



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 06:02 PM UTC

PDB ID : 4U8V / pdb_00004u8v
Title : Coupling of remote alternating-access transport mechanisms for protons and substrates in the multidrug efflux pump AcrB
Authors : Pos, K.M.
Deposited on : 2014-08-04
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

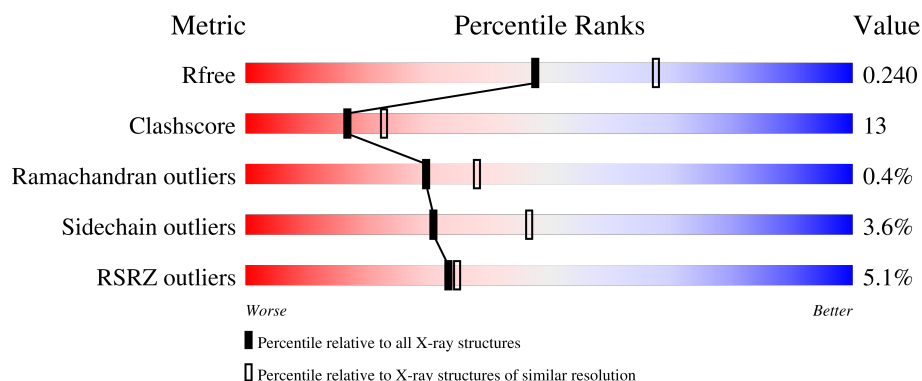
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	10% 69% 27% ..
1	B	1057	3% 76% 20% ..
1	C	1057	2% 78% 18% ..
2	D	169	4% 78% 14% 8%
2	E	169	4% 72% 18% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27546 atoms, of which 27 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1044	Total	C	N	O	S	0	0	0
			7943	5106	1316	1477	44			
1	B	1033	Total	C	N	O	S	0	0	0
			7848	5052	1296	1456	44			
1	C	1033	Total	C	N	O	S	0	0	0
			7849	5052	1296	1457	44			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	407	ASN	ASP	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	407	ASN	ASP	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	407	ASN	ASP	engineered mutation	UNP P31224
C	1050	LEU	-	expression tag	UNP P31224
C	1051	GLU	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224

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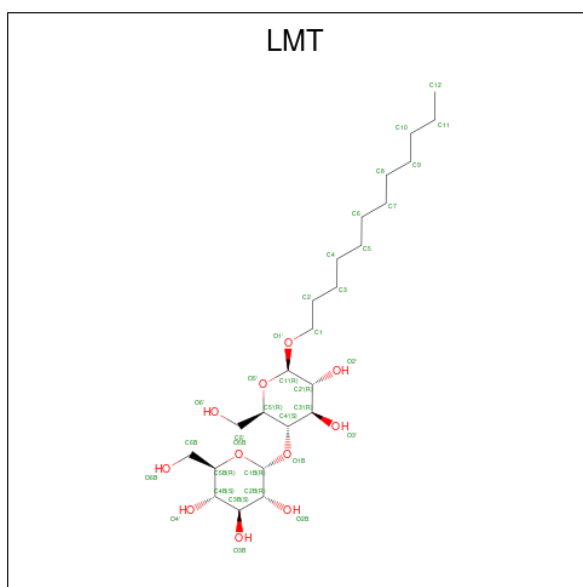
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPin.

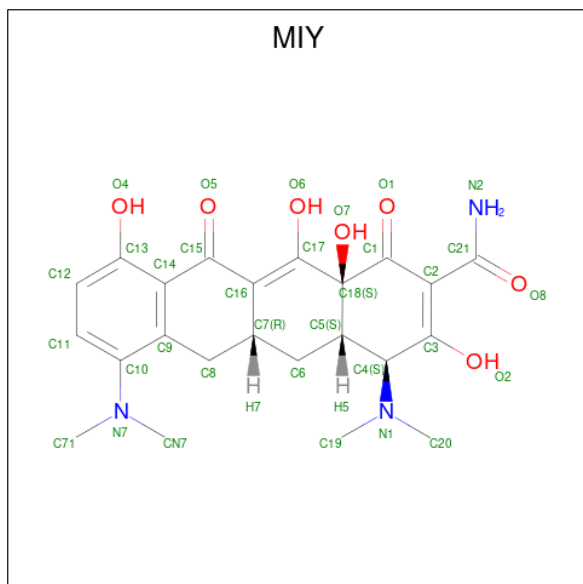
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	156	Total 1177	C 741	N 206	O 229	S 1	0	0	0
2	E	152	Total 1151	C 726	N 202	O 222	S 1	0	0	0

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



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

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



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

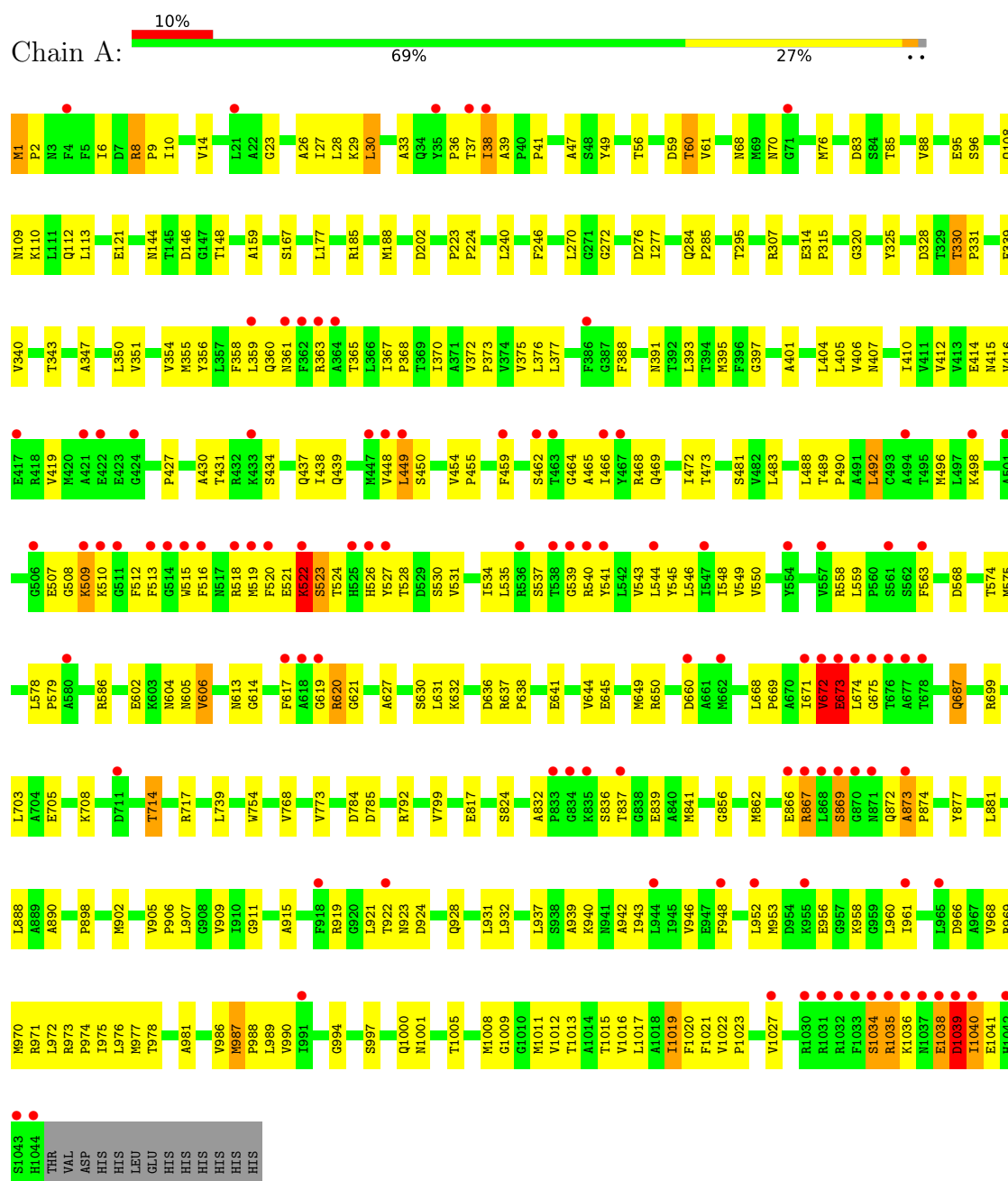
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	391	Total	O		
			391	391	0	0
5	B	376	Total	O		
			376	376	0	0
5	C	469	Total	O		
			469	469	0	0
5	D	61	Total	O		
			61	61	0	0
5	E	46	Total	O		
			46	46	0	0

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: Multidrug efflux pump subunit AcrB



[illegible]

Chain C:

78% 2% 18%

M1 M2 M3 M4 M5 M6 M7 M8 M9 M10 M11 M12 M13 M14 M15 M16 M17 M18 M19 M20

E121 E122 E123 E124 E125 E126 E127 E128 E129 E130 E131 E132 E133 E134 E135 E136 E137 E138 E139 E140

P326 P327 P328 P329 P330 P331 P332 P333 P334 P335 P336 P337 P338 P339 P340 P341 P342 P343 P344 P345

P346 P347 P348 P349 P350 P351 P352 P353 P354 P355 P356 P357 P358 P359 P360 P361 P362 P363 P364 P365

P366 P367 P368 P369 P370 P371 P372 P373 P374 P375 P376 P377 P378 P379 P380 P381 P382 P383 P384 P385

P386 P387 P388 P389 P390 P391 P392 P393 P394 P395 P396 P397 P398 P399 P400 P401 P402 P403 P404 P405

P406 P407 P408 P409 P410 P411 P412 P413 P414 P415 P416 P417 P418 P419 P420 P421 P422 P423 P424 P425

P426 P427 P428 P429 P430 P431 P432 P433 P434 P435 P436 P437 P438 P439 P440 P441 P442 P443 P444 P445

P446 P447 P448 P449 P450 P451 P452 P453 P454 P455 P456 P457 P458 P459 P460 P461 P462 P463 P464 P465

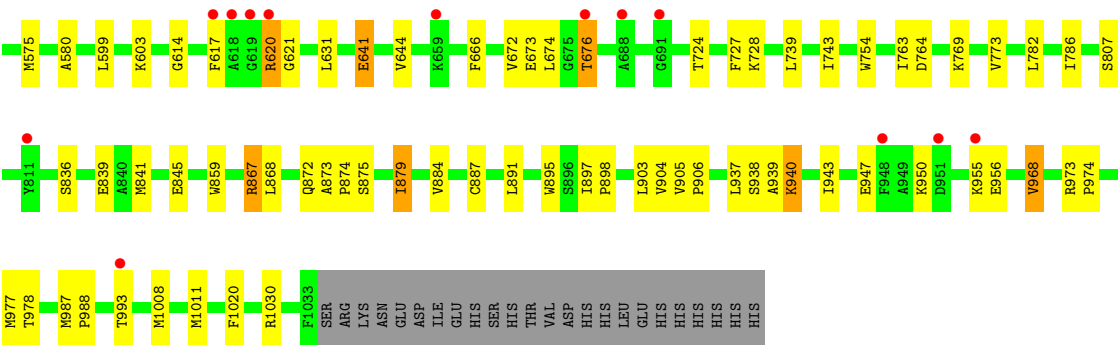
P466 P467 P468 P469 P470 P471 P472 P473 P474 P475 P476 P477 P478 P479 P480 P481 P482 P483 P484 P485

P486 P487 P488 P489 P490 P491 P492 P493 P494 P495 P496 P497 P498 P499 P500 P501 P502 P503 P504 P505

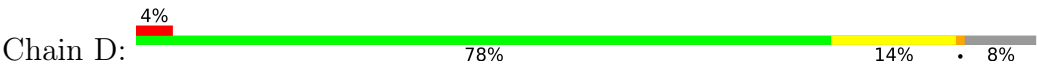
P506 P507 P508 P509 P510 P511 P512 P513 P514 P515 P516 P517 P518 P519 P520 P521 P522 P523 P524 P525

P526 P527 P528 P529 P530 P531 P532 P533 P534 P535 P536 P537 P538 P539 P540 P541 P542 P543 P544 P545

P546 P547 P548 P549



• 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	145.59Å 161.59Å 245.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 2.30 48.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.93-2.30) 99.9 (48.93-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.191 , 0.238 0.195 , 0.240	Depositor DCC
R_{free} test set	12835 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27546	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/8095	0.84	8/10991 (0.1%)
1	B	0.50	0/7998	0.83	4/10861 (0.0%)
1	C	0.52	0/7999	0.84	4/10863 (0.0%)
2	D	0.44	0/1196	0.73	0/1626
2	E	0.40	0/1170	0.72	0/1591
All	All	0.49	0/26458	0.83	16/35932 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	524	THR	N-CA-C	-8.85	101.55	111.82
1	B	426	PRO	O-C-N	6.45	124.18	121.15
1	C	325	TYR	CA-C-N	6.09	125.72	119.56
1	C	325	TYR	C-N-CA	6.09	125.72	119.56
1	B	637	ARG	CA-C-N	5.64	125.92	119.83

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	521	GLU	Peptide
1	A	522	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7943	0	8086	282	0
1	B	7848	0	8003	198	0
1	C	7849	0	8003	167	0
2	D	1177	0	1159	16	0
2	E	1151	0	1136	24	0
3	A	70	0	92	8	0
3	B	70	0	92	8	0
3	C	35	0	46	3	0
4	B	33	27	25	2	0
5	A	391	0	0	12	0
5	B	376	0	0	9	0
5	C	469	0	0	13	0
5	D	61	0	0	0	0
5	E	46	0	0	3	0
All	All	27519	27	26642	674	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 13.

The worst 5 of 674 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:GLU:HG3	1:B:977:MET:HE1	1.36	1.06
1:B:363:ARG:HD2	1:B:498:LYS:HE2	1.39	1.03
1:A:528:THR:HG21	1:A:969:ARG:HG3	1.37	1.03
1:A:38:ILE:HG12	1:A:671:ILE:HD13	1.36	1.02
2:E:34:MET:HE2	2:E:40:VAL:HG12	1.46	0.98

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%)	992 (95%)	38 (4%)	12 (1%)	10	12
1	B	1031/1057 (98%)	1007 (98%)	23 (2%)	1 (0%)	48	60
1	C	1031/1057 (98%)	1004 (97%)	26 (2%)	1 (0%)	48	60
2	D	154/169 (91%)	150 (97%)	4 (3%)	0	100	100
2	E	150/169 (89%)	145 (97%)	4 (3%)	1 (1%)	18	23
All	All	3408/3509 (97%)	3298 (97%)	95 (3%)	15 (0%)	30	38

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	522	LYS
1	A	523	SER
1	A	620	ARG
1	A	672	VAL
1	A	673	GLU

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%)	818 (96%)	32 (4%)	29	44
1	B	839/863 (97%)	805 (96%)	34 (4%)	27	41
1	C	839/863 (97%)	811 (97%)	28 (3%)	33	50
2	D	120/132 (91%)	116 (97%)	4 (3%)	33	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	117/132 (89%)	116 (99%)	1 (1%)	70 84
All	All	2765/2853 (97%)	2666 (96%)	99 (4%)	31 47

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	714	THR
1	C	158	VAL
1	B	866	GLU
1	B	1030	ARG
1	C	366	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	657	GLN
2	E	59	HIS
2	D	166	GLN
1	B	1001	ASN
1	C	526	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 ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LMT	A	1101	-	36,36,36	0.46	1 (2%)	47,47,47	0.86	1 (2%)
3	LMT	B	1101	-	36,36,36	0.44	0	47,47,47	0.97	2 (4%)
3	LMT	B	1102	-	36,36,36	0.48	1 (2%)	47,47,47	1.23	5 (10%)
3	LMT	A	1102	-	36,36,36	0.47	0	47,47,47	0.85	1 (2%)
3	LMT	C	1101	-	36,36,36	0.46	0	47,47,47	1.00	1 (2%)
4	MIY	B	1103	-	36,36,36	1.98	14 (38%)	42,58,58	2.71	17 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	A	1101	-	-	12/21/61/61	0/2/2/2
3	LMT	B	1101	-	-	9/21/61/61	0/2/2/2
3	LMT	B	1102	-	-	10/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	7/21/61/61	0/2/2/2
3	LMT	C	1101	-	-	5/21/61/61	0/2/2/2
4	MIY	B	1103	-	-	3/12/70/70	0/4/4/4

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1103	MIY	C11-C10	4.03	1.45	1.39
4	B	1103	MIY	C71-N7	3.76	1.53	1.45
4	B	1103	MIY	C4-N1	3.21	1.54	1.47
4	B	1103	MIY	CN7-N7	3.15	1.52	1.45
4	B	1103	MIY	C14-C13	-3.06	1.36	1.41

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1103	MIY	C1-C18-C17	7.59	118.78	109.88
4	B	1103	MIY	C11-C12-C13	-6.68	113.82	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1103	MIY	C15-C16-C17	6.00	123.55	118.80
4	B	1103	MIY	C12-C13-C14	5.35	126.98	120.15
4	B	1103	MIY	O5-C15-C14	-3.85	115.10	122.06

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

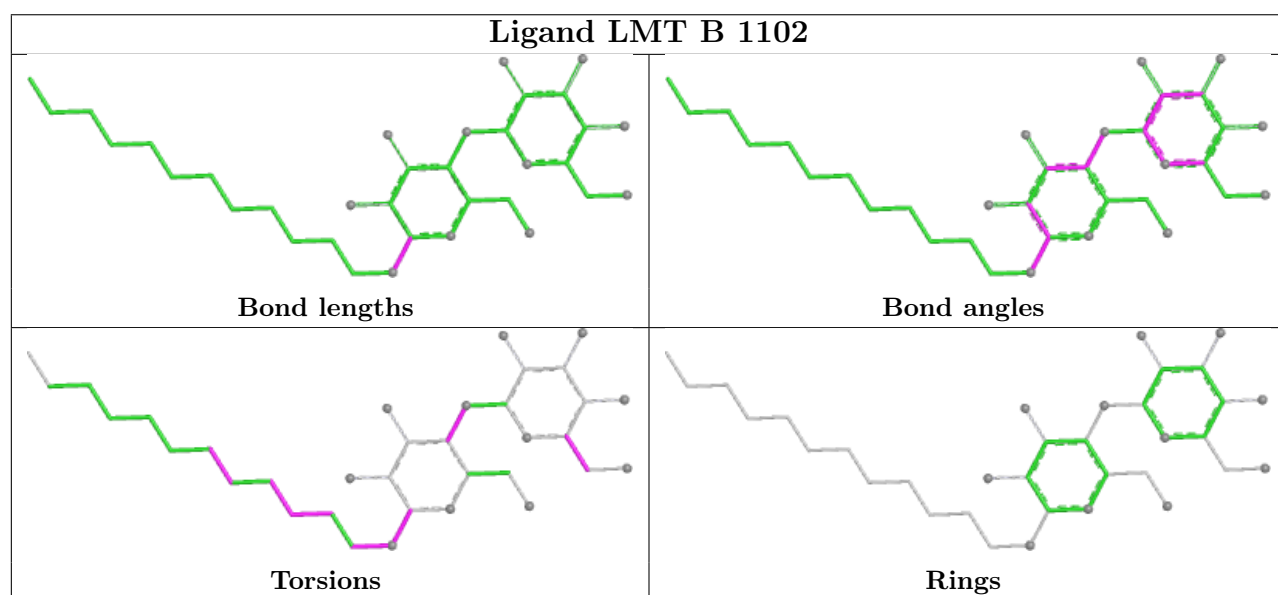
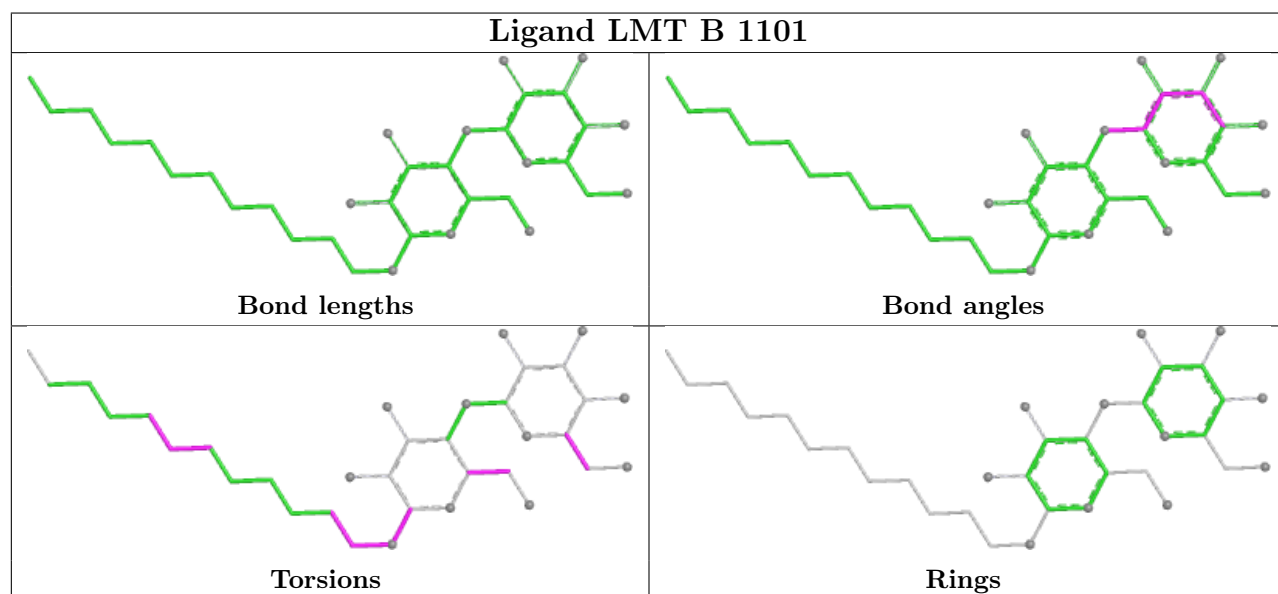
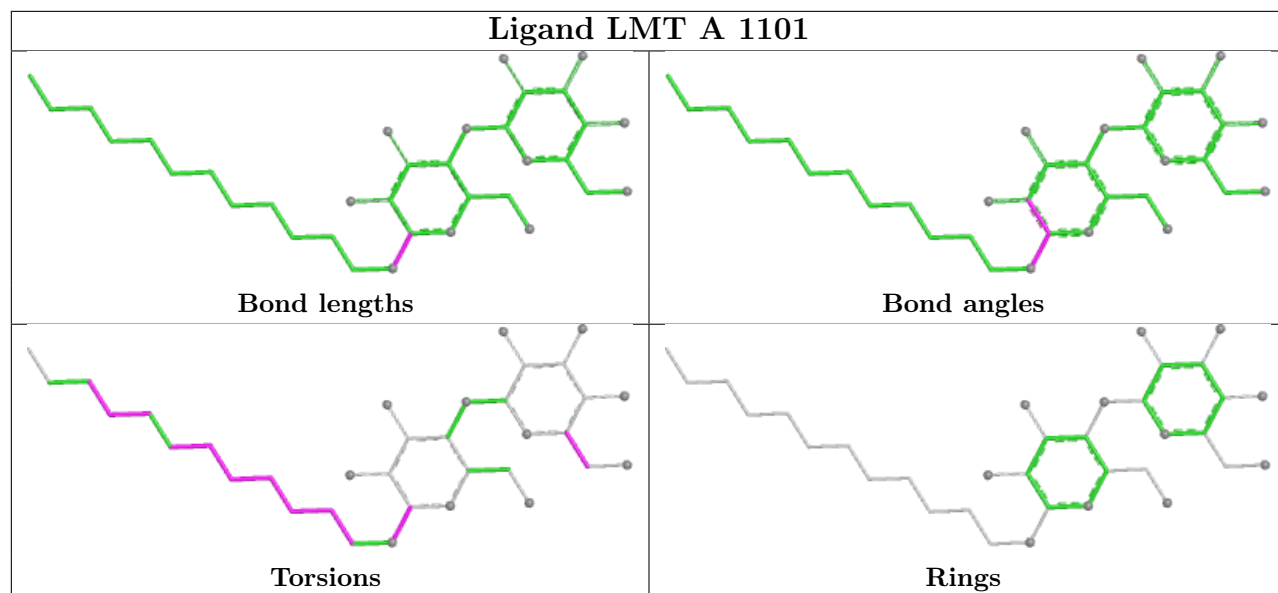
Mol	Chain	Res	Type	Atoms
3	A	1101	LMT	C2'-C1'-O1'-C1
3	B	1102	LMT	O5'-C1'-O1'-C1
3	C	1101	LMT	C2'-C1'-O1'-C1
3	B	1102	LMT	C3'-C4'-O1B-C1B
3	C	1101	LMT	O5B-C5B-C6B-O6B

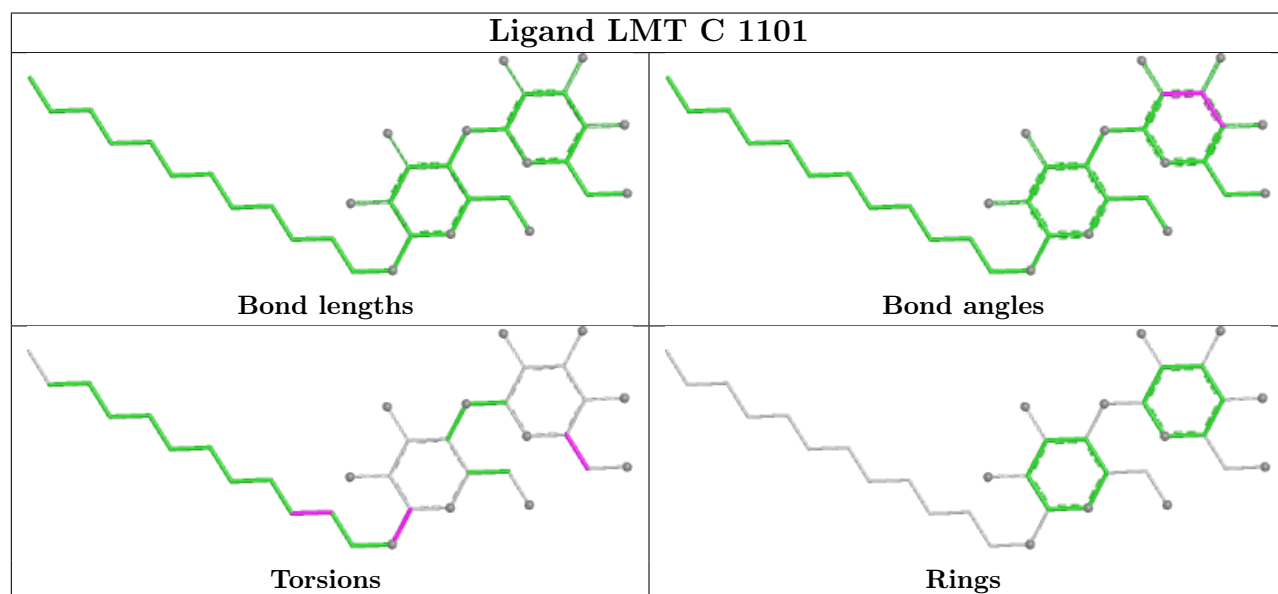
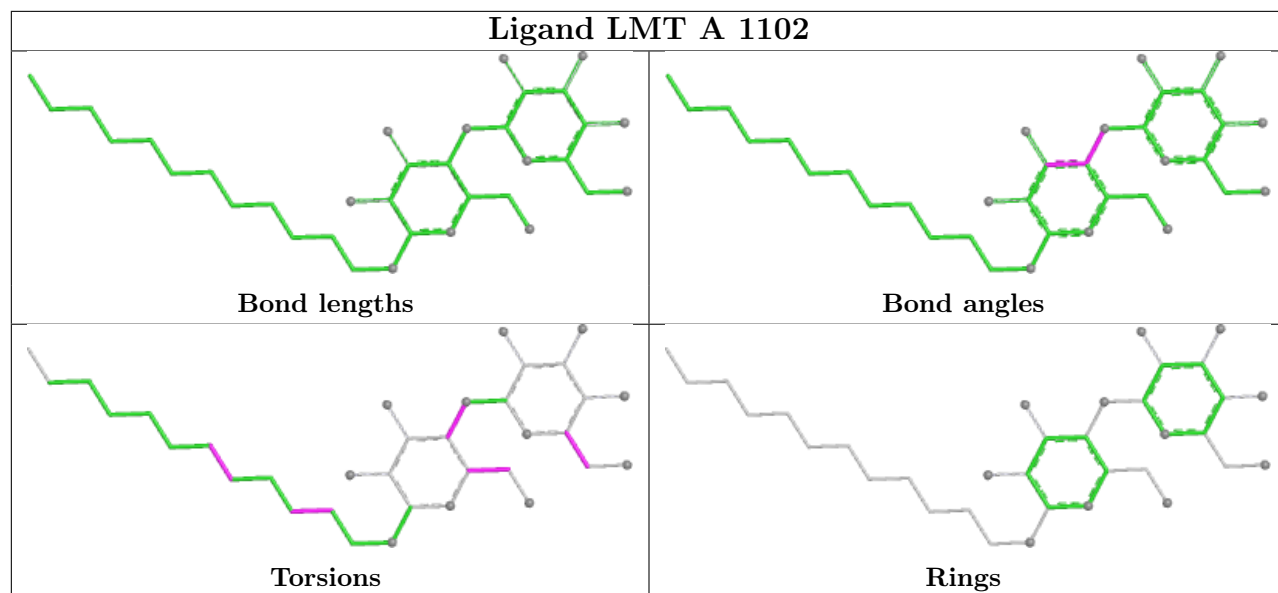
There are no ring outliers.

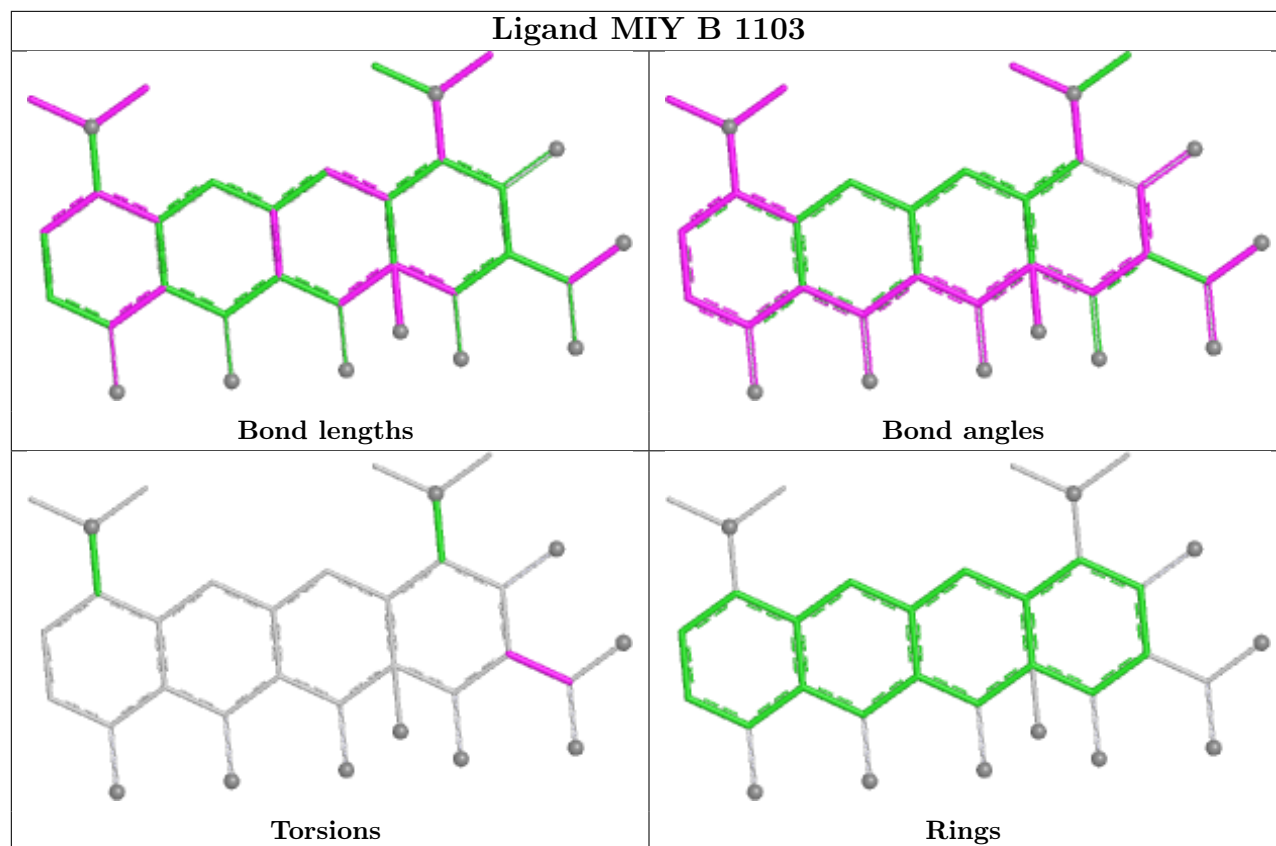
6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	LMT	3	0
3	B	1101	LMT	3	0
3	B	1102	LMT	5	0
3	A	1102	LMT	5	0
3	C	1101	LMT	3	0
4	B	1103	MIY	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.40	104 (9%) 12 14	23, 51, 115, 155	0
1	B	1033/1057 (97%)	0.09	34 (3%) 49 51	24, 48, 71, 109	0
1	C	1033/1057 (97%)	-0.08	26 (2%) 58 60	24, 43, 71, 111	0
2	D	156/169 (92%)	0.04	6 (3%) 44 46	40, 48, 74, 110	0
2	E	152/169 (89%)	0.34	6 (3%) 43 45	49, 66, 95, 120	0
All	All	3418/3509 (97%)	0.14	176 (5%) 33 35	23, 48, 92, 155	0

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	678	THR	7.9
1	A	618	ALA	7.5
1	A	672	VAL	7.1
1	A	617	PHE	6.7
1	B	617	PHE	6.6

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.

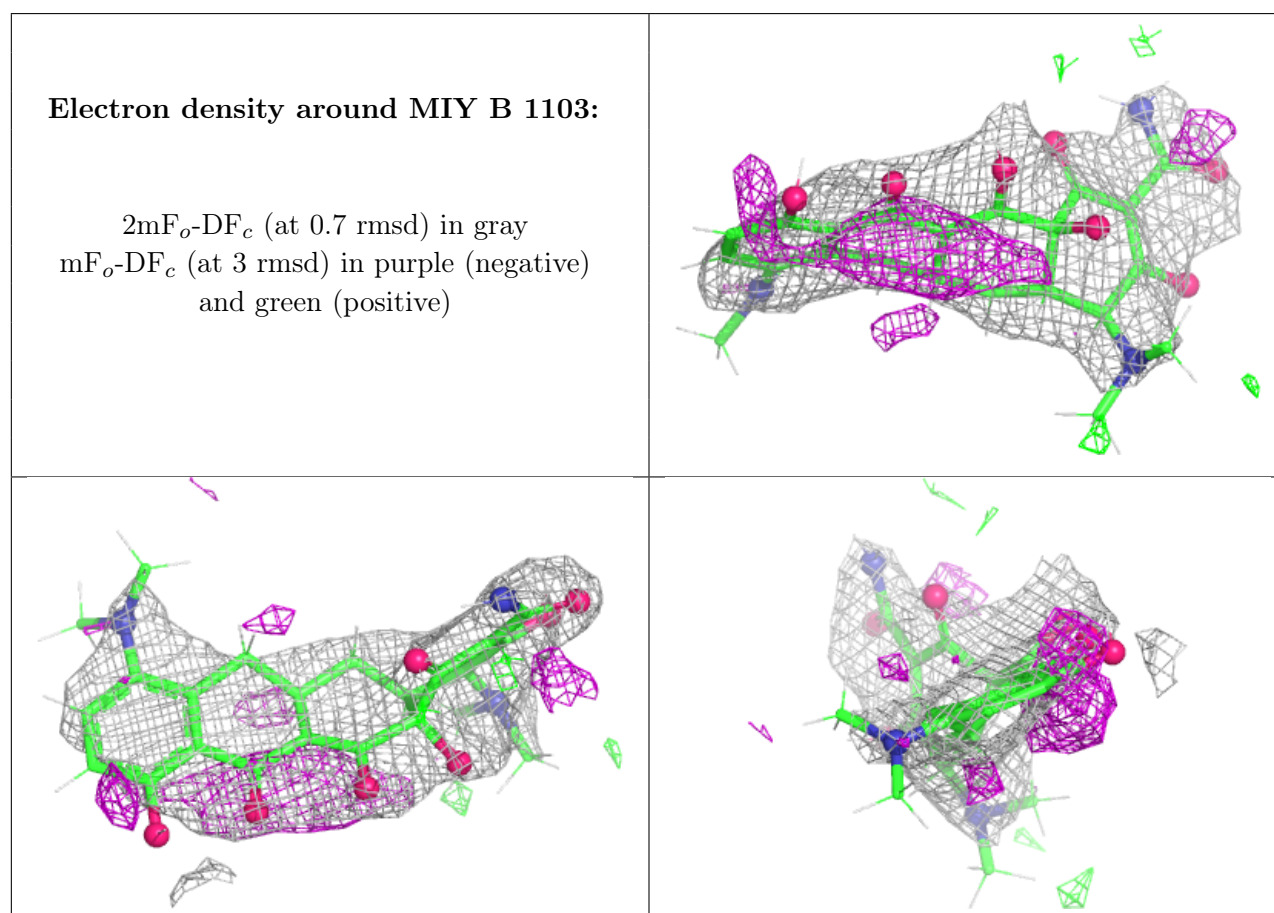
6.4 Ligands [i](#)

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.

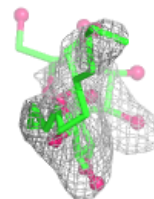
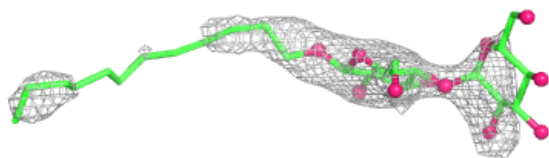
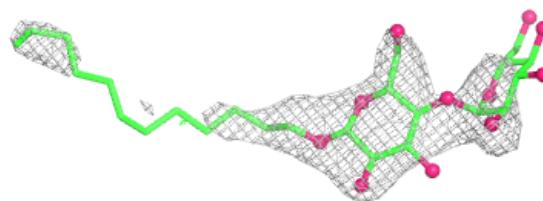
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MIY	B	1103	33/33	0.77	0.18	64,89,104,135	0
3	LMT	A	1102	35/35	0.85	0.18	83,104,125,130	0
3	LMT	B	1102	35/35	0.89	0.13	56,93,106,106	0
3	LMT	B	1101	35/35	0.90	0.14	49,70,86,88	0
3	LMT	C	1101	35/35	0.92	0.13	52,64,80,81	0
3	LMT	A	1101	35/35	0.92	0.11	45,65,90,96	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.

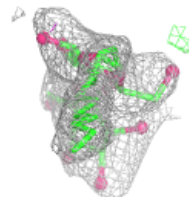
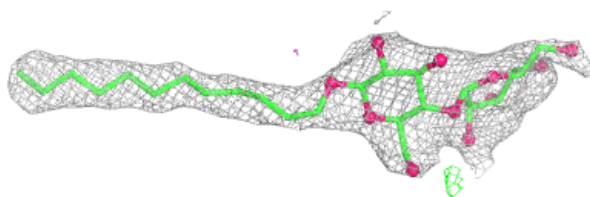
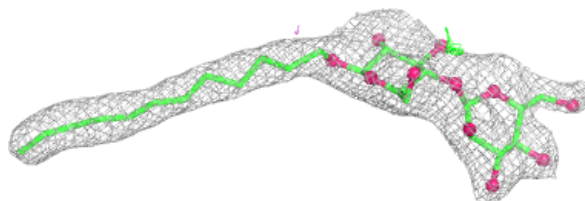


Electron density around LMT A 1102:

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

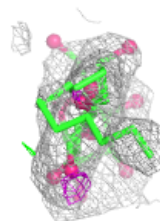
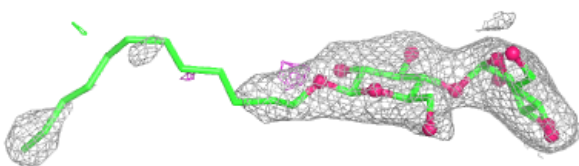
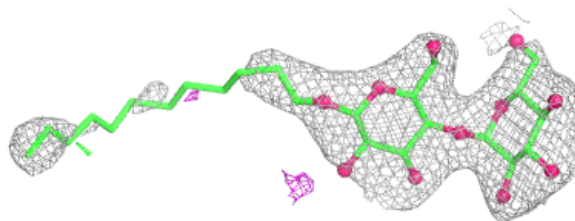
**Electron density around LMT B 1102:**

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

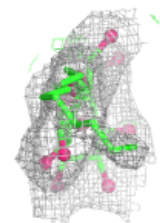
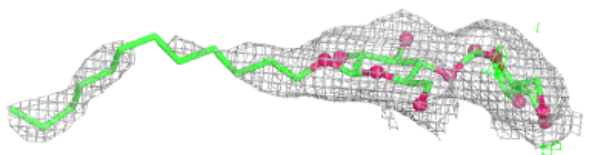
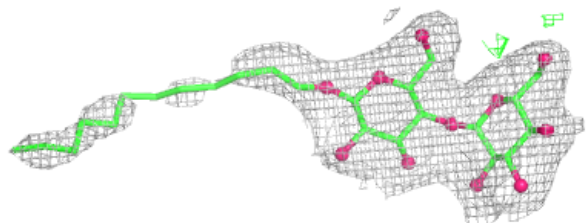


Electron density around LMT B 1101:

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

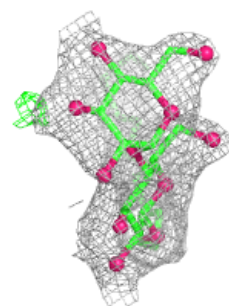
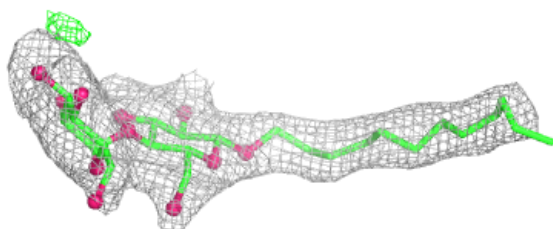
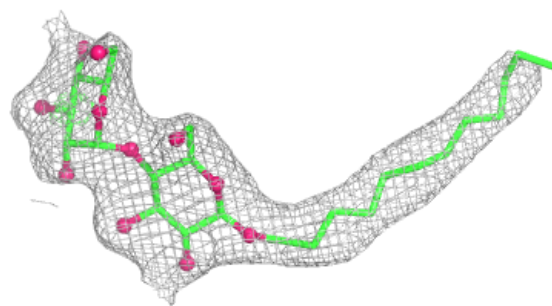
**Electron density around LMT C 1101:**

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



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 ⓘ

There are no such residues in this entry.