	1:A:828:LEU:O	2.15	0.46
1:C:903:LEU:O	1:C:906:PRO:HD2	2.16	0.46
2:D:61:GLU:HB2	5:D:217:HOH:O	2.15	0.46
2:E:97:GLU:O	2:E:101:LYS:HG3	2.15	0.46
1:A:868:LEU:O	1:A:868:LEU:HD12	2.15	0.46
1:B:897:ILE:HD13	1:B:950:LYS:HD2	1.97	0.46
1:C:669:PRO:HG3	1:C:675:GLY:O	2.16	0.46
1:A:881:LEU:HD23	1:A:881:LEU:HA	1.63	0.46
1:B:600:THR:HG22	1:B:601:LYS:N	2.29	0.46
1:C:795:ASP:OD2	1:C:797:GLN:HG3	2.16	0.46
2:D:27:ASP:OD1	2:D:62:ILE:HG13	2.14	0.46
1:A:49:TYR:CE2	1:A:60:THR:HG21	2.50	0.46
1:B:352:PHE:CD2	1:B:365:THR:HG23	2.51	0.46
1:B:527:TYR:CE2	1:B:968:VAL:CG1	2.97	0.46
1:C:334:LYS:NZ	5:C:1436:HOH:O	2.48	0.46
2:E:133:LEU:HD21	2:E:139:VAL:HG12	1.98	0.46
1:C:1016:VAL:HG12	3:C:1101:LMT:H121	1.97	0.46
1:A:247:GLY:HA2	1:A:268:ILE:CD1	2.46	0.46
1:A:672:VAL:HG13	1:A:673:GLU:H	1.81	0.46
1:B:649:MET:HE3	5:B:1798:HOH:O	2.16	0.46
1:B:893:GLU:O	1:B:893:GLU:HG3	2.16	0.46
1:C:919:ARG:HG2	1:C:919:ARG:O	2.16	0.46
1:A:368:PRO:HA	1:A:409:ALA:HB1	1.98	0.46
2:E:60:LEU:HD11	2:E:98:VAL:HG21	1.98	0.45
1:A:479:ALA:O	1:A:482:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:LYS:CG	1:A:514:GLY:H	2.29	0.45
1:C:973:ARG:HB3	1:C:974:PRO:HD3	1.97	0.45
1:B:405:LEU:HD21	1:B:477:ALA:HB1	1.96	0.45
1:A:675:GLY:HA3	1:A:862:MET:HB3	1.98	0.45
1:B:972:LEU:O	1:B:976:LEU:HG	2.15	0.45
2:E:21:ALA:CB	2:E:29:GLU:HG2	2.46	0.45
1:B:558:ARG:HG3	1:B:558:ARG:HH11	1.80	0.45
1:C:666:PHE:CE1	1:C:677:ALA:HB2	2.52	0.45
2:D:68:LYS:NZ	5:D:246:HOH:O	2.49	0.45
1:A:886:LEU:HB3	1:C:14:VAL:HG13	1.98	0.45
1:C:244:GLU:HB3	5:E:205:HOH:O	2.17	0.45
1:B:351:VAL:HG12	5:B:1322:HOH:O	2.16	0.45
1:B:408:ASP:O	1:B:412:VAL:HG23	2.17	0.45
1:B:412:VAL:O	1:B:416:VAL:HG23	2.16	0.45
1:C:355:MET:HE1	1:C:368:PRO:HB2	1.99	0.45
1:A:990:VAL:HG12	1:A:1005:THR:HG22	1.99	0.45
1:C:151:GLN:OE1	1:C:278:ILE:HG23	2.17	0.45
1:C:165:ALA:HB3	1:C:313:MET:CE	2.47	0.45
1:C:736:ALA:HB1	1:C:741:VAL:HG23	1.99	0.45
1:A:797:GLN:HG3	5:A:1611:HOH:O	2.16	0.45
1:A:712:MET:HG2	1:A:843:LEU:HD22	1.99	0.45
1:A:276:ASP:O	1:A:614:GLY:HA3	2.17	0.44
1:A:341:VAL:HG21	3:A:1101:LMT:H41	1.98	0.44
1:A:1038:GLU:HG2	1:A:1039:ASP:N	2.28	0.44
1:C:334:LYS:HE3	5:C:1494:HOH:O	2.17	0.44
1:C:736:ALA:HB1	1:C:741:VAL:CG2	2.47	0.44
1:A:509:LYS:HD2	1:A:510:LYS:N	2.31	0.44
1:B:185:ARG:HA	1:B:185:ARG:HD3	1.76	0.44
1:B:521:GLU:OE2	5:B:1841:HOH:O	2.21	0.44
1:A:465:ALA:O	1:A:469:GLN:HG2	2.16	0.44
1:A:762:PHE:CE2	1:A:764:ASP:HB2	2.53	0.44
1:C:131:LYS:NZ	5:C:1594:HOH:O	2.50	0.44
1:C:168:ARG:NE	5:C:1830:HOH:O	2.24	0.44
1:A:706:ALA:HB3	1:A:716:VAL:HG21	1.98	0.44
1:A:881:LEU:HD22	1:A:902:MET:CE	2.46	0.44
1:B:328:ASP:O	1:B:331:PRO:HD2	2.18	0.44
1:A:188:MET:HE2	1:A:773:VAL:CG1	2.46	0.44
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.52	0.44
1:B:115:MET:HB2	1:B:116:PRO:HD3	1.99	0.44
1:C:144:ASN:HA	1:C:320:GLY:O	2.18	0.44
1:C:159:ALA:HB1	1:C:181:GLN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ALA:O	1:C:751:GLY:HA2	2.17	0.44
1:B:223:PRO:HD3	1:C:275:TYR:CD1	2.52	0.44
1:A:573:MET:HE1	1:A:668:LEU:HD13	2.00	0.44
1:A:911:GLY:HA3	1:A:1013:THR:OG1	2.18	0.44
1:C:987:MET:HA	1:C:1008:MET:HE3	1.99	0.44
1:A:307:ARG:HD3	5:A:1557:HOH:O	2.17	0.44
1:B:536:ARG:NH1	3:B:1101:LMT:O3B	2.49	0.44
1:C:670:ALA:HB3	1:C:862:MET:HE2	2.00	0.44
1:A:176:GLN:HB2	5:A:1379:HOH:O	2.17	0.44
1:B:307:ARG:NH2	5:B:1549:HOH:O	2.49	0.44
1:A:713:LEU:CD2	1:A:840:ALA:HB1	2.48	0.43
1:A:991:ILE:O	1:A:991:ILE:HD12	2.18	0.43
1:A:1011:MET:O	1:A:1015:THR:HG23	2.18	0.43
1:B:876:LEU:HD23	1:B:876:LEU:HA	1.74	0.43
1:A:987:MET:HB3	1:A:988:PRO:CD	2.45	0.43
1:B:199:THR:HB	1:B:200:PRO:HD2	2.00	0.43
1:C:889:ALA:HA	1:C:894:SER:O	2.18	0.43
1:A:57:VAL:HG11	1:A:88:VAL:HG22	1.96	0.43
1:A:636:ASP:C	1:A:638:PRO:HD3	2.43	0.43
1:A:1023:PRO:O	1:A:1027:VAL:HG22	2.18	0.43
1:A:9:PRO:HD2	1:B:893:GLU:OE1	2.18	0.43
1:A:509:LYS:HD3	1:A:511:GLY:C	2.44	0.43
1:A:792:ARG:NH2	5:A:1349:HOH:O	2.48	0.43
1:A:728:LYS:HE3	1:A:730:ASP:OD1	2.18	0.43
1:B:133:SER:HB3	5:B:1371:HOH:O	2.17	0.43
1:A:958:LYS:HD3	1:A:962:GLU:OE2	2.19	0.43
1:A:987:MET:O	1:A:990:VAL:HG22	2.19	0.43
1:B:832:ALA:HB1	1:B:833:PRO:HD2	2.01	0.43
1:B:1022:VAL:N	1:B:1023:PRO:CD	2.81	0.43
1:C:895:TRP:C	1:C:898:PRO:HD2	2.43	0.43
1:B:138:MET:HE1	1:B:325:TYR:CE2	2.54	0.43
1:C:35:TYR:HB3	1:C:36:PRO:HD2	2.01	0.43
1:C:492:LEU:O	1:C:496:MET:HB3	2.18	0.43
1:C:666:PHE:CD1	1:C:677:ALA:HB2	2.53	0.43
1:B:865:GLN:NE2	5:B:1434:HOH:O	2.27	0.43
1:C:11:PHE:HD1	1:C:11:PHE:O	2.02	0.43
1:A:508:GLY:O	1:A:509:LYS:HB3	2.19	0.43
1:A:879:ILE:HG13	1:A:880:SER:N	2.33	0.43
1:B:360:GLN:HG2	1:B:513:PHE:CD1	2.54	0.43
1:B:659:LYS:HD3	1:B:659:LYS:H	1.79	0.43
1:B:708:LYS:C	1:B:710:PRO:HD3	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:LEU:HD12	1:A:492:LEU:HA	1.90	0.43
1:A:575:MET:SD	1:A:664:PHE:HE1	2.42	0.43
1:C:343:THR:HG23	1:C:988:PRO:HB2	2.00	0.43
1:A:370:ILE:O	1:A:373:PRO:HD2	2.18	0.42
1:A:507:GLU:HG2	1:A:518:ARG:HG2	2.01	0.42
1:A:583:THR:OG1	1:A:586:ARG:HG3	2.19	0.42
1:C:452:VAL:CG1	1:C:884:VAL:HG21	2.49	0.42
1:A:851:LEU:HB3	1:A:852:PRO:CD	2.49	0.42
1:A:859:TRP:HD1	1:A:867:ARG:NH2	2.17	0.42
1:B:138:MET:HE2	1:B:140:VAL:HG22	2.01	0.42
1:C:575:MET:HG2	1:C:666:PHE:CE2	2.54	0.42
2:E:31:ARG:NH1	2:E:65:VAL:HG21	2.34	0.42
1:C:1014:ALA:O	1:C:1018:ALA:CB	2.67	0.42
2:E:21:ALA:HB2	2:E:29:GLU:HG2	2.01	0.42
1:A:633:ASP:HB2	5:A:1483:HOH:O	2.19	0.42
1:C:599:LEU:O	1:C:603:LYS:HB3	2.19	0.42
2:E:68:LYS:HB2	2:E:68:LYS:HE3	1.85	0.42
2:E:94:GLU:O	2:E:98:VAL:HG23	2.19	0.42
1:A:30:LEU:HD21	1:A:384:ALA:HA	2.01	0.42
1:A:1038:GLU:C	1:A:1040:ILE:N	2.75	0.42
1:C:2:PRO:O	1:C:6:ILE:HG13	2.20	0.42
1:C:330:THR:N	1:C:331:PRO:CD	2.83	0.42
1:C:530:SER:OG	3:C:1101:LMT:H11	2.20	0.42
1:A:979:SER:O	1:A:983:ILE:HG13	2.19	0.42
1:A:1043:SER:O	1:A:1044:HIS:CB	2.67	0.42
1:B:454:VAL:HB	1:B:455:PRO:HD3	2.01	0.42
1:B:568:ASP:CG	1:B:644:VAL:HG23	2.45	0.42
1:B:897:ILE:CD1	1:B:950:LYS:HD2	2.49	0.42
1:B:6:ILE:HG23	1:B:494:ALA:CB	2.49	0.42
1:B:420:MET:CE	1:B:427:PRO:HD3	2.50	0.42
1:C:115:MET:N	1:C:116:PRO:HD2	2.34	0.42
1:C:947:GLU:HG3	1:C:948:PHE:N	2.34	0.42
1:A:362:PHE:O	1:A:366:LEU:HB2	2.19	0.42
1:A:509:LYS:HD2	1:A:511:GLY:N	2.35	0.42
1:B:139:VAL:O	1:B:326:PRO:HD2	2.19	0.42
1:C:671:ILE:N	1:C:862:MET:HE1	2.35	0.42
1:A:1027:VAL:HG23	1:A:1028:VAL:N	2.35	0.42
1:B:420:MET:CE	1:B:427:PRO:CD	2.97	0.42
1:A:519:MET:O	1:A:523:SER:OG	2.35	0.41
1:B:904:VAL:HG11	1:B:942:ALA:HB2	2.01	0.41
1:B:1030:ARG:HA	1:B:1030:ARG:HD2	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:SER:O	1:C:438:ILE:HG12	2.20	0.41
2:E:63:VAL:HG21	2:E:95:ILE:HD13	2.02	0.41
1:A:84:SER:HB2	5:A:1780:HOH:O	2.20	0.41
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.89	0.41
1:B:777:ALA:O	1:B:781:MET:HG2	2.20	0.41
1:A:38:ILE:C	1:A:38:ILE:HD12	2.44	0.41
1:C:32:VAL:HA	1:C:390:ILE:O	2.21	0.41
1:C:398:MET:O	1:C:402:ILE:HG12	2.20	0.41
2:E:42:ALA:O	2:E:50:PRO:HD3	2.19	0.41
1:A:405:LEU:HD21	1:A:477:ALA:HB1	2.02	0.41
1:A:454:VAL:N	1:A:455:PRO:CD	2.83	0.41
1:A:713:LEU:HG	1:A:843:LEU:HD23	2.02	0.41
1:A:788:ASP:HB2	5:A:1781:HOH:O	2.19	0.41
1:A:911:GLY:CA	1:A:1013:THR:HG21	2.51	0.41
1:C:671:ILE:HB	1:C:674:LEU:HD11	2.02	0.41
1:C:944:LEU:O	1:C:971:ARG:HG3	2.21	0.41
1:A:423:GLU:OE1	1:A:425:LEU:HD11	2.21	0.41
1:A:572:PHE:HE1	1:A:631:LEU:HD21	1.85	0.41
1:A:185:ARG:HA	1:A:185:ARG:HD3	1.82	0.41
1:A:356:TYR:HD1	1:A:365:THR:HG21	1.85	0.41
1:B:1024:VAL:O	1:B:1028:VAL:HG22	2.19	0.41
2:D:91:GLY:HA2	2:D:128:ILE:HD12	2.02	0.41
1:A:514:GLY:O	1:A:518:ARG:HG3	2.20	0.41
1:A:754:TRP:CH2	1:A:780:ARG:HA	2.55	0.41
1:B:451:ALA:HB2	1:B:883:VAL:HG12	2.03	0.41
1:B:483:LEU:HD23	1:B:483:LEU:HA	1.90	0.41
1:B:674:LEU:C	1:B:676:THR:H	2.28	0.41
1:C:671:ILE:HG13	1:C:862:MET:CE	2.35	0.41
1:A:909:VAL:HG22	1:A:931:LEU:HD11	2.03	0.41
1:A:578:LEU:HB3	1:A:579:PRO:CD	2.51	0.41
1:A:680:PHE:HZ	1:A:716:VAL:HG12	1.86	0.41
1:A:1038:GLU:O	1:A:1040:ILE:N	2.54	0.41
1:B:169:THR:O	1:B:172:VAL:HG13	2.20	0.41
1:B:169:THR:OG1	1:B:309:GLU:HG3	2.21	0.41
1:B:219:LEU:HD23	1:C:754:TRP:CZ3	2.56	0.41
1:B:307:ARG:NE	5:B:1549:HOH:O	2.21	0.41
1:B:420:MET:HE2	1:B:499:PRO:HA	1.95	0.41
1:B:489:THR:N	1:B:490:PRO:CD	2.83	0.41
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.36	0.41
1:C:154:ILE:O	1:C:158:VAL:HG23	2.21	0.41
1:C:168:ARG:NH2	5:C:1830:HOH:O	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:502:LYS:NZ	5:C:1203:HOH:O	2.33	0.41
2:D:129:VAL:O	2:D:133:LEU:HG	2.21	0.41
1:A:483:LEU:CD2	1:A:487:ILE:HD12	2.51	0.41
1:A:919:ARG:HD3	1:A:1005:THR:HG21	2.02	0.41
1:B:189:ASN:HA	1:B:190:PRO:HD2	1.87	0.41
1:C:483:LEU:HD23	1:C:483:LEU:HA	1.91	0.41
1:C:587:THR:CG2	1:C:622:GLN:O	2.69	0.41
1:C:868:LEU:O	1:C:872:GLN:HG2	2.20	0.41
1:A:578:LEU:HB3	1:A:579:PRO:HD2	2.03	0.40
1:B:247:GLY:HA2	1:B:268:ILE:CD1	2.50	0.40
1:B:324:VAL:CG1	1:B:326:PRO:HD3	2.49	0.40
1:C:841:MET:O	1:C:845:GLU:HG3	2.21	0.40
1:B:754:TRP:CH2	1:B:780:ARG:HA	2.56	0.40
2:E:82:THR:O	2:E:85:HIS:HB2	2.21	0.40
1:A:68:ASN:O	1:A:110:LYS:HB3	2.22	0.40
1:A:522:LYS:HD2	1:A:522:LYS:HA	1.83	0.40
1:B:527:TYR:CZ	1:B:968:VAL:HG13	2.55	0.40
1:C:987:MET:HB3	1:C:988:PRO:HD3	2.03	0.40
1:A:716:VAL:O	1:A:716:VAL:HG23	2.21	0.40
1:C:63:GLN:O	1:C:67:GLN:HG2	2.21	0.40
1:A:99:ASP:OD1	1:A:101:ASP:HB2	2.21	0.40
1:A:456:MET:HG2	1:A:467:TYR:HB3	2.03	0.40
1:A:866:GLU:C	1:A:868:LEU:N	2.79	0.40
1:C:683:GLU:O	1:C:857:TYR:HA	2.21	0.40
1:C:764:ASP:HB3	1:C:769:LYS:HD2	2.03	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	1042/1057 (99%)	1004 (96%)	33 (3%)	5 (0%)	24 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1031/1057 (98%)	995 (96%)	28 (3%)	8 (1%)	16	11
1	C	1031/1057 (98%)	1000 (97%)	30 (3%)	1 (0%)	48	46
2	D	154/169 (91%)	151 (98%)	3 (2%)	0	100	100
2	E	150/169 (89%)	146 (97%)	4 (3%)	0	100	100
All	All	3408/3509 (97%)	3296 (97%)	98 (3%)	14 (0%)	30	27

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	659	LYS
1	B	672	VAL
1	C	510	LYS
1	A	509	LYS
1	A	510	LYS
1	A	673	GLU
1	B	872	GLN
1	A	869	SER
1	B	673	GLU
1	B	676	THR
1	B	679	GLY
1	A	1038	GLU
1	B	671	ILE
1	B	870	GLY

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	842/862 (98%)	810 (96%)	32 (4%)	29	29
1	B	838/862 (97%)	810 (97%)	28 (3%)	33	34
1	C	838/862 (97%)	815 (97%)	23 (3%)	39	42
2	D	120/132 (91%)	116 (97%)	4 (3%)	33	34
2	E	117/132 (89%)	115 (98%)	2 (2%)	53	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2755/2850 (97%)	2666 (97%)	89 (3%)	34 35

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	THR
1	A	85	THR
1	A	121	GLU
1	A	127	VAL
1	A	148	THR
1	A	229	GLN
1	A	255	GLN
1	A	270	LEU
1	A	330	THR
1	A	365	THR
1	A	428	LYS
1	A	429	GLU
1	A	449	LEU
1	A	452	VAL
1	A	466	ILE
1	A	478	MET
1	A	483	LEU
1	A	492	LEU
1	A	519	MET
1	A	630	SER
1	A	659	LYS
1	A	672	VAL
1	A	674	LEU
1	A	815	ARG
1	A	868	LEU
1	A	872	GLN
1	A	879	ILE
1	A	946	VAL
1	A	968	VAL
1	A	971	ARG
1	A	984	LEU
1	A	987	MET
1	B	1	MET
1	B	30	LEU
1	B	48	SER
1	B	88	VAL
1	B	121	GLU

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Mol	Chain	Res	Type
1	B	172	VAL
1	B	225	VAL
1	B	314	GLU
1	B	324	VAL
1	B	365	THR
1	B	428	LYS
1	B	439	GLN
1	B	498	LYS
1	B	633	ASP
1	B	648	THR
1	B	659	LYS
1	B	660	ASP
1	B	674	LEU
1	B	678	THR
1	B	714	THR
1	B	748	THR
1	B	801	PHE
1	B	867	ARG
1	B	881	LEU
1	B	921	LEU
1	B	951	ASP
1	B	968	VAL
1	B	986	VAL
1	C	96	SER
1	C	121	GLU
1	C	127	VAL
1	C	129	VAL
1	C	152	GLU
1	C	255	GLN
1	C	324	VAL
1	C	372	VAL
1	C	392	THR
1	C	417	GLU
1	C	448	VAL
1	C	452	VAL
1	C	482	VAL
1	C	498	LYS
1	C	564	LEU
1	C	587	THR
1	C	620	ARG
1	C	674	LEU
1	C	773	VAL

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Mol	Chain	Res	Type
1	C	901	VAL
1	C	948	PHE
1	C	951	ASP
1	C	993	THR
2	D	61	GLU
2	D	139	VAL
2	D	154	ILE
2	D	166	GLN
2	E	45	VAL
2	E	94	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	737	GLN
1	A	797	GLN
1	A	1001	ASN
1	B	70	ASN
1	B	108	GLN
1	B	112	GLN
1	B	120	GLN
1	B	197	GLN
1	B	439	GLN
1	B	687	GLN
1	B	830	GLN
1	C	74	ASN
1	C	81	ASN
1	C	89	GLN
1	C	124	GLN
1	C	577	GLN
1	C	830	GLN
2	E	69	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
4	MIY	B	1102	-	36,36,36	1.73	10 (27%)	42,58,58	2.60	18 (42%)
3	LMT	C	1101	-	36,36,36	0.44	0	47,47,47	0.92	2 (4%)
3	LMT	A	1101	-	36,36,36	0.48	0	47,47,47	0.87	2 (4%)
3	LMT	B	1101	-	36,36,36	0.41	0	47,47,47	0.89	1 (2%)

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
4	MIY	B	1102	-	-	0/12/70/70	0/4/4/4
3	LMT	C	1101	-	-	7/21/61/61	0/2/2/2
3	LMT	A	1101	-	-	11/21/61/61	0/2/2/2
3	LMT	B	1101	-	-	6/21/61/61	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1102	MIY	C11-C10	3.51	1.45	1.39
4	B	1102	MIY	C18-C1	-3.01	1.51	1.55
4	B	1102	MIY	C7-C16	-2.78	1.48	1.51
4	B	1102	MIY	C18-C17	2.77	1.54	1.52
4	B	1102	MIY	C14-C13	-2.71	1.37	1.41
4	B	1102	MIY	C4-N1	2.61	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1102	MIY	O4-C13	2.57	1.41	1.36
4	B	1102	MIY	CN7-N7	2.44	1.51	1.45
4	B	1102	MIY	C21-N2	2.37	1.40	1.33
4	B	1102	MIY	C2-C21	2.30	1.52	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1102	MIY	C11-C12-C13	-6.85	113.65	120.50
4	B	1102	MIY	C1-C18-C17	6.51	117.52	109.88
4	B	1102	MIY	C12-C13-C14	5.20	126.79	120.15
4	B	1102	MIY	C15-C16-C17	5.09	122.83	118.80
4	B	1102	MIY	O5-C15-C14	-4.09	114.67	122.06
4	B	1102	MIY	C11-C10-N7	-3.45	116.90	121.65
4	B	1102	MIY	O7-C18-C17	-3.29	104.89	110.14
4	B	1102	MIY	C18-C17-C16	3.20	126.32	123.06
4	B	1102	MIY	O6-C17-C16	-2.86	117.96	123.52
4	B	1102	MIY	C18-C1-C2	2.75	120.12	115.75
4	B	1102	MIY	O8-C21-N2	-2.75	116.73	122.89
4	B	1102	MIY	O2-C3-C2	-2.75	118.33	122.93
4	B	1102	MIY	C9-C10-N7	2.63	122.01	118.87
4	B	1102	MIY	C19-N1-C4	2.43	119.64	114.10
3	A	1101	LMT	C1B-O1B-C4'	-2.34	112.42	117.98
3	C	1101	LMT	C4B-C3B-C2B	-2.33	106.73	110.83
4	B	1102	MIY	C71-N7-CN7	2.19	123.22	116.18
3	C	1101	LMT	C1B-O1B-C4'	-2.15	112.89	117.98
3	A	1101	LMT	O5B-C5B-C4B	2.10	113.48	109.70
4	B	1102	MIY	O4-C13-C12	-2.09	113.77	119.36
4	B	1102	MIY	CN7-N7-C10	2.09	121.63	115.16
4	B	1102	MIY	C21-C2-C1	-2.06	118.53	120.97
3	B	1101	LMT	C4B-C3B-C2B	-2.01	107.30	110.83

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	LMT	O5'-C1'-O1'-C1
3	A	1101	LMT	O5B-C5B-C6B-O6B
3	B	1101	LMT	O5'-C1'-O1'-C1
3	A	1101	LMT	C4B-C5B-C6B-O6B
3	A	1101	LMT	C2'-C1'-O1'-C1
3	B	1101	LMT	C2'-C1'-O1'-C1

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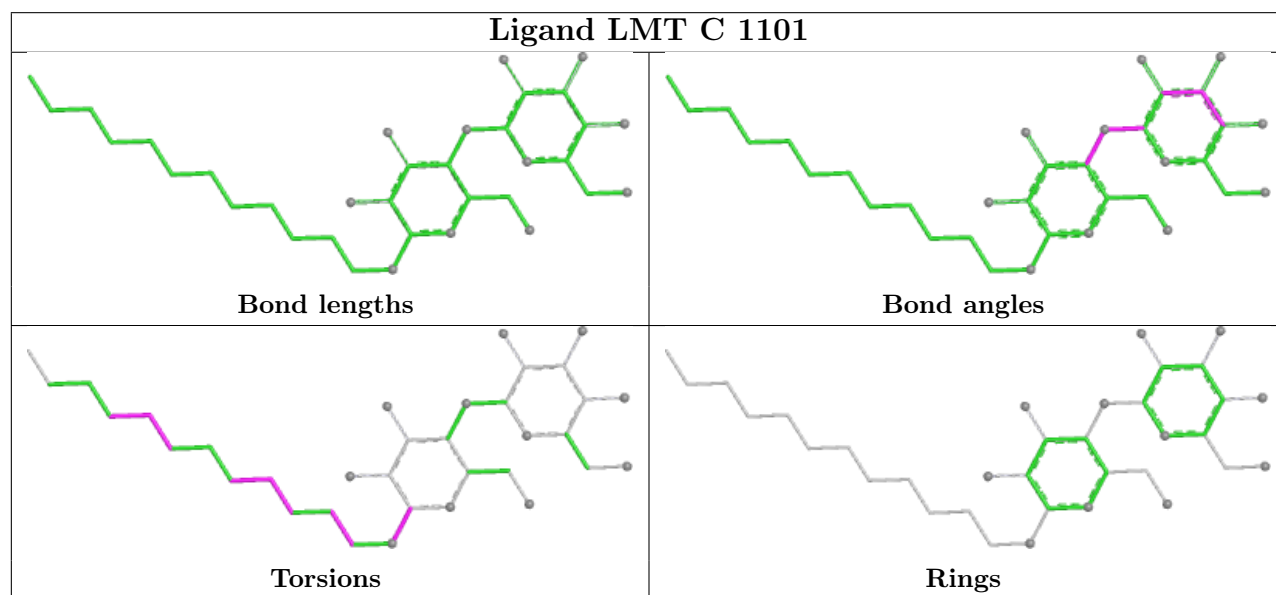
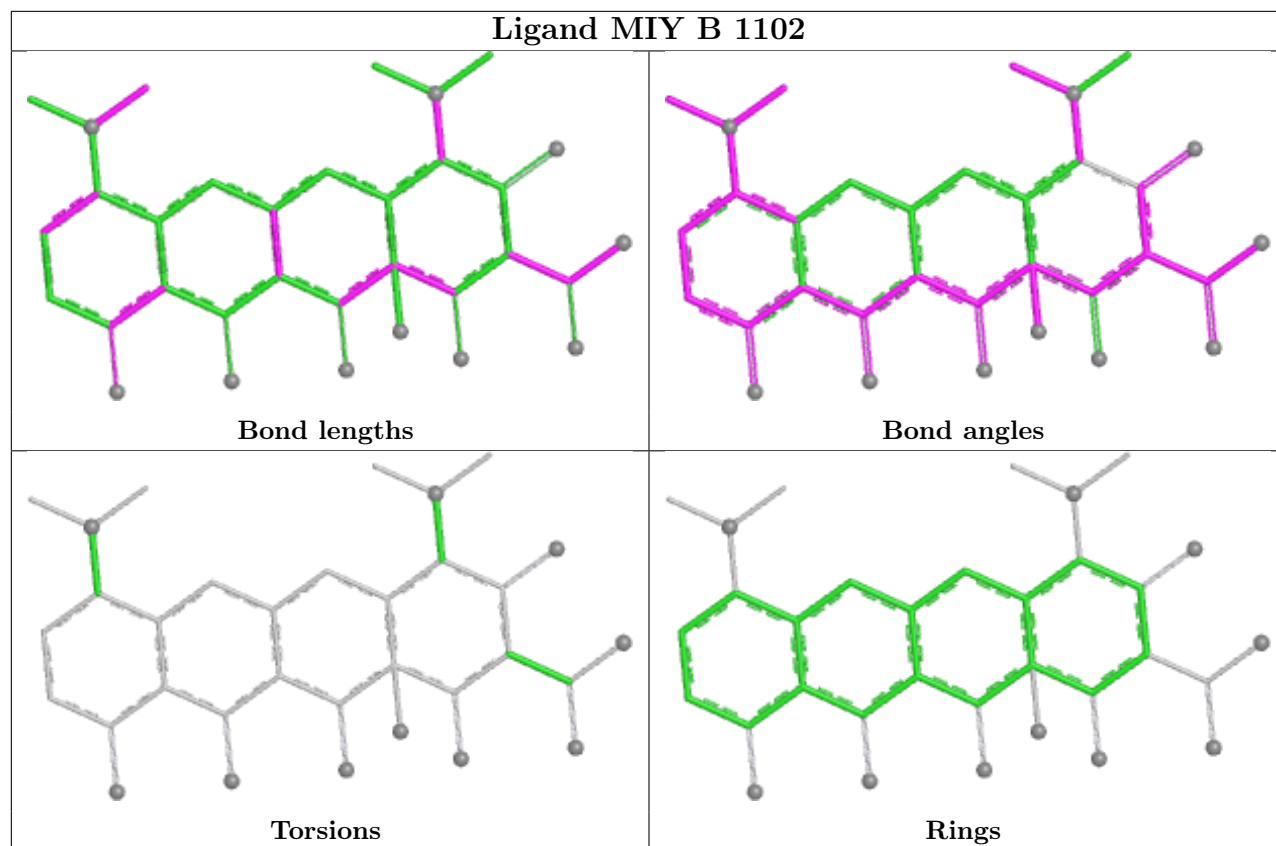
Mol	Chain	Res	Type	Atoms
3	C	1101	LMT	O5'-C1'-O1'-C1
3	C	1101	LMT	C2'-C1'-O1'-C1
3	A	1101	LMT	C7-C8-C9-C10
3	A	1101	LMT	C3-C4-C5-C6
3	B	1101	LMT	C6-C7-C8-C9
3	C	1101	LMT	C7-C8-C9-C10
3	C	1101	LMT	C3-C4-C5-C6
3	C	1101	LMT	O1'-C1-C2-C3
3	C	1101	LMT	C6-C7-C8-C9
3	A	1101	LMT	C2-C3-C4-C5
3	B	1101	LMT	O1'-C1-C2-C3
3	A	1101	LMT	C6-C7-C8-C9
3	B	1101	LMT	C1-C2-C3-C4
3	A	1101	LMT	O1'-C1-C2-C3
3	C	1101	LMT	C2-C3-C4-C5
3	A	1101	LMT	C9-C10-C11-C12
3	B	1101	LMT	C4B-C5B-C6B-O6B
3	A	1101	LMT	C11-C10-C9-C8

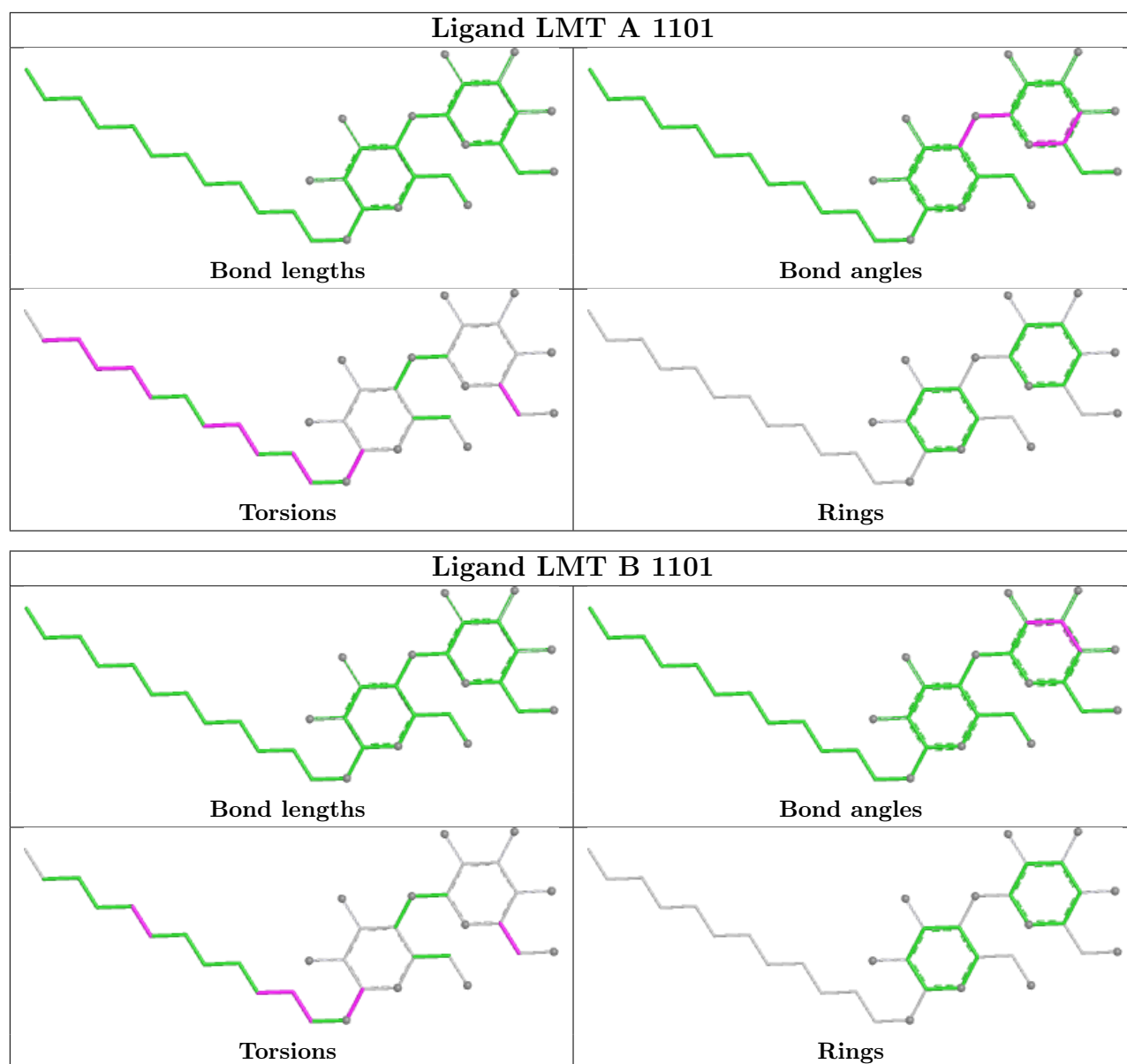
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1101	LMT	2	0
3	A	1101	LMT	3	0
3	B	1101	LMT	3	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	1044/1057 (98%)	0.42	114 (10%) 10 9	13, 41, 98, 164	0
1	B	1033/1057 (97%)	0.02	38 (3%) 45 44	15, 35, 61, 107	0
1	C	1033/1057 (97%)	0.00	31 (3%) 52 51	16, 33, 62, 101	0
2	D	156/169 (92%)	-0.15	5 (3%) 50 49	25, 34, 57, 94	0
2	E	152/169 (89%)	0.85	8 (5%) 32 31	34, 53, 83, 115	0
All	All	3418/3509 (97%)	0.16	196 (5%) 29 28	13, 36, 77, 164	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	672	VAL	7.8
1	A	868	LEU	7.2
1	B	877	TYR	6.7
1	B	677	ALA	6.5
1	C	362	PHE	6.3
1	A	670	ALA	6.2
1	A	678	THR	6.2
1	B	676	THR	6.0
1	B	675	GLY	5.6
1	B	134	SER	5.4
1	A	870	GLY	5.3
1	A	869	SER	5.1
1	A	668	LEU	5.1
1	A	865	GLN	5.1
1	A	1040	ILE	5.1
1	A	669	PRO	5.1
1	A	873	ALA	4.9
1	A	676	THR	4.8
1	A	1044	HIS	4.8
1	B	678	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	811	TYR	4.6
1	A	918	PHE	4.6
1	A	675	GLY	4.5
1	A	674	LEU	4.5
2	E	166	GLN	4.4
1	C	7	ASP	4.3
1	A	362	PHE	4.3
1	A	617	PHE	4.2
1	B	868	LEU	4.2
1	A	459	PHE	4.1
1	C	954	ASP	4.1
1	A	867	ARG	4.0
1	C	948	PHE	3.9
1	A	877	TYR	3.9
1	A	449	LEU	3.8
1	B	674	LEU	3.8
1	A	38	ILE	3.7
1	A	879	ILE	3.7
1	B	671	ILE	3.7
1	C	618	ALA	3.7
1	A	980	LEU	3.6
1	B	508	GLY	3.6
1	A	37	THR	3.5
1	B	563	PHE	3.4
1	C	955	LYS	3.4
1	A	427	PRO	3.4
1	C	743	ILE	3.4
1	A	566	ASP	3.4
1	C	620	ARG	3.3
1	C	951	ASP	3.3
1	A	441	ALA	3.3
1	A	513	PHE	3.3
1	C	96	SER	3.3
1	A	871	ASN	3.3
1	A	463	THR	3.2
1	A	520	PHE	3.2
1	A	462	SER	3.2
1	A	515	TRP	3.2
1	B	618	ALA	3.2
1	A	508	GLY	3.2
1	A	618	ALA	3.1
1	A	619	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	510	LYS	3.1
2	D	13	ASP	3.1
1	A	511	GLY	3.1
1	A	361	ASN	3.1
1	A	933	THR	3.0
1	C	617	PHE	3.0
1	A	500	ILE	3.0
1	A	539	GLY	3.0
1	A	866	GLU	3.0
1	C	674	LEU	3.0
1	A	499	PRO	3.0
1	A	538	THR	2.9
1	B	874	PRO	2.9
1	B	620	ARG	2.9
1	A	516	PHE	2.9
1	C	510	LYS	2.9
1	A	667	ASN	2.9
1	C	28	LEU	2.9
1	A	872	GLN	2.8
1	A	1027	VAL	2.8
1	A	1033	PHE	2.8
1	C	659	LYS	2.8
2	D	166	GLN	2.8
1	A	512	PHE	2.8
1	A	677	ALA	2.8
1	A	359	LEU	2.8
1	A	914	LEU	2.8
1	A	534	ILE	2.8
1	A	1035	ARG	2.7
1	A	1038	GLU	2.7
1	C	403	GLY	2.7
1	A	1036	LYS	2.7
1	C	494	ALA	2.7
1	A	514	GLY	2.7
1	B	689	GLY	2.7
1	B	870	GLY	2.7
1	B	869	SER	2.7
1	A	660	ASP	2.7
1	A	461	GLY	2.7
1	A	1037	ASN	2.7
1	A	961	ILE	2.6
2	E	164	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	540	ARG	2.6
1	A	671	ILE	2.6
1	A	71	GLY	2.6
1	A	966	ASP	2.6
2	D	12	SER	2.6
1	A	541	TYR	2.6
1	B	672	VAL	2.6
2	D	11	GLY	2.6
1	B	867	ARG	2.6
1	C	366	LEU	2.6
2	E	97	GLU	2.5
2	E	127	GLU	2.5
1	B	635	ALA	2.5
1	A	425	LEU	2.5
2	D	14	LEU	2.5
1	C	173	GLY	2.5
1	A	438	ILE	2.5
1	A	501	ALA	2.5
2	E	24	ALA	2.5
1	B	662	MET	2.5
1	B	634	TRP	2.5
1	C	130	GLU	2.4
1	A	536	ARG	2.4
1	B	332	PHE	2.4
1	A	1019	ILE	2.4
1	B	660	ASP	2.4
1	B	561	SER	2.4
1	A	522	LYS	2.4
1	A	402	ILE	2.4
1	A	510	LYS	2.4
1	A	467	TYR	2.3
1	B	407	ASP	2.3
1	A	1034	SER	2.3
1	A	489	THR	2.3
1	C	513	PHE	2.3
1	C	97	GLY	2.3
2	E	34	MET	2.3
1	B	617	PHE	2.3
1	C	897	ILE	2.3
1	A	554	TYR	2.3
1	A	1042	HIS	2.2
1	B	133	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	871	ASN	2.2
2	E	31	ARG	2.2
1	A	967	ALA	2.2
1	C	511	GLY	2.2
1	A	956	GLU	2.2
1	B	628	PHE	2.2
1	C	71	GLY	2.2
1	A	364	ALA	2.2
1	B	866	GLU	2.2
1	A	542	LEU	2.2
1	A	439	GLN	2.2
1	A	620	ARG	2.2
1	A	531	VAL	2.2
1	A	673	GLU	2.2
1	A	518	ARG	2.2
1	A	407	ASP	2.2
1	B	386	PHE	2.1
1	C	370	ILE	2.1
1	A	405	LEU	2.1
1	B	405	LEU	2.1
2	E	68	LYS	2.1
1	A	519	MET	2.1
1	A	431	THR	2.1
1	A	445	ILE	2.1
1	A	831	ALA	2.1
1	A	958	LYS	2.1
1	A	970	MET	2.1
1	A	2	PRO	2.1
1	C	148	THR	2.1
1	A	563	PHE	2.1
1	B	873	ALA	2.1
1	A	881	LEU	2.1
1	A	993	THR	2.1
1	A	498	LYS	2.1
1	A	502	LYS	2.1
1	A	955	LYS	2.1
1	C	29	LYS	2.1
1	A	421	ALA	2.1
1	A	363	ARG	2.0
1	B	837	THR	2.0
1	B	556	PHE	2.0
1	A	496	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	537	SER	2.0
1	A	1043	SER	2.0
1	B	132	SER	2.0
1	A	480	LEU	2.0
1	A	972	LEU	2.0
1	C	546	LEU	2.0
1	C	952	LEU	2.0
1	A	1039	ASP	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](#)

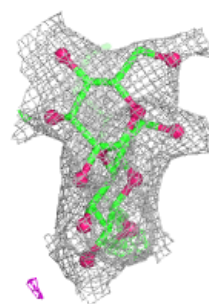
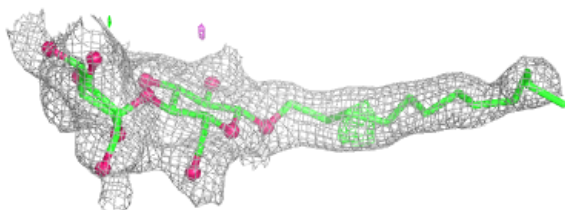
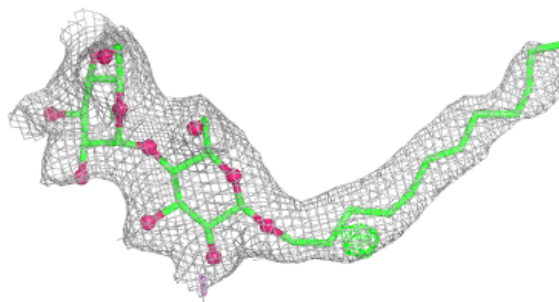
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	1101	35/35	0.87	0.13	46,66,89,93	0
4	MIY	B	1102	33/33	0.88	0.11	46,63,90,103	0
3	LMT	B	1101	35/35	0.91	0.13	44,56,85,91	0
3	LMT	C	1101	35/35	0.92	0.12	48,57,71,72	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.

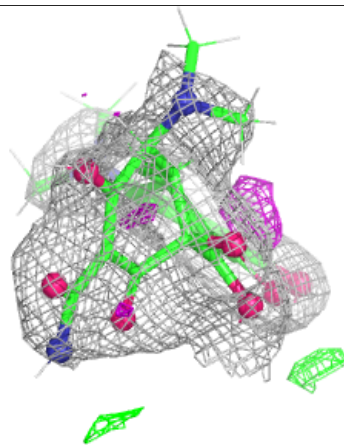
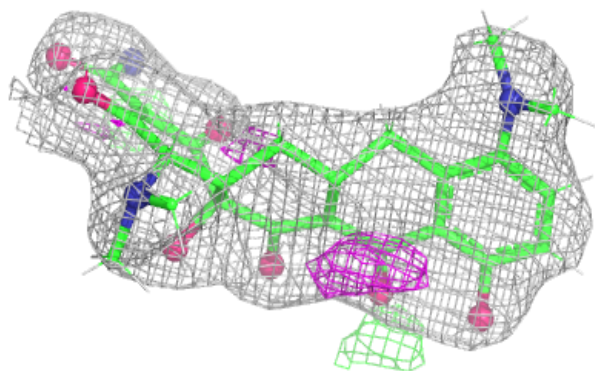
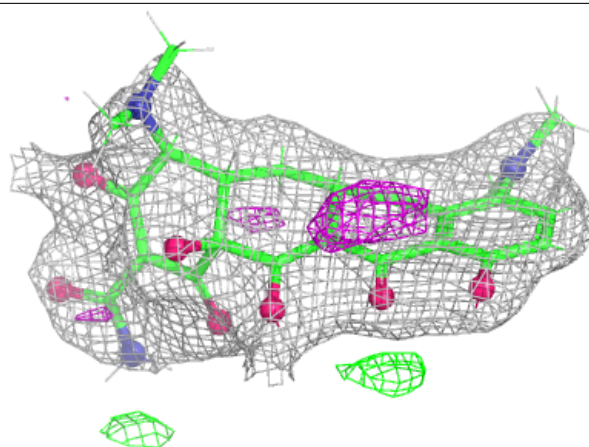
Electron density around LMT A 1101:

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



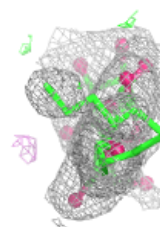
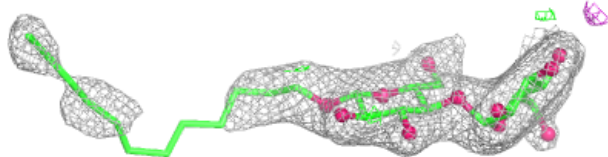
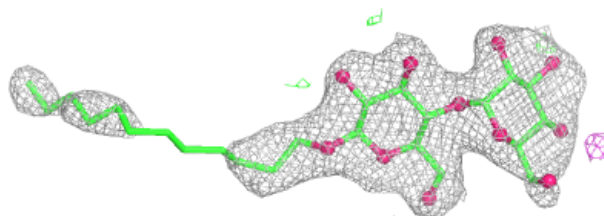
Electron density around MIY B 1102:

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

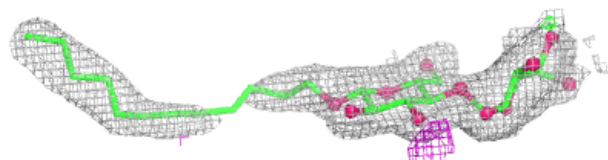
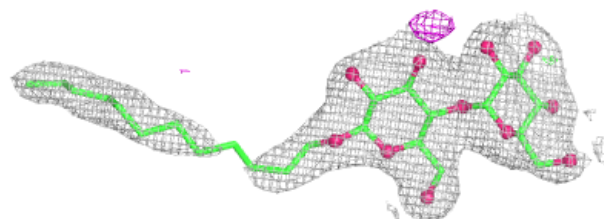


Electron density around LMT B 1101:

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

**Electron density around LMT C 1101:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.