



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:59 AM UTC

PDB ID : 4ZJQ / pdb_00004zjq
Title : Crystal structure of AcrB deletion mutant in complex with antibiotic in P21 space group
Authors : Ababou, A.; Koronakis, V.
Deposited on : 2015-04-29
Resolution : 3.59 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

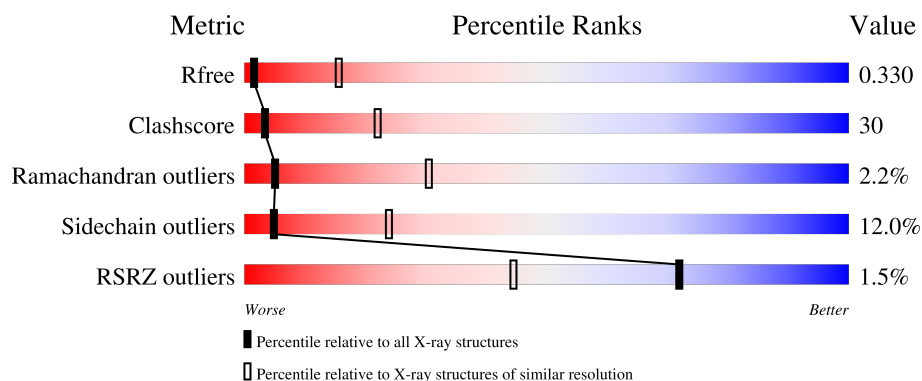
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	1044	% 46% 45% 8% .
1	B	1044	44% 47% 8% .
1	C	1044	2% 40% 49% 9% ..
1	D	1044	% 43% 47% 8% ..
1	E	1044	% 45% 46% 8% .

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Mol	Chain	Length	Quality of chain
1	F	1044	3% 39% 50% 9% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 47697 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	1038	Total	C	N	O	S	0	0	0
			7893	5072	1306	1472	43			
1	B	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			
1	C	1036	Total	C	N	O	S	0	0	0
			7877	5063	1302	1469	43			
1	D	1038	Total	C	N	O	S	0	0	0
			7893	5072	1306	1472	43			
1	E	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			
1	F	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			

There are 36 discrepancies between the modelled and reference sequences:

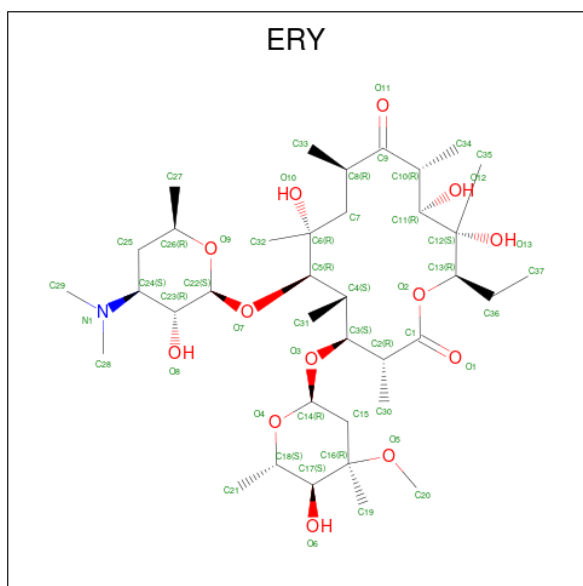
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	GLY	PHE	engineered mutation	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	PHE	deletion	UNP P31224
A	?	-	ALA	deletion	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	ARG	deletion	UNP P31224
B	?	GLY	PHE	engineered mutation	UNP P31224
B	?	-	GLY	deletion	UNP P31224
B	?	-	PHE	deletion	UNP P31224
B	?	-	ALA	deletion	UNP P31224
B	?	-	GLY	deletion	UNP P31224
B	?	-	ARG	deletion	UNP P31224
C	?	GLY	PHE	engineered mutation	UNP P31224
C	?	-	GLY	deletion	UNP P31224
C	?	-	PHE	deletion	UNP P31224
C	?	-	ALA	deletion	UNP P31224
C	?	-	GLY	deletion	UNP P31224

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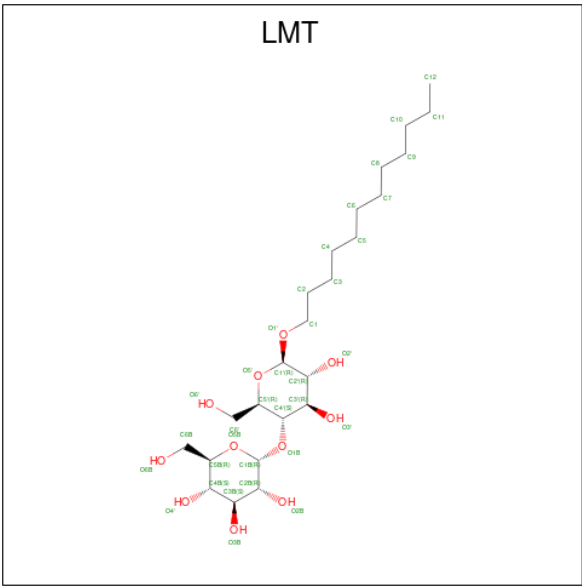
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP P31224
D	?	GLY	PHE	engineered mutation	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	PHE	deletion	UNP P31224
D	?	-	ALA	deletion	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	ARG	deletion	UNP P31224
E	?	GLY	PHE	engineered mutation	UNP P31224
E	?	-	GLY	deletion	UNP P31224
E	?	-	PHE	deletion	UNP P31224
E	?	-	ALA	deletion	UNP P31224
E	?	-	GLY	deletion	UNP P31224
E	?	-	ARG	deletion	UNP P31224
F	?	GLY	PHE	engineered mutation	UNP P31224
F	?	-	GLY	deletion	UNP P31224
F	?	-	PHE	deletion	UNP P31224
F	?	-	ALA	deletion	UNP P31224
F	?	-	GLY	deletion	UNP P31224
F	?	-	ARG	deletion	UNP P31224

- Molecule 2 is ERYTHROMYCIN A (CCD ID: ERY) (formula: $C_{37}H_{67}NO_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			51	37	1	13		
2	D	1	Total	C	N	O	0	0
			51	37	1	13		

- 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	C	1	Total	C	O	0	0
			35	24	11		
3	D	1	Total	C	O	0	0
			35	24	11		
3	D	1	Total	C	O	0	0
			35	24	11		
3	E	1	Total	C	O	0	0
			35	24	11		
3	F	1	Total	C	O	0	0
			35	24	11		

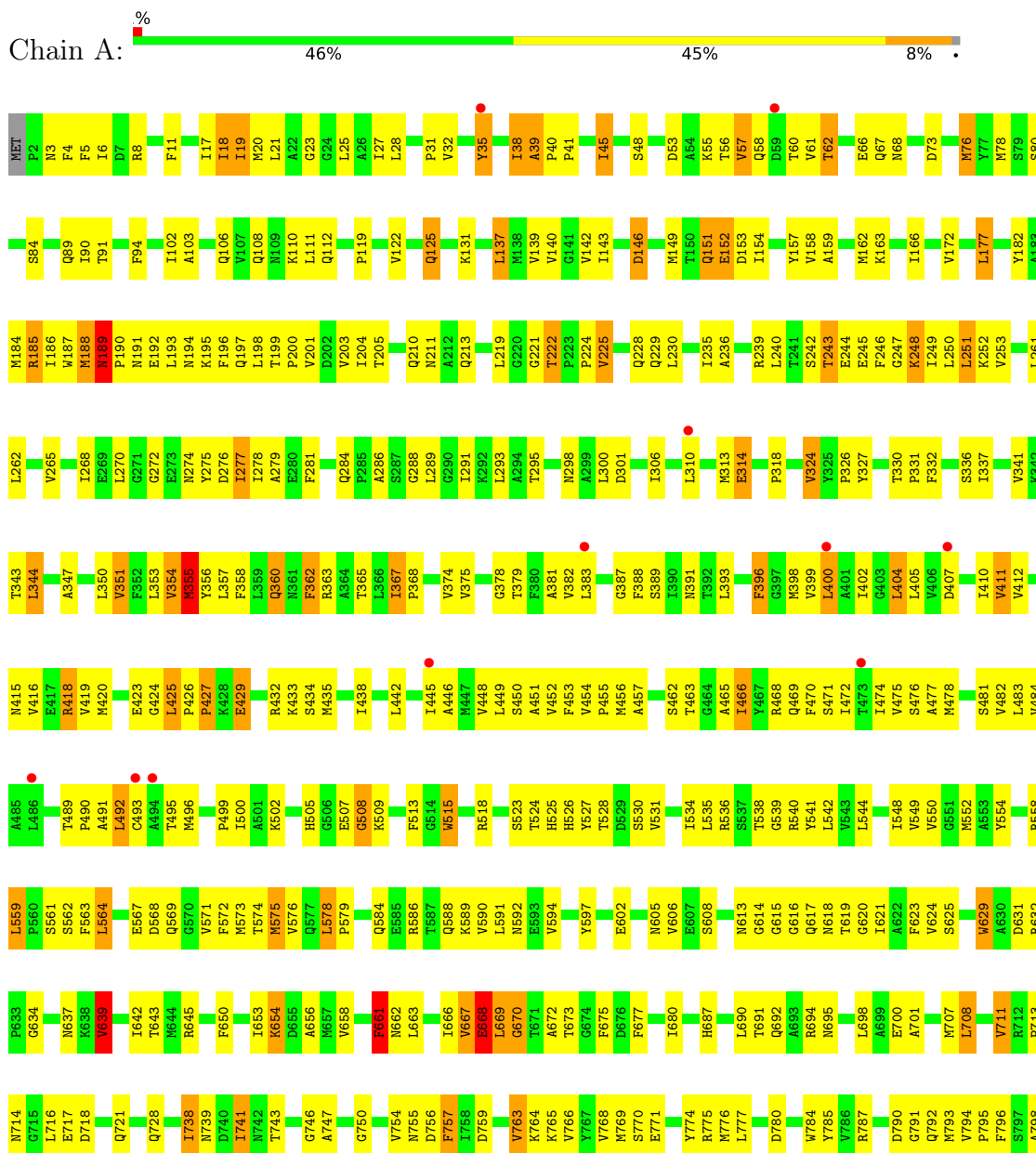
- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

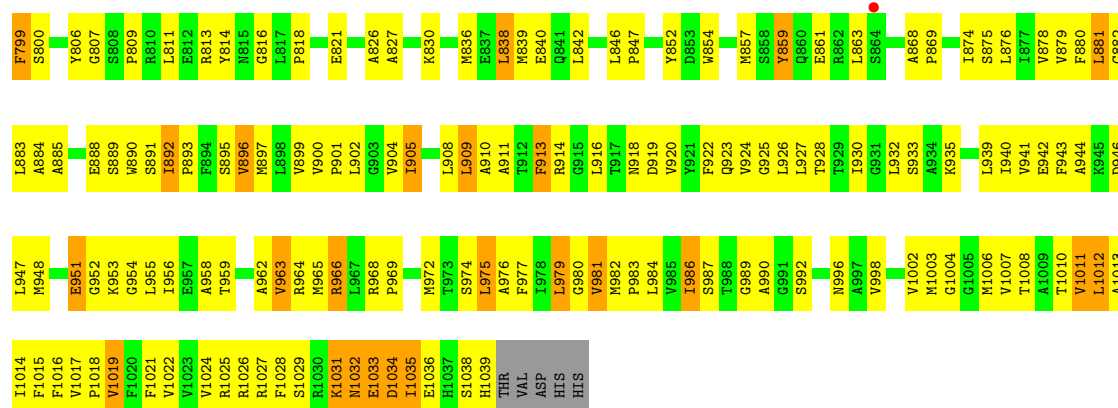
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ni	0	0
			1	1		
4	C	1	Total	Ni	0	0
			1	1		
4	E	1	Total	Ni	0	0
			1	1		

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.

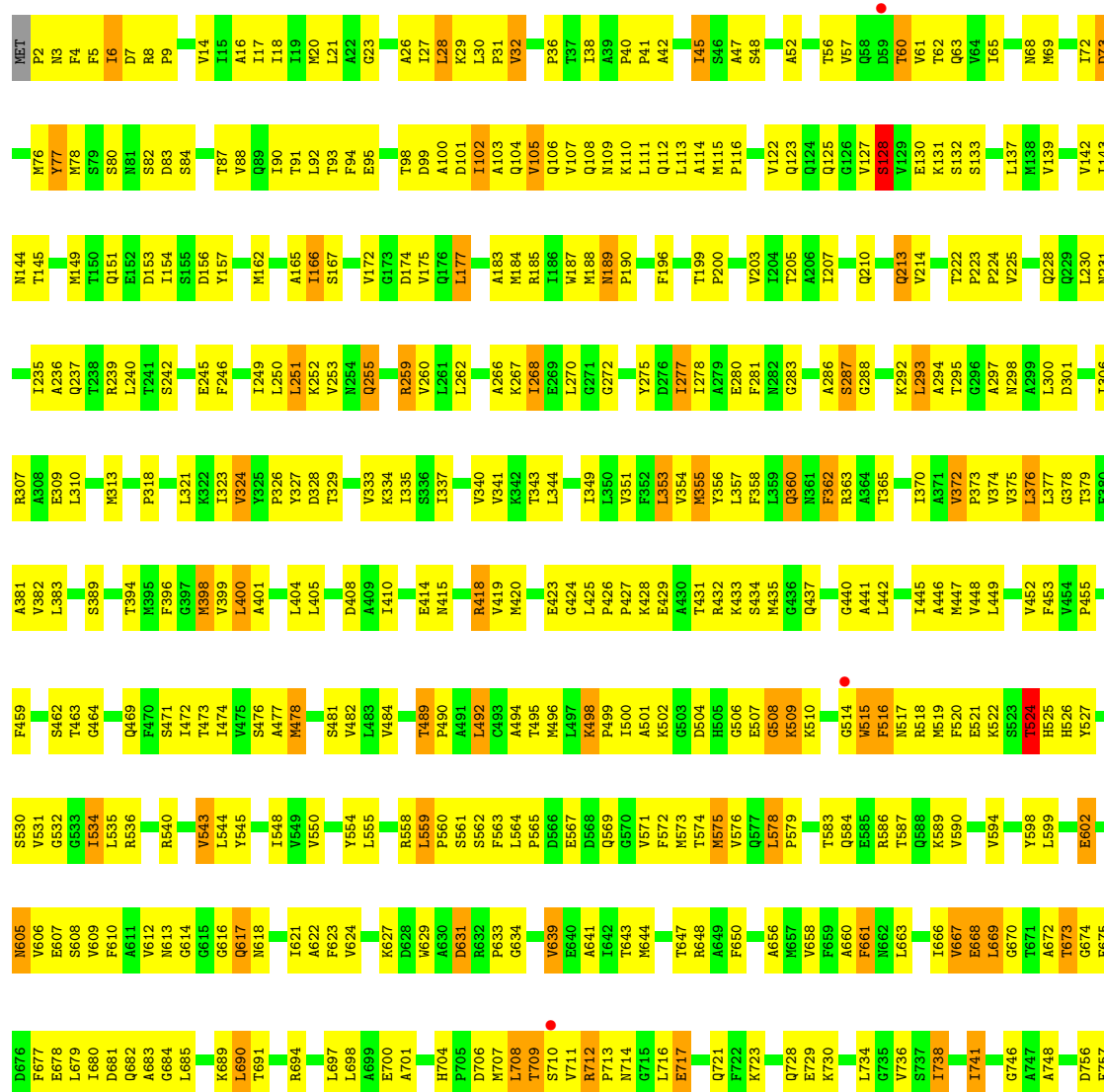
• Molecule 1: Multidrug efflux pump subunit AcrB

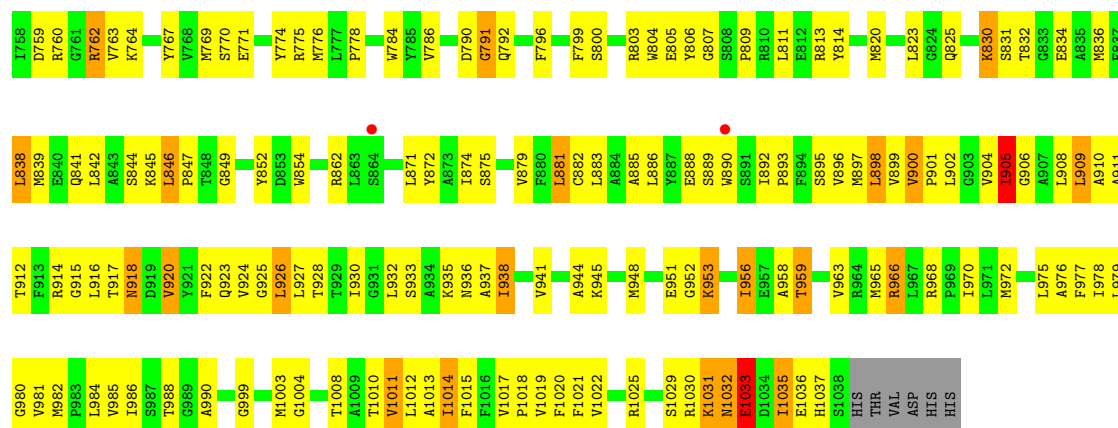




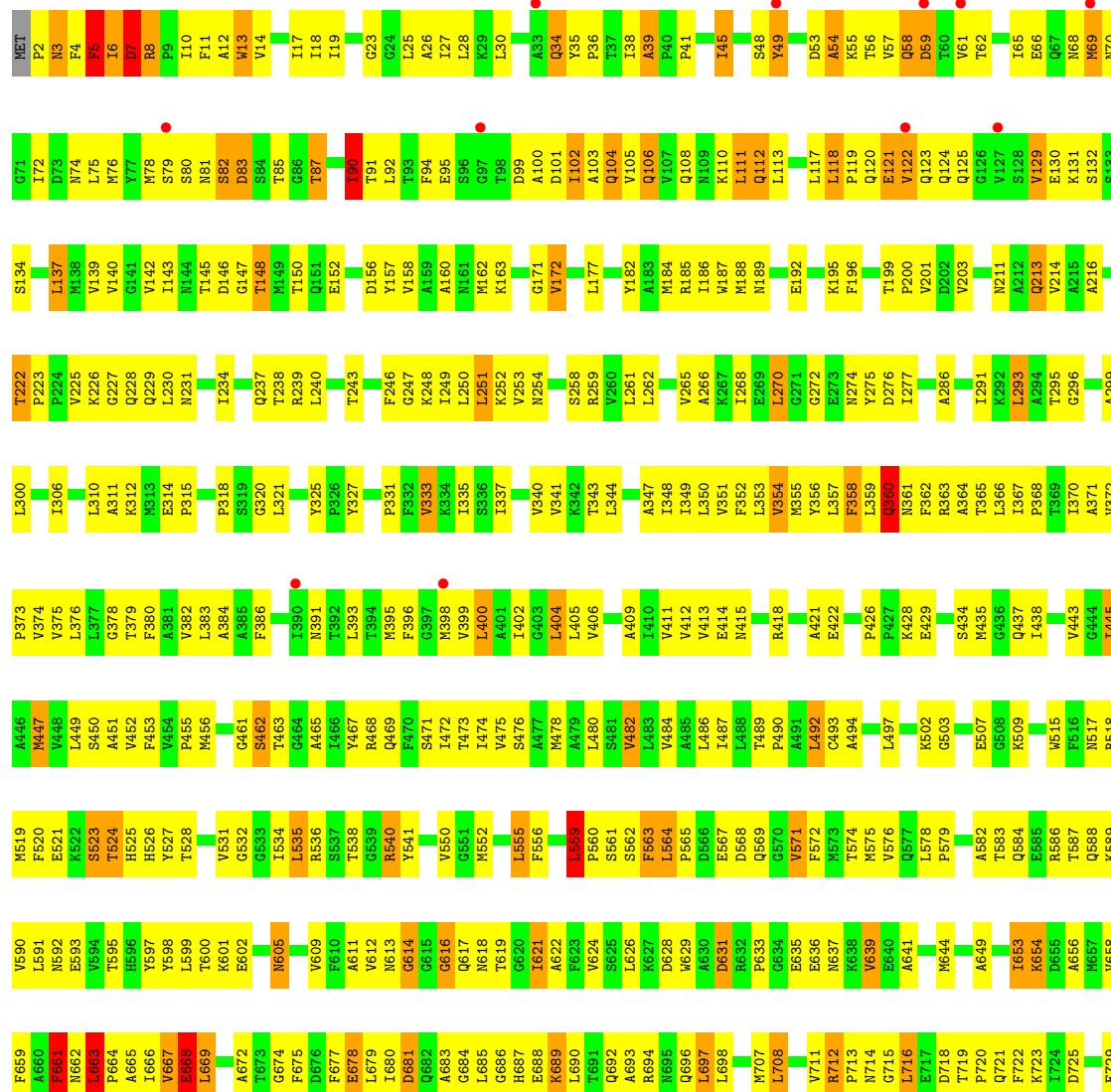
• Molecule 1: Multidrug efflux pump subunit AcrB

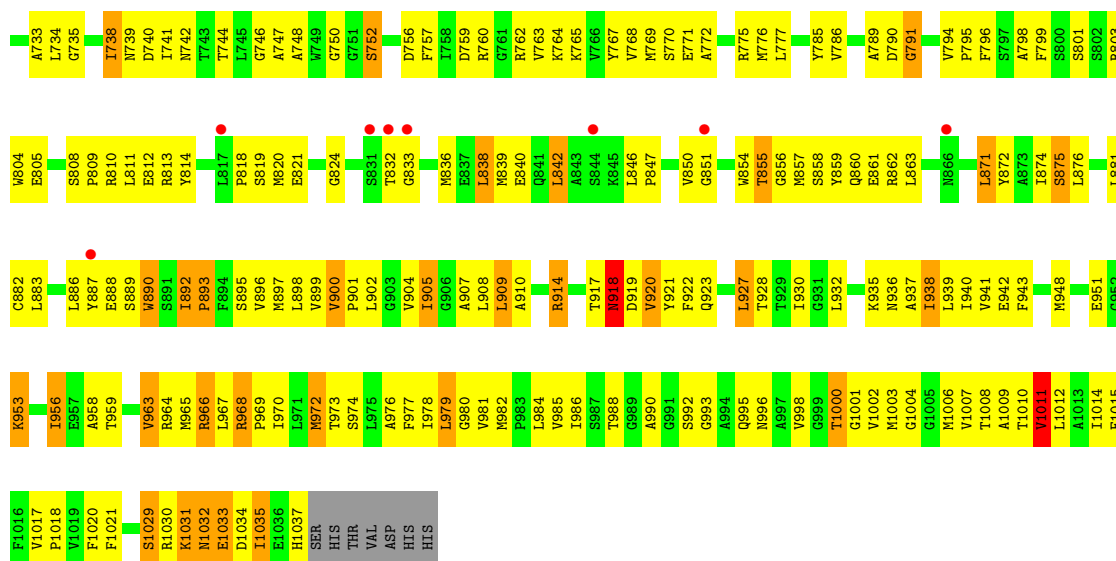
Chain B: 44% 47% 8%



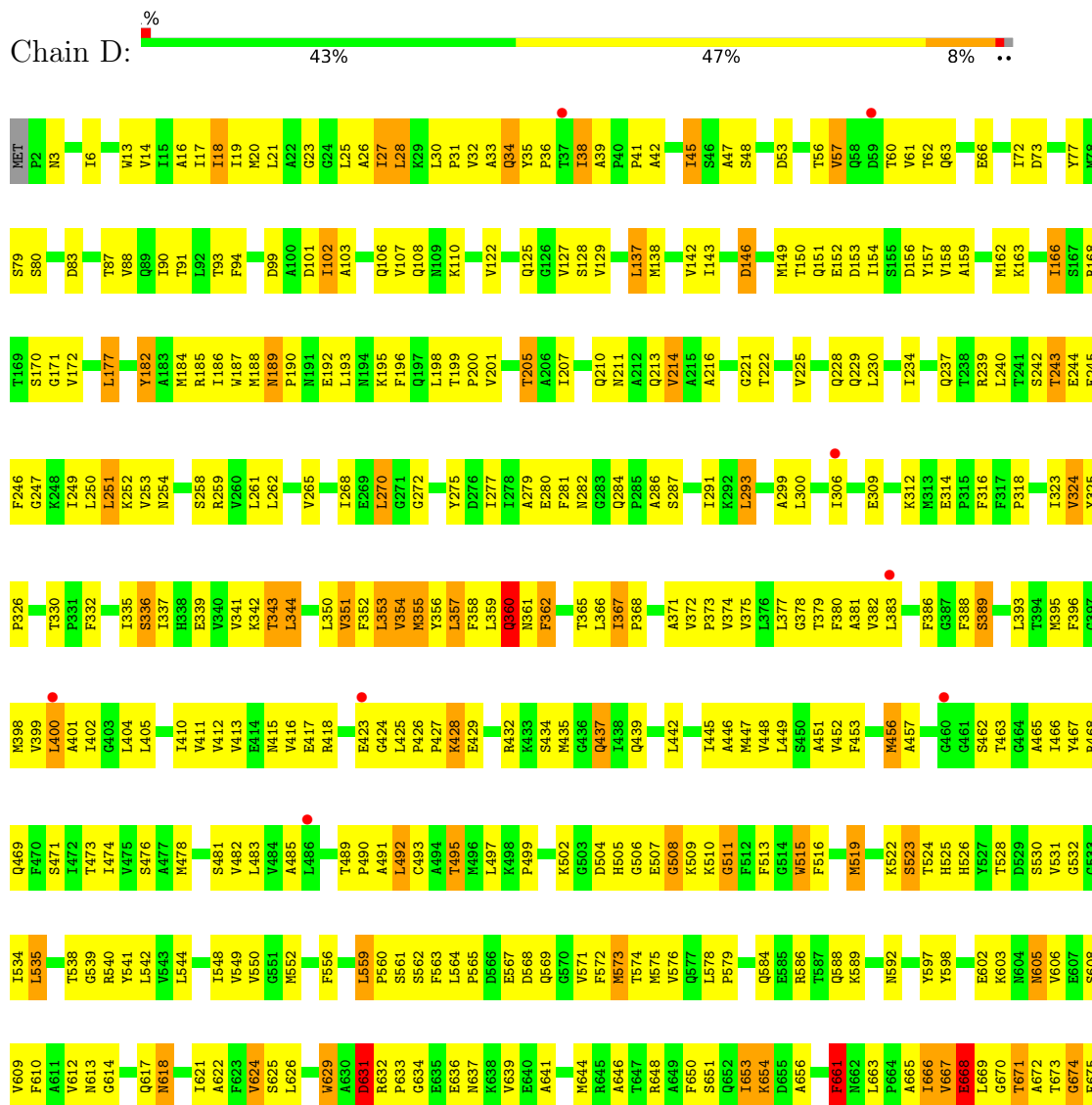


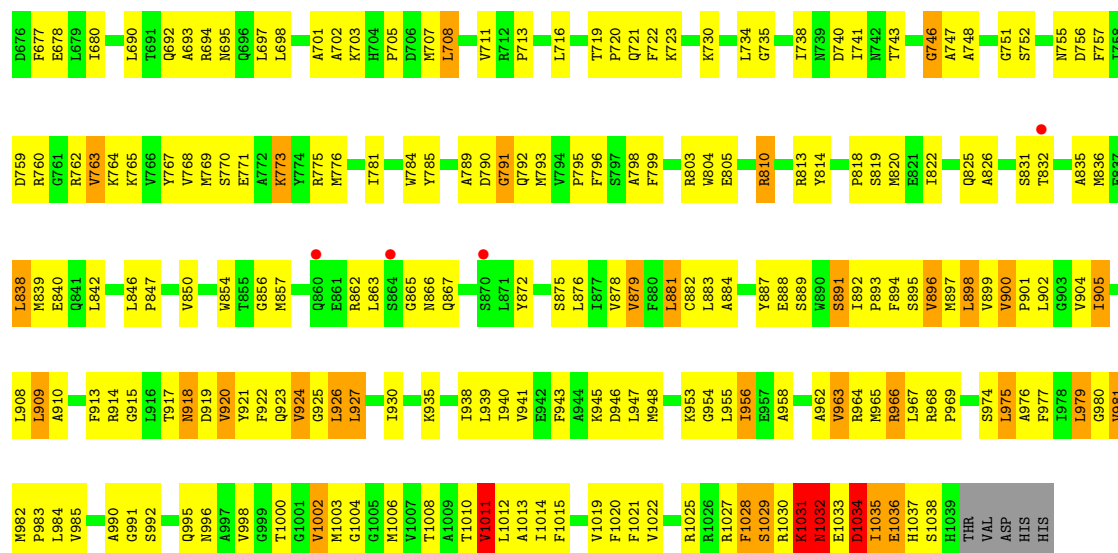
• Molecule 1: Multidrug efflux pump subunit AcrB



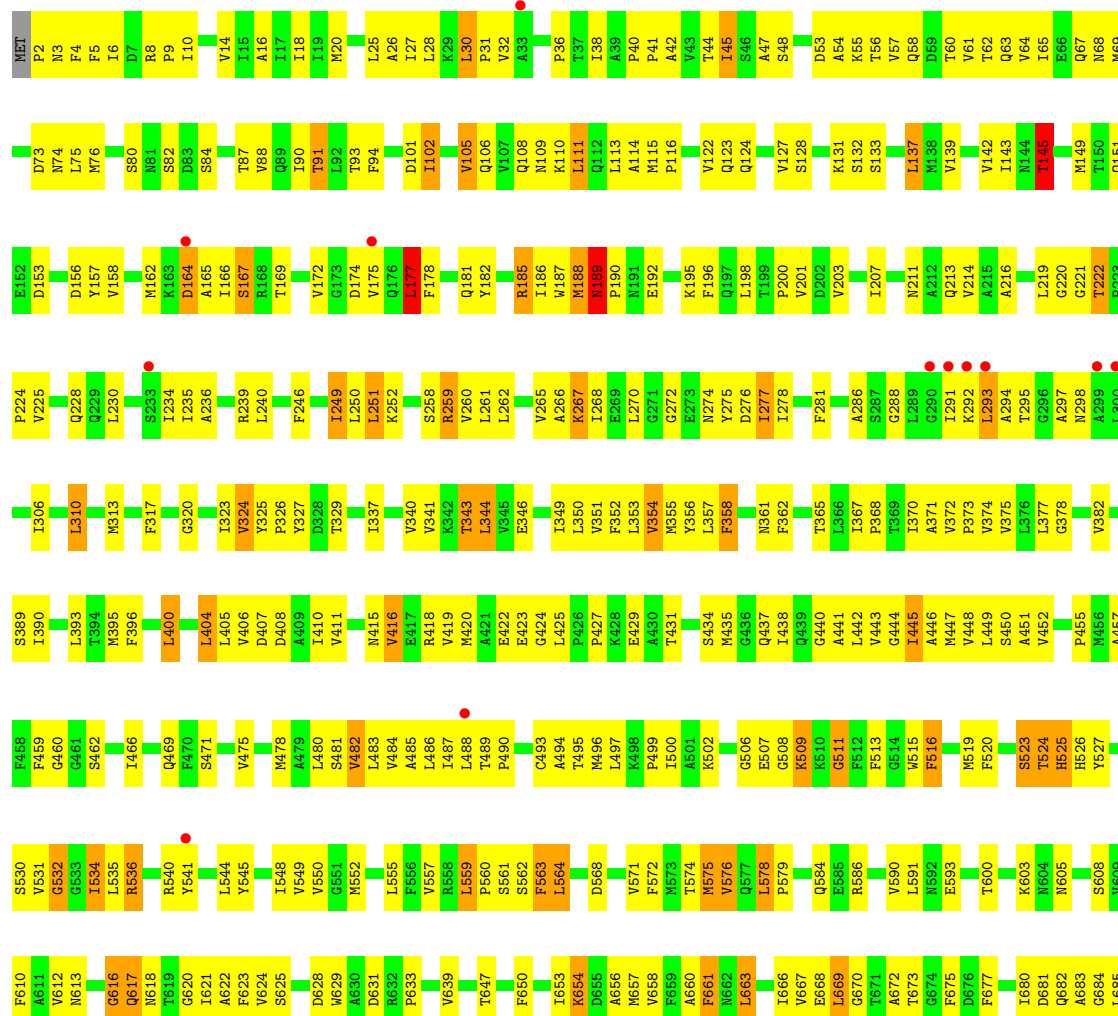
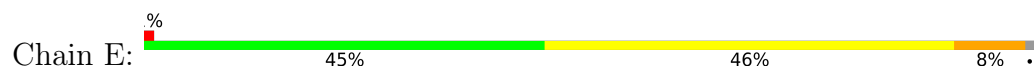


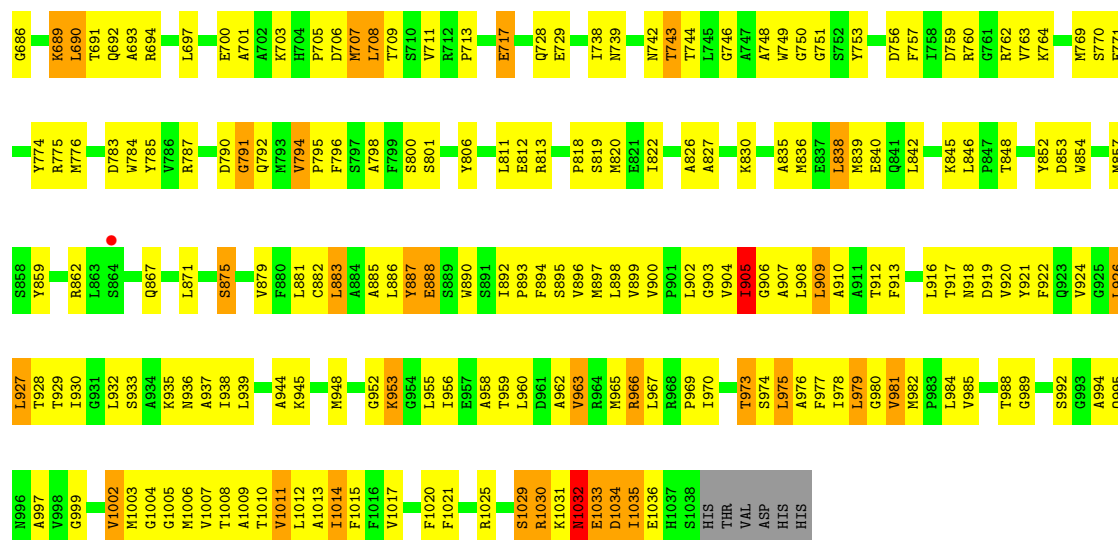
● Molecule 1: Multidrug efflux pump subunit AcrB



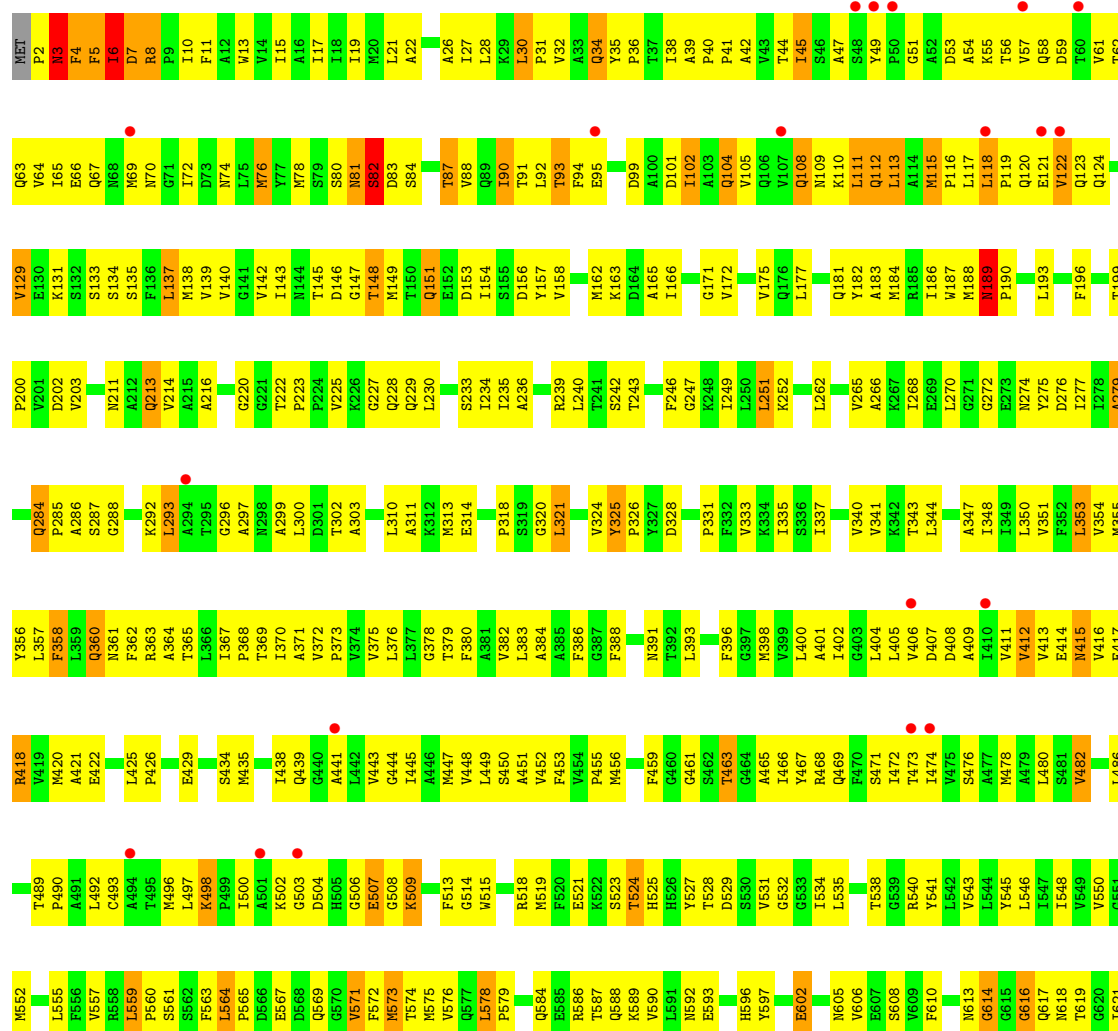


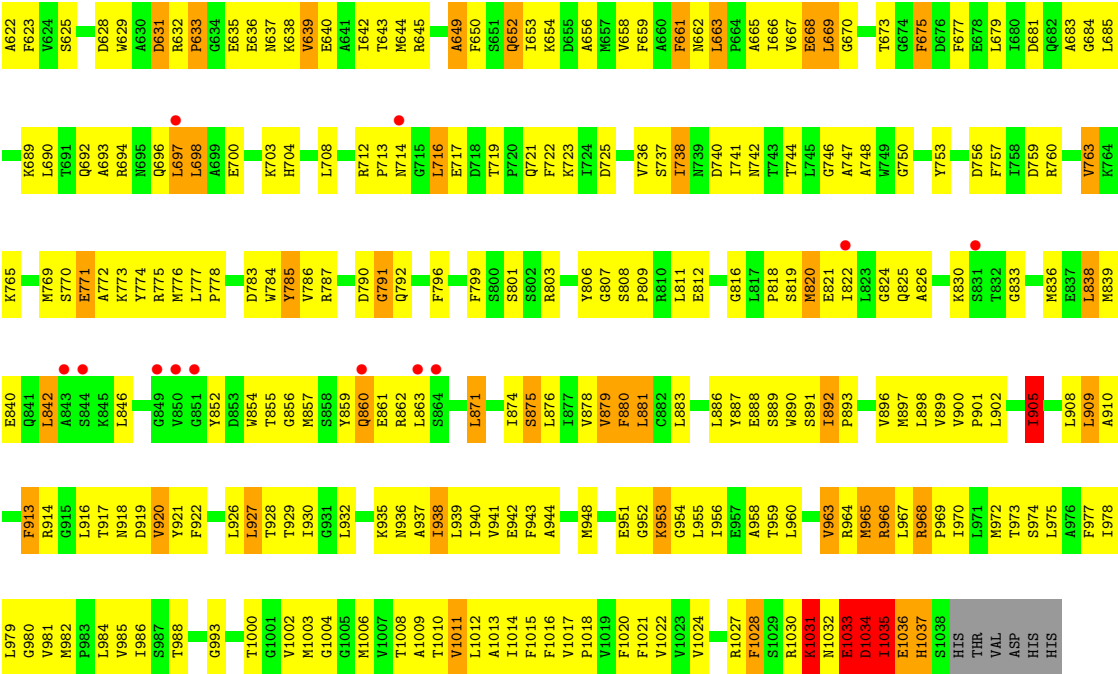
• Molecule 1: Multidrug efflux pump subunit AcrB





• Molecule 1: Multidrug efflux pump subunit AcrB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	150.06Å 154.57Å 215.74Å 90.00° 92.42° 90.00°	Depositor
Resolution (Å)	19.96 – 3.59 19.96 – 3.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.96-3.59) 95.8 (19.96-3.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.246 , 0.319 0.264 , 0.330	Depositor DCC
R_{free} test set	5715 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	110.6	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.055 for -k,-h,-l 0.070 for k,h,-l 0.068 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	47697	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9200e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ERY, NI, 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	0.80	2/8043 (0.0%)	1.22	39/10922 (0.4%)
1	B	0.80	5/8032 (0.1%)	1.18	32/10907 (0.3%)
1	C	0.82	3/8026 (0.0%)	1.29	78/10899 (0.7%)
1	D	0.75	1/8043 (0.0%)	1.18	39/10922 (0.4%)
1	E	0.76	1/8032 (0.0%)	1.18	36/10907 (0.3%)
1	F	0.77	1/8032 (0.0%)	1.23	57/10907 (0.5%)
All	All	0.78	13/48208 (0.0%)	1.22	281/65464 (0.4%)

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	1
1	B	0	1
1	D	0	1
1	F	0	2
All	All	0	5

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	900	VAL	CA-CB	10.18	1.59	1.54
1	B	372	VAL	CA-CB	9.89	1.59	1.54
1	A	1017	VAL	CA-CB	-9.55	1.49	1.54
1	B	900	VAL	CA-CB	6.75	1.57	1.54
1	C	122	VAL	CA-CB	5.84	1.61	1.54

The worst 5 of 281 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	559	LEU	CA-C-N	13.01	133.16	119.76
1	E	559	LEU	C-N-CA	13.01	133.16	119.76
1	F	118	LEU	CA-C-N	11.24	133.89	119.84
1	F	118	LEU	C-N-CA	11.24	133.89	119.84
1	C	118	LEU	CA-C-N	10.89	133.45	119.84

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1034	ASP	Peptide
1	B	1033	GLU	Peptide
1	D	1032	ASN	Peptide
1	F	1033	GLU	Peptide
1	F	1034	ASP	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	7893	0	8034	472	0
1	B	7883	0	8027	470	0
1	C	7877	0	8022	521	0
1	D	7893	0	8034	500	0
1	E	7883	0	8027	497	0
1	F	7883	0	8027	535	0
2	A	51	0	67	5	0
2	D	51	0	67	4	0
3	A	70	0	92	7	0
3	B	35	0	46	7	0
3	C	35	0	46	1	0
3	D	70	0	92	13	0
3	E	35	0	46	11	0
3	F	35	0	46	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
All	All	47697	0	48673	2908	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 30.

The worst 5 of 2908 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:F:34:GLN:HB2	1:F:333:VAL:HG22	1.45	0.98
1:D:344:LEU:HD22	1:D:402:ILE:HD11	1.45	0.97
1:B:213:GLN:HG2	1:B:239:ARG:HG3	1.44	0.96
1:C:893:PRO:HA	1:C:896:VAL:HG12	1.43	0.96
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.47	0.93

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	1036/1044 (99%)	902 (87%)	117 (11%)	17 (2%)	7	36
1	B	1035/1044 (99%)	896 (87%)	117 (11%)	22 (2%)	5	31
1	C	1034/1044 (99%)	896 (87%)	119 (12%)	19 (2%)	6	34
1	D	1036/1044 (99%)	894 (86%)	116 (11%)	26 (2%)	4	28
1	E	1035/1044 (99%)	894 (86%)	116 (11%)	25 (2%)	4	29
1	F	1035/1044 (99%)	891 (86%)	118 (11%)	26 (2%)	4	28
All	All	6211/6264 (99%)	5373 (86%)	703 (11%)	135 (2%)	5	30

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	987	SER
1	A	1033	GLU
1	B	357	LEU

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Mol	Chain	Res	Type
1	B	508	GLY
1	B	672	ALA

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	846/852 (99%)	742 (88%)	104 (12%)	4	23
1	B	845/852 (99%)	751 (89%)	94 (11%)	6	27
1	C	844/852 (99%)	736 (87%)	108 (13%)	4	22
1	D	846/852 (99%)	743 (88%)	103 (12%)	5	23
1	E	845/852 (99%)	754 (89%)	91 (11%)	6	28
1	F	845/852 (99%)	735 (87%)	110 (13%)	4	21
All	All	5071/5112 (99%)	4461 (88%)	610 (12%)	5	24

5 of 610 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	661	PHE
1	F	763	VAL
1	E	743	THR
1	E	654	LYS
1	F	115	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	996	ASN
1	F	34	GLN
1	F	577	GLN
1	C	613	ASN
1	C	592	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 for Mogul analysis.

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$
2	ERY	A	1101	-	53,53,53	1.16	3 (5%)	82,82,82	1.91	18 (21%)
3	LMT	D	1102	-	36,36,36	1.80	9 (25%)	47,47,47	1.42	7 (14%)
3	LMT	E	1101	-	36,36,36	1.89	10 (27%)	47,47,47	1.63	8 (17%)
2	ERY	D	1101	-	53,53,53	1.29	3 (5%)	82,82,82	2.08	31 (37%)
3	LMT	C	1101	-	36,36,36	1.78	9 (25%)	47,47,47	1.43	6 (12%)
3	LMT	B	2100	-	36,36,36	1.72	10 (27%)	47,47,47	1.94	14 (29%)
3	LMT	F	2100	-	36,36,36	1.73	9 (25%)	47,47,47	1.12	2 (4%)
3	LMT	A	1102	-	36,36,36	1.76	10 (27%)	47,47,47	1.15	4 (8%)
3	LMT	D	1103	-	36,36,36	1.91	9 (25%)	47,47,47	1.32	8 (17%)
3	LMT	A	1103	-	36,36,36	1.87	9 (25%)	47,47,47	1.60	9 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ERY	A	1101	-	-	33/72/107/107	0/3/3/3
3	LMT	D	1102	-	-	11/21/61/61	0/2/2/2
3	LMT	E	1101	-	-	10/21/61/61	0/2/2/2
2	ERY	D	1101	-	-	47/72/107/107	0/3/3/3
3	LMT	C	1101	-	-	12/21/61/61	0/2/2/2
3	LMT	B	2100	-	-	11/21/61/61	0/2/2/2
3	LMT	F	2100	-	-	11/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	12/21/61/61	0/2/2/2
3	LMT	D	1103	-	-	15/21/61/61	0/2/2/2
3	LMT	A	1103	-	-	14/21/61/61	0/2/2/2

The worst 5 of 81 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	ERY	O2-C1	5.54	1.47	1.34
2	A	1101	ERY	O2-C1	5.27	1.46	1.34
3	A	1103	LMT	O5'-C5'	4.54	1.55	1.44
3	D	1103	LMT	O5'-C5'	4.47	1.55	1.44
3	E	1101	LMT	O1'-C1'	4.32	1.47	1.40

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1103	LMT	O5B-C5B-C4B	5.57	119.73	109.70
3	E	1101	LMT	C1B-C2B-C3B	-5.46	98.53	110.01
2	D	1101	ERY	C20-O5-C16	5.39	128.48	117.51
3	C	1101	LMT	C4B-C3B-C2B	5.04	119.67	110.83
2	D	1101	ERY	C12-C11-C10	5.00	122.25	116.40

There are no chirality outliers.

5 of 176 torsion outliers are listed below:

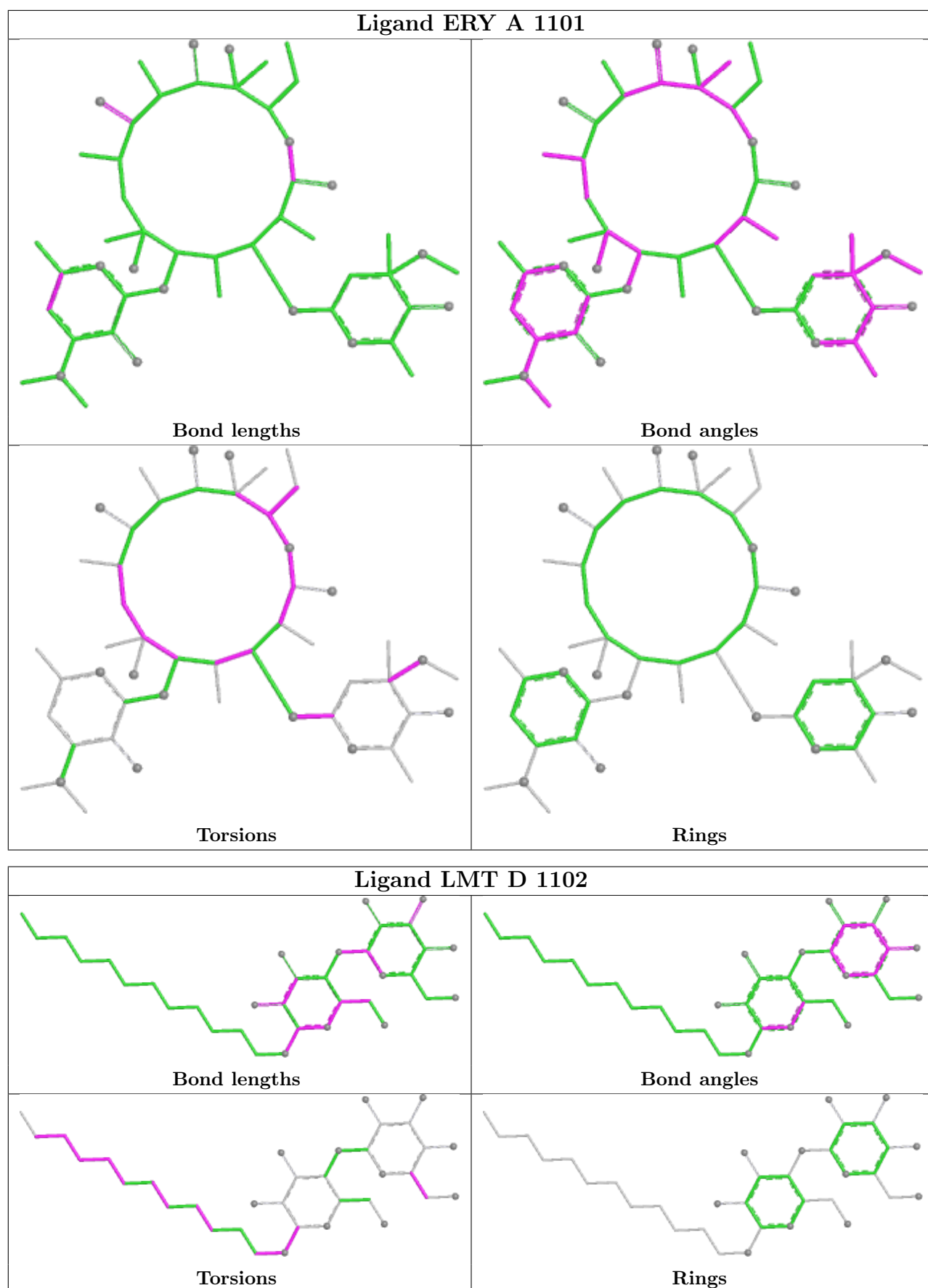
Mol	Chain	Res	Type	Atoms
2	A	1101	ERY	C11-C12-C13-O2
2	A	1101	ERY	C11-C12-C13-C36
2	A	1101	ERY	C35-C12-C13-O2
2	A	1101	ERY	C35-C12-C13-C36
2	A	1101	ERY	O13-C12-C13-O2

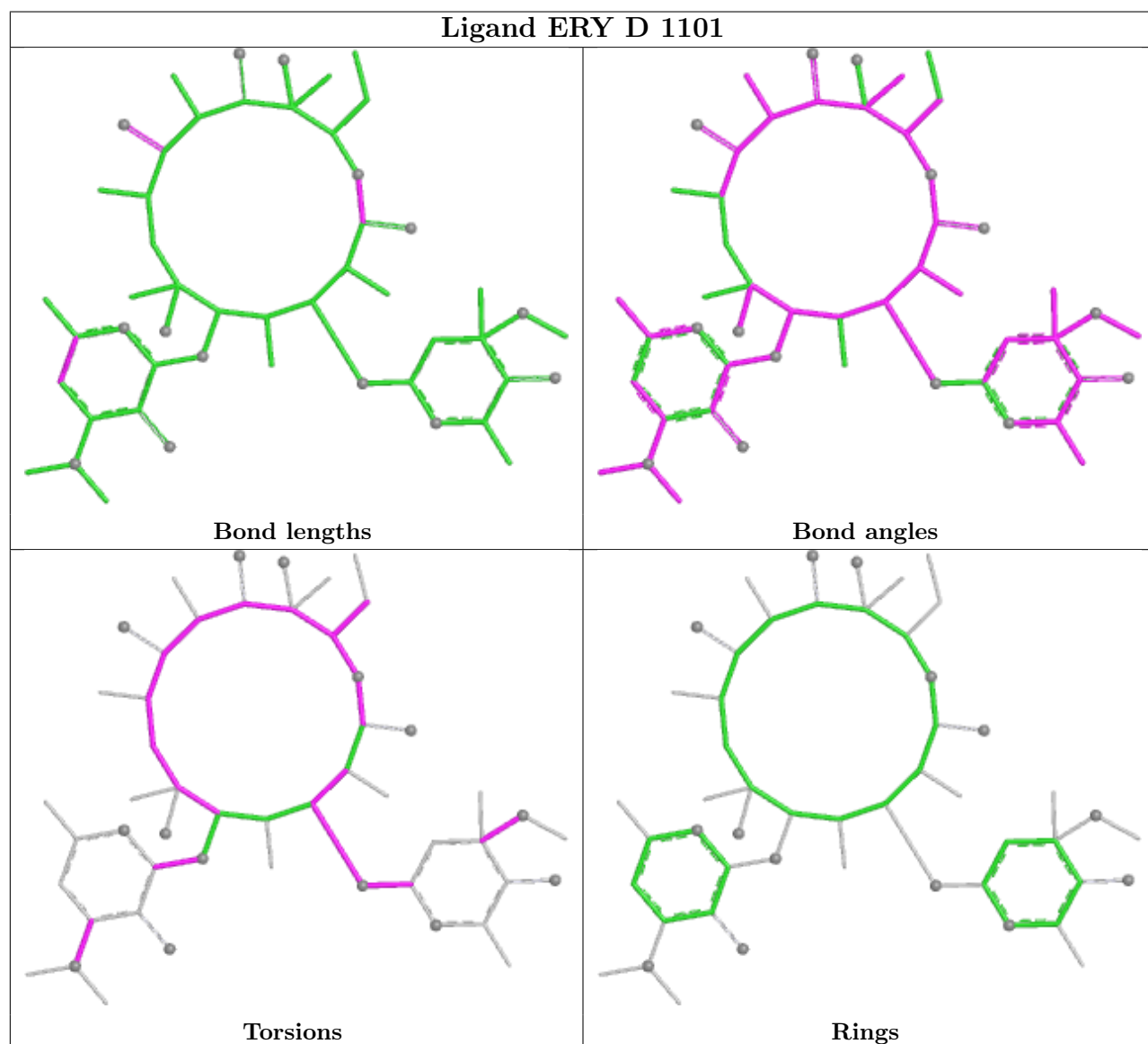
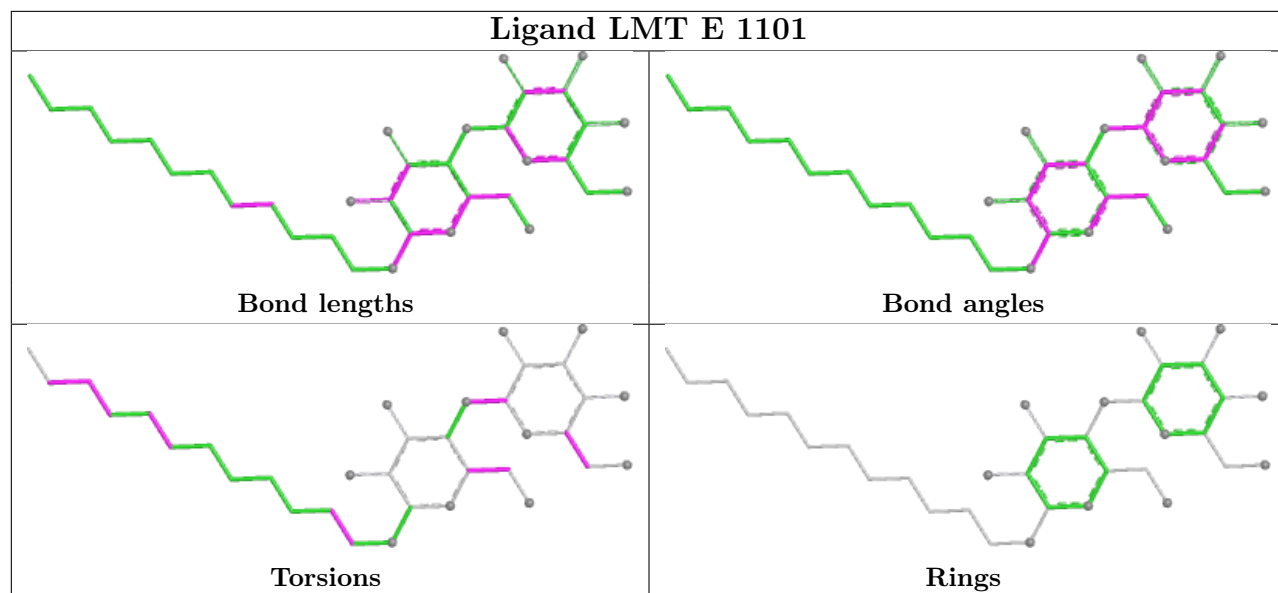
There are no ring outliers.

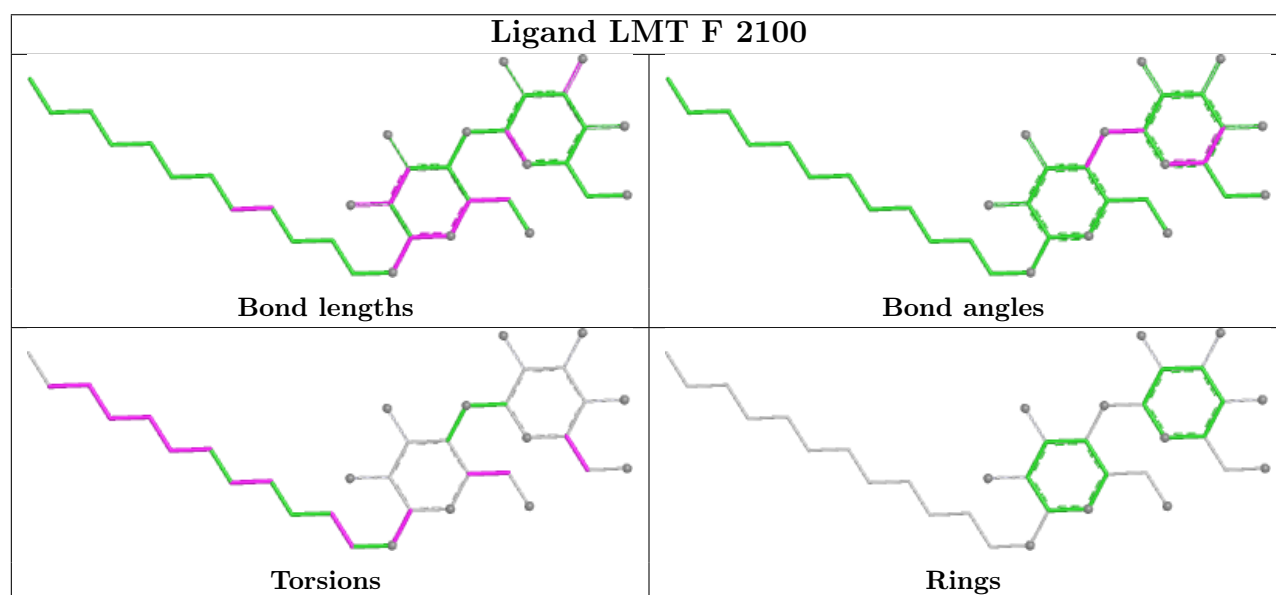
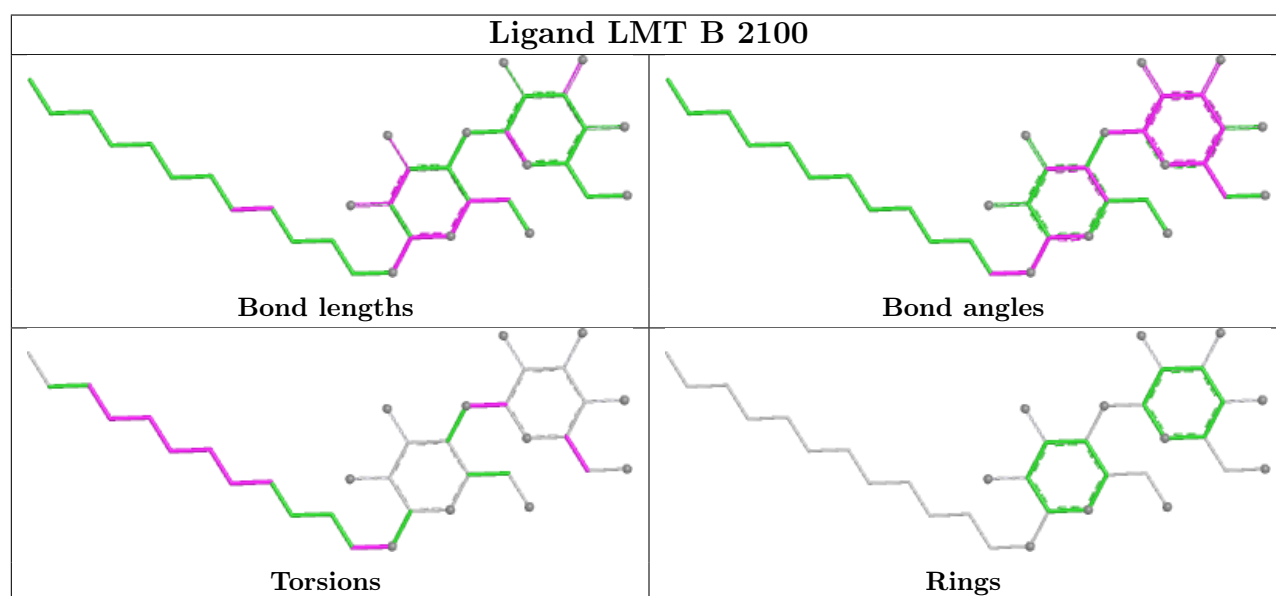
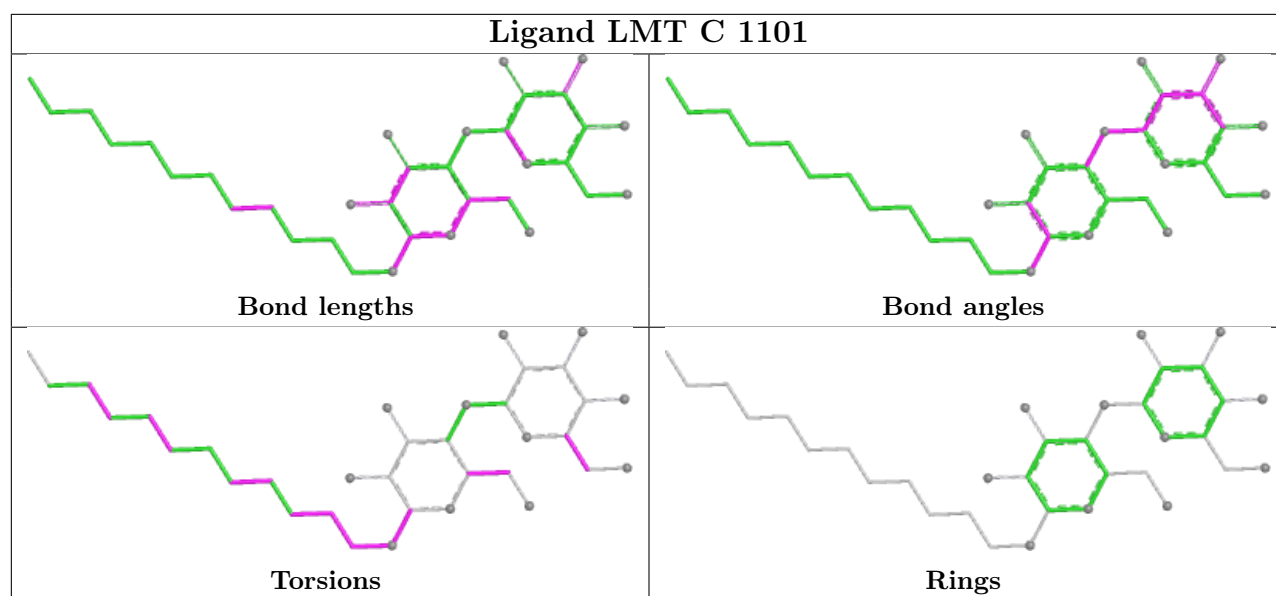
10 monomers are involved in 50 short contacts:

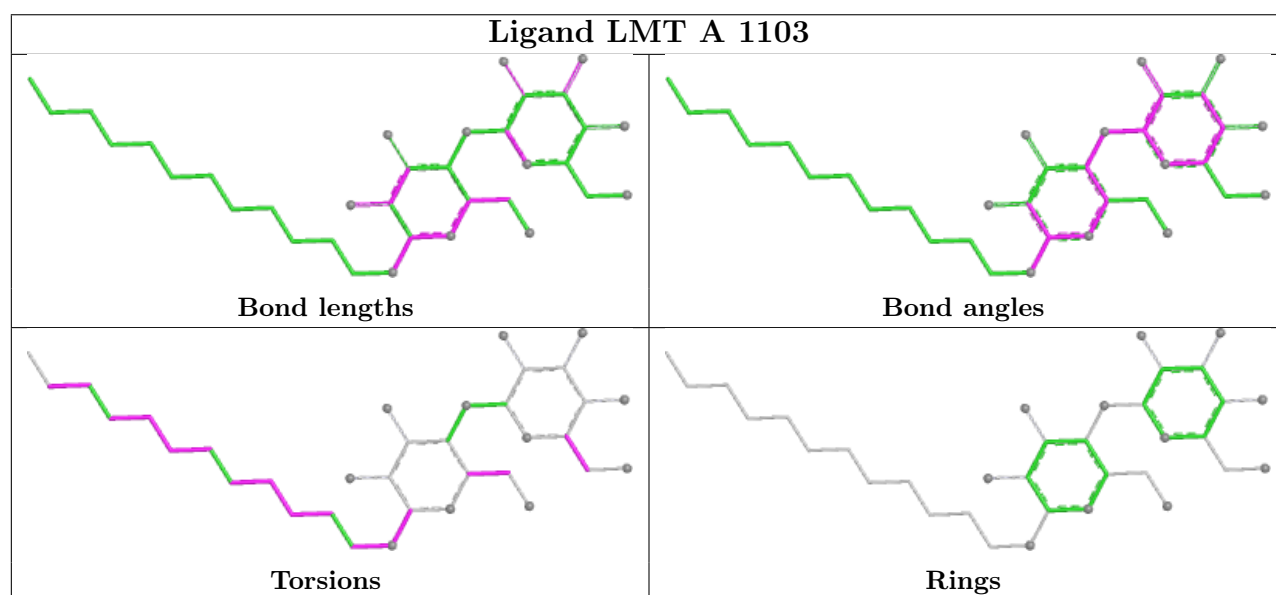
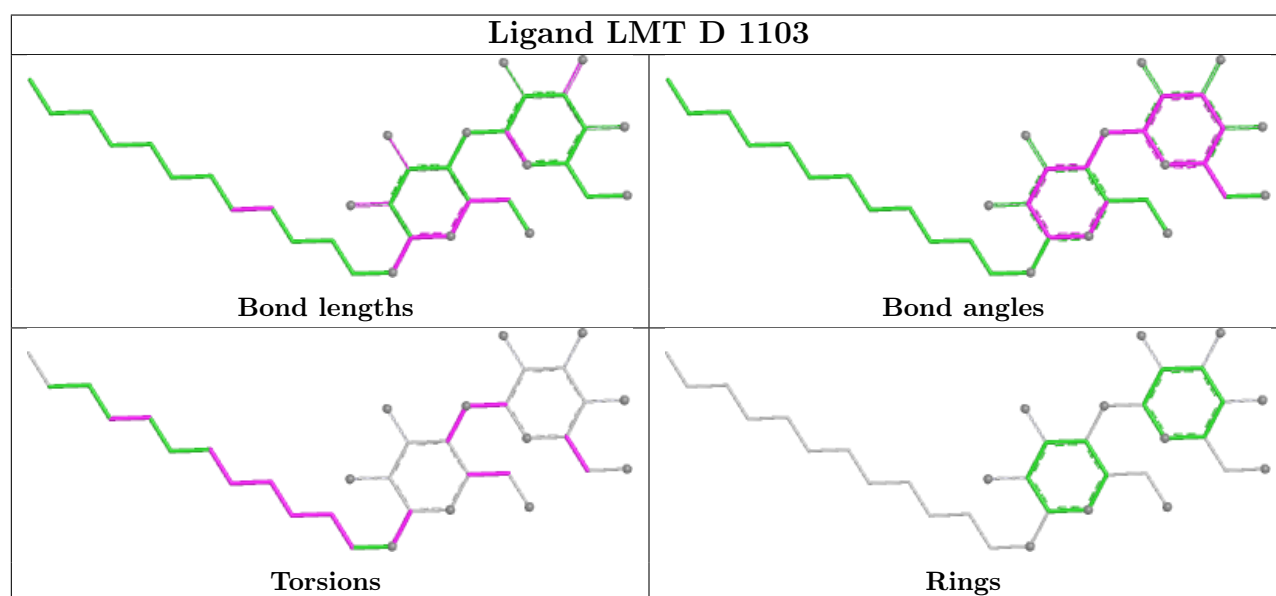
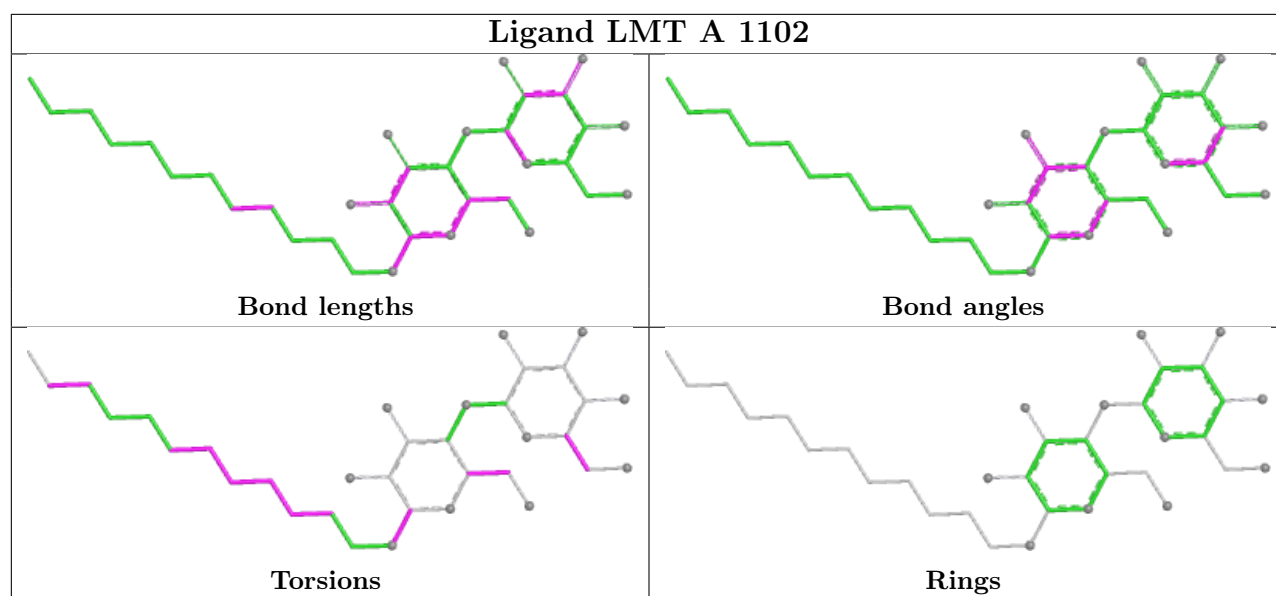
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	ERY	5	0
3	D	1102	LMT	6	0
3	E	1101	LMT	11	0
2	D	1101	ERY	4	0
3	C	1101	LMT	1	0
3	B	2100	LMT	7	0
3	F	2100	LMT	2	0
3	A	1102	LMT	5	0
3	D	1103	LMT	7	0
3	A	1103	LMT	2	0

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 [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	1038/1044 (99%)	-0.19	12 (1%) 76 50	36, 75, 109, 154	0
1	B	1037/1044 (99%)	-0.28	5 (0%) 87 66	31, 73, 111, 150	0
1	C	1036/1044 (99%)	-0.13	19 (1%) 67 40	35, 76, 112, 139	0
1	D	1038/1044 (99%)	-0.20	12 (1%) 76 50	34, 84, 123, 154	0
1	E	1037/1044 (99%)	-0.14	13 (1%) 75 48	46, 87, 118, 148	0
1	F	1037/1044 (99%)	-0.01	32 (3%) 51 29	41, 85, 119, 143	0
All	All	6223/6264 (99%)	-0.16	93 (1%) 72 44	31, 81, 116, 154	0

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	501	ALA	5.7
1	E	291	ILE	5.5
1	C	851	GLY	4.7
1	D	59	ASP	4.6
1	C	122	VAL	4.5

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

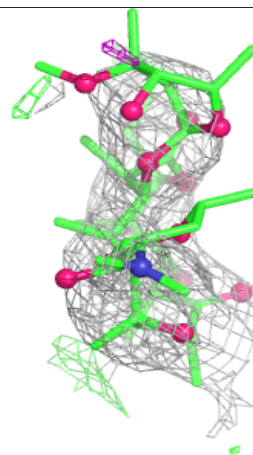
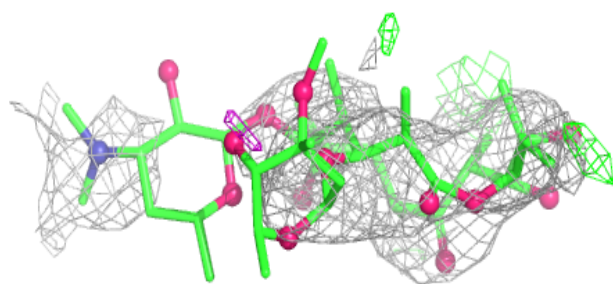
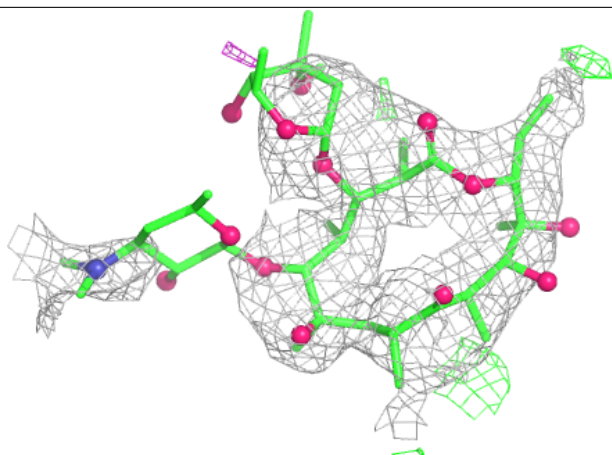
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	ERY	D	1101	51/51	0.56	0.16	62,93,101,108	51
2	ERY	A	1101	51/51	0.70	0.15	81,93,101,104	51
3	LMT	D	1103	35/35	0.71	0.16	77,92,105,106	0
3	LMT	C	1101	35/35	0.86	0.09	62,75,83,87	0
3	LMT	F	2100	35/35	0.87	0.09	49,75,87,96	0
3	LMT	B	2100	35/35	0.88	0.09	34,66,78,87	0
3	LMT	A	1103	35/35	0.88	0.12	65,90,106,109	0
3	LMT	D	1102	35/35	0.89	0.08	38,74,82,84	0
3	LMT	E	1101	35/35	0.90	0.08	63,72,86,108	0
3	LMT	A	1102	35/35	0.93	0.07	49,70,79,82	0
4	NI	A	1104	1/1	0.99	0.02	67,67,67,67	0
4	NI	E	1102	1/1	0.99	0.04	73,73,73,73	0
4	NI	C	1102	1/1	1.00	0.02	77,77,77,77	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.

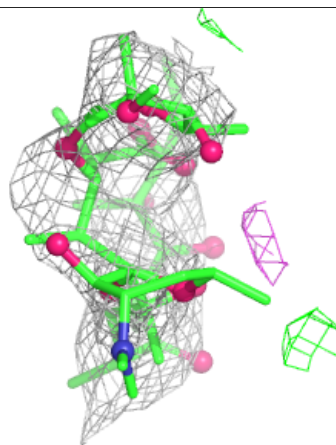
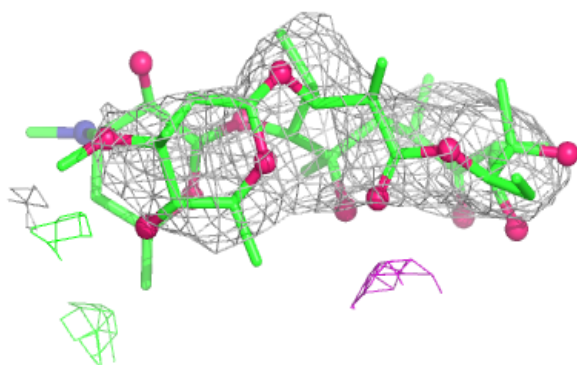
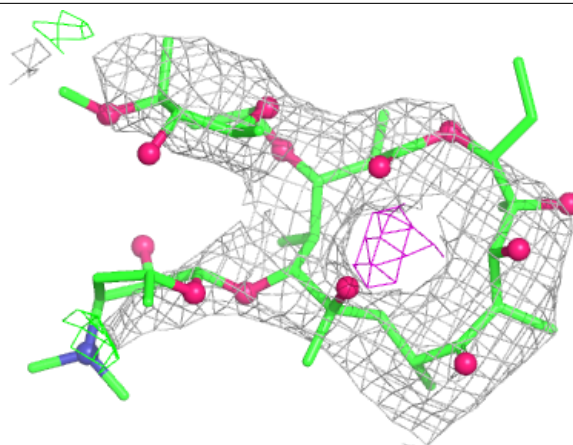
Electron density around ERY D 1101:

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

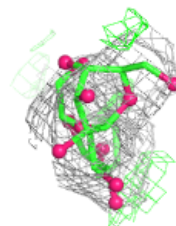
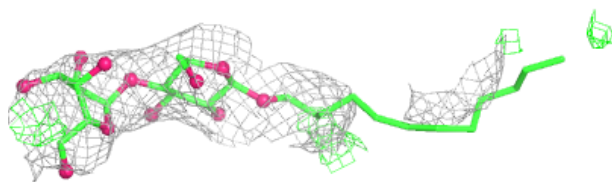
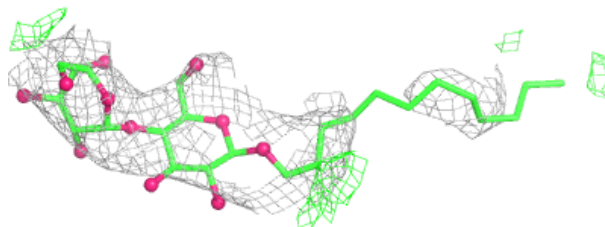


Electron density around ERY A 1101:

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

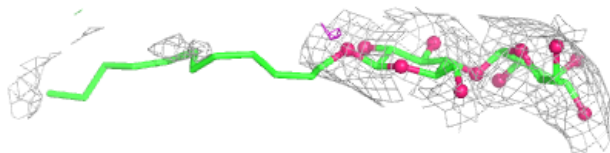
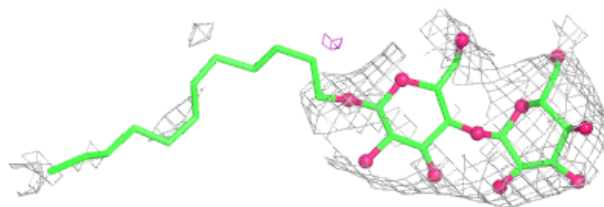
**Electron density around LMT D 1103:**

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

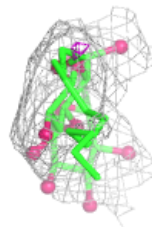
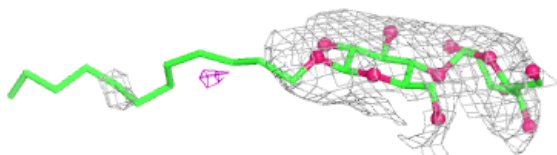
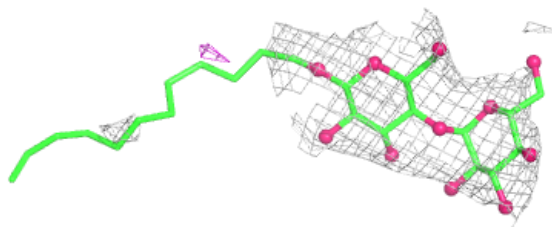


Electron density around LMT C 1101:

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

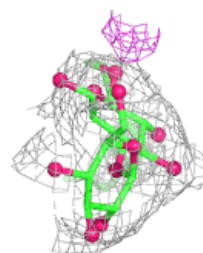
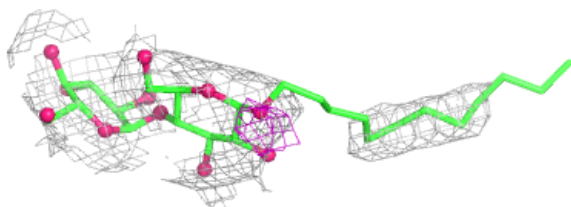
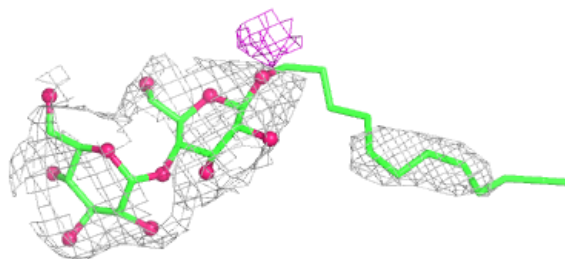
**Electron density around LMT F 2100:**

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

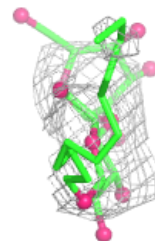
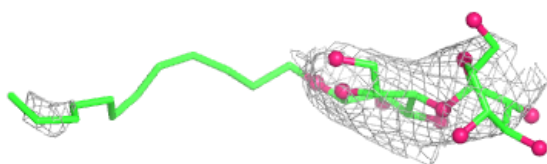
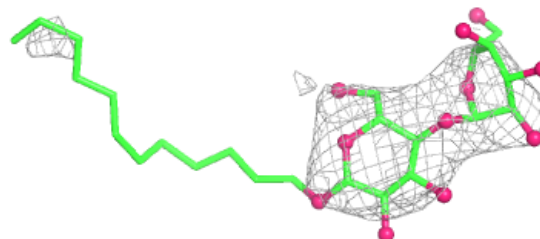


Electron density around LMT B 2100:

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

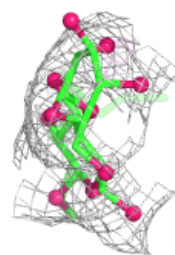
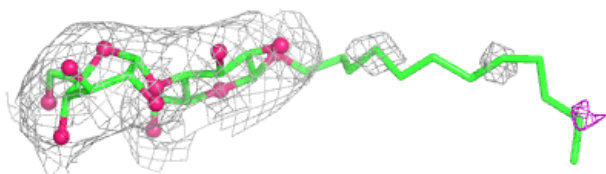
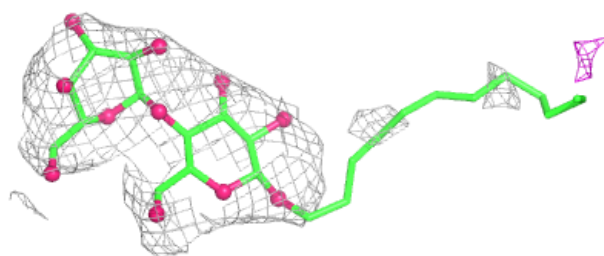
**Electron density around LMT A 1103:**

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

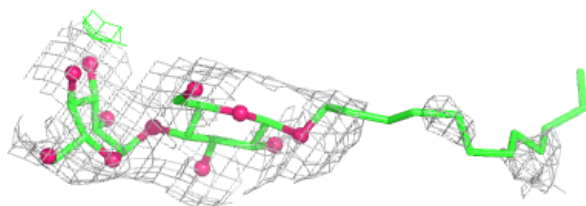
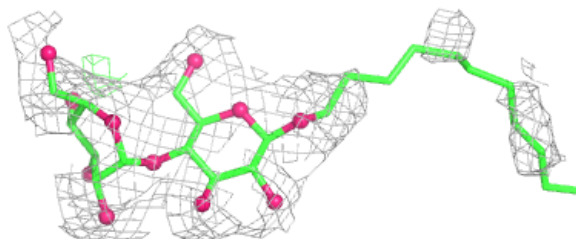


Electron density around LMT D 1102:

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

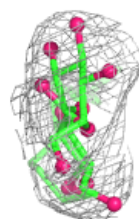
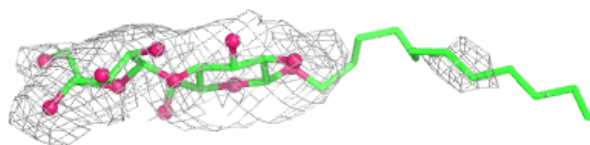
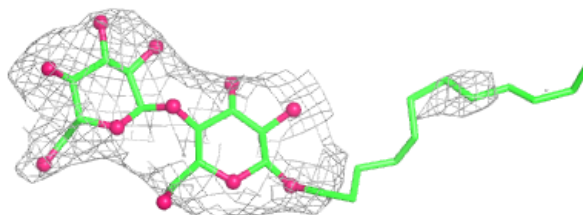
**Electron density around LMT E 1101:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.