



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2025 – 12:21 pm GMT

PDB ID : 9HCI / pdb_00009hci
Title : structure of the double Cys-substituted cross-linked AcrB variant
S562C_T837C
Authors : Brandstaetter, L.; Mueller, R.T.; Pos, K.M.
Deposited on : 2024-11-10
Resolution : 2.60 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

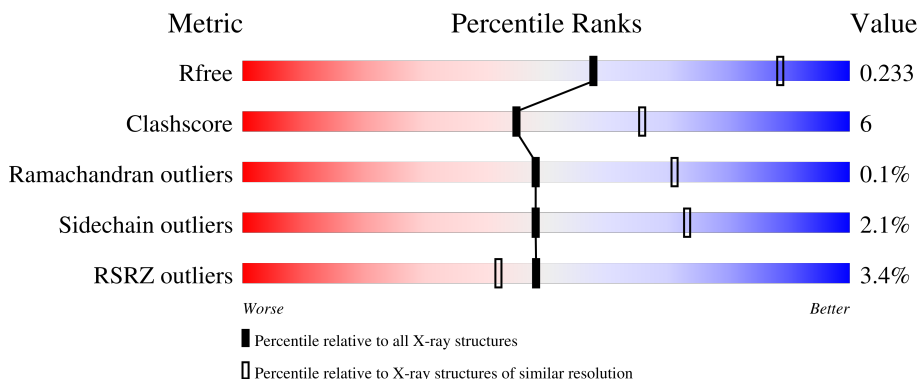
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	<div> <div>5%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>
1	B	1057	<div> <div>4%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
1	C	1057	<div> <div>2%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
2	D	169	<div> <div>%</div> <div>84%</div> <div>7%</div> <div>8%</div> </div>
2	E	169	<div> <div>%</div> <div>83%</div> <div>7%</div> <div>9%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	D10	C	1117	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 27769 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1044	Total	C	N	O	S	0	0	0
			7942	5105	1315	1476	46			
1	B	1033	Total	C	N	O	S	0	1	0
			7856	5056	1296	1457	47			
1	C	1033	Total	C	N	O	S	0	0	0
			7848	5051	1295	1456	46			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	562	CYS	SER	engineered mutation	UNP P31224
A	837	CYS	THR	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	562	CYS	SER	engineered mutation	UNP P31224
B	837	CYS	THR	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	562	CYS	SER	engineered mutation	UNP P31224
C	837	CYS	THR	engineered mutation	UNP P31224
C	1050	LEU	-	expression tag	UNP P31224

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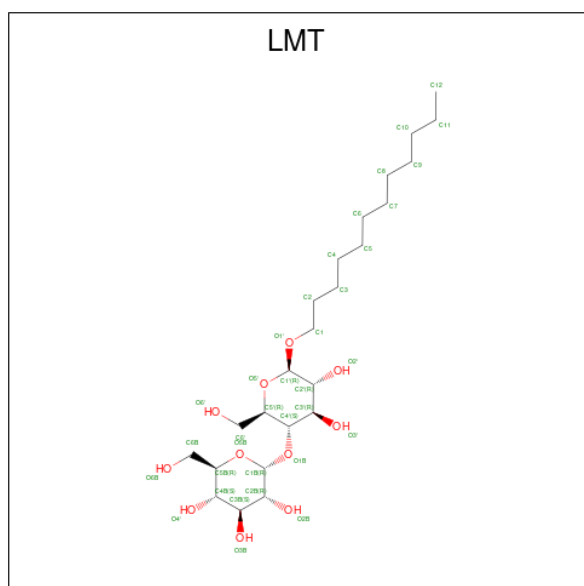
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1051	GLU	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	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	155	Total	C	N	O	S	0	0	0
			1173	739	205	228	1			
2	E	153	Total	C	N	O	S	0	0	0
			1159	732	203	223	1			

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



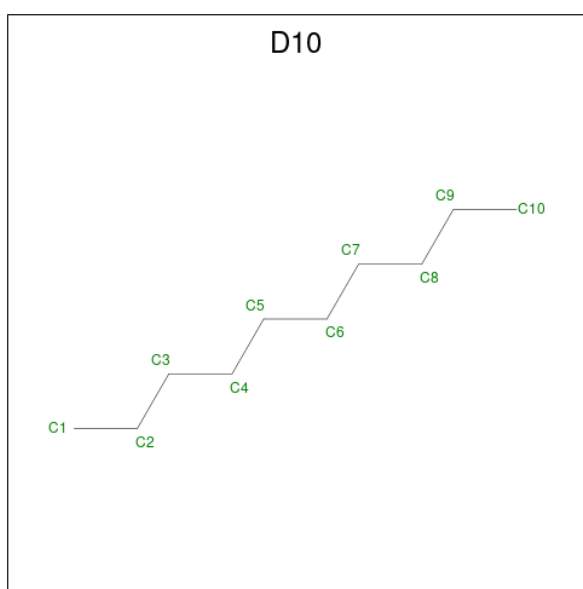
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		

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

- Molecule 4 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$).



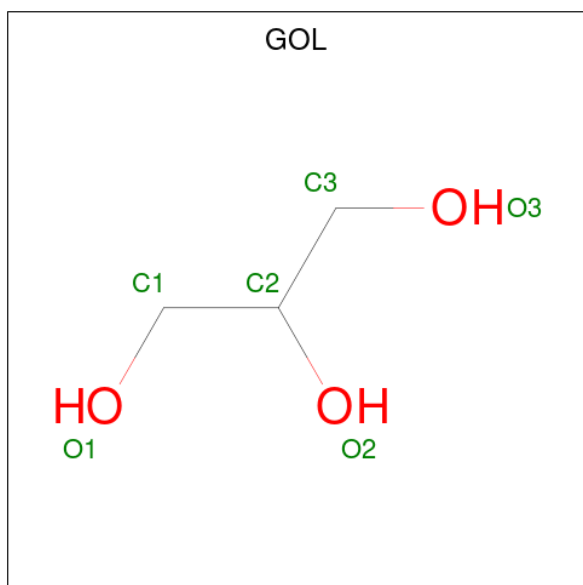
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 10 10	0	0
4	B	1	Total C 10 10	0	0
4	B	1	Total C 10 10	0	0
4	B	1	Total C 10 10	0	0
4	B	1	Total C 10 10	0	0
4	C	1	Total C 10 10	0	0
4	C	1	Total C 10 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C 10 10	0	0
4	C	1	Total C 10 10	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



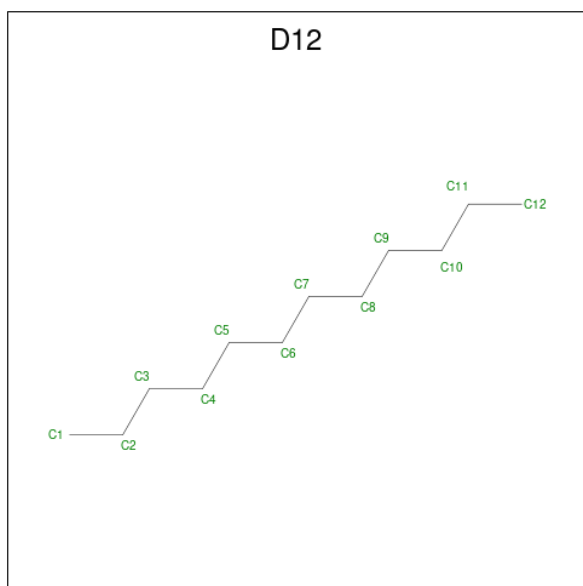
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

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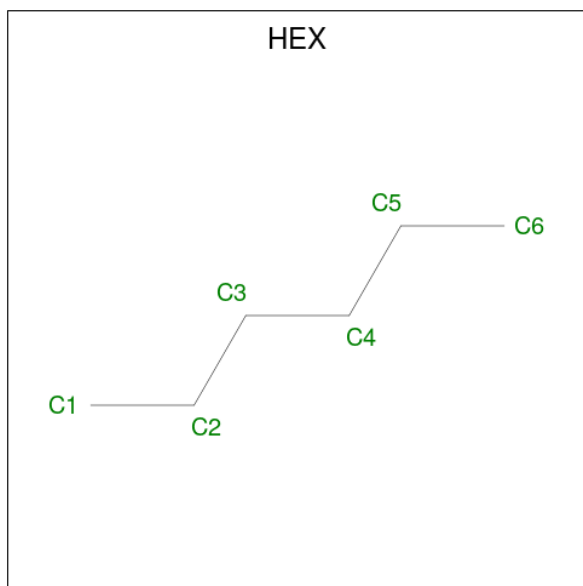
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



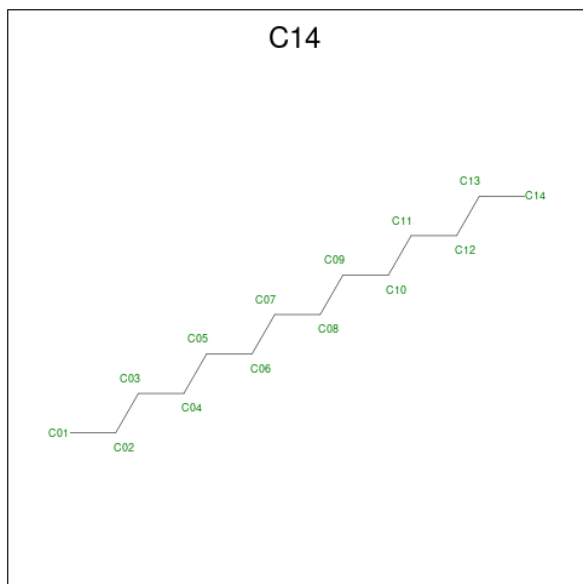
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 12 12	0	0
6	B	1	Total C 12 12	0	0
6	C	1	Total C 12 12	0	0
6	C	1	Total C 12 12	0	0

- Molecule 7 is HEXANE (CCD ID: HEX) (formula: C_6H_{14}).



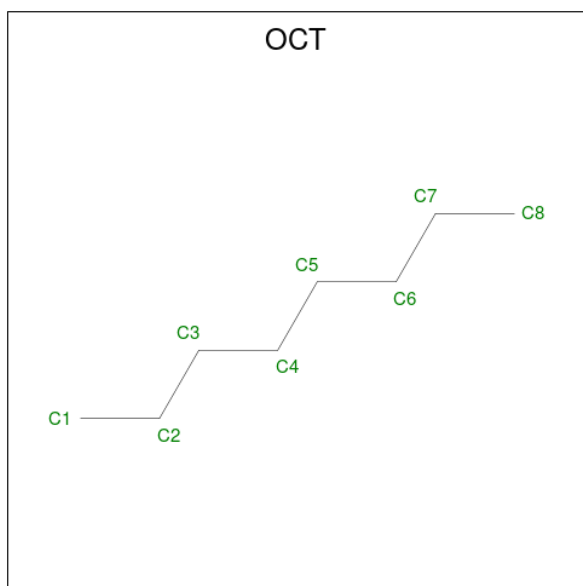
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C 6 6	0	0
7	C	1	Total C 6 6	0	0
7	C	1	Total C 6 6	0	0

- Molecule 8 is TETRADECANE (CCD ID: C14) (formula: $C_{14}H_{30}$).



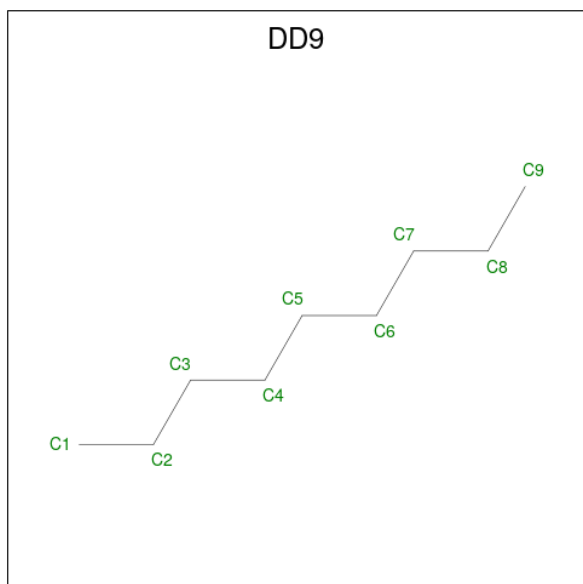
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C 14 14	0	0

- Molecule 9 is N-OCTANE (CCD ID: OCT) (formula: C_8H_{18}).



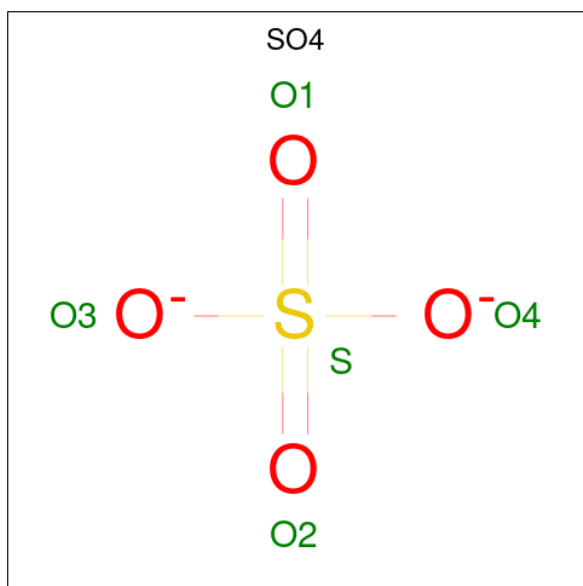
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C 8 8	0	0
9	C	1	Total C 8 8	0	0

- Molecule 10 is nonane (CCD ID: DD9) (formula: C_9H_{20}).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total C 9 9	0	0

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total O S 5 4 1	0	0

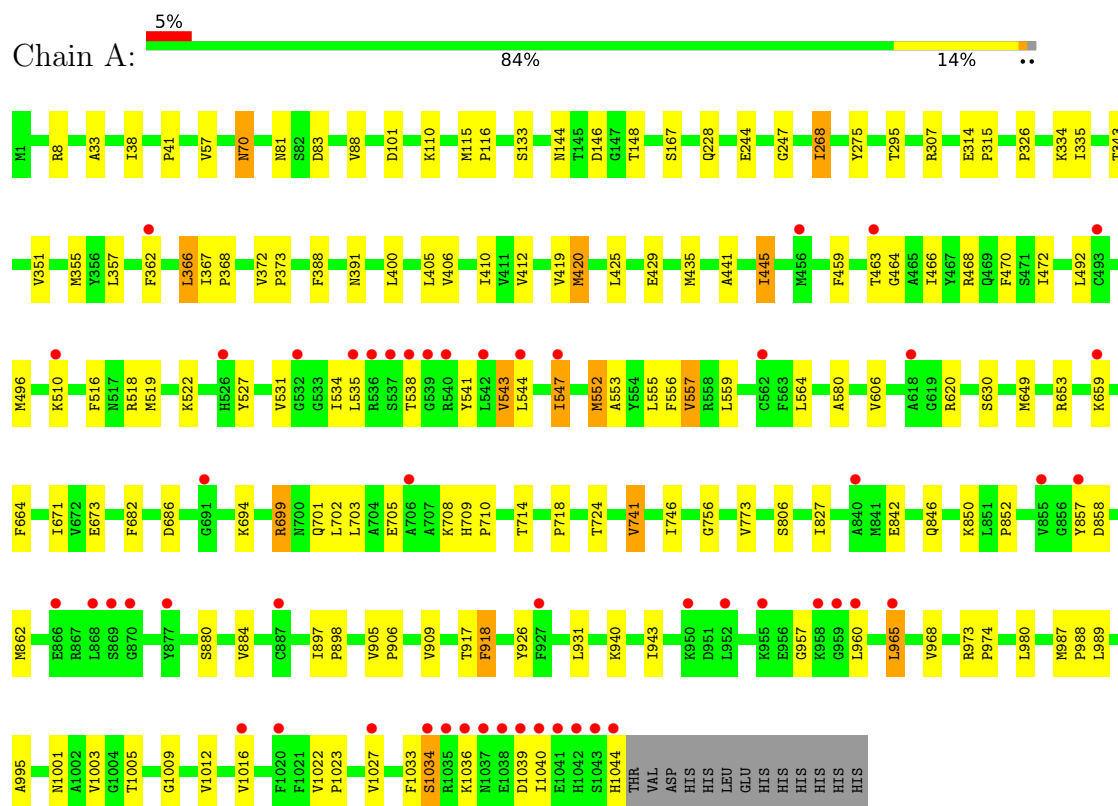
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	434	Total O 434 434	0	0
12	B	288	Total O 288 288	0	0
12	C	389	Total O 389 389	0	0
12	D	53	Total O 53 53	0	0
12	E	51	Total O 51 51	0	0

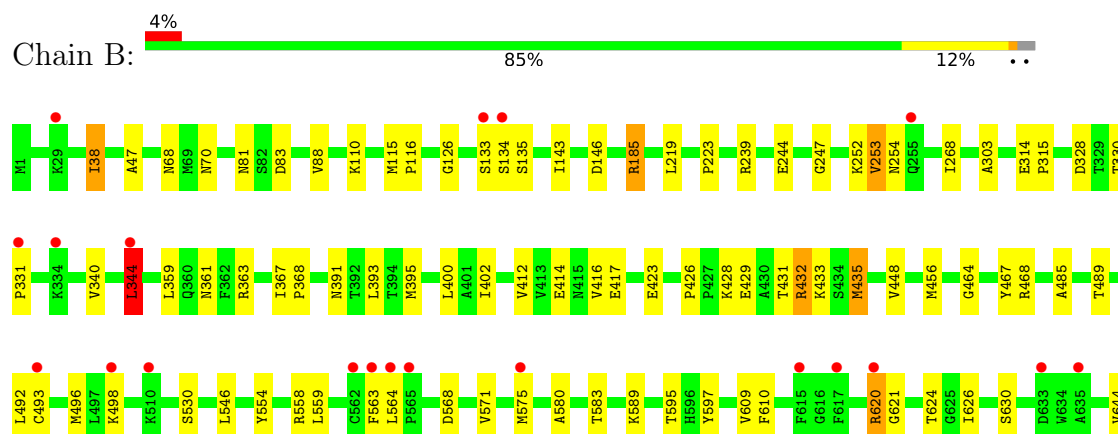
3 Residue-property plots

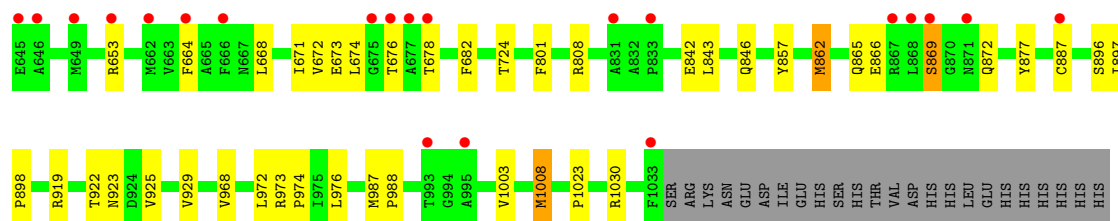
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Multidrug efflux pump subunit AcrB

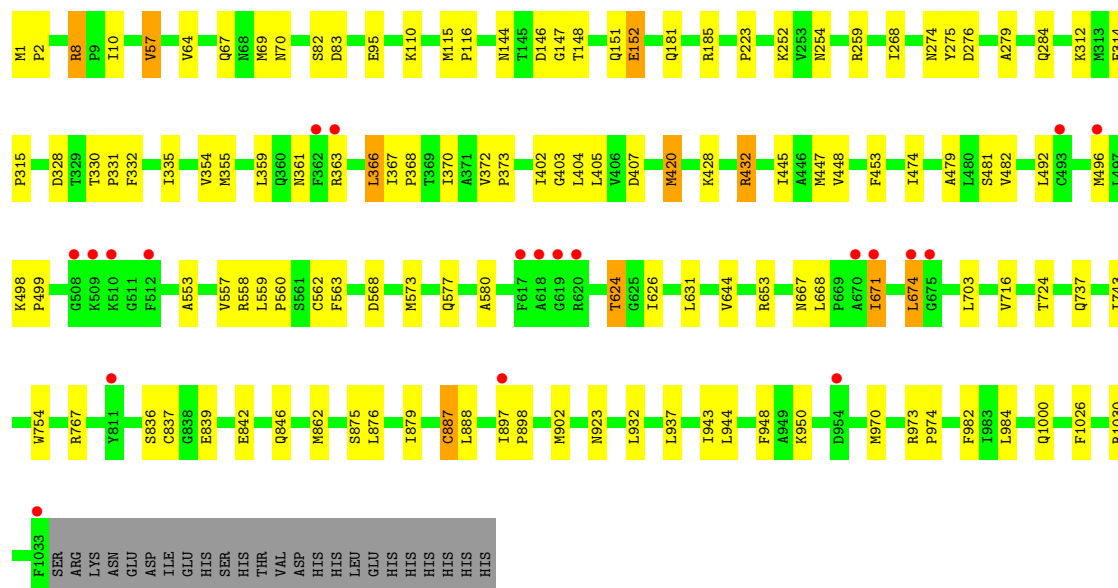
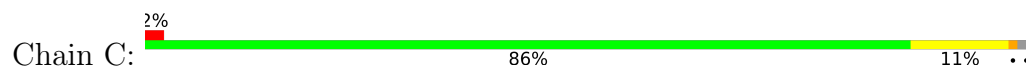


• Molecule 1: Multidrug efflux pump subunit AcrB

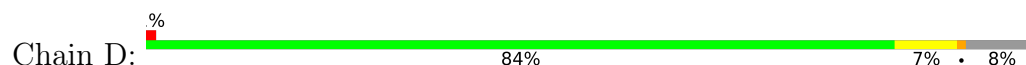




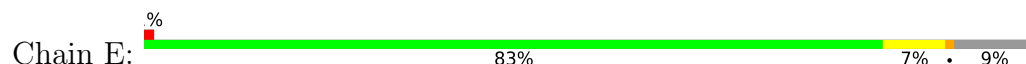
• Molecule 1: Multidrug efflux pump subunit AcrB



• 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	145.71Å 165.30Å 244.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.69 – 2.60 47.69 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.69-2.60) 100.0 (47.69-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.61Å)	Xtriage
Refinement program	PDB-REDO 8.11	Depositor
R, R_{free}	0.190 , 0.230 0.197 , 0.233	Depositor DCC
R_{free} test set	9291 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.905	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27769	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: D12, GOL, DD9, SO4, D10, HEX, OCT, C14, 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	0.70	3/8094 (0.0%)	0.93	5/10989 (0.0%)
1	B	0.69	3/8006 (0.0%)	0.94	9/10871 (0.1%)
1	C	0.69	3/7998 (0.0%)	0.91	3/10861 (0.0%)
2	D	0.69	1/1192 (0.1%)	0.93	1/1621 (0.1%)
2	E	0.64	0/1178	0.96	1/1602 (0.1%)
All	All	0.69	10/26468 (0.0%)	0.93	19/35944 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	6
1	C	0	5
2	D	0	1
All	All	0	17

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	34	MET	SD-CE	-9.91	1.54	1.79
1	A	552	MET	SD-CE	-8.35	1.58	1.79
1	C	420	MET	SD-CE	-8.28	1.58	1.79
1	B	435	MET	SD-CE	-7.93	1.59	1.79
1	A	445	ILE	CG1-CD1	-6.18	1.27	1.51
1	C	69	MET	SD-CE	-5.79	1.65	1.79
1	B	1008	MET	SD-CE	5.30	1.92	1.79
1	C	268	ILE	CG1-CD1	-5.21	1.31	1.51
1	A	268	ILE	CG1-CD1	-5.13	1.31	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	344	LEU	CB-CG	5.08	1.63	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	ASN	CA-CB-CG	-7.26	105.34	112.60
1	C	83	ASP	CA-CB-CG	6.16	118.76	112.60
1	B	244	GLU	CB-CG-CD	5.85	122.54	112.60
2	E	110	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	610	PHE	CA-CB-CG	5.78	119.58	113.80
1	B	83	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	146	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	144	ASN	CA-CB-CG	-5.66	106.94	112.60
1	B	328	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	101	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	38	ILE	N-CA-CB	-5.54	104.31	111.90
1	A	83	ASP	CA-CB-CG	5.50	118.11	112.60
1	B	146	ASP	CA-CB-CG	5.50	118.09	112.60
1	B	185	ARG	CB-CG-CD	-5.36	98.97	111.30
1	C	1000	GLN	OE1-CD-NE2	-5.28	117.32	122.60
2	D	110	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	869	SER	N-CA-C	5.17	118.84	112.54
1	A	664	PHE	CA-CB-CG	5.14	118.94	113.80
1	C	328	ASP	CA-CB-CG	5.12	117.72	112.60

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	468	ARG	Sidechain
1	A	620	ARG	Sidechain
1	A	699	ARG	Sidechain
1	A	8	ARG	Sidechain
1	A	957	GLY	Peptide
1	B	1030	ARG	Sidechain
1	B	239	ARG	Sidechain
1	B	432	ARG	Sidechain
1	B	620	ARG	Sidechain
1	B	808	ARG	Sidechain
1	B	919	ARG	Sidechain
1	C	259	ARG	Sidechain
1	C	432	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	558	ARG	Sidechain
1	C	653	ARG	Sidechain
1	C	8	ARG	Sidechain
2	D	123	ARG	Sidechain

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	7942	0	8080	121	0
1	B	7856	0	8007	91	0
1	C	7848	0	7999	85	0
2	D	1173	0	1156	9	0
2	E	1159	0	1147	9	0
3	A	175	0	230	9	0
3	B	70	0	92	3	0
3	C	35	0	46	0	0
4	A	10	0	22	0	0
4	B	40	0	88	0	0
4	C	40	0	88	0	0
5	A	12	0	16	1	0
5	B	48	0	64	0	0
5	C	18	0	24	2	0
5	D	18	0	24	0	0
6	A	12	0	26	0	0
6	B	12	0	26	0	0
6	C	24	0	52	0	0
7	B	6	0	14	0	0
7	C	12	0	28	0	0
8	C	14	0	30	0	0
9	C	16	0	36	0	0
10	C	9	0	20	0	0
11	C	5	0	0	0	0
12	A	434	0	0	12	0
12	B	288	0	0	7	0
12	C	389	0	0	4	0
12	D	53	0	0	1	0
12	E	51	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	27769	0	27315	311	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 6.

All (311) 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:343:THR:HG21	1:A:989:LEU:CD1	1.74	1.17
1:A:580:ALA:HB1	1:A:724:THR:HG22	1.30	1.13
1:A:580:ALA:CB	1:A:724:THR:HG22	2.00	0.90
1:C:146:ASP:OD1	1:C:148:THR:HG23	1.73	0.88
1:A:445:ILE:CD1	1:A:943:ILE:HG21	2.04	0.87
1:A:694:LYS:O	12:A:1201:HOH:O	1.91	0.87
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.05	0.86
2:E:41:ASN:HD21	2:E:72:ASP:H	1.20	0.85
1:A:518:ARG:O	1:A:522:LYS:HG2	1.76	0.84
1:C:671:ILE:HD11	1:C:674:LEU:HD23	1.59	0.83
1:A:343:THR:HG21	1:A:989:LEU:HD11	1.59	0.81
1:C:573:MET:HE3	1:C:626:ILE:HD11	1.61	0.81
3:B:1114:LMT:H5'	3:B:1114:LMT:O5B	1.81	0.79
1:A:357:LEU:HD21	1:A:516:PHE:CZ	2.17	0.79
1:A:343:THR:CG2	1:A:989:LEU:CD1	2.59	0.78
1:B:416:VAL:HG21	1:B:493:CYS:SG	2.24	0.77
1:A:862:MET:HG3	12:A:1506:HOH:O	1.85	0.77
1:C:152:GLU:OE1	12:C:1201:HOH:O	2.04	0.76
1:A:343:THR:HG21	1:A:989:LEU:HD12	1.66	0.76
1:A:649:MET:SD	1:A:653:ARG:NH1	2.61	0.74
1:B:468:ARG:NH1	12:B:1201:HOH:O	2.18	0.74
1:B:968:VAL:HG11	1:B:1023:PRO:HG3	1.67	0.74
1:B:363:ARG:HD3	1:B:496:MET:O	1.88	0.73
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.70	0.73
1:B:416:VAL:HG11	1:B:493:CYS:SG	2.29	0.73
1:C:181:GLN:HE22	1:C:767:ARG:HE	1.34	0.73
1:B:653:ARG:HG3	1:B:653:ARG:HH11	1.54	0.72
1:B:344:LEU:HD12	1:B:402:ILE:HD11	1.72	0.72
2:E:34:MET:HE2	2:E:34:MET:HA	1.69	0.72
1:B:423:GLU:OE2	1:B:433:LYS:HE2	1.90	0.72
1:B:133:SER:HB2	12:B:1253:HOH:O	1.94	0.67
1:B:133:SER:CB	12:B:1253:HOH:O	2.41	0.67
2:D:34:MET:HE1	2:D:40:VAL:CG1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:VAL:HG22	1:B:887:CYS:SG	2.35	0.67
1:C:151:GLN:HG2	12:C:1447:HOH:O	1.93	0.67
1:C:312:LYS:NZ	12:C:1202:HOH:O	2.28	0.67
1:A:559:LEU:HD21	1:A:917:THR:CG2	2.25	0.66
1:C:70:ASN:O	1:C:110:LYS:NZ	2.29	0.66
1:A:445:ILE:HD11	1:A:943:ILE:HG21	1.77	0.65
1:A:555:LEU:O	1:A:559:LEU:HD23	1.96	0.65
1:B:340:VAL:HG21	1:B:395[A]:MET:HB3	1.78	0.65
1:B:330:THR:N	1:B:331:PRO:HD2	2.12	0.65
1:A:559:LEU:HD21	1:A:917:THR:HG23	1.78	0.65
1:C:453:PHE:CE2	1:C:474:ILE:HG21	2.31	0.65
1:A:535:LEU:HD12	1:A:965:LEU:HD21	1.78	0.65
1:A:1001:ASN:O	1:A:1005:THR:HG23	1.96	0.64
1:C:147:GLY:HA2	12:C:1384:HOH:O	1.96	0.64
1:A:412:VAL:HG13	1:A:435:MET:CE	2.28	0.64
1:B:219:LEU:HD23	1:C:754:TRP:CZ3	2.33	0.63
1:A:880:SER:O	1:A:884:VAL:HG23	1.99	0.63
1:A:357:LEU:C	1:A:357:LEU:HD23	2.22	0.63
1:C:671:ILE:HD11	1:C:674:LEU:CD2	2.27	0.63
1:A:709:HIS:ND1	12:A:1207:HOH:O	2.31	0.63
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.80	0.63
1:B:412:VAL:HG13	1:B:435:MET:CE	2.30	0.62
1:A:535:LEU:CD1	1:A:965:LEU:HD21	2.29	0.62
1:C:948:PHE:CE2	1:C:970:MET:HE3	2.35	0.62
3:B:1114:LMT:O5B	3:B:1114:LMT:C5'	2.48	0.62
1:C:562:CYS:HB2	1:C:837:CYS:SG	2.39	0.62
1:A:445:ILE:HG21	1:A:940:LYS:HG3	1.82	0.61
1:B:877:TYR:OH	3:B:1114:LMT:O5'	2.18	0.61
1:A:850:LYS:NZ	12:A:1203:HOH:O	2.20	0.61
1:B:568:ASP:CG	1:B:644:VAL:HG23	2.26	0.61
2:E:34:MET:HE1	2:E:40:VAL:HG12	1.81	0.61
1:A:556:PHE:HZ	3:A:1102:LMT:H2O2	1.46	0.61
1:C:577:GLN:HE22	1:C:624:THR:HG22	1.65	0.61
1:A:355:MET:HE2	1:A:355:MET:HA	1.82	0.60
1:A:699:ARG:HD2	1:A:718:PRO:HB3	1.83	0.60
2:E:27:ASP:HA	2:E:62:ILE:HD11	1.83	0.60
1:B:435:MET:HE2	12:B:1212:HOH:O	2.01	0.60
1:C:568:ASP:CG	1:C:644:VAL:HG23	2.25	0.60
1:C:420:MET:CE	1:C:499:PRO:HA	2.31	0.60
1:A:968:VAL:HG11	1:A:1023:PRO:HG3	1.82	0.60
1:C:479:ALA:O	1:C:482:VAL:HG12	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:VAL:CG2	1:C:984:LEU:HD12	2.32	0.59
1:A:412:VAL:HG13	1:A:435:MET:HE1	1.83	0.59
1:C:973:ARG:HB3	1:C:974:PRO:HD3	1.84	0.59
1:A:445:ILE:HD11	1:A:943:ILE:CG2	2.32	0.59
1:A:441:ALA:O	1:A:445:ILE:HG12	2.02	0.58
1:B:653:ARG:HG3	1:B:653:ARG:NH1	2.18	0.58
1:A:307:ARG:HD2	12:A:1562:HOH:O	2.03	0.58
1:A:705:GLU:OE2	1:A:708:LYS:HE2	2.03	0.58
1:B:575:MET:HE3	1:B:664:PHE:CZ	2.39	0.57
1:C:363:ARG:HH21	1:C:498:LYS:HD2	1.70	0.57
2:E:14:LEU:HD13	2:E:14:LEU:C	2.30	0.57
1:B:400:LEU:HD21	1:B:1003:VAL:HG13	1.86	0.57
1:B:448:VAL:CG2	1:B:887:CYS:SG	2.93	0.57
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.87	0.56
1:B:412:VAL:HG13	1:B:435:MET:HE1	1.86	0.56
1:C:355:MET:SD	1:C:368:PRO:HB2	2.45	0.56
1:A:960:LEU:CD2	1:A:1027:VAL:HG12	2.35	0.56
1:C:553:ALA:O	1:C:557:VAL:HG23	2.05	0.56
1:A:343:THR:HG21	1:A:989:LEU:HD13	1.80	0.56
1:C:836:SER:OG	1:C:839:GLU:HG3	2.06	0.56
1:B:554:TYR:CE1	1:B:558:ARG:NE	2.74	0.56
1:A:334:LYS:HE2	12:A:1582:HOH:O	2.05	0.56
1:A:247:GLY:HA2	1:A:268:ILE:HD12	1.88	0.55
1:A:852:PRO:HA	12:A:1532:HOH:O	2.06	0.55
1:C:560:PRO:HB2	1:C:836:SER:HB3	1.88	0.55
1:B:580:ALA:HB1	1:B:724:THR:HG22	1.88	0.55
1:C:366:LEU:O	1:C:370:ILE:HG12	2.06	0.55
1:C:146:ASP:CG	1:C:148:THR:HG23	2.31	0.55
1:C:897:ILE:HB	1:C:898:PRO:HD3	1.89	0.55
1:C:274:ASN:HD22	1:C:276:ASP:H	1.55	0.55
1:C:445:ILE:HD11	1:C:944:LEU:HD21	1.89	0.55
1:B:972:LEU:O	1:B:976:LEU:HD23	2.06	0.55
1:C:404:LEU:HD21	1:C:937:LEU:HD21	1.89	0.54
1:A:167:SER:HB3	1:B:70:ASN:HB3	1.89	0.54
1:A:544:LEU:HA	1:A:547:ILE:CG1	2.37	0.54
1:B:563:PHE:O	1:B:925:VAL:HG23	2.06	0.54
1:B:391:ASN:HD22	1:B:393:LEU:H	1.56	0.54
1:A:842:GLU:O	1:A:846:GLN:HG3	2.07	0.54
1:A:741:VAL:HG23	1:A:746:ILE:HD11	1.90	0.54
1:B:671:ILE:O	1:B:674:LEU:HD23	2.08	0.54
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:563:PHE:HD2	1:C:862:MET:HE1	1.74	0.53
1:A:466:ILE:HD13	1:A:564:LEU:HD21	1.90	0.53
1:B:361:ASN:HB2	1:B:498:LYS:CE	2.38	0.53
1:A:400:LEU:HD12	1:A:470:PHE:HE1	1.71	0.53
1:B:671:ILE:CG2	1:B:674:LEU:HD22	2.39	0.53
1:B:252:LYS:HE2	1:B:254:ASN:ND2	2.23	0.53
1:A:534:ILE:HG23	1:A:541:TYR:CE2	2.44	0.53
1:A:553:ALA:O	1:A:557:VAL:HG22	2.09	0.52
1:A:534:ILE:HG23	1:A:541:TYR:CD2	2.44	0.52
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.91	0.52
1:A:931:LEU:HD23	3:A:1102:LMT:H41	1.90	0.52
1:A:244:GLU:HB3	12:D:346:HOH:O	2.08	0.52
1:A:343:THR:CG2	1:A:989:LEU:HD13	2.38	0.52
1:B:589:LYS:HE3	12:B:1429:HOH:O	2.10	0.52
1:C:448:VAL:HG11	1:C:943:ILE:HD11	1.91	0.52
1:B:431:THR:OG1	1:B:493:CYS:SG	2.46	0.52
1:B:862:MET:HE1	12:B:1231:HOH:O	2.09	0.52
1:B:973:ARG:HB3	1:B:974:PRO:HD3	1.90	0.52
1:C:372:VAL:HA	1:C:405:LEU:HD11	1.93	0.51
1:A:702:LEU:HD23	1:A:827:ILE:HD13	1.92	0.51
1:A:400:LEU:HD12	1:A:470:PHE:CE1	2.46	0.51
1:A:960:LEU:HD21	1:A:1027:VAL:HG12	1.92	0.51
1:B:344:LEU:CD1	1:B:402:ILE:HD11	2.40	0.51
2:D:34:MET:HE2	2:D:69:ASN:HB2	1.91	0.51
1:A:133:SER:OG	1:A:673:GLU:O	2.28	0.51
1:B:340:VAL:HG21	1:B:395[B]:MET:HB3	1.92	0.51
1:C:743:ILE:N	1:C:743:ILE:CD1	2.74	0.51
1:B:344:LEU:HD12	1:B:402:ILE:CD1	2.41	0.51
1:C:359:LEU:O	1:C:361:ASN:N	2.37	0.51
1:C:403:GLY:O	1:C:407:ASP:OD1	2.29	0.51
1:A:552:MET:HE3	1:A:906:PRO:HB3	1.93	0.51
1:B:400:LEU:HD13	1:B:929:VAL:HG12	1.93	0.50
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.92	0.50
1:C:363:ARG:NH2	1:C:498:LYS:HD2	2.25	0.50
1:A:552:MET:CE	1:A:906:PRO:HA	2.41	0.50
1:B:253:VAL:CG1	1:C:737:GLN:HE22	2.24	0.50
1:B:595:THR:HG23	1:B:609:VAL:HB	1.94	0.50
1:B:671:ILE:HB	1:B:674:LEU:CD2	2.42	0.50
3:A:1109:LMT:H12	3:A:1109:LMT:O2'	2.11	0.50
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.92	0.50
1:C:185:ARG:HH12	5:C:1114:GOL:C3	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LEU:HA	1:A:547:ILE:HD11	1.93	0.49
1:A:960:LEU:C	1:A:960:LEU:HD23	2.37	0.49
1:C:447:MET:HG3	1:C:887:CYS:SG	2.52	0.49
2:D:34:MET:HE2	2:D:69:ASN:CB	2.42	0.49
1:C:743:ILE:N	1:C:743:ILE:HD12	2.27	0.49
1:B:47:ALA:HB3	1:B:88:VAL:CG1	2.42	0.49
1:B:133:SER:HA	12:B:1253:HOH:O	2.13	0.49
1:A:70:ASN:O	1:A:110:LYS:HE3	2.12	0.49
1:A:41:PRO:HB3	1:A:295:THR:HG21	1.95	0.49
1:C:420:MET:HE2	1:C:499:PRO:HA	1.94	0.49
1:A:57:VAL:HG13	1:A:88:VAL:HG22	1.93	0.48
1:A:556:PHE:HZ	3:A:1102:LMT:O2'	1.94	0.48
1:A:686:ASP:O	12:A:1202:HOH:O	2.20	0.48
1:B:597:TYR:CD1	1:B:597:TYR:C	2.91	0.48
2:D:82:THR:OG1	2:D:85:HIS:HD2	1.96	0.48
1:B:38:ILE:HD13	1:B:671:ILE:HD13	1.96	0.48
1:B:428:LYS:NZ	1:B:432:ARG:CZ	2.77	0.48
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.95	0.48
1:A:552:MET:HE2	1:A:909:VAL:HB	1.95	0.48
1:A:909:VAL:HA	1:A:931:LEU:HD11	1.96	0.48
1:C:274:ASN:ND2	1:C:276:ASP:H	2.11	0.48
2:E:30:VAL:HG21	2:E:62:ILE:HD12	1.96	0.48
1:B:359:LEU:HD22	1:B:417:GLU:HG3	1.95	0.47
1:B:464:GLY:O	1:B:468:ARG:HB2	2.13	0.47
1:C:57:VAL:CG1	1:C:82:SER:HB3	2.44	0.47
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.95	0.47
1:A:987:MET:HB3	1:A:988:PRO:HD3	1.96	0.47
1:A:412:VAL:HG13	1:A:435:MET:HE3	1.96	0.47
1:B:70:ASN:O	1:B:110:LYS:HE3	2.15	0.47
1:A:1009:GLY:O	1:A:1012:VAL:HG22	2.14	0.47
1:A:705:GLU:CD	1:A:708:LYS:HE2	2.40	0.47
1:B:987:MET:HE1	1:B:1008:MET:SD	2.54	0.47
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.97	0.47
1:C:1026:PHE:O	1:C:1030:ARG:HG2	2.15	0.47
1:A:445:ILE:CD1	1:A:943:ILE:CG2	2.84	0.47
1:C:948:PHE:HE2	1:C:970:MET:HE3	1.79	0.46
2:E:34:MET:HE1	2:E:40:VAL:CG1	2.44	0.46
1:A:701:GLN:HA	12:A:1578:HOH:O	2.15	0.46
1:B:185:ARG:HD3	1:B:185:ARG:HA	1.72	0.46
1:C:314:GLU:N	1:C:315:PRO:CD	2.78	0.46
1:A:314:GLU:N	1:A:315:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:MET:HE1	2:D:40:VAL:HG12	1.97	0.46
1:B:223:PRO:HD3	1:C:275:TYR:CD1	2.50	0.46
1:C:144:ASN:HD21	1:C:148:THR:H	1.64	0.46
1:C:151:GLN:OE1	1:C:279:ALA:O	2.34	0.45
1:A:926:TYR:HB3	1:A:1003:VAL:HG23	1.98	0.45
1:C:492:LEU:O	1:C:496:MET:HB2	2.17	0.45
1:A:351:VAL:HG11	1:A:406:VAL:HG21	1.99	0.45
1:B:563:PHE:CZ	1:B:925:VAL:HG22	2.50	0.45
1:C:420:MET:HE1	1:C:499:PRO:HA	1.97	0.45
1:C:703:LEU:HD23	1:C:716:VAL:HG12	1.99	0.45
1:A:931:LEU:HD23	3:A:1102:LMT:C4	2.47	0.45
3:A:1105:LMT:H6'2	12:A:1266:HOH:O	2.16	0.45
1:B:247:GLY:HA2	1:B:268:ILE:HD12	1.98	0.45
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.97	0.45
1:B:426:PRO:HG2	1:B:429:GLU:OE1	2.16	0.45
1:A:228:GLN:O	1:B:583:THR:HG21	2.17	0.45
1:A:148:THR:HG21	12:A:1232:HOH:O	2.17	0.45
1:B:314:GLU:N	1:B:315:PRO:CD	2.79	0.45
1:B:575:MET:CE	1:B:664:PHE:CZ	3.00	0.45
1:B:842:GLU:O	1:B:846:GLN:HG3	2.17	0.44
1:A:57:VAL:HG11	1:A:88:VAL:HG22	1.94	0.44
1:B:563:PHE:CE1	1:B:925:VAL:HG22	2.52	0.44
1:A:57:VAL:HG13	1:A:88:VAL:CG2	2.47	0.44
1:A:659:LYS:H	1:A:659:LYS:HD2	1.81	0.44
1:A:1033:PHE:O	1:A:1034:SER:CB	2.66	0.44
1:B:219:LEU:HD23	1:C:754:TRP:HZ3	1.77	0.44
1:C:568:ASP:OD2	1:C:644:VAL:HG23	2.17	0.44
1:C:897:ILE:HD11	1:C:950:LYS:HE3	1.99	0.44
2:D:34:MET:CE	2:D:69:ASN:CB	2.95	0.44
1:B:133:SER:OG	1:B:135:SER:OG	2.34	0.44
1:B:668:LEU:HD23	1:B:672:VAL:CG1	2.48	0.44
1:A:1044:HIS:CG	1:A:1044:HIS:O	2.71	0.44
1:C:185:ARG:HH12	5:C:1114:GOL:H32	1.82	0.44
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.99	0.44
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.53	0.44
1:A:459:PHE:HB2	1:A:464:GLY:HA2	2.00	0.44
1:A:544:LEU:O	1:A:547:ILE:HG13	2.18	0.43
1:A:960:LEU:HD23	1:A:960:LEU:O	2.18	0.43
1:B:897:ILE:N	1:B:898:PRO:CD	2.82	0.43
1:C:573:MET:CE	1:C:626:ILE:HD11	2.42	0.43
1:C:875:SER:O	1:C:879:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ASN:HB2	1:B:498:LYS:HE2	2.01	0.43
1:C:876:LEU:HD21	1:C:932:LEU:HD11	2.01	0.43
2:D:49:THR:H	2:D:52:HIS:CD2	2.37	0.43
1:A:543:VAL:O	1:A:547:ILE:HG12	2.19	0.43
1:A:708:LYS:C	1:A:710:PRO:HD3	2.44	0.43
1:C:64:VAL:O	1:C:67:GLN:HG2	2.18	0.43
1:C:902:MET:HE2	1:C:902:MET:HA	2.00	0.42
1:A:559:LEU:HD21	1:A:917:THR:HG22	2.00	0.42
3:A:1109:LMT:H6D	1:B:872:GLN:HB3	2.01	0.42
1:B:492:LEU:O	1:B:496:MET:HB2	2.19	0.42
1:B:865:GLN:O	1:B:869:SER:N	2.38	0.42
1:A:355:MET:CE	1:A:410:ILE:HD11	2.50	0.42
1:A:555:LEU:HD22	1:A:917:THR:HG21	2.00	0.42
1:C:428:LYS:HZ1	1:C:432:ARG:NH2	2.17	0.42
1:C:559:LEU:HD23	1:C:923:ASN:HB2	2.00	0.42
1:A:38:ILE:HD11	1:A:671:ILE:CD1	2.49	0.42
1:B:361:ASN:HB2	1:B:498:LYS:HE3	2.00	0.42
1:B:416:VAL:HG22	1:B:431:THR:HA	2.00	0.42
1:B:485:ALA:HA	1:B:489:THR:OG1	2.20	0.42
1:C:448:VAL:CG1	1:C:888:LEU:HD21	2.50	0.42
2:D:115:THR:H	2:D:118:HIS:HD2	1.67	0.42
1:B:668:LEU:HD23	1:B:672:VAL:HG11	2.00	0.42
1:C:57:VAL:HG13	1:C:82:SER:HB3	2.02	0.42
1:A:326:PRO:O	1:A:630:SER:HB2	2.20	0.42
1:A:492:LEU:O	1:A:496:MET:HB2	2.20	0.42
1:A:897:ILE:N	1:A:898:PRO:CD	2.83	0.42
3:A:1105:LMT:C6B	12:A:1266:HOH:O	2.68	0.42
1:B:671:ILE:HG22	1:B:674:LEU:HD22	2.01	0.42
1:A:703:LEU:HD13	1:A:718:PRO:HD3	2.02	0.42
3:A:1103:LMT:O4'	1:C:8:ARG:NH1	2.53	0.42
1:A:335:ILE:HG22	1:A:995:ALA:HB3	2.02	0.41
1:C:403:GLY:HA3	1:C:982:PHE:HA	2.02	0.41
1:A:429:GLU:OE1	1:A:429:GLU:N	2.52	0.41
1:B:115:MET:N	1:B:116:PRO:CD	2.83	0.41
1:B:559:LEU:HD23	1:B:923:ASN:HB2	2.01	0.41
1:C:671:ILE:CG1	1:C:671:ILE:O	2.68	0.41
2:D:82:THR:H	2:D:85:HIS:CD2	2.39	0.41
1:C:842:GLU:O	1:C:846:GLN:HG3	2.20	0.41
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.55	0.41
1:C:447:MET:CG	1:C:887:CYS:SG	3.09	0.41
1:A:388:PHE:HE2	1:A:472:ILE:HB	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:GLY:HA3	5:A:1106:GOL:H32	2.03	0.41
1:C:671:ILE:O	1:C:671:ILE:HG13	2.20	0.41
1:A:115:MET:HB2	1:A:116:PRO:HD3	2.03	0.41
1:A:527:TYR:O	1:A:531:VAL:HG23	2.20	0.41
1:B:303:ALA:HB2	1:B:330:THR:HG21	2.03	0.41
1:B:426:PRO:HG2	1:B:429:GLU:CD	2.45	0.41
1:B:428:LYS:HZ1	1:B:432:ARG:CZ	2.32	0.41
1:C:330:THR:N	1:C:331:PRO:CD	2.84	0.41
2:E:67:LEU:HD21	2:E:73:VAL:HG23	2.01	0.41
1:A:362:PHE:O	1:A:366:LEU:HD23	2.20	0.41
1:A:559:LEU:CD2	1:A:917:THR:HG22	2.51	0.41
1:A:918:PHE:CD1	1:A:918:PHE:C	2.99	0.41
1:B:621:GLY:O	1:B:624:THR:HG22	2.20	0.41
1:C:631:LEU:HD11	1:C:644:VAL:HG22	2.03	0.41
1:B:414:GLU:OE1	1:B:974:PRO:HG3	2.20	0.41
1:A:33:ALA:O	1:A:391:ASN:HA	2.21	0.41
1:A:275:TYR:CD1	1:C:223:PRO:HD3	2.56	0.41
1:A:420:MET:HG3	1:A:425:LEU:O	2.21	0.41
1:A:741:VAL:CG2	1:A:746:ILE:HD11	2.49	0.41
1:A:806:SER:HB2	2:E:112:ASN:CG	2.46	0.41
1:A:965:LEU:HD23	1:A:965:LEU:N	2.35	0.40
1:B:568:ASP:OD2	1:B:644:VAL:HG23	2.21	0.40
1:C:332:PHE:HA	1:C:335:ILE:HG22	2.03	0.40
1:A:1022:VAL:N	1:A:1023:PRO:CD	2.84	0.40
1:B:676:THR:HG22	1:B:678:THR:HG22	2.04	0.40
1:C:252:LYS:HE3	1:C:254:ASN:ND2	2.36	0.40
1:A:115:MET:HE3	1:A:115:MET:HB3	1.95	0.40
1:A:535:LEU:HD22	1:A:1027:VAL:HG21	2.04	0.40
1:A:980:LEU:HD13	1:A:980:LEU:HA	1.98	0.40
1:B:429:GLU:OE1	1:B:429:GLU:N	2.53	0.40
1:C:667:ASN:OD1	1:C:668:LEU:N	2.54	0.40
1:C:115:MET:HB2	1:C:116:PRO:HD3	2.01	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%)	1024 (98%)	16 (2%)	2 (0%)	44	66
1	B	1032/1057 (98%)	1011 (98%)	21 (2%)	0	100	100
1	C	1031/1057 (98%)	1009 (98%)	22 (2%)	0	100	100
2	D	153/169 (90%)	152 (99%)	1 (1%)	0	100	100
2	E	151/169 (89%)	149 (99%)	2 (1%)	0	100	100
All	All	3409/3509 (97%)	3345 (98%)	62 (2%)	2 (0%)	48	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1034	SER
1	A	1036	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	850/863 (98%)	827 (97%)	23 (3%)	40	66
1	B	840/863 (97%)	821 (98%)	19 (2%)	45	71
1	C	839/863 (97%)	827 (99%)	12 (1%)	62	82
2	D	120/132 (91%)	118 (98%)	2 (2%)	56	78
2	E	118/132 (89%)	117 (99%)	1 (1%)	79	91
All	All	2767/2853 (97%)	2710 (98%)	57 (2%)	48	73

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	81	ASN

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Mol	Chain	Res	Type
1	A	366	LEU
1	A	405	LEU
1	A	419	VAL
1	A	420	MET
1	A	463	THR
1	A	510	LYS
1	A	519	MET
1	A	538	THR
1	A	543	VAL
1	A	547	ILE
1	A	557	VAL
1	A	606	VAL
1	A	714	THR
1	A	741	VAL
1	A	773	VAL
1	A	858	ASP
1	A	918	PHE
1	A	965	LEU
1	A	1016	VAL
1	A	1039	ASP
1	A	1040	ILE
1	B	81	ASN
1	B	134	SER
1	B	143	ILE
1	B	253	VAL
1	B	344	LEU
1	B	530	SER
1	B	546	LEU
1	B	564	LEU
1	B	571	VAL
1	B	620	ARG
1	B	626	ILE
1	B	630	SER
1	B	673	GLU
1	B	801	PHE
1	B	843	LEU
1	B	862	MET
1	B	866	GLU
1	B	896	SER
1	B	922	THR
1	C	10	ILE
1	C	57	VAL

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Mol	Chain	Res	Type
1	C	95	GLU
1	C	152	GLU
1	C	284	GLN
1	C	366	LEU
1	C	402	ILE
1	C	481	SER
1	C	624	THR
1	C	671	ILE
1	C	674	LEU
1	C	887	CYS
2	D	53	LEU
2	D	61	GLU
2	E	73	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	70	ASN
1	A	81	ASN
1	A	89	GLN
1	A	109	ASN
1	A	120	GLN
1	A	218	GLN
1	A	231	ASN
1	A	415	ASN
1	A	526	HIS
1	A	687	GLN
1	A	744	ASN
1	A	1001	ASN
1	B	3	ASN
1	B	58	GLN
1	B	70	ASN
1	B	108	GLN
1	B	218	GLN
1	B	254	ASN
1	B	391	ASN
1	B	687	GLN
1	B	709	HIS
1	B	744	ASN
1	B	865	GLN
1	B	1001	ASN

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Mol	Chain	Res	Type
1	C	34	GLN
1	C	58	GLN
1	C	81	ASN
1	C	104	GLN
1	C	108	GLN
1	C	144	ASN
1	C	181	GLN
1	C	197	GLN
1	C	237	GLN
1	C	254	ASN
1	C	274	ASN
1	C	505	HIS
1	C	577	GLN
1	C	737	GLN
1	C	865	GLN
1	C	1000	GLN
1	C	1001	ASN
2	D	52	HIS
2	D	85	HIS
2	D	89	HIS
2	D	92	HIS
2	D	112	ASN
2	D	118	HIS
2	E	41	ASN
2	E	92	HIS
2	E	118	HIS
2	E	125	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

45 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	D10	C	1117	-	9,9,9	0.50	0	8,8,8	0.54	0
7	HEX	B	1113	-	5,5,5	0.62	0	4,4,4	0.25	0
6	D12	A	1107	-	11,11,11	0.53	0	10,10,10	0.39	0
6	D12	C	1108	-	11,11,11	0.68	0	10,10,10	0.23	0
3	LMT	B	1109	-	36,36,36	0.41	0	47,47,47	0.67	0
5	GOL	B	1115	-	5,5,5	0.08	0	5,5,5	0.22	0
5	GOL	A	1108	-	5,5,5	0.10	0	5,5,5	0.30	0
5	GOL	B	1104	-	5,5,5	0.08	0	5,5,5	0.29	0
9	OCT	C	1106	-	7,7,7	0.36	0	6,6,6	0.82	0
4	D10	B	1103	-	9,9,9	0.72	0	8,8,8	0.39	0
10	DD9	C	1111	-	8,8,8	0.48	0	7,7,7	0.56	0
5	GOL	D	201	-	5,5,5	0.12	0	5,5,5	0.39	0
3	LMT	A	1103	-	36,36,36	0.28	0	47,47,47	0.59	0
3	LMT	A	1102	-	36,36,36	0.26	0	47,47,47	0.49	0
5	GOL	D	202	-	5,5,5	0.08	0	5,5,5	0.23	0
9	OCT	C	1104	-	7,7,7	0.73	0	6,6,6	0.70	0
4	D10	A	1104	-	9,9,9	0.58	0	8,8,8	0.43	0
4	D10	C	1116	-	9,9,9	0.60	0	8,8,8	0.51	0
5	GOL	B	1102	-	5,5,5	0.14	0	5,5,5	0.31	0
5	GOL	B	1106	-	5,5,5	0.08	0	5,5,5	0.18	0
3	LMT	A	1101	-	36,36,36	0.33	0	47,47,47	0.53	0
7	HEX	C	1112	-	5,5,5	0.49	0	4,4,4	0.26	0
5	GOL	B	1101	-	5,5,5	0.11	0	5,5,5	0.28	0
3	LMT	A	1109	-	36,36,36	0.25	0	47,47,47	0.72	1 (2%)
5	GOL	C	1114	-	5,5,5	0.16	0	5,5,5	0.53	0
5	GOL	C	1113	-	5,5,5	0.10	0	5,5,5	0.27	0
5	GOL	D	203	-	5,5,5	0.12	0	5,5,5	0.39	0
8	C14	C	1101	-	13,13,13	0.51	0	12,12,12	0.51	0
5	GOL	B	1107	-	5,5,5	0.19	0	5,5,5	0.61	0
4	D10	C	1109	-	9,9,9	0.59	0	8,8,8	0.30	0
3	LMT	C	1103	-	36,36,36	0.42	0	47,47,47	0.53	0
4	D10	C	1107	-	9,9,9	0.55	0	8,8,8	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	D10	B	1105	-	9,9,9	0.57	0	8,8,8	0.18	0
7	HEX	C	1110	-	5,5,5	0.50	0	4,4,4	0.34	0
4	D10	B	1110	-	9,9,9	0.48	0	8,8,8	0.57	0
5	GOL	A	1106	-	5,5,5	0.13	0	5,5,5	0.26	0
5	GOL	B	1108	-	5,5,5	0.09	0	5,5,5	0.32	0
5	GOL	C	1102	-	5,5,5	0.18	0	5,5,5	0.69	0
6	D12	C	1105	-	11,11,11	0.59	0	10,10,10	0.52	0
11	SO4	C	1115	-	4,4,4	0.36	0	6,6,6	0.07	0
5	GOL	B	1116	-	5,5,5	0.15	0	5,5,5	0.35	0
3	LMT	A	1105	-	36,36,36	0.43	0	47,47,47	0.80	1 (2%)
3	LMT	B	1114	-	36,36,36	0.26	0	47,47,47	0.79	2 (4%)
4	D10	B	1112	-	9,9,9	0.61	0	8,8,8	0.42	0
6	D12	B	1111	-	11,11,11	0.69	0	10,10,10	0.23	0

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	D10	C	1117	-	-	3/7/7/7	-
7	HEX	B	1113	-	-	0/3/3/3	-
6	D12	A	1107	-	-	5/9/9/9	-
6	D12	C	1108	-	-	2/9/9/9	-
3	LMT	B	1109	-	-	10/21/61/61	0/2/2/2
5	GOL	B	1115	-	-	2/4/4/4	-
5	GOL	A	1108	-	-	2/4/4/4	-
5	GOL	B	1104	-	-	1/4/4/4	-
9	OCT	C	1106	-	-	1/5/5/5	-
4	D10	B	1103	-	-	2/7/7/7	-
10	DD9	C	1111	-	-	3/6/6/6	-
5	GOL	D	201	-	-	0/4/4/4	-
3	LMT	A	1103	-	-	11/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	6/21/61/61	0/2/2/2
5	GOL	D	202	-	-	0/4/4/4	-
9	OCT	C	1104	-	-	0/5/5/5	-
4	D10	A	1104	-	-	2/7/7/7	-
4	D10	C	1116	-	-	0/7/7/7	-
5	GOL	B	1102	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	1106	-	-	2/4/4/4	-
3	LMT	A	1101	-	-	6/21/61/61	0/2/2/2
7	HEX	C	1112	-	-	3/3/3/3	-
5	GOL	B	1101	-	-	2/4/4/4	-
3	LMT	A	1109	-	-	11/21/61/61	0/2/2/2
5	GOL	C	1114	-	-	4/4/4/4	-
5	GOL	C	1113	-	-	2/4/4/4	-
5	GOL	D	203	-	-	0/4/4/4	-
8	C14	C	1101	-	-	3/11/11/11	-
5	GOL	B	1107	-	-	2/4/4/4	-
4	D10	C	1109	-	-	2/7/7/7	-
3	LMT	C	1103	-	-	8/21/61/61	0/2/2/2
4	D10	C	1107	-	-	0/7/7/7	-
4	D10	B	1105	-	-	5/7/7/7	-
7	HEX	C	1110	-	-	0/3/3/3	-
4	D10	B	1110	-	-	0/7/7/7	-
5	GOL	A	1106	-	-	2/4/4/4	-
5	GOL	B	1108	-	-	2/4/4/4	-
5	GOL	C	1102	-	-	0/4/4/4	-
6	D12	C	1105	-	-	1/9/9/9	-
5	GOL	B	1116	-	-	0/4/4/4	-
3	LMT	A	1105	-	-	9/21/61/61	0/2/2/2
3	LMT	B	1114	-	-	13/21/61/61	0/2/2/2
4	D10	B	1112	-	-	2/7/7/7	-
6	D12	B	1111	-	-	0/9/9/9	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1114	LMT	C1B-O1B-C4'	2.68	124.59	117.96
3	B	1114	LMT	C1'-O5'-C5'	2.38	118.37	113.69
3	A	1109	LMT	O1'-C1'-C2'	2.24	111.80	108.30
3	A	1105	LMT	C2'-C3'-C4'	2.10	114.48	109.68

There are no chirality outliers.

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1103	LMT	C2-C1-O1'-C1'
3	A	1105	LMT	C2B-C1B-O1B-C4'
3	A	1105	LMT	O5'-C1'-O1'-C1
3	A	1105	LMT	C2-C1-O1'-C1'
3	A	1109	LMT	C2'-C1'-O1'-C1
3	B	1114	LMT	C2'-C1'-O1'-C1
3	C	1103	LMT	C2-C1-O1'-C1'
5	A	1108	GOL	O1-C1-C2-C3
5	B	1102	GOL	O1-C1-C2-C3
5	B	1106	GOL	O1-C1-C2-C3
5	B	1107	GOL	O1-C1-C2-O2
5	B	1107	GOL	O1-C1-C2-C3
5	B	1108	GOL	O1-C1-C2-C3
5	B	1115	GOL	C1-C2-C3-O3
3	A	1105	LMT	O5B-C1B-O1B-C4'
3	B	1114	LMT	O5B-C1B-O1B-C4'
3	B	1114	LMT	C5'-C4'-O1B-C1B
3	B	1109	LMT	O5B-C5B-C6B-O6B
3	B	1109	LMT	O5'-C5'-C6'-O6'
3	B	1109	LMT	C4B-C5B-C6B-O6B
3	B	1109	LMT	C4'-C5'-C6'-O6'
3	B	1114	LMT	C4'-C5'-C6'-O6'
3	C	1103	LMT	O1'-C1-C2-C3
3	A	1103	LMT	O5'-C1'-O1'-C1
3	B	1114	LMT	O5'-C1'-O1'-C1
3	A	1103	LMT	C4'-C5'-C6'-O6'
3	A	1105	LMT	C3'-C4'-O1B-C1B
3	B	1109	LMT	C7-C8-C9-C10
3	A	1101	LMT	C11-C10-C9-C8
3	A	1109	LMT	C4-C5-C6-C7
3	A	1109	LMT	O1'-C1-C2-C3
6	A	1107	D12	C2-C3-C4-C5
3	A	1103	LMT	C2'-C1'-O1'-C1
3	B	1114	LMT	C2-C3-C4-C5
4	B	1105	D10	C4-C5-C6-C7
3	A	1109	LMT	O5'-C5'-C6'-O6'
3	B	1114	LMT	C3-C4-C5-C6
7	C	1112	HEX	C2-C3-C4-C5
5	A	1106	GOL	O1-C1-C2-C3
5	B	1101	GOL	O1-C1-C2-C3
5	C	1113	GOL	O1-C1-C2-C3
5	C	1114	GOL	O1-C1-C2-C3
5	C	1114	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	1103	LMT	C5-C6-C7-C8
3	A	1105	LMT	C5'-C4'-O1B-C1B
3	B	1109	LMT	C2-C1-O1'-C1'
3	B	1109	LMT	O1'-C1-C2-C3
4	B	1105	D10	C6-C7-C8-C9
5	A	1106	GOL	O1-C1-C2-O2
5	B	1101	GOL	O1-C1-C2-O2
5	B	1102	GOL	O1-C1-C2-O2
5	B	1106	GOL	O1-C1-C2-O2
5	B	1108	GOL	O1-C1-C2-O2
5	B	1115	GOL	O2-C2-C3-O3
3	A	1109	LMT	C11-C10-C9-C8
4	B	1112	D10	C3-C4-C5-C6
3	A	1102	LMT	O5B-C5B-C6B-O6B
3	B	1109	LMT	C4-C5-C6-C7
3	B	1114	LMT	O5'-C5'-C6'-O6'
3	A	1109	LMT	O5'-C1'-O1'-C1
10	C	1111	DD9	C2-C3-C4-C5
3	C	1103	LMT	C1-C2-C3-C4
3	B	1114	LMT	O5B-C5B-C6B-O6B
3	A	1105	LMT	C1-C2-C3-C4
4	A	1104	D10	C2-C3-C4-C5
7	C	1112	HEX	C3-C4-C5-C6
3	A	1102	LMT	C2-C3-C4-C5
4	B	1105	D10	C5-C6-C7-C8
5	A	1108	GOL	O1-C1-C2-O2
5	C	1114	GOL	O2-C2-C3-O3
3	A	1102	LMT	C9-C10-C11-C12
3	A	1101	LMT	C2'-C1'-O1'-C1
6	A	1107	D12	C1-C2-C3-C4
6	A	1107	D12	C4-C5-C6-C7
10	C	1111	DD9	C3-C4-C5-C6
4	C	1117	D10	C3-C4-C5-C6
3	C	1103	LMT	C5-C6-C7-C8
3	A	1103	LMT	O5'-C5'-C6'-O6'
3	B	1114	LMT	C2-C1-O1'-C1'
3	A	1103	LMT	O5B-C5B-C6B-O6B
3	A	1109	LMT	C9-C10-C11-C12
8	C	1101	C14	C01-C02-C03-C04
9	C	1106	OCT	C2-C3-C4-C5
3	A	1103	LMT	C7-C8-C9-C10
6	A	1107	D12	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	C	1103	LMT	C9-C10-C11-C12
3	A	1101	LMT	C1-C2-C3-C4
3	A	1105	LMT	C11-C10-C9-C8
6	C	1108	D12	C11-C10-C9-C8
4	C	1109	D10	C5-C6-C7-C8
3	A	1109	LMT	C2-C3-C4-C5
3	A	1101	LMT	O5'-C1'-O1'-C1
5	B	1104	GOL	O2-C2-C3-O3
5	C	1113	GOL	O1-C1-C2-O2
3	A	1103	LMT	O1'-C1-C2-C3
3	A	1103	LMT	C4-C5-C6-C7
4	B	1103	D10	C2-C3-C4-C5
3	C	1103	LMT	C6-C7-C8-C9
3	A	1101	LMT	C7-C8-C9-C10
4	B	1105	D10	C2-C3-C4-C5
4	B	1112	D10	C4-C5-C6-C7
3	C	1103	LMT	C4-C5-C6-C7
4	B	1105	D10	C7-C8-C9-C10
6	C	1108	D12	C9-C10-C11-C12
3	B	1109	LMT	C5-C6-C7-C8
4	C	1117	D10	C7-C8-C9-C10
3	B	1114	LMT	C1-C2-C3-C4
3	A	1102	LMT	C6-C7-C8-C9
3	A	1103	LMT	C1-C2-C3-C4
3	A	1109	LMT	C7-C8-C9-C10
3	B	1114	LMT	C11-C10-C9-C8
3	A	1105	LMT	C4-C5-C6-C7
6	C	1105	D12	C7-C8-C9-C10
4	C	1117	D10	C4-C5-C6-C7
4	B	1103	D10	C1-C2-C3-C4
8	C	1101	C14	C10-C11-C12-C13
3	B	1109	LMT	C1-C2-C3-C4
7	C	1112	HEX	C1-C2-C3-C4
4	C	1109	D10	C4-C5-C6-C7
3	A	1102	LMT	C7-C8-C9-C10
4	A	1104	D10	C1-C2-C3-C4
3	B	1114	LMT	C6-C7-C8-C9
3	A	1109	LMT	C4'-C5'-C6'-O6'
3	A	1109	LMT	C1-C2-C3-C4
6	A	1107	D12	C7-C8-C9-C10
3	A	1102	LMT	O5'-C5'-C6'-O6'
5	C	1114	GOL	O1-C1-C2-O2

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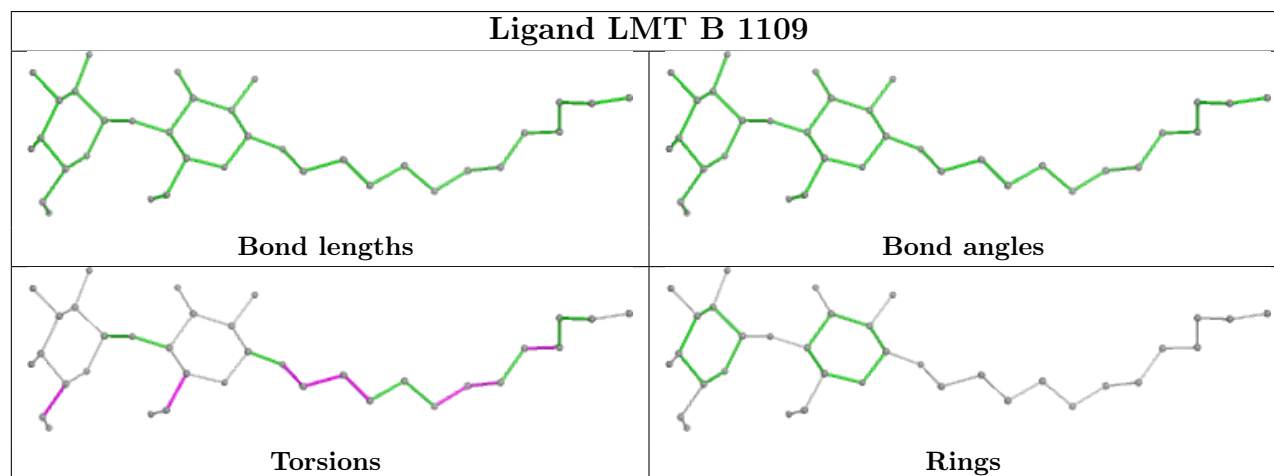
Mol	Chain	Res	Type	Atoms
3	C	1103	LMT	C7-C8-C9-C10
8	C	1101	C14	C05-C06-C07-C08
3	A	1101	LMT	C6-C7-C8-C9
10	C	1111	DD9	C5-C6-C7-C8

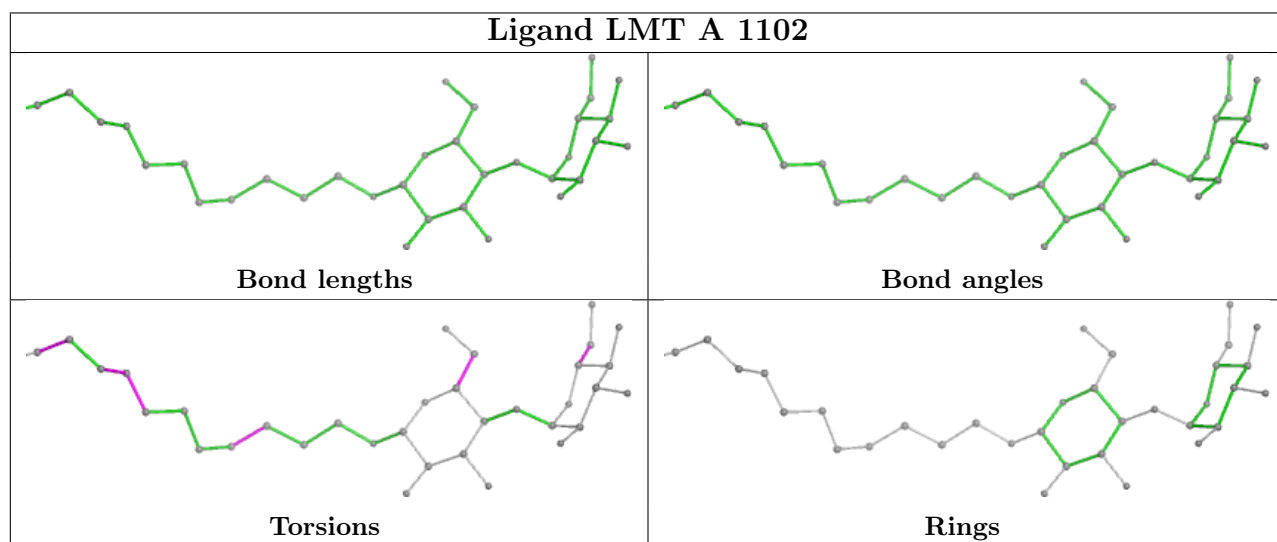
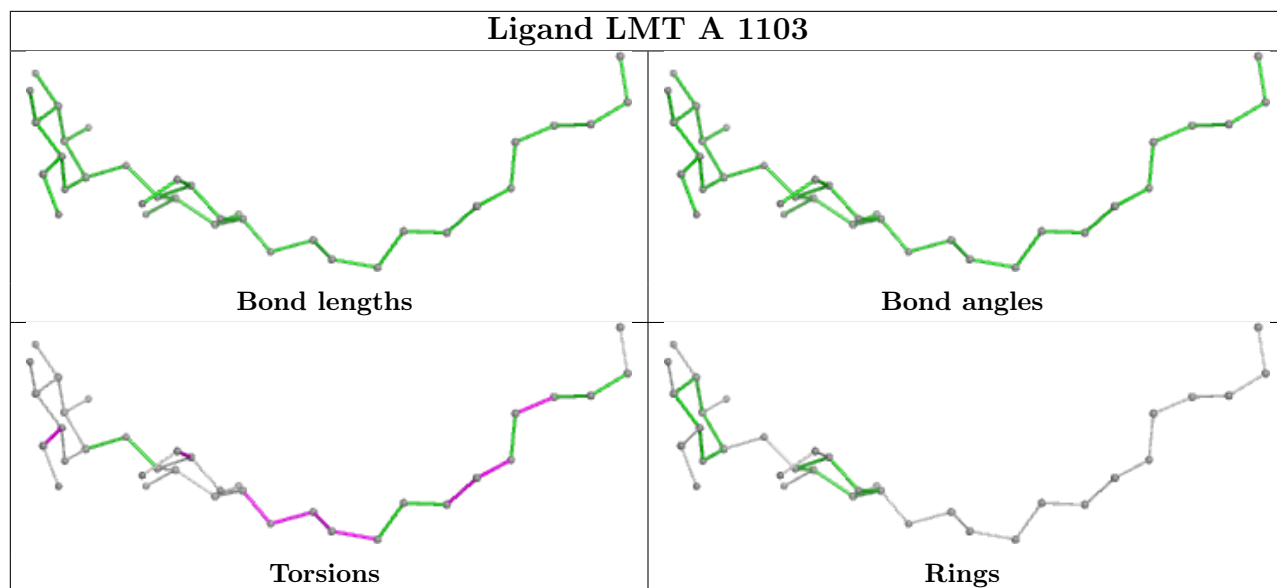
There are no ring outliers.

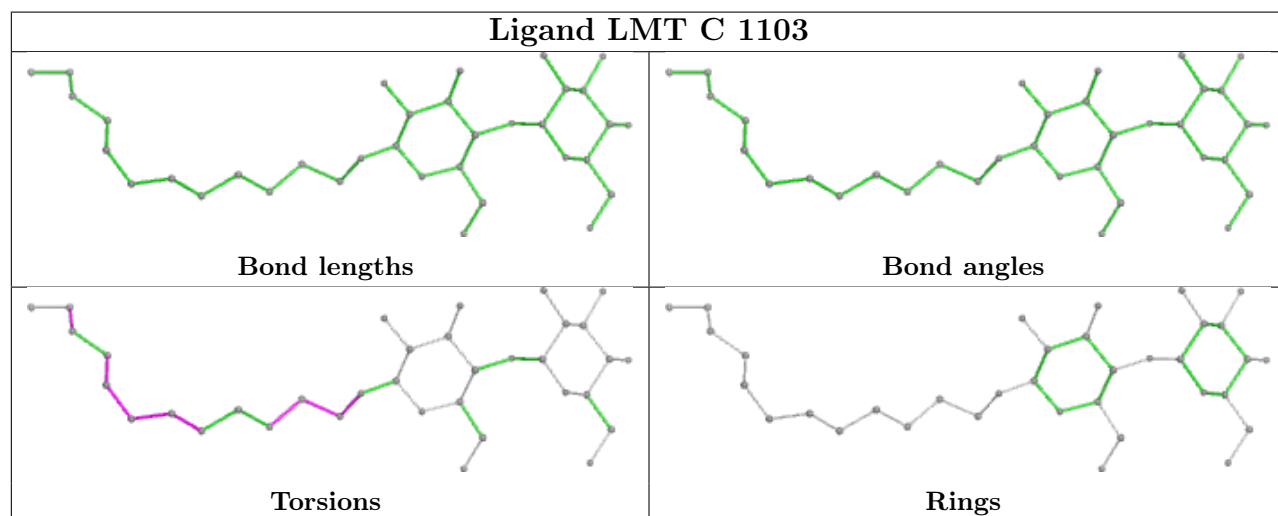
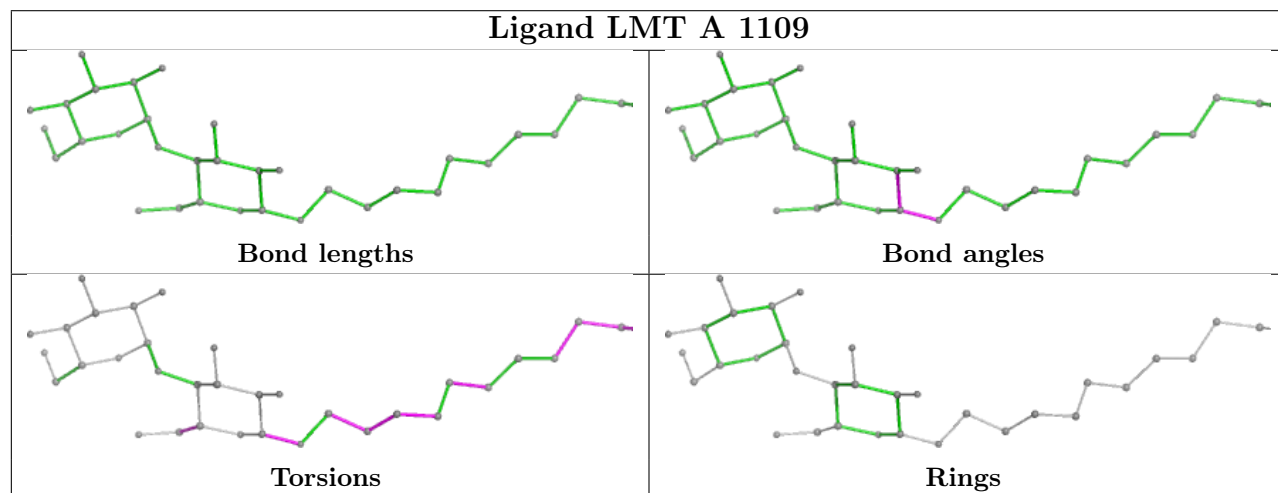
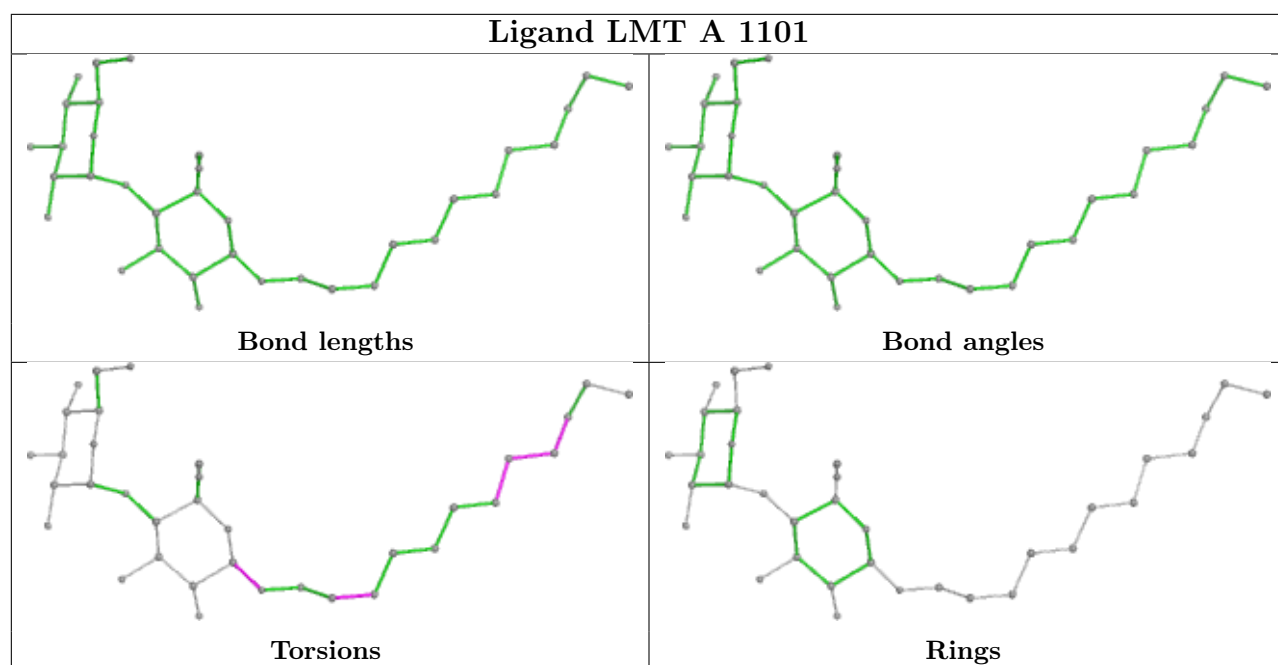
7 monomers are involved in 15 short contacts:

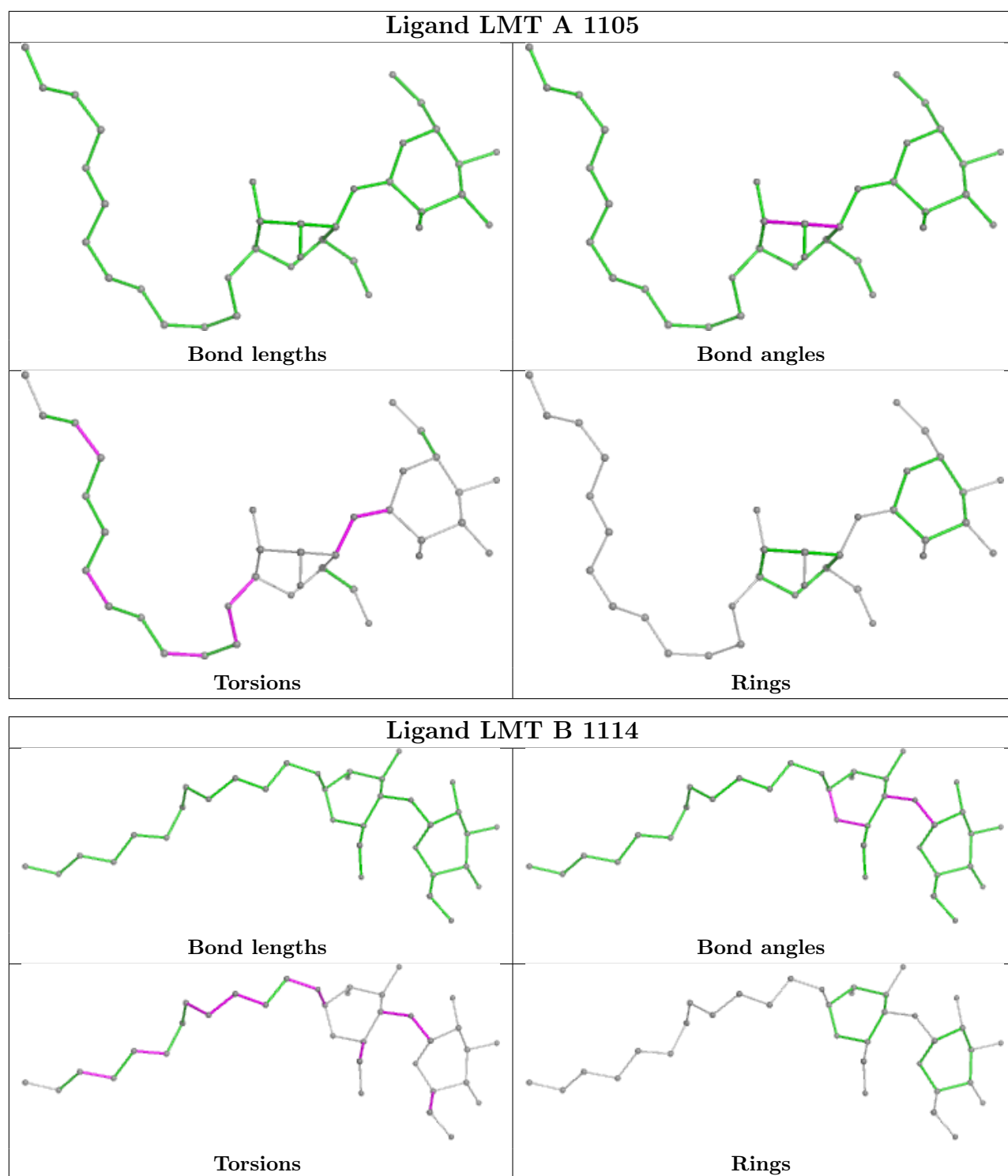
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1103	LMT	1	0
3	A	1102	LMT	4	0
3	A	1109	LMT	2	0
5	C	1114	GOL	2	0
5	A	1106	GOL	1	0
3	A	1105	LMT	2	0
3	B	1114	LMT	3	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.03	52 (4%)	35	30	15, 41, 104, 177	0
1	B	1033/1057 (97%)	-0.12	41 (3%)	43	37	13, 43, 79, 124	1 (0%)
1	C	1033/1057 (97%)	-0.31	20 (1%)	66	61	13, 38, 75, 123	0
2	D	155/169 (91%)	-0.43	2 (1%)	74	70	26, 38, 64, 90	0
2	E	153/169 (90%)	-0.15	2 (1%)	74	70	26, 46, 86, 106	0
All	All	3418/3509 (97%)	-0.15	117 (3%)	48	42	13, 41, 88, 177	1 (0%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	618	ALA	5.7
1	A	1040	ILE	5.4
1	B	868	LEU	4.8
1	A	659	LYS	4.3
1	A	539	GLY	4.3
1	A	538	THR	4.3
1	A	887	CYS	4.0
2	E	14	LEU	4.0
1	A	1036	LYS	3.9
1	C	811	TYR	3.9
1	B	575	MET	3.8
1	A	540	ARG	3.8
1	B	563	PHE	3.8
1	A	493	CYS	3.7
1	A	952	LEU	3.7
1	B	133	SER	3.7
1	B	662	MET	3.6
1	A	869	SER	3.5
1	C	670	ALA	3.5
1	A	1037	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	666	PHE	3.5
1	B	869	SER	3.4
1	B	615	PHE	3.4
1	A	362	PHE	3.4
1	B	676	THR	3.4
1	C	1033	PHE	3.3
1	A	1044	HIS	3.2
1	C	493	CYS	3.2
1	B	867	ARG	3.1
1	B	887	CYS	3.1
1	A	840	ALA	3.1
1	A	562	CYS	3.1
1	A	868	LEU	3.1
1	A	510	LYS	3.0
1	A	542	LEU	2.9
1	A	1038	GLU	2.9
1	A	1035	ARG	2.9
1	A	535	LEU	2.9
1	B	134	SER	2.9
1	B	675	GLY	2.9
1	B	871	ASN	2.9
1	A	532	GLY	2.8
1	A	866	GLU	2.8
1	B	562	CYS	2.8
1	C	620	ARG	2.8
2	D	166	GLN	2.8
1	C	674	LEU	2.8
1	A	1034	SER	2.7
1	B	995	ALA	2.7
1	B	649	MET	2.7
1	A	1043	SER	2.7
1	B	677	ALA	2.7
1	C	363	ARG	2.7
1	C	362	PHE	2.7
1	A	857	TYR	2.6
1	A	958	LYS	2.6
1	C	617	PHE	2.6
1	A	870	GLY	2.6
1	B	633	ASP	2.6
1	B	993	THR	2.6
1	A	1039	ASP	2.6
1	A	855	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	510	LYS	2.6
1	A	965	LEU	2.6
2	D	12	SER	2.5
1	B	493	CYS	2.5
1	A	955	LYS	2.5
1	C	675	GLY	2.5
1	B	646	ALA	2.5
1	A	1016	VAL	2.5
2	E	166	GLN	2.5
1	A	691	GLY	2.4
1	B	635	ALA	2.4
1	B	645	GLU	2.4
1	C	508	GLY	2.4
1	A	544	LEU	2.4
1	B	331	PRO	2.4
1	B	1033	PHE	2.4
1	A	463	THR	2.3
1	B	831	ALA	2.3
1	C	619	GLY	2.3
1	B	510	LYS	2.3
1	B	833	PRO	2.3
1	A	1042	HIS	2.3
1	B	344	LEU	2.3
1	B	565	PRO	2.3
1	A	950	LYS	2.3
1	C	509	LYS	2.3
1	A	706	ALA	2.3
1	A	536	ARG	2.2
1	A	456	MET	2.2
1	B	664	PHE	2.2
1	A	618	ALA	2.2
1	B	653	ARG	2.2
1	B	29	LYS	2.2
1	A	877	TYR	2.2
1	C	954	ASP	2.2
1	A	537	SER	2.1
1	A	1020	PHE	2.1
1	B	617	PHE	2.1
1	C	897	ILE	2.1
1	B	620	ARG	2.1
1	B	498	LYS	2.1
1	A	927	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	960	LEU	2.1
1	B	564	LEU	2.1
1	A	959	GLY	2.1
1	A	1041	GLU	2.1
1	B	678	THR	2.1
1	A	547	ILE	2.0
1	C	671	ILE	2.0
1	A	1027	VAL	2.0
1	C	512	PHE	2.0
1	B	334	LYS	2.0
1	A	526	HIS	2.0
1	C	496	MET	2.0
1	B	255	GLN	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(\AA^2)	Q<0.9
4	D10	C	1117	10/10	0.67	0.41	53,72,96,104	0
6	D12	A	1107	12/12	0.67	0.33	44,57,82,93	0
5	GOL	A	1108	6/6	0.68	0.17	73,93,100,108	0
6	D12	C	1105	12/12	0.68	0.29	42,63,86,88	0
4	D10	B	1103	10/10	0.70	0.30	40,55,67,71	0
9	OCT	C	1104	8/8	0.70	0.24	41,53,64,70	0
4	D10	B	1112	10/10	0.71	0.35	41,64,97,100	0
6	D12	B	1111	12/12	0.71	0.27	43,59,74,75	0
4	D10	C	1107	10/10	0.72	0.34	53,76,87,98	0
4	D10	C	1116	10/10	0.72	0.39	31,76,92,97	0

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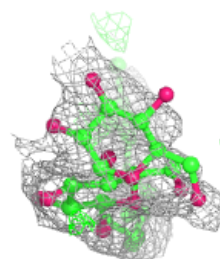
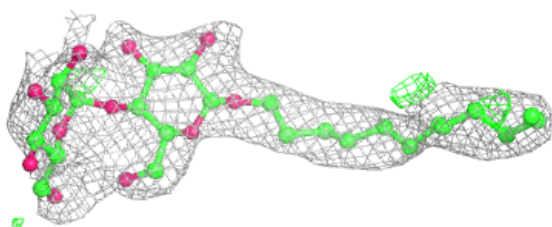
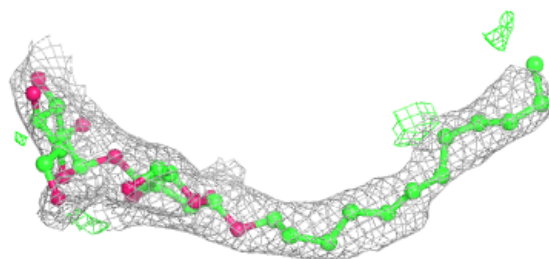
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	HEX	B	1113	6/6	0.75	0.24	46,51,57,60	0
4	D10	B	1105	10/10	0.78	0.33	41,69,78,98	0
6	D12	C	1108	12/12	0.78	0.21	37,47,65,73	0
8	C14	C	1101	14/14	0.80	0.29	62,75,90,96	0
4	D10	C	1109	10/10	0.80	0.28	52,63,98,107	0
5	GOL	B	1104	6/6	0.82	0.15	57,70,74,76	0
7	HEX	C	1112	6/6	0.83	0.29	47,58,71,76	0
4	D10	A	1104	10/10	0.83	0.26	33,56,93,99	0
7	HEX	C	1110	6/6	0.83	0.26	32,41,50,55	0
5	GOL	B	1101	6/6	0.84	0.15	40,47,61,65	0
3	LMT	A	1103	35/35	0.86	0.14	49,76,113,136	0
3	LMT	B	1109	35/35	0.86	0.17	46,75,105,109	0
4	D10	B	1110	10/10	0.86	0.17	45,55,65,70	0
3	LMT	B	1114	35/35	0.86	0.20	59,120,173,188	0
3	LMT	A	1102	35/35	0.86	0.22	69,112,167,197	0
9	OCT	C	1106	8/8	0.86	0.27	27,39,58,59	0
10	DD9	C	1111	9/9	0.86	0.25	26,59,78,85	0
5	GOL	B	1102	6/6	0.88	0.24	38,65,91,115	0
3	LMT	A	1105	35/35	0.89	0.17	36,85,136,148	0
5	GOL	C	1102	6/6	0.89	0.19	45,53,72,98	0
5	GOL	C	1113	6/6	0.89	0.18	61,67,68,70	0
5	GOL	D	202	6/6	0.89	0.14	31,47,68,74	0
3	LMT	A	1109	35/35	0.89	0.15	47,87,138,155	0
5	GOL	B	1108	6/6	0.91	0.14	39,53,69,73	0
5	GOL	D	203	6/6	0.92	0.14	43,50,57,84	0
3	LMT	C	1103	35/35	0.92	0.15	33,58,127,128	0
5	GOL	C	1114	6/6	0.92	0.10	14,18,20,22	0
3	LMT	A	1101	35/35	0.92	0.11	30,50,119,133	0
11	SO4	C	1115	5/5	0.92	0.19	56,59,73,135	0
5	GOL	B	1116	6/6	0.93	0.15	43,51,64,112	0
5	GOL	D	201	6/6	0.94	0.11	45,56,59,78	0
5	GOL	B	1107	6/6	0.94	0.09	22,29,35,37	0
5	GOL	B	1115	6/6	0.94	0.15	44,56,70,81	0
5	GOL	A	1106	6/6	0.96	0.10	19,34,47,56	0
5	GOL	B	1106	6/6	0.96	0.14	29,43,53,110	0

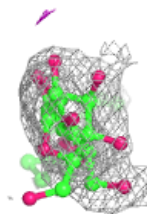
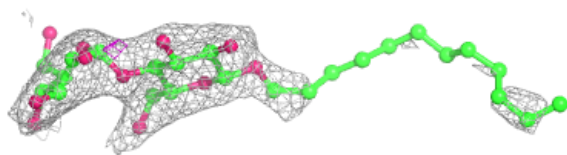
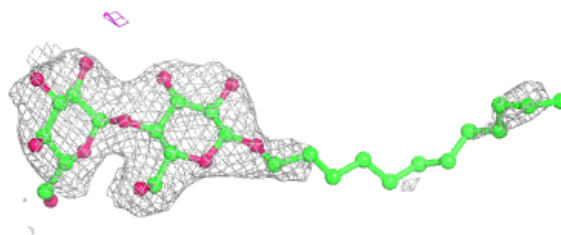
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT A 1103:

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

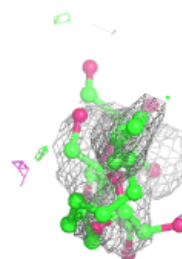
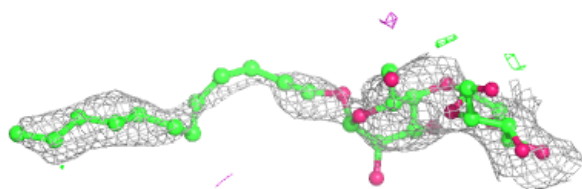
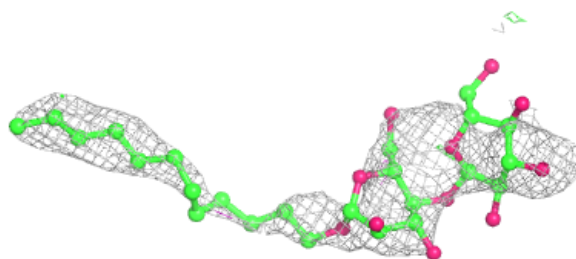
**Electron density around LMT B 1109:**

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

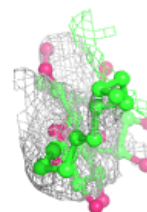
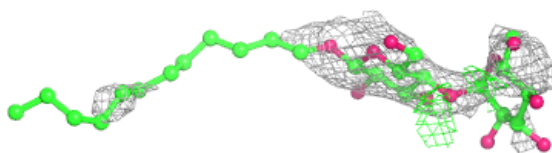
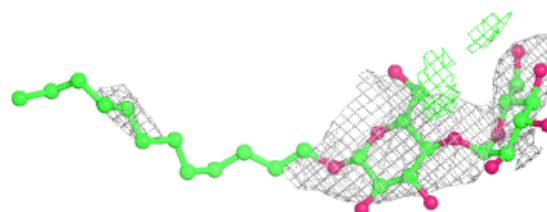


Electron density around LMT B 1114:

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

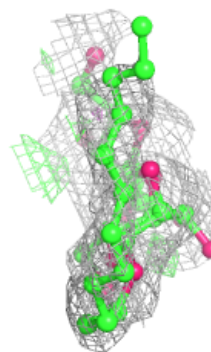
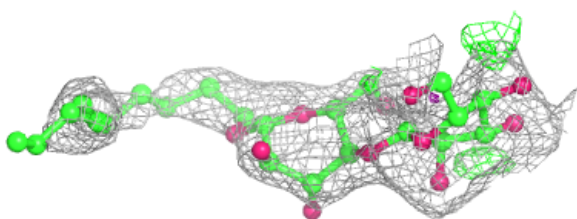
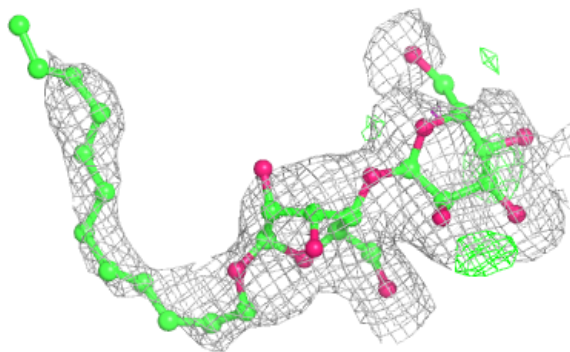
**Electron density around LMT A 1102:**

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

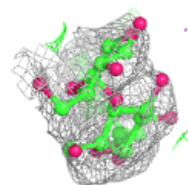
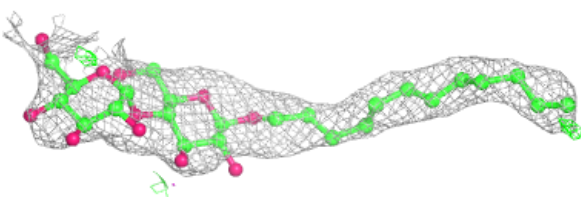
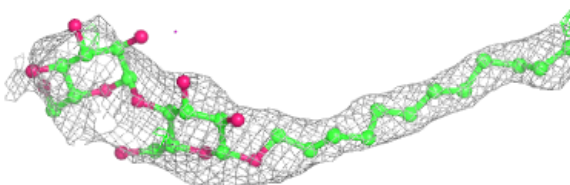


Electron density around LMT A 1105:

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

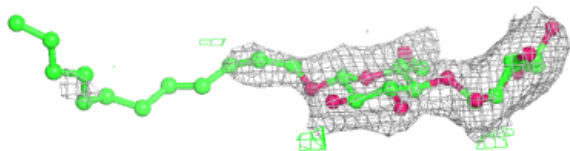
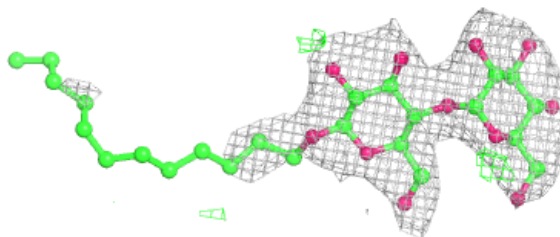
**Electron density around LMT A 1109:**

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

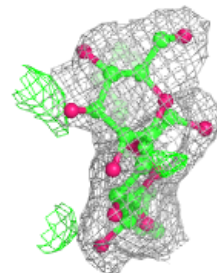
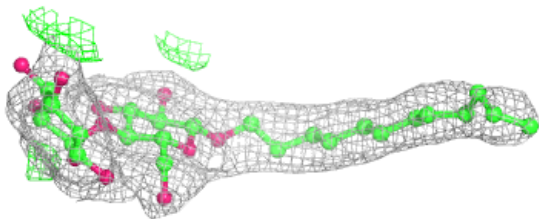
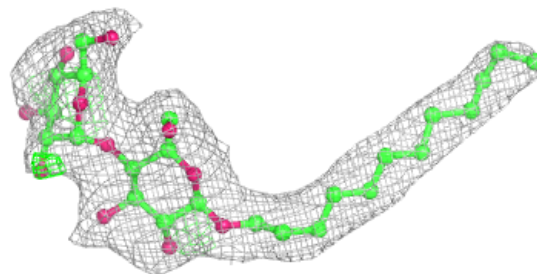


Electron density around LMT C 1103:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.