Full wwPDB X-ray Structure Validation Report (i)

Mar 6, 2026 – 02:34 PM UTC

PDB ID	:	4AYT / pdb_00004ayt
Title	:	STRUCTURE OF THE HUMAN MITOCHONDRIAL ABC TRANSPORTER, ABCB10
Authors	:	Pike, A.C.W.; Shintre, C.A.; Li, Q.; Kim, J.; von Delft, F.; Barr, A.J.; Das, S.; Chaikuad, A.; Xia, X.; Quigley, A.; Dong, Y.; Dong, L.; Krojer, T.; Vollmar, M.; Muniz, J.R.C.; Bray, J.E.; Berridge, G.; Chalk, R.; Gileadi, O.; Burgess-Brown, N.; Shrestha, L.; Goubin, S.; Yang, J.; Mahajan, P.; Mukhopadhyay, S.; Bullock, A.N.; Arrowsmith, C.H.; Weigelt, J.; Bountra, C.; Edwards, A.M.; Carpenter, E.P.
Deposited on	:	2012-06-22
Resolution	:	2.85 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 (1)) were used in the production of this report:

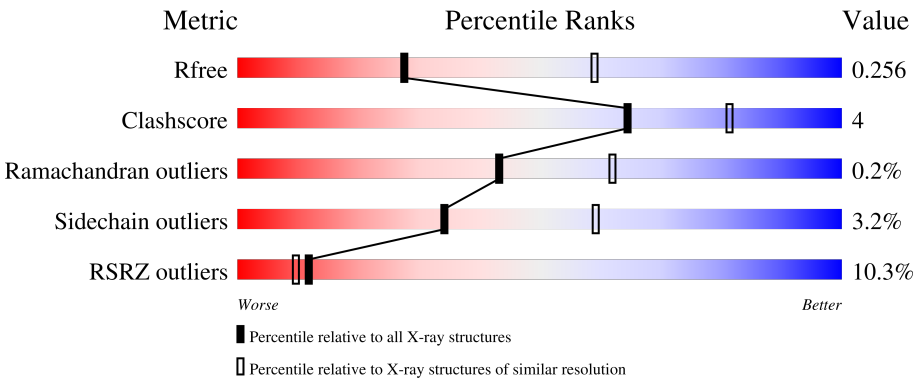
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)

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 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	595	10% 80% 14% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

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

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
6	CDL	A	1721	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4502 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.

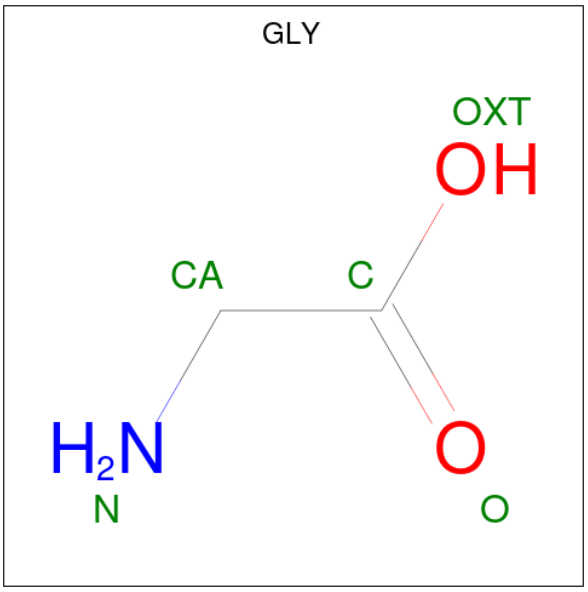
- Molecule 1 is a protein called ATP-BINDING CASSETTE SUB-FAMILY B MEMBER 10 MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	564	4236	2710	724	786	16	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	MET	-	expression tag	UNP Q9NRK6
A	739	ALA	-	expression tag	UNP Q9NRK6
A	740	GLU	-	expression tag	UNP Q9NRK6
A	741	ASN	-	expression tag	UNP Q9NRK6
A	742	LEU	-	expression tag	UNP Q9NRK6
A	743	TYR	-	expression tag	UNP Q9NRK6
A	744	PHE	-	expression tag	UNP Q9NRK6
A	745	GLN	-	expression tag	UNP Q9NRK6

- Molecule 2 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).

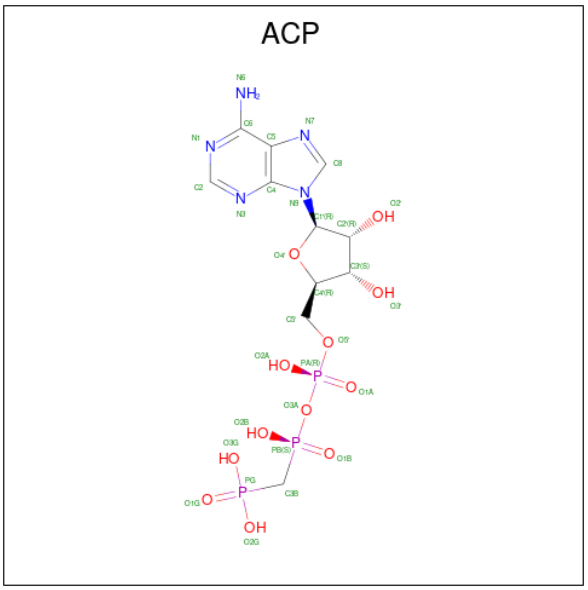


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	5	2	1	2	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

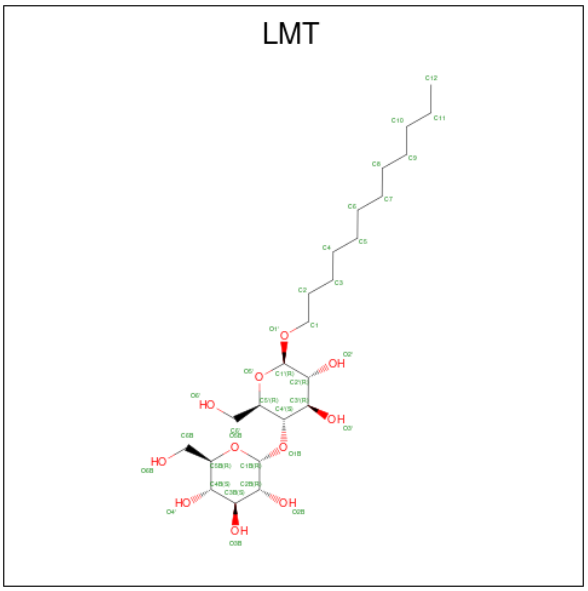
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0

- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



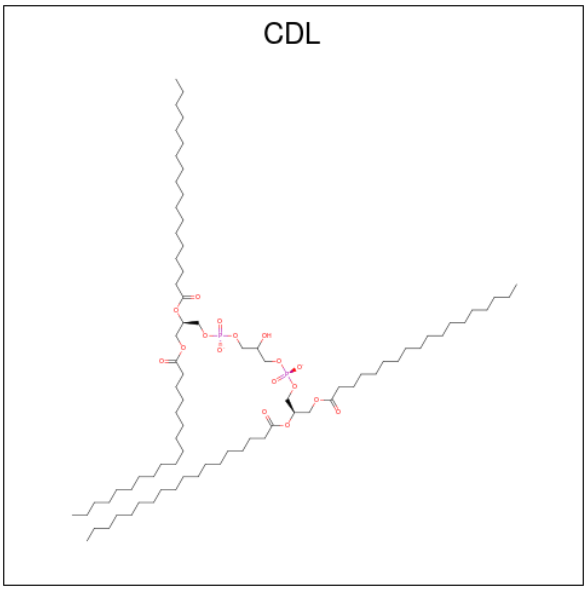
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	11	5	12	3	0	0

- Molecule 5 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 35 24 11	0	0
5	A	1	Total C 12 12	0	0
5	A	1	Total C O 35 24 11	0	0

- Molecule 6 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O P 74 55 17 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 18 18	0	0

- Molecule 7 is water.

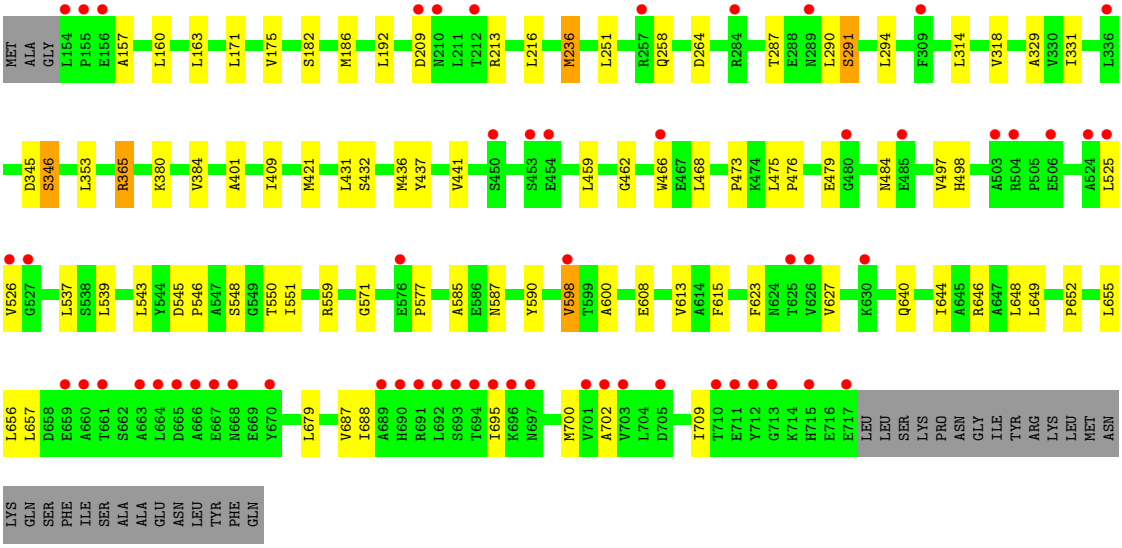
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	55	Total O 55 55	0	0

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: ATP-BINDING CASSETTE SUB-FAMILY B MEMBER 10 MITOCHONDRIAL

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	175.11Å 175.11Å 49.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.55 – 2.85 50.55 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.55-2.85) 99.4 (50.55-2.85)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.201 , 0.248 0.214 , 0.256	Depositor DCC
R_{free} test set	1064 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4502	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: LMT, MG, ACP, CDL

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	0.86	1/4312 (0.0%)	1.46	20/5849 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	MET	SD-CE	-5.78	1.65	1.79

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	432	SER	CA-C-N	6.39	129.17	120.54
1	A	432	SER	C-N-CA	6.39	129.17	120.54
1	A	484	ASN	CA-CB-CG	5.90	118.50	112.60
1	A	608	GLU	CA-C-N	5.52	128.02	120.46
1	A	608	GLU	C-N-CA	5.52	128.02	120.46
1	A	695	ILE	CA-C-N	5.51	127.98	120.54
1	A	695	ILE	C-N-CA	5.51	127.98	120.54
1	A	615	PHE	CA-CB-CG	5.31	119.11	113.80
1	A	600	ALA	CA-C-N	5.29	127.37	120.28
1	A	600	ALA	C-N-CA	5.29	127.37	120.28
1	A	264	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	401	ALA	CA-C-N	5.23	127.24	120.44
1	A	401	ALA	C-N-CA	5.23	127.24	120.44
1	A	545	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	543	LEU	N-CA-C	-5.18	105.70	112.23
1	A	543	LEU	CA-C-N	5.14	130.54	122.21
1	A	543	LEU	C-N-CA	5.14	130.54	122.21
1	A	365	ARG	CA-C-N	5.07	128.79	120.63
1	A	365	ARG	C-N-CA	5.07	128.79	120.63
1	A	345	ASP	CA-CB-CG	5.04	117.64	112.60

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	4236	0	4267	34	0
2	A	5	0	2	0	0
3	A	1	0	0	0	0
4	A	31	0	14	0	0
5	A	82	0	115	2	0
6	A	92	0	133	1	0
7	A	55	0	0	0	0
All	All	4502	0	4531	35	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (35) 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:192:LEU:HD23	1:A:436:MET:HE1	1.64	0.79
1:A:236:MET:HE2	1:A:291:SER:HB3	1.75	0.69
1:A:537:LEU:HD22	1:A:656:LEU:HB3	1.73	0.69
1:A:421:MET:HE2	1:A:431:LEU:HD22	1.79	0.63
1:A:476:PRO:HB3	1:A:479:GLU:HG2	1.87	0.57
1:A:550:THR:HG22	1:A:559:ARG:HH21	1.69	0.56
1:A:585:ALA:HB2	1:A:623:PHE:HB3	1.90	0.52
1:A:258:GLN:HA	1:A:473:PRO:HB3	1.91	0.52
1:A:157:ALA:HA	1:A:160:LEU:HD12	1.93	0.51
1:A:353:LEU:HD22	1:A:380:LYS:HD2	1.93	0.50
1:A:171:LEU:HD21	1:A:287:THR:HG22	1.93	0.50
5:A:1724:LMT:H5B	5:A:1724:LMT:H6D	1.93	0.49
1:A:498:HIS:HB2	1:A:548:SER:HB3	1.93	0.49
1:A:182:SER:O	1:A:186:MET:HG2	2.12	0.49
1:A:598:VAL:HG11	1:A:649:LEU:HD21	1.94	0.48
1:A:437:TYR:O	1:A:441:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:LEU:HB3	1:A:688:ILE:HG13	1.95	0.48
1:A:497:VAL:HG13	1:A:546:PRO:HB3	1.96	0.48
1:A:587:ASN:O	1:A:646:ARG:HD3	2.13	0.48
1:A:329:ALA:HB2	6:A:1721:CDL:H462	1.97	0.46
1:A:577:PRO:HG2	1:A:640:GLN:HA	1.97	0.45
1:A:702:ALA:HB1	1:A:709:ILE:HD12	1.99	0.45
1:A:655:LEU:HD21	1:A:657:LEU:HD21	2.00	0.43
1:A:251:LEU:HD11	1:A:468:LEU:HD12	2.01	0.43
1:A:290:LEU:O	1:A:294:LEU:HB2	2.18	0.42
1:A:644:ILE:HG23	1:A:679:LEU:HD22	2.01	0.41
1:A:160:LEU:HD11	1:A:459:LEU:HD21	2.03	0.41
1:A:409:ILE:HG13	5:A:1724:LMT:H122	2.03	0.41
1:A:590:TYR:HB3	1:A:646:ARG:HD2	2.03	0.41
1:A:571:GLY:HA3	1:A:652:PRO:HG3	2.03	0.41
1:A:346:SER:HB3	1:A:384:VAL:HG22	2.03	0.40
1:A:209:ASP:HB3	1:A:213:ARG:NH1	2.36	0.40
1:A:462:GLY:O	1:A:466:TRP:HD1	2.04	0.40
1:A:539:LEU:HB3	1:A:551:ILE:HD11	2.03	0.40
1:A:314:LEU:O	1:A:318:VAL:HG23	2.22	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	563/595 (95%)	550 (98%)	12 (2%)	1 (0%)	43 62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	627	VAL

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	441/489 (90%)	427 (97%)	14 (3%)	34 59

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	LEU
1	A	175	VAL
1	A	216	LEU
1	A	291	SER
1	A	331	ILE
1	A	346	SER
1	A	365	ARG
1	A	475	LEU
1	A	526	VAL
1	A	598	VAL
1	A	613	VAL
1	A	648	LEU
1	A	687	VAL
1	A	700	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	299	GLN
1	A	344	GLN
1	A	352	GLN
1	A	489	GLN
1	A	562	ASN
1	A	640	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	$\#\|Z\| > 2$
5	LMT	A	1723	-	11,11,36	0.34	0	10,10,47	0.26	0
4	ACP	A	900	3	31,33,33	0.51	1 (3%)	47,52,52	0.90	3 (6%)
5	LMT	A	1720	-	36,36,36	0.20	0	47,47,47	0.36	0
5	LMT	A	1724	-	36,36,36	0.24	0	47,47,47	0.46	0
6	CDL	A	1727	-	17,17,99	0.96	1 (5%)	16,16,111	1.02	2 (12%)
2	GLY	A	1717	-	4,4,4	1.01	0	3,4,4	0.84	0
6	CDL	A	1721	-	73,73,99	0.73	2 (2%)	79,85,111	0.63	4 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LMT	A	1723	-	-	3/9/9/61	-
4	ACP	A	900	3	-	3/19/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LMT	A	1720	-	-	6/21/61/61	0/2/2/2
5	LMT	A	1724	-	-	6/21/61/61	0/2/2/2
6	CDL	A	1727	-	-	8/15/15/110	-
6	CDL	A	1721	-	1/1/9/9	29/84/84/110	-
2	GLY	A	1717	-	-	2/2/2/2	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1721	CDL	C39-C38	-3.90	1.32	1.51
6	A	1721	CDL	C79-C78	-3.89	1.32	1.51
6	A	1727	CDL	C19-C18	-3.54	1.34	1.51
4	A	900	ACP	PB-O3A	2.38	1.61	1.58

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	900	ACP	O1B-PB-C3B	3.20	117.47	109.05
6	A	1727	CDL	C19-C18-C17	2.94	129.24	114.37
4	A	900	ACP	O2A-PA-O5'	-2.86	94.61	107.57
6	A	1727	CDL	C20-C19-C18	2.76	128.34	114.37
6	A	1721	CDL	C39-C38-C37	2.40	126.49	114.37
6	A	1721	CDL	C80-C79-C78	2.32	126.09	114.37
6	A	1721	CDL	C79-C78-C77	2.28	125.89	114.37
4	A	900	ACP	O3A-PA-O1A	2.25	117.47	110.70
6	A	1721	CDL	C40-C39-C38	2.21	125.56	114.37

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1721	CDL	CA4

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1721	CDL	CA3-OA5-PA1-OA2
6	A	1721	CDL	CA3-OA5-PA1-OA4
6	A	1721	CDL	CB2-OB2-PB2-OB3
6	A	1721	CDL	CB2-OB2-PB2-OB5
6	A	1721	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
6	A	1721	CDL	CA4-CA6-OA8-CA7
6	A	1727	CDL	C17-C18-C19-C20
6	A	1721	CDL	O1-C1-CB2-OB2
2	A	1717	GLY	OXT-C-CA-N
2	A	1717	GLY	O-C-CA-N
5	A	1723	LMT	C7-C8-C9-C10
5	A	1720	LMT	C2-C3-C4-C5
5	A	1720	LMT	C2-C1-O1'-C1'
5	A	1720	LMT	C1-C2-C3-C4
6	A	1727	CDL	C11-C12-C13-C14
6	A	1721	CDL	CA2-C1-CB2-OB2
5	A	1724	LMT	C7-C8-C9-C10
6	A	1727	CDL	C21-C22-C23-C24
5	A	1723	LMT	C5-C6-C7-C8
5	A	1724	LMT	C11-C10-C9-C8
5	A	1724	LMT	C4-C5-C6-C7
6	A	1727	CDL	C14-C15-C16-C17
5	A	1724	LMT	O1'-C1-C2-C3
6	A	1721	CDL	OB6-CB4-CB6-OB8
5	A	1720	LMT	C7-C8-C9-C10
4	A	900	ACP	C5'-O5'-PA-O3A
6	A	1721	CDL	CA3-OA5-PA1-OA3
6	A	1721	CDL	CB2-OB2-PB2-OB4
6	A	1721	CDL	CB3-OB5-PB2-OB2
6	A	1721	CDL	CB3-OB5-PB2-OB3
5	A	1720	LMT	C5-C6-C7-C8
5	A	1720	LMT	C3-C4-C5-C6
6	A	1721	CDL	OB5-CB3-CB4-CB6
6	A	1721	CDL	OA5-CA3-CA4-OA6
6	A	1727	CDL	C20-C21-C22-C23
6	A	1721	CDL	C79-C80-C81-C82
6	A	1721	CDL	C39-C40-C41-C42
6	A	1721	CDL	OB5-CB3-CB4-OB6
6	A	1721	CDL	C31-C32-C33-C34
5	A	1724	LMT	C3-C4-C5-C6
6	A	1721	CDL	C80-C81-C82-C83
6	A	1721	CDL	CB3-CB4-CB6-OB8
6	A	1727	CDL	C19-C20-C21-C22
6	A	1721	CDL	CA3-CA4-OA6-CA5
6	A	1721	CDL	CA6-CA4-OA6-CA5
6	A	1721	CDL	CB3-CB4-OB6-CB5
6	A	1721	CDL	CB6-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
5	A	1723	LMT	C6-C7-C8-C9
6	A	1721	CDL	C40-C41-C42-C43
6	A	1727	CDL	C22-C23-C24-C25
4	A	900	ACP	PG-C3B-PB-O1B
6	A	1721	CDL	OA5-CA3-CA4-CA6
6	A	1727	CDL	C12-C13-C14-C15
5	A	1724	LMT	C9-C10-C11-C12
4	A	900	ACP	PB-O3A-PA-O2A
6	A	1721	CDL	C12-C11-CA5-OA6
6	A	1721	CDL	C12-C11-CA5-OA7

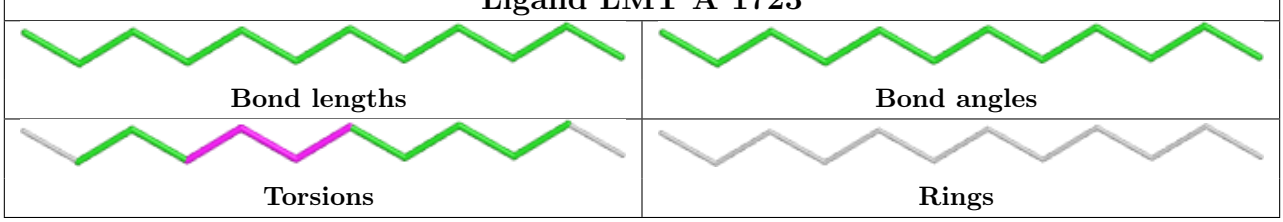
There are no ring outliers.

2 monomers are involved in 3 short contacts:

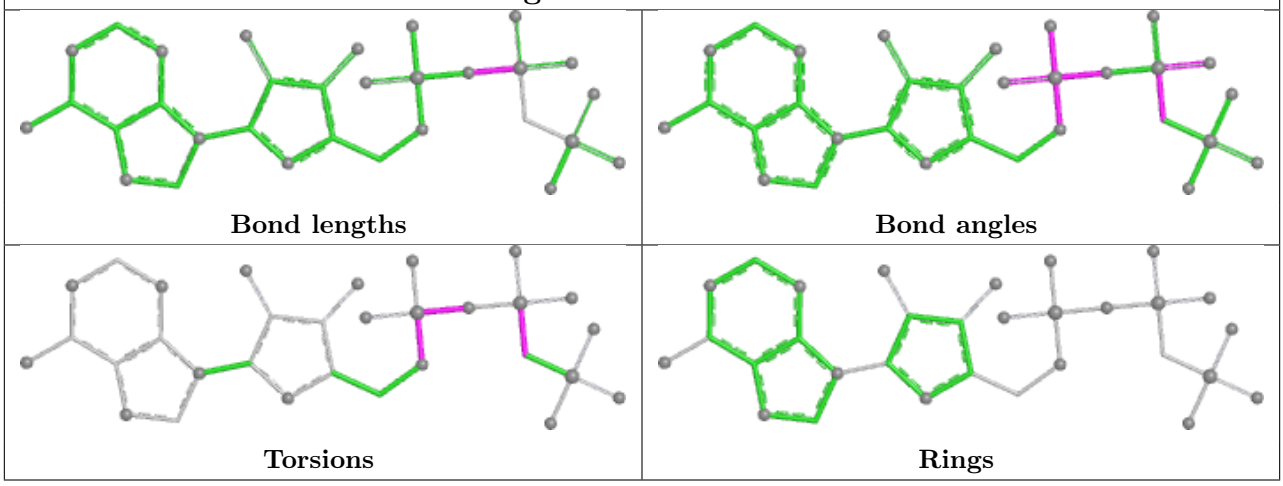
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1724	LMT	2	0
6	A	1721	CDL	1	0

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.

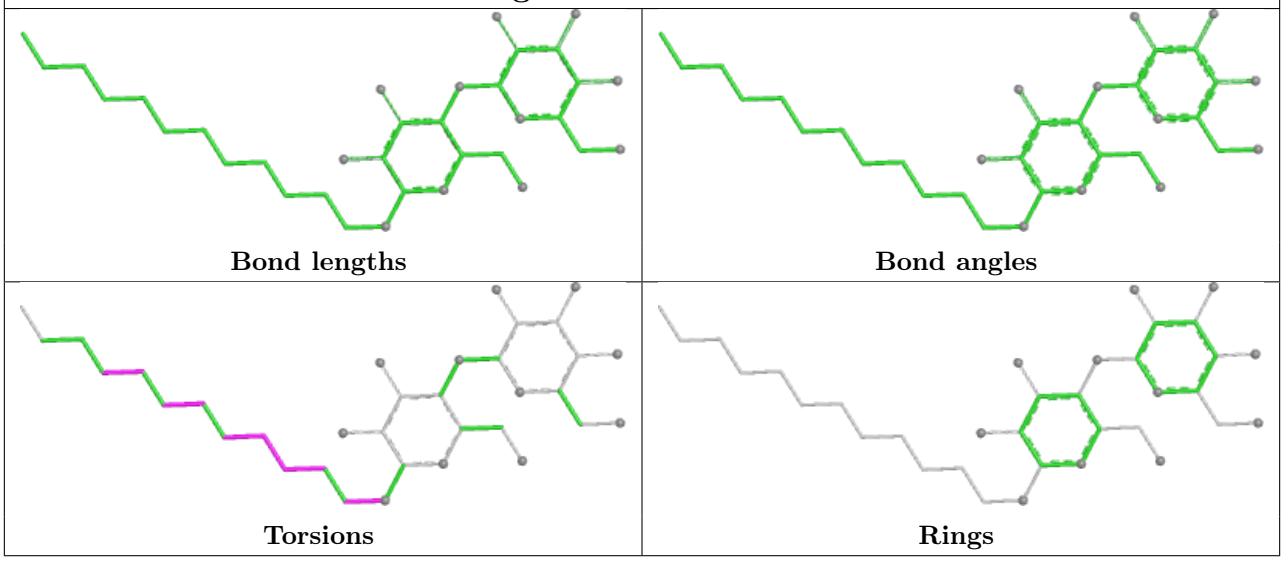
Ligand LMT A 1723



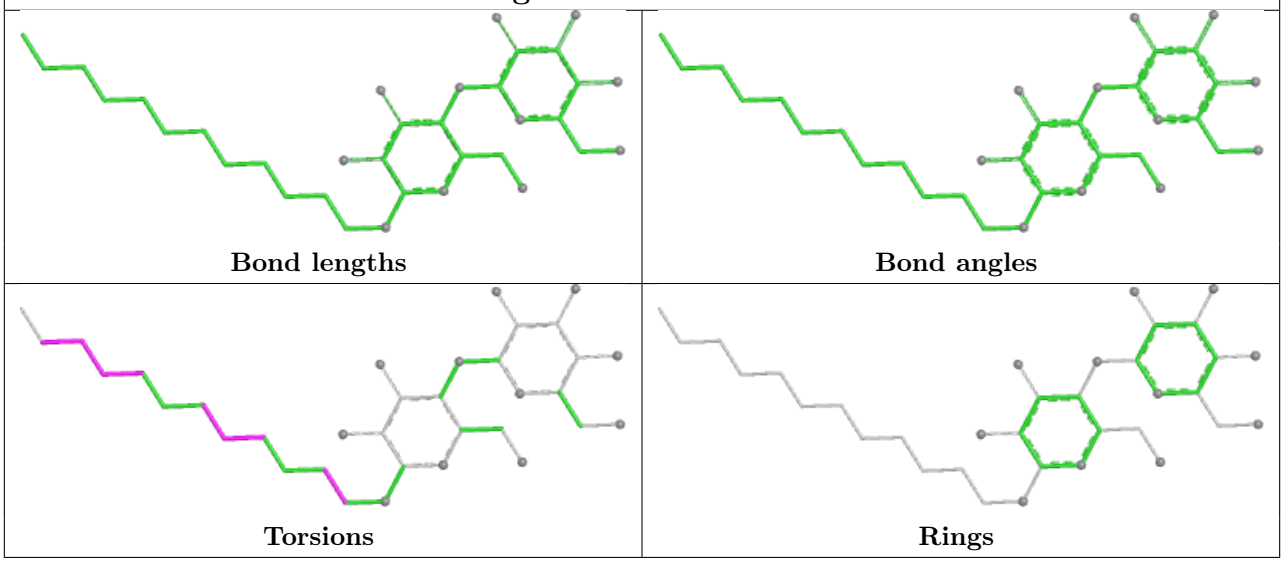
Ligand ACP A 900

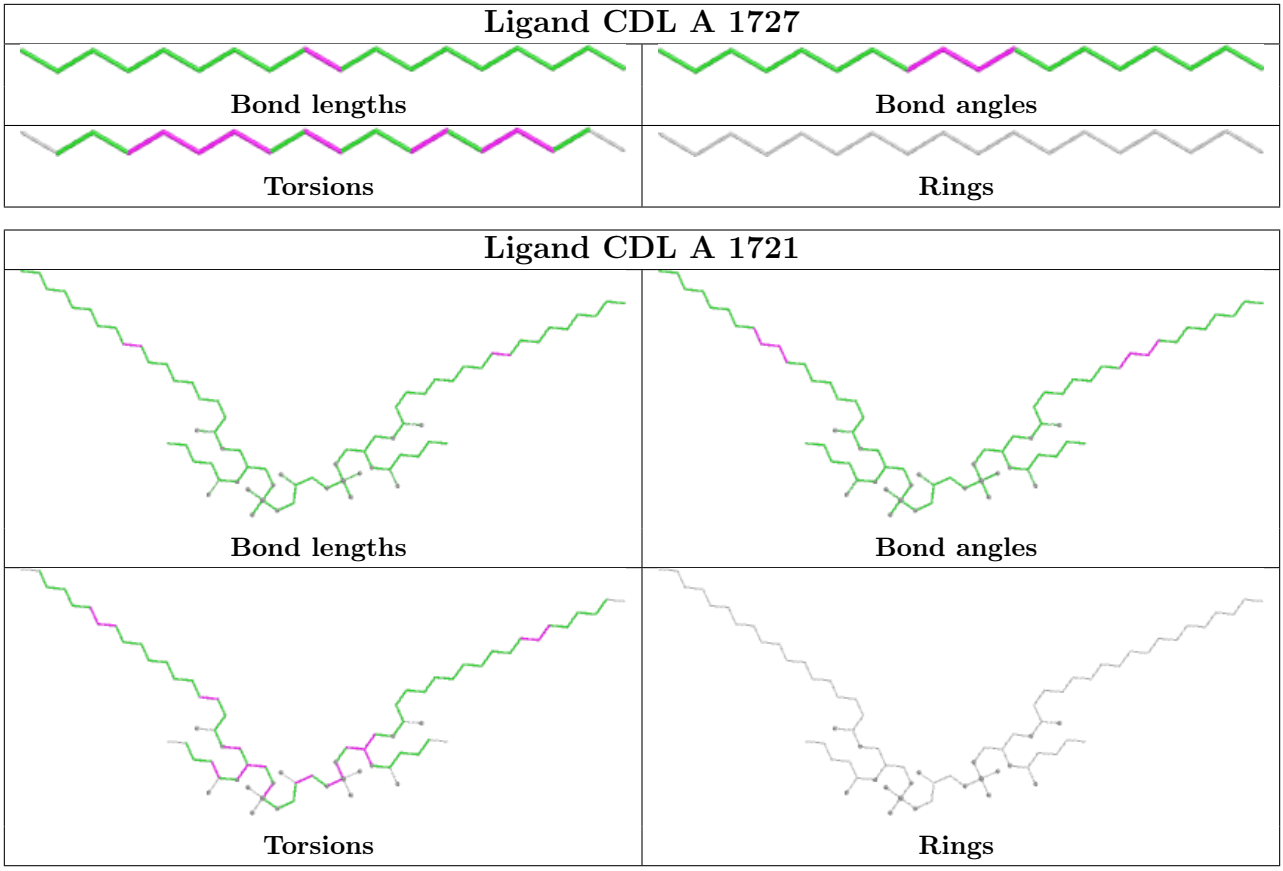


Ligand LMT A 1720



Ligand LMT A 1724





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	564/595 (94%)	0.49	58 (10%)	12	10	25, 52, 84, 115	1 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	689	ALA	6.5
1	A	453	SER	6.5
1	A	526	VAL	6.3
1	A	454	GLU	5.8
1	A	713	GLY	5.4
1	A	209	ASP	5.2
1	A	309	PHE	4.7
1	A	154	LEU	4.7
1	A	284	ARG	4.6
1	A	503	ALA	4.4
1	A	690	HIS	4.4
1	A	156	GLU	4.3
1	A	703	VAL	4.3
1	A	705	ASP	4.1
1	A	663	ALA	4.1
1	A	692	LEU	4.0
1	A	717	GLU	4.0
1	A	710	THR	4.0
1	A	691	ARG	3.9
1	A	695	ILE	3.9
1	A	701	VAL	3.8
1	A	693	SER	3.8
1	A	210	ASN	3.6
1	A	715	HIS	3.6
1	A	524	ALA	3.6
1	A	466	TRP	3.6
1	A	485	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	527	GLY	3.4
1	A	694	THR	3.4
1	A	668	ASN	3.3
1	A	450	SER	3.2
1	A	667	GLU	3.1
1	A	702	ALA	3.0
1	A	696	LYS	2.9
1	A	697	ASN	2.9
1	A	711	GLU	2.8
1	A	665	ASP	2.7
1	A	630	LYS	2.7
1	A	506	GLU	2.7
1	A	155	PRO	2.6
1	A	289	ASN	2.6
1	A	664	LEU	2.6
1	A	480	GLY	2.6
1	A	525	LEU	2.5
1	A	659	GLU	2.4
1	A	670	TYR	2.4
1	A	504	ARG	2.4
1	A	336	LEU	2.3
1	A	626	VAL	2.3
1	A	666	ALA	2.3
1	A	625	THR	2.2
1	A	257	ARG	2.2
1	A	660	ALA	2.1
1	A	576	GLU	2.1
1	A	212	THR	2.1
1	A	661	THR	2.1
1	A	598	VAL	2.0
1	A	712	TYR	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)

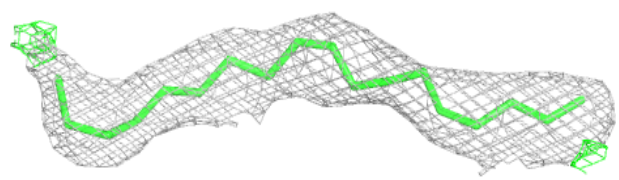
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

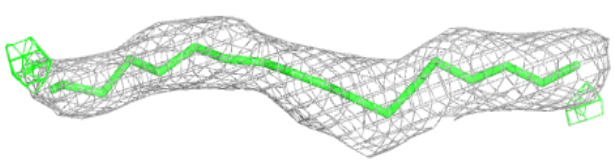
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLY	A	1717	5/5	0.62	0.19	82,84,88,104	0
3	MG	A	801	1/1	0.77	0.12	77,77,77,77	0
6	CDL	A	1727	18/100	0.86	0.18	54,62,67,67	0
5	LMT	A	1723	12/35	0.87	0.22	52,60,63,63	0
4	ACP	A	900	31/31	0.88	0.12	69,87,101,102	0
5	LMT	A	1724	35/35	0.91	0.12	45,51,64,66	0
5	LMT	A	1720	35/35	0.91	0.13	49,65,75,75	0
6	CDL	A	1721	74/100	0.93	0.13	52,62,68,69	74

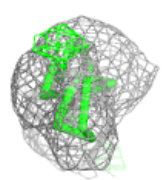
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CDL A 1727:

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

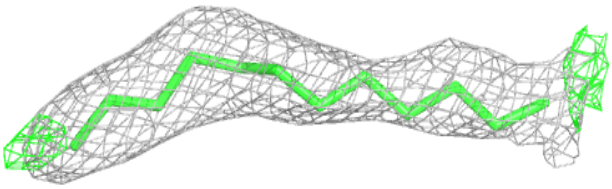


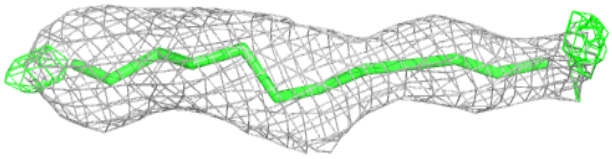


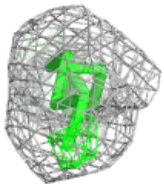


Electron density around LMT A 1723:

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

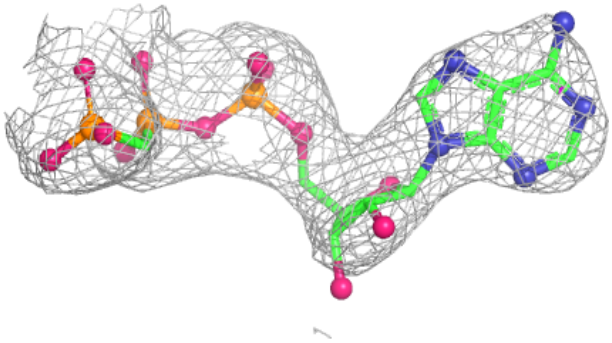


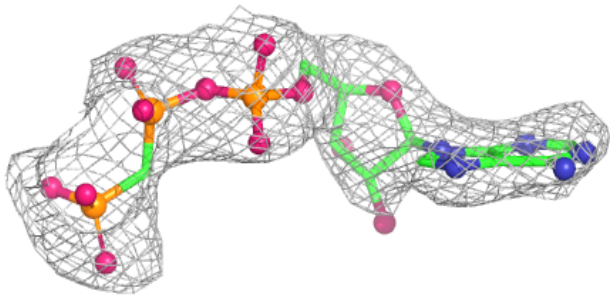


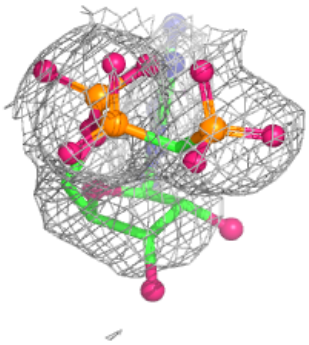


Electron density around ACP A 900:

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

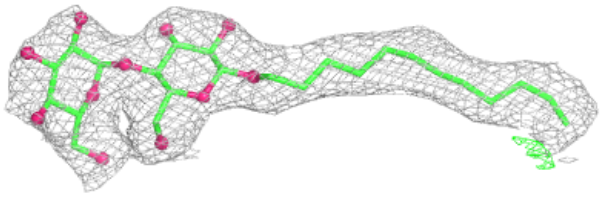


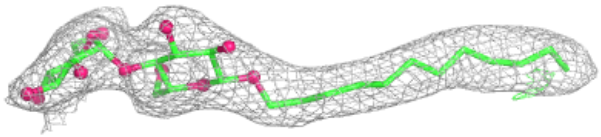


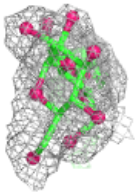


Electron density around LMT A 1724:

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

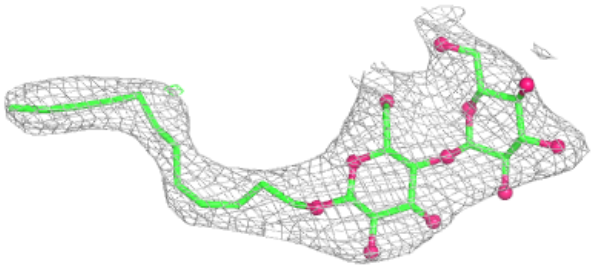


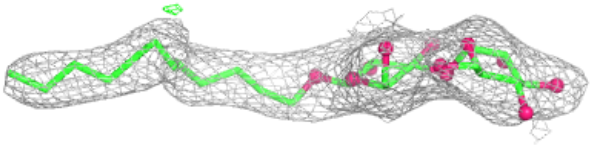


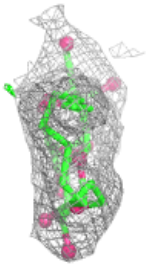


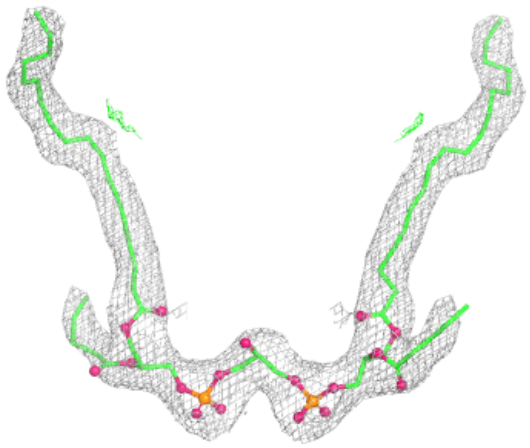
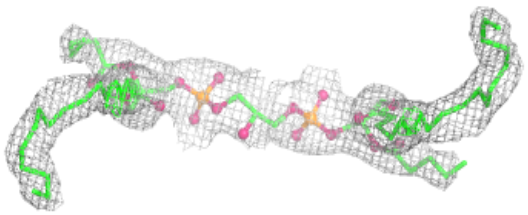
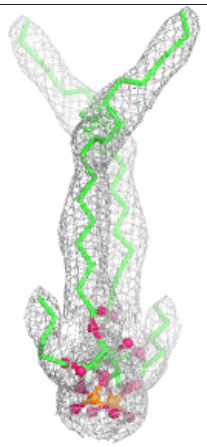
Electron density around LMT A 1720:

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







Electron density around CDL A 1721: $2mF_o$-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.