



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:56 AM UTC

PDB ID : 6ZO6 / pdb_00006zo6
Title : Minocycline binding to the deep binding pocket of AcrB-G619P
Authors : Tam, H.K.; Foong, W.E.; Pos, K.M.
Deposited on : 2020-07-07
Resolution : 2.35 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

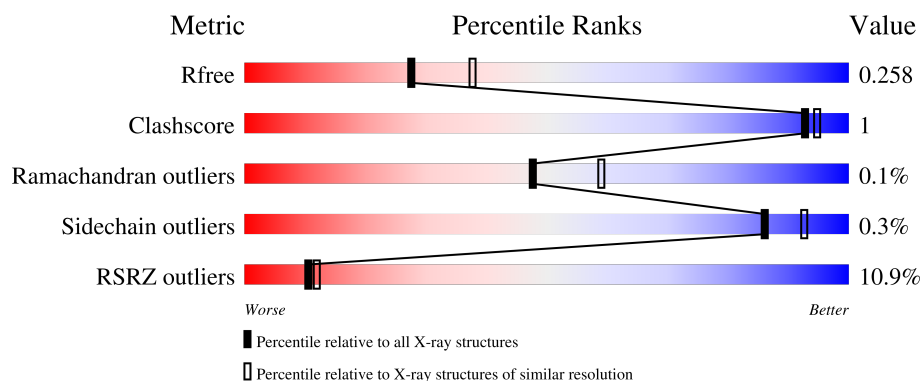
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	15% 93% 6%
1	B	1057	10% 93% 5%
1	C	1057	5% 94% •
2	D	169	7% 90% 8%
2	E	169	22% 89% 9%

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 28139 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	1042	Total	C	N	O	S	0	4	0
			7961	5119	1319	1479	44			
1	B	1033	Total	C	N	O	S	0	5	0
			7883	5074	1301	1463	45			
1	C	1034	Total	C	N	O	S	0	3	0
			7881	5071	1301	1465	44			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	619	PRO	GLY	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	619	PRO	GLY	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	619	PRO	GLY	engineered mutation	UNP P31224
C	1050	LEU	-	expression tag	UNP P31224
C	1051	GLU	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224

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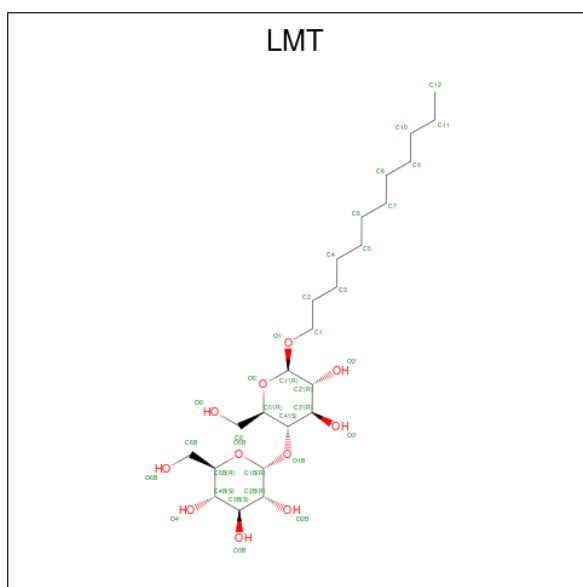
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

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

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



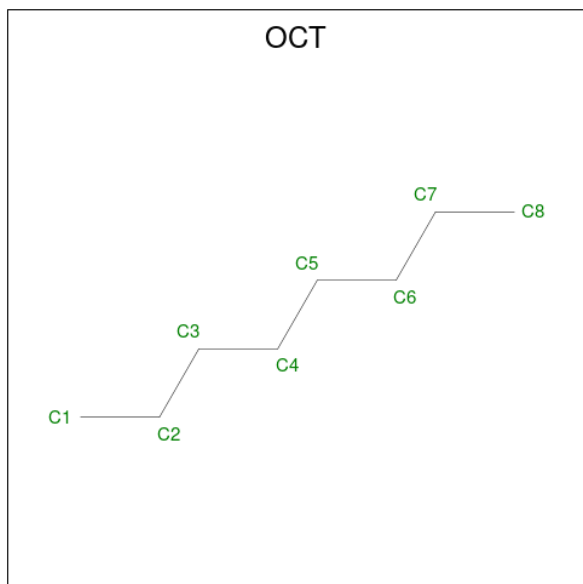
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		

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

- Molecule 4 is N-OCTANE (CCD ID: OCT) (formula: C_8H_{18}).

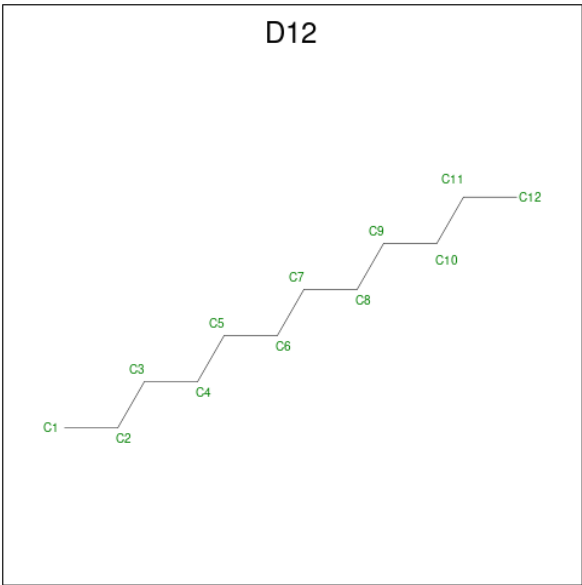


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			8	8		
4	C	1	Total	C	0	0
			8	8		
4	C	1	Total	C	0	0
			8	8		

- Molecule 5 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (CCD ID: DDQ) (formula: $C_{12}H_{27}NO$).

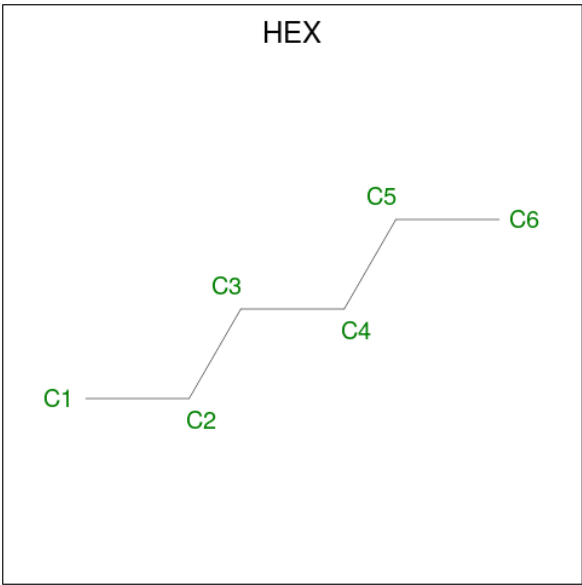
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0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

- Molecule 7 is DODECANE (CCD ID: D12) (formula: C₁₂H₂₆).



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

- Molecule 8 is HEXANE (CCD ID: HEX) (formula: C₆H₁₄).



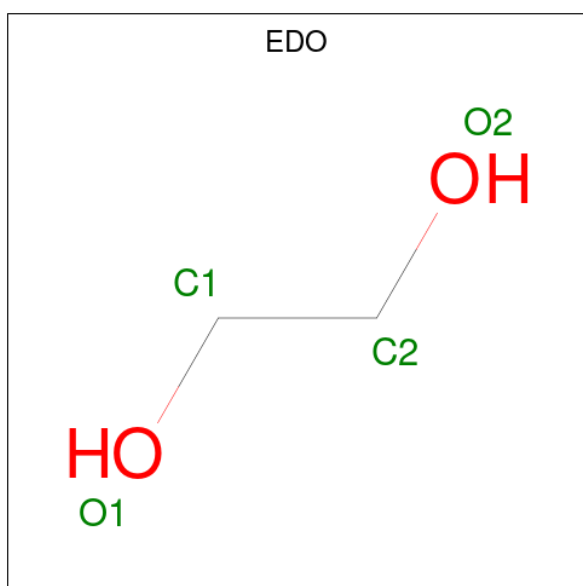
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	C	0	0
			6	6		

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

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



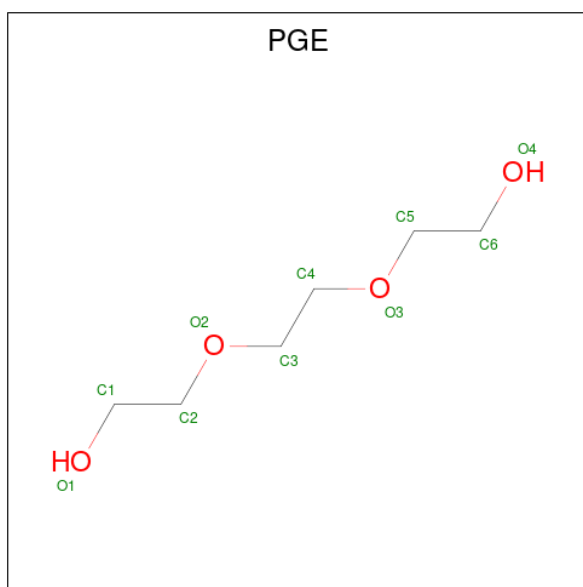
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0

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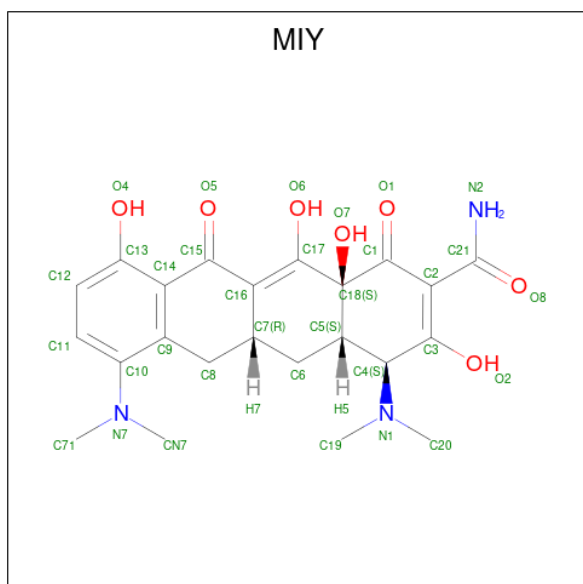
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



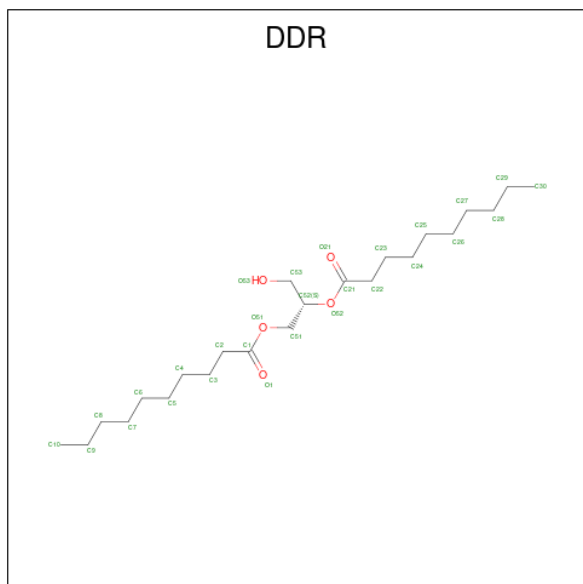
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			10	6	4		
10	C	1	Total	C	O	0	0
			10	6	4		

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



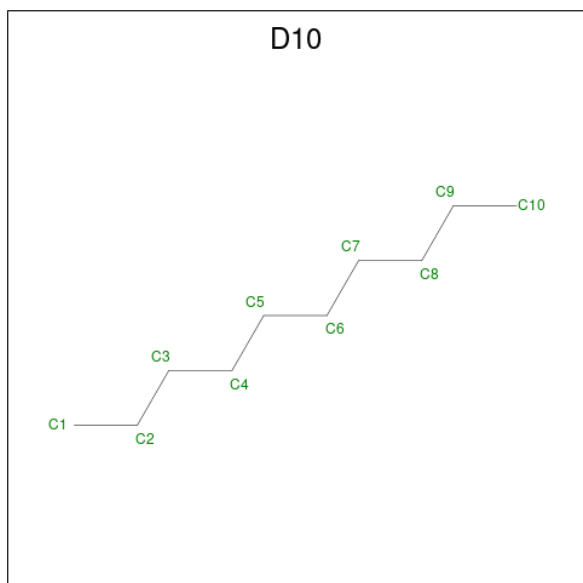
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			33	23	3	7		

- Molecule 12 is (2S)-3-hydroxypropane-1,2-diyl didecanoate (CCD ID: DDR) (formula: $C_{23}H_{44}O_5$).



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

- Molecule 13 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$).

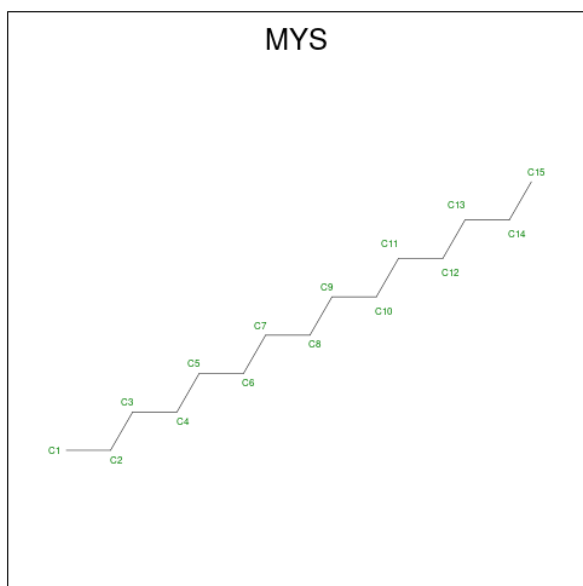


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C 10 10	0	0
13	B	1	Total C 10 10	0	0
13	B	1	Total C 10 10	0	0
13	C	1	Total C 10 10	0	0
13	C	1	Total C 10 10	0	0

- Molecule 14 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

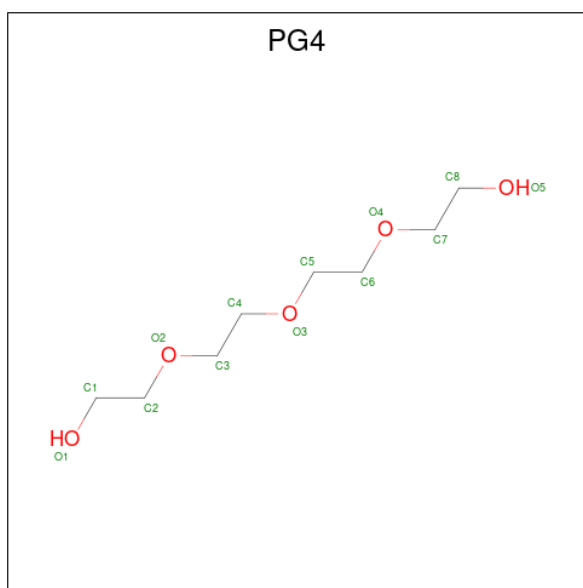
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total Cl 1 1	0	0
14	C	2	Total Cl 2 2	0	0

- Molecule 15 is PENTADECANE (CCD ID: MYS) (formula: C₁₅H₃₂).



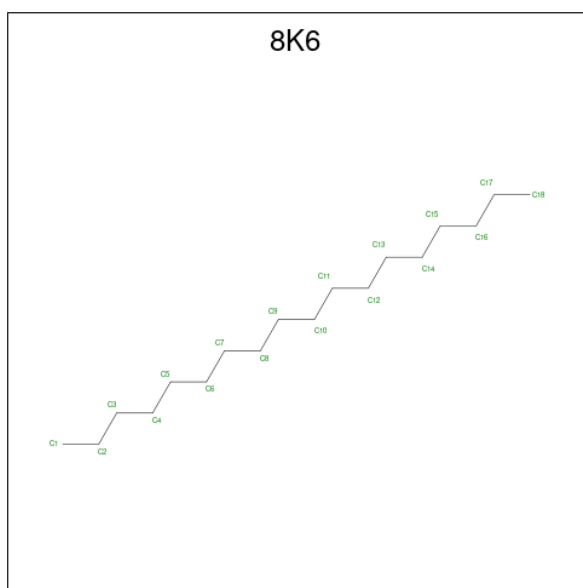
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total C 15 15	0	0
15	B	1	Total C 15 15	0	0

- Molecule 16 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



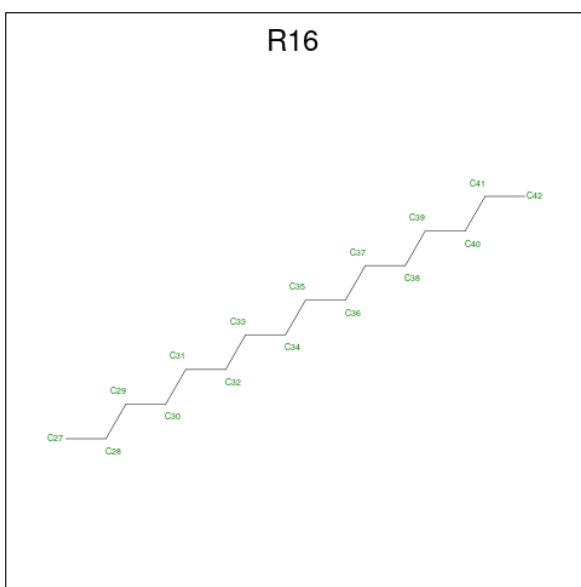
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 17 is Octadecane (CCD ID: 8K6) (formula: $C_{18}H_{38}$).



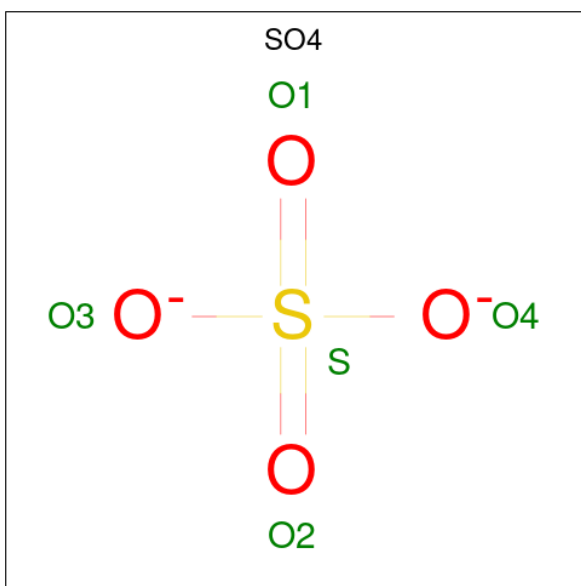
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	B	1	Total	C	0	0
			18	18		

- Molecule 18 is HEXADECANE (CCD ID: R16) (formula: $C_{16}H_{34}$).



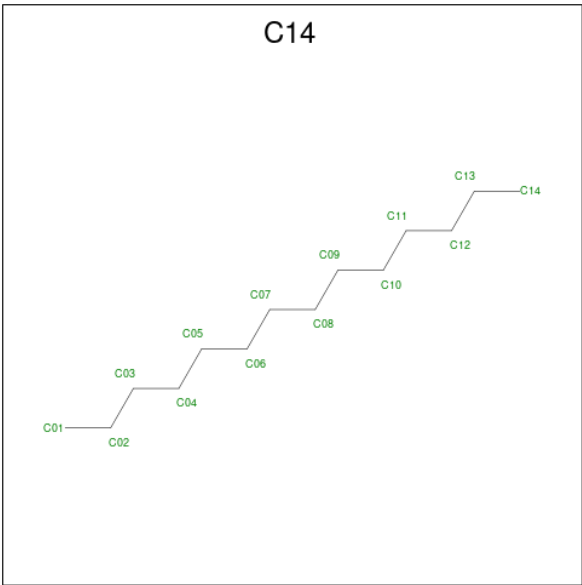
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	B	1	Total	C	0	0
			16	16		

- Molecule 19 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



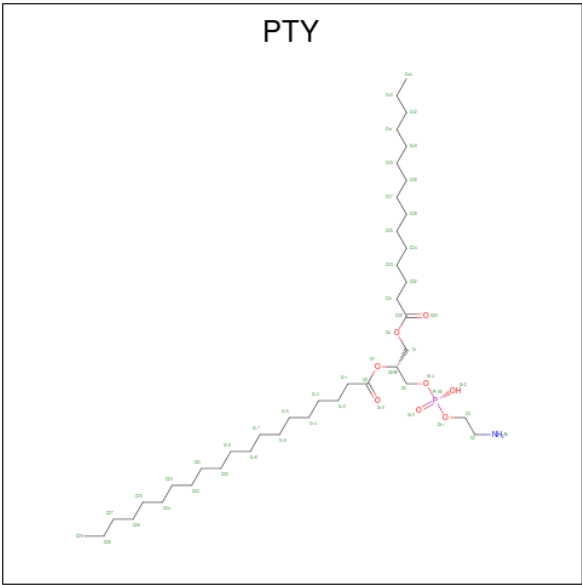
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 20 is TETRADECANE (CCD ID: C14) (formula: C₁₄H₃₀).



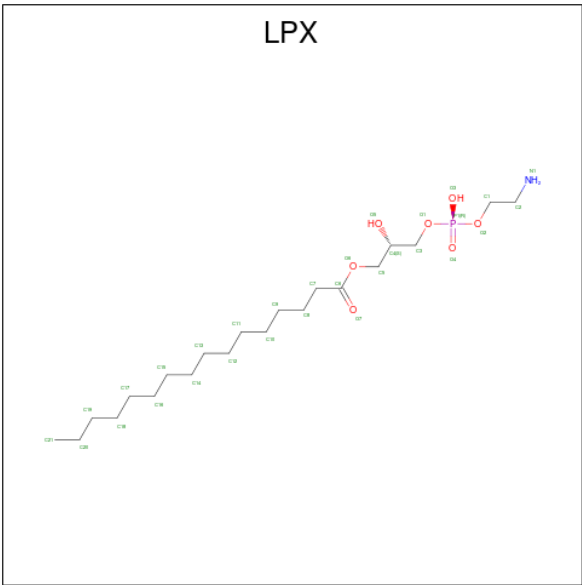
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	C	1	Total	C			0	0
			14	14				

- Molecule 21 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



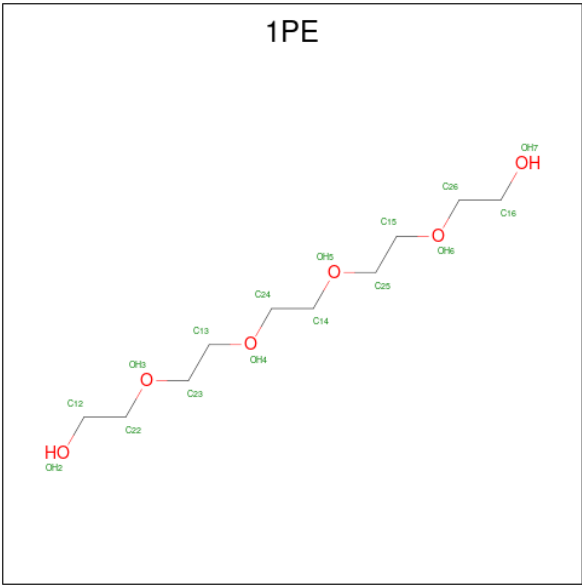
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 22 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: $C_{21}H_{44}NO_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total	C	N	O	P	0	0
			30	21	1	7	1		

- Molecule 23 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	O	0	0
			16	10	6		

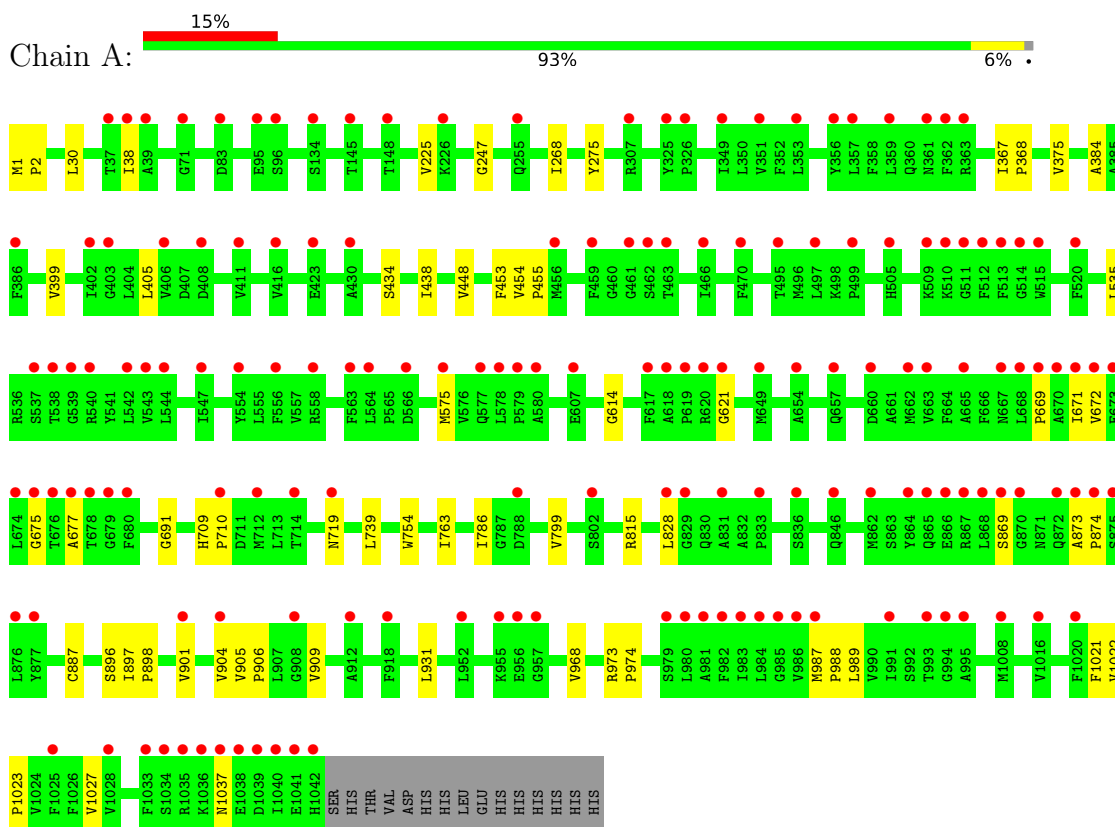
- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	380	Total 380	O 380	0	0
24	B	348	Total 348	O 348	0	0
24	C	401	Total 401	O 401	0	0
24	D	37	Total 37	O 37	0	0
24	E	22	Total 22	O 22	0	0

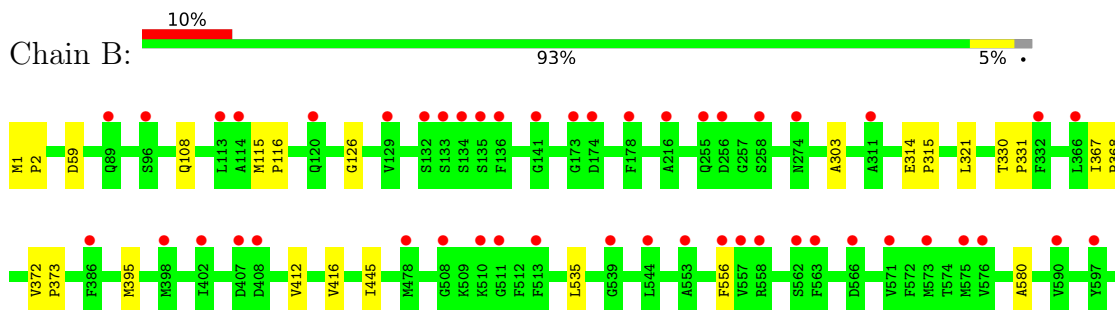
3 Residue-property plots [i](#)

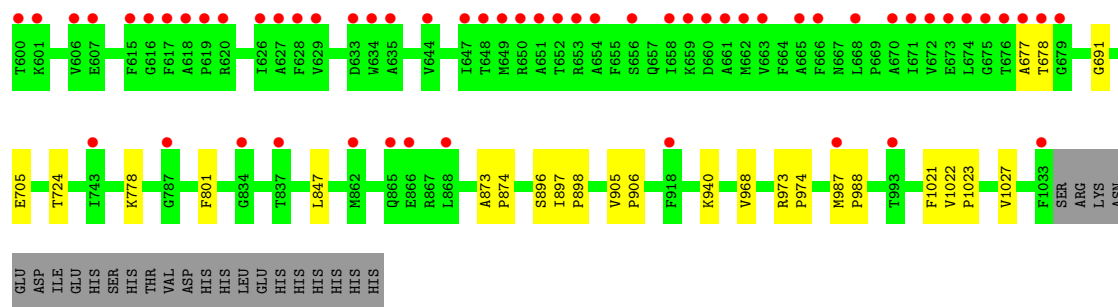
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

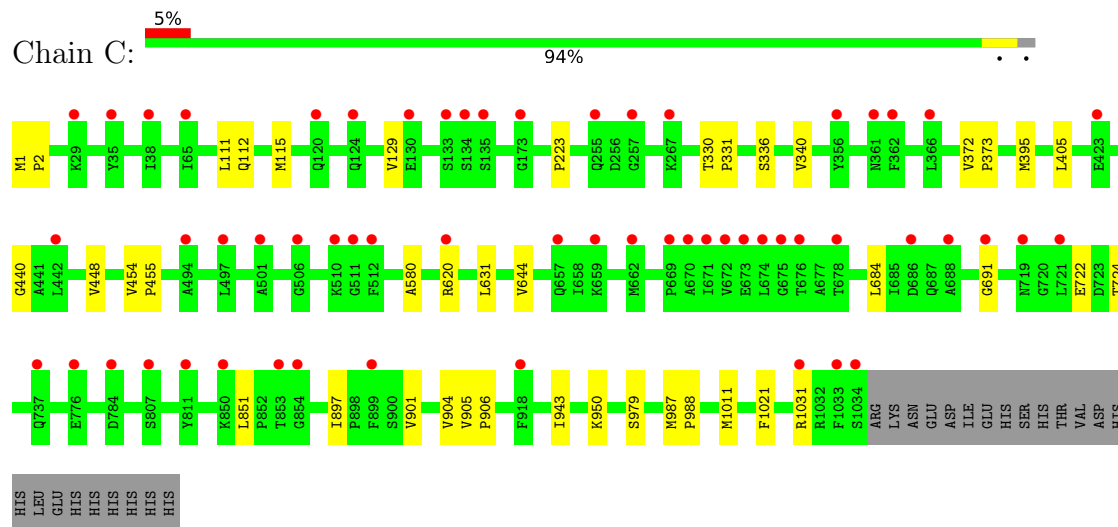


• Molecule 1: Multidrug efflux pump subunit AcrB

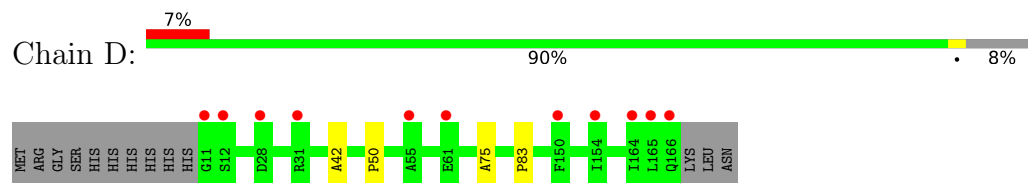




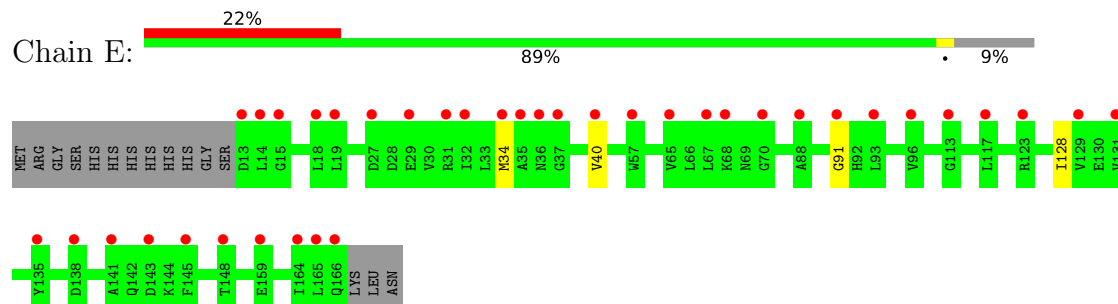
- Molecule 1: Multidrug efflux pump subunit AcrB



- 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	146.28Å 161.01Å 245.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 2.35 49.36 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.36-2.35) 100.0 (49.36-2.35)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.231 , 0.257 0.233 , 0.258	Depositor DCC
R_{free} test set	12080 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.9	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	0.93	EDS
Total number of atoms	28139	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DDR, 1PE, EDO, SO4, D12, LMT, PG4, C14, 8K6, R16, MIY, GOL, PTY, D10, LPX, MYS, PGE, HEX, DDQ, OCT, CL

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	1.04	0/8122	1.57	8/11027 (0.1%)
1	B	1.04	0/8043	1.57	6/10923 (0.1%)
1	C	1.04	0/8035	1.56	3/10912 (0.0%)
2	D	1.04	0/1196	1.58	0/1626
2	E	1.03	0/1186	1.61	0/1613
All	All	1.04	0/26582	1.57	17/36101 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	896	SER	CA-C-N	7.36	124.88	120.24
1	B	896	SER	C-N-CA	7.36	124.88	120.24
1	A	896	SER	CA-C-N	7.23	124.79	120.24
1	A	896	SER	C-N-CA	7.23	124.79	120.24
1	B	691	GLY	CA-C-O	-5.70	118.35	122.45
1	B	1021	PHE	CA-C-N	5.57	123.75	120.24
1	B	1021	PHE	C-N-CA	5.57	123.75	120.24
1	C	1021	PHE	CA-C-N	5.56	123.74	120.24
1	C	1021	PHE	C-N-CA	5.56	123.74	120.24
1	C	691	GLY	CA-C-O	-5.55	118.45	122.45
1	A	691	GLY	CA-C-O	-5.53	118.47	122.45
1	A	1021	PHE	CA-C-N	5.48	123.69	120.24
1	A	1021	PHE	C-N-CA	5.48	123.69	120.24
1	B	126	GLY	CA-C-O	-5.26	118.36	122.52
1	A	675	GLY	CA-C-O	-5.22	118.39	122.52
1	A	453	PHE	CA-C-N	5.18	124.47	120.33
1	A	453	PHE	C-N-CA	5.18	124.47	120.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7961	0	8115	30	0
1	B	7883	0	8043	28	0
1	C	7881	0	8032	24	0
2	D	1177	0	1159	2	0
2	E	1167	0	1151	2	0
3	A	105	0	138	0	0
3	B	70	0	92	0	0
3	C	35	0	46	0	0
4	A	8	0	18	0	0
4	C	16	0	36	0	0
5	A	14	0	27	0	0
5	B	28	0	54	0	0
5	C	28	0	54	0	0
6	A	36	0	48	0	0
6	B	24	0	32	0	0
6	C	18	0	24	0	0
6	E	6	0	8	0	0
7	A	12	0	26	0	0
7	C	24	0	52	0	0
8	A	6	0	14	0	0
8	B	18	0	42	0	0
8	C	12	0	28	0	0
9	A	12	0	18	0	0
9	B	40	0	60	0	0
9	C	32	0	48	0	0
9	D	12	0	18	0	0
10	A	10	0	14	0	0
10	C	10	0	14	0	0
11	B	33	0	24	0	0
12	B	28	0	44	0	0
13	B	30	0	66	0	0
13	C	20	0	44	0	0
14	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	C	2	0	0	0	0
15	B	30	0	64	0	0
16	B	13	0	18	3	0
17	B	18	0	38	0	0
18	B	16	0	34	0	0
19	B	5	0	0	0	0
20	C	14	0	30	1	0
21	C	50	0	79	0	0
22	C	30	0	43	0	0
23	C	16	0	22	0	0
24	A	380	0	0	0	0
24	B	348	0	0	0	0
24	C	401	0	0	0	0
24	D	37	0	0	0	0
24	E	22	0	0	0	0
All	All	28139	0	27917	81	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 1.

All (81) 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:C:979:SER:HA	1:C:1011:MET:HE3	1.80	0.64
1:A:968:VAL:HG11	1:A:1023:PRO:HG3	1.80	0.62
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.82	0.62
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.82	0.60
1:B:395[B]:MET:HA	1:B:395[B]:MET:HE2	1.85	0.59
1:C:901:VAL:O	1:C:904:VAL:HG12	2.03	0.59
2:E:34:MET:SD	2:E:40:VAL:HG12	2.46	0.56
1:B:580:ALA:HB1	1:B:724:THR:HG22	1.87	0.56
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.87	0.55
1:A:709:HIS:N	1:A:710:PRO:HD3	2.23	0.54
1:B:303:ALA:HB2	1:B:330:THR:HG21	1.90	0.54
1:B:108:GLN:CG	1:C:112:GLN:HG3	2.40	0.52
1:C:897:ILE:HD11	1:C:950:LYS:HG2	1.91	0.51
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.93	0.50
1:B:968:VAL:HG11	1:B:1023:PRO:HG3	1.93	0.50
1:A:38:ILE:HD11	1:A:671:ILE:HD13	1.95	0.49
1:C:580:ALA:HB1	1:C:724:THR:HA	1.94	0.49
1:C:440:GLY:HA2	20:C:1101:C14:H061	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:PRO:HD2	1:A:672:VAL:HG22	1.96	0.48
1:A:897:ILE:N	1:A:898:PRO:CD	2.77	0.48
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.95	0.48
16:B:1120:PG4:H51	1:C:115:MET:HG3	1.96	0.48
1:A:247:GLY:HA2	1:A:268:ILE:CD1	2.45	0.47
1:C:330:THR:N	1:C:331:PRO:CD	2.78	0.47
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.96	0.46
1:A:909:VAL:HA	1:A:931:LEU:HD11	1.97	0.46
1:C:111:LEU:HD22	1:C:129:VAL:CG2	2.46	0.46
1:B:445:ILE:HD13	1:B:940:LYS:HG3	1.98	0.46
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.97	0.46
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.98	0.46
1:B:115:MET:HG3	16:B:1120:PG4:H21	1.98	0.46
1:A:987:MET:N	1:A:988:PRO:CD	2.79	0.46
1:B:677:ALA:O	1:B:678:THR:OG1	2.23	0.45
1:B:303:ALA:CB	1:B:330:THR:HG21	2.47	0.45
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.99	0.45
1:B:897:ILE:N	1:B:898:PRO:CD	2.80	0.45
2:D:42:ALA:O	2:D:50:PRO:HD3	2.16	0.45
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.31	0.45
1:B:987:MET:N	1:B:988:PRO:CD	2.80	0.45
1:A:30:LEU:HD21	1:A:384:ALA:HA	1.99	0.45
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.99	0.44
1:B:330:THR:N	1:B:331:PRO:CD	2.81	0.44
1:B:367:ILE:HB	1:B:368:PRO:HD3	2.00	0.44
1:A:1022:VAL:N	1:A:1023:PRO:CD	2.81	0.44
1:A:448:VAL:HG22	1:A:887:CYS:HB3	2.00	0.44
1:B:115:MET:N	1:B:116:PRO:CD	2.80	0.44
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.99	0.44
1:A:719:ASN:HB2	1:A:828:LEU:HG	2.00	0.43
1:C:684:LEU:HD11	1:C:851:LEU:CD1	2.48	0.43
1:B:108:GLN:HG3	1:C:112:GLN:HG3	1.99	0.43
1:C:336:SER:O	1:C:340:VAL:HG23	2.18	0.43
1:B:314:GLU:HB2	1:B:315:PRO:HD3	2.01	0.43
1:C:722[B]:GLU:HA	1:C:722[B]:GLU:OE1	2.18	0.43
1:B:1:MET:HB3	1:B:2:PRO:HD3	2.00	0.43
1:C:631:LEU:HD11	1:C:644:VAL:HG22	2.01	0.43
1:A:454:VAL:N	1:A:455:PRO:CD	2.82	0.43
1:B:535:LEU:HD22	1:B:1027:VAL:HG21	2.01	0.42
1:C:905:VAL:HB	1:C:906:PRO:HD3	2.01	0.42
1:C:395:MET:HA	1:C:395:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:GLY:HA2	1:A:621:GLY:O	2.20	0.42
1:A:901:VAL:O	1:A:904:VAL:HG22	2.19	0.42
1:A:763:ILE:HD11	1:B:59:ASP:HB3	2.02	0.42
1:C:454:VAL:HB	1:C:455:PRO:HD3	2.01	0.42
1:A:1:MET:HB2	1:A:2:PRO:HD3	2.02	0.42
1:B:412:VAL:O	1:B:416:VAL:HG23	2.20	0.41
1:C:448:VAL:HG11	1:C:943:ILE:HD11	2.03	0.41
1:A:275:TYR:CD1	1:C:223:PRO:HD3	2.55	0.41
2:D:75:ALA:O	2:D:83:PRO:HD3	2.20	0.41
1:A:739:LEU:HD13	1:A:799:VAL:HG11	2.02	0.41
16:B:1120:PG4:H31	1:C:112:GLN:HG2	2.03	0.41
1:A:434:SER:O	1:A:438:ILE:HG13	2.21	0.41
1:A:535:LEU:HD22	1:A:1027:VAL:HG21	2.03	0.41
1:A:754:TRP:CZ2	1:A:786:ILE:HD13	2.55	0.41
2:E:91:GLY:HA2	2:E:128:ILE:CD1	2.51	0.41
1:A:973:ARG:N	1:A:974:PRO:HD2	2.36	0.40
1:C:372:VAL:HB	1:C:373:PRO:CD	2.51	0.40
1:B:395[B]:MET:HE2	1:B:395[B]:MET:CA	2.51	0.40
1:A:905:VAL:O	1:A:909:VAL:HG23	2.22	0.40
1:B:973:ARG:N	1:B:974:PRO:HD2	2.36	0.40
1:C:405:LEU:C	1:C:405:LEU:HD12	2.46	0.40
1:A:225:VAL:HG11	1:B:778:LYS:HA	2.04	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	1044/1057 (99%)	1013 (97%)	28 (3%)	3 (0%)	36	43
1	B	1036/1057 (98%)	1013 (98%)	23 (2%)	0	100	100
1	C	1035/1057 (98%)	1012 (98%)	23 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	154/169 (91%)	151 (98%)	3 (2%)	0	100	100
2	E	152/169 (90%)	149 (98%)	3 (2%)	0	100	100
All	All	3421/3509 (98%)	3338 (98%)	80 (2%)	3 (0%)	48	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1037	ASN
1	A	677	ALA
1	A	869	SER

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	853/864 (99%)	850 (100%)	3 (0%)	84	91
1	B	845/864 (98%)	842 (100%)	3 (0%)	84	91
1	C	844/864 (98%)	841 (100%)	3 (0%)	84	91
2	D	120/132 (91%)	120 (100%)	0	100	100
2	E	119/132 (90%)	119 (100%)	0	100	100
All	All	2781/2856 (97%)	2772 (100%)	9 (0%)	86	92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	575	MET
1	A	815[A]	ARG
1	A	815[B]	ARG
1	B	321	LEU
1	B	556	PHE
1	B	801	PHE
1	C	620	ARG
1	C	1031[A]	ARG

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Mol	Chain	Res	Type
1	C	1031[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	ASN
1	A	237	GLN
1	A	254	ASN
1	A	584	GLN
1	A	588	GLN
1	A	605	ASN
1	A	797	GLN
1	B	58	GLN
1	B	81	ASN
1	B	194	ASN
1	B	584	GLN
1	C	58	GLN
1	C	63	GLN
1	C	89	GLN
1	C	194	ASN
1	C	505	HIS
1	C	577	GLN
1	C	692	HIS
2	D	92	HIS
2	D	125	HIS
2	E	125	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 83 ligands modelled in this entry, 3 are monoatomic - leaving 80 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
9	EDO	A	1115	-	3,3,3	0.06	0	2,2,2	0.12	0
17	8K6	B	1131	-	17,17,17	0.17	0	16,16,16	0.06	0
9	EDO	A	1114	-	3,3,3	0.07	0	2,2,2	0.09	0
13	D10	C	1109	-	9,9,9	0.10	0	8,8,8	0.15	0
13	D10	B	1108	-	9,9,9	0.09	0	8,8,8	0.06	0
9	EDO	B	1129	-	3,3,3	0.06	0	2,2,2	0.09	0
11	MIY	B	1101	-	36,36,36	1.08	2 (5%)	42,58,58	1.05	2 (4%)
8	HEX	B	1116	-	5,5,5	0.13	0	4,4,4	0.11	0
5	DDQ	C	1106	-	11,13,13	2.25	2 (18%)	12,15,15	0.44	0
12	DDR	B	1104	-	27,27,27	1.24	2 (7%)	29,29,29	1.09	2 (6%)
7	D12	C	1115	-	11,11,11	0.26	0	10,10,10	0.45	0
10	PGE	A	1117	-	9,9,9	0.14	0	8,8,8	0.13	0
3	LMT	C	1102	-	36,36,36	0.43	0	47,47,47	0.48	0
9	EDO	D	202	-	3,3,3	0.06	0	2,2,2	0.09	0
19	SO4	B	1133	-	4,4,4	0.35	0	6,6,6	0.08	0
6	GOL	B	1113	-	5,5,5	0.09	0	5,5,5	0.28	0
6	GOL	A	1111	-	5,5,5	0.09	0	5,5,5	0.25	0
9	EDO	C	1127	-	3,3,3	0.06	0	2,2,2	0.11	0
7	D12	A	1112	-	11,11,11	0.24	0	10,10,10	0.49	0
8	HEX	C	1118	-	5,5,5	0.12	0	4,4,4	0.11	0
8	HEX	B	1117	-	5,5,5	0.13	0	4,4,4	0.13	0
6	GOL	C	1112	-	5,5,5	0.08	0	5,5,5	0.24	0
16	PG4	B	1120	-	12,12,12	0.16	0	11,11,11	0.09	0
9	EDO	B	1123	-	3,3,3	0.07	0	2,2,2	0.13	0
6	GOL	B	1112	-	5,5,5	0.09	0	5,5,5	0.26	0
9	EDO	B	1130	-	3,3,3	0.07	0	2,2,2	0.11	0
5	DDQ	B	1106	-	11,13,13	2.29	2 (18%)	12,15,15	0.35	0
6	GOL	A	1109	-	5,5,5	0.09	0	5,5,5	0.25	0
5	DDQ	B	1105	-	11,13,13	2.25	2 (18%)	12,15,15	0.57	0
22	LPX	C	1119	-	29,29,29	0.28	0	31,33,33	0.37	0
9	EDO	B	1126	-	3,3,3	0.06	0	2,2,2	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	R16	B	1132	-	15,15,15	0.09	0	14,14,14	0.07	0
4	OCT	A	1104	-	7,7,7	0.10	0	6,6,6	0.07	0
9	EDO	C	1124	-	3,3,3	0.06	0	2,2,2	0.09	0
5	DDQ	C	1107	-	11,13,13	2.24	2 (18%)	12,15,15	0.49	0
9	EDO	C	1128	-	3,3,3	0.07	0	2,2,2	0.11	0
3	LMT	A	1103	-	36,36,36	0.47	0	47,47,47	0.61	0
9	EDO	B	1128	-	3,3,3	0.06	0	2,2,2	0.10	0
6	GOL	A	1110	-	5,5,5	0.08	0	5,5,5	0.26	0
15	MYS	B	1119	-	14,14,14	0.25	0	13,13,13	0.52	0
9	EDO	C	1121	-	3,3,3	0.06	0	2,2,2	0.10	0
3	LMT	A	1101	-	36,36,36	0.44	0	47,47,47	0.63	0
13	D10	B	1109	-	9,9,9	0.09	0	8,8,8	0.07	0
3	LMT	A	1102	-	36,36,36	0.47	0	47,47,47	0.67	0
9	EDO	C	1125	-	3,3,3	0.06	0	2,2,2	0.10	0
6	GOL	A	1107	-	5,5,5	0.08	0	5,5,5	0.26	0
9	EDO	D	201	-	3,3,3	0.06	0	2,2,2	0.08	0
9	EDO	C	1123	-	3,3,3	0.06	0	2,2,2	0.09	0
3	LMT	B	1103	-	36,36,36	0.50	0	47,47,47	0.85	2 (4%)
9	EDO	C	1126	-	3,3,3	0.06	0	2,2,2	0.10	0
3	LMT	B	1102	-	36,36,36	0.44	0	47,47,47	0.49	0
6	GOL	B	1111	-	5,5,5	0.09	0	5,5,5	0.26	0
9	EDO	B	1122	-	3,3,3	0.06	0	2,2,2	0.08	0
7	D12	C	1116	-	11,11,11	0.25	0	10,10,10	0.50	0
6	GOL	B	1110	-	5,5,5	0.08	0	5,5,5	0.24	0
21	PTY	C	1103	-	49,49,49	0.26	0	52,54,54	0.35	0
4	OCT	C	1105	-	7,7,7	0.09	0	6,6,6	0.07	0
13	D10	B	1107	-	9,9,9	0.09	0	8,8,8	0.07	0
5	DDQ	A	1105	-	11,13,13	2.27	2 (18%)	12,15,15	0.48	0
8	HEX	A	1113	-	5,5,5	0.13	0	4,4,4	0.11	0
9	EDO	B	1124	-	3,3,3	0.06	0	2,2,2	0.12	0
23	1PE	C	1120	-	15,15,15	0.49	0	14,14,14	0.24	0
10	PGE	C	1129	-	9,9,9	0.15	0	8,8,8	0.11	0
6	GOL	A	1108	-	5,5,5	0.08	0	5,5,5	0.25	0
9	EDO	A	1116	-	3,3,3	0.06	0	2,2,2	0.11	0
13	D10	C	1108	-	9,9,9	0.09	0	8,8,8	0.06	0
4	OCT	C	1104	-	7,7,7	0.11	0	6,6,6	0.11	0
20	C14	C	1101	-	13,13,13	0.09	0	12,12,12	0.09	0
15	MYS	B	1118	-	14,14,14	0.22	0	13,13,13	0.58	0
8	HEX	B	1115	-	5,5,5	0.12	0	4,4,4	0.15	0
9	EDO	B	1121	-	3,3,3	0.05	0	2,2,2	0.09	0
9	EDO	D	203	-	3,3,3	0.06	0	2,2,2	0.11	0
9	EDO	C	1122	-	3,3,3	0.06	0	2,2,2	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	C	1110	-	5,5,5	0.09	0	5,5,5	0.27	0
8	HEX	C	1117	-	5,5,5	0.13	0	4,4,4	0.12	0
6	GOL	A	1106	-	5,5,5	0.08	0	5,5,5	0.24	0
9	EDO	B	1125	-	3,3,3	0.06	0	2,2,2	0.11	0
6	GOL	C	1111	-	5,5,5	0.10	0	5,5,5	0.27	0
6	GOL	E	201	-	5,5,5	0.09	0	5,5,5	0.26	0
9	EDO	B	1127	-	3,3,3	0.06	0	2,2,2	0.12	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
9	EDO	A	1115	-	-	1/1/1/1	-
17	8K6	B	1131	-	-	9/15/15/15	-
9	EDO	A	1114	-	-	1/1/1/1	-
13	D10	C	1109	-	-	6/7/7/7	-
13	D10	B	1108	-	-	2/7/7/7	-
9	EDO	B	1129	-	-	0/1/1/1	-
11	MIY	B	1101	-	-	2/12/70/70	0/4/4/4
8	HEX	B	1116	-	-	2/3/3/3	-
5	DDQ	C	1106	-	-	5/11/11/11	-
12	DDR	B	1104	-	-	12/29/29/29	-
7	D12	C	1115	-	-	4/9/9/9	-
10	PGE	A	1117	-	-	4/7/7/7	-
3	LMT	C	1102	-	-	7/21/61/61	0/2/2/2
9	EDO	D	202	-	-	1/1/1/1	-
6	GOL	B	1113	-	-	2/4/4/4	-
6	GOL	A	1111	-	-	2/4/4/4	-
9	EDO	C	1127	-	-	1/1/1/1	-
7	D12	A	1112	-	-	4/9/9/9	-
8	HEX	C	1118	-	-	1/3/3/3	-
8	HEX	B	1117	-	-	2/3/3/3	-
6	GOL	C	1112	-	-	2/4/4/4	-
16	PG4	B	1120	-	-	5/10/10/10	-
9	EDO	B	1123	-	-	1/1/1/1	-
6	GOL	B	1112	-	-	0/4/4/4	-
9	EDO	B	1130	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DDQ	B	1106	-	-	9/11/11/11	-
6	GOL	A	1109	-	-	0/4/4/4	-
5	DDQ	B	1105	-	-	3/11/11/11	-
22	LPX	C	1119	-	-	15/31/31/31	-
9	EDO	B	1126	-	-	1/1/1/1	-
18	R16	B	1132	-	-	9/13/13/13	-
4	OCT	A	1104	-	-	2/5/5/5	-
9	EDO	C	1124	-	-	1/1/1/1	-
5	DDQ	C	1107	-	-	6/11/11/11	-
9	EDO	C	1128	-	-	0/1/1/1	-
3	LMT	A	1103	-	-	14/21/61/61	0/2/2/2
9	EDO	B	1128	-	-	1/1/1/1	-
6	GOL	A	1110	-	-	0/4/4/4	-
15	MYS	B	1119	-	-	3/12/12/12	-
9	EDO	C	1121	-	-	0/1/1/1	-
3	LMT	A	1101	-	-	9/21/61/61	0/2/2/2
13	D10	B	1109	-	-	4/7/7/7	-
3	LMT	A	1102	-	-	12/21/61/61	0/2/2/2
9	EDO	C	1125	-	-	0/1/1/1	-
6	GOL	A	1107	-	-	2/4/4/4	-
9	EDO	D	201	-	-	0/1/1/1	-
9	EDO	C	1123	-	-	1/1/1/1	-
3	LMT	B	1103	-	-	7/21/61/61	0/2/2/2
9	EDO	C	1126	-	-	1/1/1/1	-
3	LMT	B	1102	-	-	8/21/61/61	0/2/2/2
6	GOL	B	1111	-	-	0/4/4/4	-
9	EDO	B	1122	-	-	1/1/1/1	-
7	D12	C	1116	-	-	3/9/9/9	-
6	GOL	B	1110	-	-	2/4/4/4	-
21	PTY	C	1103	-	-	23/53/53/53	-
4	OCT	C	1105	-	-	3/5/5/5	-
13	D10	B	1107	-	-	1/7/7/7	-
5	DDQ	A	1105	-	-	7/11/11/11	-
8	HEX	A	1113	-	-	1/3/3/3	-
9	EDO	B	1124	-	-	1/1/1/1	-
23	1PE	C	1120	-	-	8/13/13/13	-
10	PGE	C	1129	-	-	5/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	1108	-	-	2/4/4/4	-
9	EDO	A	1116	-	-	1/1/1/1	-
13	D10	C	1108	-	-	3/7/7/7	-
4	OCT	C	1104	-	-	4/5/5/5	-
20	C14	C	1101	-	-	6/11/11/11	-
15	MYS	B	1118	-	-	2/12/12/12	-
8	HEX	B	1115	-	-	1/3/3/3	-
9	EDO	B	1121	-	-	1/1/1/1	-
9	EDO	D	203	-	-	1/1/1/1	-
9	EDO	C	1122	-	-	1/1/1/1	-
6	GOL	C	1110	-	-	0/4/4/4	-
8	HEX	C	1117	-	-	1/3/3/3	-
6	GOL	A	1106	-	-	2/4/4/4	-
9	EDO	B	1125	-	-	1/1/1/1	-
6	GOL	C	1111	-	-	4/4/4/4	-
6	GOL	E	201	-	-	0/4/4/4	-
9	EDO	B	1127	-	-	0/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1106	DDQ	O1-N1	-6.96	1.25	1.42
5	A	1105	DDQ	O1-N1	-6.82	1.25	1.42
5	C	1106	DDQ	O1-N1	-6.80	1.25	1.42
5	B	1105	DDQ	O1-N1	-6.79	1.25	1.42
5	C	1107	DDQ	O1-N1	-6.72	1.25	1.42
11	B	1101	MIY	C21-N2	5.19	1.48	1.33
12	B	1104	DDR	O51-C1	4.30	1.45	1.33
12	B	1104	DDR	O52-C21	4.24	1.46	1.34
5	A	1105	DDQ	C1-N1	-3.07	1.48	1.51
5	C	1107	DDQ	C1-N1	-3.03	1.48	1.51
5	B	1105	DDQ	C1-N1	-2.98	1.48	1.51
5	C	1106	DDQ	C1-N1	-2.95	1.48	1.51
5	B	1106	DDQ	C1-N1	-2.87	1.48	1.51
11	B	1101	MIY	O5-C15	2.31	1.28	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1104	DDR	O52-C21-C22	3.66	119.40	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1103	LMT	O1B-C4'-C3'	3.25	115.50	107.23
12	B	1104	DDR	O51-C1-C2	2.60	119.78	111.83
11	B	1101	MIY	C15-C16-C17	2.57	120.83	118.80
3	B	1103	LMT	C1B-C2B-C3B	2.34	114.92	110.01
11	B	1101	MIY	O7-C18-C17	-2.28	106.49	110.14

There are no chirality outliers.

All (270) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1105	DDQ	C2-C1-N1-O1
5	B	1106	DDQ	C2-C1-N1-CM2
5	B	1106	DDQ	N1-C1-C2-C3
5	C	1106	DDQ	N1-C1-C2-C3
6	A	1106	GOL	C1-C2-C3-O3
6	A	1108	GOL	C1-C2-C3-O3
6	B	1113	GOL	C1-C2-C3-O3
21	C	1103	PTY	C11-C8-O7-C6
22	C	1119	LPX	C3-O1-P1-O2
22	C	1119	LPX	O2-C1-C2-N1
3	B	1103	LMT	C3'-C4'-O1B-C1B
12	B	1104	DDR	O1-C1-O51-C51
22	C	1119	LPX	O7-C6-O6-C5
12	B	1104	DDR	C2-C1-O51-C51
3	A	1103	LMT	O5B-C5B-C6B-O6B
22	C	1119	LPX	C7-C6-O6-C5
3	A	1101	LMT	O5B-C5B-C6B-O6B
3	C	1102	LMT	O5'-C5'-C6'-O6'
21	C	1103	PTY	O10-C8-O7-C6
3	A	1103	LMT	C4B-C5B-C6B-O6B
3	B	1102	LMT	O5'-C5'-C6'-O6'
23	C	1120	1PE	OH4-C13-C23-OH3
3	A	1101	LMT	O5'-C1'-O1'-C1
3	A	1102	LMT	O5'-C1'-O1'-C1
3	A	1103	LMT	O5'-C1'-O1'-C1
3	A	1101	LMT	C4B-C5B-C6B-O6B
3	C	1102	LMT	C4'-C5'-C6'-O6'
22	C	1119	LPX	C15-C16-C17-C18
23	C	1120	1PE	OH5-C14-C24-OH4
3	B	1102	LMT	C4'-C5'-C6'-O6'
3	A	1101	LMT	C2'-C1'-O1'-C1
3	A	1102	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
3	A	1103	LMT	C2'-C1'-O1'-C1
3	A	1102	LMT	C5'-C4'-O1B-C1B
6	B	1113	GOL	O2-C2-C3-O3
22	C	1119	LPX	C6-C7-C8-C9
10	A	1117	PGE	O3-C5-C6-O4
3	A	1103	LMT	O5'-C5'-C6'-O6'
22	C	1119	LPX	C17-C18-C19-C20
3	A	1103	LMT	C4'-C5'-C6'-O6'
22	C	1119	LPX	O5-C4-C5-O6
10	C	1129	PGE	O1-C1-C2-O2
16	B	1120	PG4	O4-C7-C8-O5
10	A	1117	PGE	O2-C3-C4-O3
12	B	1104	DDR	C22-C21-O52-C52
22	C	1119	LPX	C3-C4-C5-O6
12	B	1104	DDR	O21-C21-O52-C52
12	B	1104	DDR	C21-C22-C23-C24
6	A	1107	GOL	C1-C2-C3-O3
6	A	1111	GOL	C1-C2-C3-O3
6	B	1110	GOL	C1-C2-C3-O3
6	C	1111	GOL	C1-C2-C3-O3
6	C	1112	GOL	O1-C1-C2-C3
3	B	1102	LMT	O1'-C1-C2-C3
10	A	1117	PGE	O1-C1-C2-O2
3	A	1103	LMT	C11-C10-C9-C8
5	C	1106	DDQ	C6-C7-C8-C9
13	B	1109	D10	C6-C7-C8-C9
3	A	1101	LMT	C3-C4-C5-C6
3	A	1101	LMT	C4-C5-C6-C7
3	C	1102	LMT	C6-C7-C8-C9
7	C	1115	D12	C2-C3-C4-C5
6	A	1108	GOL	O2-C2-C3-O3
13	B	1108	D10	C4-C5-C6-C7
16	B	1120	PG4	O3-C5-C6-O4
5	B	1106	DDQ	C4-C5-C6-C7
3	B	1103	LMT	C11-C10-C9-C8
18	B	1132	R16	C35-C36-C37-C38
3	A	1102	LMT	C1-C2-C3-C4
13	B	1107	D10	C4-C5-C6-C7
21	C	1103	PTY	C38-C39-C40-C41
8	B	1116	HEX	C2-C3-C4-C5
21	C	1103	PTY	C25-C26-C27-C28
3	A	1102	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
21	C	1103	PTY	C16-C17-C18-C19
3	B	1103	LMT	C1-C2-C3-C4
3	C	1102	LMT	C5-C6-C7-C8
9	A	1114	EDO	O1-C1-C2-O2
9	B	1128	EDO	O1-C1-C2-O2
9	C	1122	EDO	O1-C1-C2-O2
3	A	1102	LMT	C3'-C4'-O1B-C1B
21	C	1103	PTY	C31-C30-O4-C1
3	A	1103	LMT	C6-C7-C8-C9
21	C	1103	PTY	C32-C33-C34-C35
21	C	1103	PTY	C33-C34-C35-C36
5	A	1105	DDQ	C4-C5-C6-C7
15	B	1119	MYS	C9-C10-C11-C12
5	B	1106	DDQ	C1-C2-C3-C4
3	A	1102	LMT	C5-C6-C7-C8
5	B	1106	DDQ	C5-C6-C7-C8
20	C	1101	C14	C10-C11-C12-C13
5	C	1106	DDQ	C4-C5-C6-C7
13	C	1109	D10	C2-C3-C4-C5
13	B	1109	D10	C4-C5-C6-C7
20	C	1101	C14	C03-C04-C05-C06
3	B	1102	LMT	C5-C6-C7-C8
4	A	1104	OCT	C2-C3-C4-C5
16	B	1120	PG4	C5-C6-O4-C7
7	A	1112	D12	C6-C7-C8-C9
5	B	1106	DDQ	C2-C3-C4-C5
5	B	1106	DDQ	C3-C4-C5-C6
21	C	1103	PTY	O30-C30-O4-C1
17	B	1131	8K6	C7-C8-C9-C10
22	C	1119	LPX	C11-C10-C9-C8
20	C	1101	C14	C08-C09-C10-C11
13	C	1108	D10	C4-C5-C6-C7
3	A	1102	LMT	C4-C5-C6-C7
21	C	1103	PTY	C19-C20-C21-C22
22	C	1119	LPX	C11-C12-C13-C14
12	B	1104	DDR	C26-C27-C28-C29
3	B	1102	LMT	C3-C4-C5-C6
6	A	1107	GOL	O2-C2-C3-O3
21	C	1103	PTY	C18-C19-C20-C21
17	B	1131	8K6	C4-C5-C6-C7
5	A	1105	DDQ	C6-C7-C8-C9
12	B	1104	DDR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	A	1101	LMT	C2-C3-C4-C5
7	C	1115	D12	C5-C6-C7-C8
17	B	1131	8K6	C3-C4-C5-C6
3	B	1102	LMT	C11-C10-C9-C8
4	C	1105	OCT	C4-C5-C6-C7
5	C	1107	DDQ	C3-C4-C5-C6
13	C	1109	D10	C3-C4-C5-C6
9	A	1115	EDO	O1-C1-C2-O2
9	B	1123	EDO	O1-C1-C2-O2
9	B	1125	EDO	O1-C1-C2-O2
9	B	1126	EDO	O1-C1-C2-O2
9	C	1126	EDO	O1-C1-C2-O2
9	D	202	EDO	O1-C1-C2-O2
3	A	1103	LMT	C2-C3-C4-C5
13	C	1108	D10	C2-C3-C4-C5
3	A	1101	LMT	O5'-C5'-C6'-O6'
3	A	1102	LMT	O1'-C1-C2-C3
21	C	1103	PTY	C17-C18-C19-C20
21	C	1103	PTY	C37-C38-C39-C40
15	B	1119	MYS	C6-C7-C8-C9
21	C	1103	PTY	C20-C21-C22-C23
5	B	1106	DDQ	C7-C8-C9-C10
17	B	1131	8K6	C9-C10-C11-C12
4	C	1104	OCT	C5-C6-C7-C8
20	C	1101	C14	C11-C12-C13-C14
13	B	1109	D10	C2-C3-C4-C5
18	B	1132	R16	C37-C38-C39-C40
4	C	1105	OCT	C2-C3-C4-C5
5	C	1106	DDQ	C3-C4-C5-C6
21	C	1103	PTY	C24-C25-C26-C27
10	C	1129	PGE	O3-C5-C6-O4
23	C	1120	1PE	OH7-C16-C26-OH6
6	A	1106	GOL	O2-C2-C3-O3
13	B	1108	D10	C2-C3-C4-C5
17	B	1131	8K6	C2-C3-C4-C5
13	B	1109	D10	C3-C4-C5-C6
3	B	1103	LMT	O5B-C1B-O1B-C4'
21	C	1103	PTY	O14-C5-C6-C1
8	B	1116	HEX	C3-C4-C5-C6
5	C	1106	DDQ	C7-C8-C9-C10
3	A	1102	LMT	C6-C7-C8-C9
20	C	1101	C14	C04-C05-C06-C07

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Mol	Chain	Res	Type	Atoms
16	B	1120	PG4	O2-C3-C4-O3
5	B	1105	DDQ	C4-C5-C6-C7
17	B	1131	8K6	C1-C2-C3-C4
15	B	1118	MYS	C9-C10-C11-C12
12	B	1104	DDR	C51-C52-C53-O53
5	B	1105	DDQ	C7-C8-C9-C10
9	B	1130	EDO	O1-C1-C2-O2
5	C	1107	DDQ	C2-C3-C4-C5
21	C	1103	PTY	C23-C24-C25-C26
22	C	1119	LPX	C13-C14-C15-C16
13	C	1109	D10	C1-C2-C3-C4
7	A	1112	D12	C7-C8-C9-C10
18	B	1132	R16	C28-C29-C30-C31
22	C	1119	LPX	C14-C15-C16-C17
12	B	1104	DDR	O52-C52-C53-O53
3	A	1103	LMT	C5-C6-C7-C8
3	B	1103	LMT	C3-C4-C5-C6
12	B	1104	DDR	C2-C3-C4-C5
16	B	1120	PG4	C4-C3-O2-C2
7	A	1112	D12	C3-C4-C5-C6
13	C	1109	D10	C4-C5-C6-C7
23	C	1120	1PE	C23-C13-OH4-C24
10	A	1117	PGE	C4-C3-O2-C2
23	C	1120	1PE	C16-C26-OH6-C15
17	B	1131	8K6	C14-C15-C16-C17
21	C	1103	PTY	O14-C5-C6-O7
12	B	1104	DDR	C27-C28-C29-C30
9	A	1116	EDO	O1-C1-C2-O2
9	B	1121	EDO	O1-C1-C2-O2
3	A	1103	LMT	C4-C5-C6-C7
5	A	1105	DDQ	C2-C1-N1-CM2
5	B	1106	DDQ	C2-C1-N1-CM1
8	B	1115	HEX	C3-C4-C5-C6
12	B	1104	DDR	C23-C24-C25-C26
21	C	1103	PTY	C41-C42-C43-C44
17	B	1131	8K6	C5-C6-C7-C8
7	C	1116	D12	C11-C10-C9-C8
8	B	1117	HEX	C3-C4-C5-C6
13	C	1109	D10	C7-C8-C9-C10
13	C	1108	D10	C6-C7-C8-C9
18	B	1132	R16	C39-C40-C41-C42
13	C	1109	D10	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
11	B	1101	MIY	C1-C2-C21-N2
21	C	1103	PTY	C3-O11-P1-O13
22	C	1119	LPX	C3-O1-P1-O4
8	C	1118	HEX	C2-C3-C4-C5
7	C	1115	D12	C6-C7-C8-C9
6	A	1111	GOL	O2-C2-C3-O3
6	B	1110	GOL	O2-C2-C3-O3
6	C	1112	GOL	O1-C1-C2-O2
3	B	1103	LMT	C2B-C1B-O1B-C4'
22	C	1119	LPX	C10-C11-C12-C13
5	C	1107	DDQ	N1-C1-C2-C3
18	B	1132	R16	C31-C32-C33-C34
10	C	1129	PGE	C1-C2-O2-C3
5	C	1107	DDQ	C1-C2-C3-C4
9	B	1122	EDO	O1-C1-C2-O2
9	C	1123	EDO	O1-C1-C2-O2
9	D	203	EDO	O1-C1-C2-O2
3	B	1102	LMT	C7-C8-C9-C10
23	C	1120	1PE	C25-C15-OH6-C26
10	C	1129	PGE	C3-C4-O3-C5
4	C	1104	OCT	C3-C4-C5-C6
15	B	1119	MYS	C3-C4-C5-C6
3	C	1102	LMT	C4-C5-C6-C7
5	A	1105	DDQ	C5-C6-C7-C8
3	A	1101	LMT	C6-C7-C8-C9
21	C	1103	PTY	C26-C27-C28-C29
7	C	1116	D12	C6-C7-C8-C9
18	B	1132	R16	C27-C28-C29-C30
4	C	1105	OCT	C1-C2-C3-C4
5	A	1105	DDQ	C1-C2-C3-C4
21	C	1103	PTY	C6-C5-O14-P1
4	C	1104	OCT	C4-C5-C6-C7
7	A	1112	D12	C1-C2-C3-C4
3	A	1102	LMT	C2-C3-C4-C5
23	C	1120	1PE	C14-C24-OH4-C13
5	C	1107	DDQ	C5-C6-C7-C8
21	C	1103	PTY	C34-C35-C36-C37
3	A	1102	LMT	C11-C10-C9-C8
18	B	1132	R16	C34-C35-C36-C37
7	C	1116	D12	C7-C8-C9-C10
5	C	1107	DDQ	C4-C5-C6-C7
8	A	1113	HEX	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	A	1103	LMT	C2-C1-O1'-C1'
9	C	1127	EDO	O1-C1-C2-O2
3	C	1102	LMT	C2-C3-C4-C5
6	C	1111	GOL	O1-C1-C2-C3
20	C	1101	C14	C07-C08-C09-C10
8	B	1117	HEX	C2-C3-C4-C5
6	C	1111	GOL	O2-C2-C3-O3
4	A	1104	OCT	C1-C2-C3-C4
18	B	1132	R16	C30-C31-C32-C33
4	C	1104	OCT	C2-C3-C4-C5
8	C	1117	HEX	C3-C4-C5-C6
9	B	1124	EDO	O1-C1-C2-O2
9	C	1124	EDO	O1-C1-C2-O2
18	B	1132	R16	C38-C39-C40-C41
10	C	1129	PGE	C6-C5-O3-C4
17	B	1131	8K6	C15-C16-C17-C18
15	B	1118	MYS	C10-C11-C12-C13
3	B	1102	LMT	C2-C1-O1'-C1'
3	B	1103	LMT	C2-C1-O1'-C1'
23	C	1120	1PE	OH2-C12-C22-OH3
3	A	1103	LMT	C3-C4-C5-C6
11	B	1101	MIY	C3-C2-C21-N2
5	A	1105	DDQ	C7-C8-C9-C10
5	B	1105	DDQ	C6-C7-C8-C9
3	C	1102	LMT	O1'-C1-C2-C3
6	C	1111	GOL	O1-C1-C2-O2
3	A	1103	LMT	C9-C10-C11-C12
7	C	1115	D12	C11-C10-C9-C8

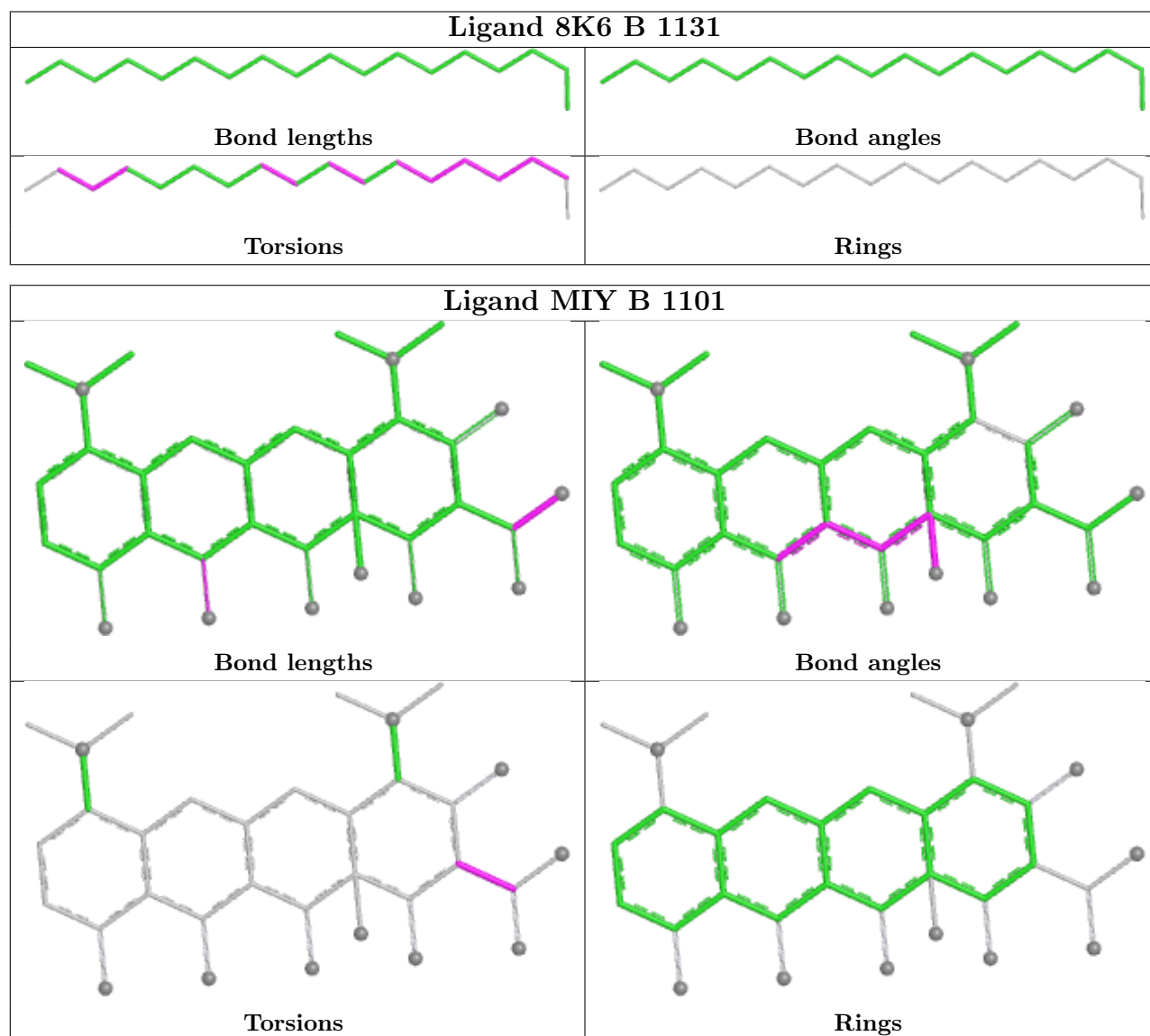
There are no ring outliers.

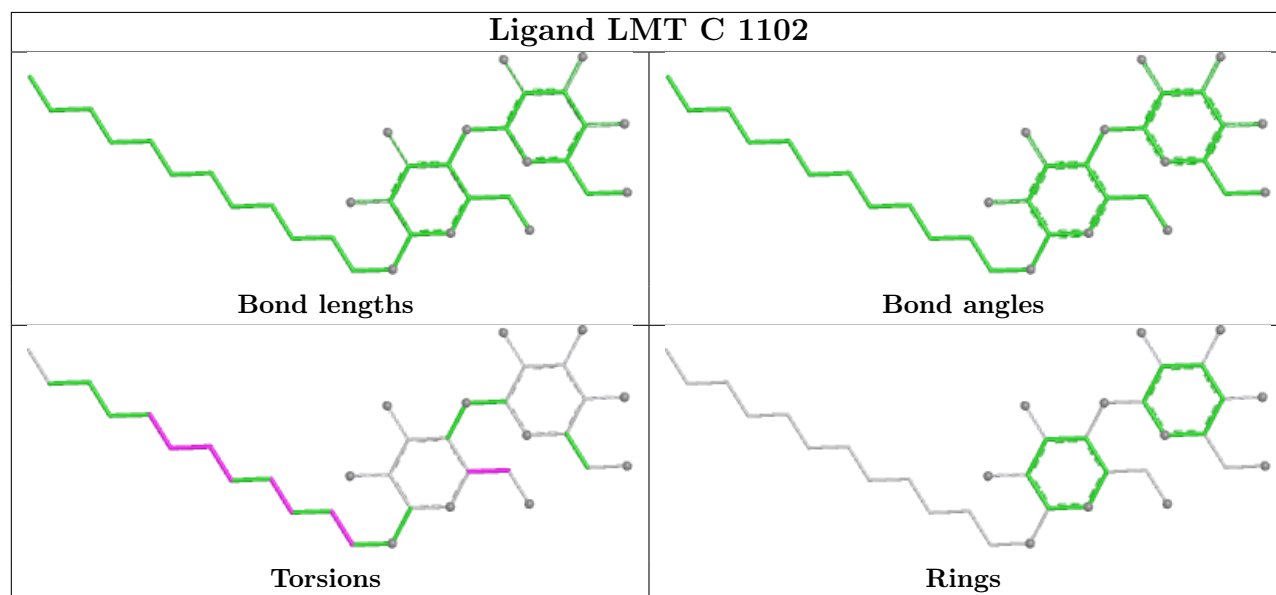
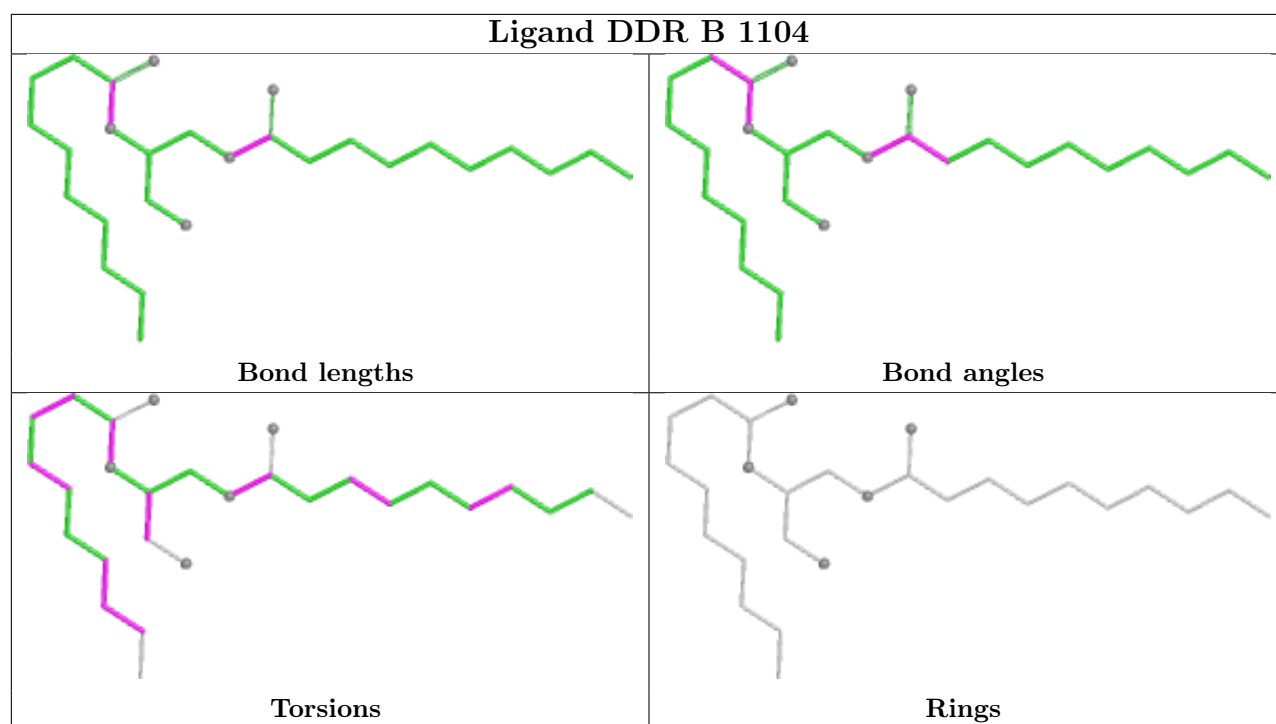
2 monomers are involved in 4 short contacts:

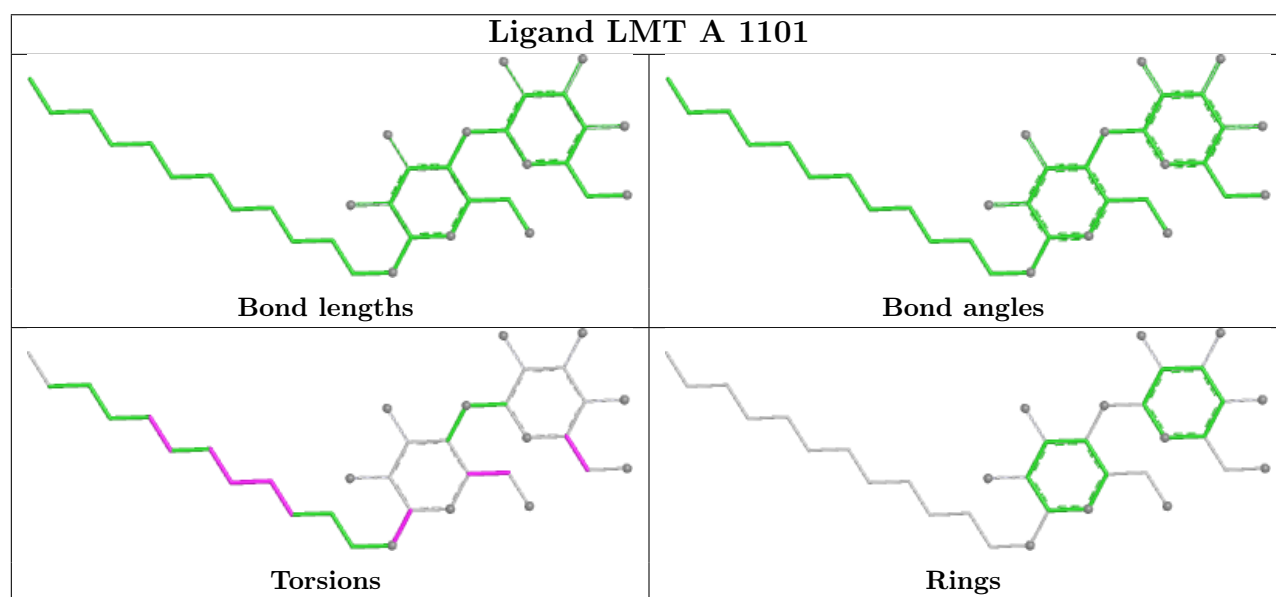
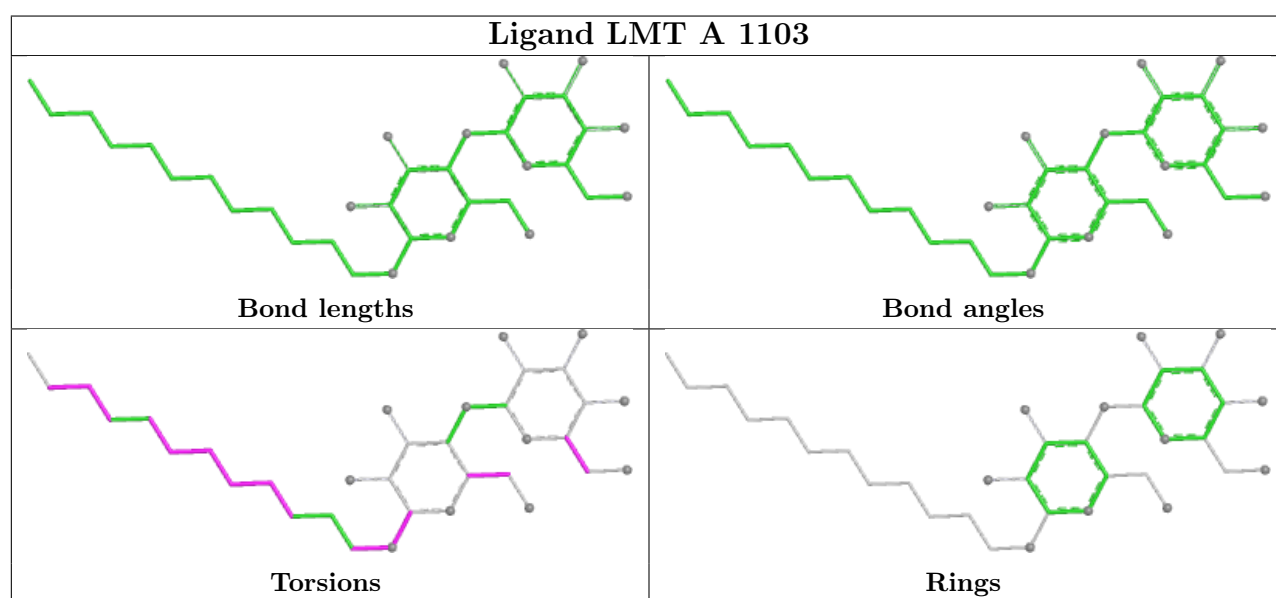
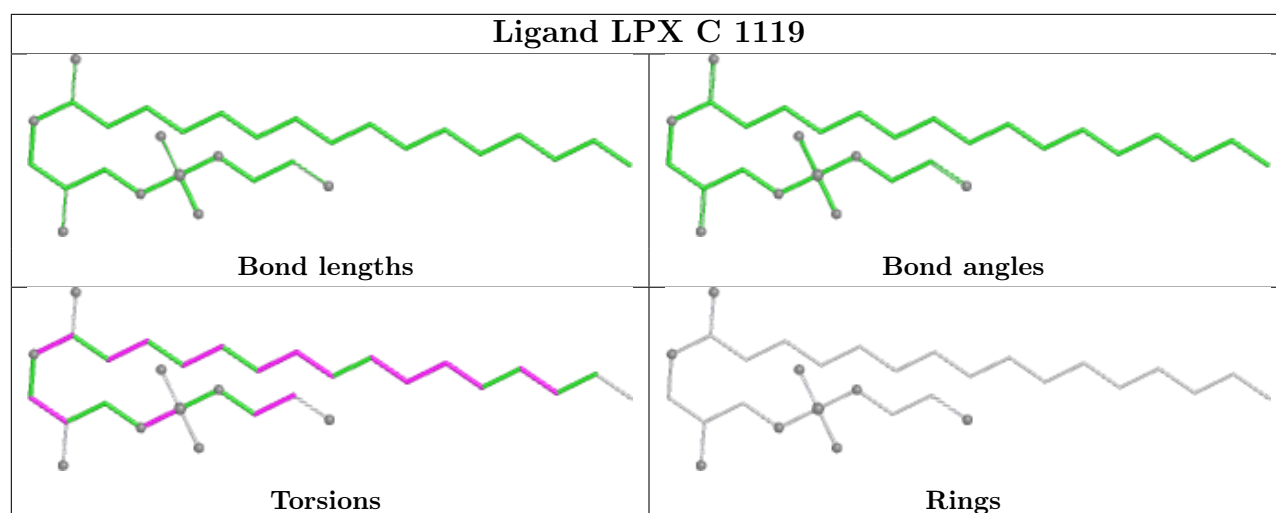
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1120	PG4	3	0
20	C	1101	C14	1	0

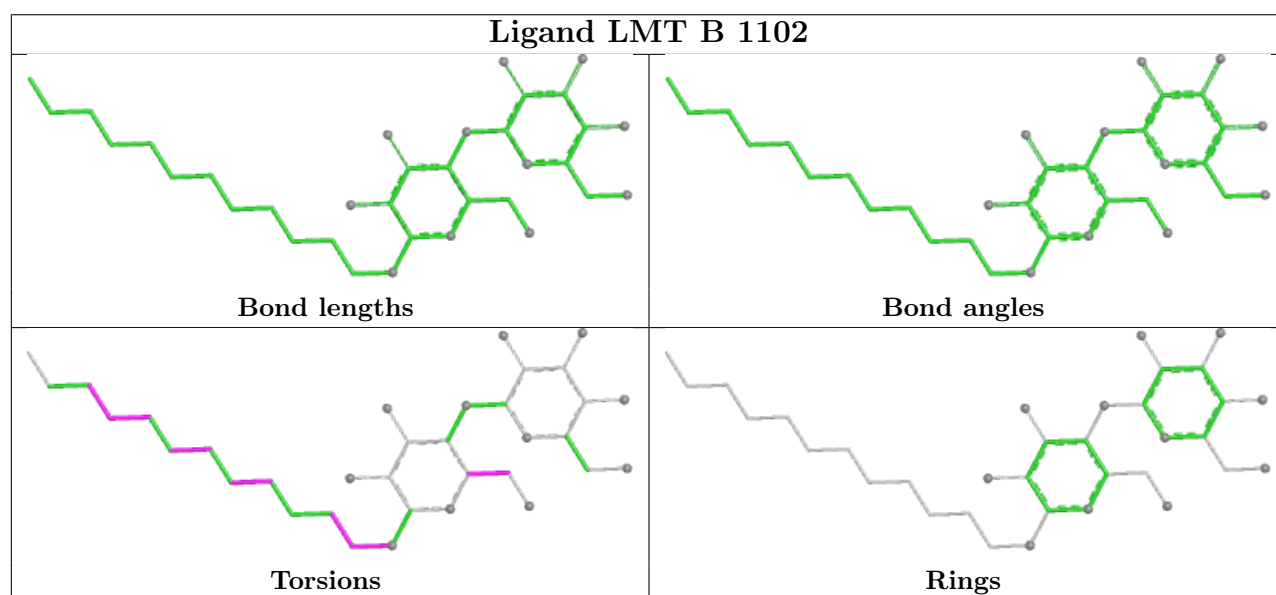
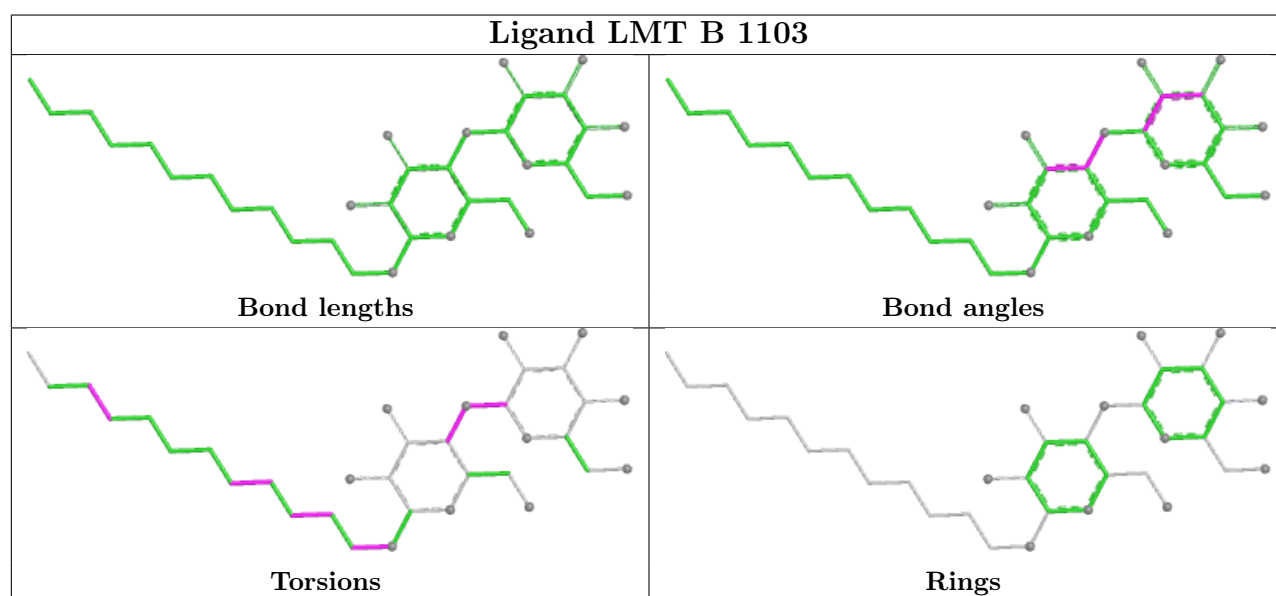
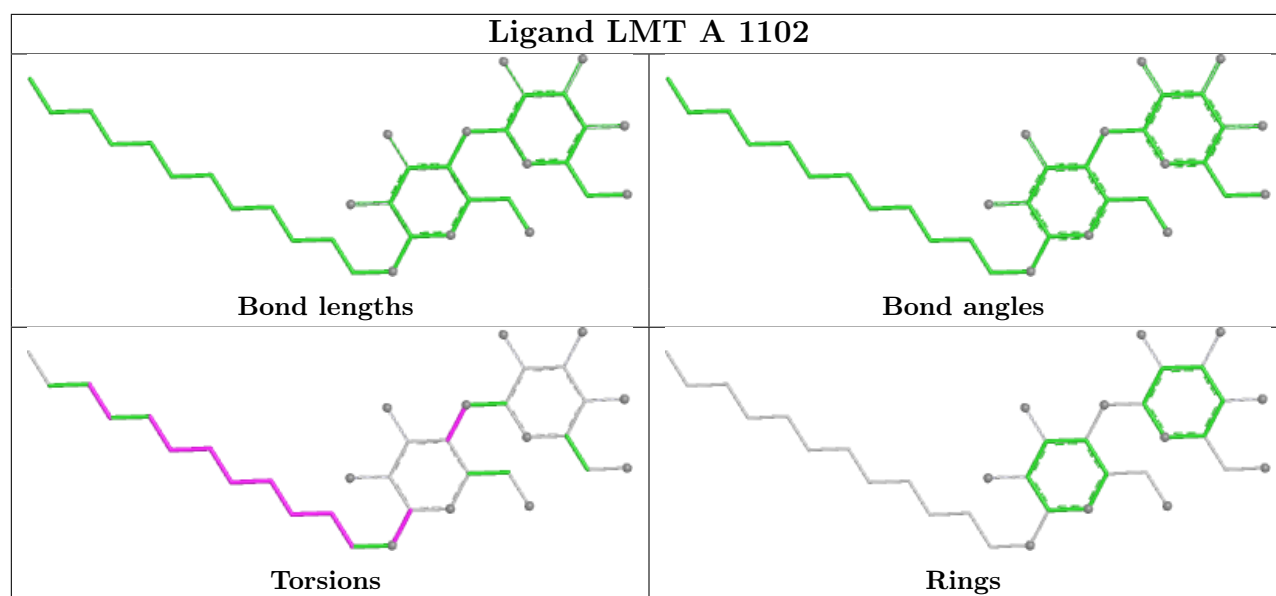
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

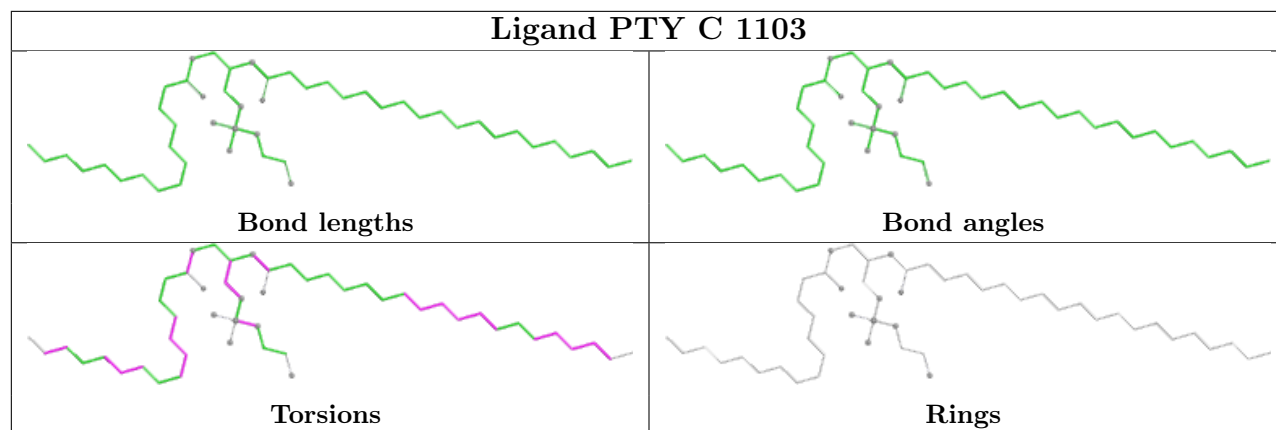
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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	1042/1057 (98%)	1.05	161 (15%)	5 5	16, 48, 79, 106	6 (0%)
1	B	1033/1057 (97%)	0.95	106 (10%)	12 13	18, 47, 66, 82	8 (0%)
1	C	1034/1057 (97%)	0.60	58 (5%)	30 35	20, 39, 55, 65	5 (0%)
2	D	156/169 (92%)	0.80	11 (7%)	22 25	38, 47, 67, 79	0
2	E	154/169 (91%)	1.46	38 (24%)	2 1	42, 58, 80, 82	0
All	All	3419/3509 (97%)	0.89	374 (10%)	10 12	16, 45, 71, 106	19 (0%)

All (374) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	617	PHE	13.5
1	B	134	SER	8.3
1	A	868	LEU	8.1
1	A	1040	ILE	7.9
1	A	668	LEU	7.7
1	A	672	VAL	7.5
1	A	670	ALA	7.2
1	A	617	PHE	7.0
1	A	673	GLU	6.9
1	B	677	ALA	6.7
1	B	618	ALA	6.7
1	C	362	PHE	6.4
1	A	675	GLY	6.3
1	C	671	ILE	6.2
1	B	678	THR	6.2
1	C	675	GLY	6.1
1	A	674	LEU	5.8
1	C	674	LEU	5.8
1	B	616	GLY	5.7
1	A	677	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	673	GLU	5.4
1	A	678	THR	5.4
1	A	676	THR	5.3
1	B	674	LEU	5.0
1	A	1038	GLU	4.9
1	C	670	ALA	4.9
1	B	634	TRP	4.8
1	A	866	GLU	4.7
1	A	873	ALA	4.7
1	B	672	VAL	4.6
1	A	38	ILE	4.6
1	A	918	PHE	4.5
1	A	362	PHE	4.5
1	A	37	THR	4.4
2	E	34	MET	4.4
1	A	980	LEU	4.3
1	B	662	MET	4.3
1	A	1042	HIS	4.2
1	A	679	GLY	4.2
1	A	671	ILE	4.2
1	A	462	SER	4.2
1	A	1039	ASP	4.1
1	B	615	PHE	4.0
1	B	628	PHE	4.0
1	B	868	LEU	4.0
1	A	459	PHE	4.0
1	B	633	ASP	3.9
1	C	811	TYR	3.9
1	B	666	PHE	3.8
1	B	573	MET	3.8
1	B	675	GLY	3.8
1	A	865	GLN	3.8
1	B	133	SER	3.8
1	C	1034	SER	3.7
1	B	366	LEU	3.7
1	C	124	GLN	3.7
1	A	994	GLY	3.7
1	A	995	ALA	3.7
1	B	575	MET	3.7
1	A	511	GLY	3.6
2	E	35	ALA	3.6
1	B	649	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	853	THR	3.6
1	A	542	LEU	3.6
1	B	676	THR	3.6
1	A	619	PRO	3.5
1	B	659	LYS	3.5
1	A	563	PHE	3.5
1	A	660	ASP	3.5
1	B	332	PHE	3.4
1	A	510	LYS	3.4
1	A	1035	ARG	3.4
1	A	669	PRO	3.4
1	A	662	MET	3.4
1	B	563	PHE	3.4
1	C	899	PHE	3.4
1	C	1031[A]	ARG	3.4
1	A	575	MET	3.3
1	A	543	VAL	3.3
2	E	141	ALA	3.3
1	A	1036	LYS	3.3
1	C	918	PHE	3.3
1	A	877	TYR	3.3
1	B	987	MET	3.2
1	B	673	GLU	3.2
1	A	538	THR	3.2
1	A	520	PHE	3.2
1	B	660	ASP	3.2
1	B	619	PRO	3.2
1	A	618	ALA	3.2
1	A	463	THR	3.2
1	A	874	PRO	3.1
1	B	258	SER	3.1
2	E	15	GLY	3.1
1	A	864	TYR	3.0
1	B	255	GLN	3.0
2	D	11	GLY	3.0
2	E	70	GLY	3.0
1	B	510	LYS	3.0
1	A	359	LEU	3.0
1	B	407	ASP	3.0
1	B	654	ALA	3.0
1	B	644	VAL	3.0
2	D	164	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	135	SER	3.0
1	C	669	PRO	3.0
1	A	461	GLY	3.0
2	E	165	LEU	2.9
1	B	658	ILE	2.9
1	A	470	PHE	2.9
1	B	132	SER	2.9
1	C	35	TYR	2.9
1	A	403	GLY	2.9
1	B	173	GLY	2.9
1	C	510	LYS	2.9
1	A	981	ALA	2.9
1	B	553	ALA	2.9
1	C	1033	PHE	2.9
2	E	123	ARG	2.9
1	B	576	VAL	2.9
2	E	129	VAL	2.9
1	B	600	THR	2.9
1	A	537	SER	2.8
1	A	955	LYS	2.8
1	A	580	ALA	2.8
1	C	361	ASN	2.8
1	A	867	ARG	2.8
1	B	627	ALA	2.8
1	B	866	GLU	2.8
1	A	361	ASN	2.8
1	A	957	GLY	2.8
1	B	787	GLY	2.8
2	E	166	GLN	2.8
1	B	665	ALA	2.8
1	B	648	THR	2.8
1	C	784	ASP	2.8
2	E	27	ASP	2.8
1	A	663	VAL	2.8
1	A	869	SER	2.7
1	A	985	GLY	2.7
1	B	656	SER	2.7
1	C	854	GLY	2.7
1	A	862	MET	2.7
1	A	876	LEU	2.7
1	B	620	ARG	2.7
2	D	31	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	68	LYS	2.7
1	B	862	MET	2.7
1	B	129	VAL	2.7
1	B	671	ILE	2.7
1	C	776	GLU	2.7
1	A	556	PHE	2.7
1	B	513	PHE	2.7
1	B	653	ARG	2.7
1	A	984	LEU	2.7
1	B	661	ALA	2.6
1	C	120	GLN	2.6
2	D	28	ASP	2.6
2	E	138	ASP	2.6
1	A	539	GLY	2.6
1	A	499	PRO	2.6
1	C	135	SER	2.6
1	A	577	GLN	2.6
1	B	178	PHE	2.6
1	B	597	TYR	2.6
1	A	495	THR	2.6
1	A	983	ILE	2.6
1	A	952	LEU	2.6
1	B	566	ASP	2.6
1	C	719	ASN	2.6
1	A	1033	PHE	2.6
1	A	904	VAL	2.6
1	A	987	MET	2.6
1	C	423	GLU	2.6
1	A	1037	ASN	2.6
1	A	514	GLY	2.6
1	B	571	VAL	2.6
1	A	509	LYS	2.6
1	A	1041	GLU	2.5
2	E	31	ARG	2.5
1	A	39	ALA	2.5
1	A	719	ASN	2.5
1	B	408	ASP	2.5
1	A	979	SER	2.5
2	E	40	VAL	2.5
1	A	515	TRP	2.5
1	A	875	SER	2.5
2	D	166	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	466	ILE	2.5
2	D	154	ILE	2.5
2	E	164	ILE	2.5
1	A	540	ARG	2.5
1	C	497	LEU	2.5
1	B	216	ALA	2.5
1	C	691	GLY	2.5
1	A	255	GLN	2.5
1	B	629	VAL	2.5
1	C	672	VAL	2.5
1	A	828	LEU	2.5
1	B	635	ALA	2.5
1	A	802	SER	2.4
1	A	325	TYR	2.4
1	A	564	LEU	2.4
1	C	662	MET	2.4
1	A	872	GLN	2.4
1	B	607	GLU	2.4
1	B	834	GLY	2.4
1	B	96	SER	2.4
1	A	986	VAL	2.4
1	B	136	PHE	2.4
1	B	544	LEU	2.4
1	B	668	LEU	2.4
1	A	665	ALA	2.4
1	A	710	PRO	2.4
1	A	547	ILE	2.4
2	E	65	VAL	2.4
1	A	846	GLN	2.4
1	C	255	GLN	2.4
2	E	13	ASP	2.4
1	B	539	GLY	2.4
1	A	1034	SER	2.4
1	A	416	VAL	2.4
1	B	478	MET	2.4
1	A	353	LEU	2.4
2	E	57	TRP	2.4
1	A	908	GLY	2.3
1	C	257	GLY	2.3
2	E	91	GLY	2.3
1	A	993	THR	2.3
1	A	513	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	145	PHE	2.3
1	A	423	GLU	2.3
1	A	956	GLU	2.3
1	B	865	GLN	2.3
1	A	430	ALA	2.3
1	A	145	THR	2.3
1	A	712	MET	2.3
1	B	650	ARG	2.3
1	B	663	VAL	2.3
2	D	150	PHE	2.3
1	C	267	LYS	2.3
1	B	141	GLY	2.3
1	C	173	GLY	2.3
1	C	356	TYR	2.3
1	A	307	ARG	2.3
1	C	512	PHE	2.3
1	A	544	LEU	2.3
1	C	442	LEU	2.3
2	D	165	LEU	2.3
1	A	566	ASP	2.3
1	C	506	GLY	2.3
2	E	37	GLY	2.3
1	A	620	ARG	2.3
1	C	134	SER	2.3
1	B	626	ILE	2.3
1	B	647	ILE	2.3
1	C	850	LYS	2.3
1	A	512	PHE	2.2
1	A	680	PHE	2.2
1	B	113	LEU	2.2
1	B	590	VAL	2.3
1	B	606	VAL	2.3
2	E	14	LEU	2.2
1	B	511	GLY	2.2
1	A	654	ALA	2.2
1	B	311	ALA	2.2
1	A	148	THR	2.2
1	A	356	TYR	2.2
1	B	652	THR	2.2
1	A	357	LEU	2.2
1	A	982	PHE	2.2
1	B	557	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	131	VAL	2.2
1	B	398	MET	2.2
1	A	621	GLY	2.2
1	B	670	ALA	2.2
1	B	837	THR	2.2
1	A	96	SER	2.2
1	A	554	TYR	2.2
1	A	1020	PHE	2.2
1	A	363	ARG	2.2
1	B	174	ASP	2.2
1	B	274	ASN	2.2
1	A	833	PRO	2.2
1	A	829	GLY	2.2
1	A	870	GLY	2.2
1	C	130	GLU	2.2
1	C	494	ALA	2.2
2	E	88	ALA	2.2
1	C	133	SER	2.2
2	E	135	TYR	2.2
1	A	578	LEU	2.2
1	C	38	ILE	2.2
2	E	18	LEU	2.2
2	E	19	LEU	2.2
1	A	667	ASN	2.2
1	B	918	PHE	2.2
1	B	601	LYS	2.2
1	A	657	GLN	2.2
1	B	89	GLN	2.2
1	B	679	GLY	2.2
1	B	651	ALA	2.2
1	C	676	THR	2.2
1	C	688	ALA	2.2
2	D	12	SER	2.2
1	B	743	ILE	2.1
2	E	67	LEU	2.1
1	A	83	ASP	2.1
1	A	1008	MET	2.1
1	A	351	VAL	2.1
1	A	408	ASP	2.1
1	A	1028	VAL	2.1
1	C	686	ASP	2.1
2	E	159	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	120	GLN	2.1
2	D	55	ALA	2.1
1	A	497	LEU	2.1
1	C	29	LYS	2.1
1	C	366	LEU	2.1
2	E	32	ILE	2.1
1	A	95	GLU	2.1
1	B	256	ASP	2.1
1	A	406	VAL	2.1
1	A	411	VAL	2.1
1	A	901	VAL	2.1
2	E	96	VAL	2.1
1	B	386	PHE	2.1
1	A	71	GLY	2.1
1	C	511	GLY	2.1
1	B	558	ARG	2.1
1	A	134	SER	2.1
2	E	148	THR	2.1
1	A	912	ALA	2.1
1	C	721	LEU	2.1
2	D	61	GLU	2.1
1	A	349	ILE	2.1
1	A	326	PRO	2.1
1	A	579	PRO	2.1
1	A	1025	PHE	2.1
1	B	508	GLY	2.1
2	E	113	GLY	2.1
1	A	558	ARG	2.1
1	C	620	ARG	2.1
1	B	114	ALA	2.1
1	C	501	ALA	2.1
1	C	737	GLN	2.1
2	E	93	LEU	2.1
1	A	788	ASP	2.1
1	B	556	PHE	2.1
1	A	714	THR	2.0
1	A	836	SER	2.0
1	B	993	THR	2.0
1	C	678	THR	2.0
1	A	649	MET	2.0
2	E	29	GLU	2.0
1	C	657	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	36	ASN	2.0
1	A	402	ILE	2.0
1	C	65	ILE	2.0
1	A	1016	VAL	2.0
1	A	386	PHE	2.0
1	B	1033	PHE	2.0
1	A	456	MET	2.0
1	A	607	GLU	2.0
1	B	562	SER	2.0
1	C	807	SER	2.0
1	A	831	ALA	2.0
1	A	505	HIS	2.0
2	E	117	LEU	2.0
2	E	143	ASP	2.0
1	A	991	ILE	2.0
1	B	402	ILE	2.0
1	A	226	LYS	2.0
1	C	659	LYS	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
8	HEX	C	1117	6/6	0.44	0.33	50,50,50,50	0
5	DDQ	C	1107	14/14	0.59	0.26	50,51,53,53	0
9	EDO	C	1125	4/4	0.60	0.31	56,56,56,57	0
20	C14	C	1101	14/14	0.60	0.27	47,47,48,48	0
9	EDO	C	1122	4/4	0.62	0.32	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	D10	C	1109	10/10	0.64	0.30	53,53,53,53	0
13	D10	B	1109	10/10	0.65	0.27	45,45,45,45	0
4	OCT	C	1104	8/8	0.66	0.25	46,46,46,46	0
3	LMT	B	1103	35/35	0.66	0.26	105,107,109,109	0
8	HEX	B	1117	6/6	0.68	0.26	45,45,45,45	0
23	1PE	C	1120	16/16	0.68	0.28	71,71,72,72	0
5	DDQ	B	1106	14/14	0.69	0.24	50,51,52,52	0
6	GOL	B	1113	6/6	0.69	0.23	64,65,65,65	0
17	8K6	B	1131	18/18	0.70	0.23	44,45,45,45	0
8	HEX	C	1118	6/6	0.70	0.24	44,44,44,44	0
9	EDO	B	1128	4/4	0.70	0.26	56,56,56,57	0
10	PGE	A	1117	10/10	0.71	0.29	72,73,73,73	0
9	EDO	A	1114	4/4	0.71	0.23	59,59,59,59	0
6	GOL	B	1112	6/6	0.72	0.20	73,74,74,74	0
5	DDQ	A	1105	14/14	0.73	0.36	95,95,96,96	0
4	OCT	C	1105	8/8	0.73	0.25	46,47,47,47	0
11	MIY	B	1101	33/33	0.74	0.21	76,76,77,77	0
7	D12	C	1115	12/12	0.74	0.31	60,61,62,62	0
15	MYS	B	1119	15/15	0.75	0.32	71,71,72,72	0
9	EDO	B	1127	4/4	0.75	0.23	63,64,64,64	0
6	GOL	E	201	6/6	0.76	0.27	67,67,67,67	0
9	EDO	B	1126	4/4	0.76	0.27	67,67,67,67	0
9	EDO	A	1116	4/4	0.77	0.24	63,63,63,63	0
5	DDQ	B	1105	14/14	0.77	0.27	68,70,73,73	0
8	HEX	B	1115	6/6	0.77	0.34	68,68,69,69	0
9	EDO	C	1128	4/4	0.77	0.23	58,58,58,58	0
9	EDO	D	202	4/4	0.78	0.26	56,56,56,56	0
13	D10	B	1108	10/10	0.78	0.21	45,45,45,45	0
9	EDO	B	1129	4/4	0.79	0.25	56,56,56,56	0
8	HEX	B	1116	6/6	0.79	0.25	54,54,55,55	0
9	EDO	D	203	4/4	0.80	0.20	56,56,56,57	0
21	PTY	C	1103	50/50	0.80	0.26	71,73,75,75	0
9	EDO	B	1123	4/4	0.80	0.20	62,63,63,63	0
13	D10	B	1107	10/10	0.81	0.31	68,68,68,68	0
7	D12	C	1116	12/12	0.81	0.19	43,43,43,43	0
9	EDO	C	1127	4/4	0.81	0.22	62,62,62,62	0
9	EDO	A	1115	4/4	0.81	0.29	70,70,70,70	0
9	EDO	D	201	4/4	0.81	0.21	67,67,67,67	0
6	GOL	A	1110	6/6	0.81	0.21	65,65,65,65	0
18	R16	B	1132	16/16	0.81	0.17	42,43,44,44	0
6	GOL	B	1111	6/6	0.81	0.20	76,76,76,77	0
9	EDO	B	1125	4/4	0.81	0.26	65,65,65,65	0

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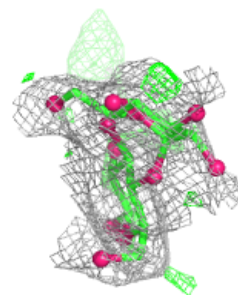
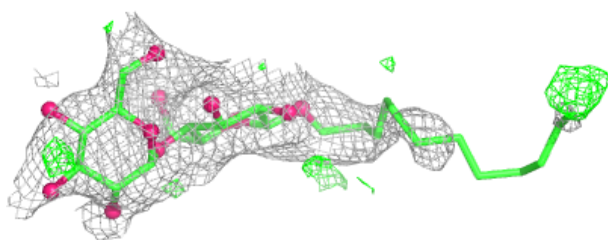
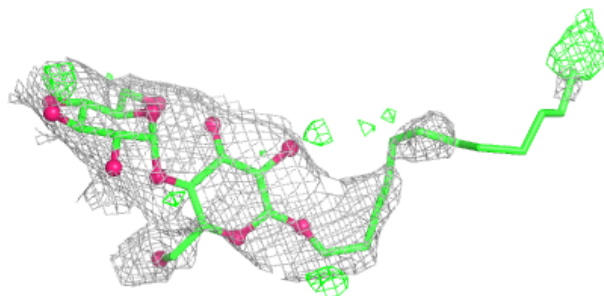
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	EDO	C	1124	4/4	0.81	0.26	67,67,67,67	0
6	GOL	C	1112	6/6	0.82	0.16	65,65,65,65	0
3	LMT	A	1103	35/35	0.82	0.19	83,84,88,88	0
3	LMT	A	1101	35/35	0.82	0.20	73,81,85,86	0
9	EDO	C	1121	4/4	0.82	0.20	60,60,61,61	0
3	LMT	B	1102	35/35	0.83	0.19	69,71,78,78	0
16	PG4	B	1120	13/13	0.83	0.20	58,59,60,60	0
6	GOL	A	1106	6/6	0.83	0.15	46,47,47,47	0
9	EDO	B	1122	4/4	0.83	0.27	68,68,68,69	0
6	GOL	A	1109	6/6	0.83	0.19	73,74,74,74	0
8	HEX	A	1113	6/6	0.83	0.29	65,65,65,66	0
5	DDQ	C	1106	14/14	0.83	0.26	72,73,75,75	0
3	LMT	A	1102	35/35	0.84	0.18	70,78,83,83	0
10	PGE	C	1129	10/10	0.84	0.21	65,65,66,66	0
22	LPX	C	1119	30/30	0.85	0.21	76,78,79,79	0
15	MYS	B	1118	15/15	0.86	0.23	67,68,68,68	0
6	GOL	A	1108	6/6	0.86	0.20	70,70,70,70	0
7	D12	A	1112	12/12	0.86	0.24	61,61,61,61	0
9	EDO	B	1124	4/4	0.87	0.20	49,49,49,49	0
13	D10	C	1108	10/10	0.87	0.21	60,60,60,60	0
6	GOL	A	1111	6/6	0.87	0.15	64,65,65,65	0
12	DDR	B	1104	28/28	0.88	0.20	67,71,71,72	0
4	OCT	A	1104	8/8	0.88	0.25	76,76,76,76	0
3	LMT	C	1102	35/35	0.88	0.16	60,62,66,66	0
9	EDO	B	1121	4/4	0.88	0.20	61,61,61,62	0
9	EDO	C	1126	4/4	0.88	0.16	56,56,56,57	0
6	GOL	C	1111	6/6	0.89	0.14	50,50,50,51	0
6	GOL	A	1107	6/6	0.90	0.13	45,45,46,46	0
6	GOL	C	1110	6/6	0.90	0.11	33,33,33,33	0
6	GOL	B	1110	6/6	0.90	0.15	47,48,48,48	0
19	SO4	B	1133	5/5	0.91	0.11	71,71,72,72	0
9	EDO	C	1123	4/4	0.92	0.16	57,57,57,58	0
9	EDO	B	1130	4/4	0.92	0.15	54,54,54,54	0
14	CL	C	1114	1/1	0.95	0.20	65,65,65,65	0
14	CL	C	1113	1/1	0.98	0.18	57,57,57,57	0
14	CL	B	1114	1/1	0.98	0.14	55,55,55,55	0

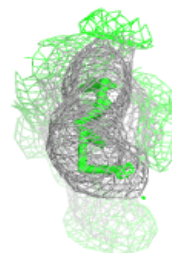
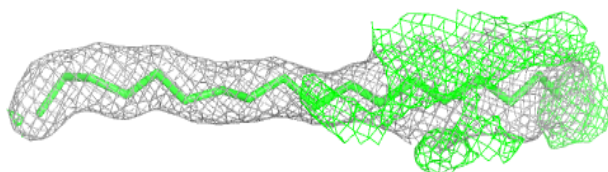
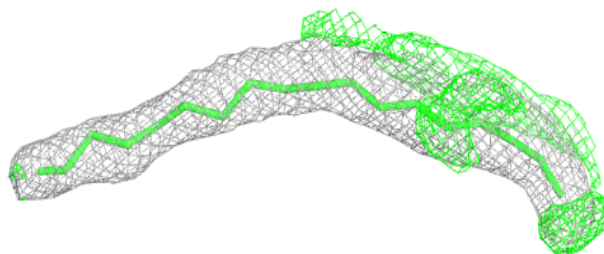
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT 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)

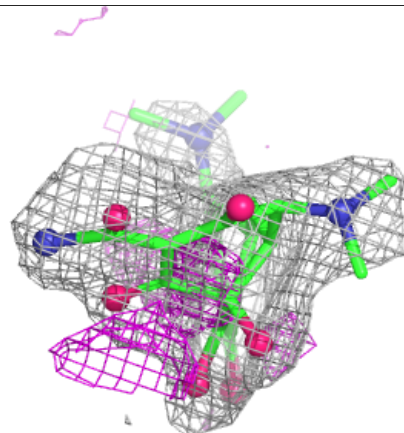
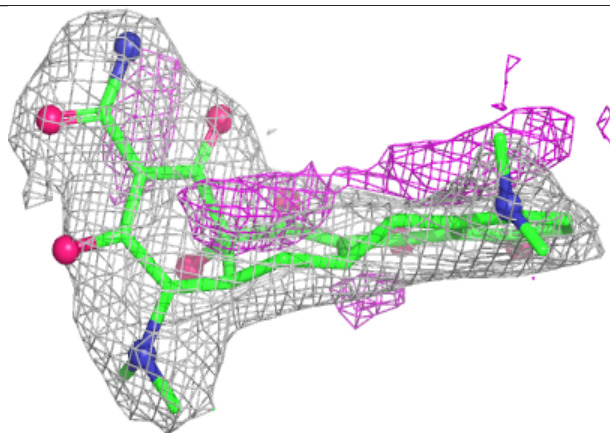
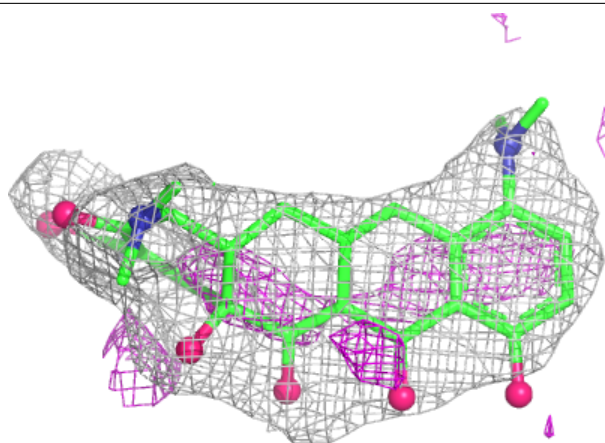
**Electron density around 8K6 B 1131:**

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



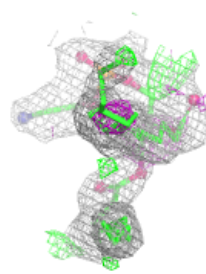
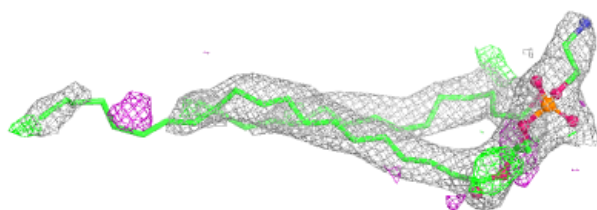
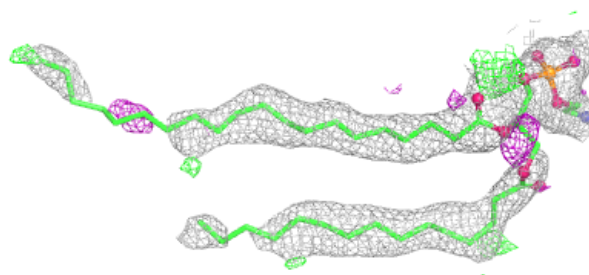
Electron density around MIY B 1101:

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

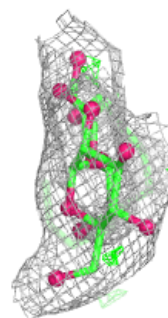
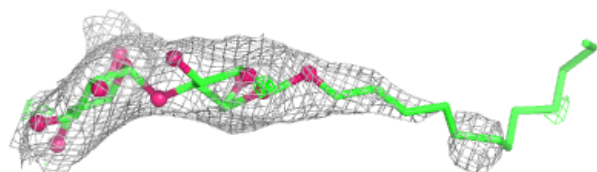
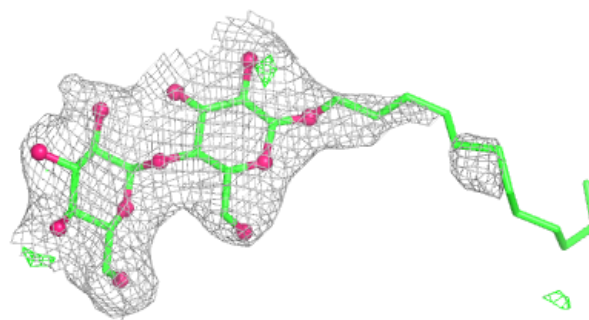


Electron density around PTY C 1103:

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

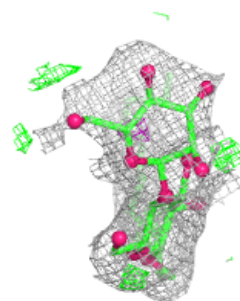
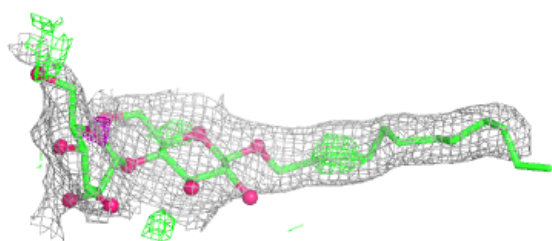
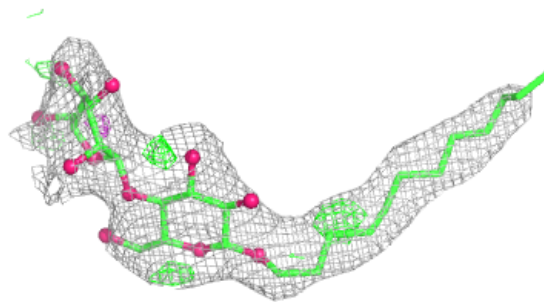
**Electron density around LMT A 1103:**

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

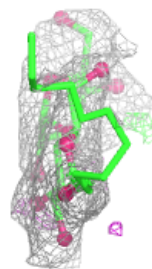
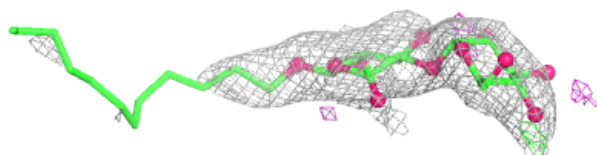
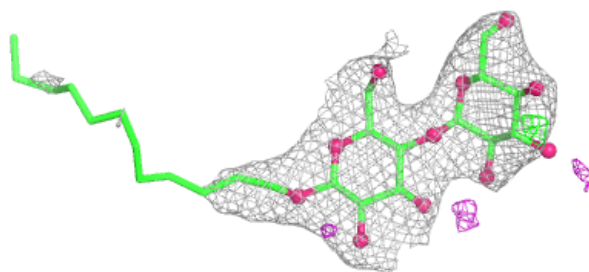


Electron density around LMT A 1101:

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

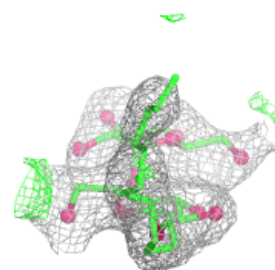
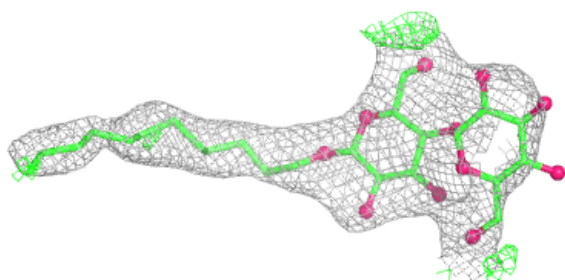
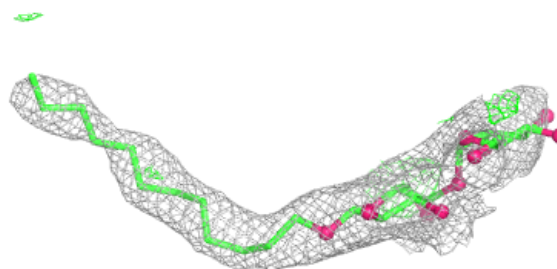
**Electron density around LMT B 1102:**

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

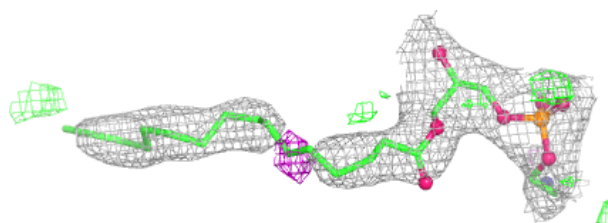
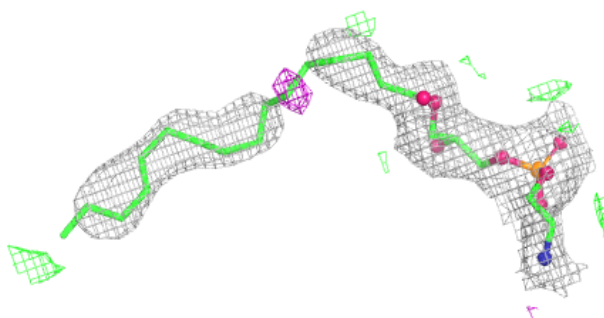


Electron density around LMT A 1102:

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

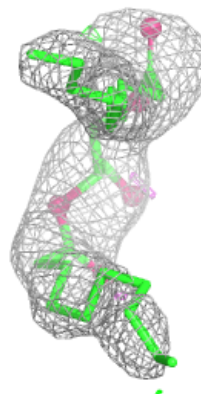
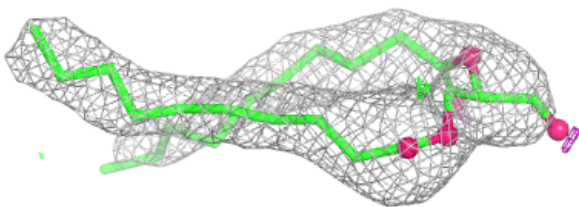
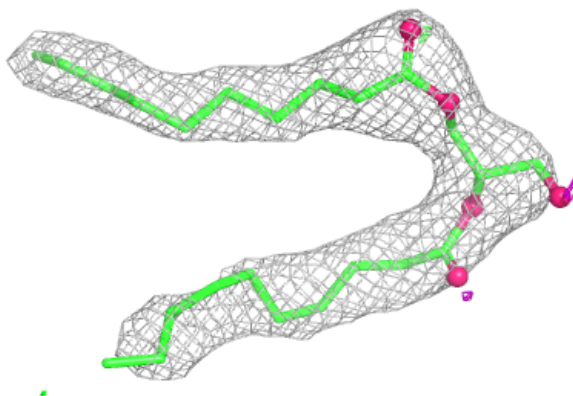
**Electron density around LPX C 1119:**

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

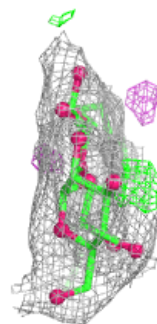
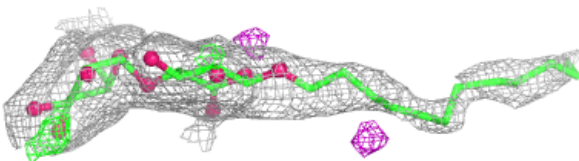
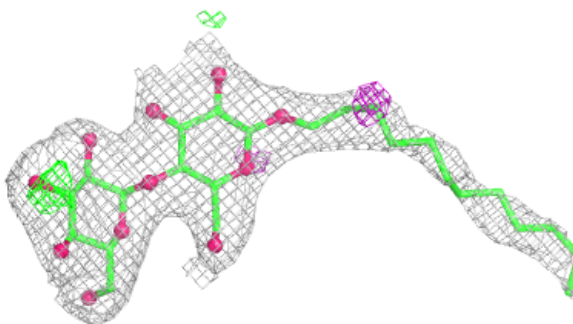


Electron density around DDR B 1104:

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

**Electron density around LMT 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.