



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:41 am BST

PDB ID : 6AJH
Title : Crystal structure of mycolic acid transporter MmpL3 from Mycobacterium smegmatis complexed with AU1235
Authors : Zhang, B.; Li, J.; Yang, X.L.; Wu, L.J.; Yang, H.T.; Rao, Z.H.
Deposited on : 2018-08-27
Resolution : 2.82 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 : 2.11
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) : 2.11

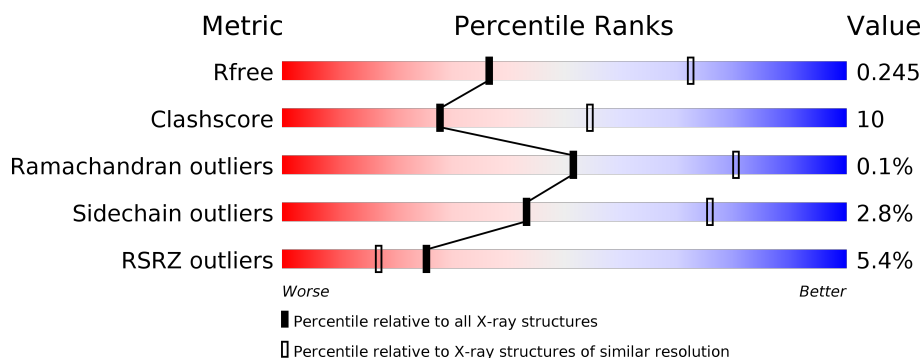
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	943	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7189 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 Drug exporters of the RND superfamily-like protein, Endolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	900	Total	C	N	O	S	0	0	0
			6952	4482	1182	1256	32			

There are 37 discrepancies between the modelled and reference sequences:

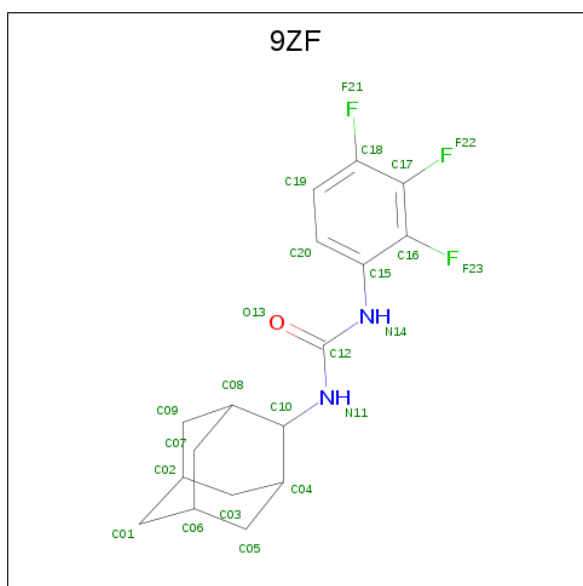
Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	expression tag	UNP I7G2R2
A	-11	PRO	-	expression tag	UNP I7G2R2
A	-10	GLU	-	expression tag	UNP I7G2R2
A	-9	VAL	-	expression tag	UNP I7G2R2
A	-8	VAL	-	expression tag	UNP I7G2R2
A	-7	GLY	-	expression tag	UNP I7G2R2
A	-6	SER	-	expression tag	UNP I7G2R2
A	-5	TYR	-	expression tag	UNP I7G2R2
A	-4	PHE	-	expression tag	UNP I7G2R2
A	-3	GLN	-	expression tag	UNP I7G2R2
A	-2	SER	-	expression tag	UNP I7G2R2
A	-1	ASN	-	expression tag	UNP I7G2R2
A	0	ALA	-	expression tag	UNP I7G2R2
A	749	GLU	-	linker	UNP I7G2R2
A	750	PHE	-	linker	UNP I7G2R2
A	803	THR	CYS	engineered mutation	UNP D9IEF7
A	846	ALA	CYS	engineered mutation	UNP D9IEF7
A	911	GLU	-	expression tag	UNP D9IEF7
A	912	PHE	-	expression tag	UNP D9IEF7
A	913	HIS	-	expression tag	UNP D9IEF7
A	914	LEU	-	expression tag	UNP D9IEF7
A	915	GLY	-	expression tag	UNP D9IEF7
A	916	GLY	-	expression tag	UNP D9IEF7
A	917	ILE	-	expression tag	UNP D9IEF7
A	918	LYS	-	expression tag	UNP D9IEF7
A	919	ALA	-	expression tag	UNP D9IEF7
A	920	PHE	-	expression tag	UNP D9IEF7

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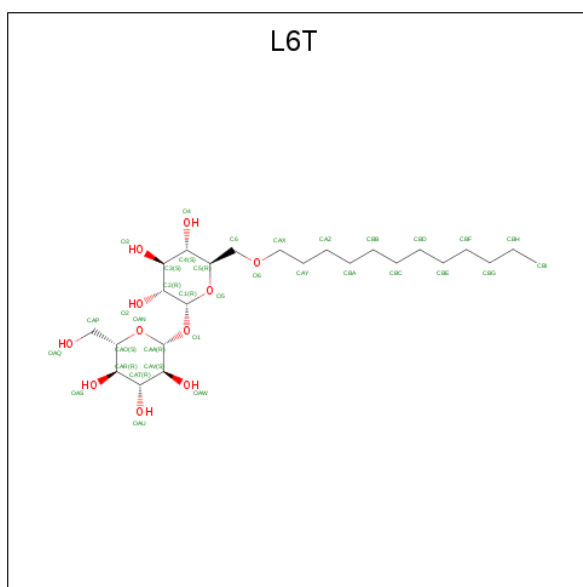
Chain	Residue	Modelled	Actual	Comment	Reference
A	921	HIS	-	expression tag	UNP D9IEF7
A	922	HIS	-	expression tag	UNP D9IEF7
A	923	HIS	-	expression tag	UNP D9IEF7
A	924	HIS	-	expression tag	UNP D9IEF7
A	925	HIS	-	expression tag	UNP D9IEF7
A	926	HIS	-	expression tag	UNP D9IEF7
A	927	HIS	-	expression tag	UNP D9IEF7
A	928	HIS	-	expression tag	UNP D9IEF7
A	929	HIS	-	expression tag	UNP D9IEF7
A	930	HIS	-	expression tag	UNP D9IEF7

- Molecule 2 is 1-(2-adamantyl)-3-[2,3,4-tris(fluoranyl)phenyl]urea (three-letter code: 9ZF) (formula: C₁₇H₁₉F₃N₂O).



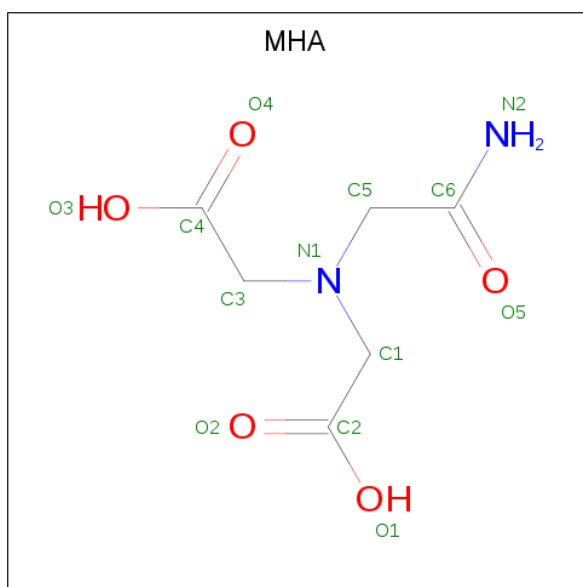
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			23	17	3	2	1		

- Molecule 3 is alpha-D-glucopyranosyl 6-O-dodecyl-alpha-D-glucopyranoside (three-letter code: L6T) (formula: C₂₄H₄₆O₁₁).



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

- Molecule 4 is (CARBAMOYLMETHYL-CARBOXYMETHYL-AMINO)-ACETIC ACID (three-letter code: MHA) (formula: $C_6H_{10}N_2O_5$).

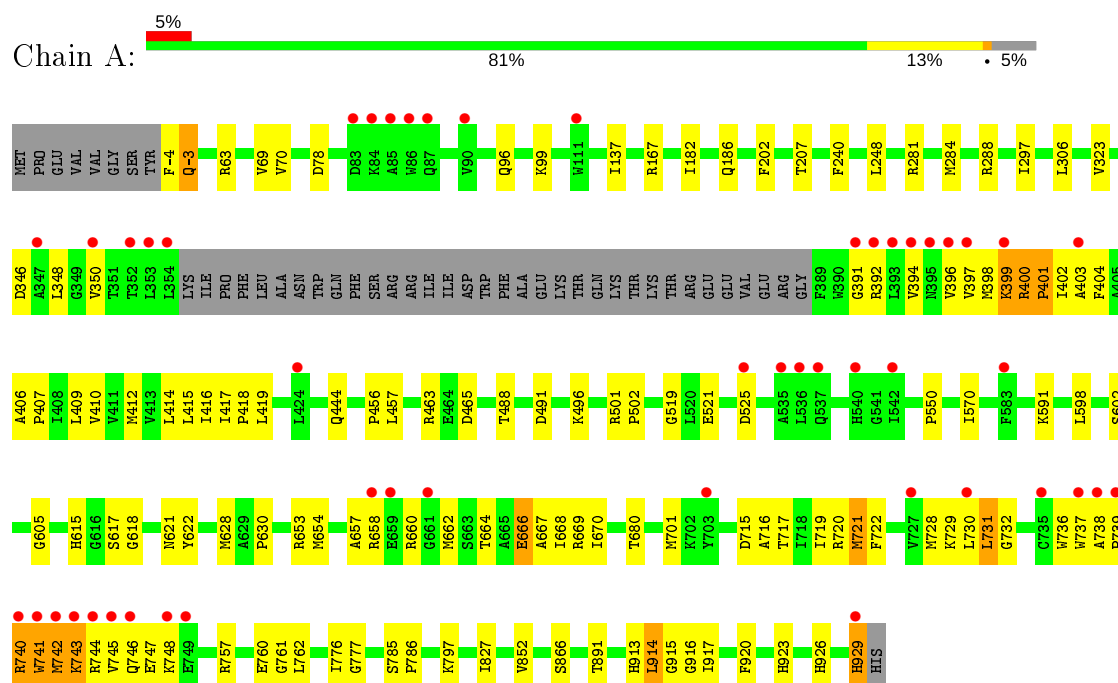


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			13	6	2	5		
4	A	1	Total	C	N	O	0	0
			13	6	2	5		
4	A	1	Total	C	N	O	0	0
			13	6	2	5		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Drug exporters of the RND superfamily-like protein, Endolysin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.97Å 141.17Å 144.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.48 – 2.82 45.51 – 2.82	Depositor EDS
% Data completeness (in resolution range)	98.7 (43.48-2.82) 98.7 (45.51-2.82)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.219 , 0.247 0.222 , 0.245	Depositor DCC
R_{free} test set	2118 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7189	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: L6T, 9ZF, MHA

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	0.29	0/7097	0.46	1/9642 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	916	GLY	N-CA-C	6.96	130.49	113.10

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	6952	0	7111	136	0
2	A	23	0	0	0	0
3	A	175	0	0	21	0
4	A	39	0	24	7	0
All	All	7189	0	7135	142	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 10.

All (142) 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:738:ALA:HB2	1:A:743:LYS:CD	1.23	1.66
1:A:738:ALA:CB	1:A:743:LYS:HD3	1.16	1.59
1:A:202:PHE:CE2	1:A:350:VAL:HG13	1.39	1.52
1:A:917:ILE:HD11	1:A:920:PHE:CE1	1.61	1.34
1:A:917:ILE:HD11	1:A:920:PHE:CD1	1.70	1.27
1:A:202:PHE:HE2	1:A:350:VAL:CG1	1.52	1.22
1:A:738:ALA:HB2	1:A:743:LYS:HD2	1.24	1.11
1:A:738:ALA:HB3	1:A:743:LYS:HD3	1.37	1.00
1:A:202:PHE:HZ	1:A:350:VAL:HA	1.26	0.99
1:A:738:ALA:CB	1:A:743:LYS:CD	2.03	0.96
1:A:202:PHE:CE2	1:A:350:VAL:CG1	2.36	0.95
1:A:917:ILE:CD1	1:A:920:PHE:CE1	2.52	0.93
1:A:202:PHE:CZ	1:A:350:VAL:HG13	2.09	0.87
1:A:202:PHE:CZ	1:A:350:VAL:HA	2.11	0.85
1:A:615:HIS:ND1	3:A:1005:L6T:CAP	2.40	0.84
1:A:653:ARG:NH2	3:A:1004:L6T:OAQ	2.11	0.84
1:A:399:LYS:HE3	1:A:400:ARG:HB2	1.57	0.83
1:A:917:ILE:CD1	1:A:920:PHE:CD1	2.59	0.82
1:A:207:THR:HG21	1:A:346:ASP:HA	1.63	0.80
1:A:398:MET:SD	1:A:729:LYS:NZ	2.54	0.80
3:A:1005:L6T:O2	4:A:1009:MHA:O5	1.99	0.79
1:A:738:ALA:HB1	1:A:743:LYS:HD3	1.57	0.77
1:A:797:LYS:HG2	1:A:929:HIS:CE1	2.19	0.77
1:A:406:ALA:HB3	1:A:407:PRO:HD3	1.67	0.75
1:A:621:ASN:OD1	3:A:1006:L6T:CAR	2.35	0.75
1:A:664:THR:HG1	1:A:736:TRP:HH2	1.33	0.74
1:A:664:THR:OG1	1:A:736:TRP:CH2	2.41	0.74
1:A:288:ARG:HB3	3:A:1004:L6T:OAW	1.88	0.74
1:A:240:PHE:HB3	3:A:1002:L6T:CBI	2.18	0.73
1:A:731:LEU:HD23	1:A:731:LEU:N	2.04	0.73
3:A:1005:L6T:CAO	4:A:1009:MHA:HC32	2.19	0.72
3:A:1005:L6T:C3	4:A:1009:MHA:O4	2.37	0.72
1:A:398:MET:HA	1:A:729:LYS:NZ	2.06	0.71
1:A:653:ARG:NH2	3:A:1004:L6T:CAP	2.54	0.71
1:A:657:ALA:HB3	1:A:667:ALA:HB1	1.73	0.70
1:A:615:HIS:CE1	3:A:1005:L6T:CAP	2.75	0.70
1:A:739:PRO:O	1:A:740:ARG:HG3	1.92	0.70
1:A:917:ILE:HD11	1:A:920:PHE:HE1	1.51	0.68
1:A:628:MET:HG3	1:A:630:PRO:HD2	1.74	0.68
1:A:202:PHE:HZ	1:A:350:VAL:CA	2.06	0.68
1:A:653:ARG:HH22	3:A:1004:L6T:CAP	2.05	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:PRO:O	1:A:742:MET:HB2	1.95	0.67
1:A:417:ILE:HG13	1:A:418:PRO:HD3	1.76	0.66
1:A:914:LEU:HD12	1:A:915:GLY:O	1.97	0.65
1:A:664:THR:OG1	1:A:736:TRP:CZ3	2.48	0.65
1:A:717:THR:O	1:A:721:MET:HG3	1.96	0.65
1:A:740:ARG:NH2	1:A:742:MET:SD	2.70	0.64
1:A:401:PRO:CG	1:A:730:LEU:HD11	2.28	0.64
1:A:914:LEU:C	1:A:914:LEU:HD12	2.17	0.64
1:A:618:GLY:N	4:A:1009:MHA:O3	2.24	0.63
1:A:240:PHE:CB	3:A:1002:L6T:CBI	2.76	0.62
1:A:406:ALA:N	1:A:407:PRO:CD	2.64	0.60
1:A:396:VAL:O	1:A:399:LYS:HG3	2.02	0.59
1:A:69:VAL:HB	1:A:137:ILE:HB	1.85	0.59
1:A:297:ILE:HG21	1:A:323:VAL:HG21	1.85	0.58
1:A:306:LEU:HD11	1:A:570:ILE:HD12	1.85	0.58
1:A:591:LYS:HE3	1:A:728:MET:HG3	1.84	0.58
1:A:653:ARG:NH1	3:A:1004:L6T:OAQ	2.36	0.58
1:A:491:ASP:OD2	1:A:496:LYS:NZ	2.33	0.58
1:A:746:GLN:H	1:A:746:GLN:CD	2.08	0.57
1:A:917:ILE:O	1:A:917:ILE:HG13	2.03	0.57
1:A:657:ALA:HB3	1:A:667:ALA:CB	2.35	0.57
1:A:396:VAL:O	1:A:399:LYS:CG	2.54	0.56
1:A:744:ARG:HG2	1:A:745:VAL:O	2.06	0.56
1:A:96:GLN:HG2	1:A:99:LYS:HZ1	1.71	0.56
1:A:410:VAL:O	1:A:414:LEU:HD22	2.07	0.55
1:A:488:THR:HG22	1:A:521:GLU:HG3	1.88	0.55
1:A:729:LYS:O	1:A:732:GLY:HA2	2.07	0.54
1:A:738:ALA:HB1	1:A:743:LYS:HB2	1.88	0.54
1:A:414:LEU:O	1:A:417:ILE:HG13	2.07	0.54
4:A:1009:MHA:O3	4:A:1009:MHA:HC52	2.05	0.54
1:A:664:THR:OG1	1:A:736:TRP:HH2	1.85	0.54
1:A:739:PRO:C	1:A:740:ARG:CG	2.76	0.54
1:A:716:ALA:O	1:A:720:ARG:NH2	2.41	0.54
3:A:1004:L6T:C6	3:A:1004:L6T:C2	2.86	0.53
1:A:797:LYS:HG2	1:A:929:HIS:HE1	1.73	0.53
1:A:167:ARG:NH1	1:A:444:GLN:OE1	2.43	0.52
1:A:653:ARG:CZ	3:A:1004:L6T:OAQ	2.58	0.52
1:A:415:LEU:O	1:A:605:GLY:HA3	2.09	0.52
1:A:394:VAL:O	1:A:398:MET:HG2	2.10	0.52
3:A:1004:L6T:CAV	3:A:1004:L6T:CAP	2.86	0.52
1:A:717:THR:O	1:A:721:MET:CG	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ARG:HA	1:A:284:MET:HE2	1.91	0.51
1:A:598:LEU:O	1:A:602:SER:OG	2.25	0.50
1:A:401:PRO:CB	1:A:730:LEU:HD11	2.41	0.50
1:A:757:ARG:HG3	1:A:762:LEU:HB2	1.94	0.50
1:A:721:MET:HB2	1:A:722:PHE:CE2	2.47	0.49
1:A:721:MET:HB2	1:A:722:PHE:CD2	2.47	0.49
1:A:412:MET:O	1:A:416:ILE:HG13	2.12	0.49
1:A:731:LEU:N	1:A:731:LEU:CD2	2.73	0.49
1:A:654:MET:SD	1:A:668:ILE:HA	2.53	0.48
1:A:391:GLY:HA2	1:A:394:VAL:HG12	1.95	0.47
1:A:914:LEU:HG	1:A:914:LEU:O	2.14	0.47
1:A:737:TRP:CD2	1:A:739:PRO:HD3	2.50	0.47
1:A:653:ARG:CZ	3:A:1004:L6T:CAP	2.92	0.47
1:A:398:MET:HA	1:A:729:LYS:HZ2	1.76	0.47
1:A:913:HIS:CE1	1:A:915:GLY:HA2	2.51	0.46
1:A:737:TRP:CH2	1:A:739:PRO:HG3	2.51	0.46
1:A:666:GLU:O	1:A:670:ILE:HG12	2.16	0.46
1:A:866:SER:OG	4:A:1008:MHA:N2	2.49	0.46
1:A:657:ALA:CB	1:A:667:ALA:CB	2.94	0.45
1:A:398:MET:HA	1:A:729:LYS:HZ1	1.79	0.45
1:A:729:LYS:O	1:A:732:GLY:CA	2.65	0.45
1:A:182:ILE:O	1:A:186:GLN:HG2	2.16	0.45
1:A:739:PRO:C	1:A:740:ARG:HG3	2.36	0.45
1:A:463:ARG:HG2	1:A:465:ASP:OD1	2.17	0.44
1:A:747:GLU:N	1:A:747:GLU:CD	2.69	0.44
1:A:621:ASN:OD1	3:A:1006:L6T:OAS	2.35	0.44
1:A:284:MET:O	1:A:288:ARG:HD3	2.18	0.44
1:A:653:ARG:NH1	3:A:1004:L6T:CAP	2.81	0.44
1:A:63:ARG:NH1	3:A:1002:L6T:OAW	2.51	0.43
1:A:917:ILE:CG1	1:A:920:PHE:CE1	3.01	0.43
1:A:664:THR:HG21	1:A:732:GLY:O	2.18	0.43
1:A:746:GLN:OE1	1:A:746:GLN:N	2.51	0.43
1:A:415:LEU:O	1:A:418:PRO:HD2	2.19	0.43
1:A:740:ARG:CZ	1:A:742:MET:SD	3.06	0.43
1:A:760:GLU:OE2	1:A:923:HIS:HB3	2.19	0.43
1:A:715:ASP:HA	1:A:719:ILE:HB	2.01	0.42
1:A:456:PRO:HA	1:A:519:GLY:HA2	2.01	0.42
1:A:501:ARG:HA	1:A:502:PRO:HD3	1.94	0.42
1:A:525:ASP:OD1	1:A:525:ASP:N	2.52	0.42
1:A:401:PRO:HG2	1:A:730:LEU:HD11	2.02	0.42
1:A:457:LEU:HD21	1:A:550:PRO:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:ARG:HB2	1:A:741:TRP:H	1.37	0.42
1:A:776:ILE:HG12	1:A:777:GLY:H	1.84	0.42
1:A:891:THR:HG22	4:A:1007:MHA:HC32	2.00	0.42
1:A:680:THR:HG23	1:A:720:ARG:HH12	1.84	0.42
1:A:419:LEU:HB2	1:A:605:GLY:HA2	2.01	0.41
1:A:746:GLN:N	1:A:746:GLN:CD	2.73	0.41
1:A:914:LEU:CD1	1:A:915:GLY:O	2.68	0.41
1:A:240:PHE:HB2	3:A:1002:L6T:CBI	2.50	0.41
1:A:403:ALA:O	1:A:407:PRO:HG2	2.20	0.41
1:A:397:VAL:HG13	1:A:404:PHE:CD2	2.56	0.41
1:A:926:HIS:ND1	1:A:926:HIS:O	2.53	0.41
1:A:761:GLY:HA3	1:A:920:PHE:CE1	2.55	0.41
1:A:617:SER:HA	1:A:622:TYR:CE2	2.55	0.41
1:A:827:ILE:HD11	1:A:852:VAL:HG21	2.03	0.41
1:A:207:THR:HG23	1:A:348:LEU:O	2.20	0.41
1:A:248:LEU:HD22	1:A:701:MET:HE1	2.03	0.41
1:A:785:SER:HA	1:A:786:PRO:HD3	1.84	0.41
1:A:-4:PHE:C	1:A:-3:GLN:HG3	2.40	0.41
1:A:392:ARG:O	1:A:396:VAL:HG23	2.21	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	896/943 (95%)	878 (98%)	17 (2%)	1 (0%)	51 80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	738/777 (95%)	717 (97%)	21 (3%)	43 76

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	GLN
1	A	70	VAL
1	A	78	ASP
1	A	399	LYS
1	A	400	ARG
1	A	402	ILE
1	A	409	LEU
1	A	658	ARG
1	A	660	ARG
1	A	662	MET
1	A	666	GLU
1	A	669	ARG
1	A	721	MET
1	A	731	LEU
1	A	740	ARG
1	A	741	TRP
1	A	742	MET
1	A	743	LYS
1	A	748	LYS
1	A	914	LEU
1	A	929	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-3	GLN
1	A	913	HIS
1	A	929	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	L6T	A	1005	-	36,36,36	1.43	6 (16%)	47,47,47	0.91	2 (4%)
2	9ZF	A	1001	-	26,26,26	1.81	3 (11%)	37,39,39	2.38	8 (21%)
3	L6T	A	1004	-	36,36,36	1.44	6 (16%)	47,47,47	0.84	1 (2%)
4	MHA	A	1007	-	6,12,12	1.65	1 (16%)	9,15,15	1.87	4 (44%)
4	MHA	A	1009	-	6,12,12	0.63	0	9,15,15	2.19	2 (22%)
3	L6T	A	1003	-	36,36,36	1.29	5 (13%)	47,47,47	1.41	8 (17%)
4	MHA	A	1008	-	6,12,12	1.66	1 (16%)	9,15,15	1.83	4 (44%)
3	L6T	A	1006	-	36,36,36	1.44	6 (16%)	47,47,47	0.81	0
3	L6T	A	1002	-	36,36,36	1.53	7 (19%)	47,47,47	1.02	3 (6%)

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	L6T	A	1005	-	-	13/20/60/60	0/2/2/2
2	9ZF	A	1001	-	-	0/8/36/36	0/5/4/4
3	L6T	A	1004	-	-	13/20/60/60	0/2/2/2
4	MHA	A	1007	-	-	3/8/12/12	-
4	MHA	A	1009	-	-	6/8/12/12	-
3	L6T	A	1003	-	-	12/20/60/60	0/2/2/2
4	MHA	A	1008	-	-	1/8/12/12	-
3	L6T	A	1006	-	-	8/20/60/60	0/2/2/2
3	L6T	A	1002	-	-	7/20/60/60	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	9ZF	C09-C08	-5.38	1.40	1.53
2	A	1001	9ZF	C12-N11	4.32	1.44	1.35
2	A	1001	9ZF	C12-N14	4.13	1.46	1.37
3	A	1004	L6T	OAN-CAO	3.99	1.54	1.44
3	A	1006	L6T	OAN-CAO	3.95	1.53	1.44
3	A	1005	L6T	OAN-CAO	3.95	1.53	1.44
3	A	1002	L6T	CAP-CAO	-3.75	1.39	1.51
3	A	1003	L6T	OAN-CAO	3.47	1.52	1.44
3	A	1002	L6T	CAV-CAT	-3.31	1.43	1.52
3	A	1004	L6T	CAP-CAO	-3.12	1.41	1.51
3	A	1006	L6T	CAP-CAO	-3.10	1.41	1.51
4	A	1008	MHA	C6-N2	3.09	1.42	1.32
3	A	1005	L6T	CAP-CAO	-3.09	1.41	1.51
4	A	1007	MHA	C6-N2	3.08	1.42	1.32
3	A	1003	L6T	CAP-CAO	-3.02	1.41	1.51
3	A	1002	L6T	OAN-CAO	2.92	1.51	1.44
3	A	1002	L6T	CAT-CAR	-2.83	1.45	1.52
3	A	1002	L6T	C3-C2	-2.78	1.45	1.52
3	A	1002	L6T	C4-C3	-2.72	1.45	1.52
3	A	1002	L6T	CAA-CAV	-2.67	1.44	1.52
3	A	1006	L6T	O5-C1	2.54	1.48	1.41
3	A	1004	L6T	O5-C1	2.49	1.48	1.41
3	A	1005	L6T	O5-C1	2.49	1.48	1.41
3	A	1003	L6T	CAV-CAT	-2.42	1.46	1.52
3	A	1003	L6T	C3-C2	-2.39	1.46	1.52
3	A	1004	L6T	CAV-CAT	-2.31	1.46	1.52
3	A	1003	L6T	CAA-CAV	-2.31	1.45	1.52
3	A	1006	L6T	CAV-CAT	-2.29	1.46	1.52
3	A	1005	L6T	CAV-CAT	-2.27	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1006	L6T	OAN-CAA	2.12	1.47	1.41
3	A	1004	L6T	OAN-CAA	2.11	1.47	1.41
3	A	1005	L6T	OAW-CAV	2.09	1.47	1.43
3	A	1006	L6T	OAW-CAV	2.06	1.47	1.43
3	A	1005	L6T	OAN-CAA	2.05	1.47	1.41
3	A	1004	L6T	OAW-CAV	2.05	1.47	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	9ZF	C07-C06-C01	-8.28	94.02	109.65
2	A	1001	9ZF	C03-C04-C10	-7.80	94.59	109.56
4	A	1009	MHA	C2-C1-N1	-4.60	106.94	113.48
3	A	1003	L6T	CAA-OAN-CAO	-4.09	105.66	113.69
4	A	1009	MHA	C6-C5-N1	-3.99	107.46	114.38
2	A	1001	9ZF	N14-C12-N11	3.80	119.07	113.76
3	A	1003	L6T	CAV-CAT-CAR	3.09	116.22	110.82
2	A	1001	9ZF	C09-C02-C03	-3.07	103.86	109.65
3	A	1003	L6T	CAT-CAR-CAO	2.91	115.42	110.24
4	A	1007	MHA	C5-C6-N2	2.77	120.23	115.86
2	A	1001	9ZF	C07-C06-C05	2.71	114.77	109.65
4	A	1008	MHA	C2-C1-N1	-2.66	109.69	113.48
3	A	1005	L6T	CAA-O1-C1	-2.63	109.72	114.42
3	A	1004	L6T	CAA-O1-C1	-2.62	109.74	114.42
3	A	1003	L6T	CAP-CAO-CAR	-2.61	106.90	113.00
4	A	1007	MHA	C4-C3-N1	-2.54	109.87	113.48
4	A	1008	MHA	C6-C5-N1	-2.54	109.97	114.38
4	A	1008	MHA	C5-C6-N2	2.52	119.84	115.86
4	A	1007	MHA	C6-C5-N1	-2.51	110.01	114.38
2	A	1001	9ZF	C05-C04-C10	2.47	114.30	109.56
3	A	1003	L6T	OAN-CAO-CAR	-2.45	105.24	109.69
2	A	1001	9ZF	O13-C12-N11	-2.39	118.26	122.62
3	A	1002	L6T	O5-C5-C6	2.38	111.47	106.67
4	A	1008	MHA	C4-C3-N1	-2.36	110.12	113.48
3	A	1003	L6T	O1-C1-C2	2.32	114.11	108.10
3	A	1005	L6T	CAT-CAR-CAO	2.31	114.36	110.24
4	A	1007	MHA	C2-C1-N1	-2.27	110.25	113.48
3	A	1003	L6T	CAA-O1-C1	-2.17	110.55	114.42
3	A	1003	L6T	C3-C4-C5	2.13	114.04	110.24
2	A	1001	9ZF	C05-C04-C03	2.12	112.68	109.05
3	A	1002	L6T	CAP-CAO-CAR	-2.03	108.24	113.00
3	A	1002	L6T	O4-C4-C3	-2.01	105.70	110.35

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1005	L6T	C5-C6-O6-CAX
4	A	1009	MHA	C4-C3-N1-C5
3	A	1003	L6T	C2-C1-O1-CAA
3	A	1005	L6T	CBE-CBF-CBG-CBH
3	A	1003	L6T	OAN-CAO-CAP-OAQ
3	A	1003	L6T	CAR-CAO-CAP-OAQ
3	A	1005	L6T	O5-C1-O1-CAA
3	A	1005	L6T	OAN-CAA-O1-C1
3	A	1003	L6T	O5-C5-C6-O6
3	A	1003	L6T	C4-C5-C6-O6
3	A	1005	L6T	O6-CAX-CAY-CAZ
3	A	1005	L6T	CAY-CAZ-CBA-CBB
4	A	1009	MHA	N1-C5-C6-N2
3	A	1005	L6T	C2-C1-O1-CAA
3	A	1005	L6T	CAV-CAA-O1-C1
3	A	1006	L6T	C2-C1-O1-CAA
3	A	1004	L6T	CBB-CBC-CBD-CBE
3	A	1006	L6T	CBA-CBB-CBC-CBD
3	A	1002	L6T	CAZ-CBA-CBB-CBC
3	A	1006	L6T	CAZ-CBA-CBB-CBC
3	A	1005	L6T	CAX-CAY-CAZ-CBA
3	A	1004	L6T	CAY-CAZ-CBA-CBB
3	A	1006	L6T	CAX-CAY-CAZ-CBA
3	A	1002	L6T	CBD-CBE-CBF-CBG
3	A	1006	L6T	O5-C1-O1-CAA
3	A	1003	L6T	CBE-CBF-CBG-CBH
3	A	1003	L6T	CBD-CBE-CBF-CBG
3	A	1006	L6T	CBC-CBD-CBE-CBF
3	A	1006	L6T	CBB-CBC-CBD-CBE
3	A	1005	L6T	CBA-CBB-CBC-CBD
3	A	1004	L6T	CBA-CBB-CBC-CBD
4	A	1009	MHA	N1-C5-C6-O5
3	A	1004	L6T	CBD-CBE-CBF-CBG
4	A	1009	MHA	C4-C3-N1-C1
3	A	1004	L6T	CBF-CBG-CBH-CBI
3	A	1002	L6T	O5-C5-C6-O6
4	A	1009	MHA	C2-C1-N1-C3
3	A	1004	L6T	CBC-CBD-CBE-CBF
3	A	1002	L6T	O6-CAX-CAY-CAZ
4	A	1007	MHA	C4-C3-N1-C1

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Mol	Chain	Res	Type	Atoms
4	A	1009	MHA	C2-C1-N1-C5
3	A	1002	L6T	C5-C6-O6-CAX
3	A	1002	L6T	CAX-CAY-CAZ-CBA
3	A	1004	L6T	CAY-CAX-O6-C6
3	A	1002	L6T	CBF-CBG-CBH-CBI
3	A	1004	L6T	C4-C5-C6-O6
3	A	1004	L6T	CAR-CAO-CAP-OAQ
3	A	1005	L6T	CBC-CBD-CBE-CBF
3	A	1004	L6T	CBE-CBF-CBG-CBH
3	A	1005	L6T	CAR-CAO-CAP-OAQ
3	A	1003	L6T	C5-C6-O6-CAX
3	A	1003	L6T	O6-CAX-CAY-CAZ
4	A	1007	MHA	C4-C3-N1-C5
4	A	1007	MHA	C2-C1-N1-C5
3	A	1003	L6T	CAY-CAX-O6-C6
3	A	1005	L6T	OAN-CAO-CAP-OAQ
3	A	1004	L6T	OAN-CAO-CAP-OAQ
3	A	1004	L6T	CAV-CAA-O1-C1
3	A	1004	L6T	O6-CAX-CAY-CAZ
3	A	1003	L6T	CAX-CAY-CAZ-CBA
3	A	1006	L6T	CAY-CAZ-CBA-CBB
3	A	1003	L6T	CBF-CBG-CBH-CBI
4	A	1008	MHA	C2-C1-N1-C3

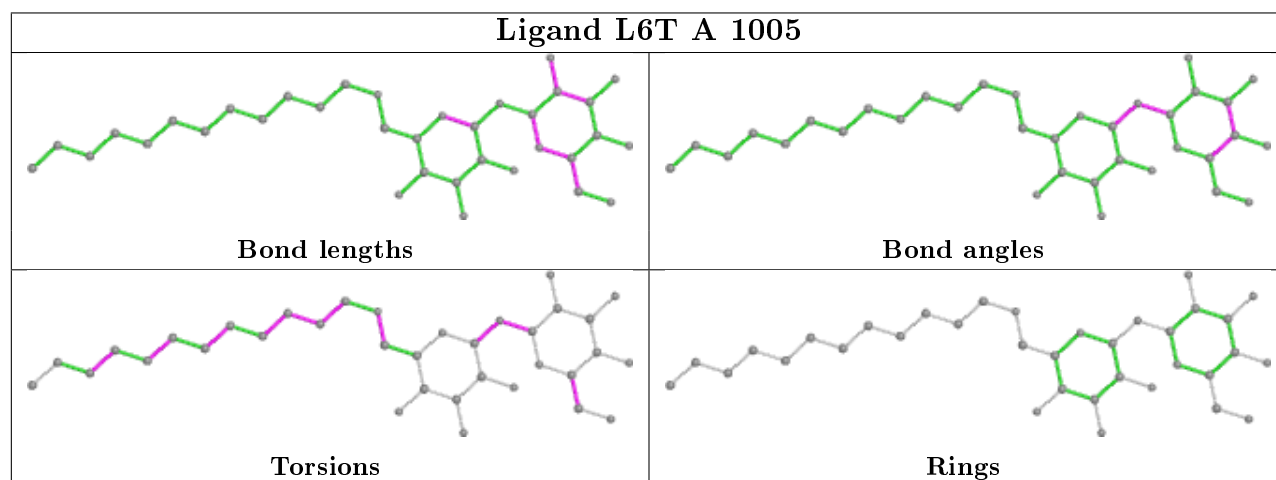
There are no ring outliers.

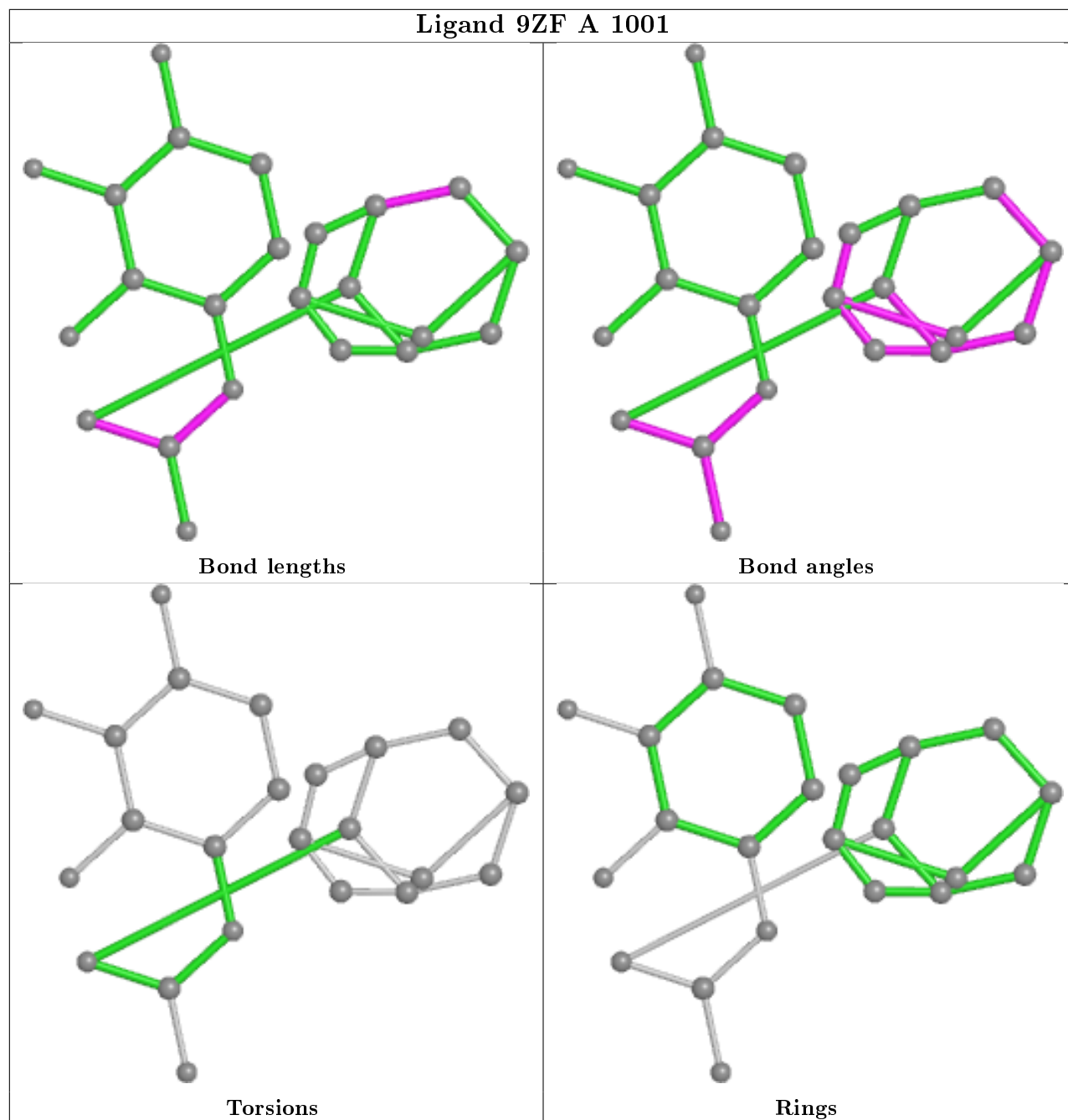
7 monomers are involved in 25 short contacts:

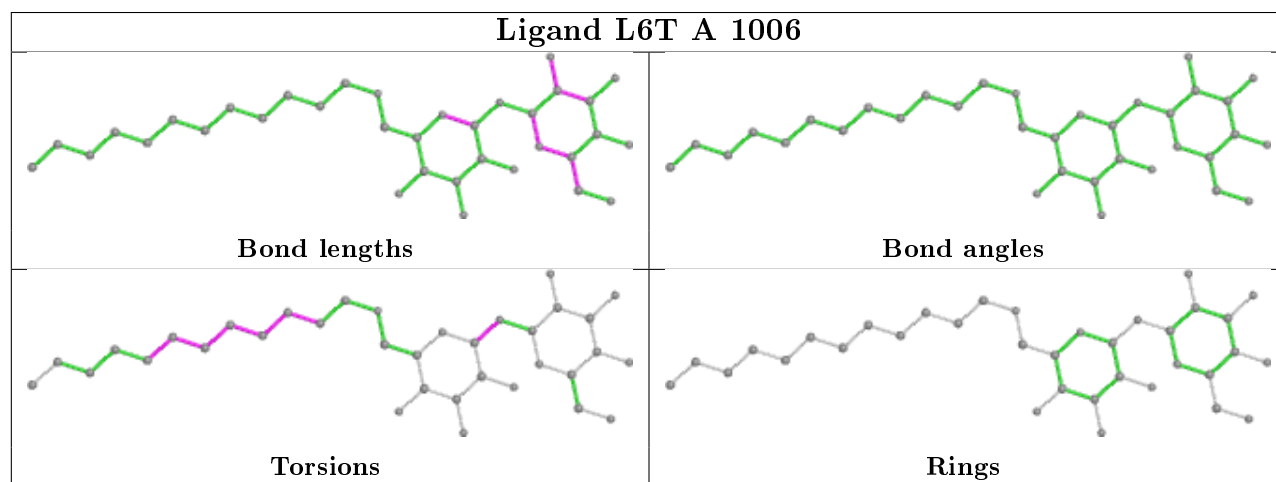
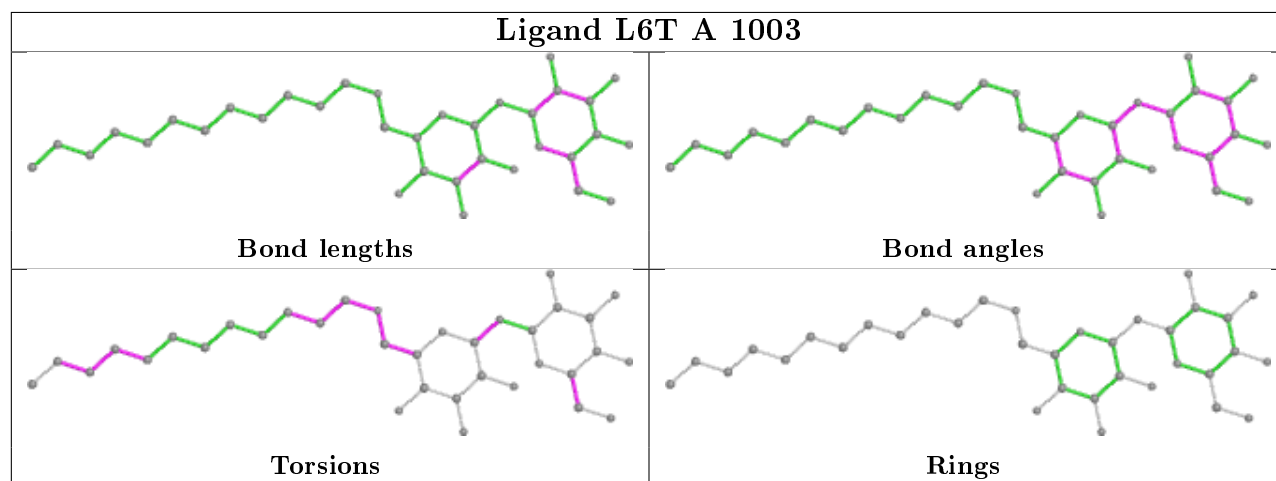
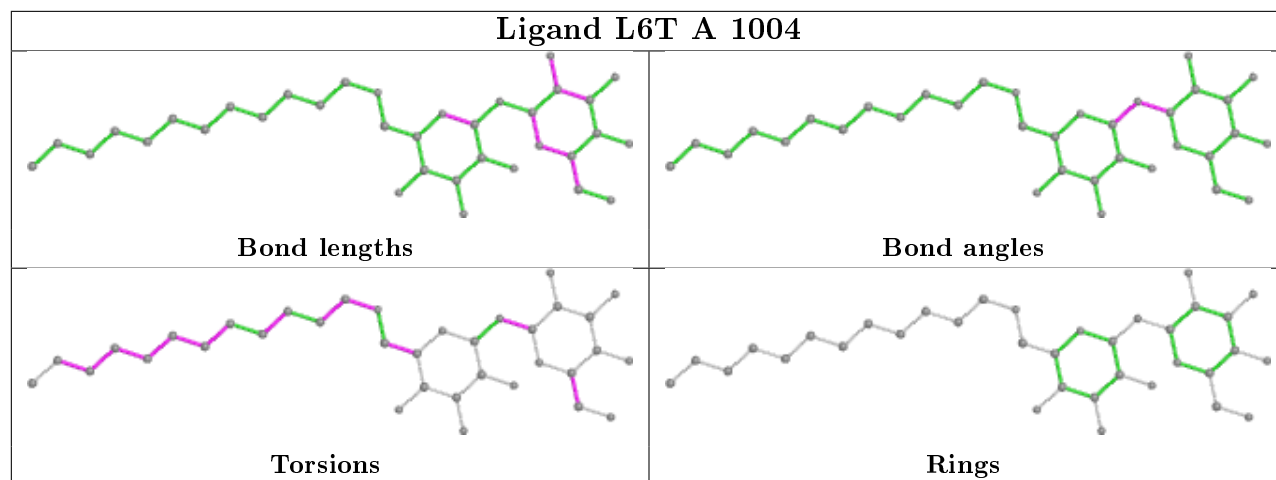
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1005	L6T	5	0
3	A	1004	L6T	10	0
4	A	1007	MHA	1	0
4	A	1009	MHA	5	0
4	A	1008	MHA	1	0
3	A	1006	L6T	2	0
3	A	1002	L6T	4	0

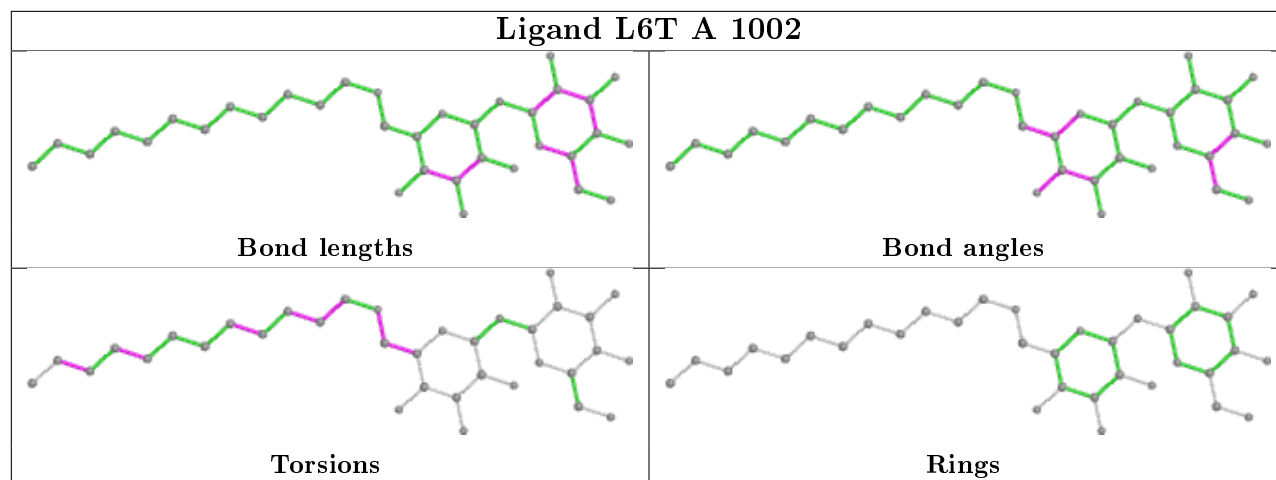
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	900/943 (95%)	0.09	49 (5%) 25 17	37, 66, 138, 234	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	746	GLN	7.8
1	A	738	ALA	7.0
1	A	745	VAL	6.3
1	A	744	ARG	6.0
1	A	742	MET	5.3
1	A	354	LEU	5.0
1	A	737	TRP	4.8
1	A	353	LEU	4.7
1	A	743	LYS	4.5
1	A	391	GLY	4.4
1	A	396	VAL	4.3
1	A	659	GLU	3.9
1	A	741	TRP	3.9
1	A	393	LEU	3.8
1	A	399	LYS	3.8
1	A	929	HIS	3.8
1	A	394	VAL	3.6
1	A	739	PRO	3.6
1	A	85	ALA	3.5
1	A	395	ASN	3.5
1	A	86	TRP	3.4
1	A	730	LEU	3.4
1	A	536	LEU	3.3
1	A	352	THR	3.3
1	A	525	ASP	3.1
1	A	83	ASP	2.9
1	A	90	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	347	ALA	2.8
1	A	397	VAL	2.8
1	A	350	VAL	2.8
1	A	111	TRP	2.7
1	A	740	ARG	2.5
1	A	748	LYS	2.5
1	A	749	GLU	2.5
1	A	537	GLN	2.5
1	A	392	ARG	2.4
1	A	424	LEU	2.4
1	A	583	PHE	2.4
1	A	727	VAL	2.4
1	A	403	ALA	2.4
1	A	535	ALA	2.3
1	A	540	HIS	2.3
1	A	735	CYS	2.3
1	A	661	GLY	2.1
1	A	87	GLN	2.1
1	A	658	ARG	2.1
1	A	542	ILE	2.1
1	A	84	LYS	2.1
1	A	703	TYR	2.1

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 carbohydrates 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.

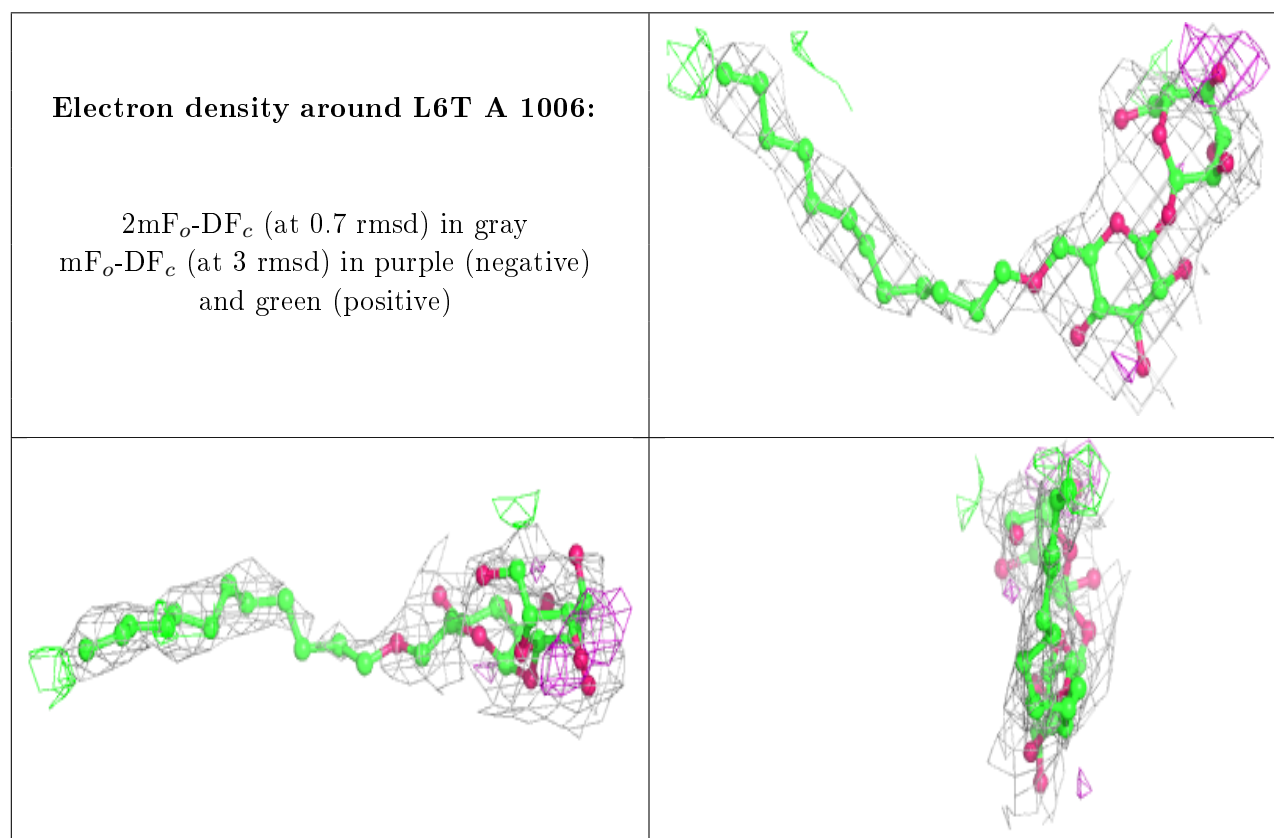
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MHA	A	1009	13/13	0.58	0.31	123,142,152,158	0

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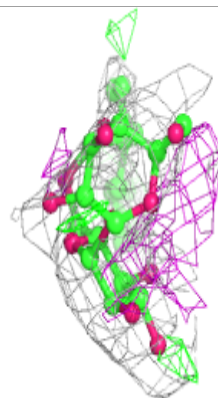
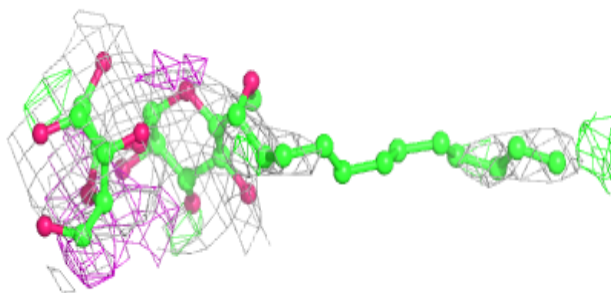
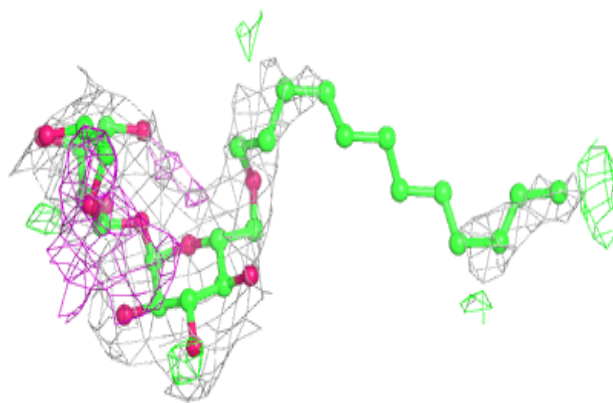
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	L6T	A	1006	35/35	0.72	0.29	58,132,147,149	0
3	L6T	A	1005	35/35	0.81	0.39	75,130,148,150	0
3	L6T	A	1003	35/35	0.85	0.29	44,125,164,166	0
3	L6T	A	1004	35/35	0.85	0.22	77,107,120,135	0
4	MHA	A	1008	13/13	0.93	0.23	64,70,78,84	0
3	L6T	A	1002	35/35	0.94	0.21	38,76,102,111	0
2	9ZF	A	1001	23/23	0.95	0.23	82,86,91,94	0
4	MHA	A	1007	13/13	0.96	0.14	59,64,74,79	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.

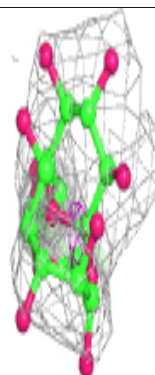
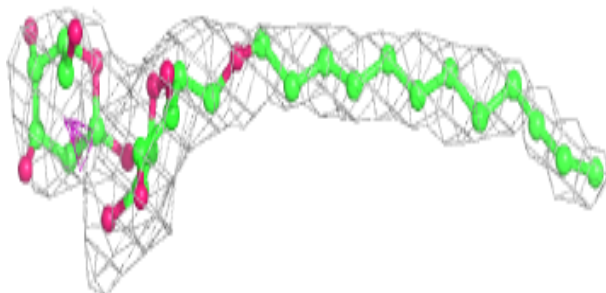
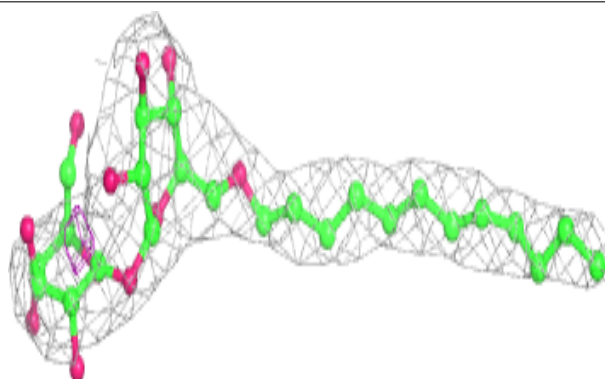


Electron density around L6T A 1005:

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

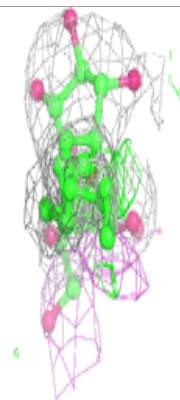
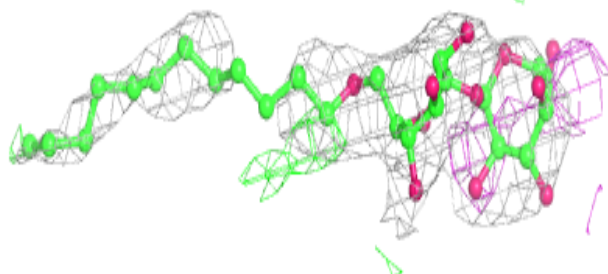
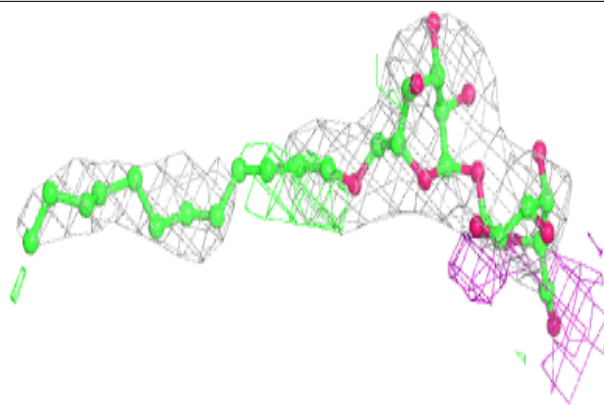
**Electron density around L6T A 1003:**

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

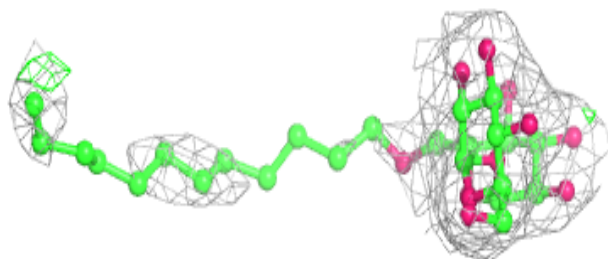
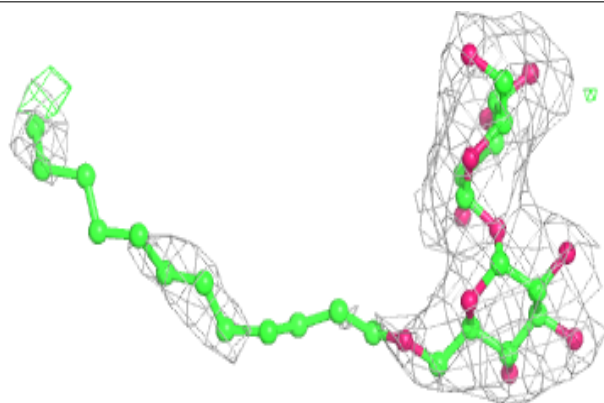


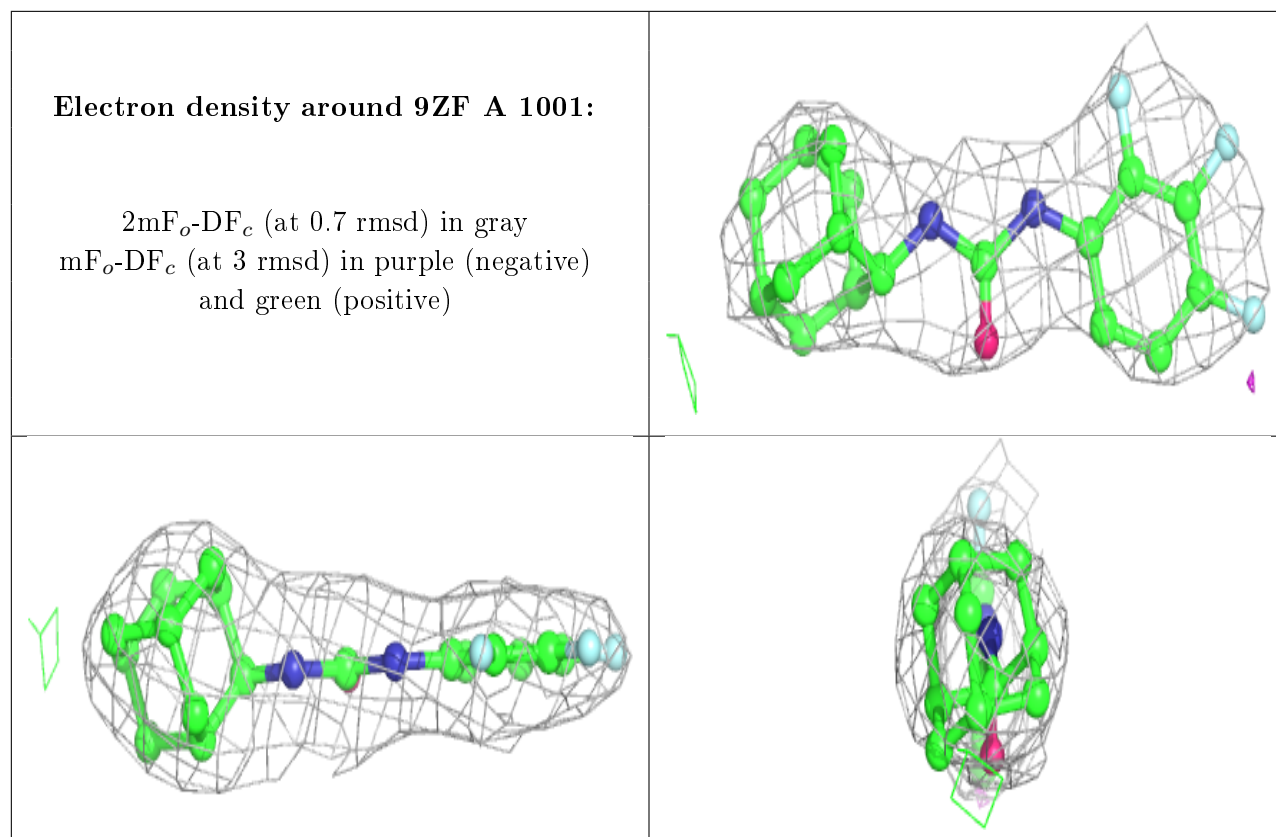
Electron density around L6T A 1004:

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

**Electron density around L6T A 1002:**

$2mF_o-DF_c$ (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.