



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:03 AM UTC

PDB ID : 4DX6 / pdb_00004dx6
Title : Transport of drugs by the multidrug transporter AcrB involves an access and a deep binding pocket that are separated by a switch-loop
Authors : Eicher, T.; Cha, H.; Seeger, M.A.; Brandstaetter, L.; El-Delik, J.; Bohnert, J.A.; Kern, W.V.; Verrey, F.; Gruetter, M.G.; Diederichs, K.; Pos, K.M.
Deposited on : 2012-02-27
Resolution : 2.90 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:

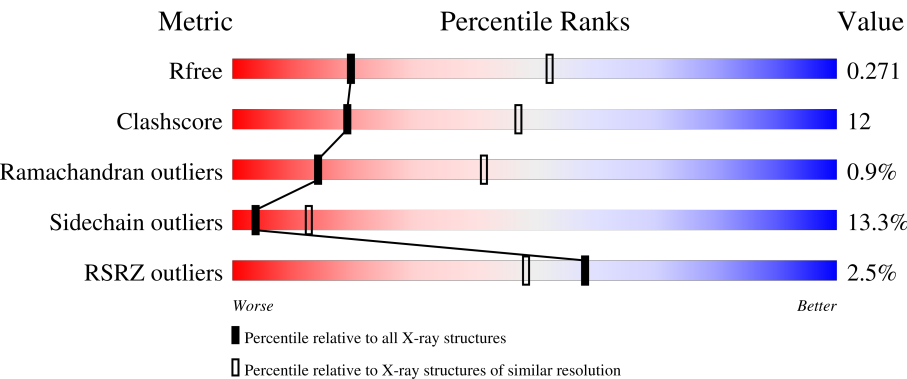
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	3% 63% 30% 6% .
1	B	1057	3% 68% 24% 5% .
1	C	1057	2% 65% 28% . .
2	D	169	% 70% 18% 8% .

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Mol	Chain	Length	Quality of chain
2	E	169	2% 54% 29% 7% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26232 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
			7947	5108	1316	1479	44			
1	B	1033	Total	C	N	O	S	0	0	0
			7853	5054	1296	1459	44			
1	C	1034	Total	C	N	O	S	0	0	0
			7859	5057	1297	1461	44			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	616	ASN	GLY	conflict	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	616	ASN	GLY	conflict	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	616	ASN	GLY	conflict	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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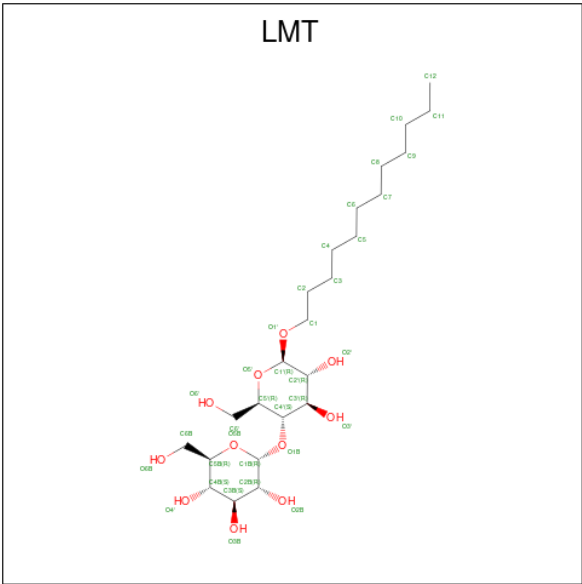
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- 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: C₂₄H₄₆O₁₁).



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	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		

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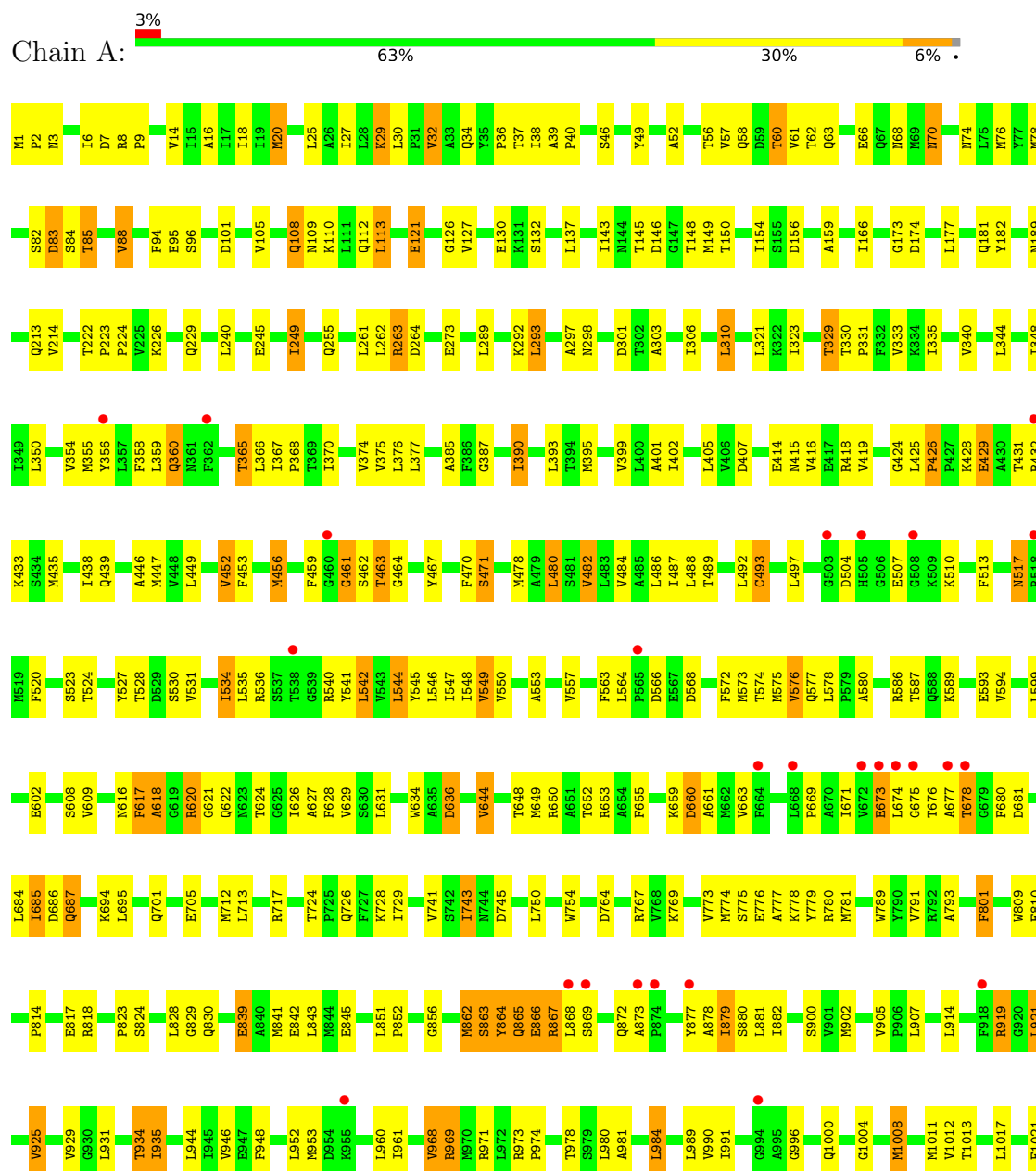
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		

3 Residue-property plots [i](#)

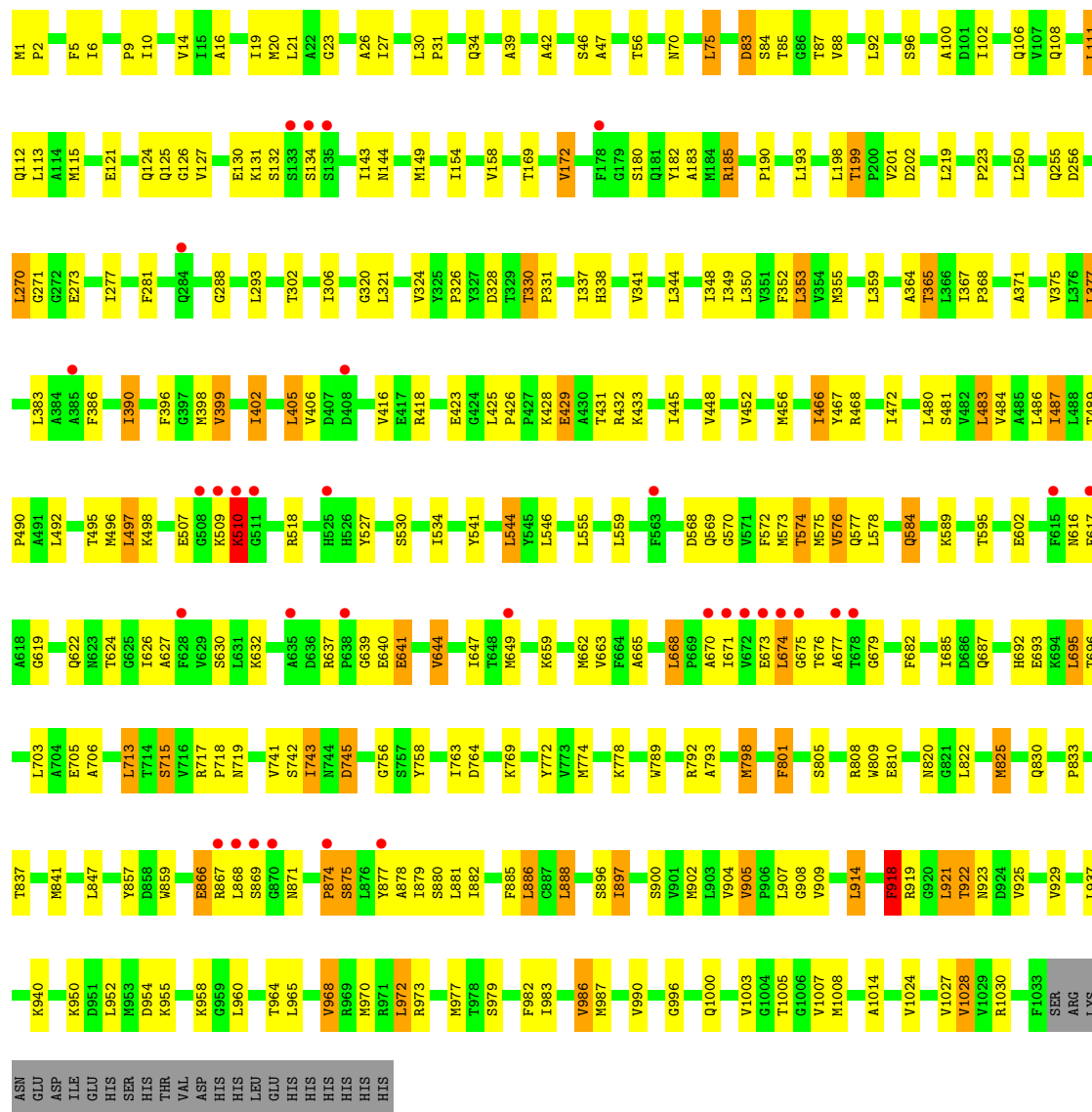
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Acriflavine resistance protein B



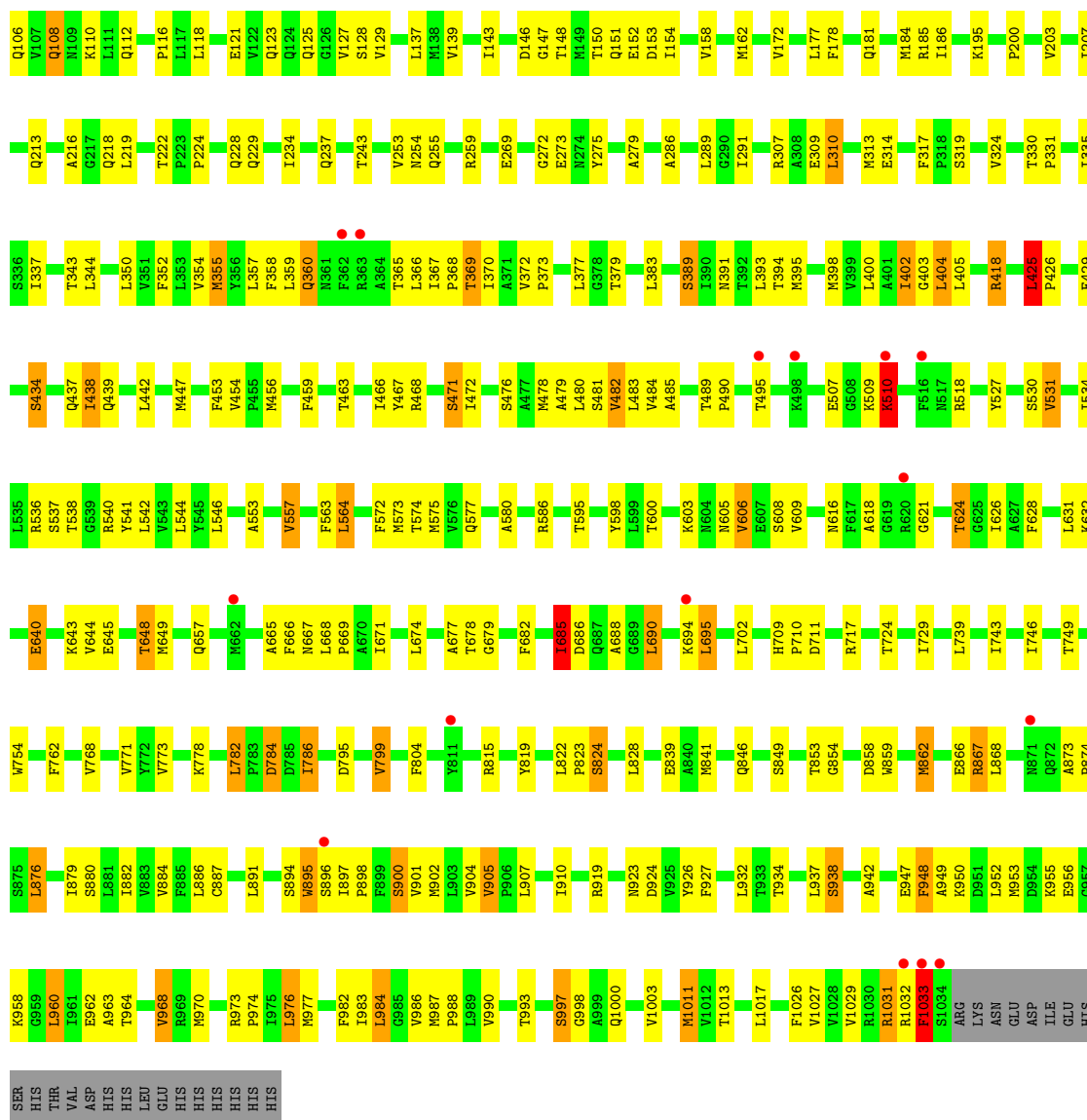


● Molecule 1: Acriflavine resistance protein B

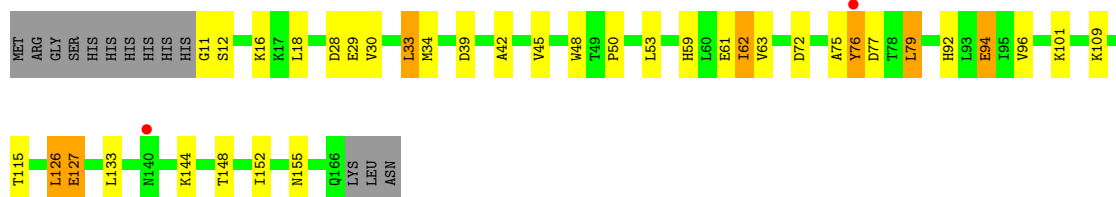


● Molecule 1: Acriflavine resistance protein B



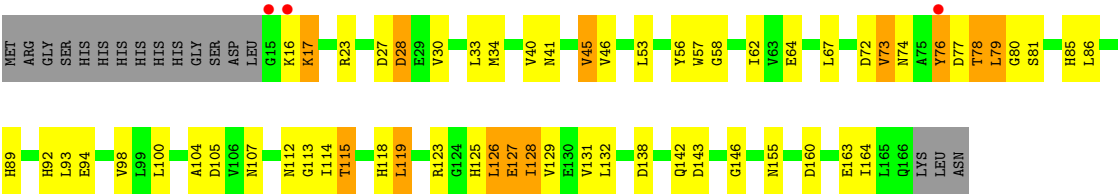


• Molecule 2: DARPIN



• Molecule 2: DARPIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	145.69Å 165.45Å 245.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 2.90 49.28 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.28-2.90) 100.0 (49.28-2.90)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, R_{free}	0.209 , 0.270 0.208 , 0.271	Depositor DCC
R_{free} test set	12616 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	26232	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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

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	0.57	0/8099	0.96	10/10997 (0.1%)
1	B	0.54	0/8003	0.94	15/10869 (0.1%)
1	C	0.58	1/8009 (0.0%)	0.97	23/10877 (0.2%)
2	D	0.51	0/1196	0.87	0/1626
2	E	0.53	0/1170	0.95	2/1591 (0.1%)
All	All	0.56	1/26477 (0.0%)	0.95	50/35960 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	905	VAL	CA-CB	5.17	1.57	1.54

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	ASP	N-CA-C	6.86	118.54	108.86
1	B	425	LEU	CA-C-N	6.79	124.55	119.66
1	B	425	LEU	C-N-CA	6.79	124.55	119.66
1	A	273	GLU	N-CA-C	-6.66	103.95	111.07
1	C	74	ASN	N-CA-C	6.37	120.30	111.90
1	C	997	SER	N-CA-C	-6.24	105.70	113.38
1	B	277	ILE	N-CA-C	6.03	116.55	107.75
1	B	674	LEU	N-CA-C	5.99	123.55	110.80
1	A	685	ILE	N-CA-C	5.89	116.36	108.11
1	B	487	ILE	CB-CA-C	-5.89	105.81	111.05
1	B	869	SER	N-CA-C	5.88	117.35	110.41
1	A	622	GLN	N-CA-C	-5.86	105.89	114.39
1	C	799	VAL	CA-C-N	5.69	125.45	119.76
1	C	799	VAL	C-N-CA	5.69	125.45	119.76
1	B	288	GLY	N-CA-C	5.68	119.87	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	998	GLY	N-CA-C	-5.66	105.94	112.50
2	E	17	LYS	N-CA-C	-5.56	106.34	113.01
1	A	644	VAL	N-CA-C	5.55	116.19	110.36
1	B	83	ASP	N-CA-C	5.49	117.60	109.69
1	C	49	TYR	CA-C-N	5.45	125.76	119.93
1	C	49	TYR	C-N-CA	5.45	125.76	119.93
1	C	367	ILE	CA-C-N	-5.45	114.16	120.04
1	C	367	ILE	C-N-CA	-5.45	114.16	120.04
1	C	782	LEU	CA-C-N	5.42	126.62	119.84
1	C	782	LEU	C-N-CA	5.42	126.62	119.84
1	C	137	LEU	N-CA-C	-5.42	105.45	111.36
1	B	498	LYS	CA-C-N	5.37	125.37	119.89
1	B	498	LYS	C-N-CA	5.37	125.37	119.89
1	B	386	PHE	N-CA-C	-5.36	106.33	112.92
1	C	685	ILE	N-CA-C	5.35	115.60	108.11
1	C	1033	PHE	N-CA-C	5.33	117.42	108.73
1	A	865	GLN	CA-C-N	5.31	131.26	121.70
1	A	865	GLN	C-N-CA	5.31	131.26	121.70
1	B	570	GLY	N-CA-C	-5.24	108.45	114.69
1	C	425	LEU	CA-C-N	5.24	123.43	119.66
1	C	425	LEU	C-N-CA	5.24	123.43	119.66
1	A	426	PRO	O-C-N	5.23	123.71	121.31
1	C	905	VAL	CA-C-N	-5.21	114.30	119.56
1	C	905	VAL	C-N-CA	-5.21	114.30	119.56
1	A	661	ALA	N-CA-C	5.19	116.18	108.60
1	B	905	VAL	N-CA-C	5.19	119.15	112.67
1	A	249	ILE	N-CA-CB	5.18	116.69	110.31
1	C	679	GLY	N-CA-C	5.18	117.82	111.45
2	E	104	ALA	N-CA-C	5.16	118.28	110.64
1	C	454	VAL	CA-C-N	-5.15	113.62	119.28
1	C	454	VAL	C-N-CA	-5.15	113.62	119.28
1	B	644	VAL	N-CA-C	5.12	115.73	110.36
1	B	1007	VAL	N-CA-C	-5.09	106.18	111.58
1	C	538	THR	N-CA-C	5.06	117.45	111.33
1	C	895	TRP	N-CA-C	-5.03	107.54	113.97

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	7947	0	8087	226	0
1	B	7853	0	8004	164	0
1	C	7859	0	8009	188	0
2	D	1177	0	1159	25	0
2	E	1151	0	1136	40	0
3	A	70	0	92	4	0
3	B	105	0	138	4	0
3	C	70	0	92	3	0
All	All	26232	0	26717	624	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 (624) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:GLY:H	1:A:624:THR:HG21	1.31	0.95
1:A:968:VAL:HG21	1:A:1023:PRO:HG3	1.57	0.86
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.59	0.84
1:C:616:ASN:HB3	1:C:618:ALA:H	1.41	0.84
1:A:764:ASP:OD2	1:A:769:LYS:NZ	2.16	0.79
1:A:350:LEU:HD23	1:A:984:LEU:HD13	1.65	0.79
1:B:696:THR:HG22	1:B:825:MET:HE1	1.65	0.79
1:A:580:ALA:HB1	1:A:724:THR:HG22	1.64	0.78
1:A:674:LEU:HB3	1:A:675:GLY:HA2	1.65	0.78
1:A:867:ARG:HB3	1:A:868:LEU:HB2	1.64	0.78
1:C:876:LEU:HD11	1:C:932:LEU:HD11	1.65	0.78
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.65	0.76
1:A:356:TYR:HA	1:A:365:THR:HG21	1.67	0.76
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.66	0.76
1:B:324:VAL:HG23	1:B:326:PRO:HD3	1.66	0.75
1:A:866:GLU:HB2	1:A:867:ARG:HA	1.69	0.75
1:C:563:PHE:HB2	1:C:866:GLU:HG3	1.67	0.74
1:B:866:GLU:OE2	3:B:1103:LMT:O4'	2.07	0.72
1:C:572:PHE:HE2	1:C:631:LEU:HD21	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:979:SER:O	1:B:983:ILE:HG12	1.90	0.72
1:A:575:MET:HE3	1:A:616:ASN:HD22	1.53	0.71
1:A:14:VAL:HG22	1:B:886:LEU:HD12	1.73	0.71
1:B:990:VAL:HG13	1:B:1005:THR:HG22	1.72	0.70
1:A:775:SER:HB3	1:A:780:ARG:HD3	1.73	0.70
1:A:809:TRP:HE1	2:E:78:THR:HG23	1.57	0.70
2:E:46:VAL:O	2:E:78:THR:HG22	1.92	0.70
1:B:919:ARG:NH2	1:B:990:VAL:O	2.26	0.69
1:B:897:ILE:O	1:B:900:SER:OG	2.11	0.68
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.76	0.68
1:A:56:THR:O	1:A:60:THR:HB	1.94	0.68
1:C:960:LEU:HD22	1:C:1027:VAL:HG22	1.76	0.67
2:E:115:THR:OG1	2:E:118:HIS:ND1	2.27	0.67
1:A:74:ASN:HB3	1:A:95:GLU:HB2	1.76	0.67
1:B:973:ARG:HG2	1:B:977:MET:HE2	1.77	0.67
1:B:445:ILE:HG21	1:B:940:LYS:HE2	1.75	0.67
1:C:357:LEU:O	1:C:360:GLN:NE2	2.28	0.67
1:C:867:ARG:HG2	1:C:867:ARG:HH11	1.60	0.66
1:A:459:PHE:HB2	1:A:464:GLY:HA2	1.78	0.66
1:B:574:THR:HG23	1:B:627:ALA:HB3	1.78	0.65
1:C:536:ARG:NH2	3:C:1102:LMT:O3B	2.28	0.65
1:C:907:LEU:HD22	1:C:1017:LEU:HD23	1.79	0.65
1:B:987:MET:HG2	1:B:1008:MET:HE3	1.79	0.65
1:A:602:GLU:OE1	1:A:650:ARG:NH1	2.30	0.65
1:B:950:LYS:NZ	1:B:954:ASP:OD1	2.25	0.64
1:B:47:ALA:HB2	1:B:127:VAL:HG13	1.80	0.64
1:B:742:SER:HB3	1:B:745:ASP:HB2	1.79	0.64
1:A:934:THR:HG22	1:A:1011:MET:HE3	1.80	0.64
2:E:28:ASP:OD1	2:E:28:ASP:N	2.31	0.64
1:A:70:ASN:O	1:A:110:LYS:HE3	1.98	0.63
1:B:108:GLN:HG3	1:C:112:GLN:HG3	1.79	0.63
1:A:616:ASN:O	1:A:618:ALA:N	2.31	0.63
1:C:104:GLN:HE22	1:C:108:GLN:HG3	1.63	0.63
1:A:534:ILE:HB	1:A:541:TYR:CZ	2.34	0.63
1:B:584:GLN:HB3	1:B:622:GLN:HG2	1.81	0.63
1:C:393:LEU:HD13	1:C:466:ILE:HG23	1.81	0.62
1:B:527:TYR:CE2	1:B:968:VAL:HG13	2.34	0.62
1:C:104:GLN:NE2	1:C:108:GLN:HG3	2.13	0.62
2:E:56:TYR:HB2	2:E:86:LEU:HD13	1.81	0.62
1:C:49:TYR:HB3	1:C:57:VAL:HG22	1.80	0.62
1:A:137:LEU:O	1:A:329:THR:OG1	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:THR:HA	1:B:665:ALA:HA	1.82	0.62
1:B:507:GLU:O	1:B:518:ARG:NH1	2.32	0.61
1:C:150:THR:O	1:C:154:ILE:HG13	2.00	0.61
1:B:26:ALA:O	1:B:30:LEU:HB2	2.01	0.61
1:A:109:ASN:O	1:A:112:GLN:HG2	2.01	0.61
1:A:674:LEU:HB3	1:A:675:GLY:CA	2.31	0.61
1:A:355:MET:HB3	1:A:365:THR:HB	1.83	0.61
1:A:669:PRO:HG2	1:A:674:LEU:HD21	1.83	0.61
1:C:8:ARG:NH2	3:C:1101:LMT:O4'	2.33	0.61
1:B:405:LEU:HD22	1:B:481:SER:HB2	1.82	0.60
1:A:416:VAL:HG22	1:A:431:THR:HA	1.84	0.60
1:C:575:MET:HG3	1:C:666:PHE:HE1	1.65	0.60
1:B:124:GLN:NE2	1:B:758:TYR:O	2.34	0.60
2:E:123:ARG:HG2	2:E:125:HIS:CE1	2.37	0.60
1:B:885:PHE:HD1	1:B:902:MET:HE1	1.66	0.60
1:A:355:MET:HE2	1:A:355:MET:HA	1.84	0.59
1:B:75:LEU:HD21	1:B:92:LEU:HB3	1.84	0.59
1:B:801:PHE:O	1:B:805:SER:OG	2.19	0.59
2:E:126:LEU:HD12	2:E:126:LEU:H	1.66	0.59
1:C:150:THR:HG23	1:C:153:ASP:H	1.67	0.59
1:C:151:GLN:HE21	1:C:286:ALA:H	1.49	0.59
1:A:16:ALA:HB2	1:A:488:LEU:HD22	1.83	0.59
1:B:375:VAL:HG22	1:B:484:VAL:HG21	1.85	0.59
1:B:576:VAL:HB	1:B:663:VAL:HG22	1.85	0.59
2:E:74:ASN:HD21	2:E:105:ASP:H	1.49	0.59
1:A:213:GLN:HG3	1:B:56:THR:HG23	1.84	0.58
1:A:989:LEU:HD22	1:A:1000:GLN:HB3	1.84	0.58
1:B:134:SER:OG	1:B:673:GLU:OE2	2.21	0.58
1:A:189:ASN:ND2	1:A:779:TYR:OH	2.37	0.58
1:A:649:MET:HE1	1:A:653:ARG:HH11	1.69	0.58
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.68	0.58
1:A:774:MET:HG2	1:A:775:SER:H	1.68	0.58
1:A:29:LYS:HE3	3:B:1102:LMT:H1'	1.86	0.58
1:C:370:ILE:O	1:C:373:PRO:HD2	2.04	0.58
1:A:907:LEU:HD22	1:A:1017:LEU:HB3	1.85	0.58
1:C:690:LEU:HD21	1:C:854:GLY:HA3	1.85	0.58
1:A:101:ASP:O	1:A:105:VAL:HG23	2.04	0.58
1:A:461:GLY:O	1:A:463:THR:N	2.37	0.57
1:A:980:LEU:O	1:A:984:LEU:HB2	2.03	0.57
1:A:839:GLU:HA	1:A:842:GLU:HB3	1.86	0.57
1:B:952:LEU:HD22	1:B:958:LYS:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ASN:O	1:C:110:LYS:NZ	2.38	0.57
1:B:871:ASN:HD22	3:B:1102:LMT:H6'1	1.69	0.57
1:C:540:ARG:NH2	3:C:1102:LMT:O6'	2.38	0.57
1:A:34:GLN:HB2	1:A:333:VAL:HG22	1.87	0.57
1:A:686:ASP:HB3	1:A:823:PRO:HB2	1.87	0.57
1:A:878:ALA:O	1:A:882:ILE:HG12	2.05	0.57
1:A:166:ILE:HD12	1:A:306:ILE:HG23	1.87	0.56
1:B:897:ILE:HD12	1:B:950:LYS:HD2	1.87	0.56
1:C:355:MET:HE3	1:C:368:PRO:HG2	1.87	0.56
2:E:67:LEU:HD21	2:E:73:VAL:HG23	1.86	0.56
1:A:535:LEU:HD22	1:A:1027:VAL:HG21	1.88	0.56
1:C:904:VAL:HG13	1:C:938:SER:HB2	1.86	0.56
1:A:401:ALA:O	1:A:405:LEU:HG	2.05	0.56
1:C:186:ILE:HB	1:C:773:VAL:HG12	1.87	0.56
1:A:636:ASP:OD2	1:A:636:ASP:N	2.39	0.56
1:A:726:GLN:N	1:A:810:GLU:O	2.33	0.56
2:E:94:GLU:O	2:E:98:VAL:HG23	2.05	0.56
1:A:867:ARG:H	1:A:868:LEU:HB2	1.71	0.56
1:B:396:PHE:HA	1:B:399:VAL:HG13	1.88	0.56
1:A:609:VAL:HG22	1:A:629:VAL:HG22	1.88	0.56
1:C:150:THR:HG22	1:C:153:ASP:OD1	2.06	0.56
1:A:27:ILE:HD13	3:A:1101:LMT:H61	1.88	0.56
1:A:146:ASP:HB2	1:A:148:THR:HG23	1.87	0.56
1:B:673:GLU:O	1:B:675:GLY:N	2.38	0.56
2:E:58:GLY:HA3	2:E:92:HIS:CE1	2.42	0.55
1:A:255:GLN:CD	1:A:255:GLN:H	2.14	0.55
1:B:1024:VAL:O	1:B:1028:VAL:HG12	2.06	0.55
1:C:365:THR:O	1:C:369:THR:OG1	2.24	0.55
1:C:531:VAL:HA	1:C:534:ILE:HB	1.88	0.55
1:C:563:PHE:O	1:C:924:ASP:HB2	2.07	0.55
1:A:996:GLY:O	1:A:1000:GLN:HG3	2.06	0.55
1:A:1011:MET:HE2	1:A:1011:MET:HA	1.88	0.55
1:A:415:ASN:OD1	1:A:418:ARG:NH1	2.39	0.55
1:B:715:SER:O	1:B:717:ARG:NH1	2.38	0.55
2:E:34:MET:HA	2:E:34:MET:HE3	1.88	0.55
1:A:3:ASN:HA	1:A:6:ILE:HD12	1.88	0.55
1:B:352:PHE:HD2	1:B:353:LEU:HD13	1.72	0.55
1:C:682:PHE:HB2	1:C:859:TRP:CZ3	2.41	0.55
2:D:126:LEU:H	2:D:126:LEU:HD12	1.71	0.55
2:E:30:VAL:O	2:E:34:MET:HB2	2.07	0.55
1:A:49:TYR:CE2	1:A:121:GLU:HG3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:692:HIS:O	1:B:696:THR:HG23	2.07	0.55
1:C:379:THR:HG23	1:C:476:SER:HB2	1.89	0.54
1:C:507:GLU:HG2	1:C:518:ARG:HG2	1.89	0.54
2:D:29:GLU:O	2:D:33:LEU:HD12	2.08	0.54
2:D:48:TRP:CD1	2:D:77:ASP:HB3	2.40	0.54
1:A:354:VAL:HG21	1:A:981:ALA:HA	1.88	0.54
1:A:453:PHE:O	1:A:471:SER:OG	2.24	0.54
1:C:151:GLN:NE2	1:C:286:ALA:H	2.05	0.54
1:C:372:VAL:HA	1:C:405:LEU:HD11	1.88	0.54
1:A:20:MET:HG3	1:A:377:LEU:HD13	1.88	0.54
1:A:1008:MET:O	1:A:1012:VAL:HG23	2.07	0.54
1:A:393:LEU:HD22	1:A:470:PHE:HE1	1.72	0.54
1:A:573:MET:HE1	1:A:628:PHE:CE1	2.42	0.54
1:B:144:ASN:HB2	1:B:154:ILE:HD11	1.89	0.54
1:B:877:TYR:HE2	3:B:1103:LMT:H11	1.72	0.54
2:D:34:MET:HE2	2:D:34:MET:HA	1.90	0.54
2:E:113:GLY:O	2:E:143:ASP:HA	2.08	0.54
1:C:485:ALA:HA	1:C:489:THR:OG1	2.08	0.54
1:A:864:TYR:C	1:A:867:ARG:HB2	2.33	0.54
1:A:63:GLN:CD	1:C:768:VAL:HG23	2.33	0.53
1:A:574:THR:HB	1:A:627:ALA:HB3	1.89	0.53
1:A:576:VAL:HG22	1:A:663:VAL:HG22	1.90	0.53
1:A:777:ALA:O	1:A:781:MET:HG2	2.09	0.53
1:C:36:PRO:O	1:C:38:ILE:HG23	2.08	0.53
1:C:181:GLN:O	1:C:272:GLY:HA2	2.08	0.53
1:C:203:VAL:O	1:C:207:ILE:HG13	2.08	0.53
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.90	0.53
1:B:10:ILE:HD12	1:C:895:TRP:NE1	2.23	0.53
1:C:882:ILE:O	1:C:886:LEU:HG	2.08	0.53
1:A:456:MET:HG3	1:A:467:TYR:HB3	1.89	0.53
1:A:1022:VAL:HA	1:A:1025:PHE:HD1	1.74	0.53
1:B:328:ASP:OD1	1:B:330:THR:HB	2.08	0.53
1:C:418:ARG:HH12	1:C:970:MET:HG2	1.74	0.53
1:C:648:THR:HG22	1:C:665:ALA:HB1	1.90	0.53
1:A:366:LEU:O	1:A:370:ILE:HG12	2.08	0.53
1:B:42:ALA:HB3	1:B:132:SER:HB2	1.91	0.53
1:B:416:VAL:HG21	1:B:431:THR:HG22	1.91	0.53
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.43	0.53
1:A:865:GLN:HA	1:A:866:GLU:C	2.33	0.53
1:C:438:ILE:HG12	1:C:442:LEU:HG	1.91	0.53
1:A:166:ILE:HD11	1:A:310:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ASN:HA	1:C:6:ILE:HD12	1.91	0.52
1:C:600:THR:O	1:C:603:LYS:HE3	2.09	0.52
2:E:41:ASN:HD21	2:E:72:ASP:HB2	1.75	0.52
1:A:393:LEU:HD22	1:A:470:PHE:CE1	2.44	0.52
1:A:414:GLU:CD	1:A:974:PRO:HG3	2.34	0.52
1:A:426:PRO:HD2	1:A:429:GLU:HG3	1.90	0.52
1:B:83:ASP:OD2	1:B:85:THR:OG1	2.27	0.52
1:B:925:VAL:O	1:B:929:VAL:HG23	2.09	0.52
2:E:93:LEU:HD13	2:E:128:ILE:HG12	1.90	0.52
1:C:150:THR:OG1	1:C:151:GLN:N	2.41	0.52
1:A:545:TYR:O	1:A:549:VAL:HG23	2.10	0.52
1:A:960:LEU:HG	1:A:1027:VAL:HG12	1.92	0.52
1:C:309:GLU:HG3	1:C:313:MET:HE3	1.91	0.52
1:A:435:MET:O	1:A:439:GLN:HB2	2.10	0.52
1:A:573:MET:HE3	1:A:617:PHE:HZ	1.75	0.52
1:B:1:MET:HE2	1:B:487:ILE:HG12	1.92	0.52
1:C:667:ASN:OD1	1:C:668:LEU:N	2.42	0.52
2:E:85:HIS:NE2	2:E:114:ILE:O	2.30	0.52
2:E:89:HIS:CD2	2:E:119:LEU:HG	2.45	0.52
1:A:544:LEU:O	1:A:548:ILE:HG12	2.10	0.51
1:B:281:PHE:CZ	1:B:324:VAL:HG21	2.45	0.51
1:A:817:GLU:HB2	1:A:824:SER:O	2.11	0.51
1:A:867:ARG:HG3	1:A:868:LEU:HD13	1.92	0.51
1:A:879:ILE:HG12	1:A:880:SER:N	2.21	0.51
1:B:676:THR:OG1	1:B:679:GLY:HA3	2.09	0.51
1:C:480:LEU:O	1:C:484:VAL:HG23	2.10	0.51
1:C:949:ALA:O	1:C:953:MET:HG3	2.10	0.51
1:A:867:ARG:HB3	1:A:868:LEU:CB	2.39	0.51
1:B:423:GLU:OE1	1:B:433:LYS:NZ	2.41	0.51
1:B:584:GLN:HB3	1:B:622:GLN:CG	2.41	0.51
1:B:632:LYS:O	1:B:637:ARG:NE	2.31	0.51
1:C:102:ILE:O	1:C:106:GLN:HG3	2.10	0.51
1:C:218:GLN:HA	1:C:234:ILE:HG13	1.92	0.51
1:C:897:ILE:HB	1:C:898:PRO:HD3	1.93	0.51
1:A:310:LEU:HG	1:A:323:ILE:HD13	1.92	0.51
1:C:259:ARG:HH22	2:E:155:ASN:CG	2.17	0.51
1:C:595:THR:HG23	1:C:609:VAL:HG11	1.93	0.51
1:B:16:ALA:O	1:B:20:MET:HG3	2.10	0.51
1:B:908:GLY:HA2	1:B:1014:ALA:HB2	1.91	0.51
1:A:750:LEU:HB2	1:A:801:PHE:CZ	2.46	0.51
1:B:190:PRO:HB3	1:B:789:TRP:CE3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:ASN:HB3	1:B:619:GLY:O	2.11	0.51
1:A:865:GLN:HA	1:A:867:ARG:N	2.26	0.50
2:D:30:VAL:HG21	2:D:62:ILE:HG12	1.92	0.50
1:A:676:THR:O	1:A:678:THR:N	2.38	0.50
1:A:900:SER:HB3	1:A:1029:VAL:HG21	1.94	0.50
1:A:110:LYS:O	1:A:113:LEU:HB2	2.12	0.50
1:B:575:MET:HE1	1:B:617:PHE:HB2	1.93	0.50
1:B:223:PRO:HD3	1:C:275:TYR:CD1	2.46	0.50
1:C:873:ALA:N	1:C:874:PRO:HD2	2.27	0.50
1:A:146:ASP:CB	1:A:148:THR:HG23	2.41	0.50
1:A:149:MET:HE3	1:A:154:ILE:HG12	1.94	0.50
1:B:355:MET:O	1:B:359:LEU:HB2	2.12	0.50
1:A:594:VAL:HA	1:A:655:PHE:CE1	2.47	0.50
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.93	0.50
1:C:564:LEU:HD12	1:C:926:TYR:CE1	2.47	0.50
1:B:960:LEU:HD21	1:B:1027:VAL:HA	1.93	0.50
1:C:575:MET:HG3	1:C:666:PHE:CE1	2.46	0.50
1:A:14:VAL:O	1:A:18:ILE:HG12	2.12	0.50
1:C:45:ILE:HG12	1:C:129:VAL:HG22	1.93	0.50
1:C:531:VAL:HG21	1:C:968:VAL:HG11	1.93	0.50
1:C:645:GLU:O	1:C:649:MET:HB2	2.12	0.50
2:D:94:GLU:CD	2:D:94:GLU:H	2.18	0.50
1:A:263:ARG:NH2	2:D:155:ASN:O	2.43	0.49
1:C:644:VAL:O	1:C:648:THR:OG1	2.29	0.49
2:E:160:ASP:O	2:E:163:GLU:HG2	2.12	0.49
1:B:39:ALA:HB2	1:B:673:GLU:HG2	1.94	0.49
1:C:784:ASP:OD2	1:C:784:ASP:N	2.43	0.49
1:A:775:SER:OG	1:A:789:TRP:HZ2	1.95	0.49
2:E:89:HIS:O	2:E:123:ARG:HD2	2.13	0.49
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.12	0.49
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.12	0.49
1:B:30:LEU:HB3	1:B:390:ILE:HD12	1.95	0.49
1:A:303:ALA:HB2	1:A:330:THR:HG21	1.94	0.49
1:B:875:SER:O	1:B:879:ILE:HG12	2.11	0.49
1:B:149:MET:HE2	1:B:154:ILE:HD13	1.94	0.49
2:D:48:TRP:HD1	2:D:77:ASP:HB3	1.77	0.49
2:E:56:TYR:HD1	2:E:57:TRP:CE3	2.30	0.49
1:A:85:THR:HG21	1:A:620:ARG:HG2	1.95	0.49
1:C:395:MET:HE2	1:C:395:MET:HA	1.93	0.49
1:C:573:MET:HB2	1:C:666:PHE:CE2	2.48	0.49
1:C:997:SER:HA	1:C:1000:GLN:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:PRO:O	1:C:335:ILE:HG22	2.13	0.49
1:B:573:MET:HE2	1:B:668:LEU:HD22	1.95	0.48
1:B:809:TRP:NE1	2:D:79:LEU:HD22	2.28	0.48
1:B:866:GLU:O	1:B:868:LEU:N	2.46	0.48
1:B:426:PRO:HD2	1:B:429:GLU:HG3	1.95	0.48
1:B:573:MET:HB2	1:B:573:MET:HE3	1.61	0.48
1:C:352:PHE:HD1	1:C:369:THR:HG21	1.78	0.48
1:C:640:GLU:HA	1:C:643:LYS:HG2	1.95	0.48
1:C:948:PHE:CE1	1:C:970:MET:HE2	2.48	0.48
2:E:23:ARG:HB2	2:E:53:LEU:HD13	1.94	0.48
2:E:76:TYR:H	2:E:76:TYR:HD2	1.61	0.48
1:B:677:ALA:C	1:B:679:GLY:H	2.22	0.48
1:B:792:ARG:HB2	1:B:798:MET:HE1	1.96	0.48
1:C:880:SER:O	1:C:884:VAL:HG23	2.12	0.48
1:C:983:ILE:HG13	1:C:1011:MET:HG2	1.95	0.48
1:A:544:LEU:HA	1:A:547:ILE:HD12	1.95	0.48
1:A:578:LEU:HD13	1:A:587:THR:HG23	1.96	0.48
1:A:594:VAL:HG13	1:A:655:PHE:CZ	2.49	0.48
1:C:228:GLN:HG3	1:C:229:GLN:N	2.27	0.48
2:D:148:THR:O	2:D:152:ILE:HG12	2.13	0.48
2:E:160:ASP:O	2:E:164:ILE:HG13	2.14	0.48
1:A:527:TYR:CE1	1:A:968:VAL:HG13	2.48	0.48
2:D:72:ASP:HB3	2:D:75:ALA:HB2	1.96	0.48
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.44	0.48
1:A:68:ASN:O	1:A:110:LYS:HB3	2.13	0.48
1:A:530:SER:O	1:A:534:ILE:HG23	2.14	0.48
1:C:1029:VAL:C	1:C:1031:ARG:H	2.22	0.48
1:C:309:GLU:O	1:C:313:MET:HG3	2.12	0.47
1:B:180:SER:HB2	1:B:273:GLU:HG3	1.95	0.47
1:B:964:THR:O	1:B:968:VAL:HB	2.14	0.47
1:C:573:MET:HE3	1:C:573:MET:HB3	1.80	0.47
2:E:125:HIS:O	2:E:129:VAL:HG23	2.13	0.47
2:E:127:GLU:O	2:E:131:VAL:HG23	2.14	0.47
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.97	0.47
1:A:528:THR:HG21	1:A:969:ARG:HB3	1.97	0.47
1:B:371:ALA:O	1:B:375:VAL:HG23	2.13	0.47
1:B:918:PHE:CD1	1:B:918:PHE:C	2.92	0.47
1:C:418:ARG:CZ	1:C:970:MET:HE3	2.44	0.47
1:A:360:GLN:HG3	1:A:513:PHE:CD1	2.49	0.47
1:B:982:PHE:O	1:B:986:VAL:HG13	2.15	0.47
2:E:27:ASP:HA	2:E:62:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:PHE:CD1	1:B:487:ILE:HG23	2.50	0.47
1:C:459:PHE:CE1	1:C:876:LEU:HD23	2.50	0.47
1:A:293:LEU:HD22	1:A:297:ALA:HB3	1.97	0.47
1:B:448:VAL:O	1:B:452:VAL:HG23	2.15	0.47
1:C:686:ASP:HB2	1:C:695:LEU:HG	1.97	0.47
2:D:12:SER:O	2:D:16:LYS:HG2	2.15	0.47
1:A:358:PHE:HE2	1:A:520:PHE:HE1	1.62	0.47
1:C:20:MET:HG2	1:C:377:LEU:HD12	1.96	0.47
1:C:621:GLY:O	1:C:624:THR:HB	2.14	0.47
1:A:2:PRO:O	1:A:6:ILE:HG13	2.15	0.47
1:A:527:TYR:HE1	1:A:968:VAL:HG13	1.80	0.47
1:A:1043:SER:HA	1:A:1044:HIS:HA	1.57	0.47
1:B:616:ASN:HB2	1:B:624:THR:HB	1.96	0.47
1:C:61:VAL:O	1:C:65:ILE:HG13	2.14	0.47
1:A:572:PHE:HE1	1:A:631:LEU:HD21	1.80	0.47
1:A:919:ARG:NH2	1:A:990:VAL:O	2.48	0.47
1:A:1038:GLU:CD	1:A:1039:ASP:HA	2.40	0.47
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.96	0.47
1:A:919:ARG:HB3	1:A:921:LEU:HD22	1.97	0.46
1:C:151:GLN:NE2	1:C:279:ALA:O	2.47	0.46
1:C:358:PHE:CD1	1:C:977:MET:HG2	2.50	0.46
1:C:841:MET:HE3	1:C:859:TRP:CD2	2.50	0.46
2:E:77:ASP:O	2:E:80:GLY:N	2.48	0.46
3:A:1102:LMT:H5B	3:A:1102:LMT:H6D	1.96	0.46
1:B:154:ILE:O	1:B:158:VAL:HG23	2.15	0.46
2:D:92:HIS:O	2:D:96:VAL:HG23	2.14	0.46
1:A:680:PHE:CZ	1:A:829:GLY:HA3	2.51	0.46
1:A:132:SER:HB3	1:A:173:GLY:HA3	1.96	0.46
1:C:984:LEU:HD12	1:C:987:MET:HG3	1.98	0.46
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.76	0.46
1:A:925:VAL:O	1:A:929:VAL:HG22	2.16	0.46
1:C:509:LYS:HA	1:C:510:LYS:HD2	1.98	0.46
1:B:377:LEU:HD12	1:B:377:LEU:HA	1.75	0.46
1:C:33:ALA:O	1:C:337:ILE:HD11	2.16	0.46
1:C:958:LYS:HB2	1:C:963:ALA:HB2	1.98	0.46
1:A:108:GLN:O	1:A:108:GLN:HG3	2.16	0.46
1:A:809:TRP:NE1	2:E:78:THR:HG23	2.26	0.46
1:B:905:VAL:O	1:B:909:VAL:HG23	2.15	0.46
1:B:986:VAL:O	1:B:990:VAL:HG23	2.15	0.46
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.97	0.46
1:B:14:VAL:HG13	1:C:886:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ALA:HB1	1:B:131:LYS:HD3	1.98	0.46
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.97	0.46
1:A:407:ASP:HB2	1:A:978:THR:HG21	1.98	0.46
1:A:1021:PHE:HB3	1:A:1025:PHE:CE1	2.51	0.46
1:A:449:LEU:HB3	1:A:478:MET:HE1	1.97	0.46
1:A:774:MET:HG2	1:A:775:SER:N	2.30	0.46
1:A:459:PHE:CE2	1:A:873:ALA:HB2	2.51	0.45
1:C:383:LEU:HD12	1:C:383:LEU:HA	1.79	0.45
1:C:200:PRO:HD2	1:C:749:THR:HG23	1.98	0.45
3:A:1102:LMT:H41	3:A:1102:LMT:H72	1.56	0.45
1:B:534:ILE:HG23	1:B:541:TYR:CE1	2.51	0.45
2:E:123:ARG:HG2	2:E:125:HIS:HE1	1.79	0.45
1:A:156:ASP:HB2	1:A:182:TYR:CD1	2.51	0.45
1:C:685:ILE:HD11	1:C:858:ASP:HB2	1.97	0.45
1:C:846:GLN:O	1:C:849:SER:OG	2.34	0.45
1:A:416:VAL:HG11	1:A:431:THR:HG22	1.99	0.45
1:A:687:GLN:HG3	1:A:856:GLY:N	2.30	0.45
1:A:1013:THR:HB	1:A:1017:LEU:HD23	1.97	0.45
1:B:428:LYS:HE3	1:B:432:ARG:NH2	2.32	0.45
1:C:671:ILE:H	1:C:862:MET:HE1	1.82	0.45
1:A:674:LEU:HD22	1:A:676:THR:N	2.31	0.45
1:B:111:LEU:O	1:B:115:MET:HG2	2.16	0.45
1:B:472:ILE:HD13	1:B:472:ILE:HA	1.89	0.45
1:C:139:VAL:HG13	1:C:178:PHE:HE1	1.82	0.45
1:C:425:LEU:HD12	1:C:425:LEU:HA	1.86	0.45
1:C:686:ASP:HB3	1:C:823:PRO:HB2	1.97	0.45
1:A:83:ASP:OD2	1:A:85:THR:HG23	2.16	0.45
1:A:395:MET:O	1:A:399:VAL:HG23	2.17	0.45
1:A:589:LYS:O	1:A:593:GLU:HG3	2.17	0.45
1:A:780:ARG:HG3	1:A:780:ARG:HH11	1.82	0.45
1:A:877:TYR:HA	1:A:880:SER:HB3	1.97	0.45
1:B:448:VAL:HG21	1:B:888:LEU:HD13	1.98	0.45
1:B:874:PRO:HG2	1:B:875:SER:H	1.82	0.45
1:C:479:ALA:O	1:C:482:VAL:HG13	2.17	0.45
1:A:575:MET:HE3	1:A:616:ASN:ND2	2.29	0.45
1:A:867:ARG:CB	1:A:868:LEU:HB2	2.41	0.45
1:C:973:ARG:HB3	1:C:974:PRO:HD3	1.98	0.45
1:A:517:ASN:N	1:A:517:ASN:HD22	2.15	0.45
1:A:546:LEU:O	1:A:550:VAL:HG23	2.17	0.45
1:B:185:ARG:HA	1:B:185:ARG:HD2	1.74	0.44
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:918:PHE:C	1:B:918:PHE:HD1	2.25	0.44
1:C:400:LEU:O	1:C:404:LEU:HD22	2.17	0.44
2:E:100:LEU:HA	2:E:100:LEU:HD23	1.74	0.44
1:A:674:LEU:HD23	1:A:674:LEU:HA	1.71	0.44
1:B:402:ILE:HD12	1:B:402:ILE:HA	1.74	0.44
1:B:878:ALA:O	1:B:882:ILE:HG13	2.17	0.44
1:A:449:LEU:O	1:A:452:VAL:HG13	2.18	0.44
1:A:463:THR:O	1:A:467:TYR:HD2	1.99	0.44
1:A:673:GLU:OE1	1:A:865:GLN:NE2	2.51	0.44
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.18	0.44
1:B:527:TYR:HE2	1:B:968:VAL:HG13	1.81	0.44
1:B:575:MET:O	1:B:663:VAL:HA	2.17	0.44
1:B:764:ASP:OD2	1:B:769:LYS:NZ	2.50	0.44
1:A:818:ARG:NH2	1:A:823:PRO:HD3	2.33	0.44
1:B:9:PRO:HG3	1:B:495:THR:HG21	1.98	0.44
1:B:584:GLN:N	1:B:622:GLN:HG2	2.33	0.44
1:B:996:GLY:O	1:B:1000:GLN:HG3	2.17	0.44
1:A:599:LEU:HD23	1:A:599:LEU:HA	1.78	0.44
1:A:750:LEU:HB2	1:A:801:PHE:HZ	1.82	0.44
1:B:364:ALA:HB2	1:B:497:LEU:HD11	1.99	0.44
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.53	0.44
1:C:36:PRO:HD3	1:C:391:ASN:ND2	2.33	0.44
1:C:447:MET:SD	1:C:887:CYS:HB3	2.57	0.44
1:C:754:TRP:CZ2	1:C:786:ILE:HG13	2.52	0.44
1:A:56:THR:HG23	1:C:213:GLN:HG2	1.99	0.44
1:B:685:ILE:HG22	1:B:687:GLN:HG2	2.00	0.44
1:B:169:THR:O	1:B:172:VAL:HG13	2.17	0.44
1:B:756:GLY:HA3	1:B:774:MET:HE2	1.98	0.44
1:C:674:LEU:HD23	1:C:674:LEU:HA	1.78	0.44
1:C:900:SER:OG	1:C:1026:PHE:HA	2.17	0.44
2:D:11:GLY:N	2:D:16:LYS:HD3	2.33	0.44
1:A:76:MET:HE2	1:A:94:PHE:C	2.43	0.44
1:A:467:TYR:CZ	1:A:925:VAL:HG22	2.53	0.44
1:A:948:PHE:O	1:A:952:LEU:HG	2.18	0.44
1:B:30:LEU:HA	1:B:31:PRO:HD3	1.88	0.44
1:C:434:SER:O	1:C:438:ILE:HG23	2.17	0.44
2:D:144:LYS:HB2	2:D:144:LYS:HE3	1.82	0.44
1:A:7:ASP:C	1:A:9:PRO:HD3	2.43	0.44
1:A:27:ILE:HG23	3:A:1101:LMT:H41	2.00	0.44
1:A:375:VAL:HB	1:A:405:LEU:HD13	1.99	0.44
1:A:681:ASP:H	1:A:863:SER:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ASN:HA	1:B:320:GLY:O	2.18	0.44
1:B:492:LEU:O	1:B:496:MET:HB2	2.18	0.43
1:B:706:ALA:HB1	1:B:713:LEU:HD23	1.99	0.43
1:B:841:MET:HG2	1:B:859:TRP:CZ2	2.53	0.43
1:C:510:LYS:O	1:C:510:LYS:HG2	2.17	0.43
1:C:577:GLN:HE21	1:C:577:GLN:HB2	1.57	0.43
1:C:688:ALA:HB3	1:C:690:LEU:HD22	1.99	0.43
1:C:901:VAL:HG13	1:C:942:ALA:HB3	2.00	0.43
1:C:984:LEU:HD12	1:C:984:LEU:HA	1.77	0.43
1:A:150:THR:O	1:A:154:ILE:HG13	2.18	0.43
1:A:366:LEU:HD12	1:A:366:LEU:HA	1.79	0.43
1:B:2:PRO:HG3	1:B:486:LEU:HD23	2.01	0.43
2:E:142:GLN:HB3	2:E:146:GLY:HA2	1.99	0.43
1:C:41:PRO:HG2	1:C:94:PHE:HB2	2.00	0.43
1:C:255:GLN:OE1	1:C:255:GLN:N	2.49	0.43
2:D:76:TYR:N	2:D:76:TYR:CD2	2.86	0.43
2:D:127:GLU:H	2:D:127:GLU:HG2	1.27	0.43
1:A:531:VAL:O	1:A:535:LEU:HG	2.17	0.43
1:B:23:GLY:O	1:B:27:ILE:HG13	2.19	0.43
1:C:478:MET:O	1:C:481:SER:OG	2.35	0.43
1:C:746:ILE:HG13	1:C:804:PHE:CE2	2.54	0.43
1:A:39:ALA:HA	1:A:40:PRO:HD3	1.77	0.43
1:A:174:ASP:HB3	1:A:292:LYS:HG3	1.99	0.43
1:B:682:PHE:HD1	1:B:859:TRP:CH2	2.35	0.43
1:A:713:LEU:HD13	1:A:843:LEU:HD23	1.99	0.43
1:C:216:ALA:HB3	1:C:234:ILE:O	2.19	0.43
1:C:598:TYR:HB3	1:C:606:VAL:HG21	2.01	0.43
1:A:36:PRO:O	1:A:38:ILE:HG23	2.18	0.43
1:A:298:ASN:HB3	1:A:301:ASP:HB2	2.01	0.43
1:A:586:ARG:HH12	1:A:660:ASP:HB3	1.84	0.43
1:A:1008:MET:HE2	1:A:1008:MET:HB3	1.81	0.43
1:B:125:GLN:NE2	1:B:772:TYR:OH	2.52	0.43
1:B:530:SER:O	1:B:534:ILE:HG13	2.19	0.43
1:A:415:ASN:O	1:A:419:VAL:HG23	2.19	0.43
1:B:641:GLU:H	1:B:641:GLU:HG3	1.49	0.43
1:B:866:GLU:C	1:B:868:LEU:H	2.27	0.43
1:C:398:MET:O	1:C:402:ILE:HG12	2.18	0.43
1:C:527:TYR:CE2	1:C:968:VAL:HG13	2.54	0.43
2:D:76:TYR:N	2:D:76:TYR:HD2	2.17	0.43
1:A:375:VAL:HG11	1:A:405:LEU:HD22	2.01	0.42
1:B:302:THR:O	1:B:306:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:ASP:OD2	1:B:644:VAL:HG23	2.19	0.42
1:C:102:ILE:HD13	1:C:102:ILE:HA	1.79	0.42
1:C:350:LEU:O	1:C:354:VAL:HG23	2.19	0.42
1:A:1030:ARG:HD2	1:A:1030:ARG:HA	1.86	0.42
1:A:1038:GLU:OE2	1:A:1039:ASP:HA	2.19	0.42
1:B:352:PHE:HE1	1:B:365:THR:HG21	1.83	0.42
1:B:418:ARG:HD2	1:B:970:MET:HG2	2.00	0.42
1:B:741:VAL:HG22	1:B:793:ALA:HB2	2.02	0.42
1:C:553:ALA:O	1:C:557:VAL:HG22	2.18	0.42
1:A:428:LYS:O	1:A:432:ARG:HB2	2.19	0.42
1:A:573:MET:HE1	1:A:628:PHE:HE1	1.83	0.42
1:A:684:LEU:O	1:A:824:SER:HA	2.18	0.42
1:C:259:ARG:NH2	2:E:155:ASN:OD1	2.33	0.42
2:D:59:HIS:O	2:D:63:VAL:HG23	2.20	0.42
1:A:330:THR:OG1	1:A:331:PRO:HD3	2.19	0.42
1:A:547:ILE:O	1:A:550:VAL:HB	2.18	0.42
1:B:328:ASP:CG	1:B:331:PRO:HD3	2.44	0.42
1:C:575:MET:HE3	1:C:575:MET:HB3	1.89	0.42
1:C:984:LEU:O	1:C:987:MET:HB2	2.19	0.42
1:A:675:GLY:HA2	1:A:862:MET:HE2	2.01	0.42
1:C:31:PRO:HB2	1:C:389:SER:HB3	2.01	0.42
1:C:403:GLY:HA3	1:C:982:PHE:HA	2.00	0.42
1:C:527:TYR:O	1:C:530:SER:HB3	2.19	0.42
1:C:669:PRO:HD3	1:C:677:ALA:C	2.44	0.42
1:A:189:ASN:ND2	1:A:779:TYR:CZ	2.88	0.42
1:A:743:ILE:H	1:A:743:ILE:HG12	1.57	0.42
1:A:1004:GLY:O	1:A:1008:MET:HB2	2.19	0.42
1:B:914:LEU:HD13	1:B:914:LEU:HA	1.92	0.42
1:A:58:GLN:HA	1:A:62:THR:OG1	2.19	0.42
1:A:370:ILE:O	1:A:374:VAL:HG23	2.20	0.42
1:A:905:VAL:HG22	1:A:935:ILE:HG23	2.02	0.42
1:B:466:ILE:HD11	1:B:671:ILE:HD12	2.02	0.42
1:B:575:MET:HE3	1:B:575:MET:HB2	1.85	0.42
2:D:18:LEU:HD23	2:D:39:ASP:O	2.19	0.42
1:A:712:MET:HB3	1:A:713:LEU:HD13	2.01	0.42
1:A:809:TRP:NE1	2:E:79:LEU:HD22	2.35	0.42
1:B:193:LEU:HB3	1:B:198:LEU:O	2.20	0.42
1:B:219:LEU:HD23	1:C:754:TRP:CZ3	2.55	0.42
1:C:456:MET:HE2	1:C:467:TYR:HB3	2.02	0.42
1:C:976:LEU:HD12	1:C:976:LEU:HA	1.83	0.42
1:A:568:ASP:CG	1:A:644:VAL:HG23	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:GLU:OE1	1:B:647:ILE:HG23	2.20	0.42
1:C:426:PRO:HG2	1:C:429:GLU:HB3	2.01	0.42
1:C:605:ASN:O	1:C:632:LYS:N	2.50	0.42
1:A:49:TYR:HB3	1:A:52:ALA:HB3	2.02	0.42
1:B:509:LYS:HG2	1:B:510:LYS:H	1.85	0.42
1:B:639:GLY:O	1:B:641:GLU:N	2.52	0.42
1:C:1:MET:O	1:C:4:PHE:HB3	2.19	0.42
1:C:185:ARG:HD3	1:C:272:GLY:O	2.20	0.42
1:C:509:LYS:HA	1:C:510:LYS:CB	2.49	0.42
2:E:119:LEU:HD12	2:E:119:LEU:HA	1.83	0.42
1:A:159:ALA:HB2	1:A:177:LEU:HD22	2.02	0.41
1:A:616:ASN:O	1:A:616:ASN:CG	2.63	0.41
1:B:541:TYR:HA	1:B:544:LEU:HB2	2.02	0.41
1:C:955:LYS:HD2	1:C:955:LYS:N	2.35	0.41
1:A:66:GLU:HG2	1:A:78:MET:HE3	2.01	0.41
1:A:261:LEU:O	1:A:264:ASP:HB2	2.21	0.41
1:A:331:PRO:O	1:A:335:ILE:HG13	2.20	0.41
1:B:199:THR:OG1	1:B:201:VAL:HB	2.20	0.41
1:B:904:VAL:O	1:B:907:LEU:HB2	2.19	0.41
1:C:57:VAL:HG21	1:C:86:GLY:CA	2.41	0.41
2:D:133:LEU:HD23	2:D:133:LEU:HA	1.80	0.41
1:A:497:LEU:HA	1:A:497:LEU:HD23	1.81	0.41
1:A:542:LEU:HA	1:A:542:LEU:HD13	1.75	0.41
1:A:701:GLN:O	1:A:705:GLU:HG2	2.21	0.41
1:A:934:THR:HG22	1:A:1011:MET:HG2	2.02	0.41
1:B:183:ALA:N	1:B:271:GLY:O	2.53	0.41
1:B:568:ASP:OD2	1:B:644:VAL:N	2.44	0.41
1:C:38:ILE:HD11	1:C:671:ILE:HG21	2.02	0.41
1:C:61:VAL:HA	1:C:118:LEU:HD22	2.03	0.41
1:C:158:VAL:HG22	1:C:162:MET:SD	2.60	0.41
2:E:17:LYS:HB2	2:E:33:LEU:HD13	2.03	0.41
1:A:344:LEU:O	1:A:348:ILE:HG13	2.20	0.41
1:B:113:LEU:HD23	1:B:113:LEU:HA	1.89	0.41
1:B:695:LEU:HD23	1:B:695:LEU:HA	1.61	0.41
1:B:921:LEU:HB3	1:B:922:THR:H	1.60	0.41
1:B:960:LEU:CD2	1:B:1027:VAL:HG22	2.50	0.41
1:C:314:GLU:HA	1:C:317:PHE:CE1	2.56	0.41
1:C:819:TYR:N	1:C:824:SER:HB3	2.34	0.41
2:E:107:ASN:HD21	2:E:138:ASP:HB2	1.85	0.41
1:A:159:ALA:HB3	1:A:181:GLN:HG3	2.01	0.41
1:B:182:TYR:HB3	1:B:270:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:THR:N	1:C:331:PRO:HD2	2.36	0.41
1:C:453:PHE:O	1:C:471:SER:OG	2.32	0.41
1:C:534:ILE:HG23	1:C:541:TYR:CE2	2.55	0.41
1:C:709:HIS:N	1:C:710:PRO:HD3	2.36	0.41
1:C:897:ILE:HD11	1:C:950:LYS:HD3	2.02	0.41
1:C:934:THR:HA	1:C:937:LEU:HD12	2.01	0.41
1:C:937:LEU:HB3	1:C:1011:MET:HE3	2.03	0.41
1:A:480:LEU:HD13	1:A:480:LEU:HA	1.84	0.41
1:A:914:LEU:HD23	1:A:914:LEU:HA	1.89	0.41
1:B:344:LEU:O	1:B:348:ILE:HG12	2.20	0.41
1:C:355:MET:HE1	1:C:369:THR:HG23	2.03	0.41
1:C:468:ARG:O	1:C:472:ILE:HG22	2.20	0.41
1:C:671:ILE:O	1:C:671:ILE:HG13	2.20	0.41
1:C:690:LEU:HB3	1:C:694:LYS:HB2	2.02	0.41
1:A:358:PHE:HE2	1:A:520:PHE:CE1	2.39	0.41
1:A:669:PRO:CG	1:A:674:LEU:HD21	2.50	0.41
1:A:851:LEU:HA	1:A:851:LEU:HD23	1.82	0.41
1:B:350:LEU:HD23	1:B:350:LEU:HA	1.84	0.41
1:C:35:TYR:CD2	1:C:671:ILE:HG22	2.56	0.41
1:A:367:ILE:HB	1:A:368:PRO:HD3	2.02	0.41
1:A:428:LYS:HG2	1:A:432:ARG:HH21	1.85	0.41
1:A:741:VAL:HG12	1:A:793:ALA:HB2	2.02	0.41
1:C:222:THR:HA	1:C:224:PRO:HD3	2.02	0.41
2:D:42:ALA:O	2:D:50:PRO:HD3	2.21	0.41
1:A:563:PHE:CD1	1:A:564:LEU:HG	2.55	0.41
1:B:483:LEU:HD13	1:B:483:LEU:HA	1.75	0.41
1:B:527:TYR:CD2	1:B:972:LEU:HG	2.56	0.41
1:B:743:ILE:H	1:B:743:ILE:HG12	1.57	0.41
1:C:146:ASP:O	1:C:148:THR:N	2.54	0.41
1:C:310:LEU:HD12	1:C:310:LEU:HA	1.94	0.41
1:C:952:LEU:O	1:C:956:GLU:HB2	2.21	0.41
1:C:1033:PHE:CD2	1:C:1033:PHE:N	2.89	0.41
1:A:864:TYR:HB3	1:A:865:GLN:H	1.74	0.41
1:B:102:ILE:O	1:B:106:GLN:HG3	2.20	0.41
1:B:126:GLY:HA3	1:C:116:PRO:CB	2.44	0.41
1:B:921:LEU:HD12	1:B:921:LEU:HA	1.82	0.41
1:C:69:MET:HG3	1:C:92:LEU:HD21	2.03	0.41
1:C:184:MET:HB2	1:C:762:PHE:CE2	2.56	0.41
1:A:355:MET:O	1:A:359:LEU:HB2	2.20	0.40
1:A:649:MET:HE1	1:A:653:ARG:HD3	2.01	0.40
1:C:907:LEU:O	1:C:910:ILE:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:76:TYR:N	2:E:76:TYR:CD2	2.88	0.40
1:B:190:PRO:HB3	1:B:789:TRP:CZ3	2.56	0.40
1:C:574:THR:OG1	1:C:598:TYR:OH	2.34	0.40
2:E:128:ILE:O	2:E:132:LEU:HG	2.21	0.40
1:A:32:VAL:HG12	1:A:390:ILE:HB	2.02	0.40
1:A:159:ALA:CB	1:A:181:GLN:HG3	2.52	0.40
1:A:745:ASP:HB3	1:A:791:VAL:HG11	2.04	0.40
1:A:841:MET:O	1:A:845:GLU:HG3	2.22	0.40
1:B:349:ILE:O	1:B:353:LEU:HD22	2.21	0.40
1:B:352:PHE:CE1	1:B:365:THR:HG21	2.56	0.40
1:B:885:PHE:CD1	1:B:902:MET:HE1	2.51	0.40
1:C:15:ILE:O	1:C:19:ILE:HG13	2.21	0.40
1:C:573:MET:HE1	1:C:628:PHE:CE1	2.56	0.40
2:D:109:LYS:HG2	2:D:115:THR:HG22	2.04	0.40
1:A:385:ALA:C	1:A:387:GLY:H	2.29	0.40
1:A:489:THR:O	1:A:493:CYS:HB2	2.21	0.40
1:B:367:ILE:HB	1:B:368:PRO:HD3	2.03	0.40
1:B:559:LEU:HD23	1:B:923:ASN:HB2	2.04	0.40
1:C:30:LEU:HA	1:C:31:PRO:HD3	1.96	0.40
1:C:65:ILE:HG22	1:C:69:MET:HE3	2.02	0.40
1:C:184:MET:HB3	1:C:771:VAL:HG22	2.03	0.40
1:C:923:ASN:OD1	1:C:927:PHE:HD2	2.05	0.40
1:C:964:THR:O	1:C:968:VAL:HB	2.21	0.40
1:C:986:VAL:O	1:C:990:VAL:HG23	2.22	0.40
1:A:84:SER:OG	1:A:814:PRO:HA	2.22	0.40
1:A:553:ALA:O	1:A:557:VAL:HG22	2.21	0.40
1:A:1039:ASP:H	1:A:1040:ILE:HD12	1.86	0.40
1:B:703:LEU:HD11	1:B:718:PRO:HG3	2.03	0.40
1:B:809:TRP:CD1	2:D:79:LEU:HD22	2.56	0.40
1:C:489:THR:OG1	1:C:490:PRO:HD3	2.21	0.40
2:D:126:LEU:HD12	2:D:126:LEU:N	2.36	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%)	963 (92%)	63 (6%)	16 (2%)	8	28
1	B	1031/1057 (98%)	954 (92%)	66 (6%)	11 (1%)	11	36
1	C	1032/1057 (98%)	963 (93%)	66 (6%)	3 (0%)	36	65
2	D	154/169 (91%)	144 (94%)	10 (6%)	0	100	100
2	E	150/169 (89%)	139 (93%)	10 (7%)	1 (1%)	18	48
All	All	3409/3509 (97%)	3163 (93%)	215 (6%)	31 (1%)	14	41

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	SER
1	A	864	TYR
1	A	866	GLU
1	A	1040	ILE
1	B	510	LYS
1	B	674	LEU
1	A	618	ALA
1	B	640	GLU
1	B	659	LYS
1	C	147	GLY
1	C	1031	ARG
1	A	424	GLY
1	A	617	PHE
1	A	634	TRP
1	A	869	SER
1	B	670	ALA
1	B	867	ARG
1	B	874	PRO
1	B	918	PHE
1	C	510	LYS
1	A	504	ASP
1	A	852	PRO
1	B	34	GLN
1	A	126	GLY
1	A	145	THR
1	A	677	ALA
1	A	1043	SER
1	B	820	ASN

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Mol	Chain	Res	Type
1	B	833	PRO
1	A	461	GLY
2	E	45	VAL

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	851/864 (98%)	726 (85%)	125 (15%)	3	10
1	B	840/864 (97%)	739 (88%)	101 (12%)	5	16
1	C	841/864 (97%)	728 (87%)	113 (13%)	4	12
2	D	120/132 (91%)	108 (90%)	12 (10%)	7	24
2	E	117/132 (89%)	101 (86%)	16 (14%)	3	12
All	All	2769/2856 (97%)	2402 (87%)	367 (13%)	4	12

All (367) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	ARG
1	A	20	MET
1	A	25	LEU
1	A	29	LYS
1	A	30	LEU
1	A	32	VAL
1	A	37	THR
1	A	46	SER
1	A	60	THR
1	A	70	ASN
1	A	82	SER
1	A	85	THR
1	A	88	VAL
1	A	96	SER
1	A	108	GLN

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Mol	Chain	Res	Type
1	A	113	LEU
1	A	121	GLU
1	A	127	VAL
1	A	130	GLU
1	A	143	ILE
1	A	214	VAL
1	A	222	THR
1	A	226	LYS
1	A	229	GLN
1	A	240	LEU
1	A	245	GLU
1	A	249	ILE
1	A	262	LEU
1	A	263	ARG
1	A	289	LEU
1	A	293	LEU
1	A	310	LEU
1	A	321	LEU
1	A	329	THR
1	A	360	GLN
1	A	365	THR
1	A	376	LEU
1	A	390	ILE
1	A	402	ILE
1	A	425	LEU
1	A	429	GLU
1	A	433	LYS
1	A	438	ILE
1	A	447	MET
1	A	452	VAL
1	A	456	MET
1	A	463	THR
1	A	471	SER
1	A	480	LEU
1	A	482	VAL
1	A	484	VAL
1	A	486	LEU
1	A	487	ILE
1	A	492	LEU
1	A	493	CYS
1	A	507	GLU
1	A	510	LYS

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Mol	Chain	Res	Type
1	A	517	ASN
1	A	523	SER
1	A	524	THR
1	A	534	ILE
1	A	536	ARG
1	A	540	ARG
1	A	542	LEU
1	A	544	LEU
1	A	549	VAL
1	A	566	ASP
1	A	576	VAL
1	A	577	GLN
1	A	608	SER
1	A	620	ARG
1	A	626	ILE
1	A	636	ASP
1	A	648	THR
1	A	652	THR
1	A	659	LYS
1	A	660	ASP
1	A	671	ILE
1	A	673	GLU
1	A	678	THR
1	A	685	ILE
1	A	687	GLN
1	A	694	LYS
1	A	695	LEU
1	A	717	ARG
1	A	728	LYS
1	A	729	ILE
1	A	743	ILE
1	A	767	ARG
1	A	773	VAL
1	A	776	GLU
1	A	778	LYS
1	A	801	PHE
1	A	828	LEU
1	A	830	GLN
1	A	839	GLU
1	A	862	MET
1	A	863	SER
1	A	867	ARG

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Mol	Chain	Res	Type
1	A	872	GLN
1	A	879	ILE
1	A	881	LEU
1	A	902	MET
1	A	919	ARG
1	A	921	LEU
1	A	925	VAL
1	A	931	LEU
1	A	934	THR
1	A	935	ILE
1	A	944	LEU
1	A	946	VAL
1	A	953	MET
1	A	961	ILE
1	A	968	VAL
1	A	969	ARG
1	A	971	ARG
1	A	973	ARG
1	A	984	LEU
1	A	991	ILE
1	A	1008	MET
1	A	1035	ARG
1	A	1040	ILE
1	A	1041	GLU
1	A	1044	HIS
1	B	6	ILE
1	B	19	ILE
1	B	21	LEU
1	B	46	SER
1	B	70	ASN
1	B	75	LEU
1	B	84	SER
1	B	87	THR
1	B	88	VAL
1	B	96	SER
1	B	111	LEU
1	B	112	GLN
1	B	121	GLU
1	B	130	GLU
1	B	143	ILE
1	B	172	VAL
1	B	185	ARG

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Mol	Chain	Res	Type
1	B	199	THR
1	B	250	LEU
1	B	255	GLN
1	B	256	ASP
1	B	270	LEU
1	B	293	LEU
1	B	321	LEU
1	B	330	THR
1	B	337	ILE
1	B	338	HIS
1	B	341	VAL
1	B	353	LEU
1	B	365	THR
1	B	377	LEU
1	B	383	LEU
1	B	390	ILE
1	B	398	MET
1	B	399	VAL
1	B	402	ILE
1	B	405	LEU
1	B	406	VAL
1	B	429	GLU
1	B	466	ILE
1	B	468	ARG
1	B	480	LEU
1	B	483	LEU
1	B	497	LEU
1	B	510	LYS
1	B	544	LEU
1	B	546	LEU
1	B	555	LEU
1	B	569	GLN
1	B	572	PHE
1	B	574	THR
1	B	576	VAL
1	B	577	GLN
1	B	578	LEU
1	B	584	GLN
1	B	589	LYS
1	B	595	THR
1	B	626	ILE
1	B	630	SER

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Mol	Chain	Res	Type
1	B	641	GLU
1	B	649	MET
1	B	662	MET
1	B	668	LEU
1	B	693	GLU
1	B	695	LEU
1	B	713	LEU
1	B	715	SER
1	B	719	ASN
1	B	743	ILE
1	B	745	ASP
1	B	763	ILE
1	B	778	LYS
1	B	798	MET
1	B	801	PHE
1	B	808	ARG
1	B	810	GLU
1	B	822	LEU
1	B	825	MET
1	B	830	GLN
1	B	837	THR
1	B	866	GLU
1	B	875	SER
1	B	880	SER
1	B	881	LEU
1	B	886	LEU
1	B	888	LEU
1	B	896	SER
1	B	897	ILE
1	B	914	LEU
1	B	918	PHE
1	B	921	LEU
1	B	922	THR
1	B	937	LEU
1	B	955	LYS
1	B	965	LEU
1	B	968	VAL
1	B	972	LEU
1	B	986	VAL
1	B	1003	VAL
1	B	1028	VAL
1	B	1030	ARG

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Mol	Chain	Res	Type
1	C	1	MET
1	C	10	ILE
1	C	18	ILE
1	C	38	ILE
1	C	75	LEU
1	C	79	SER
1	C	87	THR
1	C	95	GLU
1	C	108	GLN
1	C	121	GLU
1	C	123	GLN
1	C	125	GLN
1	C	127	VAL
1	C	128	SER
1	C	143	ILE
1	C	152	GLU
1	C	177	LEU
1	C	195	LYS
1	C	237	GLN
1	C	243	THR
1	C	253	VAL
1	C	254	ASN
1	C	269	GLU
1	C	273	GLU
1	C	289	LEU
1	C	307	ARG
1	C	310	LEU
1	C	319	SER
1	C	324	VAL
1	C	344	LEU
1	C	355	MET
1	C	359	LEU
1	C	360	GLN
1	C	366	LEU
1	C	369	THR
1	C	389	SER
1	C	394	THR
1	C	402	ILE
1	C	404	LEU
1	C	418	ARG
1	C	425	LEU
1	C	434	SER

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Mol	Chain	Res	Type
1	C	437	GLN
1	C	438	ILE
1	C	439	GLN
1	C	463	THR
1	C	471	SER
1	C	482	VAL
1	C	483	LEU
1	C	495	THR
1	C	510	LYS
1	C	531	VAL
1	C	537	SER
1	C	542	LEU
1	C	544	LEU
1	C	546	LEU
1	C	557	VAL
1	C	564	LEU
1	C	586	ARG
1	C	606	VAL
1	C	608	SER
1	C	624	THR
1	C	626	ILE
1	C	640	GLU
1	C	648	THR
1	C	657	GLN
1	C	678	THR
1	C	685	ILE
1	C	690	LEU
1	C	695	LEU
1	C	702	LEU
1	C	711	ASP
1	C	717	ARG
1	C	729	ILE
1	C	739	LEU
1	C	743	ILE
1	C	778	LYS
1	C	782	LEU
1	C	784	ASP
1	C	786	ILE
1	C	795	ASP
1	C	799	VAL
1	C	815	ARG
1	C	822	LEU

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Mol	Chain	Res	Type
1	C	824	SER
1	C	828	LEU
1	C	839	GLU
1	C	853	THR
1	C	862	MET
1	C	867	ARG
1	C	868	LEU
1	C	876	LEU
1	C	879	ILE
1	C	891	LEU
1	C	894	SER
1	C	896	SER
1	C	900	SER
1	C	902	MET
1	C	905	VAL
1	C	919	ARG
1	C	938	SER
1	C	947	GLU
1	C	948	PHE
1	C	960	LEU
1	C	962	GLU
1	C	968	VAL
1	C	976	LEU
1	C	984	LEU
1	C	993	THR
1	C	1003	VAL
1	C	1011	MET
1	C	1032	ARG
1	C	1033	PHE
2	D	28	ASP
2	D	33	LEU
2	D	45	VAL
2	D	53	LEU
2	D	61	GLU
2	D	62	ILE
2	D	76	TYR
2	D	79	LEU
2	D	94	GLU
2	D	101	LYS
2	D	126	LEU
2	D	127	GLU
2	E	16	LYS

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Mol	Chain	Res	Type
2	E	28	ASP
2	E	40	VAL
2	E	45	VAL
2	E	64	GLU
2	E	73	VAL
2	E	76	TYR
2	E	78	THR
2	E	79	LEU
2	E	81	SER
2	E	112	ASN
2	E	115	THR
2	E	119	LEU
2	E	126	LEU
2	E	127	GLU
2	E	128	ILE

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

Mol	Chain	Res	Type
1	A	58	GLN
1	A	125	GLN
1	A	237	GLN
1	A	517	ASN
1	A	747	ASN
1	A	797	GLN
1	A	1037	ASN
1	B	161	ASN
1	B	218	GLN
1	B	231	ASN
1	B	254	ASN
1	C	68	ASN
1	C	104	GLN
1	C	108	GLN
1	C	120	GLN
1	C	124	GLN
1	C	125	GLN
1	C	151	GLN
1	C	161	ASN
1	C	237	GLN
1	C	439	GLN
1	C	469	GLN
1	C	525	HIS

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Mol	Chain	Res	Type
1	C	577	GLN
1	C	596	HIS
2	D	41	ASN
2	D	69	ASN
2	D	102	ASN
2	D	155	ASN
2	E	92	HIS
2	E	125	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

7 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	1101	-	36,36,36	1.12	3 (8%)	47,47,47	1.16	3 (6%)
3	LMT	C	1102	-	36,36,36	1.18	3 (8%)	47,47,47	1.29	4 (8%)
3	LMT	B	1101	-	36,36,36	1.16	3 (8%)	47,47,47	1.31	8 (17%)
3	LMT	B	1102	-	36,36,36	1.16	3 (8%)	47,47,47	1.40	8 (17%)
3	LMT	B	1103	-	36,36,36	1.15	4 (11%)	47,47,47	1.66	14 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LMT	A	1102	-	36,36,36	1.14	3 (8%)	47,47,47	1.48	7 (14%)
3	LMT	A	1101	-	36,36,36	1.16	3 (8%)	47,47,47	1.45	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	C	1101	-	-	14/21/61/61	0/2/2/2
3	LMT	C	1102	-	-	10/21/61/61	0/2/2/2
3	LMT	B	1101	-	-	6/21/61/61	0/2/2/2
3	LMT	B	1102	-	-	15/21/61/61	0/2/2/2
3	LMT	B	1103	-	-	16/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	13/21/61/61	0/2/2/2
3	LMT	A	1101	-	-	12/21/61/61	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	LMT	O5B-C1B	4.09	1.52	1.41
3	B	1101	LMT	O5B-C1B	3.98	1.52	1.41
3	B	1102	LMT	O5B-C1B	3.95	1.52	1.41
3	B	1103	LMT	O5B-C1B	3.94	1.52	1.41
3	C	1102	LMT	O5B-C1B	3.79	1.51	1.41
3	A	1102	LMT	O5B-C1B	3.78	1.51	1.41
3	C	1101	LMT	O5B-C1B	3.48	1.50	1.41
3	A	1102	LMT	C3'-C4'	-3.03	1.44	1.52
3	B	1101	LMT	O5'-C5'	2.93	1.51	1.44
3	A	1102	LMT	O5'-C5'	2.90	1.51	1.44
3	B	1102	LMT	O5'-C5'	2.87	1.51	1.44
3	B	1102	LMT	C3'-C4'	-2.86	1.44	1.52
3	C	1102	LMT	C3'-C4'	-2.86	1.44	1.52
3	C	1101	LMT	C3'-C4'	-2.83	1.44	1.52
3	B	1101	LMT	C3'-C4'	-2.82	1.44	1.52
3	A	1101	LMT	C3'-C4'	-2.80	1.44	1.52
3	C	1102	LMT	O5'-C5'	2.75	1.51	1.44
3	B	1103	LMT	O5'-C5'	2.71	1.51	1.44
3	A	1101	LMT	O5'-C5'	2.59	1.50	1.44
3	C	1101	LMT	O5'-C5'	2.56	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1103	LMT	C3'-C4'	-2.55	1.45	1.52
3	B	1103	LMT	O1B-C4'	2.14	1.49	1.43

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1102	LMT	C1-O1'-C1'	5.03	122.27	113.68
3	A	1102	LMT	C3B-C4B-C5B	4.76	118.86	110.23
3	A	1102	LMT	C1-O1'-C1'	3.94	120.42	113.68
3	A	1101	LMT	O5'-C1'-C2'	3.78	118.14	110.37
3	A	1102	LMT	O5B-C5B-C4B	3.70	116.36	109.70
3	C	1102	LMT	C1-O1'-C1'	3.56	119.76	113.68
3	B	1103	LMT	C1-O1'-C1'	3.52	119.69	113.68
3	C	1102	LMT	O5B-C5B-C4B	3.52	116.04	109.70
3	A	1102	LMT	C4B-C3B-C2B	3.45	116.89	110.83
3	B	1103	LMT	C1B-O1B-C4'	3.38	125.99	117.98
3	B	1103	LMT	C2'-C3'-C4'	3.31	117.20	109.68
3	A	1101	LMT	C2'-C3'-C4'	3.27	117.09	109.68
3	A	1101	LMT	C1'-C2'-C3'	3.21	116.77	110.01
3	B	1102	LMT	C2'-C3'-C4'	3.16	116.85	109.68
3	A	1101	LMT	C1-O1'-C1'	3.14	119.04	113.68
3	C	1101	LMT	C1-O1'-C1'	2.97	118.76	113.68
3	B	1101	LMT	C1-O1'-C1'	2.97	118.75	113.68
3	B	1101	LMT	C2'-C3'-C4'	2.94	116.36	109.68
3	C	1101	LMT	C2'-C3'-C4'	2.85	116.15	109.68
3	B	1101	LMT	O6'-C6'-C5'	2.64	120.34	111.33
3	B	1103	LMT	O5B-C5B-C4B	2.64	114.45	109.70
3	B	1101	LMT	O5B-C5B-C4B	2.61	114.41	109.70
3	B	1103	LMT	O5B-C1B-C2B	2.59	115.69	110.37
3	B	1103	LMT	O1B-C4'-C5'	2.56	116.20	109.48
3	C	1102	LMT	O1'-C1-C2	2.54	117.99	109.37
3	A	1101	LMT	O1'-C1-C2	2.52	117.93	109.37
3	C	1102	LMT	C2'-C3'-C4'	2.52	115.40	109.68
3	B	1103	LMT	C4B-C3B-C2B	2.50	115.22	110.83
3	B	1103	LMT	O1'-C1-C2	2.45	117.68	109.37
3	B	1102	LMT	O1B-C1B-C2B	2.40	113.99	108.09
3	C	1101	LMT	O6'-C6'-C5'	2.31	119.19	111.33
3	B	1101	LMT	C1B-O5B-C5B	2.30	118.22	113.72
3	B	1101	LMT	O1'-C1-C2	2.30	117.17	109.37
3	B	1103	LMT	O1B-C1B-C2B	2.30	113.74	108.09
3	A	1102	LMT	O6'-C6'-C5'	2.29	119.12	111.33
3	B	1101	LMT	O6B-C6B-C5B	2.29	119.11	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1102	LMT	O1'-C1-C2	2.28	117.11	109.37
3	B	1103	LMT	C3'-C4'-C5'	2.27	115.97	110.93
3	B	1103	LMT	C1B-C2B-C3B	2.27	114.78	110.01
3	B	1102	LMT	C1'-C2'-C3'	2.25	114.74	110.01
3	A	1101	LMT	O5B-C5B-C4B	2.22	113.69	109.70
3	B	1103	LMT	O6'-C6'-C5'	2.21	118.87	111.33
3	B	1102	LMT	O6B-C6B-C5B	2.21	118.86	111.33
3	B	1101	LMT	O3B-C3B-C2B	2.20	115.57	110.38
3	A	1101	LMT	O6'-C6'-C5'	2.19	118.79	111.33
3	A	1102	LMT	O6B-C6B-C5B	2.18	118.74	111.33
3	B	1103	LMT	C3B-C4B-C5B	2.17	114.17	110.23
3	B	1103	LMT	O5'-C1'-C2'	2.16	114.82	110.37
3	B	1102	LMT	O5'-C1'-C2'	2.13	114.74	110.37
3	B	1102	LMT	O6'-C6'-C5'	2.06	118.34	111.33
3	A	1102	LMT	O5B-C5B-C6B	2.06	111.53	106.44

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1102	LMT	O5'-C1'-O1'-C1
3	B	1103	LMT	C2'-C1'-O1'-C1
3	C	1101	LMT	O5'-C1'-O1'-C1
3	C	1102	LMT	C2-C1-O1'-C1'
3	B	1103	LMT	C5'-C4'-O1B-C1B
3	B	1103	LMT	C2B-C1B-O1B-C4'
3	C	1102	LMT	O5'-C5'-C6'-O6'
3	B	1101	LMT	O5B-C5B-C6B-O6B
3	C	1102	LMT	C4B-C5B-C6B-O6B
3	A	1102	LMT	O5'-C1'-O1'-C1
3	B	1103	LMT	O5'-C1'-O1'-C1
3	B	1103	LMT	O5'-C5'-C6'-O6'
3	A	1102	LMT	C2-C3-C4-C5
3	A	1101	LMT	O5B-C5B-C6B-O6B
3	B	1102	LMT	O5B-C5B-C6B-O6B
3	B	1102	LMT	O5'-C5'-C6'-O6'
3	C	1101	LMT	O5B-C5B-C6B-O6B
3	B	1101	LMT	C7-C8-C9-C10
3	A	1102	LMT	C4-C5-C6-C7
3	C	1101	LMT	C2-C3-C4-C5
3	B	1102	LMT	C4B-C5B-C6B-O6B
3	A	1101	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
3	A	1102	LMT	C2'-C1'-O1'-C1
3	C	1102	LMT	O5B-C5B-C6B-O6B
3	B	1101	LMT	C4B-C5B-C6B-O6B
3	B	1102	LMT	C4'-C5'-C6'-O6'
3	A	1101	LMT	C4B-C5B-C6B-O6B
3	C	1102	LMT	C4'-C5'-C6'-O6'
3	B	1102	LMT	C2B-C1B-O1B-C4'
3	C	1101	LMT	O5'-C5'-C6'-O6'
3	A	1101	LMT	O5'-C1'-O1'-C1
3	A	1101	LMT	O1'-C1-C2-C3
3	A	1102	LMT	O1'-C1-C2-C3
3	C	1101	LMT	C2-C1-O1'-C1'
3	B	1102	LMT	C2-C3-C4-C5
3	B	1103	LMT	C5-C6-C7-C8
3	A	1102	LMT	C1-C2-C3-C4
3	B	1103	LMT	C6-C7-C8-C9
3	A	1101	LMT	C11-C10-C9-C8
3	A	1102	LMT	C11-C10-C9-C8
3	B	1103	LMT	C4B-C5B-C6B-O6B
3	B	1102	LMT	O5B-C1B-O1B-C4'
3	C	1101	LMT	C5-C6-C7-C8
3	B	1102	LMT	C2'-C1'-O1'-C1
3	A	1102	LMT	C4B-C5B-C6B-O6B
3	A	1101	LMT	C2-C3-C4-C5
3	A	1101	LMT	C1-C2-C3-C4
3	B	1103	LMT	C11-C10-C9-C8
3	B	1101	LMT	C4-C5-C6-C7
3	C	1102	LMT	C6-C7-C8-C9
3	C	1101	LMT	C4B-C5B-C6B-O6B
3	B	1102	LMT	C5-C6-C7-C8
3	C	1102	LMT	O1'-C1-C2-C3
3	A	1101	LMT	C7-C8-C9-C10
3	A	1102	LMT	C5-C6-C7-C8
3	B	1102	LMT	C3-C4-C5-C6
3	C	1101	LMT	O1'-C1-C2-C3
3	B	1103	LMT	O5B-C1B-O1B-C4'
3	B	1102	LMT	C9-C10-C11-C12
3	A	1102	LMT	C9-C10-C11-C12
3	C	1101	LMT	C3-C4-C5-C6
3	A	1101	LMT	C2-C1-O1'-C1'
3	B	1103	LMT	C2-C1-O1'-C1'
3	C	1101	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
3	A	1101	LMT	C6-C7-C8-C9
3	B	1103	LMT	C7-C8-C9-C10
3	B	1102	LMT	C6-C7-C8-C9
3	B	1103	LMT	C4'-C5'-C6'-O6'
3	B	1101	LMT	C2-C3-C4-C5
3	A	1102	LMT	C3-C4-C5-C6
3	B	1101	LMT	C1-C2-C3-C4
3	C	1101	LMT	C11-C10-C9-C8
3	C	1102	LMT	C5-C6-C7-C8
3	B	1102	LMT	C2-C1-O1'-C1'
3	C	1102	LMT	C1-C2-C3-C4
3	B	1103	LMT	C9-C10-C11-C12
3	B	1103	LMT	O5B-C5B-C6B-O6B
3	C	1102	LMT	C11-C10-C9-C8
3	A	1102	LMT	C6-C7-C8-C9
3	B	1102	LMT	C4-C5-C6-C7
3	C	1101	LMT	C4-C5-C6-C7
3	B	1103	LMT	O1'-C1-C2-C3
3	C	1101	LMT	C6-C7-C8-C9
3	A	1102	LMT	C7-C8-C9-C10
3	C	1101	LMT	C3'-C4'-O1B-C1B
3	A	1101	LMT	C9-C10-C11-C12

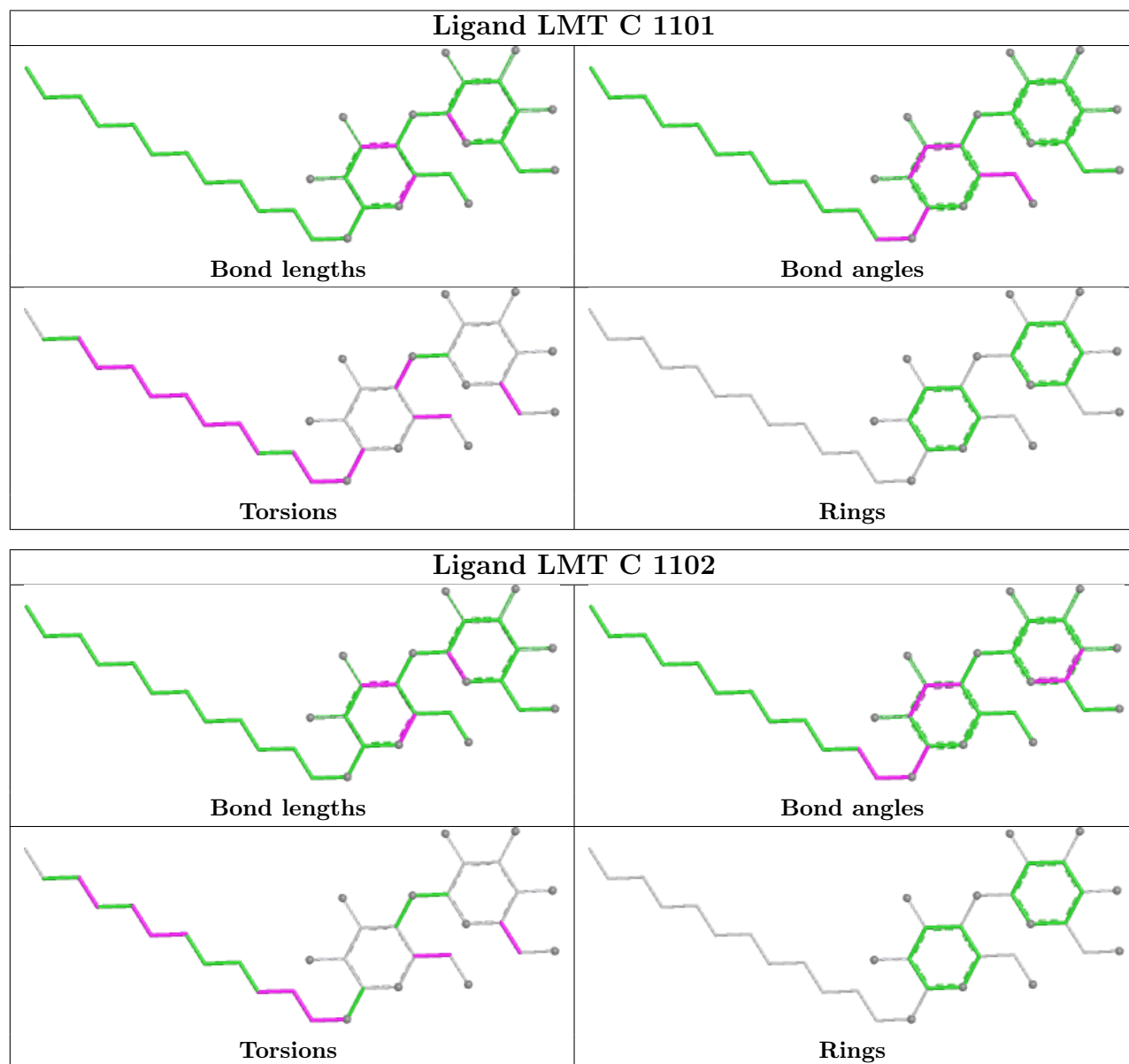
There are no ring outliers.

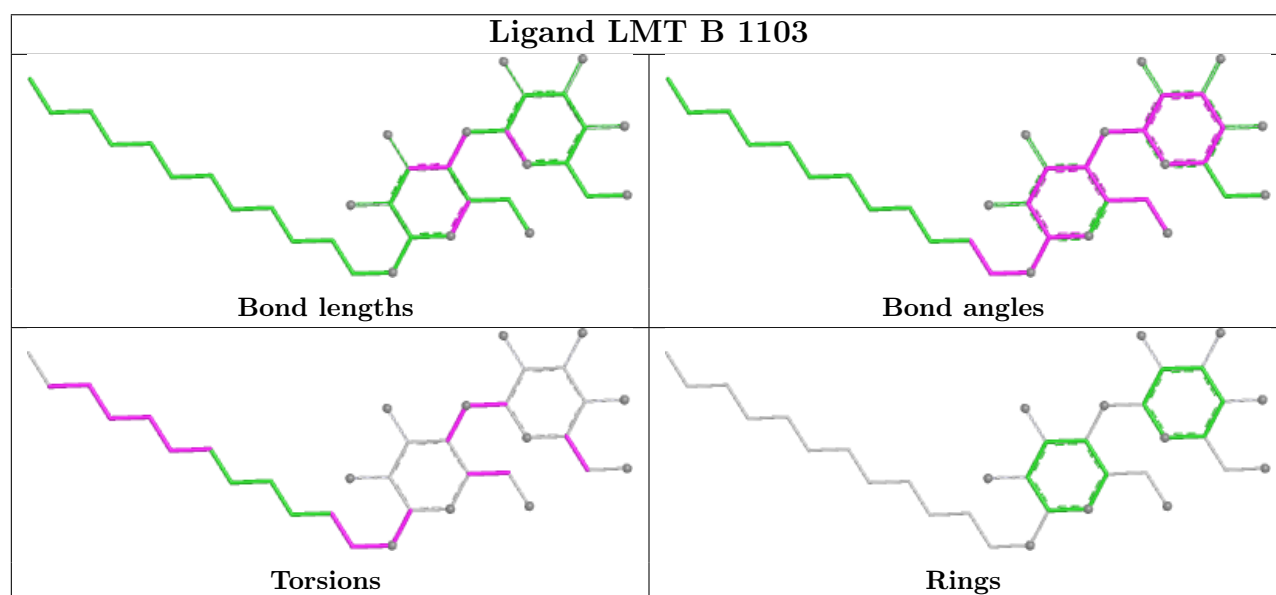
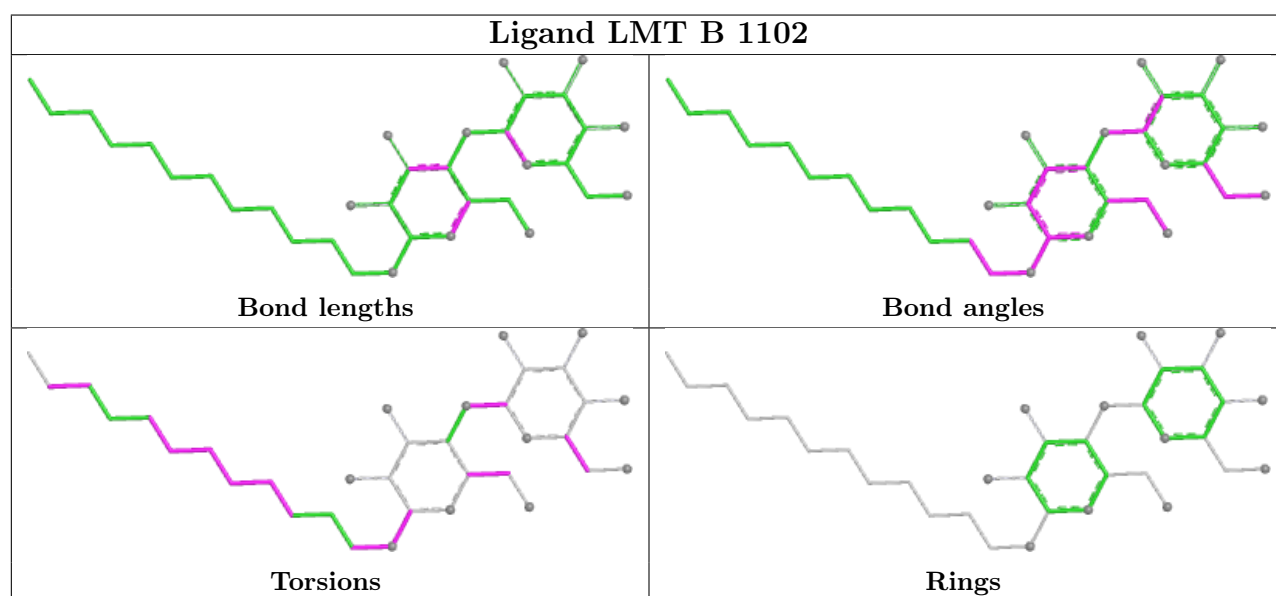
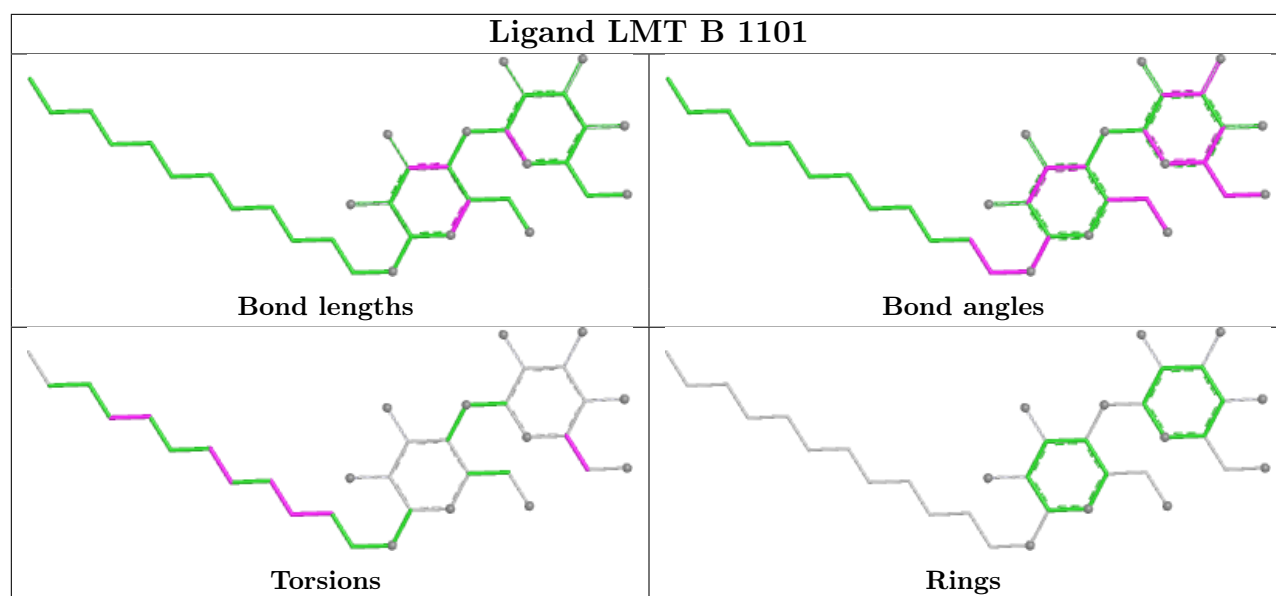
6 monomers are involved in 11 short contacts:

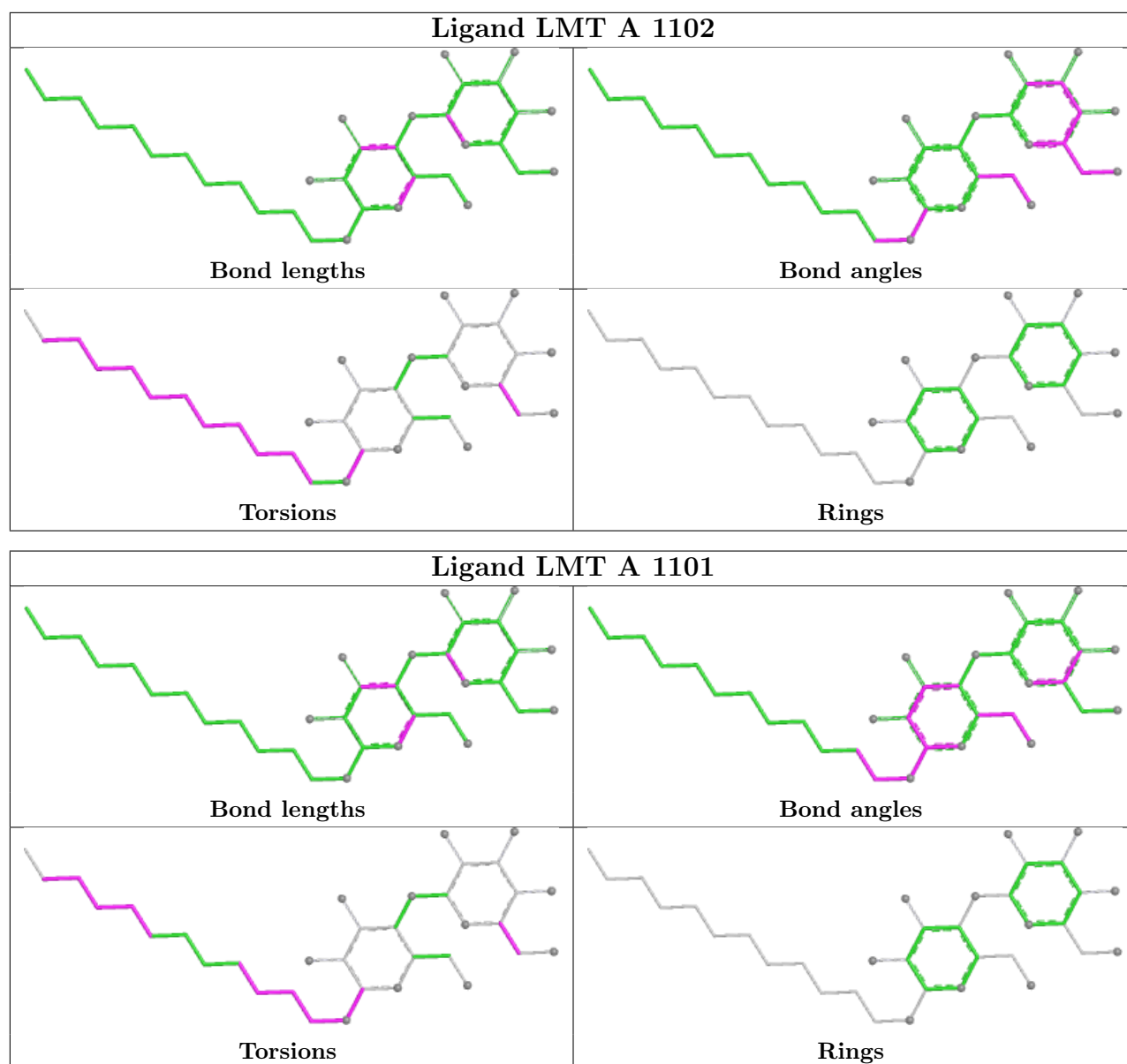
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1101	LMT	1	0
3	C	1102	LMT	2	0
3	B	1102	LMT	2	0
3	B	1103	LMT	2	0
3	A	1102	LMT	2	0
3	A	1101	LMT	2	0

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%)	-0.07	31 (2%)	52	43	13, 57, 113, 163	0
1	B	1033/1057 (97%)	-0.01	33 (3%)	50	41	24, 61, 101, 159	0
1	C	1034/1057 (97%)	-0.13	17 (1%)	70	62	17, 53, 92, 164	0
2	D	156/169 (92%)	-0.08	2 (1%)	75	67	41, 60, 90, 117	0
2	E	152/169 (89%)	0.11	3 (1%)	65	56	32, 59, 99, 119	0
All	All	3419/3509 (97%)	-0.06	86 (2%)	58	48	13, 58, 102, 164	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	674	LEU	7.2
1	B	134	SER	7.0
1	A	868	LEU	5.7
1	C	1034	SER	4.6
1	B	563	PHE	4.5
1	A	672	VAL	4.5
1	B	671	ILE	4.4
1	A	1044	HIS	4.2
1	B	675	GLY	4.2
1	B	615	PHE	4.0
1	B	678	THR	4.0
2	E	15	GLY	3.9
1	B	677	ALA	3.9
1	B	672	VAL	3.7
1	C	1032	ARG	3.7
1	A	518	ARG	3.7
1	B	867	ARG	3.5
1	C	362	PHE	3.5
1	C	1033	PHE	3.5
1	A	677	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	617	PHE	3.4
1	A	565	PRO	3.2
2	E	16	LYS	3.2
2	E	76	TYR	3.2
1	A	673	GLU	3.2
1	A	674	LEU	3.1
1	A	505	HIS	3.1
1	C	516	PHE	3.1
1	B	868	LEU	3.0
1	B	628	PHE	3.0
1	B	673	GLU	2.8
1	A	877	TYR	2.8
1	A	955	LYS	2.8
1	A	664	PHE	2.8
1	A	503	GLY	2.7
1	A	874	PRO	2.7
1	A	538	THR	2.7
1	B	133	SER	2.7
1	A	678	THR	2.7
2	D	140	ASN	2.7
1	C	694	LYS	2.6
1	C	811	TYR	2.6
1	B	670	ALA	2.6
1	A	869	SER	2.6
1	A	1034	SER	2.6
1	B	178	PHE	2.6
1	B	635	ALA	2.6
1	C	498	LYS	2.5
1	B	135	SER	2.5
1	A	668	LEU	2.5
1	A	1038	GLU	2.5
1	A	508	GLY	2.4
1	B	385	ALA	2.4
1	B	874	PRO	2.4
1	C	363	ARG	2.4
1	A	460	GLY	2.4
1	A	432	ARG	2.4
1	B	510	LYS	2.4
1	A	994	GLY	2.3
1	C	896	SER	2.3
1	C	620	ARG	2.3
1	B	870	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	871	ASN	2.3
1	A	362	PHE	2.2
1	A	873	ALA	2.2
1	C	29	LYS	2.2
1	B	408	ASP	2.2
1	B	525	HIS	2.2
1	A	675	GLY	2.2
1	C	70	ASN	2.2
1	B	284	GLN	2.2
1	C	495	THR	2.2
1	A	918	PHE	2.2
1	B	877	TYR	2.2
1	C	662	MET	2.2
1	B	649	MET	2.1
1	B	511	GLY	2.1
1	B	869	SER	2.1
1	A	1035	ARG	2.1
1	B	509	LYS	2.1
1	B	638	PRO	2.1
1	C	510	LYS	2.1
1	A	1043	SER	2.0
1	B	508	GLY	2.0
1	A	356	TYR	2.0
2	D	76	TYR	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](#)

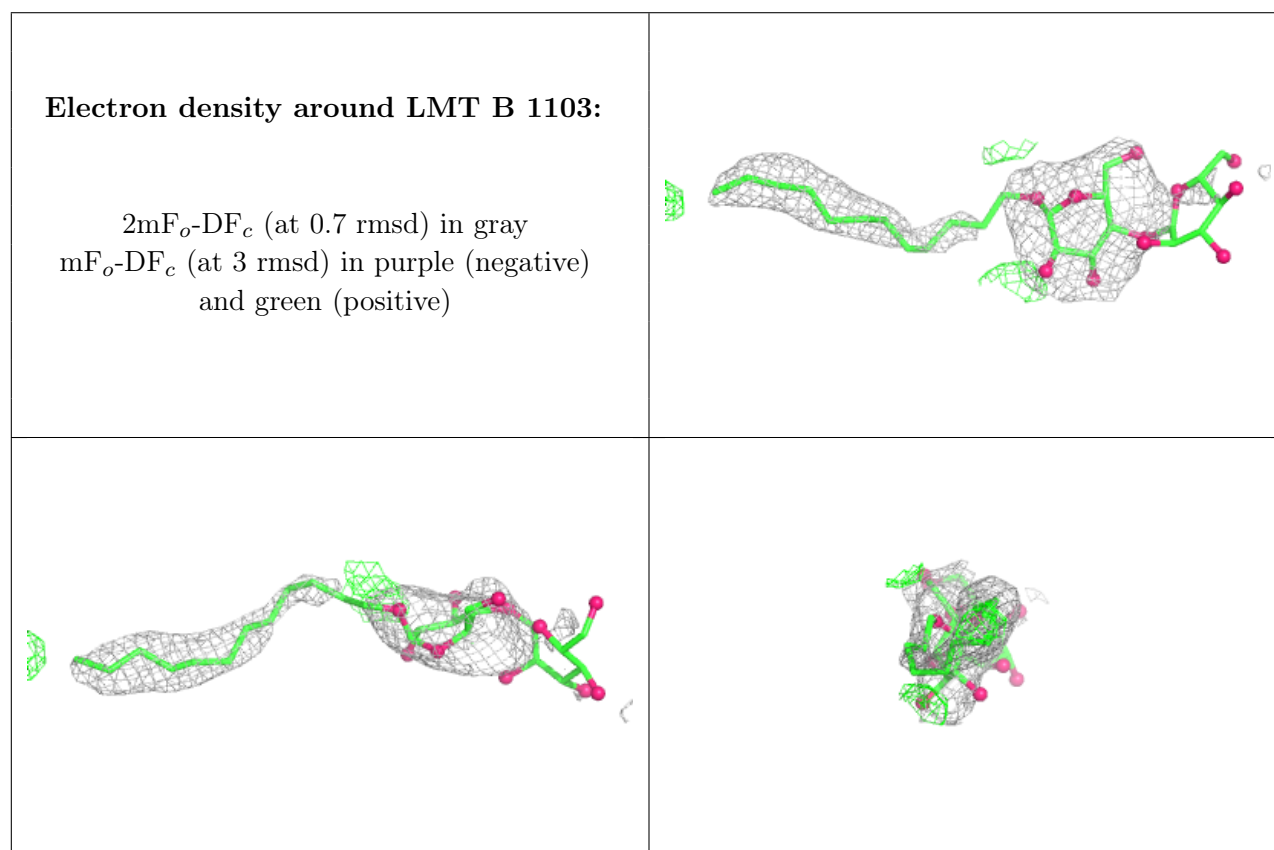
There are no oligosaccharides in this entry.

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.

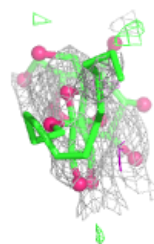
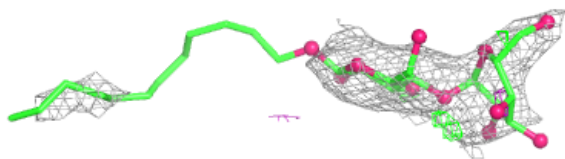
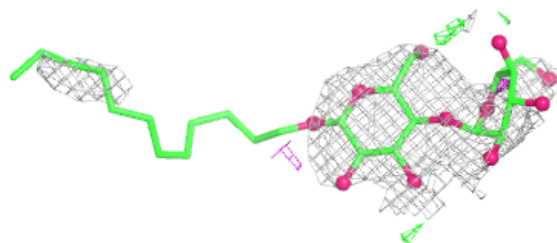
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LMT	B	1103	35/35	0.82	0.20	42,147,193,195	0
3	LMT	A	1102	35/35	0.86	0.19	90,116,154,157	0
3	LMT	B	1102	35/35	0.87	0.15	52,134,161,164	0
3	LMT	C	1101	35/35	0.87	0.14	55,97,134,136	0
3	LMT	B	1101	35/35	0.89	0.16	66,102,122,125	0
3	LMT	A	1101	35/35	0.90	0.13	32,107,156,157	0
3	LMT	C	1102	35/35	0.92	0.12	63,87,104,110	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.

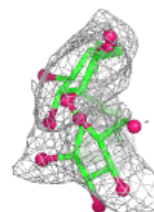
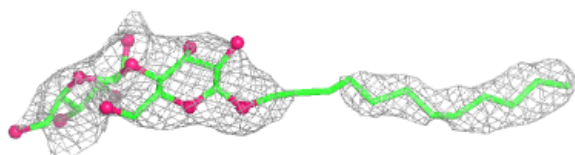
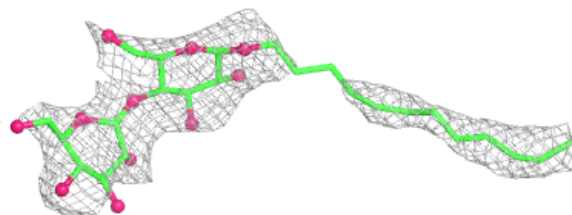


Electron density around LMT A 1102:

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

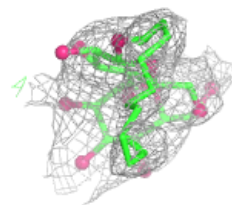
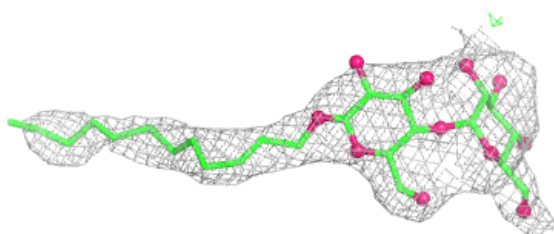
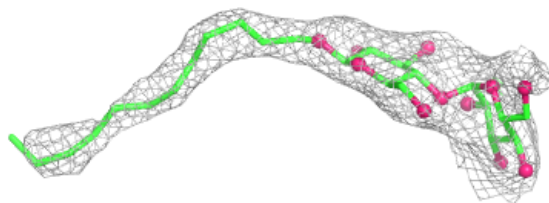
**Electron density around LMT B 1102:**

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

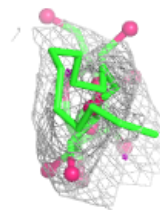
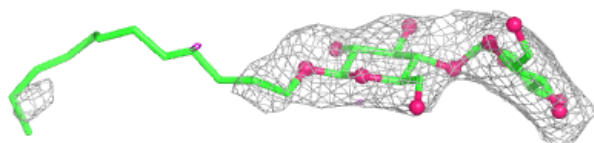
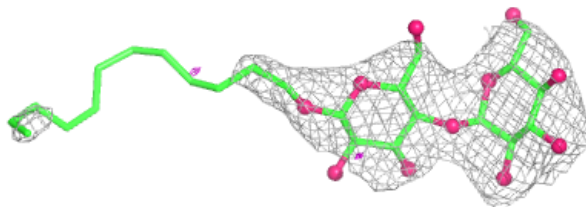


Electron density around LMT C 1101:

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

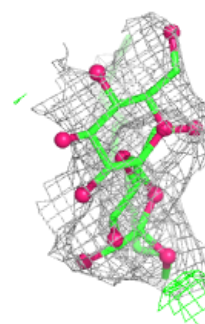
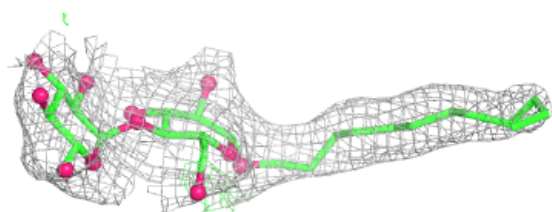
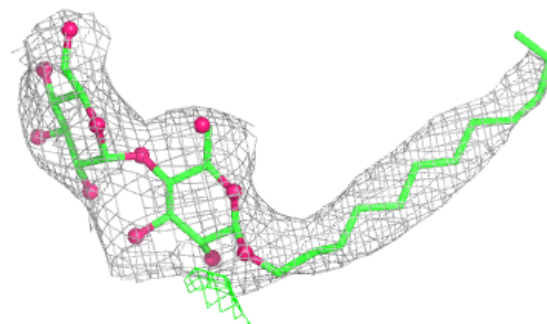
**Electron density around LMT B 1101:**

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

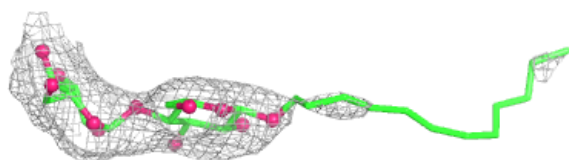
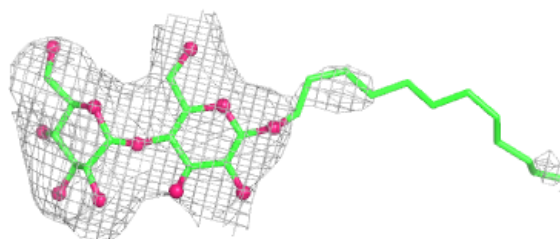


Electron density around LMT A 1101:

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

**Electron density around LMT C 1102:**

$2mF_o-DF_c$ (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.