



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:29 AM UTC

PDB ID : 6Q4N / pdb_00006q4n
Title : Fusidic acid bound AcrB_V340A
Authors : Tam, H.K.; Pos, K.M.
Deposited on : 2018-12-06
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

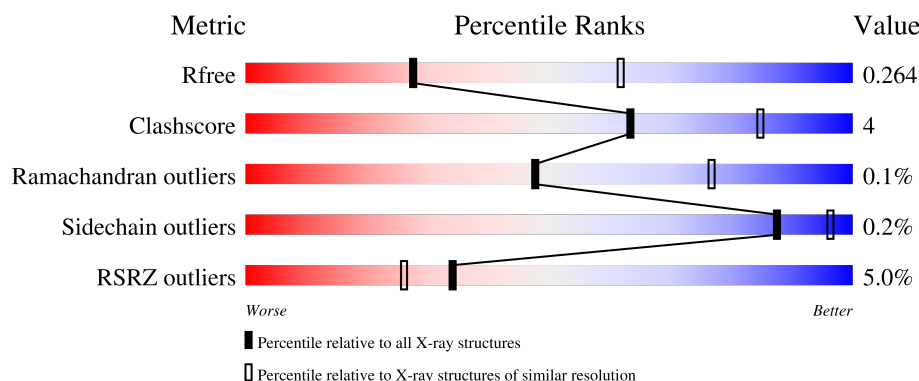
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	
1	B	1057	
1	C	1057	
2	D	169	
2	E	169	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 27045 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	1036	Total	C	N	O	S	0	1	0
			7879	5069	1302	1464	44			
1	B	1034	Total	C	N	O	S	0	0	0
			7853	5053	1296	1460	44			
1	C	1034	Total	C	N	O	S	0	1	0
			7858	5056	1297	1461	44			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	340	ALA	VAL	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	340	ALA	VAL	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	340	ALA	VAL	engineered mutation	UNP P31224
C	1050	LEU	-	expression tag	UNP P31224
C	1051	GLU	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224

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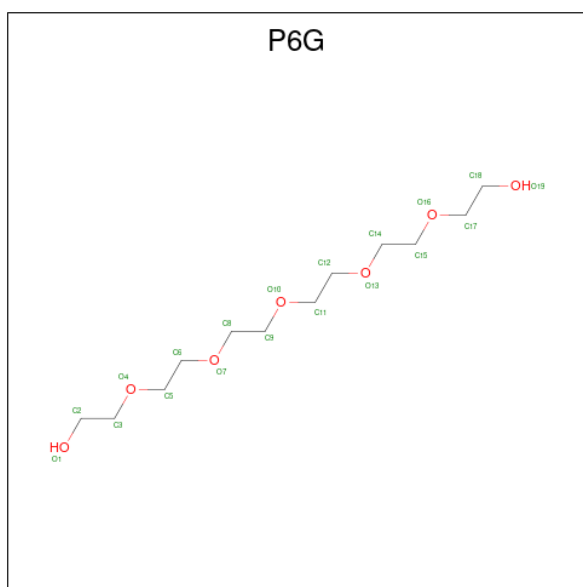
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPin.

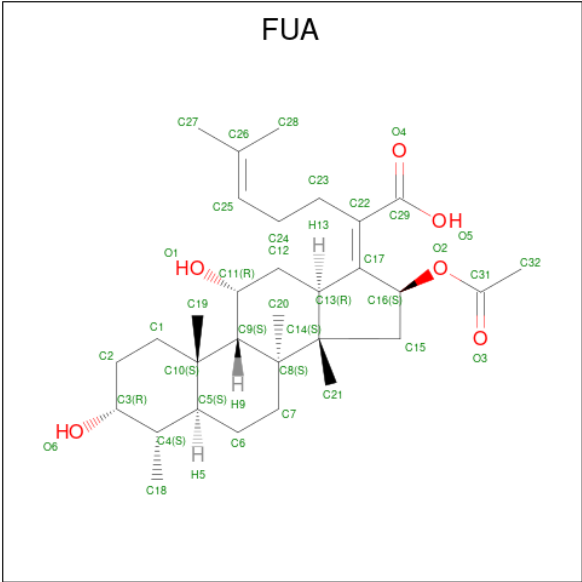
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	156	Total	C	N	O	S	0	0	0
			1177	741	206	229	1			
2	E	154	Total	C	N	O	S	0	0	0
			1167	736	204	226	1			

- Molecule 3 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



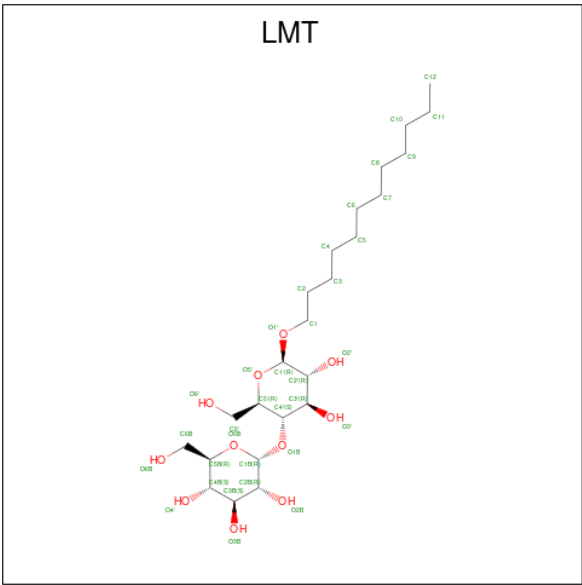
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 4 is FUSIDIC ACID (CCD ID: FUA) (formula: C₃₁H₄₈O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			37	31	6		
4	B	1	Total	C	O	0	0
			37	31	6		
4	C	1	Total	C	O	0	0
			37	31	6		

- Molecule 5 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



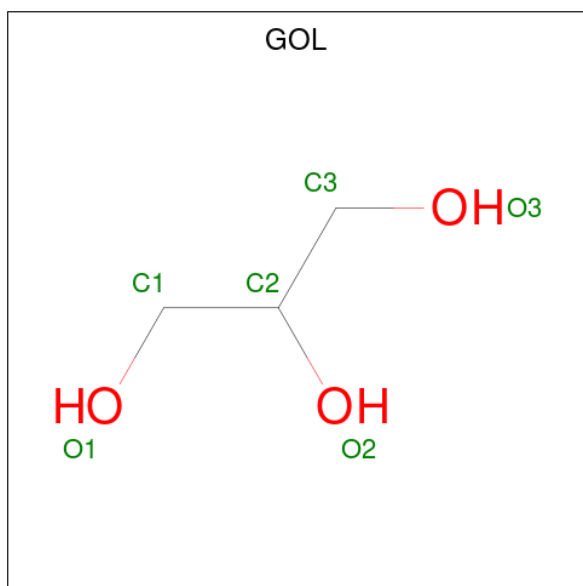
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			35	24	11		

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



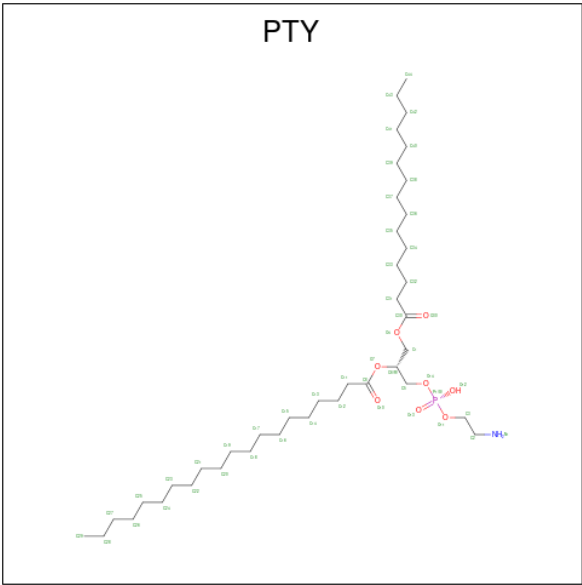
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

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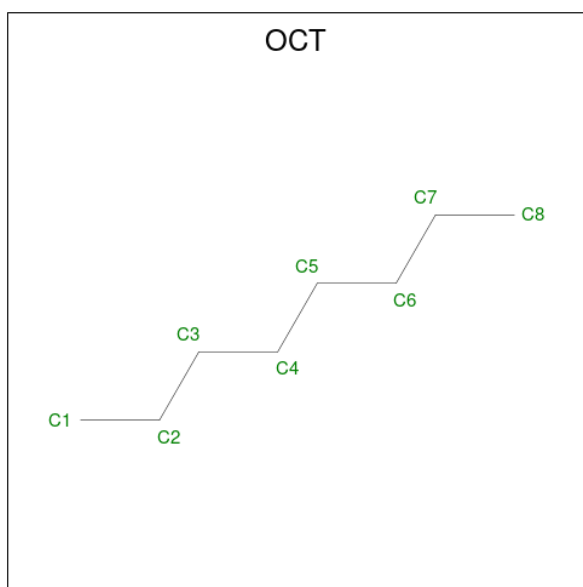
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



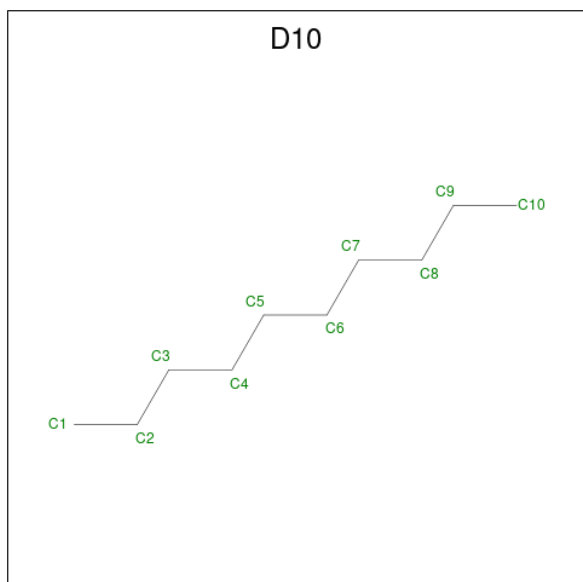
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
7	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
7	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
7	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 8 is N-OCTANE (CCD ID: OCT) (formula: C₈H₁₈).



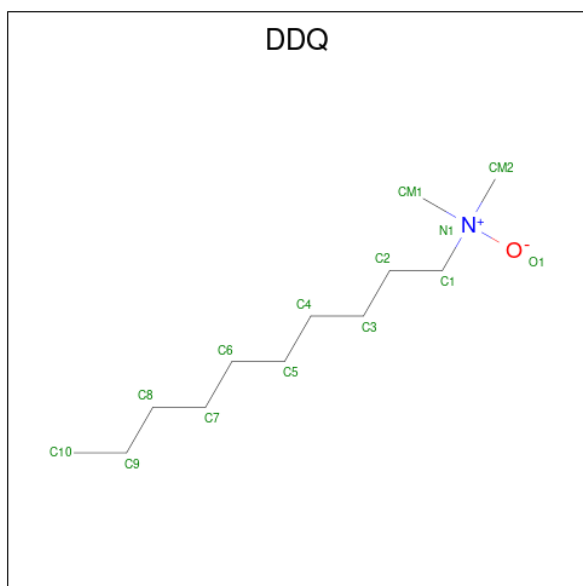
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C 8 8	0	0
8	B	1	Total C 8 8	0	0
8	C	1	Total C 8 8	0	0
8	C	1	Total C 8 8	0	0
8	C	1	Total C 8 8	0	0

- Molecule 9 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$).



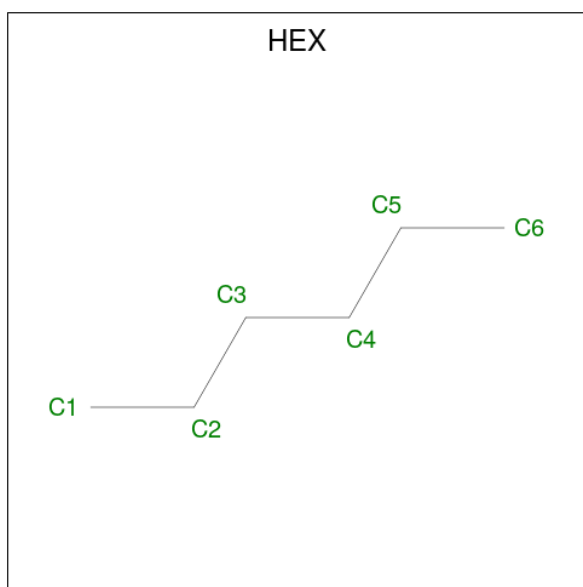
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C 10 10	0	0
9	B	1	Total C 10 10	0	0
9	B	1	Total C 10 10	0	0
9	B	1	Total C 10 10	0	0
9	C	1	Total C 10 10	0	0

- Molecule 10 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (CCD ID: DDQ) (formula: $C_{12}H_{27}NO$).



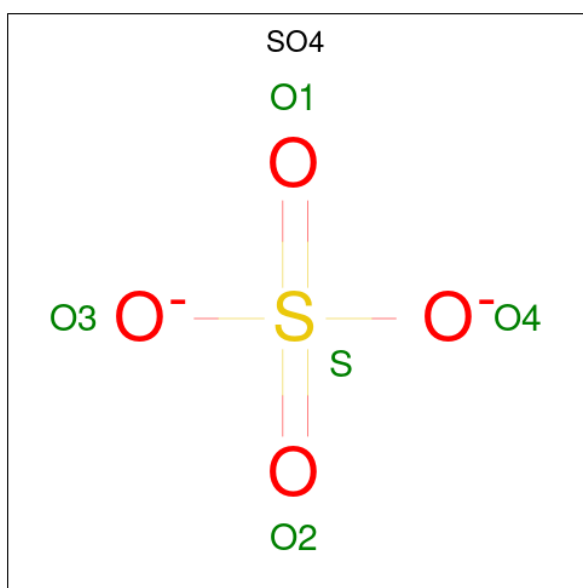
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C N O 14 12 1 1	0	0
10	C	1	Total C N O 14 12 1 1	0	0

- Molecule 11 is HEXANE (CCD ID: HEX) (formula: C_6H_{14}).



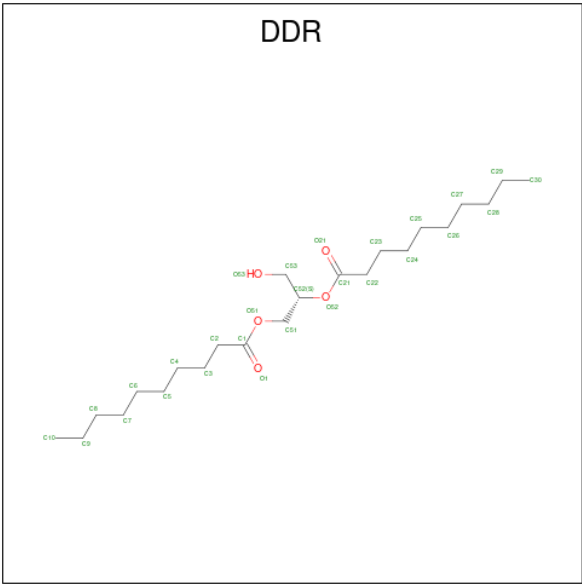
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C 6 6	0	0
11	C	1	Total C 6 6	0	0

- Molecule 12 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



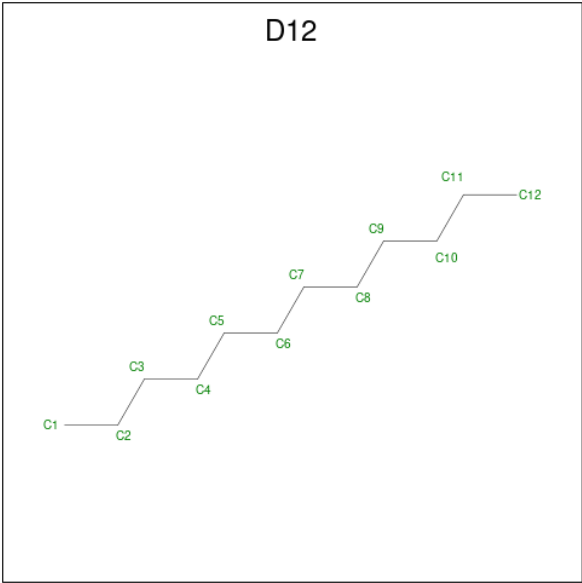
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total O S 5 4 1	0	0
12	C	1	Total O S 5 4 1	0	0

- Molecule 13 is (2S)-3-hydroxypropane-1,2-diyl didecanoate (CCD ID: DDR) (formula: C₂₃H₄₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			28	23	5		

- Molecule 14 is DODECANE (CCD ID: D12) (formula: C₁₂H₂₆).



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

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	79	Total 79	O 79	0	0
15	B	76	Total 76	O 76	0	0
15	C	105	Total 105	O 105	0	0
15	D	18	Total 18	O 18	0	0
15	E	7	Total 7	O 7	0	0

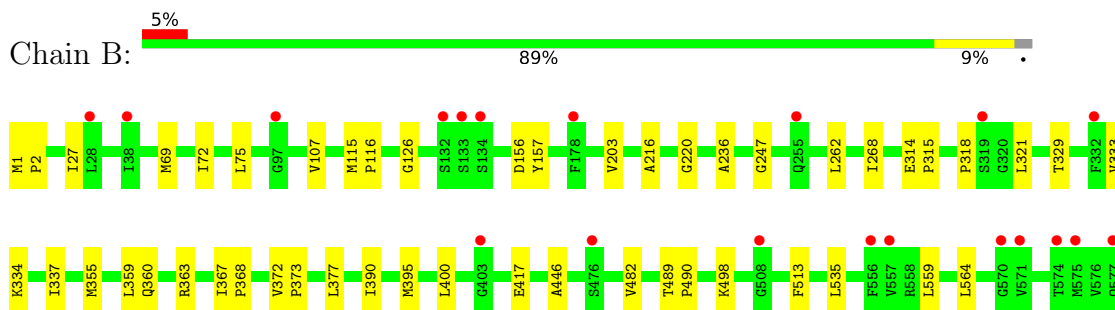
3 Residue-property plots [i](#)

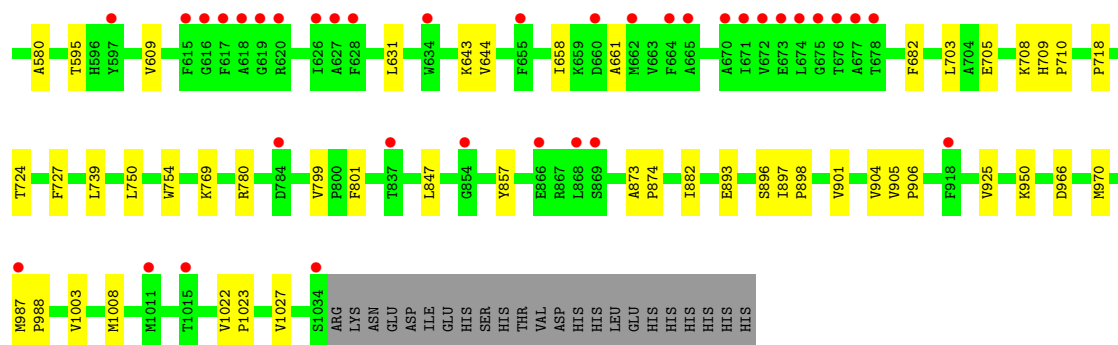
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

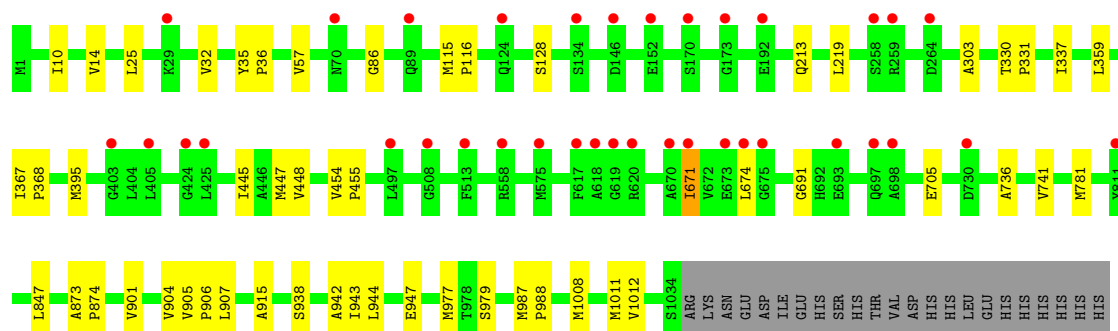


• Molecule 1: Multidrug efflux pump subunit AcrB

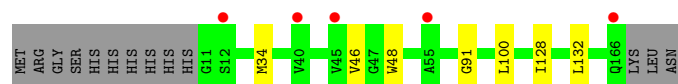
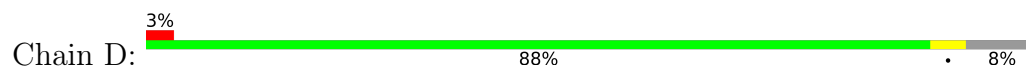




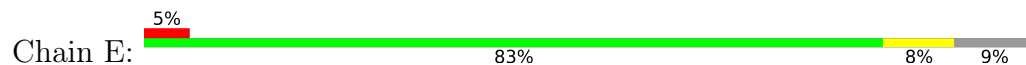
• Molecule 1: Multidrug efflux pump subunit AcrB



• 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	145.21Å 162.99Å 245.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.80 49.09 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.09-2.80) 100.0 (49.09-2.80)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.233 , 0.265 0.234 , 0.264	Depositor DCC
R_{free} test set	7105 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	27045	wwPDB-VP
Average B, all atoms (Å ²)	65.0	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, DDR, GOL, LMT, D10, P6G, D12, OCT, DDQ, HEX, FUA, PTY

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	1.01	0/8032	1.56	4/10905 (0.0%)
1	B	1.01	0/8003	1.55	2/10868 (0.0%)
1	C	1.01	0/8011	1.54	1/10879 (0.0%)
2	D	1.02	0/1196	1.57	0/1626
2	E	1.02	0/1186	1.58	0/1613
All	All	1.01	0/26428	1.55	7/35891 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	896	SER	CA-C-N	6.96	124.62	120.24
1	A	896	SER	C-N-CA	6.96	124.62	120.24
1	A	904	VAL	CA-C-N	6.16	124.12	120.24
1	A	904	VAL	C-N-CA	6.16	124.12	120.24
1	B	896	SER	CA-C-N	5.96	124.00	120.24
1	B	896	SER	C-N-CA	5.96	124.00	120.24
1	C	691	GLY	CA-C-O	-5.18	118.59	122.37

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	7879	0	8034	87	0
1	B	7853	0	8002	61	0
1	C	7858	0	8008	38	0
2	D	1177	0	1159	5	0
2	E	1167	0	1151	8	0
3	A	19	0	26	0	0
4	A	37	0	47	7	0
4	B	37	0	47	7	0
4	C	37	0	47	6	0
5	A	105	0	138	1	0
5	B	105	0	138	1	0
5	C	70	0	92	1	0
6	A	12	0	16	1	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
6	E	12	0	16	1	0
7	B	50	0	79	8	0
7	C	150	0	237	9	0
8	B	16	0	36	0	0
8	C	24	0	54	0	0
9	B	40	0	88	1	0
9	C	10	0	22	0	0
10	B	14	0	27	1	0
10	C	14	0	27	0	0
11	B	6	0	14	0	0
11	C	6	0	14	0	0
12	B	5	0	0	0	0
12	C	5	0	0	0	0
13	B	28	0	44	0	0
14	B	12	0	26	0	0
15	A	79	0	0	0	0
15	B	76	0	0	0	0
15	C	105	0	0	0	0
15	D	18	0	0	0	0
15	E	7	0	0	0	0
All	All	27045	0	27605	219	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 4.

All (219) 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)
4:B:1101:FUA:H122	4:B:1101:FUA:H232	1.54	0.89
4:A:1102:FUA:H202	4:A:1102:FUA:H5	1.54	0.88
4:C:1101:FUA:H202	4:C:1101:FUA:H5	1.62	0.81
7:C:1106:PTY:HC11	7:C:1106:PTY:H322	1.63	0.79
4:B:1101:FUA:H232	4:B:1101:FUA:C12	2.13	0.78
1:B:987:MET:HG3	1:B:1008:MET:HE1	1.66	0.77
1:C:901:VAL:O	1:C:904:VAL:HG12	1.85	0.76
7:B:1105:PTY:H282	10:B:1113:DDQ:H102	1.71	0.72
1:C:904:VAL:HG23	1:C:907:LEU:HD12	1.71	0.71
7:B:1105:PTY:H172	7:B:1105:PTY:H402	1.73	0.71
4:B:1101:FUA:H202	4:B:1101:FUA:H5	1.74	0.69
1:C:359:LEU:HG	1:C:977:MET:HE1	1.75	0.68
4:C:1101:FUA:H122	4:C:1101:FUA:H231	1.75	0.68
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.76	0.68
1:A:493:CYS:O	1:A:497:LEU:HB2	1.94	0.67
1:A:355:MET:HB2	1:A:365:THR:HG23	1.77	0.65
1:C:979:SER:HA	1:C:1011:MET:HE3	1.77	0.65
1:A:968:VAL:HG11	1:A:1023:PRO:HG3	1.77	0.65
7:C:1106:PTY:H322	7:C:1106:PTY:C1	2.27	0.65
1:B:535:LEU:HD22	1:B:1027:VAL:HG21	1.79	0.64
1:B:901:VAL:O	1:B:904:VAL:HG12	1.97	0.64
2:D:34:MET:HE2	2:D:34:MET:HA	1.80	0.63
7:B:1105:PTY:H331	7:B:1105:PTY:HC11	1.81	0.63
1:B:247:GLY:HA2	1:B:268:ILE:CD1	2.29	0.63
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.81	0.62
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.80	0.62
1:A:372:VAL:HG21	1:A:406:VAL:HG22	1.81	0.62
1:C:671:ILE:HD11	1:C:674:LEU:HD12	1.83	0.61
1:A:247:GLY:HA2	1:A:268:ILE:CD1	2.31	0.60
1:C:445:ILE:HD11	1:C:944:LEU:HD21	1.82	0.60
1:B:395:MET:HA	1:B:395:MET:HE2	1.83	0.59
1:A:527:TYR:CD2	1:A:972:LEU:HD22	2.38	0.59
2:D:91:GLY:HA2	2:D:128:ILE:CD1	2.33	0.59
4:C:1101:FUA:H272	4:C:1101:FUA:H232	1.85	0.58
1:A:113:LEU:HD11	1:C:128:SER:HB3	1.86	0.58
1:B:400:LEU:HD21	1:B:1003:VAL:HG13	1.86	0.58
1:A:919:ARG:HD3	1:A:1005:THR:HG21	1.85	0.58
1:B:580:ALA:HB1	1:B:724:THR:HG22	1.86	0.58
1:A:942:ALA:O	1:A:946:VAL:HG23	2.03	0.57
1:A:219:LEU:HD23	1:B:754:TRP:CZ3	2.39	0.56
1:A:897:ILE:N	1:A:898:PRO:HD2	2.19	0.56
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:91:GLY:HA2	2:D:128:ILE:HD12	1.87	0.56
1:A:572:PHE:HE2	1:A:631:LEU:HD21	1.71	0.55
1:C:35:TYR:HB3	1:C:36:PRO:HD2	1.88	0.55
1:B:334:LYS:HG3	4:B:1101:FUA:H281	1.87	0.55
2:E:20:GLU:HG2	6:E:201:GOL:H11	1.87	0.55
1:A:541:TYR:HA	1:A:544:LEU:HD12	1.89	0.54
2:E:14:LEU:HD23	2:E:38:ALA:HA	1.90	0.54
1:A:101:ASP:O	1:A:105:VAL:HG23	2.09	0.53
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.90	0.53
1:A:709:HIS:N	1:A:710:PRO:HD3	2.24	0.52
1:B:400:LEU:CD2	1:B:1003:VAL:HG13	2.40	0.52
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.92	0.52
1:A:676:THR:O	1:A:678:THR:N	2.43	0.52
1:A:879:ILE:O	1:A:883:VAL:HG23	2.09	0.52
1:A:652:THR:HG23	1:A:664:PHE:CB	2.39	0.52
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.92	0.52
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.91	0.51
1:C:32:VAL:HG12	1:C:337:ILE:HD13	1.92	0.51
1:B:882:ILE:HG23	9:B:1111:D10:H91	1.92	0.51
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.92	0.51
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.93	0.51
1:B:337:ILE:HG21	4:B:1101:FUA:H272	1.92	0.51
1:A:457:ALA:HB2	1:A:471:SER:CB	2.41	0.50
1:A:489:THR:HB	1:A:490:PRO:HD3	1.93	0.50
1:A:115:MET:HB2	1:A:116:PRO:HD3	1.94	0.50
1:A:837:THR:HG22	1:A:841:MET:HE3	1.93	0.50
1:A:309:GLU:HG3	1:A:313:MET:HE3	1.93	0.50
1:A:355:MET:CB	1:A:365:THR:HG23	2.42	0.50
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.47	0.50
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.41	0.50
1:A:879:ILE:HD13	1:C:25:LEU:HD11	1.94	0.50
1:C:303:ALA:HB2	1:C:330:THR:HG21	1.92	0.50
1:A:57:VAL:HG12	1:A:88:VAL:HG22	1.92	0.50
1:A:644:VAL:CG1	1:A:667:ASN:HB2	2.42	0.50
1:C:671:ILE:HD11	1:C:674:LEU:CD1	2.41	0.50
4:A:1102:FUA:H202	4:A:1102:FUA:C5	2.34	0.50
1:A:341:VAL:O	1:A:344:LEU:HB2	2.12	0.49
1:B:966:ASP:O	1:B:970:MET:HG3	2.11	0.49
1:A:390:ILE:HG21	5:A:1104:LMT:H32	1.94	0.49
1:B:220:GLY:HA2	1:C:781:MET:SD	2.52	0.49
1:B:390:ILE:HD13	5:B:1103:LMT:H31	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:VAL:HG12	4:A:1102:FUA:H323	1.95	0.49
1:C:873:ALA:HB3	1:C:874:PRO:HD3	1.95	0.49
1:A:509:LYS:O	1:A:514:GLY:HA3	2.13	0.48
1:C:448:VAL:HG11	1:C:943:ILE:HD11	1.95	0.48
2:E:91:GLY:HA2	2:E:128:ILE:HD12	1.95	0.48
1:A:879:ILE:CD1	1:C:25:LEU:HD11	2.43	0.48
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.94	0.48
1:A:987:MET:HB3	1:A:988:PRO:HD3	1.95	0.48
1:B:897:ILE:HD13	1:B:950:LYS:HD2	1.96	0.48
1:A:352:PHE:CD1	1:A:365:THR:HG22	2.49	0.48
1:A:375:VAL:HG11	1:A:405:LEU:CD2	2.42	0.48
1:A:1016:VAL:HG23	1:A:1017:LEU:HD12	1.94	0.48
1:C:1008:MET:O	1:C:1012:VAL:HG23	2.14	0.48
1:A:712:MET:SD	1:A:835:LYS:HD2	2.54	0.48
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.96	0.48
1:A:56:THR:HG23	1:C:213:GLN:HG3	1.95	0.47
4:B:1101:FUA:C12	4:B:1101:FUA:C23	2.90	0.47
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.97	0.47
1:C:330:THR:N	1:C:331:PRO:CD	2.77	0.47
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.96	0.47
2:D:46:VAL:HG23	2:D:48:TRP:CD1	2.49	0.47
1:A:973:ARG:N	1:A:974:PRO:HD2	2.29	0.47
7:B:1105:PTY:H361	7:C:1104:PTY:H371	1.95	0.47
7:B:1105:PTY:H112	7:B:1105:PTY:HC12	1.96	0.46
1:A:968:VAL:HG11	1:A:1023:PRO:CG	2.44	0.46
1:B:157:TYR:CE2	1:B:318:PRO:HD3	2.51	0.46
7:C:1106:PTY:H171	7:C:1106:PTY:H352	1.97	0.46
1:A:298:ASN:HB3	1:A:301:ASP:HB2	1.98	0.46
1:A:330:THR:N	1:A:331:PRO:CD	2.79	0.46
1:B:359:LEU:HD13	1:B:417:GLU:HG3	1.98	0.45
1:B:595:THR:HG23	1:B:609:VAL:HB	1.98	0.45
1:B:703:LEU:HD11	1:B:718:PRO:HD3	1.97	0.45
7:C:1106:PTY:C1	7:C:1106:PTY:C32	2.92	0.45
1:B:156:ASP:OD1	1:B:769:LYS:NZ	2.49	0.45
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.31	0.45
1:A:946:VAL:HG13	1:A:1026:PHE:CE1	2.52	0.45
1:B:360:GLN:HG2	1:B:513:PHE:CD2	2.50	0.45
1:B:658:ILE:HG22	1:B:661:ALA:HB3	1.99	0.45
1:A:184:MET:HG2	1:A:246:PHE:CD2	2.51	0.45
1:A:864:TYR:O	1:A:868:LEU:HD13	2.17	0.45
1:A:961:ILE:HD11	1:A:1031:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1107:GOL:H31	1:B:75:LEU:HD23	1.99	0.45
2:E:133:LEU:HD21	2:E:139:VAL:HG12	1.99	0.45
1:C:671:ILE:HD11	1:C:674:LEU:CG	2.46	0.45
4:C:1101:FUA:H202	4:C:1101:FUA:C5	2.40	0.45
1:C:10:ILE:O	1:C:14:VAL:HG23	2.17	0.45
2:E:82:THR:O	2:E:85:HIS:HB2	2.17	0.45
2:E:23:ARG:HG3	2:E:57:TRP:CD1	2.52	0.45
1:A:207:ILE:O	1:A:211:ASN:HB3	2.18	0.44
1:C:447:MET:HE1	7:C:1106:PTY:H372	1.99	0.44
1:A:482:VAL:O	1:A:486:LEU:HG	2.17	0.44
1:A:712:MET:HG2	1:A:843:LEU:HD22	1.98	0.44
1:A:901:VAL:O	1:A:904:VAL:HG22	2.17	0.44
1:B:27:ILE:CD1	1:B:377:LEU:HD22	2.47	0.44
1:B:631:LEU:HD11	1:B:644:VAL:HG22	1.98	0.44
1:B:750:LEU:HB2	1:B:801:PHE:CZ	2.52	0.44
1:B:897:ILE:N	1:B:898:PRO:HD2	2.31	0.44
1:A:838:GLY:O	1:A:842:GLU:HG3	2.17	0.44
1:A:330:THR:OG1	1:A:331:PRO:HD3	2.17	0.44
2:E:91:GLY:HA2	2:E:128:ILE:CD1	2.48	0.44
4:A:1102:FUA:O4	4:A:1102:FUA:H242	2.17	0.44
1:A:219:LEU:HD11	1:B:727:PHE:CG	2.53	0.43
1:B:395:MET:HA	1:B:395:MET:CE	2.47	0.43
1:C:395:MET:HE2	1:C:395:MET:HA	1.99	0.43
1:A:1:MET:HB2	1:A:2:PRO:HD3	2.00	0.43
1:A:184:MET:HG2	1:A:246:PHE:CE2	2.53	0.43
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.18	0.43
1:A:449:LEU:HB3	1:A:478:MET:SD	2.58	0.43
1:B:754:TRP:CH2	1:B:780:ARG:HA	2.53	0.43
7:B:1105:PTY:P1	7:B:1105:PTY:H311	2.57	0.43
1:A:506:GLY:C	1:A:508:GLY:H	2.27	0.43
4:A:1102:FUA:C5	4:A:1102:FUA:C20	2.96	0.43
1:C:705:GLU:HB3	1:C:847:LEU:HD22	2.01	0.43
1:C:915:ALA:HA	5:C:1103:LMT:H92	2.01	0.43
1:A:952:LEU:O	1:A:956:GLU:HB2	2.18	0.43
4:A:1102:FUA:O1	4:A:1102:FUA:H12	2.19	0.43
1:B:72:ILE:HD13	1:B:107:VAL:HG22	2.00	0.43
1:B:216:ALA:HB2	1:B:236:ALA:HB2	2.00	0.43
1:C:454:VAL:HB	1:C:455:PRO:HD3	2.00	0.43
1:C:904:VAL:HG11	1:C:942:ALA:HB2	2.01	0.43
4:C:1101:FUA:H232	4:C:1101:FUA:C27	2.47	0.43
2:E:108:ALA:O	2:E:116:PRO:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:VAL:HG12	1:A:667:ASN:HB2	2.01	0.42
7:C:1106:PTY:O14	7:C:1106:PTY:HC21	2.18	0.42
1:A:911:GLY:CA	1:A:1013:THR:HG21	2.49	0.42
1:B:893:GLU:O	1:B:893:GLU:HG3	2.19	0.42
1:C:671:ILE:HD11	1:C:674:LEU:HG	2.00	0.42
1:B:897:ILE:N	1:B:898:PRO:CD	2.82	0.42
1:A:359:LEU:HD13	1:A:364:ALA:HB1	2.02	0.42
1:C:736:ALA:HB1	1:C:741:VAL:HG23	2.00	0.42
1:A:754:TRP:CZ3	1:A:780:ARG:HA	2.54	0.42
1:B:709:HIS:N	1:B:710:PRO:HD3	2.34	0.42
1:B:126:GLY:HA3	1:C:116:PRO:HB3	2.02	0.42
1:B:987:MET:N	1:B:988:PRO:CD	2.82	0.42
7:B:1105:PTY:HC11	7:B:1105:PTY:C33	2.49	0.42
1:B:739:LEU:HD13	1:B:799:VAL:HG11	2.02	0.42
1:A:544:LEU:O	1:A:547:ILE:HB	2.20	0.41
1:A:968:VAL:CG1	1:A:1023:PRO:HG3	2.48	0.41
1:B:708:LYS:C	1:B:710:PRO:HD3	2.45	0.41
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.85	0.41
4:A:1102:FUA:H122	4:A:1102:FUA:C23	2.50	0.41
1:B:363:ARG:HD2	1:B:498:LYS:HE3	2.02	0.41
1:A:38:ILE:HD11	1:A:671:ILE:HD13	2.02	0.41
1:A:137:LEU:HD11	1:A:299:ALA:HB1	2.02	0.41
1:B:314:GLU:HB2	1:B:315:PRO:HD3	2.02	0.41
1:A:445:ILE:CG1	1:A:943:ILE:HG21	2.51	0.41
1:B:329:THR:O	1:B:333:VAL:HG23	2.20	0.41
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.96	0.41
1:A:445:ILE:HG12	1:A:943:ILE:HG21	2.03	0.41
1:B:203:VAL:HG13	1:B:262:LEU:CD1	2.51	0.41
1:A:405:LEU:HD21	1:A:477:ALA:HB1	2.02	0.41
1:B:355:MET:HE2	1:B:368:PRO:HG2	2.01	0.41
2:D:100:LEU:HD11	2:D:132:LEU:HD23	2.03	0.41
1:A:449:LEU:HD21	1:A:936:GLY:CA	2.51	0.41
1:B:559:LEU:HD12	1:B:559:LEU:HA	1.94	0.41
1:C:904:VAL:HG13	1:C:938:SER:HB3	2.02	0.41
1:A:578:LEU:HD23	1:A:586:ARG:HE	1.85	0.41
1:A:777:ALA:O	1:A:781:MET:HG2	2.21	0.41
1:A:168:ARG:HG2	1:B:69:MET:O	2.21	0.40
1:B:115:MET:HB2	1:B:116:PRO:HD3	2.03	0.40
1:B:318:PRO:HD2	1:B:321:LEU:HD22	2.03	0.40
1:A:905:VAL:N	1:A:906:PRO:CD	2.84	0.40
1:A:1016:VAL:HG23	1:A:1017:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:905:VAL:HB	1:C:906:PRO:HD3	2.03	0.40
1:A:157:TYR:CD2	1:A:321:LEU:HD21	2.56	0.40
1:A:326:PRO:O	1:A:630:SER:HB2	2.20	0.40
1:A:750:LEU:HB2	1:A:801:PHE:CZ	2.56	0.40
1:B:564:LEU:HD23	1:B:925:VAL:HG22	2.04	0.40
1:B:643:LYS:HA	1:B:643:LYS:HD3	1.82	0.40
7:B:1105:PTY:H382	7:C:1104:PTY:H391	2.02	0.40
1:A:946:VAL:HG13	1:A:1026:PHE:CD1	2.56	0.40
4:B:1101:FUA:H202	4:B:1101:FUA:C5	2.45	0.40
4:C:1101:FUA:H231	4:C:1101:FUA:C12	2.47	0.40
1:A:303:ALA:HB2	1:A:330:THR:HG21	2.04	0.40
1:C:115:MET:N	1:C:116:PRO:HD2	2.36	0.40
1:C:947:GLU:OE2	7:C:1106:PTY:N1	2.54	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	1035/1057 (98%)	997 (96%)	36 (4%)	2 (0%)	43	72
1	B	1032/1057 (98%)	1008 (98%)	24 (2%)	0	100	100
1	C	1033/1057 (98%)	1010 (98%)	23 (2%)	0	100	100
2	D	154/169 (91%)	152 (99%)	2 (1%)	0	100	100
2	E	152/169 (90%)	148 (97%)	4 (3%)	0	100	100
All	All	3406/3509 (97%)	3315 (97%)	89 (3%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	677	ALA

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Mol	Chain	Res	Type
1	A	538	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	842/862 (98%)	838 (100%)	4 (0%)	81	93
1	B	839/862 (97%)	839 (100%)	0	100	100
1	C	840/862 (97%)	839 (100%)	1 (0%)	88	97
2	D	120/132 (91%)	120 (100%)	0	100	100
2	E	119/132 (90%)	119 (100%)	0	100	100
All	All	2760/2850 (97%)	2755 (100%)	5 (0%)	87	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	ASP
1	A	437	GLN
1	A	801	PHE
1	A	972	LEU
1	C	671	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	ASN
1	A	237	GLN
1	A	274	ASN
1	A	361	ASN
1	A	605	ASN
1	A	687	GLN
1	B	58	GLN
1	B	70	ASN

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Mol	Chain	Res	Type
1	B	108	GLN
1	B	112	GLN
1	B	194	ASN
1	B	231	ASN
1	B	517	ASN
1	B	525	HIS
1	B	657	GLN
1	B	846	GLN
1	C	58	GLN
1	C	254	ASN
1	C	274	ASN
1	C	360	GLN
1	C	517	ASN
1	C	569	GLN
1	C	577	GLN
1	C	588	GLN
1	C	613	ASN
1	C	1001	ASN
2	D	92	HIS
2	E	122	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

40 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
5	LMT	C	1102	-	36,36,36	0.40	0	47,47,47	0.55	0
5	LMT	B	1104	-	36,36,36	0.43	0	47,47,47	0.94	2 (4%)
11	HEX	B	1114	-	5,5,5	0.13	0	4,4,4	0.11	0
6	GOL	E	201	-	5,5,5	0.09	0	5,5,5	0.25	0
9	D10	B	1112	-	9,9,9	0.12	0	8,8,8	0.07	0
10	DDQ	B	1113	-	11,13,13	2.28	2 (18%)	12,15,15	0.55	0
8	OCT	C	1109	-	7,7,7	0.10	0	6,6,6	0.07	0
11	HEX	C	1113	-	5,5,5	0.13	0	4,4,4	0.07	0
9	D10	B	1110	-	9,9,9	0.11	0	8,8,8	0.14	0
5	LMT	A	1104	-	36,36,36	0.39	0	47,47,47	1.04	3 (6%)
4	FUA	A	1102	-	39,40,40	1.67	3 (7%)	50,64,64	0.88	1 (2%)
6	GOL	A	1107	-	5,5,5	0.09	0	5,5,5	0.28	0
5	LMT	B	1103	-	36,36,36	0.47	0	47,47,47	0.68	0
9	D10	B	1111	-	9,9,9	0.14	0	8,8,8	0.13	0
8	OCT	C	1110	-	7,7,7	0.10	0	6,6,6	0.11	0
8	OCT	B	1107	-	7,7,7	0.09	0	6,6,6	0.11	0
6	GOL	E	202	-	5,5,5	0.09	0	5,5,5	0.26	0
7	PTY	C	1105	-	49,49,49	0.30	0	52,54,54	0.33	0
8	OCT	B	1108	-	7,7,7	0.11	0	6,6,6	0.17	0
12	SO4	B	1115	-	4,4,4	0.34	0	6,6,6	0.07	0
12	SO4	C	1114	-	4,4,4	0.34	0	6,6,6	0.08	0
9	D10	B	1109	-	9,9,9	0.09	0	8,8,8	0.09	0
14	D12	B	1117	-	11,11,11	0.21	0	10,10,10	0.55	0
7	PTY	B	1105	-	49,49,49	0.30	0	52,54,54	0.38	0
5	LMT	C	1103	-	36,36,36	0.54	1 (2%)	47,47,47	1.01	4 (8%)
6	GOL	A	1106	-	5,5,5	0.09	0	5,5,5	0.24	0
6	GOL	C	1107	-	5,5,5	0.09	0	5,5,5	0.26	0
9	D10	C	1111	-	9,9,9	0.11	0	8,8,8	0.05	0
4	FUA	C	1101	-	39,40,40	1.67	2 (5%)	50,64,64	1.03	4 (8%)
3	P6G	A	1101	-	18,18,18	0.51	0	17,17,17	0.20	0
10	DDQ	C	1112	-	11,13,13	2.28	2 (18%)	12,15,15	0.51	0
13	DDR	B	1116	-	27,27,27	1.23	2 (7%)	29,29,29	1.18	3 (10%)
6	GOL	B	1106	-	5,5,5	0.09	0	5,5,5	0.26	0
5	LMT	A	1105	-	36,36,36	0.43	0	47,47,47	0.57	0
7	PTY	C	1106	-	49,49,49	0.28	0	52,54,54	0.46	0
5	LMT	A	1103	-	36,36,36	0.41	0	47,47,47	0.71	1 (2%)
8	OCT	C	1108	-	7,7,7	0.10	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PTY	C	1104	-	49,49,49	0.27	0	52,54,54	0.38	0
4	FUA	B	1101	-	39,40,40	1.70	2 (5%)	50,64,64	0.94	2 (4%)
5	LMT	B	1102	-	36,36,36	0.43	0	47,47,47	0.61	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
5	LMT	C	1102	-	-	8/21/61/61	0/2/2/2
5	LMT	B	1104	-	-	6/21/61/61	0/2/2/2
11	HEX	B	1114	-	-	0/3/3/3	-
6	GOL	E	201	-	-	0/4/4/4	-
9	D10	B	1112	-	-	2/7/7/7	-
10	DDQ	B	1113	-	-	2/11/11/11	-
8	OCT	C	1109	-	-	2/5/5/5	-
11	HEX	C	1113	-	-	1/3/3/3	-
9	D10	B	1110	-	-	5/7/7/7	-
5	LMT	A	1104	-	-	4/21/61/61	0/2/2/2
4	FUA	A	1102	-	-	7/16/92/92	0/4/4/4
6	GOL	A	1107	-	-	2/4/4/4	-
5	LMT	B	1103	-	-	13/21/61/61	0/2/2/2
9	D10	B	1111	-	-	5/7/7/7	-
8	OCT	C	1110	-	-	4/5/5/5	-
8	OCT	B	1107	-	-	4/5/5/5	-
6	GOL	E	202	-	-	2/4/4/4	-
7	PTY	C	1105	-	-	25/53/53/53	-
8	OCT	B	1108	-	-	1/5/5/5	-
9	D10	B	1109	-	-	3/7/7/7	-
14	D12	B	1117	-	-	5/9/9/9	-
7	PTY	B	1105	-	-	30/53/53/53	-
5	LMT	C	1103	-	-	11/21/61/61	0/2/2/2
6	GOL	A	1106	-	-	0/4/4/4	-
6	GOL	C	1107	-	-	1/4/4/4	-
9	D10	C	1111	-	-	2/7/7/7	-
4	FUA	C	1101	-	-	5/16/92/92	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P6G	A	1101	-	-	12/16/16/16	-
10	DDQ	C	1112	-	-	3/11/11/11	-
13	DDR	B	1116	-	-	18/29/29/29	-
6	GOL	B	1106	-	-	2/4/4/4	-
5	LMT	A	1105	-	-	11/21/61/61	0/2/2/2
7	PTY	C	1106	-	-	33/53/53/53	-
5	LMT	A	1103	-	-	12/21/61/61	0/2/2/2
8	OCT	C	1108	-	-	3/5/5/5	-
7	PTY	C	1104	-	-	23/53/53/53	-
4	FUA	B	1101	-	-	5/16/92/92	0/4/4/4
5	LMT	B	1102	-	-	9/21/61/61	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1101	FUA	C29-C22	-9.96	1.33	1.47
4	C	1101	FUA	C29-C22	-9.71	1.34	1.47
4	A	1102	FUA	C29-C22	-9.51	1.34	1.47
10	B	1113	DDQ	O1-N1	-6.80	1.25	1.42
10	C	1112	DDQ	O1-N1	-6.77	1.25	1.42
13	B	1116	DDR	O51-C1	4.35	1.46	1.33
13	B	1116	DDR	O52-C21	4.07	1.45	1.34
10	B	1113	DDQ	C1-N1	-3.24	1.48	1.51
10	C	1112	DDQ	C1-N1	-3.21	1.48	1.51
4	A	1102	FUA	O5-C29	-2.64	1.23	1.30
4	C	1101	FUA	O5-C29	-2.58	1.23	1.30
4	B	1101	FUA	O5-C29	-2.56	1.23	1.30
5	C	1103	LMT	O1'-C1'	2.22	1.43	1.40
4	A	1102	FUA	C9-C11	2.03	1.57	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1116	DDR	O52-C21-C22	3.56	119.17	111.48
5	A	1104	LMT	O5'-C5'-C4'	3.11	116.15	109.72
5	B	1104	LMT	O5'-C5'-C4'	3.10	116.14	109.72
4	C	1101	FUA	C10-C5-C4	-3.05	109.50	113.20
5	A	1104	LMT	C1'-O5'-C5'	2.87	119.32	113.72
13	B	1116	DDR	O51-C1-C2	2.73	120.17	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1103	LMT	O5'-C5'-C4'	2.71	115.32	109.72
5	C	1103	LMT	C3'-C4'-C5'	2.56	116.61	110.93
5	C	1103	LMT	O5'-C1'-C2'	-2.52	105.20	110.37
4	C	1101	FUA	C6-C5-C10	2.50	114.66	111.66
13	B	1116	DDR	C52-O52-C21	-2.50	111.82	117.80
5	A	1104	LMT	C1B-O1B-C4'	-2.34	112.43	117.98
5	B	1104	LMT	C3'-C4'-C5'	2.21	115.83	110.93
4	A	1102	FUA	C24-C23-C22	2.17	117.34	112.72
4	C	1101	FUA	O2-C16-C17	2.17	114.66	108.30
4	C	1101	FUA	C18-C4-C5	2.15	116.43	112.95
4	B	1101	FUA	C7-C8-C14	2.14	112.63	110.78
4	B	1101	FUA	C14-C8-C9	-2.10	105.60	109.30
5	C	1103	LMT	C1B-C2B-C3B	2.07	114.36	110.01
5	A	1103	LMT	C1B-O1B-C4'	-2.00	113.24	117.98

There are no chirality outliers.

All (281) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	FUA	C23-C22-C29-O4
4	A	1102	FUA	C23-C22-C29-O5
4	B	1101	FUA	C23-C22-C29-O4
4	B	1101	FUA	C23-C22-C29-O5
4	B	1101	FUA	C32-C31-O2-C16
4	B	1101	FUA	O3-C31-O2-C16
4	C	1101	FUA	C23-C22-C29-O4
4	C	1101	FUA	C23-C22-C29-O5
4	C	1101	FUA	C23-C24-C25-C26
5	B	1102	LMT	C2'-C1'-O1'-C1
5	B	1102	LMT	O5'-C1'-O1'-C1
5	B	1103	LMT	C2-C1-O1'-C1'
7	B	1105	PTY	C11-C8-O7-C6
7	B	1105	PTY	C3-O11-P1-O12
7	B	1105	PTY	C3-O11-P1-O14
7	C	1104	PTY	O4-C1-C6-O7
7	C	1104	PTY	C3-O11-P1-O12
7	C	1104	PTY	C3-O11-P1-O14
7	C	1105	PTY	C11-C8-O7-C6
7	C	1105	PTY	C3-O11-P1-O13
7	C	1105	PTY	C3-O11-P1-O14
7	C	1105	PTY	C5-O14-P1-O11
7	C	1106	PTY	N1-C2-C3-O11

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Mol	Chain	Res	Type	Atoms
7	C	1106	PTY	C2-C3-O11-P1
7	C	1106	PTY	C11-C8-O7-C6
7	C	1106	PTY	C3-O11-P1-O13
7	C	1106	PTY	C3-O11-P1-O14
7	C	1106	PTY	C5-O14-P1-O11
4	A	1102	FUA	C32-C31-O2-C16
7	B	1105	PTY	C31-C30-O4-C1
7	B	1105	PTY	O30-C30-O4-C1
7	C	1106	PTY	O30-C30-O4-C1
7	B	1105	PTY	O10-C8-O7-C6
7	C	1105	PTY	O10-C8-O7-C6
7	C	1106	PTY	C31-C30-O4-C1
4	A	1102	FUA	O3-C31-O2-C16
7	C	1106	PTY	O10-C8-O7-C6
5	A	1105	LMT	O5B-C5B-C6B-O6B
5	C	1103	LMT	O5'-C5'-C6'-O6'
5	C	1103	LMT	C4'-C5'-C6'-O6'
4	A	1102	FUA	C22-C23-C24-C25
4	C	1101	FUA	C22-C23-C24-C25
3	A	1101	P6G	O4-C5-C6-O7
5	B	1103	LMT	O5'-C1'-O1'-C1
5	C	1102	LMT	O5'-C1'-O1'-C1
5	B	1103	LMT	O5'-C5'-C6'-O6'
5	A	1103	LMT	O5B-C5B-C6B-O6B
5	A	1103	LMT	C4B-C5B-C6B-O6B
3	A	1101	P6G	O7-C8-C9-O10
5	C	1103	LMT	C4B-C5B-C6B-O6B
5	C	1102	LMT	C2'-C1'-O1'-C1
5	B	1103	LMT	C4'-C5'-C6'-O6'
7	C	1105	PTY	C31-C30-O4-C1
13	B	1116	DDR	C2-C1-O51-C51
5	C	1103	LMT	O5B-C5B-C6B-O6B
3	A	1101	P6G	O13-C14-C15-O16
3	A	1101	P6G	O16-C17-C18-O19
5	A	1105	LMT	C4B-C5B-C6B-O6B
7	C	1105	PTY	C8-C11-C12-C13
5	C	1103	LMT	O5'-C1'-O1'-C1
7	B	1105	PTY	C24-C25-C26-C27
13	B	1116	DDR	C22-C21-O52-C52
7	C	1105	PTY	O30-C30-O4-C1
7	C	1106	PTY	C8-C11-C12-C13
13	B	1116	DDR	O21-C21-O52-C52

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Mol	Chain	Res	Type	Atoms
5	A	1105	LMT	O1'-C1-C2-C3
13	B	1116	DDR	O1-C1-O51-C51
5	C	1103	LMT	C2'-C1'-O1'-C1
7	B	1105	PTY	C26-C27-C28-C29
6	A	1107	GOL	O1-C1-C2-C3
6	B	1106	GOL	C1-C2-C3-O3
6	E	202	GOL	C1-C2-C3-O3
5	C	1102	LMT	C6-C7-C8-C9
9	B	1109	D10	C6-C7-C8-C9
7	C	1104	PTY	C32-C33-C34-C35
7	C	1106	PTY	C18-C19-C20-C21
7	C	1104	PTY	C18-C19-C20-C21
6	A	1107	GOL	O1-C1-C2-O2
6	B	1106	GOL	O2-C2-C3-O3
5	C	1103	LMT	C3-C4-C5-C6
5	A	1105	LMT	C3-C4-C5-C6
7	C	1104	PTY	C35-C36-C37-C38
5	A	1104	LMT	C6-C7-C8-C9
5	A	1103	LMT	C1-C2-C3-C4
5	C	1102	LMT	C7-C8-C9-C10
7	C	1104	PTY	C13-C14-C15-C16
7	C	1106	PTY	C12-C13-C14-C15
5	B	1103	LMT	C1-C2-C3-C4
5	A	1103	LMT	O5'-C5'-C6'-O6'
5	B	1103	LMT	C5-C6-C7-C8
9	B	1109	D10	C3-C4-C5-C6
3	A	1101	P6G	O10-C11-C12-O13
5	C	1103	LMT	C2-C3-C4-C5
7	C	1106	PTY	C11-C12-C13-C14
7	B	1105	PTY	C35-C36-C37-C38
7	B	1105	PTY	C40-C41-C42-C43
8	C	1110	OCT	C2-C3-C4-C5
5	B	1104	LMT	O5B-C1B-O1B-C4'
8	C	1109	OCT	C4-C5-C6-C7
5	A	1104	LMT	C4-C5-C6-C7
5	B	1104	LMT	C5-C6-C7-C8
7	C	1104	PTY	C31-C32-C33-C34
7	C	1105	PTY	C32-C33-C34-C35
4	A	1102	FUA	C29-C22-C23-C24
5	B	1104	LMT	C4-C5-C6-C7
7	C	1104	PTY	C38-C39-C40-C41
7	C	1106	PTY	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
13	B	1116	DDR	C1-C2-C3-C4
7	C	1105	PTY	C22-C23-C24-C25
5	A	1103	LMT	C2-C3-C4-C5
7	B	1105	PTY	C19-C20-C21-C22
10	C	1112	DDQ	C6-C7-C8-C9
13	B	1116	DDR	C23-C24-C25-C26
8	B	1107	OCT	C3-C4-C5-C6
7	B	1105	PTY	C34-C35-C36-C37
7	C	1105	PTY	C39-C40-C41-C42
9	C	1111	D10	C2-C3-C4-C5
5	B	1102	LMT	C6-C7-C8-C9
7	C	1106	PTY	C25-C26-C27-C28
9	B	1110	D10	C6-C7-C8-C9
5	B	1102	LMT	C5-C6-C7-C8
7	C	1104	PTY	C11-C8-O7-C6
5	C	1102	LMT	C1-C2-C3-C4
5	B	1104	LMT	C7-C8-C9-C10
7	B	1105	PTY	C20-C21-C22-C23
5	B	1102	LMT	C2-C3-C4-C5
7	C	1106	PTY	C33-C34-C35-C36
7	C	1106	PTY	C20-C21-C22-C23
10	C	1112	DDQ	C7-C8-C9-C10
8	C	1108	OCT	C3-C4-C5-C6
9	B	1109	D10	C2-C3-C4-C5
11	C	1113	HEX	C2-C3-C4-C5
5	A	1105	LMT	C5-C6-C7-C8
7	C	1105	PTY	C18-C19-C20-C21
5	B	1103	LMT	O5B-C5B-C6B-O6B
7	C	1104	PTY	C12-C13-C14-C15
7	C	1106	PTY	C23-C24-C25-C26
5	B	1103	LMT	C3-C4-C5-C6
5	A	1105	LMT	C11-C10-C9-C8
7	B	1105	PTY	C31-C32-C33-C34
14	B	1117	D12	C7-C8-C9-C10
7	B	1105	PTY	O14-C5-C6-C1
7	C	1104	PTY	O10-C8-O7-C6
7	C	1104	PTY	C40-C41-C42-C43
7	C	1105	PTY	C24-C25-C26-C27
10	C	1112	DDQ	C4-C5-C6-C7
7	C	1104	PTY	O4-C1-C6-C5
5	A	1103	LMT	C4-C5-C6-C7
4	A	1102	FUA	C17-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
7	B	1105	PTY	C17-C18-C19-C20
7	C	1106	PTY	C21-C22-C23-C24
7	C	1104	PTY	C15-C16-C17-C18
7	C	1106	PTY	C5-C6-O7-C8
7	C	1105	PTY	C25-C26-C27-C28
13	B	1116	DDR	C22-C23-C24-C25
8	C	1109	OCT	C1-C2-C3-C4
5	B	1102	LMT	O5B-C5B-C6B-O6B
7	C	1106	PTY	C38-C39-C40-C41
9	B	1111	D10	C7-C8-C9-C10
5	C	1103	LMT	C5-C6-C7-C8
13	B	1116	DDR	C27-C28-C29-C30
7	C	1105	PTY	C11-C12-C13-C14
5	B	1102	LMT	C9-C10-C11-C12
9	B	1111	D10	C1-C2-C3-C4
5	A	1103	LMT	C3-C4-C5-C6
7	C	1104	PTY	C26-C27-C28-C29
5	A	1103	LMT	C7-C8-C9-C10
13	B	1116	DDR	C7-C8-C9-C10
13	B	1116	DDR	C24-C25-C26-C27
5	C	1102	LMT	C2-C1-O1'-C1'
5	C	1103	LMT	C2-C1-O1'-C1'
14	B	1117	D12	C6-C7-C8-C9
7	C	1105	PTY	C6-C5-O14-P1
7	C	1106	PTY	C6-C5-O14-P1
8	C	1110	OCT	C1-C2-C3-C4
5	A	1105	LMT	C1-C2-C3-C4
10	B	1113	DDQ	C7-C8-C9-C10
7	C	1105	PTY	O14-C5-C6-C1
9	B	1112	D10	C4-C5-C6-C7
7	C	1106	PTY	O4-C30-C31-C32
9	B	1110	D10	C7-C8-C9-C10
9	C	1111	D10	C1-C2-C3-C4
5	C	1102	LMT	C9-C10-C11-C12
7	C	1106	PTY	C41-C42-C43-C44
7	B	1105	PTY	C21-C22-C23-C24
8	C	1110	OCT	C4-C5-C6-C7
13	B	1116	DDR	C51-C52-C53-O53
7	C	1104	PTY	C33-C34-C35-C36
7	B	1105	PTY	O14-C5-C6-O7
7	C	1105	PTY	O14-C5-C6-O7
7	B	1105	PTY	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
7	C	1104	PTY	C20-C21-C22-C23
7	C	1106	PTY	C19-C20-C21-C22
5	A	1104	LMT	C2-C3-C4-C5
8	C	1108	OCT	C2-C3-C4-C5
5	A	1105	LMT	O5'-C5'-C6'-O6'
3	A	1101	P6G	C8-C9-O10-C11
13	B	1116	DDR	C3-C4-C5-C6
14	B	1117	D12	C1-C2-C3-C4
7	C	1104	PTY	C23-C24-C25-C26
5	B	1103	LMT	C2-C3-C4-C5
10	B	1113	DDQ	C6-C7-C8-C9
7	B	1105	PTY	C25-C26-C27-C28
7	C	1105	PTY	C20-C21-C22-C23
3	A	1101	P6G	O1-C2-C3-O4
7	C	1104	PTY	C34-C35-C36-C37
5	A	1103	LMT	C11-C10-C9-C8
8	C	1110	OCT	C5-C6-C7-C8
5	A	1105	LMT	C9-C10-C11-C12
7	B	1105	PTY	C32-C33-C34-C35
7	C	1106	PTY	C24-C25-C26-C27
7	B	1105	PTY	C11-C12-C13-C14
7	B	1105	PTY	C8-C11-C12-C13
8	C	1108	OCT	C1-C2-C3-C4
3	A	1101	P6G	C15-C14-O13-C12
7	C	1105	PTY	C21-C22-C23-C24
7	C	1105	PTY	C26-C27-C28-C29
5	B	1104	LMT	C3-C4-C5-C6
5	A	1103	LMT	C5-C6-C7-C8
7	C	1105	PTY	C40-C41-C42-C43
9	B	1110	D10	C3-C4-C5-C6
13	B	1116	DDR	C2-C3-C4-C5
5	C	1103	LMT	C7-C8-C9-C10
9	B	1112	D10	C3-C4-C5-C6
5	A	1104	LMT	C4B-C5B-C6B-O6B
7	C	1106	PTY	C31-C32-C33-C34
3	A	1101	P6G	C14-C15-O16-C17
7	B	1105	PTY	C38-C39-C40-C41
7	B	1105	PTY	C3-O11-P1-O13
7	B	1105	PTY	C5-O14-P1-O13
7	C	1105	PTY	C3-O11-P1-O12
7	C	1105	PTY	C5-O14-P1-O13
7	C	1106	PTY	C5-O14-P1-O13

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Mol	Chain	Res	Type	Atoms
6	E	202	GOL	O2-C2-C3-O3
7	B	1105	PTY	C41-C42-C43-C44
7	C	1106	PTY	C16-C17-C18-C19
7	C	1104	PTY	C24-C25-C26-C27
5	B	1103	LMT	O1'-C1-C2-C3
5	B	1102	LMT	O1'-C1-C2-C3
9	B	1110	D10	C2-C3-C4-C5
7	C	1106	PTY	C15-C16-C17-C18
5	A	1105	LMT	C2-C3-C4-C5
14	B	1117	D12	C9-C10-C11-C12
5	A	1105	LMT	C4-C5-C6-C7
5	B	1103	LMT	C3'-C4'-O1B-C1B
7	C	1105	PTY	C16-C17-C18-C19
5	B	1102	LMT	O5'-C5'-C6'-O6'
5	B	1104	LMT	C1-C2-C3-C4
7	C	1106	PTY	C35-C36-C37-C38
13	B	1116	DDR	O52-C52-C53-O53
9	B	1111	D10	C5-C6-C7-C8
5	B	1103	LMT	C5'-C4'-O1B-C1B
6	C	1107	GOL	O1-C1-C2-O2
8	B	1107	OCT	C1-C2-C3-C4
14	B	1117	D12	C4-C5-C6-C7
7	B	1105	PTY	C12-C13-C14-C15
5	B	1103	LMT	C6-C7-C8-C9
7	C	1104	PTY	C21-C22-C23-C24
7	C	1106	PTY	O30-C30-C31-C32
8	B	1107	OCT	C4-C5-C6-C7
13	B	1116	DDR	C26-C27-C28-C29
9	B	1110	D10	C5-C6-C7-C8
13	B	1116	DDR	O52-C21-C22-C23
5	C	1102	LMT	C4B-C5B-C6B-O6B
9	B	1111	D10	C4-C5-C6-C7
9	B	1111	D10	C2-C3-C4-C5
13	B	1116	DDR	C25-C26-C27-C28
4	C	1101	FUA	C17-C16-O2-C31
4	B	1101	FUA	C29-C22-C23-C24
5	A	1103	LMT	C4'-C5'-C6'-O6'
7	C	1104	PTY	C25-C26-C27-C28
8	B	1107	OCT	C2-C3-C4-C5
3	A	1101	P6G	C5-C6-O7-C8
8	B	1108	OCT	C5-C6-C7-C8
7	B	1105	PTY	C36-C37-C38-C39

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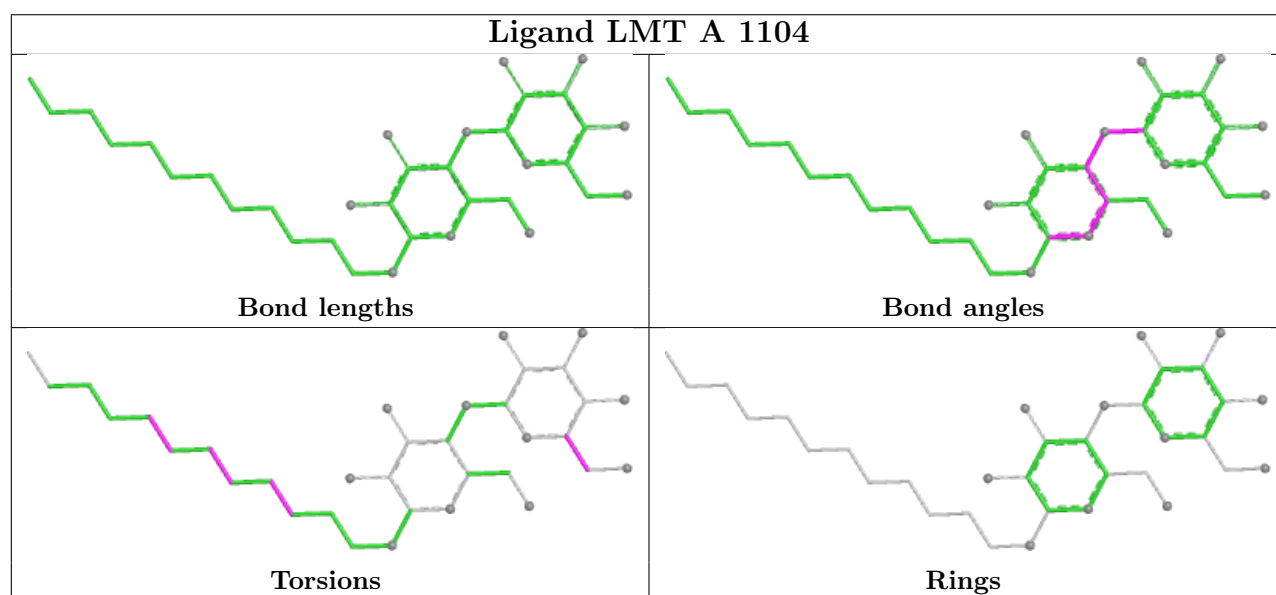
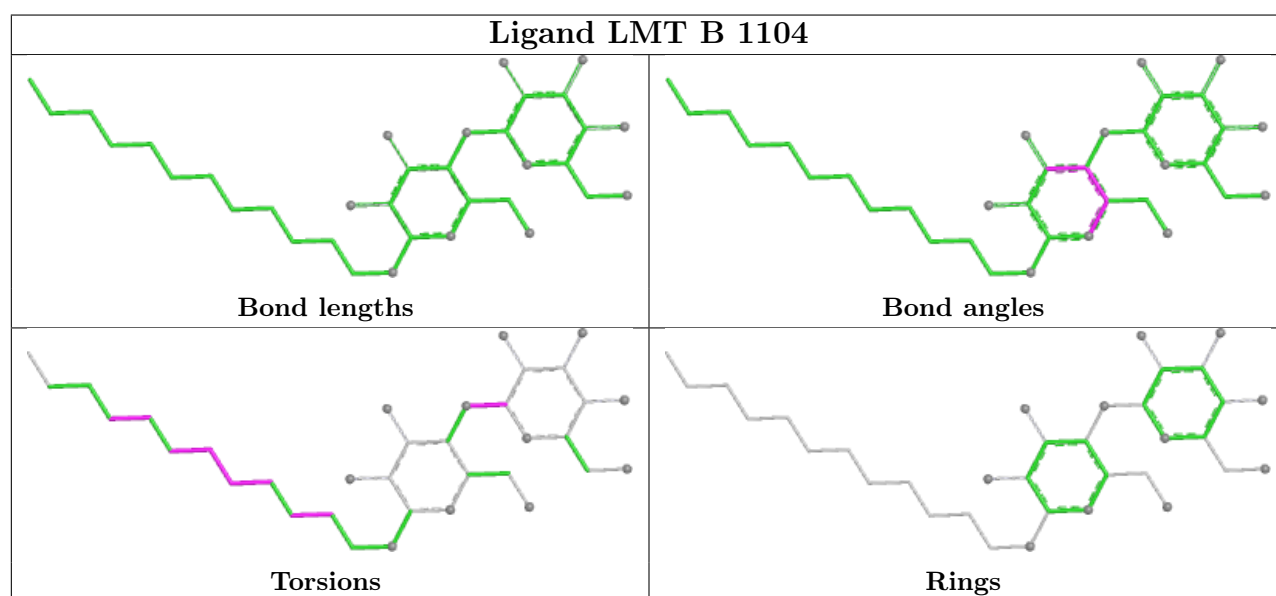
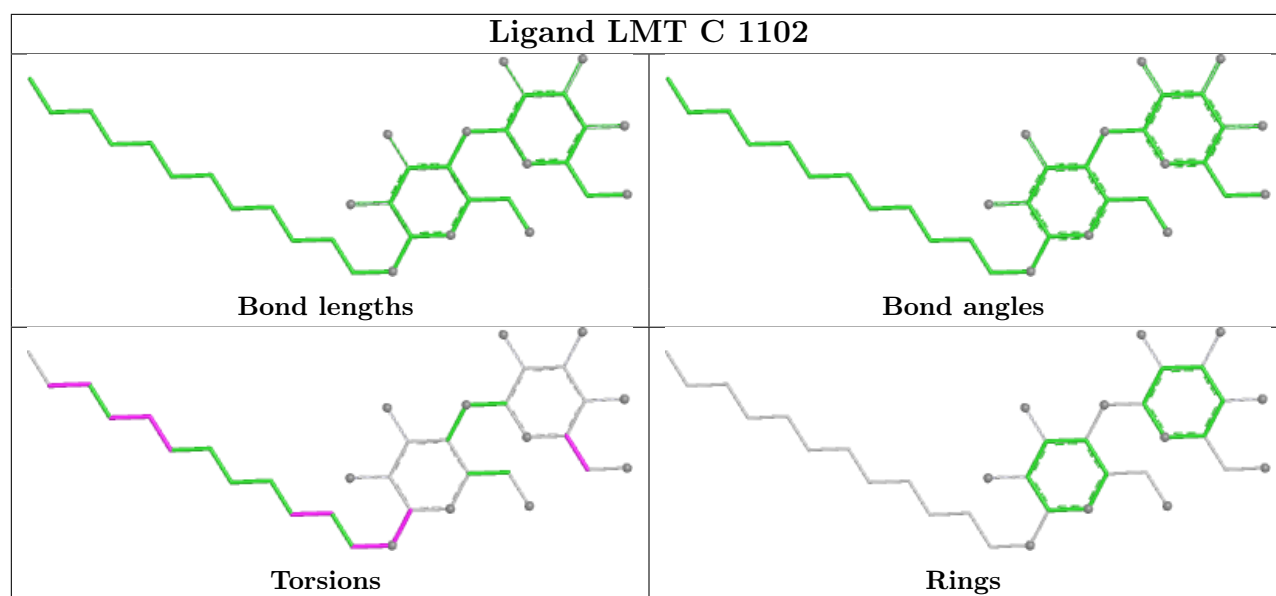
Mol	Chain	Res	Type	Atoms
5	A	1103	LMT	O5B-C1B-O1B-C4'
7	B	1105	PTY	C16-C17-C18-C19
13	B	1116	DDR	O21-C21-C22-C23
7	C	1106	PTY	C13-C14-C15-C16
3	A	1101	P6G	C2-C3-O4-C5
3	A	1101	P6G	C6-C5-O4-C3

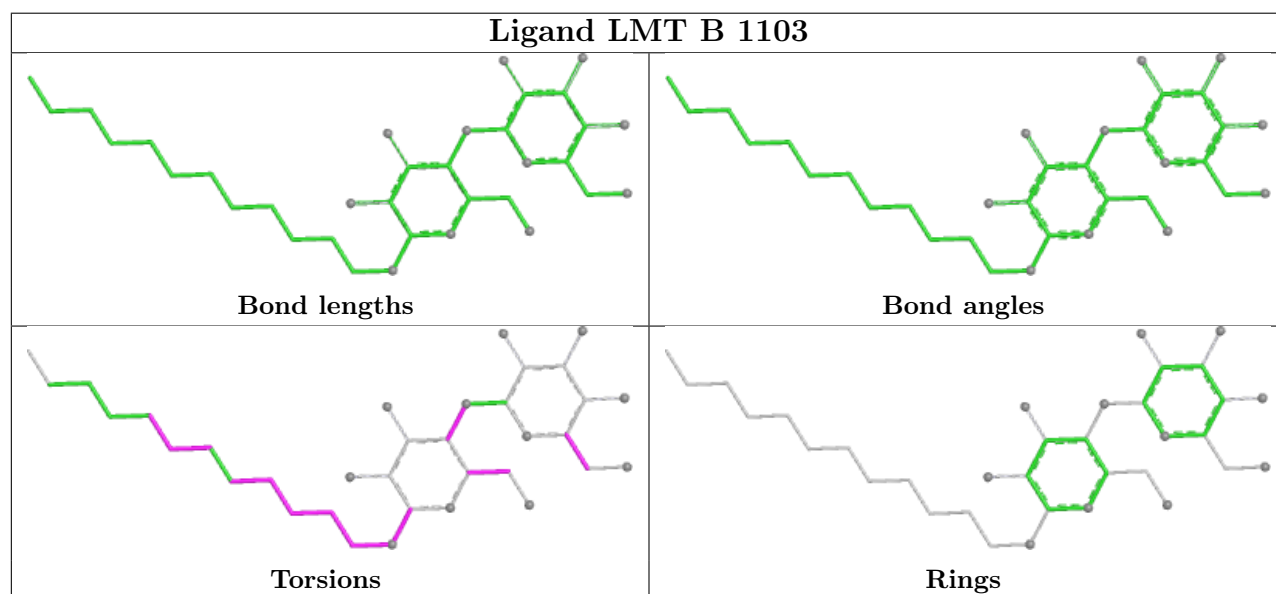
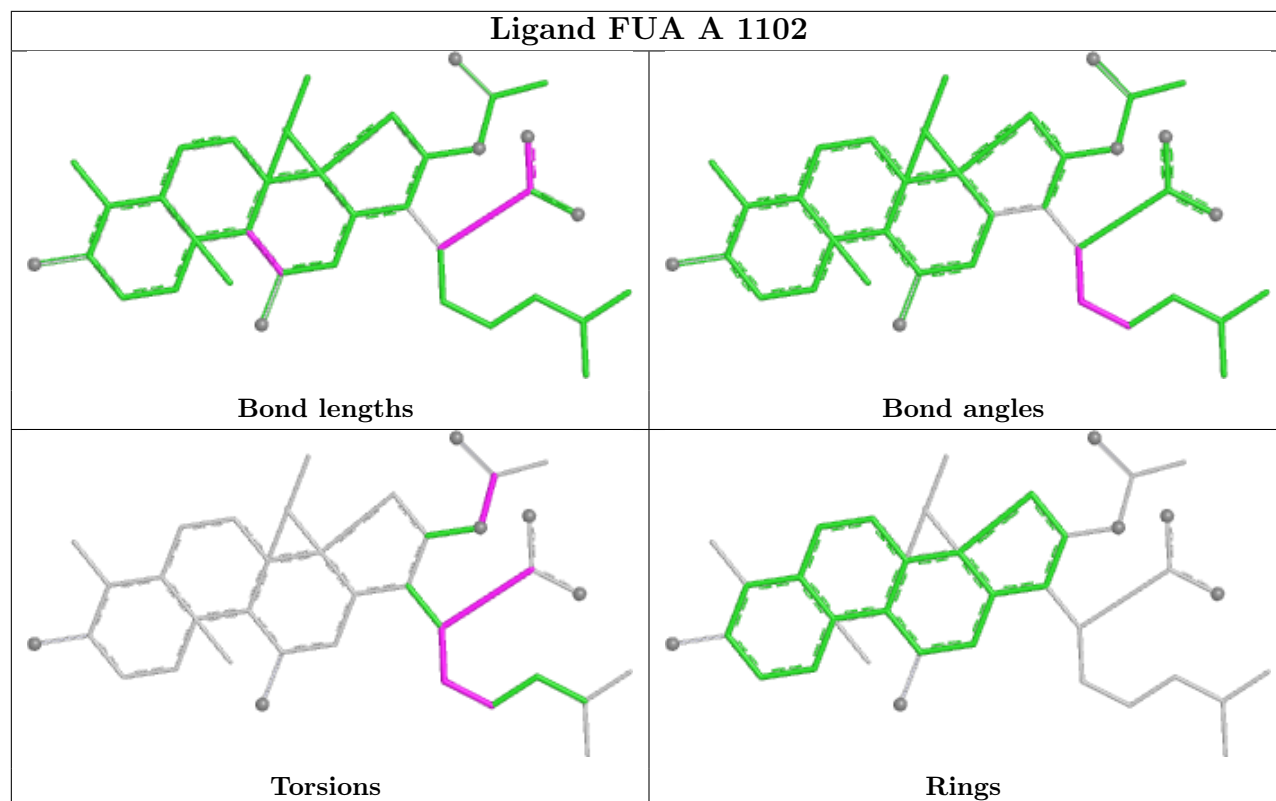
There are no ring outliers.

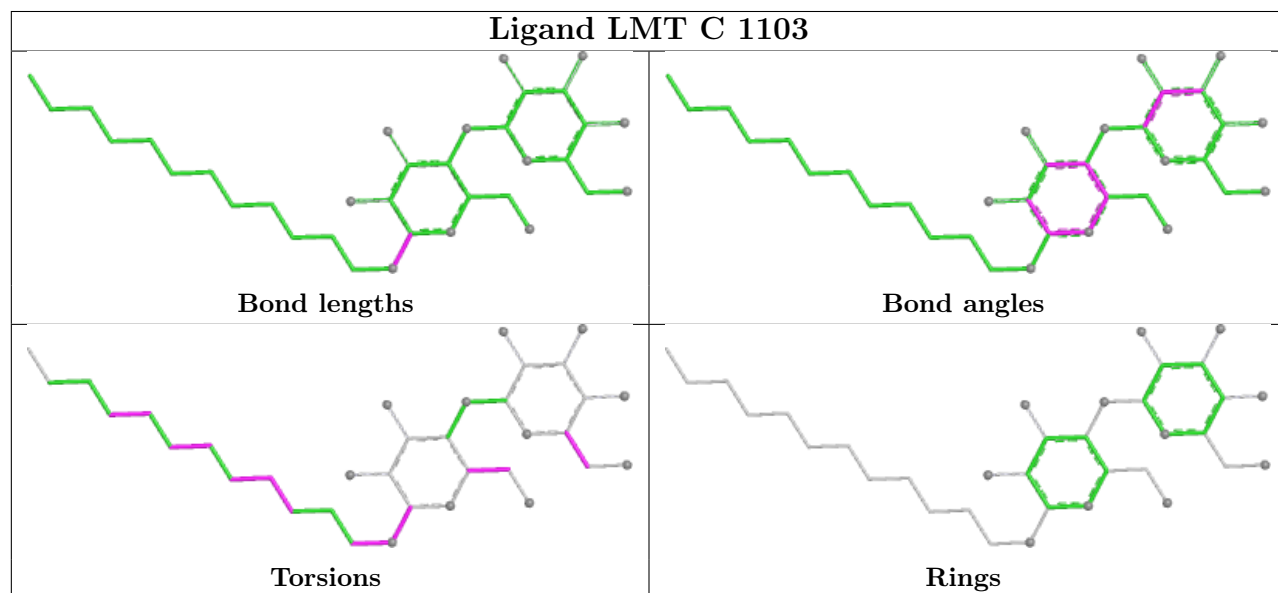
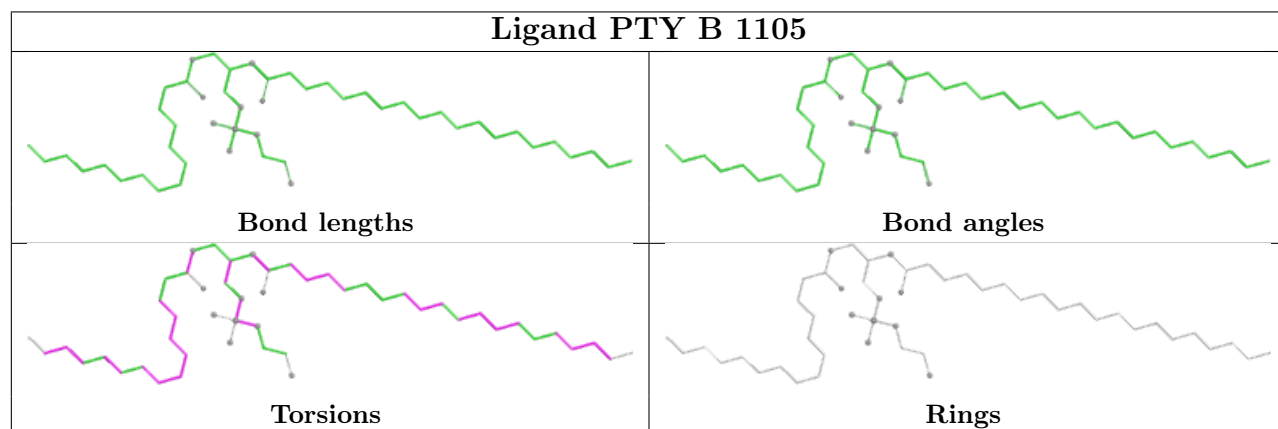
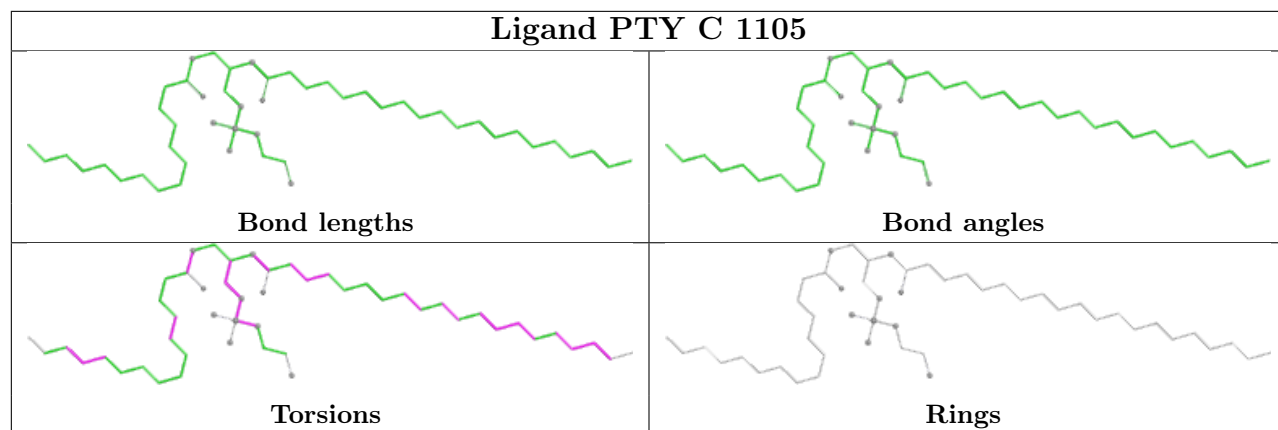
13 monomers are involved in 41 short contacts:

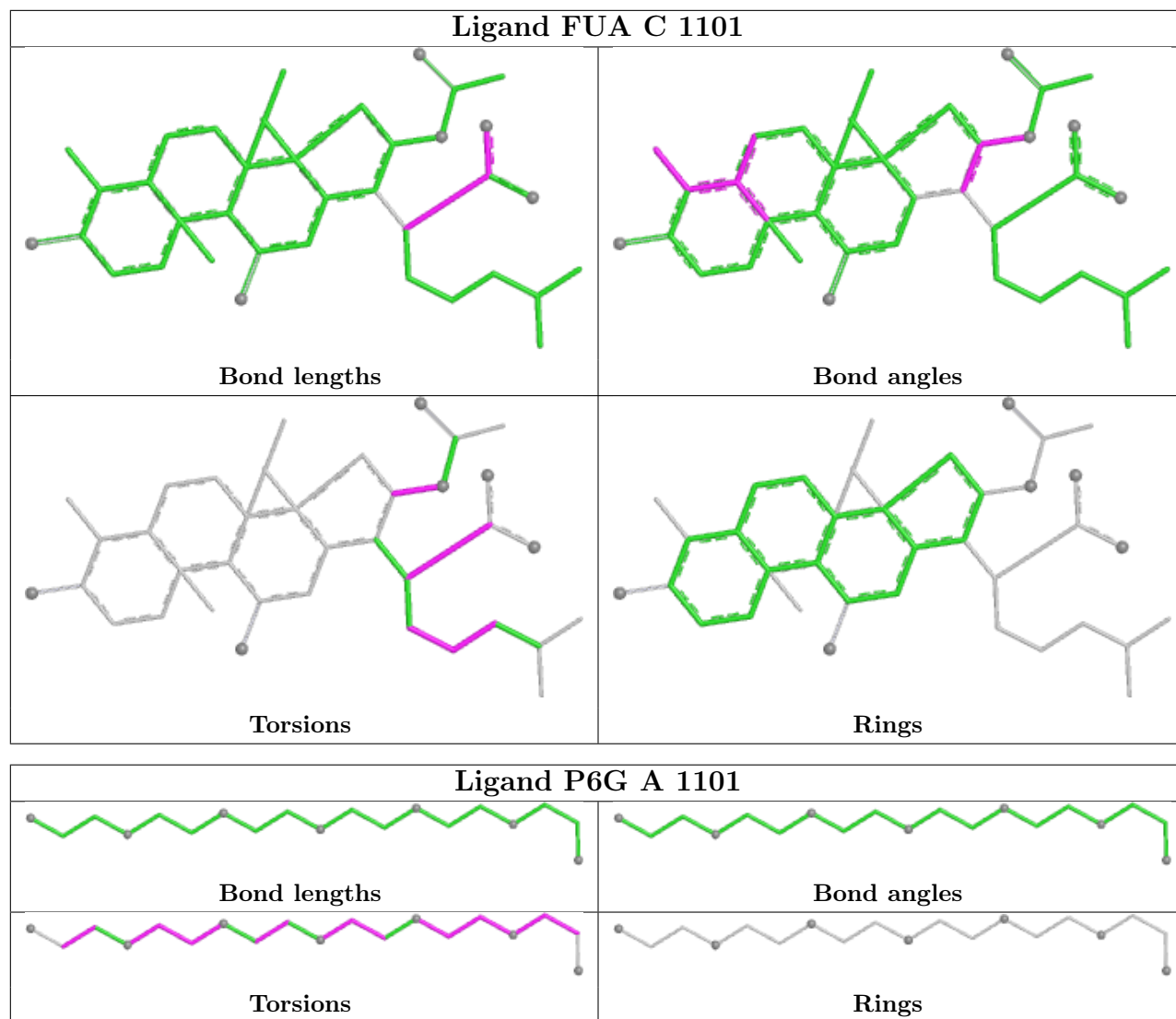
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	201	GOL	1	0
10	B	1113	DDQ	1	0
5	A	1104	LMT	1	0
4	A	1102	FUA	7	0
6	A	1107	GOL	1	0
5	B	1103	LMT	1	0
9	B	1111	D10	1	0
7	B	1105	PTY	8	0
5	C	1103	LMT	1	0
4	C	1101	FUA	6	0
7	C	1106	PTY	7	0
7	C	1104	PTY	2	0
4	B	1101	FUA	7	0

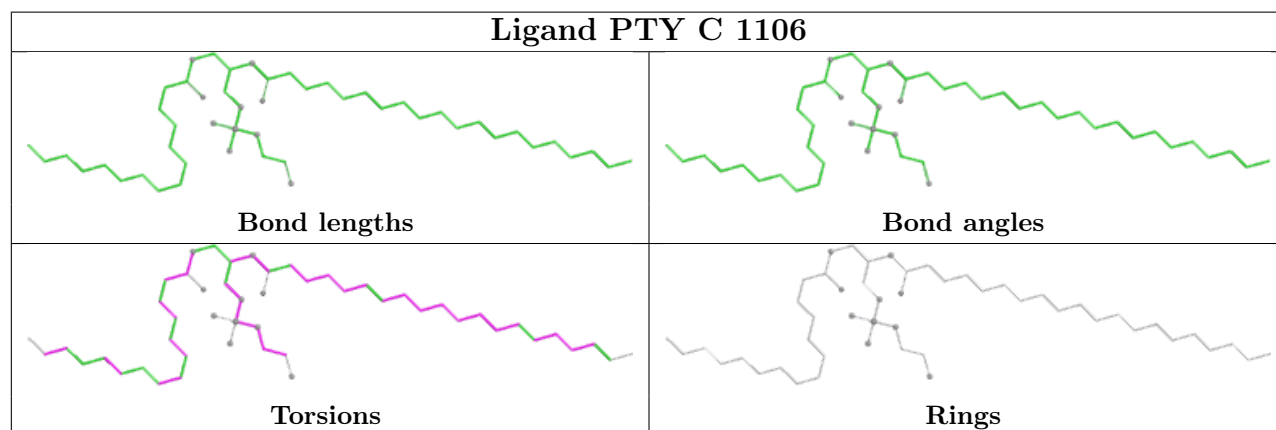
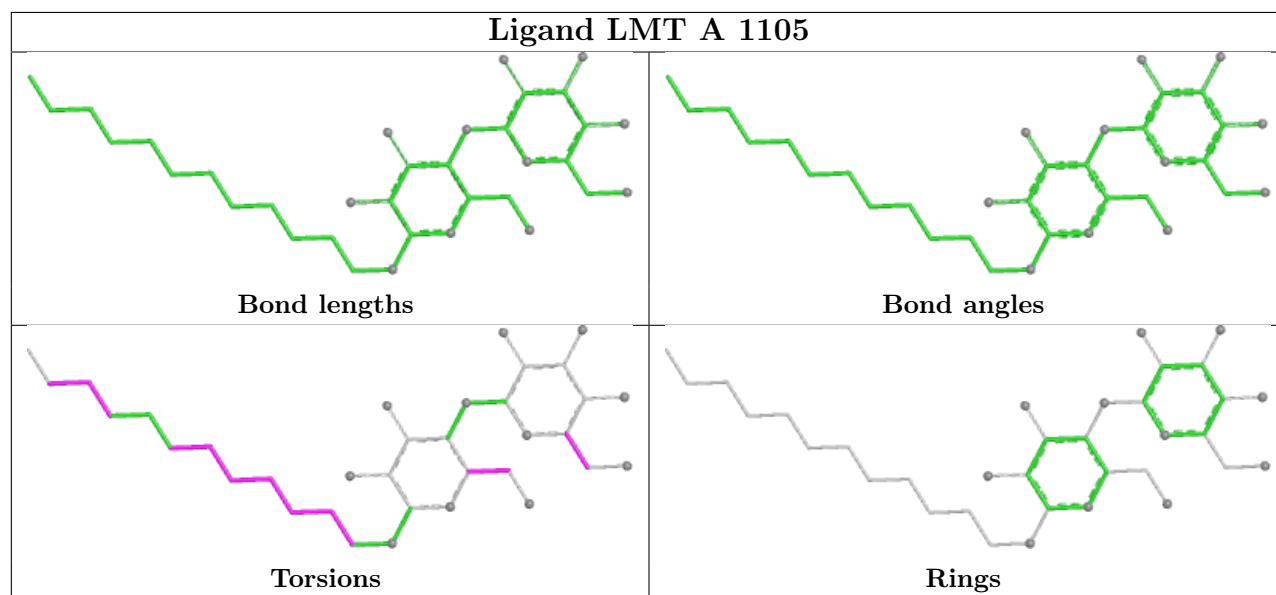
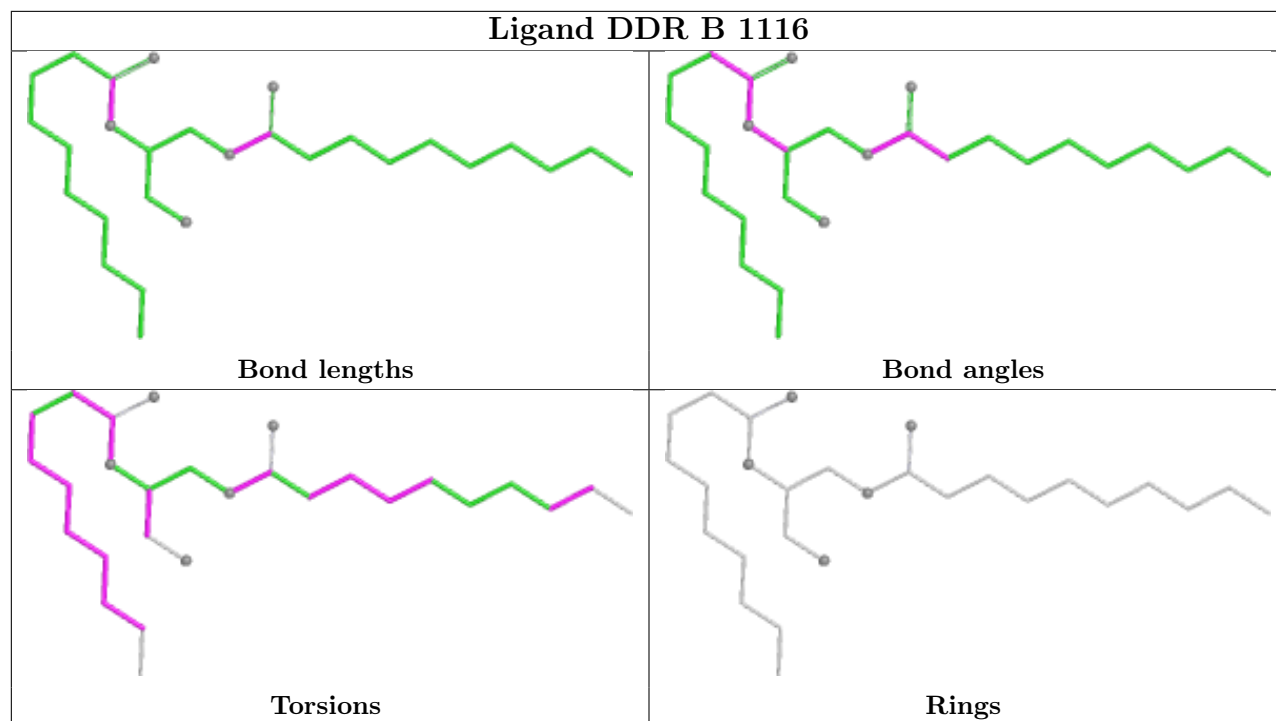
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

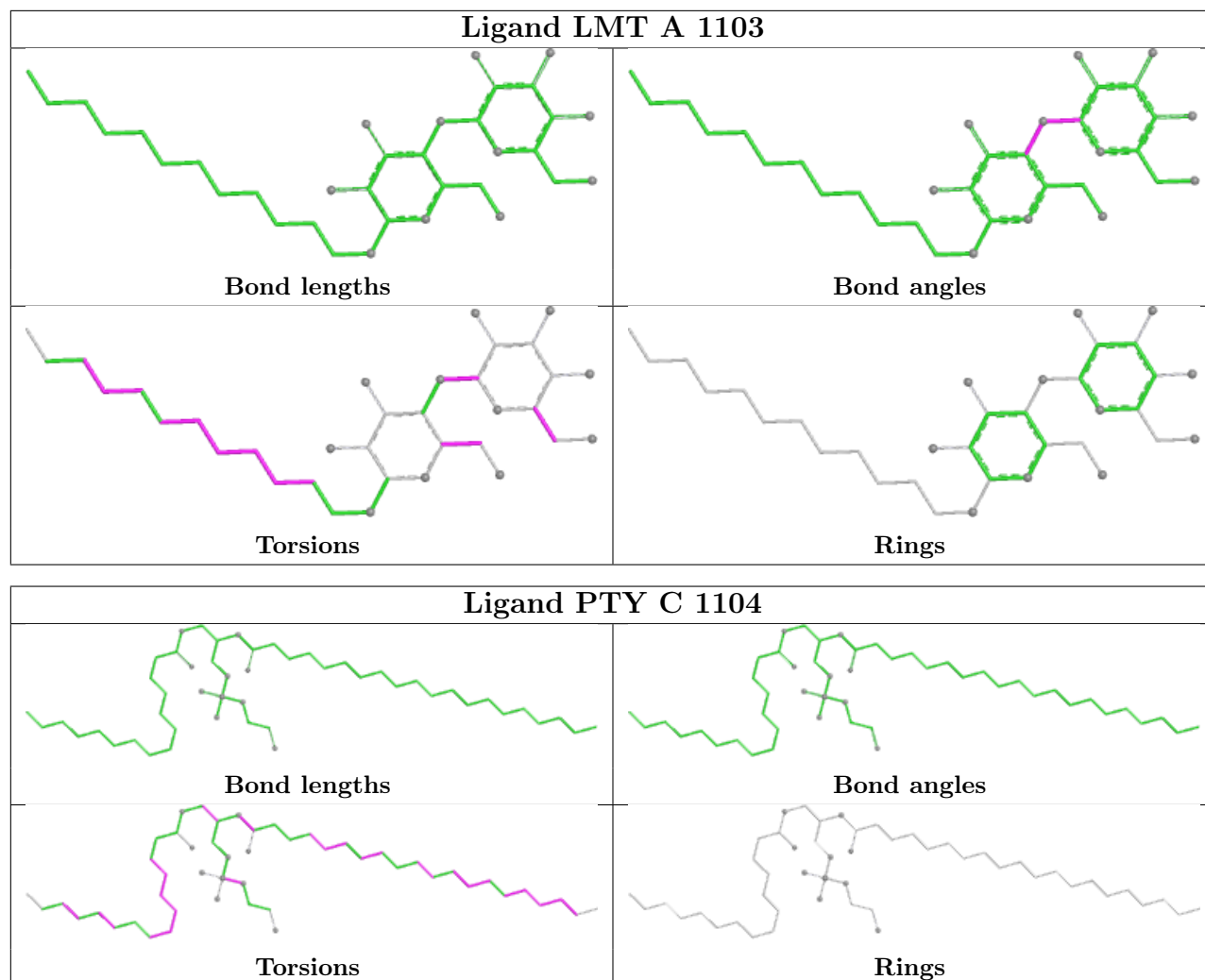


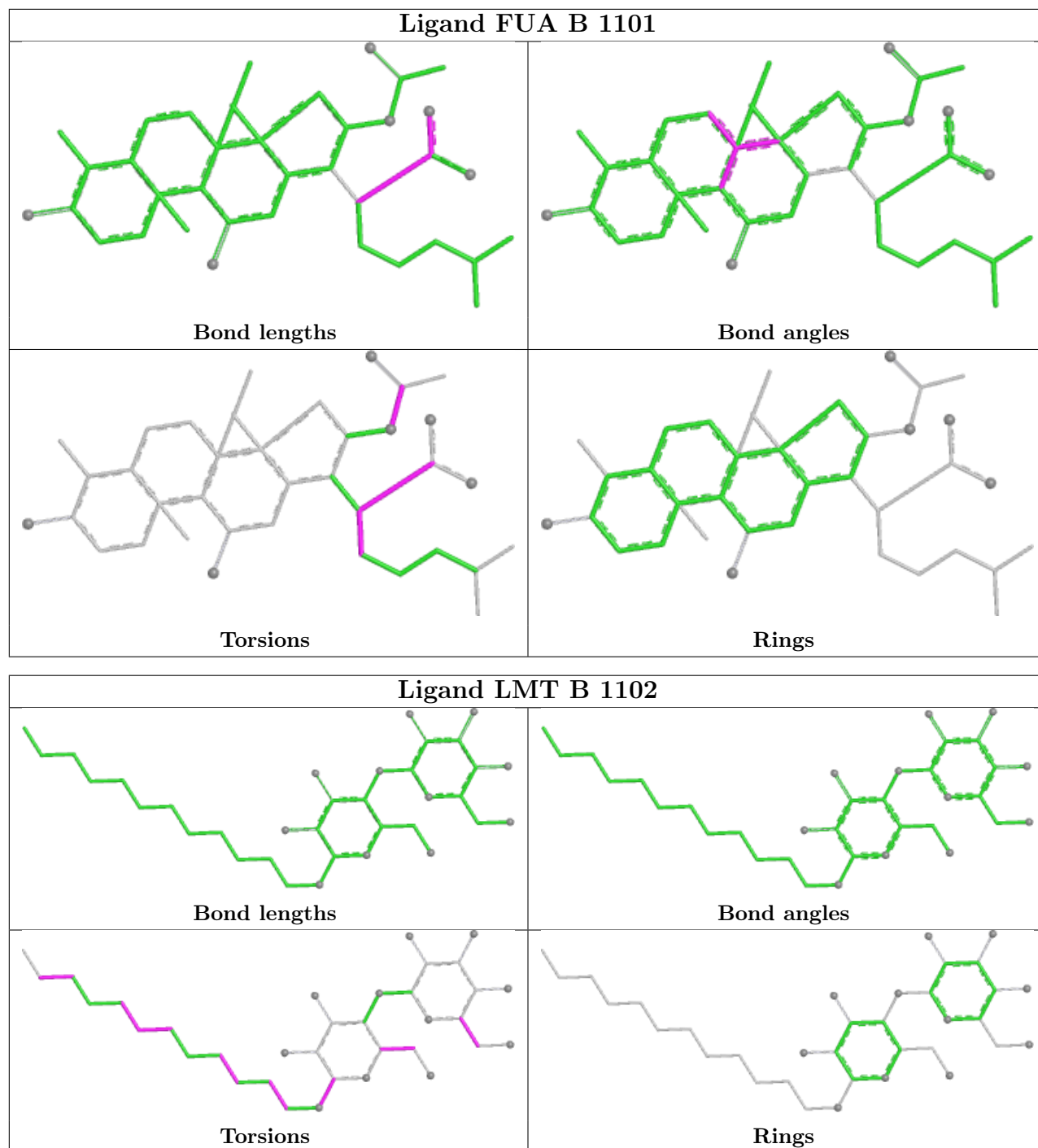












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1036/1057 (98%)	0.62	64 (6%)	26	20	31, 69, 105, 127	2 (0%)
1	B	1034/1057 (97%)	0.53	56 (5%)	31	24	40, 62, 86, 103	1 (0%)
1	C	1034/1057 (97%)	0.43	36 (3%)	47	38	35, 55, 79, 94	1 (0%)
2	D	156/169 (92%)	0.48	5 (3%)	50	40	51, 62, 81, 98	0
2	E	154/169 (91%)	0.88	9 (5%)	29	22	60, 75, 98, 104	0
All	All	3414/3509 (97%)	0.54	170 (4%)	34	26	31, 61, 94, 127	4 (0%)

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	674	LEU	6.1
1	A	868	LEU	5.3
1	A	423	GLU	5.1
1	B	671	ILE	5.0
1	A	1036	LYS	5.0
1	A	617	PHE	4.9
1	B	672	VAL	4.7
1	A	670	ALA	4.5
1	A	678	THR	4.5
1	B	617	PHE	4.4
1	B	662	MET	4.2
1	A	510	LYS	4.2
1	B	628	PHE	4.1
1	B	678	THR	4.1
1	C	671	ILE	4.1
1	A	668	LEU	4.0
1	B	575	MET	4.0
1	B	674	LEU	3.9
1	C	617	PHE	3.9
1	B	615	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	672	VAL	3.7
1	A	956	GLU	3.7
1	A	677	ALA	3.6
1	B	675	GLY	3.6
2	E	146	GLY	3.6
1	B	673	GLU	3.6
2	E	143	ASP	3.5
2	E	35	ALA	3.5
1	A	533	GLY	3.4
1	A	981	ALA	3.4
1	A	462	SER	3.4
1	B	134	SER	3.4
1	B	618	ALA	3.3
1	B	332	PHE	3.2
1	B	866	GLU	3.2
1	B	677	ALA	3.2
1	C	403	GLY	3.1
1	C	619	GLY	3.1
1	A	664	PHE	3.1
1	A	957	GLY	3.1
1	B	664	PHE	3.0
1	A	676	THR	3.0
1	A	950	LYS	2.9
1	C	674	LEU	2.9
1	C	811	TYR	2.9
1	C	146	ASP	2.9
1	B	660	ASP	2.9
1	A	869	SER	2.9
1	B	132	SER	2.9
1	B	676	THR	2.9
1	A	673	GLU	2.8
1	B	1015	THR	2.8
1	C	618	ALA	2.8
2	E	74	ASN	2.8
1	A	675	GLY	2.8
1	A	918	PHE	2.7
1	C	620	ARG	2.7
1	B	634	TRP	2.7
1	B	655	PHE	2.7
1	C	70[A]	ASN	2.7
1	A	422	GLU	2.7
1	A	955	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	877	TYR	2.7
1	A	298	ASN	2.7
1	B	577	GLN	2.7
1	A	509	LYS	2.7
1	B	403	GLY	2.7
1	A	535	LEU	2.7
1	A	499	PRO	2.6
1	B	670	ALA	2.6
1	A	513	PHE	2.6
1	C	170	SER	2.6
1	C	558	ARG	2.6
1	A	538	THR	2.6
1	B	868	LEU	2.6
1	A	802	SER	2.5
1	B	1011	MET	2.5
1	B	918	PHE	2.5
1	A	426	PRO	2.5
1	A	662	MET	2.5
1	C	192	GLU	2.5
1	B	626	ILE	2.5
1	A	386	PHE	2.5
1	A	148	THR	2.5
1	B	97	GLY	2.4
2	E	139	VAL	2.4
2	E	140	ASN	2.4
1	B	571	VAL	2.4
1	C	508	GLY	2.4
1	A	120	GLN	2.4
1	B	837	THR	2.4
1	A	353	LEU	2.4
1	C	513	PHE	2.4
1	C	673	GLU	2.4
1	C	697	GLN	2.4
1	B	508	GLY	2.4
1	C	124	GLN	2.4
1	A	671	ILE	2.4
1	A	29	LYS	2.3
1	B	620	ARG	2.3
1	C	29	LYS	2.3
2	D	166	GLN	2.3
1	A	37	THR	2.3
1	B	38	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	565	PRO	2.3
1	B	557	VAL	2.3
2	D	40	VAL	2.3
1	C	173	GLY	2.3
1	B	627	ALA	2.3
1	B	28	LEU	2.3
1	C	497	LEU	2.3
1	A	38	ILE	2.3
1	A	431	THR	2.3
1	B	665	ALA	2.3
1	C	730	ASP	2.3
1	B	574	THR	2.3
1	B	597	TYR	2.3
2	D	45	VAL	2.3
1	A	993	THR	2.3
1	B	133	SER	2.3
1	B	869	SER	2.3
1	B	1034	SER	2.3
1	A	679	GLY	2.3
1	C	424	GLY	2.3
2	D	55	ALA	2.2
1	C	425	LEU	2.2
1	A	255	GLN	2.2
1	B	854	GLY	2.2
1	A	862	MET	2.2
1	C	693	GLU	2.2
1	C	698	ALA	2.2
1	A	498	LYS	2.2
1	A	865	GLN	2.2
2	E	13	ASP	2.2
1	A	669	PRO	2.2
1	B	570	GLY	2.2
1	A	456	MET	2.2
1	C	575	MET	2.2
1	A	362	PHE	2.2
1	C	152	GLU	2.2
1	A	874	PRO	2.2
1	A	1008	MET	2.2
1	C	258	SER	2.2
1	B	556	PHE	2.2
1	A	415	ASN	2.1
1	A	649	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	784	ASP	2.1
1	B	319	SER	2.1
2	D	12	SER	2.1
1	C	259	ARG	2.1
1	C	264	ASP	2.1
1	B	619	GLY	2.1
1	C	675	GLY	2.1
1	A	418	ARG	2.1
1	A	414	GLU	2.1
1	A	438	ILE	2.1
1	C	405	LEU	2.1
1	C	134	SER	2.1
1	B	255	GLN	2.1
1	C	89	GLN	2.1
1	A	876	LEU	2.1
1	B	616	GLY	2.1
2	E	31	ARG	2.1
1	B	987	MET	2.0
1	A	984	LEU	2.0
1	A	971	ARG	2.0
1	B	178	PHE	2.0
1	B	476	SER	2.0
1	C	670	ALA	2.0
2	E	40	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

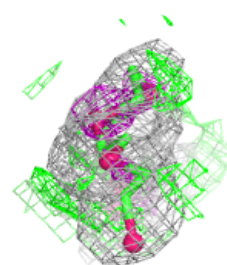
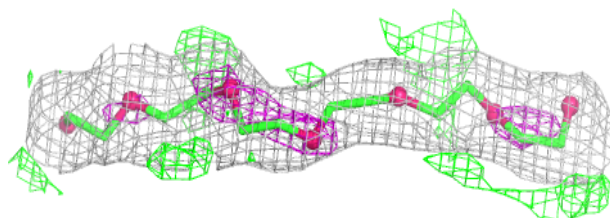
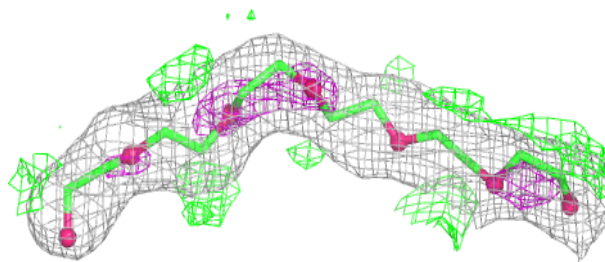
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	P6G	A	1101	19/19	0.62	0.19	45,46,47,47	0
8	OCT	C	1108	8/8	0.69	0.35	67,68,68,68	0
6	GOL	A	1106	6/6	0.71	0.29	70,71,71,72	0
7	PTY	B	1105	50/50	0.73	0.31	106,123,136,137	0
10	DDQ	B	1113	14/14	0.73	0.36	97,102,107,107	0
11	HEX	B	1114	6/6	0.73	0.29	64,64,64,64	0
5	LMT	C	1103	35/35	0.77	0.23	93,112,114,114	0
5	LMT	A	1105	35/35	0.79	0.19	107,112,116,116	0
14	D12	B	1117	12/12	0.79	0.33	85,86,87,87	0
7	PTY	C	1105	50/50	0.80	0.27	83,88,97,99	0
7	PTY	C	1106	50/50	0.80	0.30	96,112,125,127	0
7	PTY	C	1104	50/50	0.80	0.28	91,112,121,123	0
6	GOL	E	202	6/6	0.81	0.20	85,85,86,86	0
10	DDQ	C	1112	14/14	0.81	0.29	83,83,84,84	0
6	GOL	C	1107	6/6	0.81	0.20	52,53,53,54	0
8	OCT	C	1109	8/8	0.81	0.34	78,79,80,80	0
5	LMT	B	1104	35/35	0.82	0.20	91,114,123,123	0
8	OCT	C	1110	8/8	0.82	0.33	80,81,81,81	0
5	LMT	A	1104	35/35	0.82	0.21	104,117,129,130	0
5	LMT	A	1103	35/35	0.84	0.21	93,104,109,109	0
9	D10	B	1111	10/10	0.84	0.25	71,71,72,72	0
5	LMT	B	1102	35/35	0.85	0.17	83,89,94,94	0
4	FUA	A	1102	37/37	0.85	0.30	98,100,100,100	37
9	D10	B	1109	10/10	0.86	0.23	69,70,70,70	0
8	OCT	B	1107	8/8	0.86	0.33	88,90,90,90	0
8	OCT	B	1108	8/8	0.86	0.34	85,86,86,86	0
5	LMT	B	1103	35/35	0.86	0.17	84,89,90,91	0
4	FUA	C	1101	37/37	0.86	0.30	90,94,96,96	37
6	GOL	B	1106	6/6	0.86	0.24	81,82,83,83	0
13	DDR	B	1116	28/28	0.88	0.25	95,104,105,107	0
6	GOL	E	201	6/6	0.88	0.15	72,72,73,73	0
11	HEX	C	1113	6/6	0.89	0.24	33,33,33,33	0
9	D10	C	1111	10/10	0.89	0.23	73,74,74,74	0
9	D10	B	1110	10/10	0.89	0.24	73,74,74,74	0
6	GOL	A	1107	6/6	0.90	0.17	69,70,70,70	0
9	D10	B	1112	10/10	0.90	0.26	73,74,74,74	0
4	FUA	B	1101	37/37	0.90	0.18	79,81,84,84	0
5	LMT	C	1102	35/35	0.91	0.13	72,74,76,76	0
12	SO4	B	1115	5/5	0.94	0.09	82,83,83,83	0
12	SO4	C	1114	5/5	0.95	0.15	74,74,75,75	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.

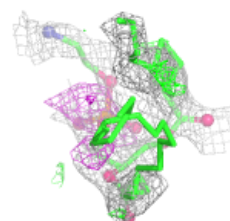
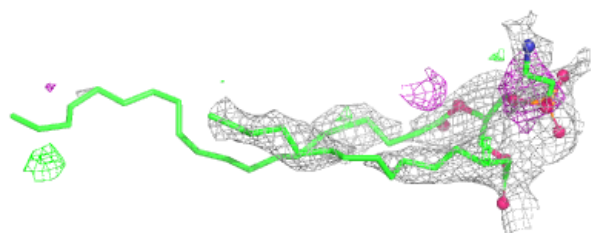
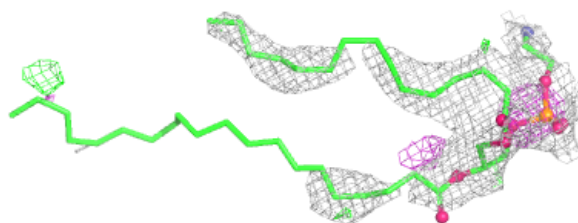
Electron density around P6G A 1101:

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



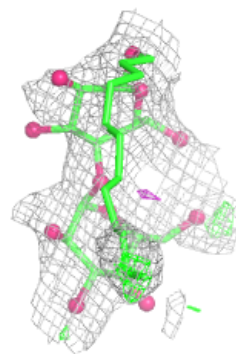
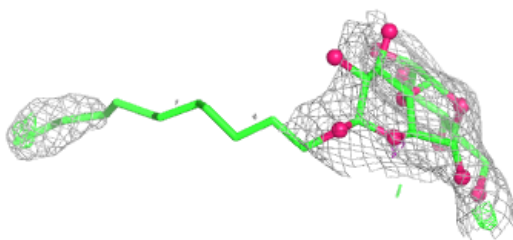
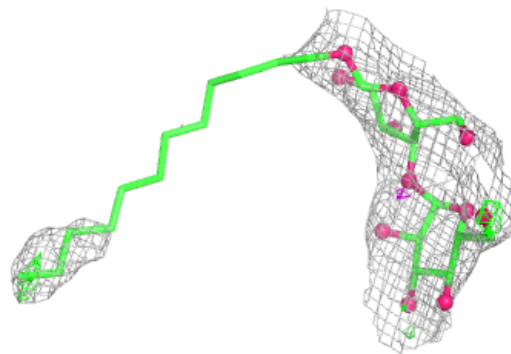
Electron density around PTY B 1105:

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

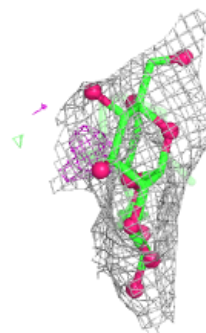
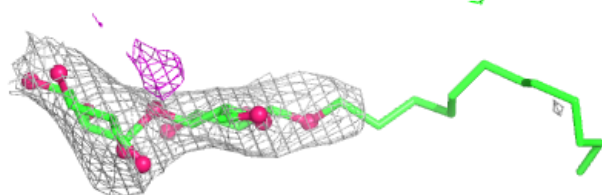
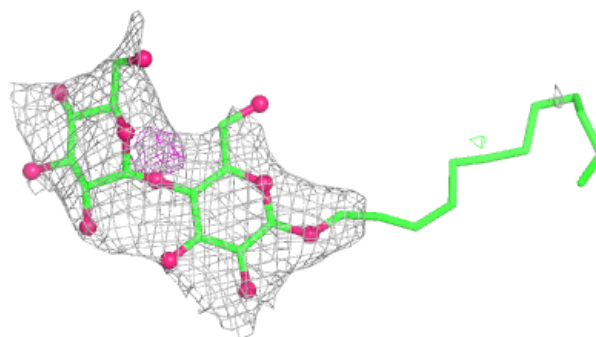


Electron density around LMT C 1103:

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

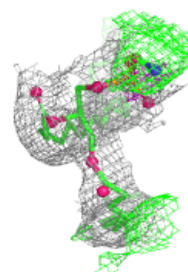
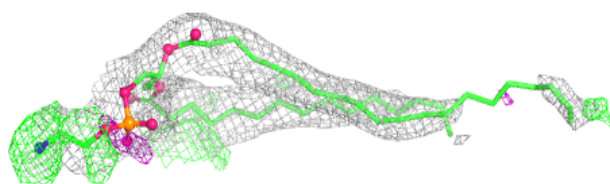
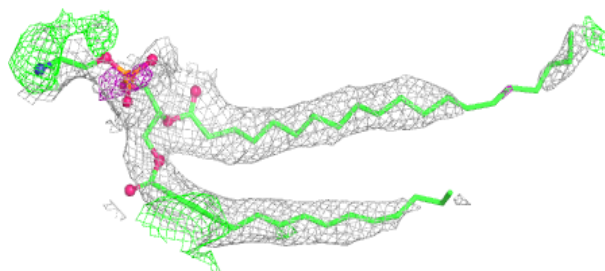
**Electron density around LMT A 1105:**

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

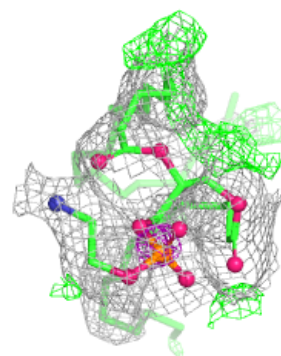
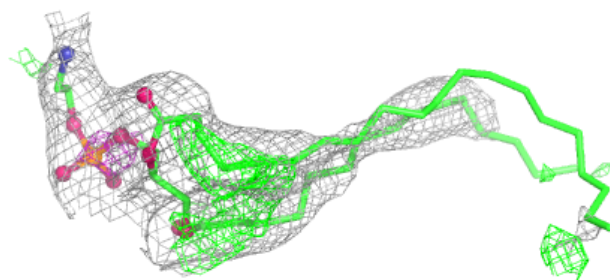
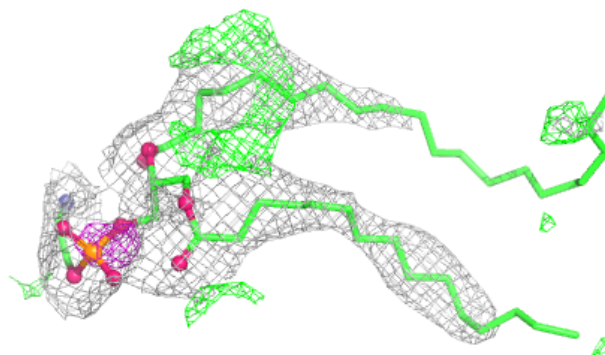


Electron density around PTY C 1105:

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

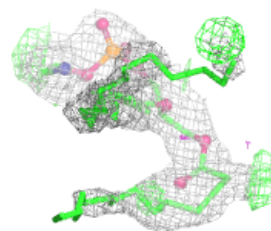
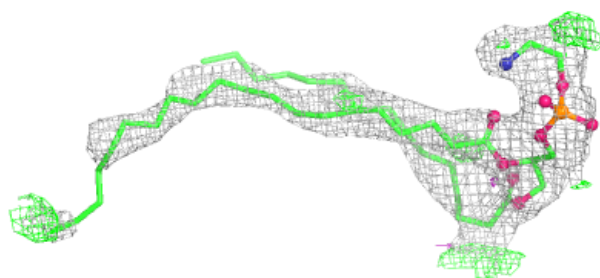
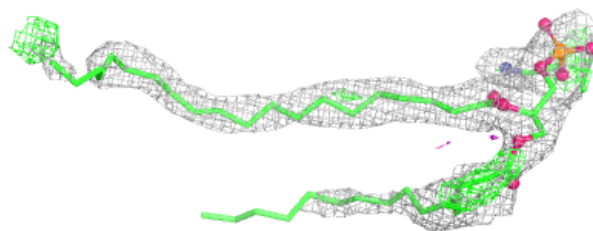
**Electron density around PTY C 1106:**

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

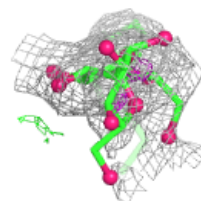
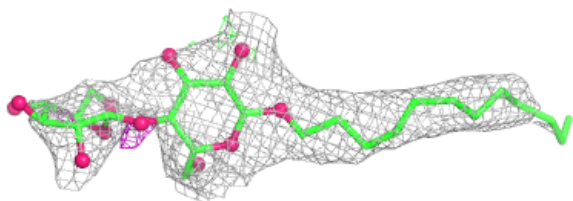
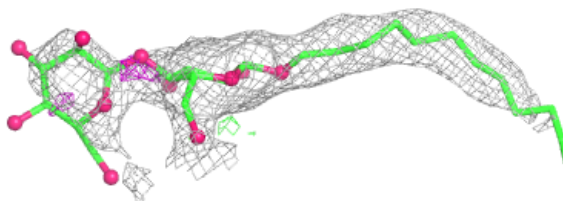


Electron density around PTY C 1104:

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

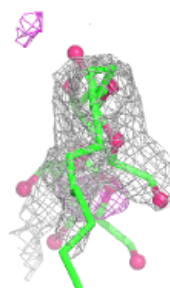
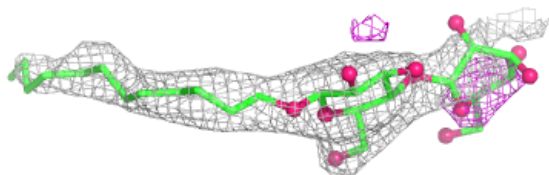
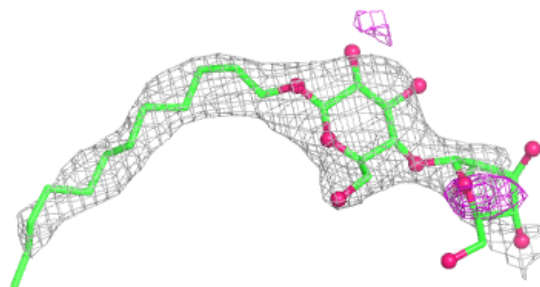
**Electron density around LMT B 1104:**

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

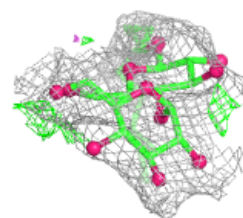
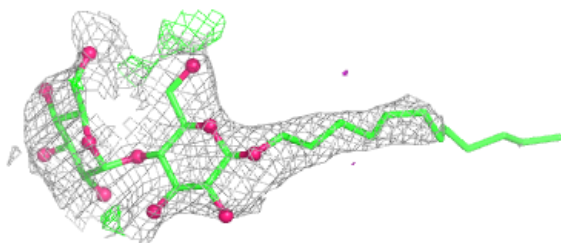
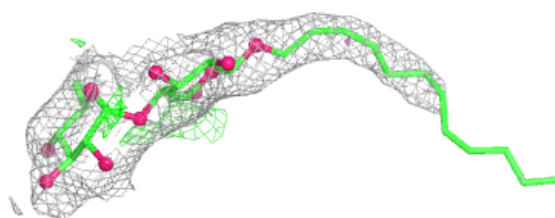


Electron density around LMT A 1104:

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

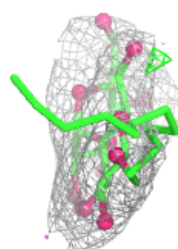
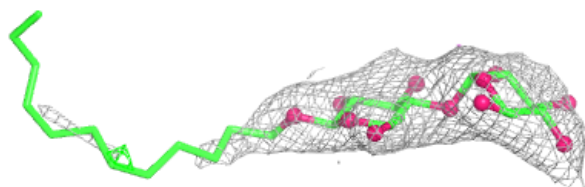
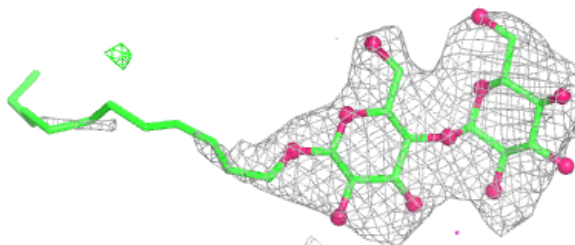
**Electron density around LMT A 1103:**

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

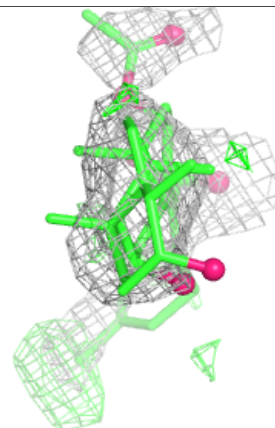
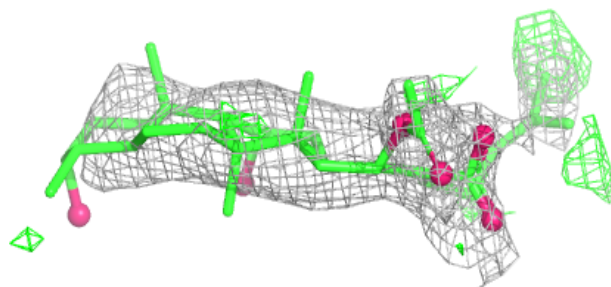
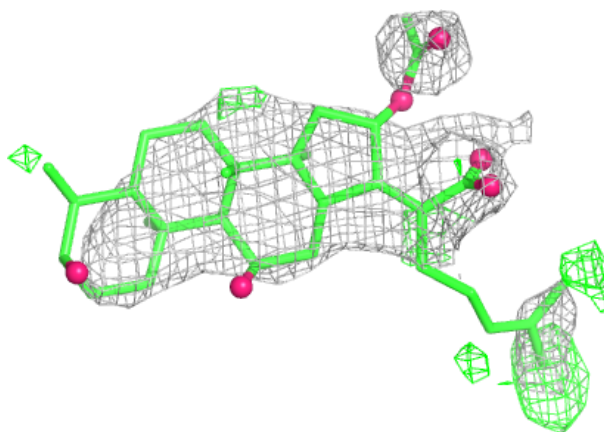


Electron density around LMT B 1102:

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

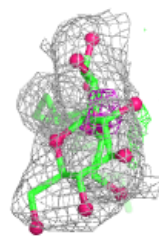
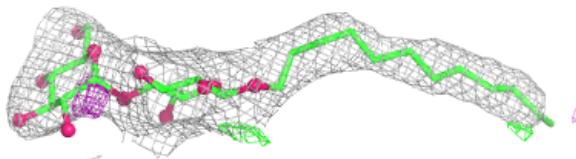
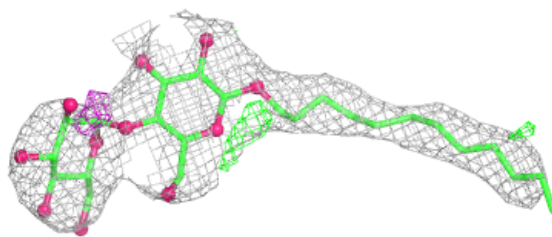
**Electron density around FUA A 1102:**

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



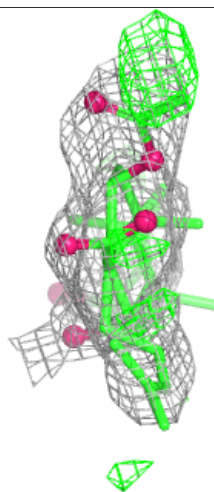
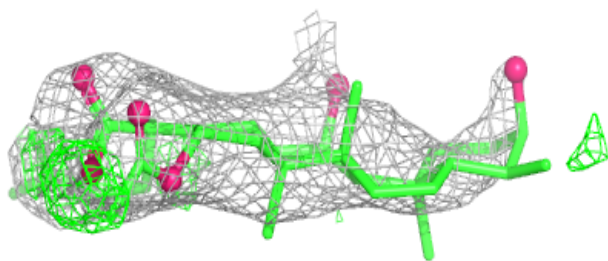
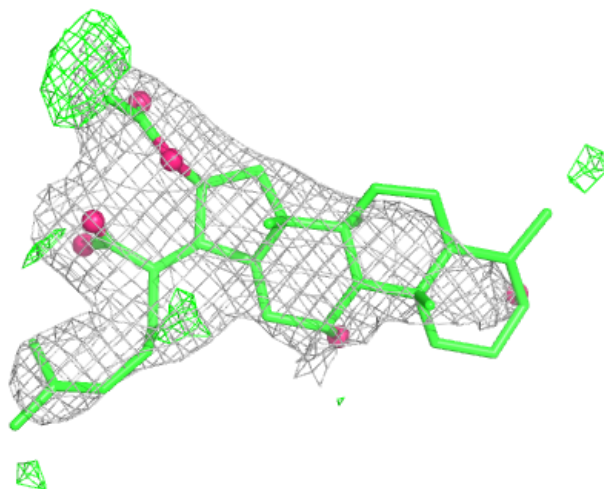
Electron density around LMT B 1103:

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



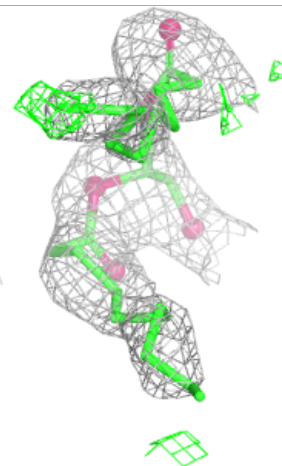
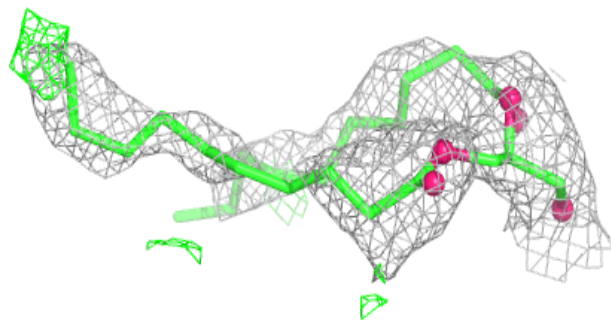
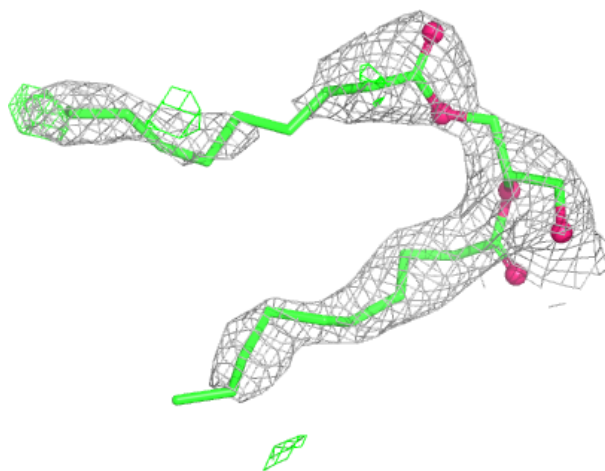
Electron density around FUA C 1101:

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



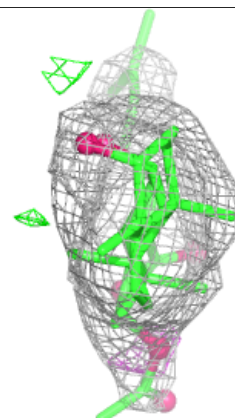
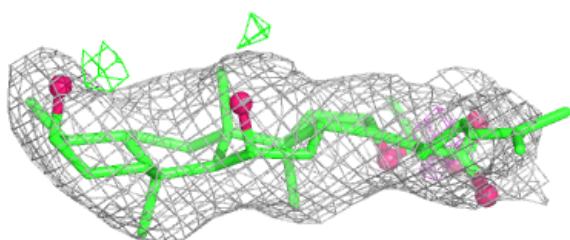
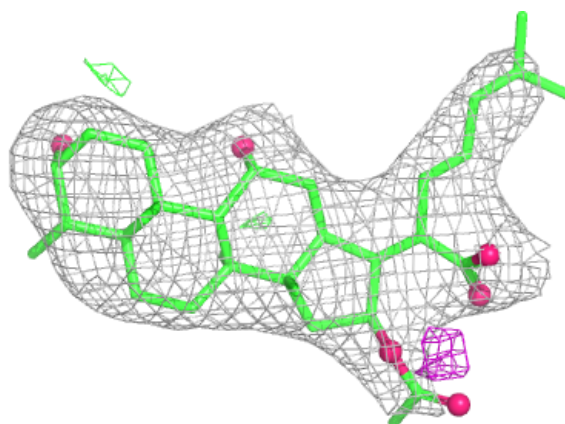
Electron density around DDR B 1116:

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

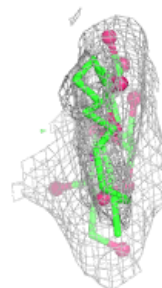
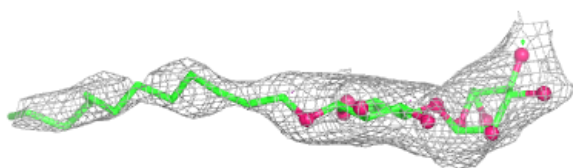
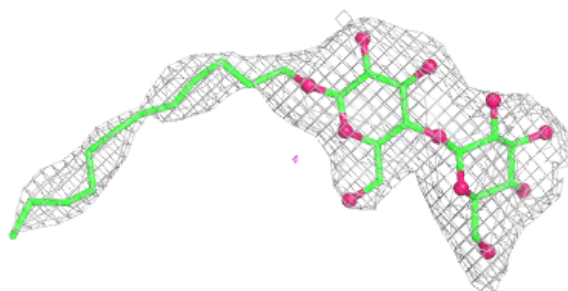


Electron density around FUA B 1101:

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

**Electron density around LMT C 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.