Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 03:33 AM BST

PDB ID	:	6L85
Title	:	The sodium-dependent phosphate transporter
Authors	:	Tsai, J.-Y.; Sun, Y.-J.
Deposited on	:	2019-11-04
Resolution	:	2.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

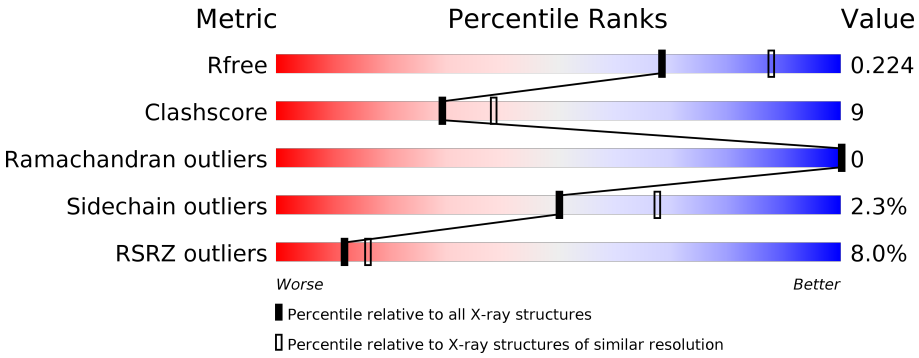
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4.dev1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	402	7% 84% 14%
1	B	402	8% 82% 17%

2 Entry composition

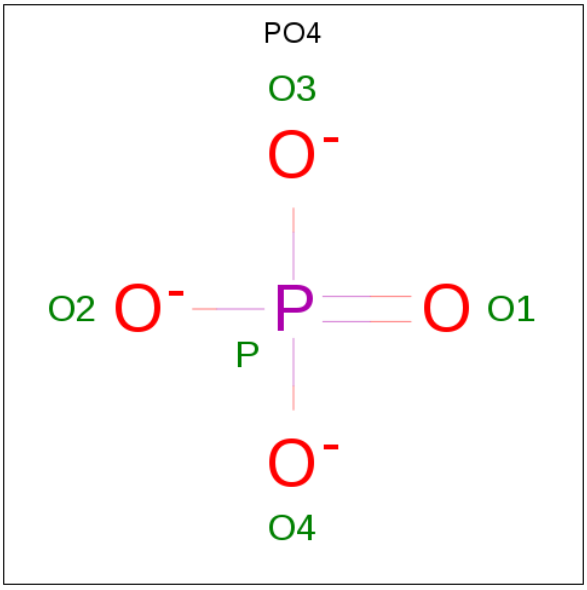
There are 6 unique types of molecules in this entry. The entry contains 6300 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphate transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			2991	1986	474	517	14			
1	B	401	Total	C	N	O	S	0	0	0
			3000	1992	476	518	14			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

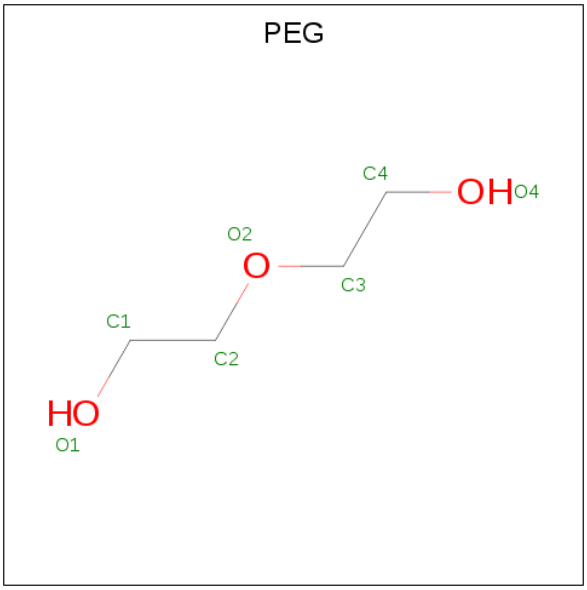


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total Na 3 3	0	0
3	A	3	Total Na 3 3	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0

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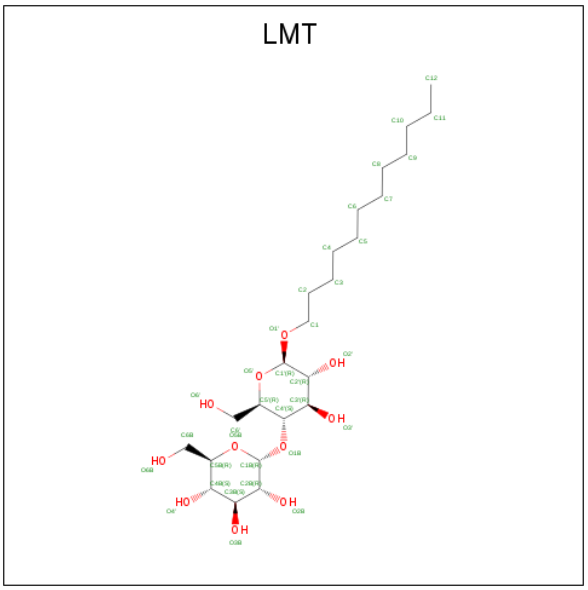
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 7 4 3	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 23 18 5	0	0
5	A	1	Total C O 23 18 5	0	0
5	B	1	Total C O 13 12 1	0	0

- Molecule 6 is water.

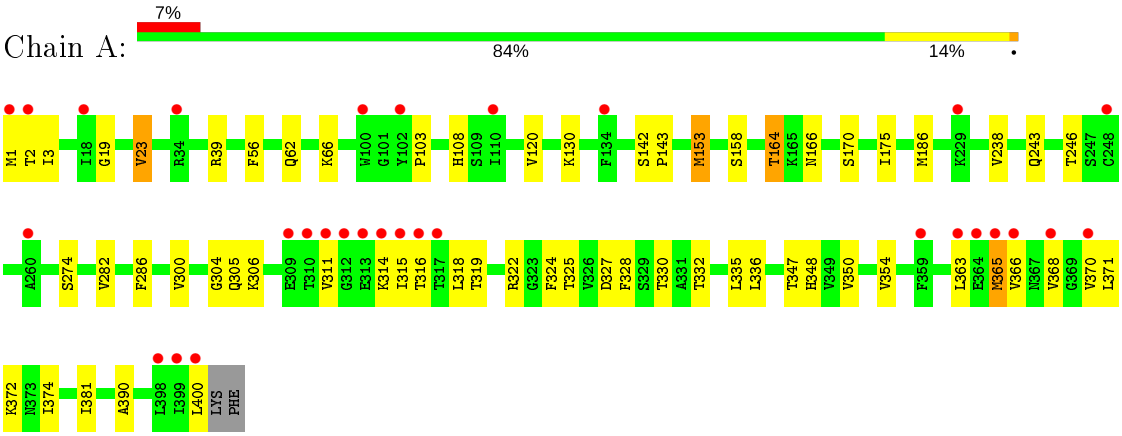
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	83	Total O 83 83	0	0
6	B	74	Total O 74 74	0	0

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.

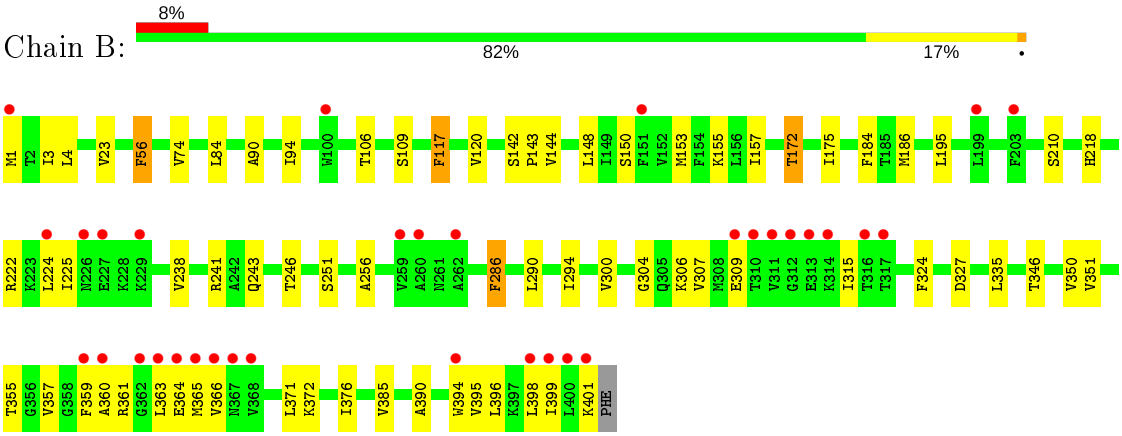
- Molecule 1: Phosphate transporter

Chain A:



- Molecule 1: Phosphate transporter

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	121.18Å 112.65Å 110.79Å 90.00° 119.36° 90.00°	Depositor
Resolution (Å)	29.40 – 2.30 29.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.40-2.30) 98.0 (29.40-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.188 , 0.224 0.188 , 0.224	Depositor DCC
R_{free} test set	2864 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	43.5	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 71.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6300	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PO4, PEG, 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	0.43	0/3053	0.58	0/4158
1	B	0.43	0/3062	0.59	0/4169
All	All	0.43	0/6115	0.58	0/8327

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	365	MET	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2991	0	3169	57	0
1	B	3000	0	3183	62	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	49	0	70	1	0
4	B	28	0	40	1	0
5	A	46	0	68	2	0
5	B	13	0	25	0	0
6	A	83	0	0	4	0
6	B	74	0	0	2	0
All	All	6300	0	6555	120	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 9.

All (120) 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:B:395:VAL:O	1:B:399:ILE:HD12	1.44	1.16
1:A:314:LYS:HE2	1:A:347:THR:HG23	1.39	1.05
1:A:103:PRO:HB3	1:A:314:LYS:HE3	1.52	0.90
1:A:315:ILE:HG23	1:A:354:VAL:HG21	1.56	0.86
1:A:243:GLN:HA	1:A:246:THR:HG22	1.59	0.85
1:B:359:PHE:HB2	1:B:361:ARG:HB2	1.60	0.82
1:B:395:VAL:O	1:B:399:ILE:CD1	2.26	0.81
1:B:361:ARG:HB3	1:B:363:LEU:HD13	1.63	0.79
1:A:314:LYS:CE	1:A:347:THR:HG23	2.12	0.78
1:B:243:GLN:HA	1:B:246:THR:HG22	1.66	0.78
1:B:363:LEU:HA	1:B:364:GLU:C	2.05	0.77
1:B:315:ILE:HA	1:B:361:ARG:HH12	1.50	0.76
1:A:315:ILE:HD12	1:A:354:VAL:CG2	2.17	0.75
1:A:23:VAL:HG11	1:A:300:VAL:HG13	1.69	0.74
1:B:359:PHE:HA	1:B:361:ARG:HD2	1.70	0.74
1:B:224:LEU:HD21	1:B:241:ARG:HG3	1.71	0.73
4:A:507:PEG:H21	4:B:508:PEG:H32	1.71	0.71
1:B:395:VAL:HG13	1:B:399:ILE:HD11	1.71	0.71
1:B:144:VAL:O	1:B:148:LEU:HG	1.93	0.69
1:B:120:VAL:HG21	1:B:390:ALA:HB1	1.75	0.68
1:B:175:ILE:HD12	1:B:238:VAL:HG12	1.75	0.67
1:A:315:ILE:HD12	1:A:354:VAL:HG23	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:VAL:O	1:B:355:THR:HG23	1.97	0.64
1:A:1:MET:SD	1:A:2:THR:N	2.71	0.63
1:A:23:VAL:HG13	1:A:300:VAL:HG22	1.80	0.63
1:B:246:THR:HG21	1:B:324:PHE:HA	1.81	0.61
1:A:365:MET:SD	1:A:366:VAL:HA	2.41	0.59
1:A:1:MET:HG3	1:A:3:ILE:HG22	1.84	0.59
1:B:184:PHE:HB2	1:B:210:SER:OG	2.02	0.59
1:A:314:LYS:HE2	1:A:347:THR:CG2	2.24	0.59
1:A:366:VAL:HG11	1:A:371:LEU:HD22	1.85	0.58
1:A:246:THR:HG21	1:A:324:PHE:HA	1.86	0.58
1:B:90:ALA:O	1:B:94:ILE:HG12	2.04	0.57
1:B:23:VAL:HB	1:B:300:VAL:HG22	1.86	0.57
1:B:74:VAL:HG11	1:B:117:PHE:HZ	1.69	0.57
1:B:218:HIS:NE2	1:B:222:ARG:HD2	2.22	0.55
1:A:39:ARG:HA	1:A:305:GLN:OE1	2.06	0.55
1:B:394:TRP:CZ2	1:B:398:LEU:HD11	2.42	0.54
1:B:364:GLU:HG2	1:B:365:MET:H	1.73	0.54
1:B:365:MET:HA	1:B:366:VAL:C	2.29	0.53
1:A:315:ILE:HD12	1:A:354:VAL:HG21	1.90	0.53
1:B:372:LYS:O	1:B:376:ILE:HG12	2.09	0.53
1:A:319:THR:OG1	1:A:322:ARG:HG3	2.09	0.52
1:A:305:GLN:HG2	1:A:306:LYS:HE3	1.92	0.52
1:B:366:VAL:HG21	1:B:371:LEU:HD13	1.91	0.51
1:B:94:ILE:HD12	1:B:106:THR:HG22	1.93	0.51
1:B:290:LEU:O	1:B:294:ILE:HG12	2.10	0.51
1:A:66:LYS:HE3	1:A:282:VAL:HG23	1.93	0.50
1:B:243:GLN:CA	1:B:246:THR:HG22	2.39	0.50
1:A:243:GLN:HA	1:A:246:THR:CG2	2.37	0.50
1:A:120:VAL:HG21	1:A:390:ALA:HB1	1.92	0.50
1:B:309:GLU:HG2	6:B:602:HOH:O	2.11	0.50
1:A:304:GLY:O	1:A:305:GLN:HB3	2.11	0.49
1:A:164:THR:HG23	1:A:166:ASN:H	1.76	0.49
1:B:172:THR:HG23	1:B:218:HIS:CE1	2.47	0.49
1:B:307:VAL:HG13	6:B:623:HOH:O	2.12	0.49
1:B:366:VAL:HG23	1:B:371:LEU:HD22	1.94	0.49
1:B:1:MET:HG2	1:B:4:LEU:HD12	1.94	0.48
1:A:23:VAL:CG1	1:A:300:VAL:HG13	2.40	0.48
1:A:243:GLN:CA	1:A:246:THR:HG22	2.38	0.48
1:B:150:SER:OG	1:B:357:VAL:HG13	2.14	0.48
1:A:246:THR:HG23	1:A:327:ASP:OD2	2.13	0.48
1:A:318:LEU:HB3	1:A:322:ARG:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:VAL:CG1	1:A:372:LYS:HE3	2.44	0.48
1:B:360:ALA:HB3	1:B:361:ARG:HA	1.95	0.47
1:A:19:GLY:O	1:A:23:VAL:HG22	2.15	0.47
1:B:243:GLN:HA	1:B:246:THR:CG2	2.40	0.47
1:A:1:MET:HG3	1:A:3:ILE:H	1.79	0.47
1:B:399:ILE:HD12	1:B:399:ILE:H	1.80	0.46
1:A:175:ILE:HD12	1:A:238:VAL:HG12	1.97	0.46
1:B:364:GLU:HG2	1:B:365:MET:N	2.30	0.46
1:B:246:THR:HG23	1:B:327:ASP:HB2	1.97	0.46
1:B:346:THR:O	1:B:350:VAL:HG23	2.15	0.46
1:B:395:VAL:HG13	1:B:399:ILE:CD1	2.43	0.46
1:B:225:ILE:HD13	1:B:238:VAL:HG21	1.96	0.46
1:B:394:TRP:CH2	1:B:398:LEU:HD11	2.51	0.45
1:A:370:VAL:O	1:A:374:ILE:HG12	2.16	0.45
1:B:94:ILE:HD11	1:B:106:THR:HA	1.98	0.45
1:A:186:MET:HG2	1:A:335:LEU:HD11	1.98	0.45
1:A:103:PRO:CB	1:A:314:LYS:HE3	2.35	0.45
1:A:120:VAL:CG2	1:A:390:ALA:HB1	2.47	0.45
1:B:363:LEU:HA	1:B:365:MET:N	2.31	0.45
1:A:142:SER:OG	1:A:143:PRO:HD3	2.17	0.45
1:B:246:THR:HG23	1:B:327:ASP:CB	2.46	0.45
1:B:153:MET:O	1:B:157:ILE:HG12	2.17	0.45
5:A:512:LMT:H12	1:B:195:LEU:HD13	1.99	0.45
1:A:330:THR:HG21	1:A:350:VAL:HG13	1.99	0.44
1:A:311:VAL:HG22	1:A:316:THR:HG21	1.99	0.44
1:A:368:VAL:HG12	1:A:372:LYS:HE3	2.00	0.44
1:A:314:LYS:CE	1:A:347:THR:CG2	2.91	0.44
5:A:513:LMT:H22	1:B:286:PHE:CZ	2.53	0.44
1:A:400:LEU:HG	6:A:643:HOH:O	2.18	0.44
1:A:153:MET:HE3	1:A:325:THR:HG23	1.99	0.43
1:A:103:PRO:HB3	1:A:314:LYS:CE	2.37	0.43
1:A:246:THR:HG23	1:A:327:ASP:CB	2.49	0.43
1:B:304:GLY:C	1:B:306:LYS:H	2.21	0.43
1:A:315:ILE:HG22	1:A:318:LEU:HD11	2.00	0.43
1:A:363:LEU:HD23	1:A:363:LEU:HA	1.89	0.43
1:B:142:SER:HB2	1:B:143:PRO:HD3	2.01	0.43
1:B:3:ILE:HD11	1:B:84:LEU:HD11	2.00	0.43
1:A:348:HIS:HD2	6:A:618:HOH:O	2.01	0.43
1:A:246:THR:HG23	1:A:327:ASP:HB2	2.01	0.42
1:A:62:GLN:NE2	6:A:606:HOH:O	2.52	0.42
1:B:224:LEU:HB3	1:B:238:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:LEU:O	1:B:401:LYS:N	2.52	0.42
1:B:395:VAL:CG1	1:B:399:ILE:HD11	2.47	0.42
1:A:332:THR:O	1:A:336:LEU:HG	2.19	0.42
1:B:396:LEU:HA	1:B:396:LEU:HD12	1.89	0.42
1:B:395:VAL:CG1	1:B:399:ILE:CD1	2.98	0.42
1:B:56:PHE:HB3	1:B:256:ALA:HB1	2.02	0.42
1:B:225:ILE:HA	1:B:225:ILE:HD12	1.90	0.42
1:A:381:ILE:HB	6:A:637:HOH:O	2.21	0.41
1:A:66:LYS:HG3	1:A:282:VAL:HG21	2.03	0.41
1:A:164:THR:HG21	1:A:170:SER:OG	2.21	0.41
1:B:186:MET:HG2	1:B:335:LEU:HD11	2.03	0.41
1:A:66:LYS:HE3	1:A:282:VAL:CG2	2.51	0.41
1:A:153:MET:HE1	1:A:328:PHE:HB3	2.03	0.40
1:A:315:ILE:HD11	1:A:350:VAL:HB	2.04	0.40
1:B:109:SER:O	1:B:385:VAL:HG11	2.20	0.40
1:B:360:ALA:H	1:B:361:ARG:HE	1.70	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	398/402 (99%)	385 (97%)	13 (3%)	0	100	100
1	B	399/402 (99%)	383 (96%)	16 (4%)	0	100	100
All	All	797/804 (99%)	768 (96%)	29 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	326/328 (99%)	317 (97%)	9 (3%)	43 60
1	B	327/328 (100%)	321 (98%)	6 (2%)	59 75
All	All	653/656 (100%)	638 (98%)	15 (2%)	50 67

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	56	PHE
1	A	108	HIS
1	A	130	LYS
1	A	153	MET
1	A	158	SER
1	A	164	THR
1	A	274	SER
1	A	286	PHE
1	B	56	PHE
1	B	117	PHE
1	B	155	LYS
1	B	172	THR
1	B	251	SER
1	B	286	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	108	HIS

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 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
4	PEG	B	508	-	6,6,6	0.73	0	5,5,5	0.27	0
2	PO4	A	501	-	4,4,4	2.30	2 (50%)	6,6,6	1.18	1 (16%)
4	PEG	A	509	-	6,6,6	0.69	0	5,5,5	0.31	0
4	PEG	B	505	-	6,6,6	0.76	0	5,5,5	0.52	0
5	LMT	B	509	-	12,12,36	0.76	0	11,11,47	0.88	0
4	PEG	A	507	-	6,6,6	0.68	0	5,5,5	0.48	0
4	PEG	A	510	-	6,6,6	0.72	0	5,5,5	0.36	0
2	PO4	B	501	-	4,4,4	0.82	0	6,6,6	0.64	0
5	LMT	A	512	-	23,23,36	0.80	1 (4%)	26,27,47	1.07	0
4	PEG	A	506	-	6,6,6	0.79	0	5,5,5	0.25	0
4	PEG	A	505	-	6,6,6	0.67	0	5,5,5	0.34	0
4	PEG	B	507	-	6,6,6	0.62	0	5,5,5	0.45	0
5	LMT	A	513	-	23,23,36	0.73	1 (4%)	26,27,47	1.57	2 (7%)
4	PEG	A	508	-	6,6,6	0.68	0	5,5,5	0.33	0
4	PEG	A	511	-	6,6,6	0.62	0	5,5,5	0.30	0
4	PEG	B	506	-	6,6,6	0.70	0	5,5,5	0.23	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
4	PEG	B	508	-	-	1/4/4/4	-
4	PEG	A	509	-	-	2/4/4/4	-
4	PEG	B	505	-	-	2/4/4/4	-
5	LMT	B	509	-	-	4/10/10/61	-
4	PEG	A	510	-	-	2/4/4/4	-
4	PEG	A	507	-	-	2/4/4/4	-
5	LMT	A	512	-	-	10/15/31/61	0/1/1/2
4	PEG	A	506	-	-	2/4/4/4	-
4	PEG	A	505	-	-	2/4/4/4	-
4	PEG	B	507	-	-	3/4/4/4	-
5	LMT	A	513	-	-	6/15/31/61	0/1/1/2
4	PEG	A	508	-	-	3/4/4/4	-
4	PEG	A	511	-	-	3/4/4/4	-
4	PEG	B	506	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PO4	P-O4	-3.20	1.45	1.54
5	A	512	LMT	O1'-C1'	2.47	1.44	1.40
2	A	501	PO4	P-O2	-2.47	1.47	1.54
5	A	513	LMT	O1'-C1'	2.18	1.43	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	513	LMT	C1'-O5'-C5'	-4.62	108.01	113.13
5	A	513	LMT	O5'-C5'-C6'	2.89	111.46	106.83
2	A	501	PO4	O4-P-O2	-2.05	101.39	107.97

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	512	LMT	C2'-C1'-O1'-C1
5	A	512	LMT	O5'-C1'-O1'-C1
5	A	512	LMT	C4'-C5'-C6'-O6'
5	A	512	LMT	O5'-C5'-C6'-O6'
5	A	513	LMT	C2'-C1'-O1'-C1

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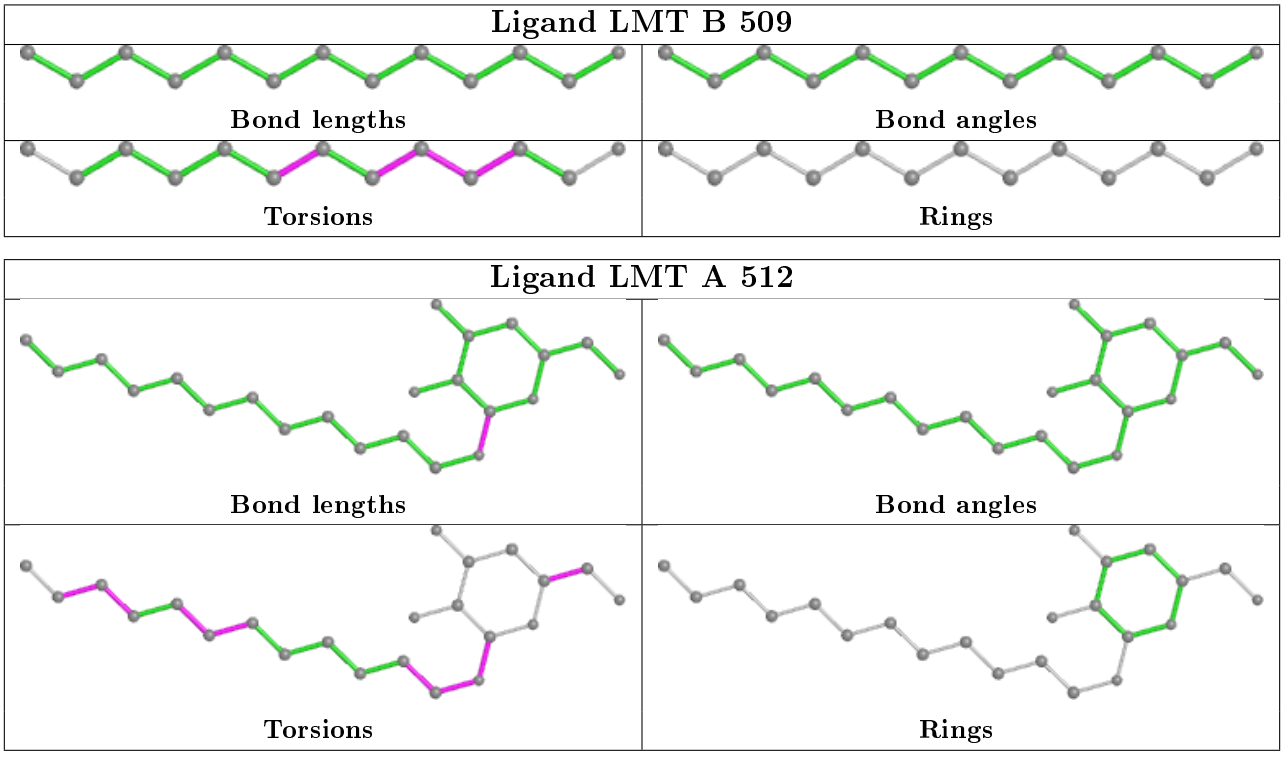
Mol	Chain	Res	Type	Atoms
5	A	513	LMT	O5'-C1'-O1'-C1
4	A	510	PEG	C4-C3-O2-C2
5	B	509	LMT	C2-C3-C4-C5
4	B	505	PEG	O2-C3-C4-O4
4	A	509	PEG	O2-C3-C4-O4
5	A	512	LMT	O1'-C1-C2-C3
5	A	513	LMT	O1'-C1-C2-C3
4	A	505	PEG	O1-C1-C2-O2
4	B	506	PEG	O2-C3-C4-O4
4	A	511	PEG	O2-C3-C4-O4
5	A	512	LMT	C6-C7-C8-C9
4	A	506	PEG	O1-C1-C2-O2
4	B	507	PEG	O1-C1-C2-O2
4	B	507	PEG	O2-C3-C4-O4
5	A	513	LMT	C7-C8-C9-C10
5	A	512	LMT	C11-C10-C9-C8
4	B	505	PEG	O1-C1-C2-O2
4	A	508	PEG	C4-C3-O2-C2
5	A	512	LMT	C2-C1-O1'-C1'
4	A	510	PEG	O1-C1-C2-O2
4	B	507	PEG	C4-C3-O2-C2
4	A	511	PEG	C1-C2-O2-C3
4	A	511	PEG	C4-C3-O2-C2
5	B	509	LMT	C5-C6-C7-C8
5	A	512	LMT	C9-C10-C11-C12
4	B	506	PEG	O1-C1-C2-O2
4	A	507	PEG	C1-C2-O2-C3
4	B	508	PEG	O2-C3-C4-O4
4	A	506	PEG	C1-C2-O2-C3
5	A	513	LMT	C5-C6-C7-C8
4	A	508	PEG	C1-C2-O2-C3
4	A	508	PEG	O1-C1-C2-O2
4	A	507	PEG	O2-C3-C4-O4
5	A	513	LMT	C3-C4-C5-C6
5	B	509	LMT	C1-C2-C3-C4
4	A	509	PEG	C4-C3-O2-C2
4	A	505	PEG	C1-C2-O2-C3
5	B	509	LMT	C3-C4-C5-C6
5	A	512	LMT	C5-C6-C7-C8

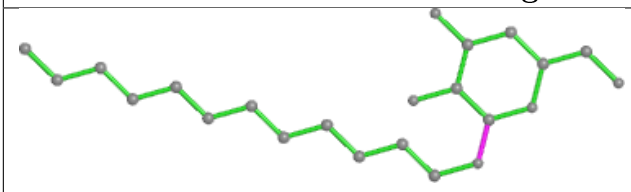
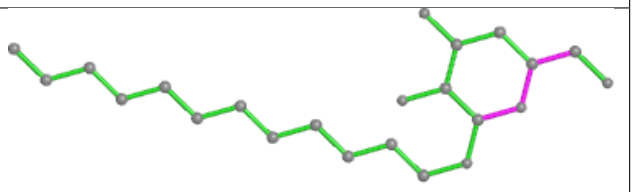
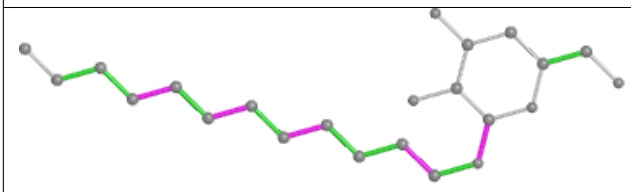
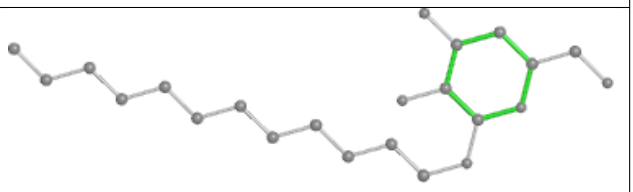
There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	508	PEG	1	0
4	A	507	PEG	1	0
5	A	512	LMT	1	0
5	A	513	LMT	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 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	400/402 (99%)	0.26	30 (7%)	14	19	32, 49, 75, 93	0
1	B	401/402 (99%)	0.19	34 (8%)	10	14	31, 46, 74, 93	0
All	All	801/804 (99%)	0.23	64 (7%)	12	16	31, 48, 74, 93	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	GLY	10.2
1	A	400	LEU	9.3
1	A	316	THR	8.3
1	A	310	THR	8.0
1	A	315	ILE	8.0
1	B	363	LEU	6.6
1	A	311	VAL	6.0
1	B	364	GLU	5.4
1	B	359	PHE	5.4
1	A	399	ILE	5.3
1	B	362	GLY	5.1
1	B	400	LEU	4.8
1	B	311	VAL	4.8
1	A	365	MET	4.7
1	B	365	MET	4.4
1	B	360	ALA	3.9
1	B	399	ILE	3.9
1	A	363	LEU	3.8
1	B	312	GLY	3.7
1	B	401	LYS	3.7
1	A	314	LYS	3.6
1	A	2	THR	3.5
1	B	317	THR	3.5
1	A	309	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	34	ARG	3.2
1	A	366	VAL	3.2
1	A	100	TRP	3.1
1	B	366	VAL	3.1
1	A	229	LYS	3.1
1	A	134	PHE	3.1
1	A	359	PHE	2.9
1	B	310	THR	2.8
1	B	227	GLU	2.8
1	A	368	VAL	2.8
1	B	259	VAL	2.8
1	A	18	ILE	2.8
1	A	317	THR	2.7
1	A	398	LEU	2.7
1	B	367	ASN	2.6
1	B	394	TRP	2.6
1	A	260	ALA	2.5
1	B	100	TRP	2.5
1	B	260	ALA	2.5
1	A	102	TYR	2.4
1	B	1	MET	2.4
1	A	370	VAL	2.4
1	B	368	VAL	2.4
1	B	224	LEU	2.3
1	B	229	LYS	2.3
1	B	398	LEU	2.3
1	B	316	THR	2.3
1	B	203	PHE	2.2
1	B	199	LEU	2.2
1	A	364	GLU	2.2
1	B	262	ALA	2.2
1	B	314	LYS	2.1
1	B	313	GLU	2.1
1	B	151	PHE	2.1
1	A	1	MET	2.1
1	A	313	GLU	2.1
1	B	309	GLU	2.1
1	B	226	ASN	2.0
1	A	248	CYS	2.0
1	A	110	ILE	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)

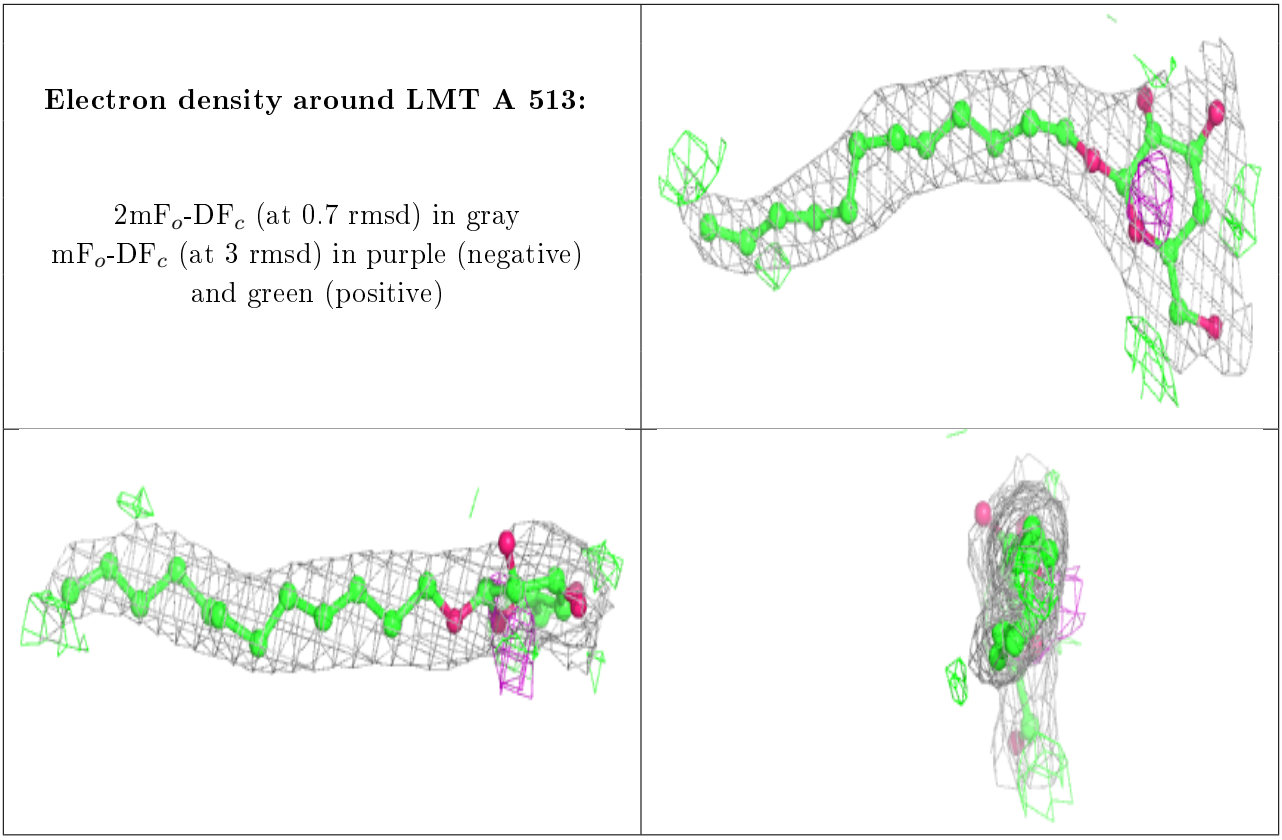
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	PEG	B	506	7/7	0.70	0.26	72,74,78,78	0
4	PEG	B	508	7/7	0.73	0.22	63,67,74,76	0
5	LMT	A	513	23/35	0.75	0.22	45,63,76,84	0
4	PEG	B	505	7/7	0.76	0.17	63,66,68,73	0
4	PEG	A	506	7/7	0.78	0.23	55,57,65,66	0
5	LMT	A	512	23/35	0.79	0.21	45,61,78,82	0
4	PEG	B	507	7/7	0.80	0.22	65,68,74,74	0
4	PEG	A	509	7/7	0.80	0.17	72,73,76,78	0
4	PEG	A	510	7/7	0.82	0.20	61,67,79,80	0
4	PEG	A	508	7/7	0.84	0.20	67,72,75,80	0
5	LMT	B	509	13/35	0.85	0.17	56,60,68,69	0
4	PEG	A	511	7/7	0.85	0.30	58,64,71,81	0
4	PEG	A	507	7/7	0.86	0.11	61,68,71,74	0
4	PEG	A	505	7/7	0.92	0.11	65,66,72,77	0
3	NA	A	504	1/1	0.96	0.08	50,50,50,50	0
3	NA	B	502	1/1	0.97	0.12	38,38,38,38	0
3	NA	A	502	1/1	0.98	0.13	46,46,46,46	0
3	NA	B	503	1/1	0.98	0.16	34,34,34,34	0
3	NA	B	504	1/1	0.98	0.06	51,51,51,51	0
2	PO4	B	501	5/5	0.99	0.16	33,34,37,38	0
3	NA	A	503	1/1	0.99	0.21	36,36,36,36	0
2	PO4	A	501	5/5	0.99	0.23	33,33,44,53	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.

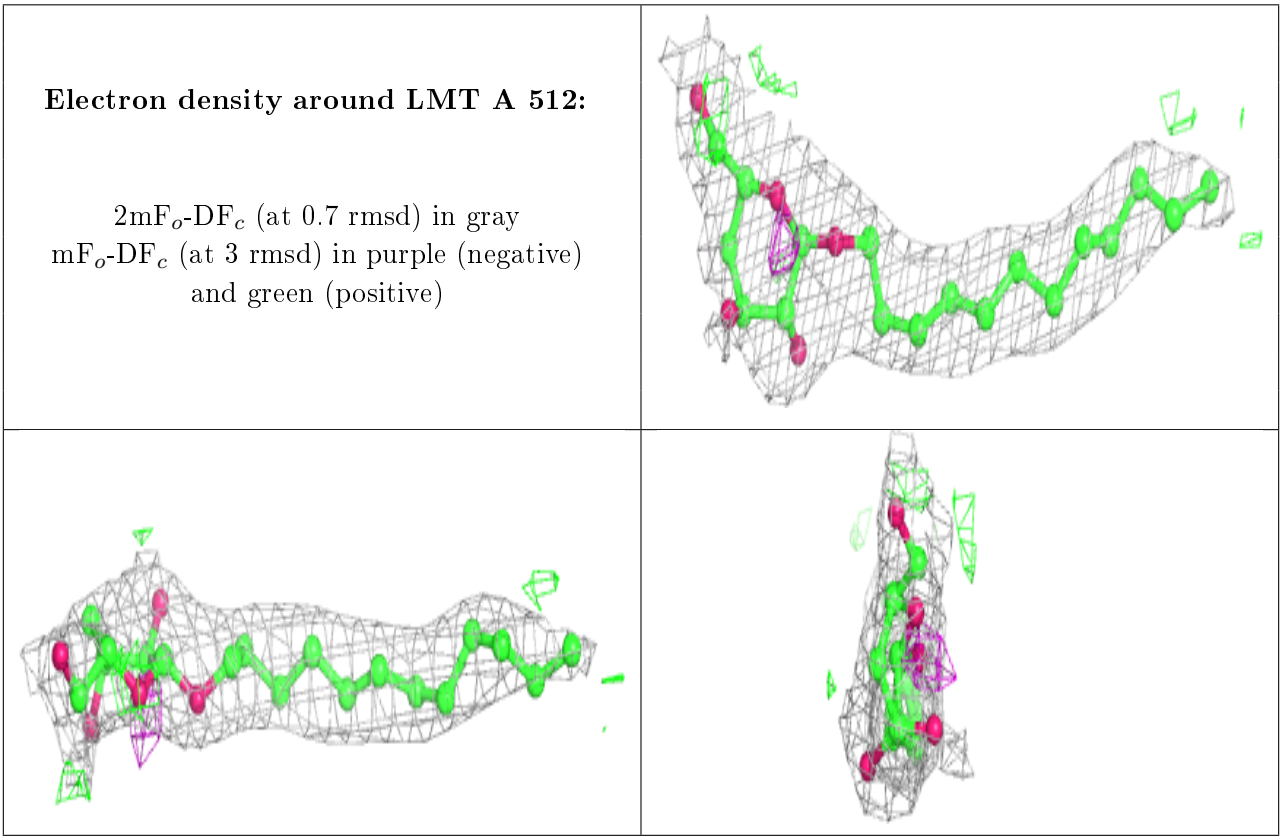
Electron density around LMT A 513:

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



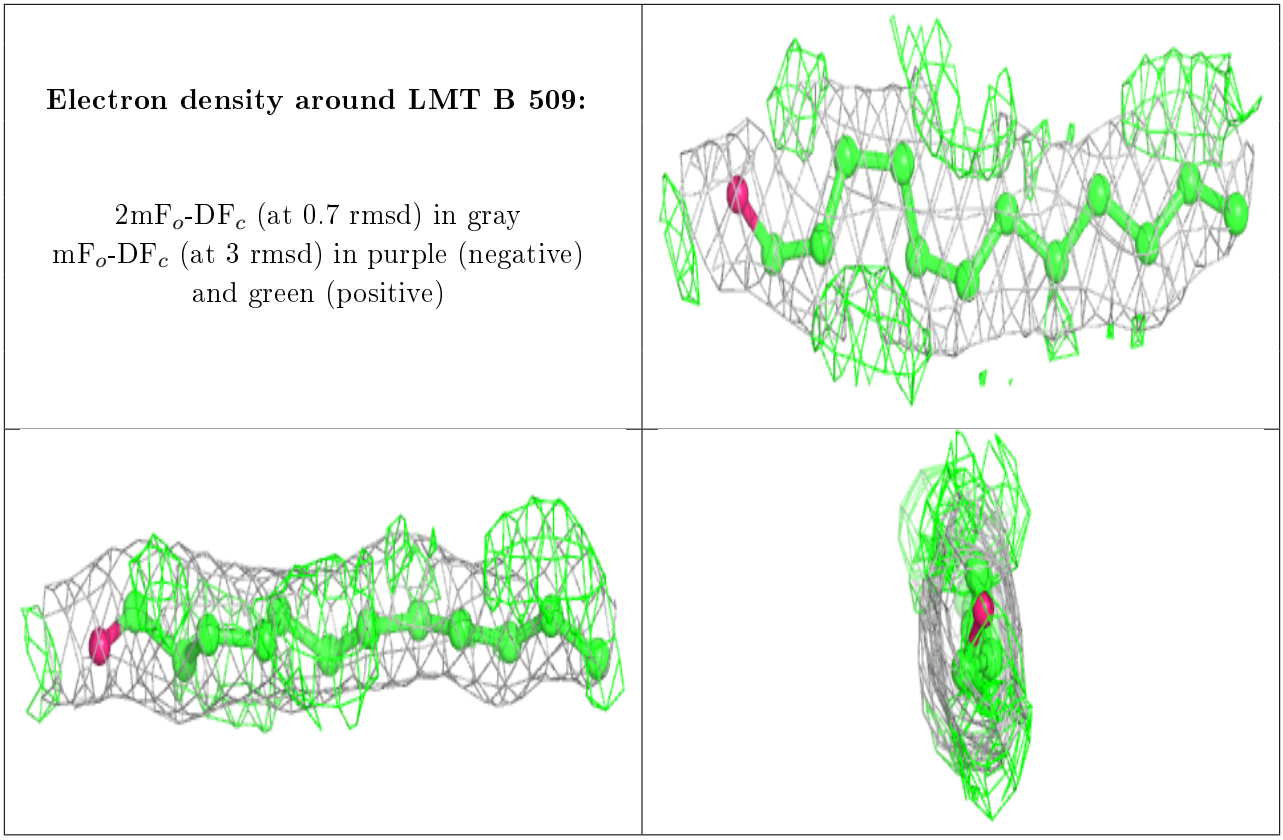
Electron density around LMT A 512:

$2mF_o$-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 509:

$2mF_o$-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

There are no such residues in this entry.