Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 11:48 PM EDT

PDB ID	:	6ZOB
Title	:	3-Formylrifamycin SV binding to the access pocket of AcrB L protomer
Authors	:	Tam, H.K.; Foong, W.E.; Pos, K.M.
Deposited on	:	2020-07-07
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 (i) 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 (i)) were used in the production of this report:

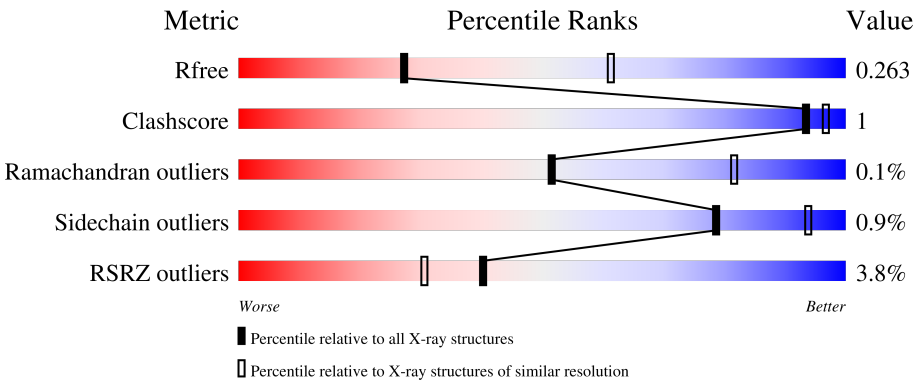
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	3% 93% 5% •
1	B	1057	4% 93% 5% •
1	C	1057	2% 93% 5% •
2	D	169	5% 91% • 9%
2	E	169	18% 88% • 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LMT	A	1206	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 26439 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
			Total	C	N	O	S			
1	A	1035	7866	5061	1300	1461	44	0	0	0
1	B	1034	7855	5055	1296	1460	44	0	0	0
1	C	1033	7849	5052	1295	1458	44	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

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

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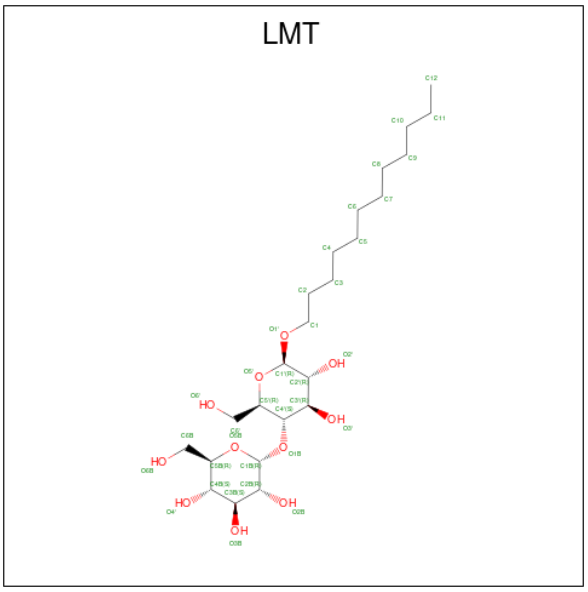
Chain	Residue	Modelled	Actual	Comment	Reference
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

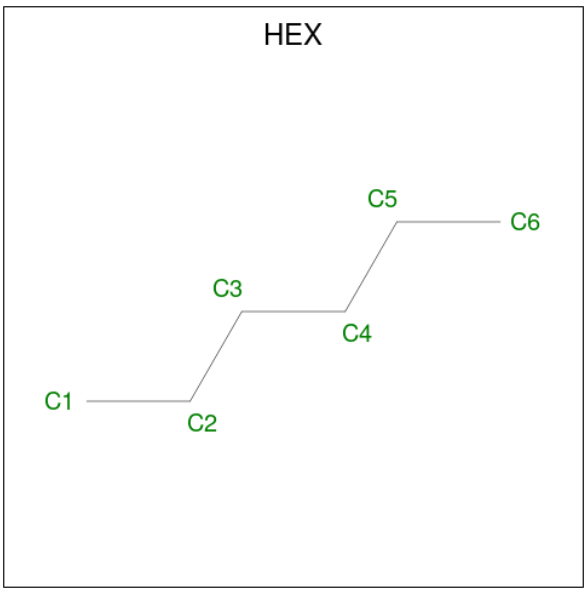
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	154	1167	736	204	226	1	0	0	0
			Total	C	N	O	S			
2	E	154	1178	742	208	227	1	0	1	0

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



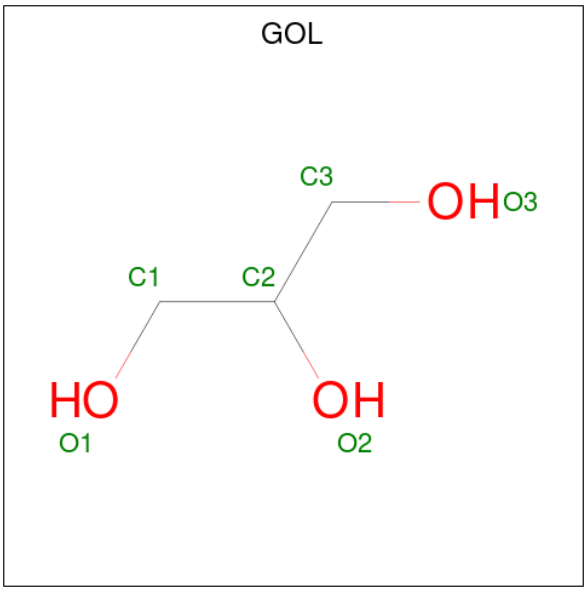
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	35	24	11	0	0
			Total	C	O		
3	A	1	35	24	11	0	0
			Total	C	O		
3	A	1	35	24	11	0	0
			Total	C	O		
3	A	1	35	24	11	0	0
			Total	C	O		
3	B	1	35	24	11	0	0
			Total	C	O		
3	C	1	35	24	11	0	0

- Molecule 4 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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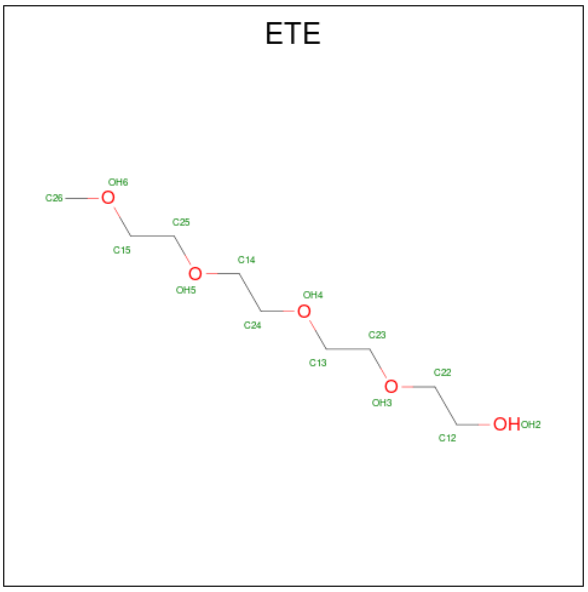
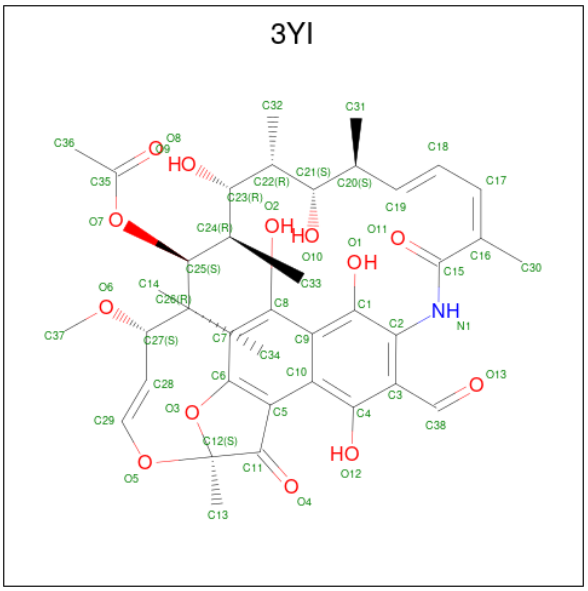
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	C	1	6	3	3	0	0
			Total	C	O		
5	D	1	6	3	3	0	0

- Molecule 6 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: ETE) (formula: $C_9H_{20}O_5$).



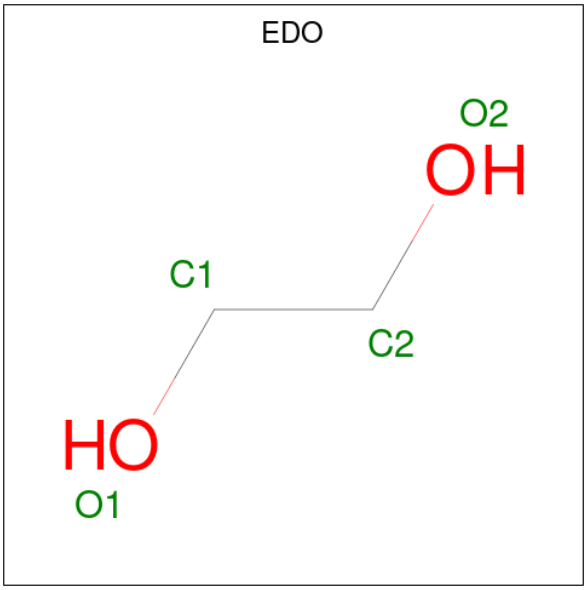
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	14	9	5	0	0

- Molecule 7 is (2S,12Z,14E,16S,17S,18R,19R,20R,21S,22R,23S,24E)-8-formyl-5,6,9,17,19-pentahydroxy-23-methoxy-2,4,12,16,18,20,22-heptam ethyl-1,11-dioxo-1,2-dihydro-2,7-(epoxypentadeca[1,11,13]trienoimino)naphtho[2,1-b]furan-21-yl acetate (three-letter code: 3YI) (formula: $C_{38}H_{47}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



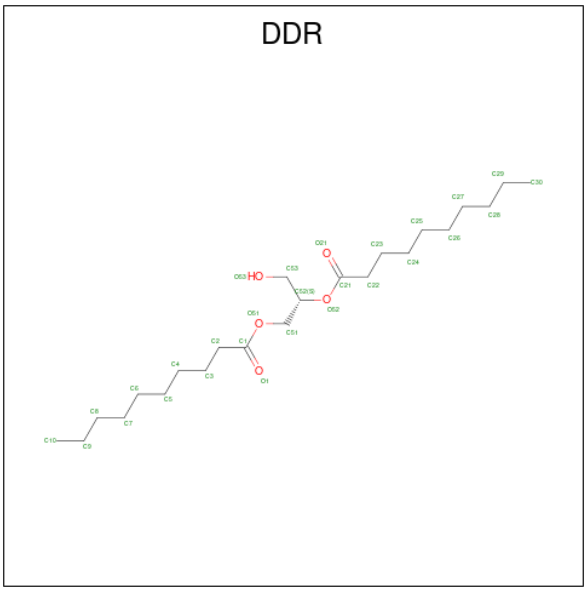
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	52	38	1	13	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



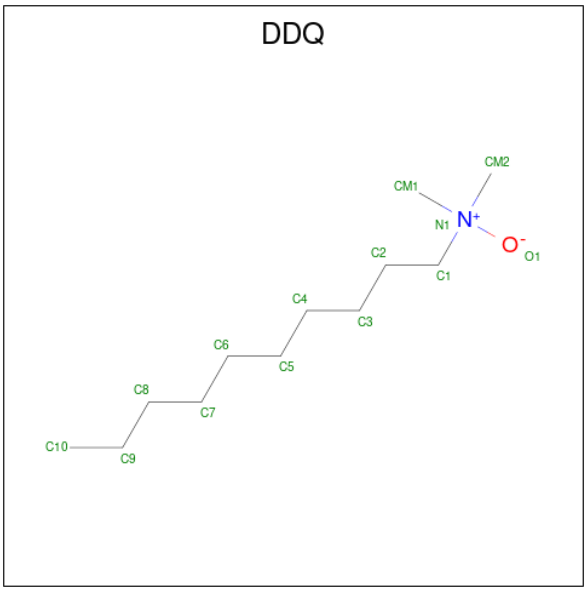
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	4	2	2	0	0

- Molecule 9 is (2S)-3-hydroxypropane-1,2-diyl didecanoate (three-letter code: DDR) (formula: $C_{23}H_{44}O_5$).



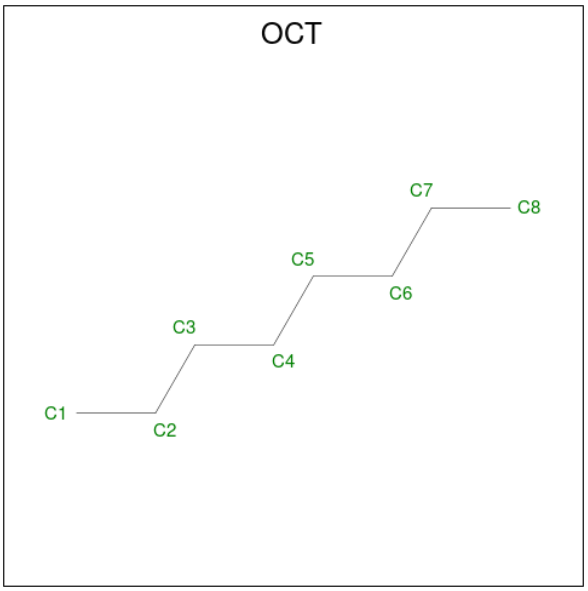
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	B	1	28	23	5	0	0

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



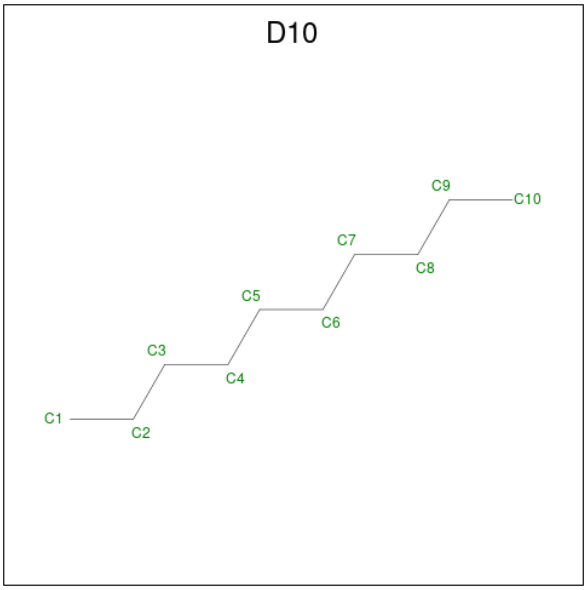
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	B	1	14	12	1	1	0	0

- Molecule 11 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



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

- Molecule 12 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



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

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
13	C	1	1	1	0	0

- Molecule 14 is water.

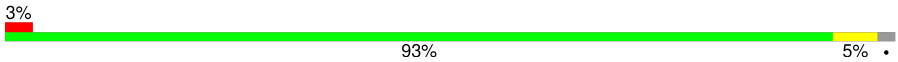
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
14	A	62	62	62	0	0
			Total	O		
14	B	30	30	30	0	0
			Total	O		
14	C	51	51	51	0	0
			Total	O		
14	D	2	2	2	0	0
			Total	O		
14	E	8	8	8	0	0

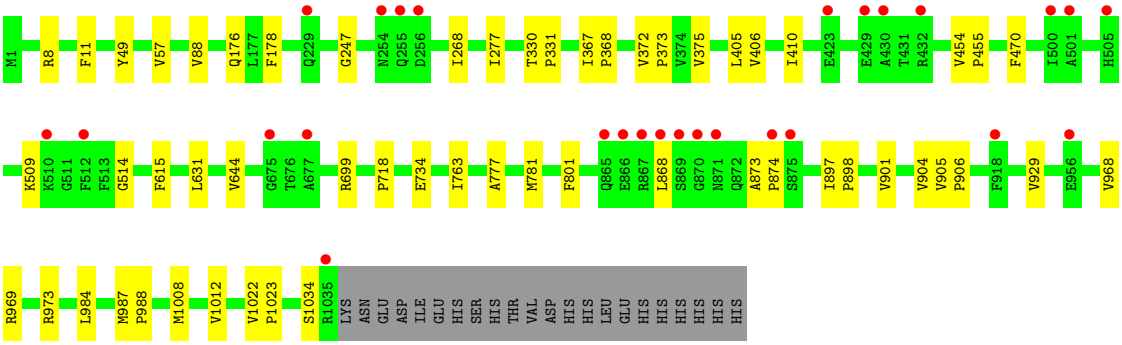
3 Residue-property plots (i)

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

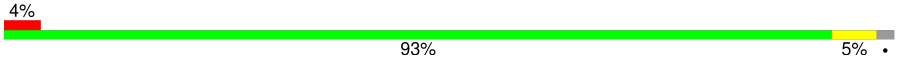
Chain A:

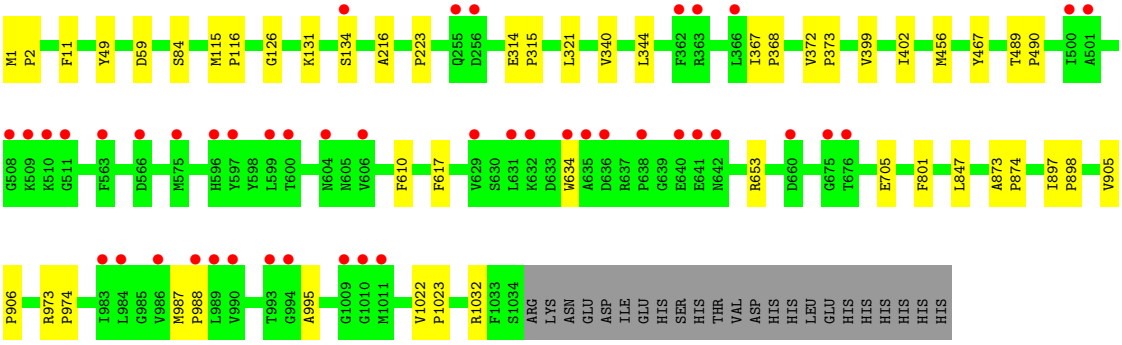




• Molecule 1: Multidrug efflux pump subunit AcrB

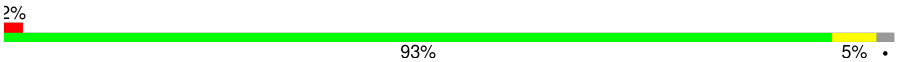
Chain B:

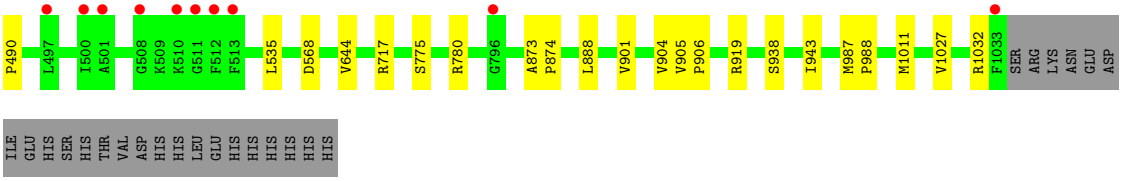




• Molecule 1: Multidrug efflux pump subunit AcrB

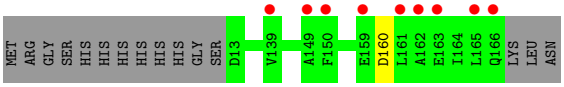
Chain C:





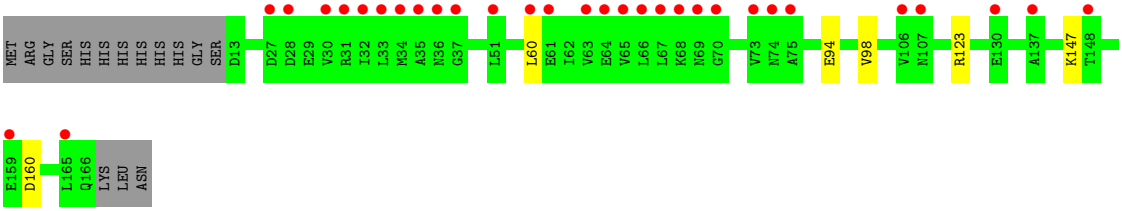
- Molecule 2: DARPIN

Chain D:



- Molecule 2: DARPIN

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	145.36Å 160.19Å 244.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.80 49.10 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.15-2.80) 100.0 (49.10-2.80)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.238 , 0.262 0.240 , 0.263	Depositor DCC
R_{free} test set	6895 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	54.8	Xtriage
Anisotropy	0.709	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	26439	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 3YI, ETE, DDR, HEX, DDQ, D10, GOL, OCT, CL, EDO, LMT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.67	0/8016	0.71	0/10885
1	B	0.68	0/8005	0.71	0/10871
1	C	0.67	0/7999	0.70	0/10863
2	D	0.68	0/1186	0.71	0/1613
2	E	0.68	0/1197	0.71	0/1627
All	All	0.67	0/26403	0.71	0/35859

There are no bond length outliers.

There are no bond angle outliers.

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	7866	0	8019	27	0
1	B	7855	0	8006	23	0
1	C	7849	0	8001	24	0
2	D	1167	0	1151	0	0
2	E	1178	0	1163	4	0
3	A	140	0	184	0	0
3	B	35	0	46	0	0
3	C	35	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	6	0	14	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	14	0	20	0	0
7	A	52	0	0	1	0
8	A	4	0	6	0	0
9	B	28	0	44	0	0
10	B	14	0	27	1	0
11	B	8	0	18	0	0
12	C	10	0	22	0	0
13	C	1	0	0	0	0
14	A	62	0	0	0	0
14	B	30	0	0	0	0
14	C	51	0	0	0	0
14	D	2	0	0	0	0
14	E	8	0	0	0	0
All	All	26439	0	26799	75	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 (75) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.81	0.62
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.82	0.61
1:C:151:GLN:NE2	1:C:279:ALA:O	2.36	0.58
1:B:344:LEU:HD22	1:B:402:ILE:HD13	1.85	0.56
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.86	0.56
1:C:115:MET:N	1:C:116:PRO:HD2	2.21	0.56
2:E:94:GLU:O	2:E:98:VAL:HG23	2.07	0.55
1:C:901:VAL:O	1:C:904:VAL:HG12	2.08	0.54
1:A:968:VAL:HG11	1:A:1023:PRO:HG3	1.90	0.53
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.93	0.50
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.92	0.50
1:A:330:THR:OG1	1:A:331:PRO:HD3	2.11	0.50
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.41	0.50
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.27	0.50
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.95	0.48
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.94	0.48
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.94	0.48
1:B:987:MET:N	1:B:988:PRO:CD	2.76	0.48
1:A:247:GLY:HA2	1:A:268:ILE:HD13	1.96	0.48
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.94	0.48
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.96	0.47
1:A:777:ALA:O	1:A:781:MET:HG2	2.15	0.47
1:B:399:VAL:O	1:B:402:ILE:HG22	2.15	0.46
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.97	0.46
1:C:535:LEU:HD22	1:C:1027:VAL:HG21	1.98	0.45
1:C:165:ALA:HB3	1:C:313:MET:CE	2.47	0.45
1:C:351:VAL:HG21	1:C:402:ILE:HG22	1.98	0.45
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.97	0.45
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.99	0.45
1:A:1022:VAL:N	1:A:1023:PRO:CD	2.80	0.45
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.97	0.45
2:E:60:LEU:HD11	2:E:98:VAL:HG21	1.98	0.45
1:C:330:THR:N	1:C:331:PRO:CD	2.80	0.44
1:A:8:ARG:HD3	10:B:1103:DDQ:HM11	1.98	0.44
1:B:634:TRP:CD2	1:B:995:ALA:HB2	2.51	0.44
1:B:897:ILE:N	1:B:898:PRO:HD2	2.31	0.44
1:A:509:LYS:O	1:A:514:GLY:HA3	2.18	0.44
1:A:454:VAL:N	1:A:455:PRO:CD	2.81	0.44
1:C:40:PRO:HB2	1:C:94:PHE:O	2.17	0.44
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.99	0.44
1:B:115:MET:N	1:B:116:PRO:CD	2.81	0.43
1:B:873:ALA:HB3	1:B:874:PRO:HD3	2.00	0.43
1:A:176:GLN:HG2	1:A:615:PHE:CE2	2.54	0.43
7:A:1208:3YI:O12	7:A:1208:3YI:O4	2.36	0.43
1:C:873:ALA:HB3	1:C:874:PRO:HD3	1.99	0.43
1:A:631:LEU:HD11	1:A:644:VAL:HG22	2.01	0.43
1:A:406:VAL:HG12	1:A:410:ILE:HD12	2.00	0.43
1:B:223:PRO:HD3	1:C:275:TYR:CD1	2.53	0.42
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.54	0.42
1:A:734:GLU:OE2	2:E:147:LYS:NZ	2.42	0.42
1:A:1008:MET:O	1:A:1012:VAL:HG23	2.20	0.42
1:A:178:PHE:HA	1:A:277:ILE:HG21	2.01	0.42
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.54	0.42
1:C:775:SER:HB3	1:C:780:ARG:HD3	2.01	0.42
1:B:489:THR:N	1:B:490:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:897:ILE:N	1:B:898:PRO:CD	2.83	0.42
1:A:901:VAL:O	1:A:904:VAL:HG22	2.20	0.41
1:C:303:ALA:HB2	1:C:330:THR:HG21	2.01	0.41
1:C:568:ASP:CG	1:C:644:VAL:HG23	2.41	0.41
2:E:123[B]:ARG:HD3	2:E:123[B]:ARG:HA	1.81	0.41
1:B:314:GLU:N	1:B:315:PRO:CD	2.83	0.41
1:B:340:VAL:O	1:B:344:LEU:HG	2.21	0.41
1:A:897:ILE:N	1:A:898:PRO:CD	2.84	0.41
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.21	0.41
1:C:398:MET:O	1:C:402:ILE:HG12	2.20	0.41
1:C:904:VAL:HG13	1:C:938:SER:HB3	2.01	0.41
1:C:489:THR:HB	1:C:490:PRO:HD3	2.02	0.41
1:A:763:ILE:HD11	1:B:59:ASP:HB3	2.02	0.41
1:C:1:MET:HB3	1:C:2:PRO:HD3	2.02	0.41
1:A:699:ARG:HD2	1:A:718:PRO:HB3	2.03	0.40
1:A:987:MET:N	1:A:988:PRO:CD	2.85	0.40
1:C:888:LEU:HD21	1:C:943:ILE:HD11	2.04	0.40
1:B:973:ARG:N	1:B:974:PRO:HD2	2.37	0.40
1:A:984:LEU:HA	1:A:987:MET:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1033/1057 (98%)	999 (97%)	32 (3%)	2 (0%)	47 78
1	B	1032/1057 (98%)	1005 (97%)	25 (2%)	2 (0%)	47 78
1	C	1031/1057 (98%)	1004 (97%)	27 (3%)	0	100 100
2	D	152/169 (90%)	147 (97%)	5 (3%)	0	100 100
2	E	153/169 (90%)	149 (97%)	4 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3401/3509 (97%)	3304 (97%)	93 (3%)	4 (0%)	51 81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	868	LEU
1	A	1034	SER
1	B	134	SER
1	B	216	ALA

5.3.2 Protein sidechains (i)

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	841/863 (98%)	836 (99%)	5 (1%)	86 96
1	B	840/863 (97%)	830 (99%)	10 (1%)	71 92
1	C	839/863 (97%)	832 (99%)	7 (1%)	81 94
2	D	119/132 (90%)	118 (99%)	1 (1%)	81 94
2	E	120/132 (91%)	119 (99%)	1 (1%)	81 94
All	All	2759/2853 (97%)	2735 (99%)	24 (1%)	78 94

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	49	TYR
1	A	801	PHE
1	A	969	ARG
1	A	973	ARG
1	B	11	PHE
1	B	49	TYR
1	B	84	SER
1	B	131	LYS
1	B	321	LEU

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Mol	Chain	Res	Type
1	B	610	PHE
1	B	617	PHE
1	B	653	ARG
1	B	801	PHE
1	B	1032	ARG
1	C	11	PHE
1	C	49	TYR
1	C	274	ASN
1	C	717	ARG
1	C	919	ARG
1	C	1011	MET
1	C	1032	ARG
2	D	160	ASP
2	E	160	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\#\|Z\| > 2$
3	LMT	A	1202	-	36,36,36	0.47	0	47,47,47	0.63	0
4	HEX	A	1204	-	5,5,5	0.13	0	4,4,4	0.15	0
3	LMT	A	1203	-	36,36,36	0.48	1 (2%)	47,47,47	0.67	0
3	LMT	B	1101	-	36,36,36	0.48	1 (2%)	47,47,47	0.64	0
8	EDO	A	1209	-	3,3,3	0.07	0	2,2,2	0.12	0
10	DDQ	B	1103	-	11,13,13	0.16	0	12,15,15	0.18	0
5	GOL	D	201	-	5,5,5	0.09	0	5,5,5	0.25	0
5	GOL	A	1205	-	5,5,5	0.09	0	5,5,5	0.31	0
7	3YI	A	1208	-	55,55,55	0.99	2 (3%)	82,83,83	1.49	7 (8%)
5	GOL	C	1103	-	5,5,5	0.08	0	5,5,5	0.23	0
11	OCT	B	1104	-	7,7,7	0.10	0	6,6,6	0.06	0
12	D10	C	1102	-	9,9,9	0.09	0	8,8,8	0.06	0
5	GOL	B	1105	-	5,5,5	0.10	0	5,5,5	0.25	0
3	LMT	C	1101	-	36,36,36	0.47	0	47,47,47	0.86	3 (6%)
9	DDR	B	1102	-	27,27,27	0.24	0	29,29,29	0.27	0
3	LMT	A	1201	-	36,36,36	0.46	0	47,47,47	0.63	0
3	LMT	A	1206	-	36,36,36	0.51	1 (2%)	47,47,47	0.72	0
6	ETE	A	1207	-	13,13,13	0.18	0	12,12,12	0.10	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
3	LMT	A	1202	-	-	6/21/61/61	0/2/2/2
4	HEX	A	1204	-	-	1/3/3/3	-
3	LMT	A	1203	-	-	11/21/61/61	0/2/2/2
3	LMT	B	1101	-	-	10/21/61/61	0/2/2/2
8	EDO	A	1209	-	-	1/1/1/1	-
10	DDQ	B	1103	-	-	7/11/11/11	-
5	GOL	D	201	-	-	2/4/4/4	-
5	GOL	A	1205	-	-	4/4/4/4	-
7	3YI	A	1208	-	-	13/57/72/72	0/4/4/4
5	GOL	C	1103	-	-	0/4/4/4	-
11	OCT	B	1104	-	-	4/5/5/5	-
12	D10	C	1102	-	-	4/7/7/7	-
5	GOL	B	1105	-	-	0/4/4/4	-
3	LMT	C	1101	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	DDR	B	1102	-	-	13/29/29/29	-
3	LMT	A	1201	-	-	12/21/61/61	0/2/2/2
3	LMT	A	1206	-	-	14/21/61/61	0/2/2/2
6	ETE	A	1207	-	-	7/11/11/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1208	3YI	C15-N1	4.26	1.44	1.35
7	A	1208	3YI	C14-C7	-2.19	1.47	1.51
3	A	1206	LMT	O1'-C1'	2.03	1.43	1.40
3	B	1101	LMT	O1'-C1'	2.02	1.43	1.40
3	A	1203	LMT	O1'-C1'	2.00	1.43	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1208	3YI	C2-C3-C4	6.41	123.26	119.19
7	A	1208	3YI	C4-C3-C38	-4.61	113.50	119.83
7	A	1208	3YI	C3-C2-C1	-3.61	118.12	120.68
3	C	1101	LMT	C1B-O5B-C5B	3.41	120.39	113.72
7	A	1208	3YI	O7-C35-C36	2.93	116.31	111.09
7	A	1208	3YI	C3-C4-C10	-2.44	119.21	121.19
7	A	1208	3YI	O4-C11-C12	2.26	125.11	120.56
3	C	1101	LMT	C3B-C4B-C5B	2.25	114.32	110.23
3	C	1101	LMT	O5B-C5B-C4B	2.16	113.59	109.70
7	A	1208	3YI	C2-N1-C15	-2.07	117.76	124.06

There are no chirality outliers.

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1205	GOL	C1-C2-C3-O3
5	D	201	GOL	C1-C2-C3-O3
7	A	1208	3YI	C26-C27-O6-C37
7	A	1208	3YI	C28-C27-O6-C37
7	A	1208	3YI	C25-C26-C27-O6
7	A	1208	3YI	C25-C26-C27-C28
7	A	1208	3YI	C34-C26-C27-O6
7	A	1208	3YI	C34-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
10	B	1103	DDQ	C2-C1-N1-CM1
10	B	1103	DDQ	N1-C1-C2-C3
7	A	1208	3YI	C36-C35-O7-C25
3	A	1206	LMT	O5B-C1B-O1B-C4'
9	B	1102	DDR	O21-C21-O52-C52
9	B	1102	DDR	O1-C1-O51-C51
3	B	1101	LMT	O5B-C5B-C6B-O6B
3	A	1202	LMT	O5'-C5'-C6'-O6'
9	B	1102	DDR	C2-C1-O51-C51
3	A	1203	LMT	O5B-C5B-C6B-O6B
3	B	1101	LMT	O5'-C5'-C6'-O6'
9	B	1102	DDR	C22-C21-O52-C52
3	A	1206	LMT	C2B-C1B-O1B-C4'
3	A	1202	LMT	C4'-C5'-C6'-O6'
3	B	1101	LMT	C4B-C5B-C6B-O6B
3	A	1203	LMT	C4B-C5B-C6B-O6B
3	A	1202	LMT	O5'-C1'-O1'-C1
3	B	1101	LMT	O5'-C1'-O1'-C1
6	A	1207	ETE	OH6-C15-C25-OH5
6	A	1207	ETE	OH5-C14-C24-OH4
3	C	1101	LMT	O5B-C5B-C6B-O6B
3	B	1101	LMT	C4'-C5'-C6'-O6'
3	C	1101	LMT	C4B-C5B-C6B-O6B
7	A	1208	3YI	O8-C35-O7-C25
3	A	1202	LMT	C2'-C1'-O1'-C1
3	B	1101	LMT	C2'-C1'-O1'-C1
3	A	1206	LMT	C2'-C1'-O1'-C1
5	A	1205	GOL	O1-C1-C2-C3
3	A	1206	LMT	O5'-C1'-O1'-C1
7	A	1208	3YI	C18-C19-C20-C31
3	A	1206	LMT	C4-C5-C6-C7
5	A	1205	GOL	O1-C1-C2-O2
5	D	201	GOL	O2-C2-C3-O3
3	A	1206	LMT	C2-C3-C4-C5
11	B	1104	OCT	C3-C4-C5-C6
9	B	1102	DDR	C2-C3-C4-C5
3	A	1206	LMT	C1-C2-C3-C4
7	A	1208	3YI	C4-C3-C38-O13
3	A	1203	LMT	C5-C6-C7-C8
10	B	1103	DDQ	C3-C4-C5-C6
3	C	1101	LMT	C5-C6-C7-C8
8	A	1209	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	1203	LMT	C7-C8-C9-C10
3	C	1101	LMT	C2-C3-C4-C5
10	B	1103	DDQ	C2-C3-C4-C5
12	C	1102	D10	C2-C3-C4-C5
3	A	1201	LMT	O1'-C1-C2-C3
10	B	1103	DDQ	C1-C2-C3-C4
12	C	1102	D10	C3-C4-C5-C6
7	A	1208	3YI	C16-C17-C18-C19
3	C	1101	LMT	C11-C10-C9-C8
3	A	1201	LMT	C5-C6-C7-C8
3	A	1206	LMT	O5'-C5'-C6'-O6'
11	B	1104	OCT	C4-C5-C6-C7
3	C	1101	LMT	O1'-C1-C2-C3
3	A	1203	LMT	O5'-C5'-C6'-O6'
3	C	1101	LMT	C9-C10-C11-C12
9	B	1102	DDR	C27-C28-C29-C30
11	B	1104	OCT	C2-C3-C4-C5
3	B	1101	LMT	O1'-C1-C2-C3
3	A	1206	LMT	C7-C8-C9-C10
3	A	1202	LMT	C9-C10-C11-C12
4	A	1204	HEX	C3-C4-C5-C6
3	A	1201	LMT	C2-C1-O1'-C1'
3	A	1203	LMT	C2-C1-O1'-C1'
3	A	1206	LMT	C2-C1-O1'-C1'
9	B	1102	DDR	C3-C4-C5-C6
3	C	1101	LMT	C3-C4-C5-C6
9	B	1102	DDR	C26-C27-C28-C29
3	A	1202	LMT	C7-C8-C9-C10
3	B	1101	LMT	C11-C10-C9-C8
6	A	1207	ETE	C14-C24-OH4-C13
9	B	1102	DDR	C6-C7-C8-C9
9	B	1102	DDR	C24-C25-C26-C27
12	C	1102	D10	C1-C2-C3-C4
10	B	1103	DDQ	C5-C6-C7-C8
3	B	1101	LMT	C5-C6-C7-C8
6	A	1207	ETE	C15-C25-OH5-C14
3	A	1201	LMT	C3'-C4'-O1B-C1B
3	A	1203	LMT	C9-C10-C11-C12
3	A	1201	LMT	C5'-C4'-O1B-C1B
3	A	1201	LMT	O5B-C1B-O1B-C4'
6	A	1207	ETE	C13-C23-OH3-C22
5	A	1205	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	1203	LMT	C2-C3-C4-C5
3	C	1101	LMT	C1-C2-C3-C4
9	B	1102	DDR	C1-C2-C3-C4
3	A	1201	LMT	C2B-C1B-O1B-C4'
6	A	1207	ETE	OH4-C13-C23-OH3
11	B	1104	OCT	C1-C2-C3-C4
3	A	1201	LMT	C3-C4-C5-C6
3	B	1101	LMT	C6-C7-C8-C9
3	A	1201	LMT	C7-C8-C9-C10
3	A	1203	LMT	O5'-C1'-O1'-C1
7	A	1208	3YI	C18-C19-C20-C21
3	A	1201	LMT	C11-C10-C9-C8
3	A	1203	LMT	C6-C7-C8-C9
6	A	1207	ETE	OH2-C12-C22-OH3
3	A	1201	LMT	C9-C10-C11-C12
3	A	1206	LMT	O1'-C1-C2-C3
3	A	1206	LMT	C9-C10-C11-C12
3	A	1206	LMT	C5'-C4'-O1B-C1B
12	C	1102	D10	C6-C7-C8-C9
10	B	1103	DDQ	C2-C1-N1-CM2
3	A	1206	LMT	C3'-C4'-O1B-C1B
9	B	1102	DDR	O51-C1-C2-C3
7	A	1208	3YI	O6-C27-C28-C29
3	A	1203	LMT	C4'-C5'-C6'-O6'
9	B	1102	DDR	O1-C1-C2-C3
3	A	1201	LMT	C2-C3-C4-C5

There are no ring outliers.

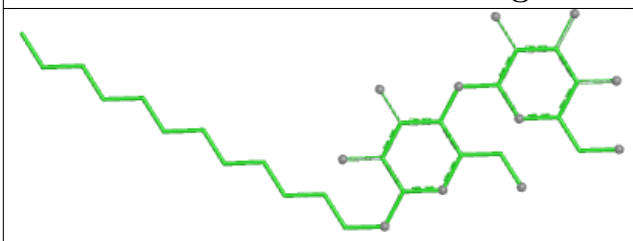
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1103	DDQ	1	0
7	A	1208	3YI	1	0

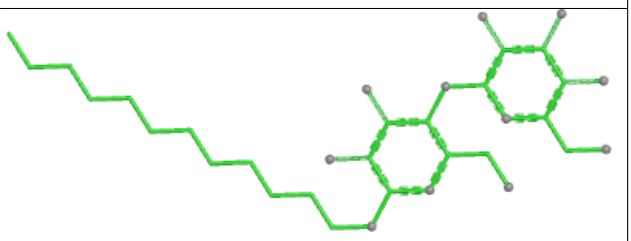
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

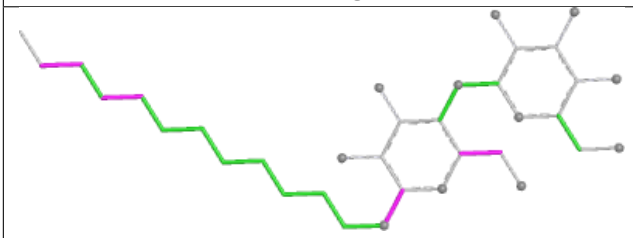
Ligand LMT A 1202



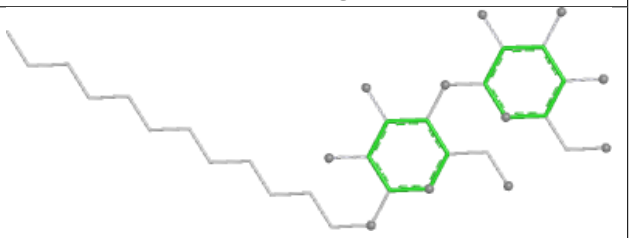
Bond lengths



Bond angles

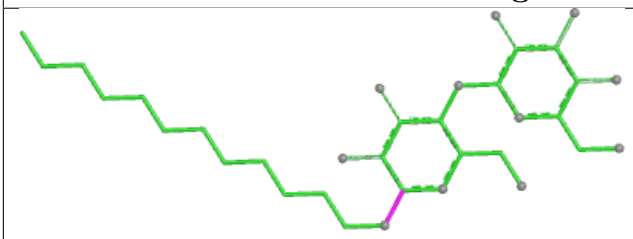


Torsions

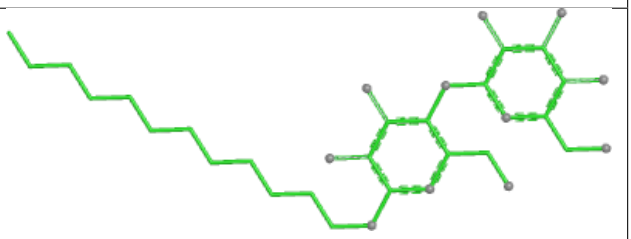


Rings

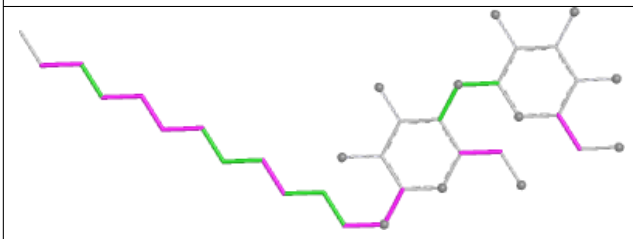
Ligand LMT A 1203



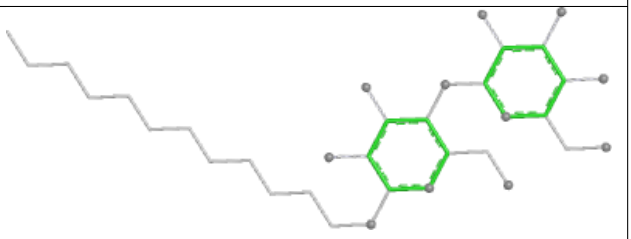
Bond lengths



Bond angles

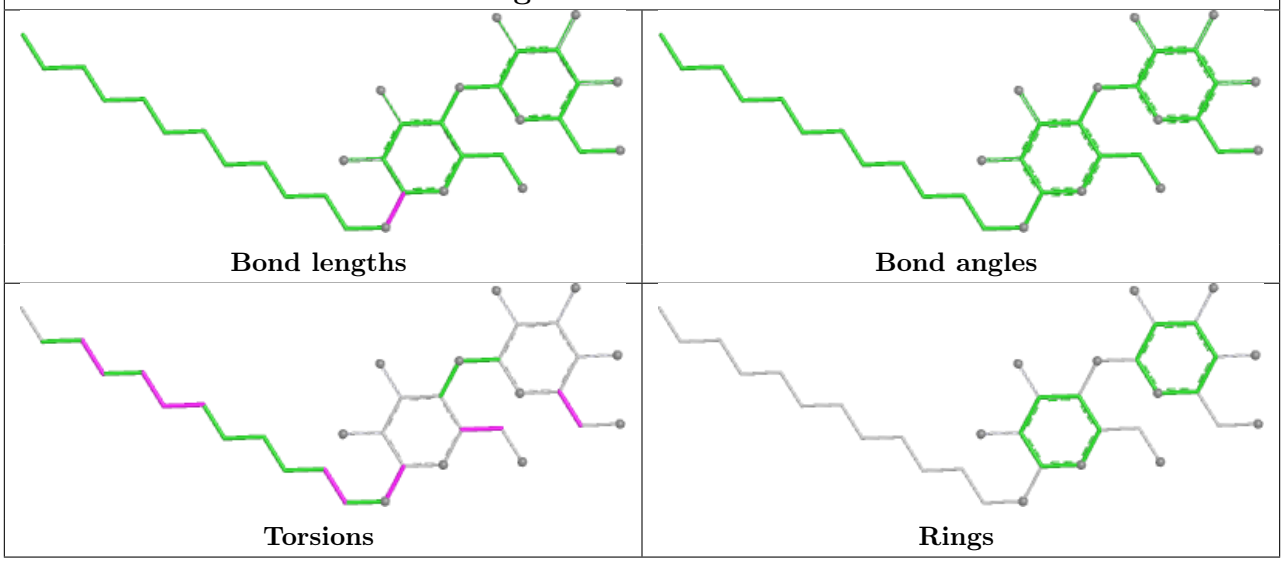


Torsions

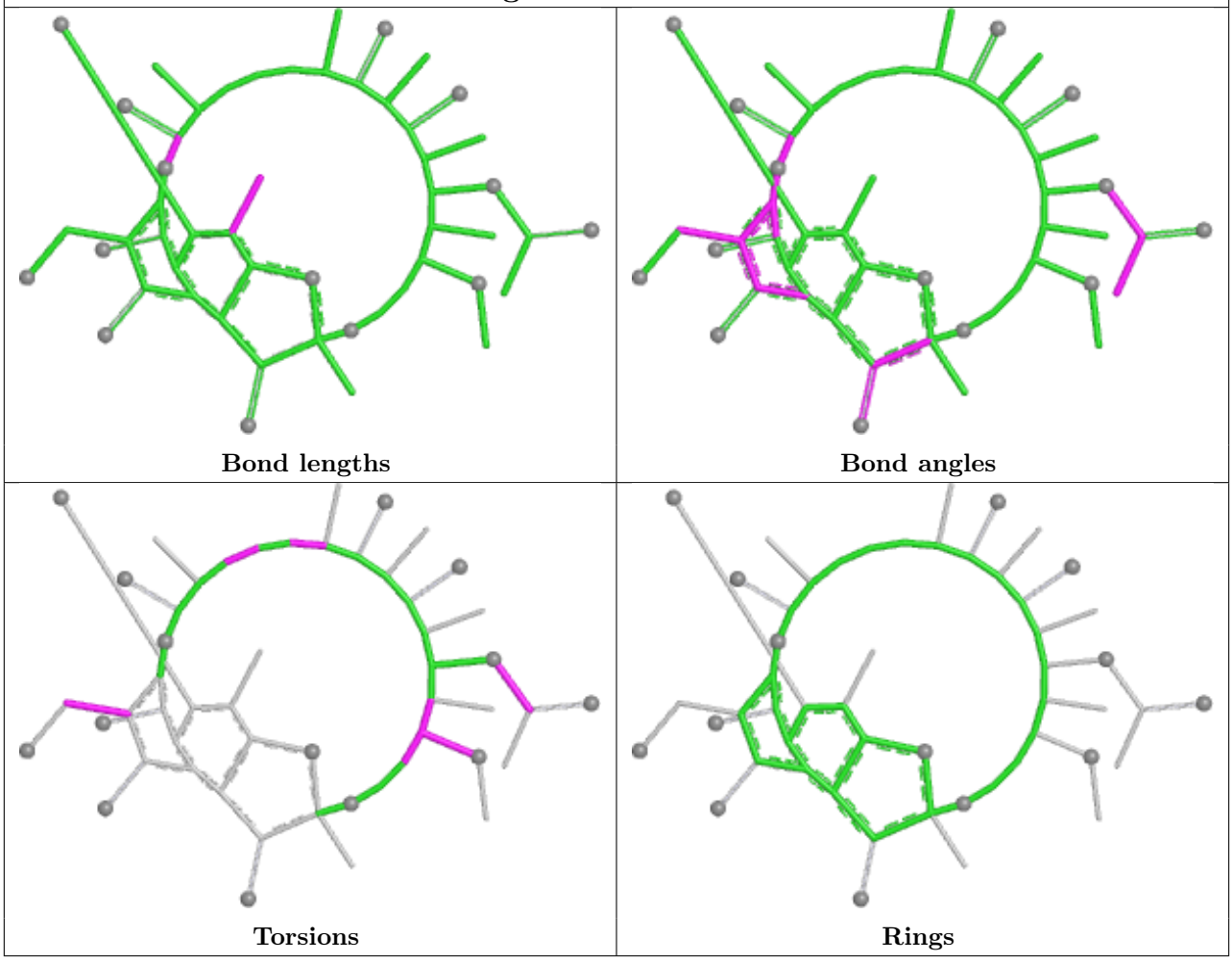


Rings

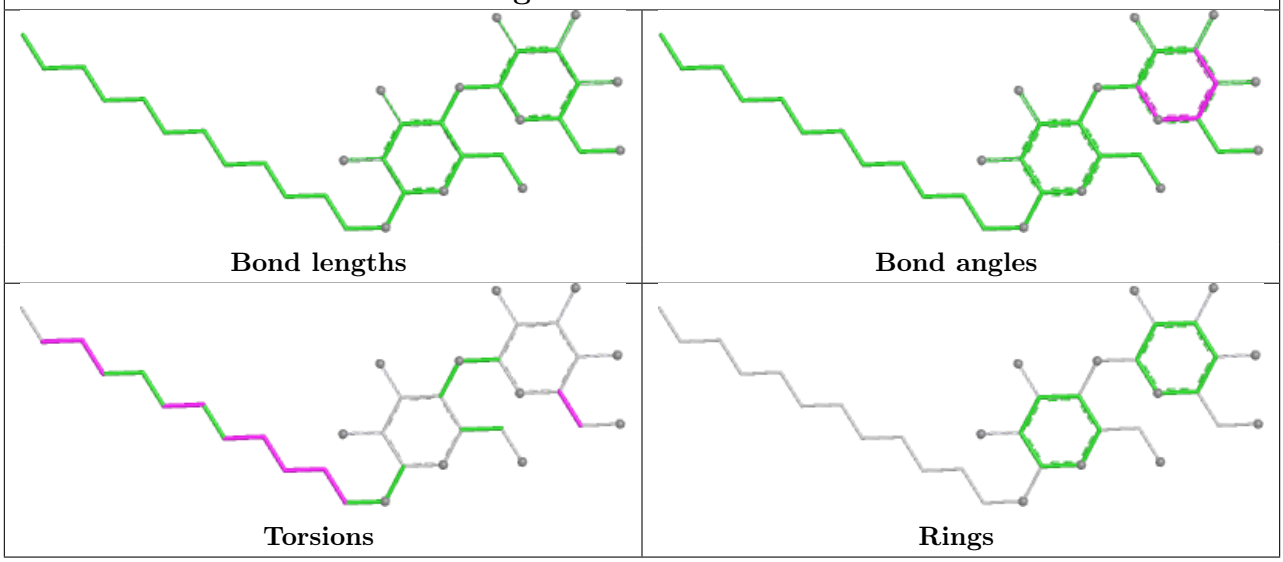
Ligand LMT B 1101



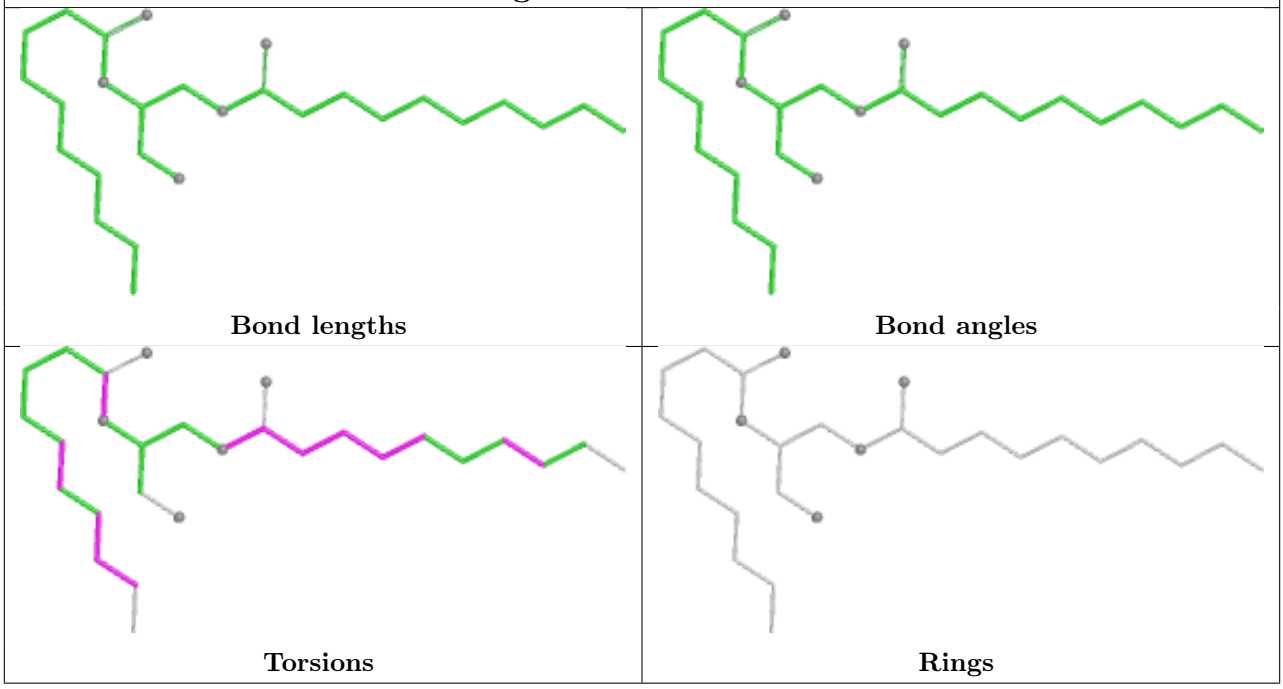
Ligand 3YI A 1208

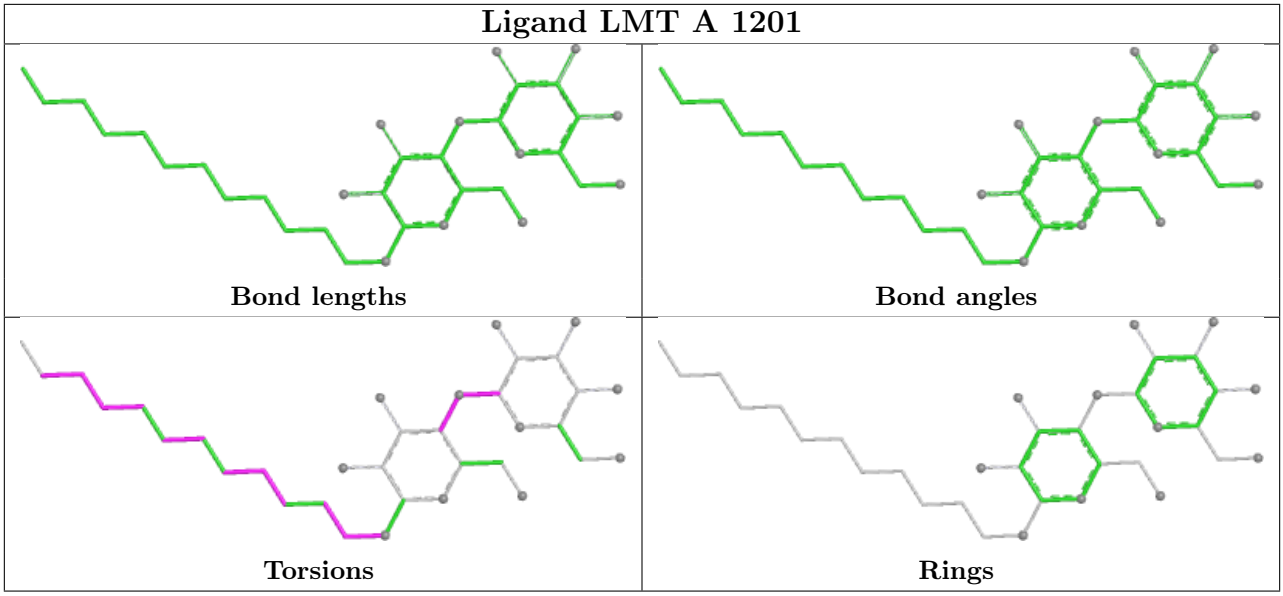


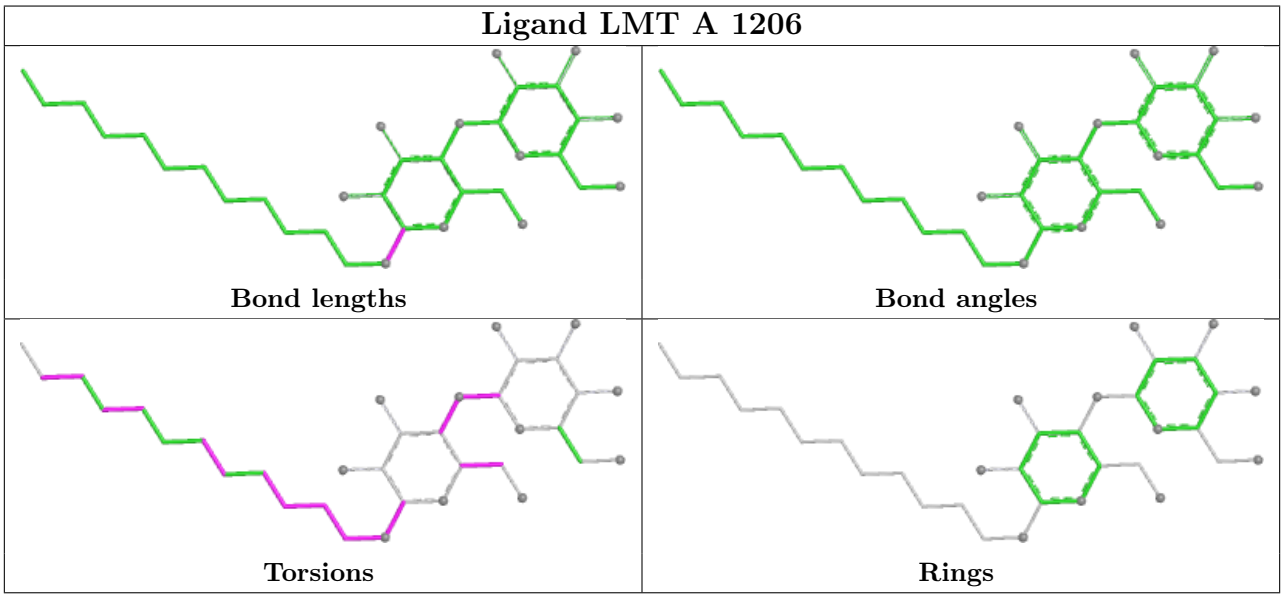
Ligand LMT C 1101



Ligand DDR B 1102







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1035/1057 (97%)	0.12	27 (2%)	56	46	40, 60, 97, 122	6 (0%)
1	B	1034/1057 (97%)	0.19	45 (4%)	34	24	41, 65, 95, 124	0
1	C	1033/1057 (97%)	0.01	17 (1%)	72	66	41, 56, 75, 86	0
2	D	154/169 (91%)	0.26	9 (5%)	23	15	57, 65, 84, 90	0
2	E	154/169 (91%)	1.03	31 (20%)	1	0	57, 70, 87, 93	0
All	All	3410/3509 (97%)	0.16	129 (3%)	40	30	40, 61, 92, 124	6 (0%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	869	SER	6.2
1	A	870	GLY	6.2
1	B	993	THR	5.5
1	B	134	SER	5.1
1	B	1009	GLY	5.1
1	A	677	ALA	5.0
1	B	989	LEU	4.6
1	B	986	VAL	4.5
1	A	868	LEU	4.4
2	E	60	LEU	4.3
2	E	34	MET	4.3
2	E	32	ILE	4.3
1	B	1010	GLY	4.3
1	B	635	ALA	4.1
2	E	27	ASP	4.1
1	B	600	THR	4.0
1	B	1011	MET	4.0
1	A	1035	ARG	3.8
2	E	67	LEU	3.8
1	B	642	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
2	E	30	VAL	3.8
1	A	429	GLU	3.7
1	C	510	LYS	3.7
1	A	866	GLU	3.7
1	B	256	ASP	3.7
2	D	166	GLN	3.6
2	D	150	PHE	3.6
1	A	871	ASN	3.6
2	E	31	ARG	3.6
1	B	641	GLU	3.6
1	A	865	GLN	3.6
1	B	510	LYS	3.5
1	C	362	PHE	3.5
1	B	640	GLU	3.5
2	E	35	ALA	3.5
1	A	675	GLY	3.5
2	E	66	LEU	3.5
1	B	366	LEU	3.4
1	A	255	GLN	3.4
1	A	874	PRO	3.3
1	A	867	ARG	3.3
1	C	501	ALA	3.3
1	A	510	LYS	3.3
1	C	255	GLN	3.3
1	B	511	GLY	3.2
1	B	596	HIS	3.2
1	A	501	ALA	3.2
1	A	875	SER	3.1
2	D	149	ALA	3.1
1	B	638	PRO	3.1
2	E	68	LYS	3.1
1	B	255	GLN	3.0
2	E	148	THR	3.0
2	D	161	LEU	3.0
1	B	563	PHE	2.9
1	A	432	ARG	2.9
1	B	636	ASP	2.9
2	E	64	GLU	2.9
2	E	37	GLY	2.9
2	E	73	VAL	2.9
2	D	163	GLU	2.8
1	C	513	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	33	LEU	2.8
2	D	162	ALA	2.8
2	E	65	VAL	2.7
1	A	918	PHE	2.7
2	E	28	ASP	2.7
1	B	606	VAL	2.7
1	B	629	VAL	2.7
1	B	599	LEU	2.7
1	A	500	ILE	2.6
1	B	675	GLY	2.6
1	B	632	LYS	2.6
1	C	197	GLN	2.6
1	C	1033	PHE	2.6
1	A	256	ASP	2.6
2	E	51	LEU	2.6
2	E	107	ASN	2.6
1	B	575	MET	2.5
2	E	70	GLY	2.5
2	E	106	VAL	2.5
1	B	508	GLY	2.5
2	E	36	ASN	2.5
1	B	501	ALA	2.5
2	D	165	LEU	2.5
1	B	994	GLY	2.4
1	C	500	ILE	2.4
1	A	512	PHE	2.4
2	E	74	ASN	2.4
1	C	257	GLY	2.4
2	E	165	LEU	2.3
1	B	634	TRP	2.3
2	E	159	GLU	2.3
1	B	631	LEU	2.3
1	B	566	ASP	2.3
1	C	511	GLY	2.3
1	B	676	THR	2.2
1	C	796	GLY	2.2
1	C	497	LEU	2.2
2	E	137	ALA	2.2
1	B	988	PRO	2.2
1	C	425	LEU	2.2
1	B	604	ASN	2.2
1	C	512	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	956	GLU	2.2
1	B	363	ARG	2.2
1	B	983	ILE	2.2
1	C	508	GLY	2.2
1	B	597	TYR	2.2
2	E	63	VAL	2.2
2	E	75	ALA	2.1
1	A	423	GLU	2.1
1	C	363	ARG	2.1
1	B	500	ILE	2.1
2	E	130	GLU	2.1
2	E	61	GLU	2.1
1	C	421	ALA	2.1
1	A	254	ASN	2.1
1	B	990	VAL	2.1
1	A	430	ALA	2.1
2	D	159	GLU	2.1
1	A	505	HIS	2.0
1	B	984	LEU	2.0
1	B	509	LYS	2.0
2	D	139	VAL	2.0
1	B	362	PHE	2.0
1	B	660	ASP	2.0
1	A	229	GLN	2.0
2	E	69	ASN	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 monosaccharides in this entry.

6.4 Ligands (i)

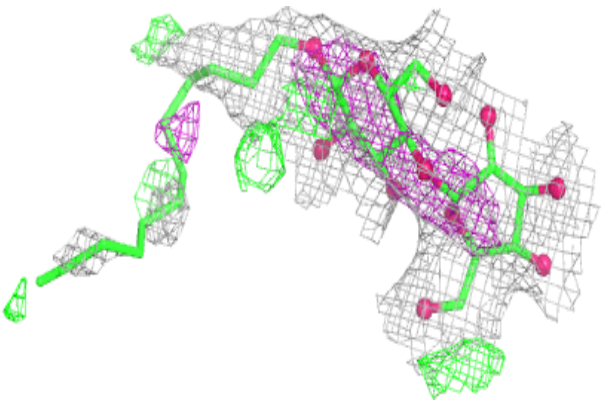
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

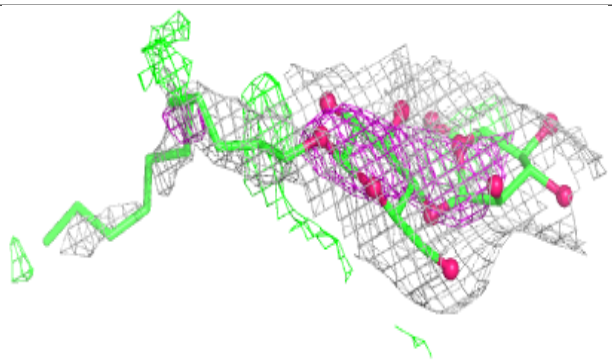
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LMT	A	1206	35/35	0.65	0.47	66,78,79,79	0
3	LMT	A	1202	35/35	0.69	0.32	81,96,102,102	0
6	ETE	A	1207	14/14	0.75	0.22	91,93,93,93	0
10	DDQ	B	1103	14/14	0.81	0.29	53,55,57,58	0
3	LMT	A	1203	35/35	0.83	0.44	100,105,106,106	0
3	LMT	C	1101	35/35	0.85	0.28	78,79,80,80	0
11	OCT	B	1104	8/8	0.85	0.17	53,53,53,53	0
5	GOL	D	201	6/6	0.86	0.34	74,74,74,74	0
3	LMT	A	1201	35/35	0.87	0.24	82,88,92,93	0
5	GOL	B	1105	6/6	0.87	0.27	75,75,75,76	0
3	LMT	B	1101	35/35	0.87	0.31	94,95,99,99	0
12	D10	C	1102	10/10	0.87	0.24	61,62,62,62	0
5	GOL	A	1205	6/6	0.90	0.32	52,53,53,53	0
9	DDR	B	1102	28/28	0.91	0.30	85,87,89,89	0
4	HEX	A	1204	6/6	0.91	0.13	48,48,48,48	0
8	EDO	A	1209	4/4	0.92	0.19	58,58,58,58	0
7	3YI	A	1208	52/52	0.93	0.18	47,49,50,50	0
5	GOL	C	1103	6/6	0.95	0.20	58,58,58,58	0
13	CL	C	1104	1/1	0.97	0.17	51,51,51,51	0

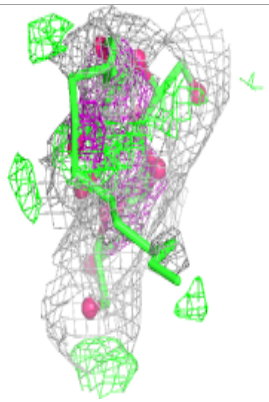
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT A 1206:

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

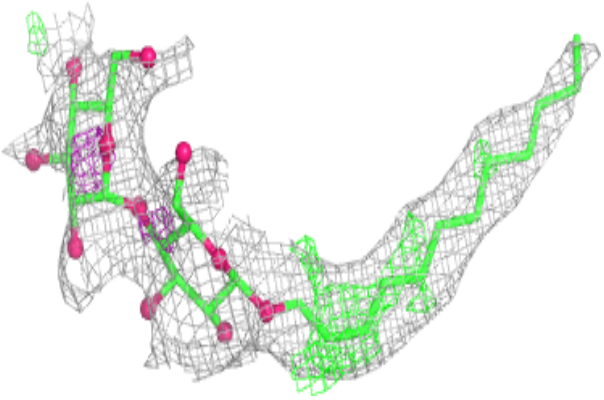


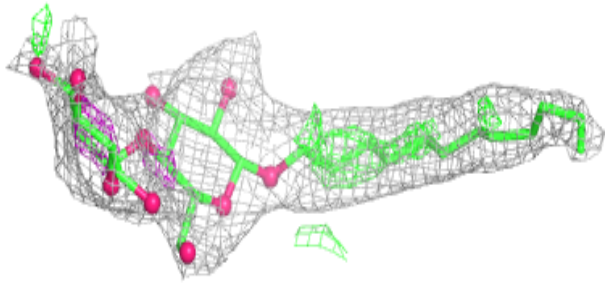


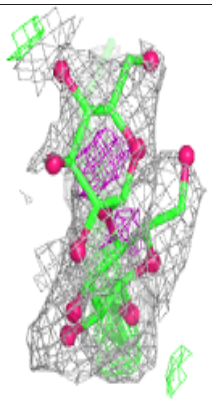


Electron density around LMT A 1202:

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

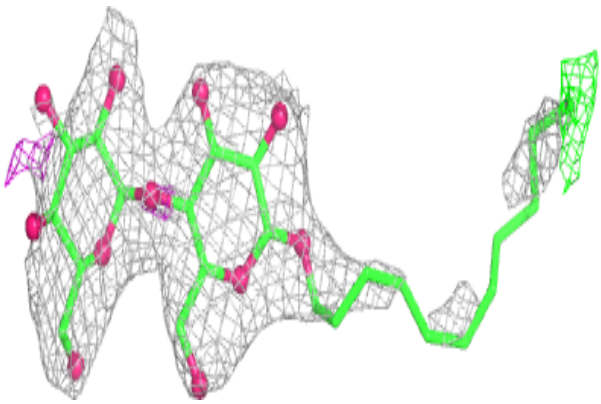


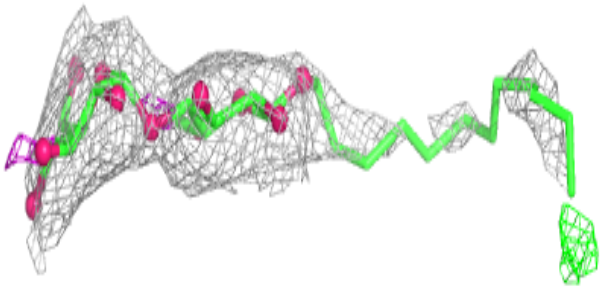


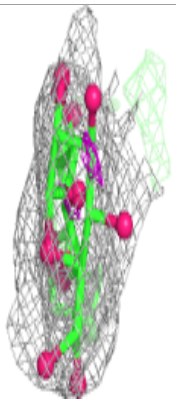


Electron density around LMT A 1203:

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

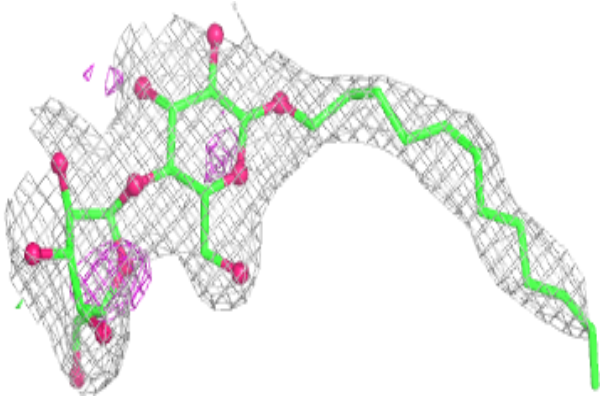


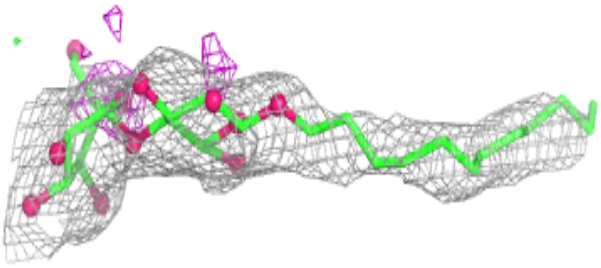


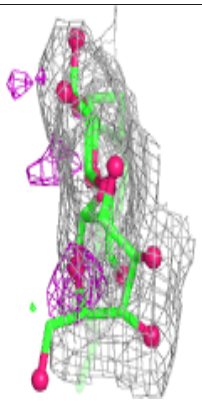


Electron density around LMT C 1101:

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

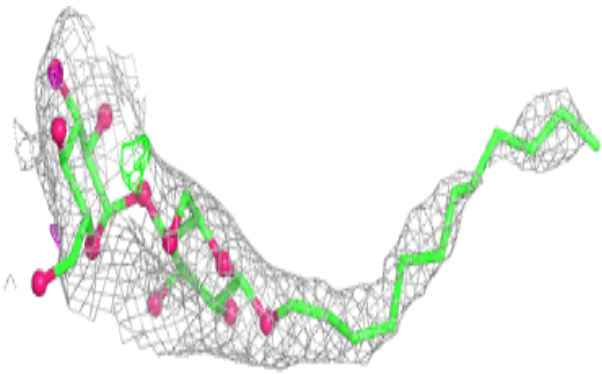


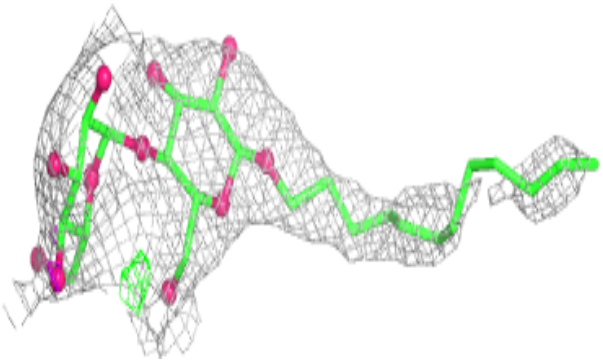


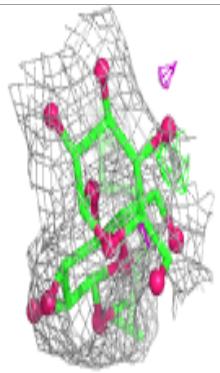


Electron density around LMT A 1201:

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

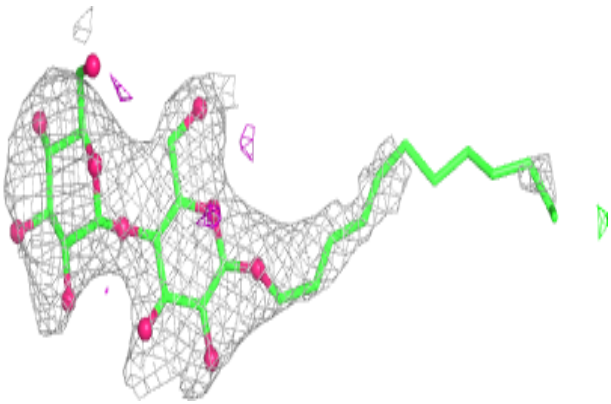


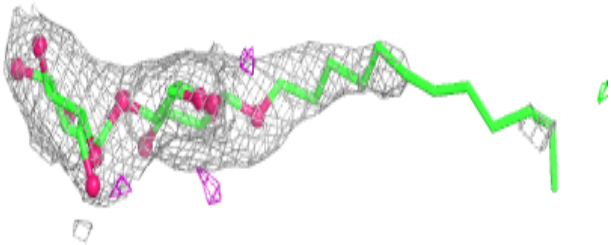


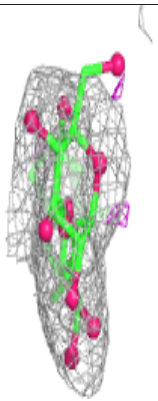


Electron density around LMT B 1101:

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

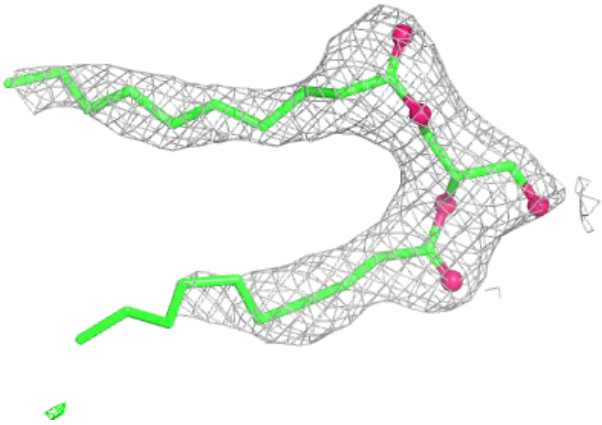


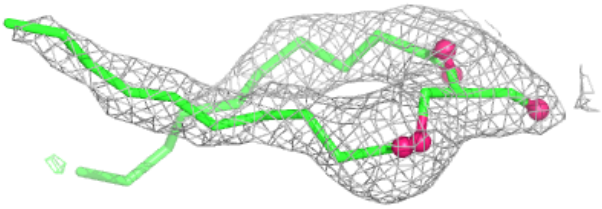


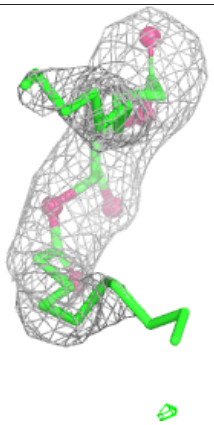


Electron density around DDR B 1102:

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

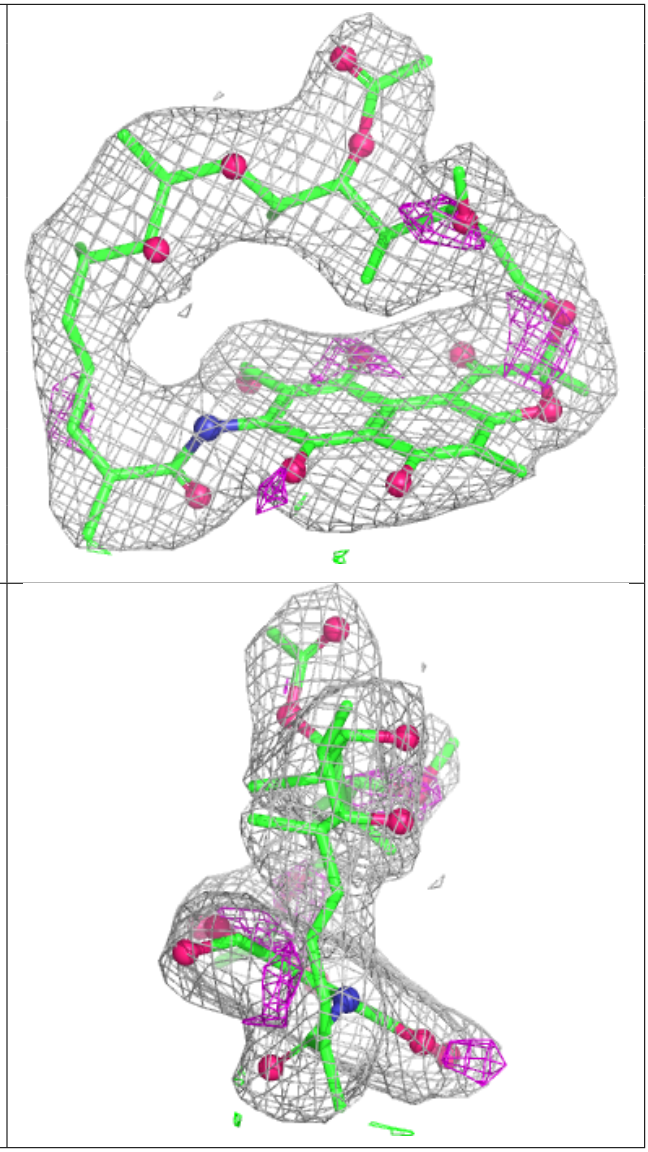






Electron density around 3YI A 1208:

$2mF_o$-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.