Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 10:12 PM JST

PDB ID	:	7C2M
Title	:	Crystal structure of mycolic acid transporter MmpL3 from Mycobacterium smegmatis complexed with NITD-349
Authors	:	Zhang, B.; Yang, X.; Hu, T.; Rao, Z.
Deposited on	:	2020-05-08
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

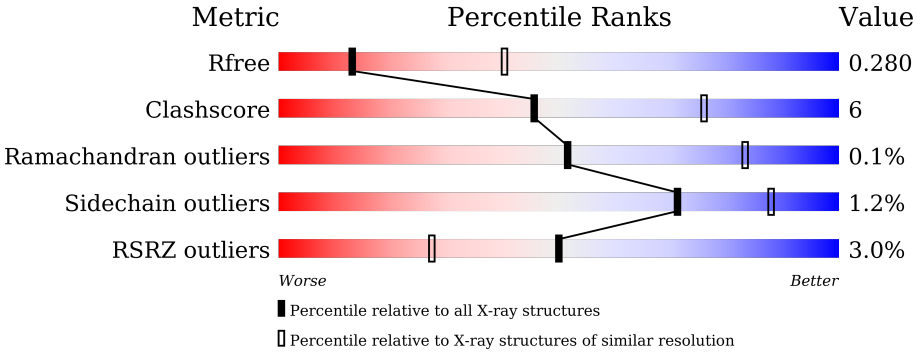
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	934	3% 81% 15% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	L6T	A	1006	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7175 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 Chimera of drug exporters of the RND superfamily-like protein and Endolysin.

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

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 A0A097J809
A	846	ALA	CYS	engineered mutation	UNP A0A097J809
A	911	GLU	-	expression tag	UNP A0A097J809
A	912	PHE	-	expression tag	UNP A0A097J809
A	913	HIS	-	expression tag	UNP A0A097J809
A	914	LEU	-	expression tag	UNP A0A097J809
A	915	GLY	-	expression tag	UNP A0A097J809
A	916	GLY	-	expression tag	UNP A0A097J809
A	917	ILE	-	expression tag	UNP A0A097J809
A	918	LYS	-	expression tag	UNP A0A097J809
A	919	ALA	-	expression tag	UNP A0A097J809
A	920	PHE	-	expression tag	UNP A0A097J809
A	921	HIS	-	expression tag	UNP A0A097J809
A	922	HIS	-	expression tag	UNP A0A097J809
A	923	HIS	-	expression tag	UNP A0A097J809
A	924	HIS	-	expression tag	UNP A0A097J809
A	925	HIS	-	expression tag	UNP A0A097J809
A	926	HIS	-	expression tag	UNP A0A097J809
A	927	HIS	-	expression tag	UNP A0A097J809

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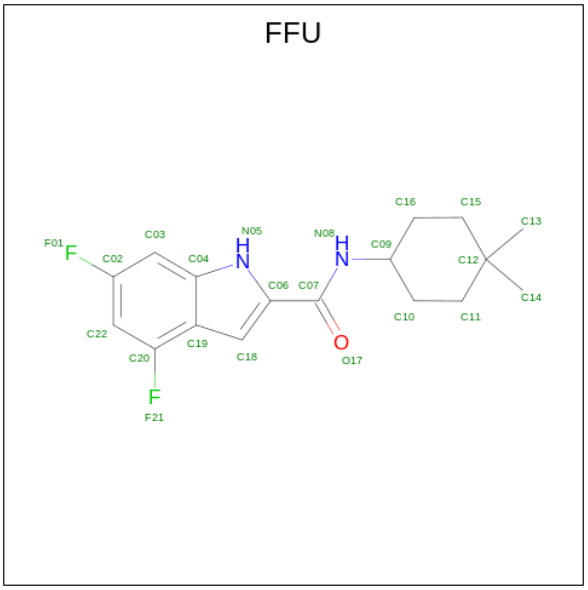
Chain	Residue	Modelled	Actual	Comment	Reference
A	928	HIS	-	expression tag	UNP A0A097J809
A	929	HIS	-	expression tag	UNP A0A097J809

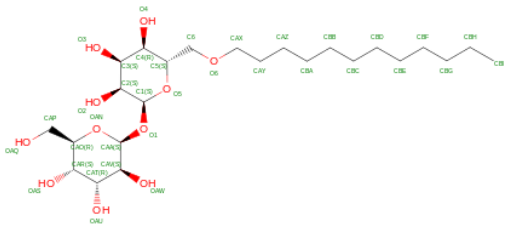
- Molecule 2 is N-(4,4-dimethylcyclohexyl)-4,6-bis(fluoranyl)-1H-indole-2-carboxamide (three-letter code: FFU) (formula: $C_{17}H_{20}F_2N_2O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	22	17	2	2	1	0	0

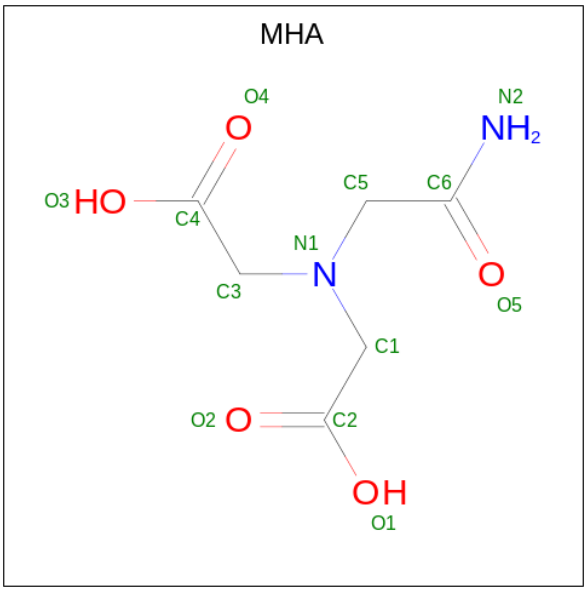
- Molecule 3 is alpha-D-glucopyranosyl 6-O-dodecyl-alpha-D-glucopyranoside (three-letter code: L6T) (formula: $C_{24}H_{46}O_{11}$).

L6T



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

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



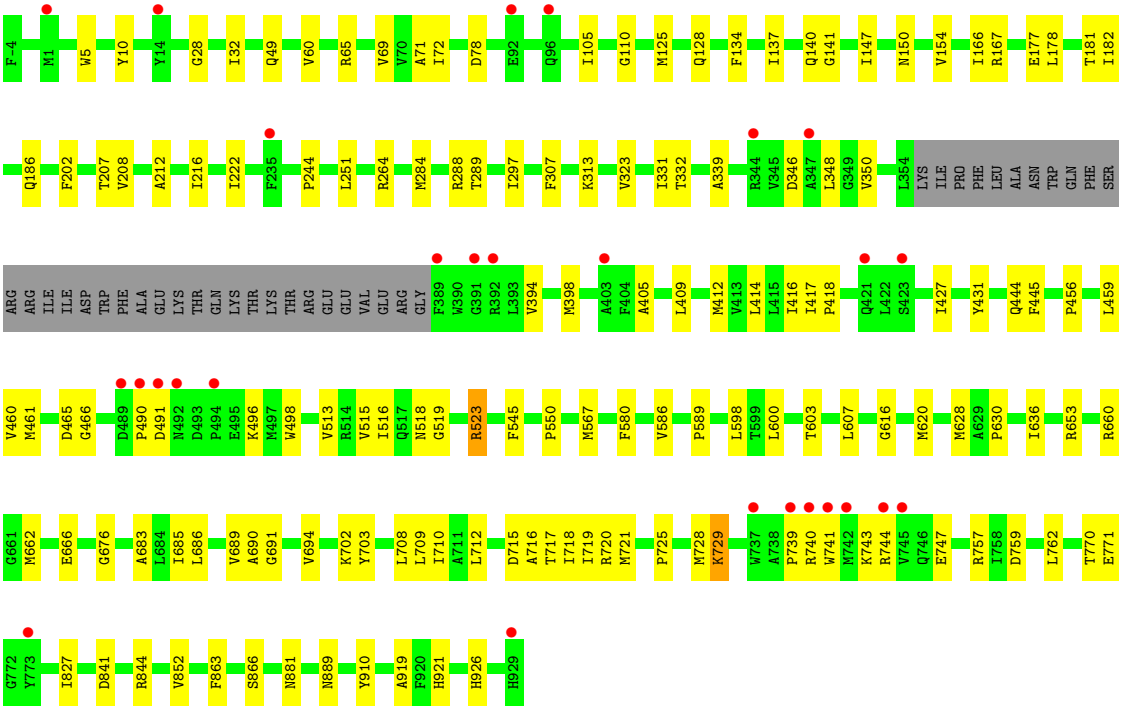
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	13	6	2	5	0	0
			Total	C	N	O		
4	A	1	13	6	2	5	0	0

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: Chimera of drug exporters of the RND superfamily-like protein and Endolysin

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.24Å 143.62Å 143.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.40 – 3.10 45.40 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.40-3.10) 99.6 (45.40-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.253 , 0.281 0.253 , 0.280	Depositor DCC
R_{free} test set	1994 reflections (6.00%)	wwPDB-VP
Wilson B-factor (Å^2)	97.8	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	7175	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: FFU, L6T, 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	0.25	0/7097	0.43	0/9642

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6952	0	7111	85	0
2	A	22	0	0	0	0
3	A	175	0	0	5	0
4	A	26	0	16	5	0
All	All	7175	0	7127	92	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 6.

All (92) 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:405:ALA:O	1:A:409:LEU:HD12	1.70	0.92
1:A:398:MET:SD	1:A:729:LYS:NZ	2.50	0.85
4:A:1008:MHA:HC11	4:A:1008:MHA:N2	1.99	0.75
3:A:1003:L6T:OAS	3:A:1003:L6T:OAQ	2.08	0.70
1:A:207:THR:HG21	1:A:346:ASP:HA	1.76	0.67
1:A:417:ILE:HG13	1:A:418:PRO:HD3	1.77	0.67
1:A:863:PHE:HA	4:A:1008:MHA:O5	1.96	0.66
1:A:10:TYR:HD1	1:A:339:ALA:HB1	1.66	0.60
1:A:628:MET:HG3	1:A:630:PRO:HD2	1.84	0.60
4:A:1008:MHA:HC11	4:A:1008:MHA:HN21	1.66	0.60
1:A:757:ARG:HG3	1:A:762:LEU:HB2	1.85	0.58
4:A:1008:MHA:HC32	4:A:1008:MHA:O2	2.03	0.58
1:A:297:ILE:HG21	1:A:323:VAL:HG21	1.86	0.58
1:A:307:PHE:O	1:A:313:LYS:NZ	2.37	0.57
1:A:398:MET:HA	1:A:729:LYS:NZ	2.18	0.57
1:A:202:PHE:HE2	1:A:350:VAL:HG13	1.69	0.56
1:A:498:TRP:H	1:A:518:ASN:HD22	1.54	0.56
1:A:771:GLU:OE1	1:A:921:HIS:NE2	2.38	0.56
1:A:72:ILE:HD11	1:A:445:PHE:HB2	1.88	0.56
1:A:49:GLN:HG3	1:A:545:PHE:HD1	1.72	0.54
1:A:716:ALA:O	1:A:720:ARG:NH2	2.40	0.54
1:A:456:PRO:HA	1:A:519:GLY:HA2	1.89	0.53
1:A:881:ASN:OD1	4:A:1008:MHA:N2	2.42	0.53
1:A:744:ARG:NE	1:A:747:GLU:OE2	2.43	0.51
1:A:178:LEU:O	1:A:181:THR:OG1	2.24	0.51
1:A:412:MET:O	1:A:416:ILE:HG13	2.12	0.50
1:A:65:ARG:NH1	1:A:141:GLY:O	2.44	0.50
1:A:140:GLN:O	1:A:150:ASN:ND2	2.44	0.50
1:A:460:VAL:HG22	1:A:515:VAL:HG22	1.94	0.50
1:A:69:VAL:HB	1:A:137:ILE:HB	1.93	0.49
1:A:827:ILE:HD11	1:A:852:VAL:HG21	1.94	0.49
1:A:715:ASP:HA	1:A:719:ILE:HB	1.94	0.49
1:A:465:ASP:OD1	1:A:466:GLY:N	2.45	0.49
1:A:686:LEU:HD23	1:A:712:LEU:HD13	1.94	0.49
1:A:71:ALA:HB1	1:A:166:ILE:HD11	1.94	0.49
1:A:414:LEU:O	1:A:417:ILE:HG12	2.12	0.49
1:A:717:THR:OG1	1:A:718:ILE:N	2.46	0.48
1:A:167:ARG:NH1	1:A:444:GLN:OE1	2.47	0.48
1:A:284:MET:O	1:A:288:ARG:HD3	2.14	0.48
1:A:491:ASP:OD2	1:A:496:LYS:NZ	2.40	0.48
1:A:694:VAL:O	1:A:702:LYS:NZ	2.35	0.47
1:A:717:THR:O	1:A:721:MET:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ILE:HD11	1:A:251:LEU:HB2	1.97	0.47
1:A:461:MET:O	1:A:513:VAL:HA	2.15	0.47
1:A:725:PRO:HA	1:A:728:MET:HE2	1.98	0.46
1:A:580:PHE:CD1	1:A:589:PRO:HG2	2.51	0.46
3:A:1002:L6T:OAQ	3:A:1002:L6T:OAS	2.34	0.46
1:A:141:GLY:HA3	1:A:147:ILE:HG12	1.98	0.45
1:A:105:ILE:HG13	1:A:154:VAL:HG11	1.98	0.45
1:A:459:LEU:HD12	1:A:516:ILE:HD11	1.97	0.45
1:A:580:PHE:HE1	1:A:586:VAL:HA	1.81	0.45
1:A:202:PHE:HZ	1:A:350:VAL:HA	1.80	0.45
1:A:616:GLY:N	3:A:1005:L6T:C6	2.80	0.45
1:A:28:GLY:O	1:A:32:ILE:HG23	2.17	0.45
1:A:739:PRO:HB2	1:A:740:ARG:HE	1.82	0.45
1:A:398:MET:HA	1:A:729:LYS:HZ1	1.81	0.44
1:A:208:VAL:HB	1:A:348:LEU:HB2	1.99	0.44
3:A:1005:L6T:C3	3:A:1005:L6T:CAA	2.93	0.44
1:A:653:ARG:HA	1:A:653:ARG:HD3	1.79	0.44
1:A:620:MET:HA	1:A:620:MET:HE2	2.00	0.44
1:A:743:LYS:HA	1:A:743:LYS:HD2	1.81	0.44
1:A:863:PHE:HB3	1:A:866:SER:HB2	2.00	0.44
1:A:523:ARG:HH22	1:A:550:PRO:HA	1.82	0.43
1:A:600:LEU:HD11	1:A:636:ILE:HA	2.00	0.43
1:A:690:ALA:O	1:A:694:VAL:HG13	2.18	0.43
1:A:177:GLU:O	1:A:181:THR:HG23	2.17	0.43
1:A:926:HIS:O	1:A:926:HIS:ND1	2.51	0.43
1:A:60:VAL:HG21	1:A:513:VAL:HB	2.00	0.43
1:A:770:THR:HG21	1:A:919:ALA:HB1	1.99	0.43
3:A:1005:L6T:O1	3:A:1005:L6T:O4	2.37	0.42
1:A:412:MET:HE3	1:A:598:LEU:HD23	2.00	0.42
1:A:841:ASP:OD1	1:A:844:ARG:NH1	2.49	0.42
1:A:182:ILE:O	1:A:186:GLN:HG2	2.19	0.42
1:A:71:ALA:O	1:A:134:PHE:HA	2.19	0.42
1:A:5:TRP:HZ2	1:A:332:THR:HG22	1.85	0.42
1:A:182:ILE:HD12	1:A:244:PRO:HG3	2.02	0.42
1:A:759:ASP:OD2	1:A:910:TYR:OH	2.26	0.42
1:A:691:GLY:O	1:A:694:VAL:HG22	2.20	0.42
1:A:694:VAL:HG11	1:A:709:LEU:HD12	2.01	0.42
1:A:289:THR:HG21	1:A:653:ARG:HH22	1.85	0.42
1:A:685:ILE:O	1:A:689:VAL:HG23	2.20	0.41
1:A:394:VAL:O	1:A:398:MET:HG2	2.20	0.41
1:A:708:LEU:HD23	1:A:708:LEU:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ILE:HG12	1:A:431:TYR:CE2	2.55	0.41
1:A:683:ALA:O	1:A:712:LEU:HD21	2.21	0.41
1:A:264:ARG:HA	1:A:264:ARG:HD3	1.87	0.41
1:A:607:LEU:HB3	1:A:703:TYR:CE1	2.56	0.41
1:A:662:MET:HG3	1:A:666:GLU:HG3	2.03	0.41
1:A:676:GLY:HA2	1:A:720:ARG:HH11	1.85	0.41
1:A:110:GLY:HA2	1:A:125:MET:SD	2.61	0.40
1:A:212:ALA:O	1:A:216:ILE:HG13	2.21	0.40
1:A:603:THR:HG23	1:A:710:ILE:HB	2.04	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	896/934 (96%)	868 (97%)	27 (3%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	490	PRO

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	738/769 (96%)	729 (99%)	9 (1%)	71 88

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

Mol	Chain	Res	Type
1	A	78	ASP
1	A	128	GLN
1	A	331	ILE
1	A	523	ARG
1	A	567	MET
1	A	660	ARG
1	A	729	LYS
1	A	741	TRP
1	A	889	ASN

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
2	FFU	A	1001	-	22,24,24	1.51	3 (13%)	31,36,36	2.32	7 (22%)
3	L6T	A	1002	-	36,36,36	1.46	7 (19%)	47,47,47	1.40	7 (14%)
4	MHA	A	1007	-	12,12,12	1.55	1 (8%)	15,15,15	1.35	1 (6%)
3	L6T	A	1003	-	36,36,36	1.64	7 (19%)	47,47,47	1.99	11 (23%)
3	L6T	A	1006	-	36,36,36	1.46	7 (19%)	47,47,47	1.34	5 (10%)
3	L6T	A	1004	-	36,36,36	1.55	8 (22%)	47,47,47	1.22	4 (8%)
3	L6T	A	1005	-	36,36,36	1.47	8 (22%)	47,47,47	1.70	7 (14%)
4	MHA	A	1008	-	12,12,12	0.85	0	15,15,15	0.84	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
2	FFU	A	1001	-	-	1/5/20/20	0/3/3/3
3	L6T	A	1002	-	-	8/20/60/60	0/2/2/2
4	MHA	A	1007	-	-	6/12/12/12	-
3	L6T	A	1003	-	-	12/20/60/60	0/2/2/2
3	L6T	A	1006	-	-	13/20/60/60	0/2/2/2
3	L6T	A	1004	-	-	10/20/60/60	0/2/2/2
3	L6T	A	1005	-	-	11/20/60/60	0/2/2/2
4	MHA	A	1008	-	-	9/12/12/12	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	FFU	C07-N08	5.26	1.45	1.34
3	A	1004	L6T	O5-C5	4.40	1.55	1.44
3	A	1002	L6T	O5-C5	4.01	1.54	1.44
4	A	1007	MHA	C6-N2	3.98	1.45	1.32
3	A	1003	L6T	C3-C2	-3.98	1.42	1.52
3	A	1006	L6T	O5-C5	3.81	1.53	1.44
3	A	1004	L6T	OAN-CAA	3.61	1.51	1.41
3	A	1003	L6T	C6-C5	-3.48	1.40	1.51
3	A	1002	L6T	OAN-CAA	3.26	1.50	1.41
3	A	1003	L6T	O1-CAA	-3.16	1.32	1.41
3	A	1003	L6T	OAN-CAA	3.09	1.49	1.41
3	A	1005	L6T	O5-C5	3.08	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1006	L6T	OAN-CAA	3.03	1.49	1.41
3	A	1005	L6T	C3-C2	-2.86	1.45	1.52
3	A	1005	L6T	C6-C5	-2.83	1.42	1.51
3	A	1002	L6T	C6-C5	-2.81	1.42	1.51
3	A	1006	L6T	C6-C5	-2.74	1.43	1.51
3	A	1003	L6T	C4-C3	-2.73	1.45	1.52
3	A	1003	L6T	O5-C5	2.72	1.51	1.44
3	A	1004	L6T	O5-C1	2.61	1.48	1.41
3	A	1003	L6T	C1-C2	-2.60	1.45	1.52
3	A	1002	L6T	O2-C2	2.51	1.48	1.43
3	A	1004	L6T	O3-C3	2.47	1.48	1.43
3	A	1005	L6T	O2-C2	2.46	1.48	1.43
3	A	1006	L6T	O3-C3	2.45	1.48	1.43
3	A	1006	L6T	O5-C1	2.44	1.48	1.41
3	A	1002	L6T	O3-C3	2.41	1.48	1.43
3	A	1006	L6T	O2-C2	2.39	1.48	1.43
3	A	1005	L6T	OAN-CAA	2.35	1.47	1.41
3	A	1006	L6T	C3-C2	-2.33	1.46	1.52
3	A	1004	L6T	C6-C5	-2.33	1.44	1.51
3	A	1004	L6T	O2-C2	2.30	1.48	1.43
3	A	1005	L6T	C4-C5	2.29	1.57	1.53
3	A	1002	L6T	O5-C1	2.26	1.47	1.41
3	A	1005	L6T	CAV-CAT	-2.20	1.46	1.52
3	A	1004	L6T	C3-C2	-2.19	1.46	1.52
3	A	1002	L6T	C3-C2	-2.12	1.46	1.52
2	A	1001	FFU	O17-C07	-2.11	1.19	1.23
2	A	1001	FFU	C22-C20	2.07	1.39	1.36
3	A	1005	L6T	O3-C3	2.06	1.47	1.43
3	A	1004	L6T	C4-C5	2.05	1.57	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	FFU	C22-C20-C19	-8.36	120.08	124.07
3	A	1003	L6T	CAA-O1-C1	-7.22	101.52	114.42
3	A	1003	L6T	CAT-CAR-CAO	-5.99	99.55	110.24
3	A	1005	L6T	C3-C4-C5	5.71	120.43	110.24
2	A	1001	FFU	C03-C02-C22	-5.22	119.97	124.09
3	A	1005	L6T	O4-C4-C3	-4.31	100.39	110.35
3	A	1006	L6T	OAN-CAO-CAR	3.96	116.88	109.69
3	A	1005	L6T	CAT-CAR-CAO	3.91	117.21	110.24
2	A	1001	FFU	F21-C20-C19	3.88	120.08	116.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1005	L6T	OAN-CAO-CAR	3.78	116.56	109.69
2	A	1001	FFU	C20-C22-C02	3.71	120.00	116.64
3	A	1002	L6T	O1-C1-C2	3.70	117.69	108.10
3	A	1004	L6T	C3-C4-C5	3.65	116.74	110.24
3	A	1006	L6T	CAT-CAR-CAO	3.60	116.67	110.24
3	A	1003	L6T	OAN-CAO-CAP	3.49	115.11	106.44
2	A	1001	FFU	C15-C12-C11	3.29	113.21	108.71
3	A	1003	L6T	OAU-CAT-CAR	-3.25	102.83	110.35
4	A	1007	MHA	C5-C6-N2	3.15	120.83	115.86
3	A	1004	L6T	C4-C3-C2	3.02	116.09	110.82
3	A	1006	L6T	CAV-CAT-CAR	2.93	115.93	110.82
3	A	1005	L6T	CAA-O1-C1	-2.92	109.20	114.42
2	A	1001	FFU	C06-N05-C04	2.82	110.33	104.45
3	A	1003	L6T	OAW-CAV-CAA	-2.78	103.30	110.05
3	A	1003	L6T	O3-C3-C2	-2.78	103.93	110.35
3	A	1005	L6T	OAU-CAT-CAV	-2.72	104.06	110.35
3	A	1002	L6T	O1-C1-O5	-2.67	103.22	110.67
3	A	1003	L6T	CAV-CAT-CAR	2.66	115.47	110.82
3	A	1003	L6T	O2-C2-C3	-2.62	104.28	110.35
3	A	1002	L6T	C1-O5-C5	-2.62	108.54	113.69
3	A	1004	L6T	O5-C5-C6	2.58	111.87	106.67
3	A	1002	L6T	O2-C2-C1	2.55	116.25	110.05
3	A	1003	L6T	O4-C4-C3	-2.52	104.51	110.35
3	A	1002	L6T	C4-C3-C2	2.44	115.08	110.82
3	A	1002	L6T	O5-C5-C6	2.40	111.51	106.67
3	A	1005	L6T	CAP-CAO-CAR	-2.39	107.40	113.00
2	A	1001	FFU	C06-C07-N08	2.35	119.57	115.20
3	A	1003	L6T	OAN-CAO-CAR	-2.16	105.77	109.69
3	A	1003	L6T	OAQ-CAP-CAO	-2.13	103.97	111.29
3	A	1002	L6T	CAV-CAT-CAR	2.10	114.49	110.82
3	A	1004	L6T	OAN-CAO-CAP	2.09	111.63	106.44
3	A	1006	L6T	C4-C3-C2	2.04	114.38	110.82
3	A	1006	L6T	O5-C5-C6	2.02	110.74	106.67

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	L6T	C2-C1-O1-CAA
3	A	1002	L6T	O5-C1-O1-CAA
3	A	1004	L6T	OAN-CAA-O1-C1
3	A	1005	L6T	C2-C1-O1-CAA

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Mol	Chain	Res	Type	Atoms
3	A	1005	L6T	O5-C1-O1-CAA
3	A	1005	L6T	CAV-CAA-O1-C1
3	A	1005	L6T	OAN-CAA-O1-C1
4	A	1007	MHA	N1-C5-C6-O5
4	A	1007	MHA	N1-C5-C6-N2
4	A	1008	MHA	C2-C1-N1-C3
4	A	1008	MHA	N1-C1-C2-O1
4	A	1008	MHA	N1-C1-C2-O2
4	A	1008	MHA	N1-C5-C6-O5
4	A	1008	MHA	N1-C5-C6-N2
3	A	1006	L6T	O5-C5-C6-O6
3	A	1003	L6T	O5-C5-C6-O6
3	A	1006	L6T	C4-C5-C6-O6
4	A	1007	MHA	N1-C3-C4-O3
4	A	1007	MHA	N1-C3-C4-O4
4	A	1007	MHA	C6-C5-N1-C1
3	A	1003	L6T	C4-C5-C6-O6
3	A	1006	L6T	O5-C1-O1-CAA
3	A	1006	L6T	CAR-CAO-CAP-OAQ
3	A	1006	L6T	O6-CAX-CAY-CAZ
3	A	1006	L6T	C2-C1-O1-CAA
4	A	1008	MHA	C6-C5-N1-C1
3	A	1003	L6T	CBA-CBB-CBC-CBD
3	A	1006	L6T	CBD-CBE-CBF-CBG
3	A	1006	L6T	CBE-CBF-CBG-CBH
3	A	1004	L6T	O5-C5-C6-O6
3	A	1002	L6T	O6-CAX-CAY-CAZ
3	A	1005	L6T	CAX-CAY-CAZ-CBA
3	A	1005	L6T	CBD-CBE-CBF-CBG
3	A	1005	L6T	O6-CAX-CAY-CAZ
3	A	1005	L6T	CBE-CBF-CBG-CBH
3	A	1002	L6T	OAN-CAO-CAP-OAQ
3	A	1006	L6T	CBC-CBD-CBE-CBF
3	A	1005	L6T	CBB-CBC-CBD-CBE
3	A	1006	L6T	CBA-CBB-CBC-CBD
3	A	1006	L6T	OAN-CAO-CAP-OAQ
3	A	1003	L6T	OAN-CAO-CAP-OAQ
3	A	1004	L6T	CAY-CAX-O6-C6
3	A	1004	L6T	OAN-CAO-CAP-OAQ
3	A	1005	L6T	CAR-CAO-CAP-OAQ
3	A	1002	L6T	O5-C5-C6-O6
3	A	1003	L6T	CAZ-CBA-CBB-CBC

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Mol	Chain	Res	Type	Atoms
3	A	1003	L6T	CAV-CAA-O1-C1
4	A	1008	MHA	C6-C5-N1-C3
3	A	1002	L6T	C4-C5-C6-O6
3	A	1003	L6T	CBE-CBF-CBG-CBH
3	A	1006	L6T	CAX-CAY-CAZ-CBA
3	A	1003	L6T	O5-C1-O1-CAA
3	A	1003	L6T	OAN-CAA-O1-C1
3	A	1004	L6T	CBC-CBD-CBE-CBF
3	A	1003	L6T	CBF-CBG-CBH-CBI
3	A	1003	L6T	C5-C6-O6-CAX
3	A	1004	L6T	CBF-CBG-CBH-CBI
3	A	1004	L6T	CBA-CBB-CBC-CBD
3	A	1005	L6T	CAY-CAZ-CBA-CBB
3	A	1002	L6T	C5-C6-O6-CAX
3	A	1004	L6T	CBB-CBC-CBD-CBE
3	A	1004	L6T	CAY-CAZ-CBA-CBB
3	A	1002	L6T	CBD-CBE-CBF-CBG
2	A	1001	FFU	C18-C06-C07-O17
3	A	1004	L6T	CBE-CBF-CBG-CBH
3	A	1006	L6T	CBB-CBC-CBD-CBE
4	A	1007	MHA	C2-C1-N1-C5
4	A	1008	MHA	C2-C1-N1-C5
4	A	1008	MHA	C4-C3-N1-C1
3	A	1003	L6T	C2-C1-O1-CAA

There are no ring outliers.

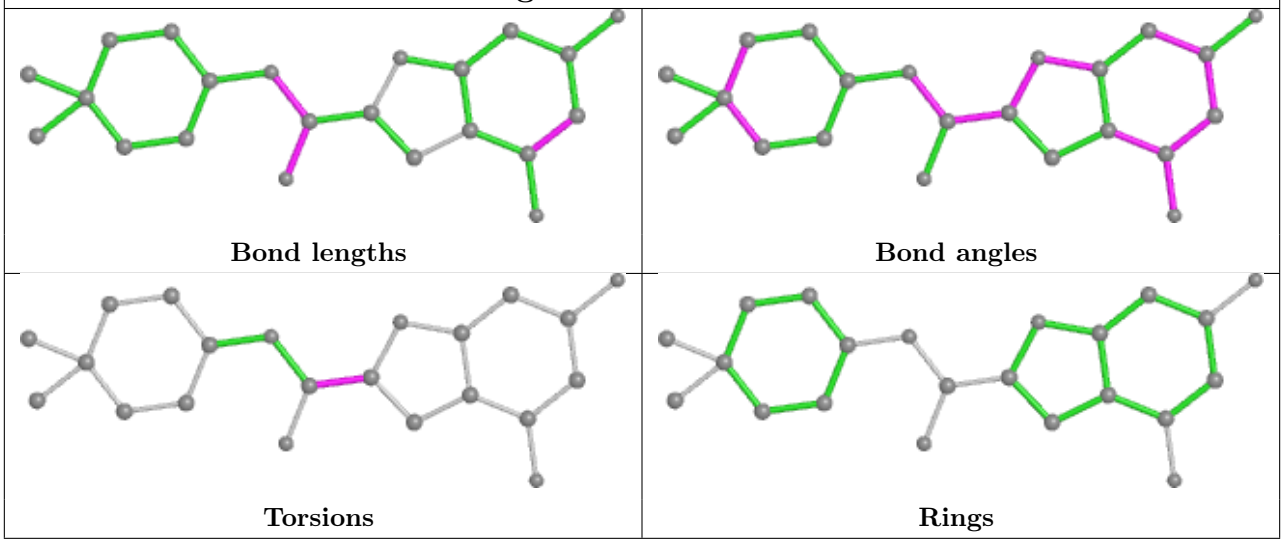
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	L6T	1	0
3	A	1003	L6T	1	0
3	A	1005	L6T	3	0
4	A	1008	MHA	5	0

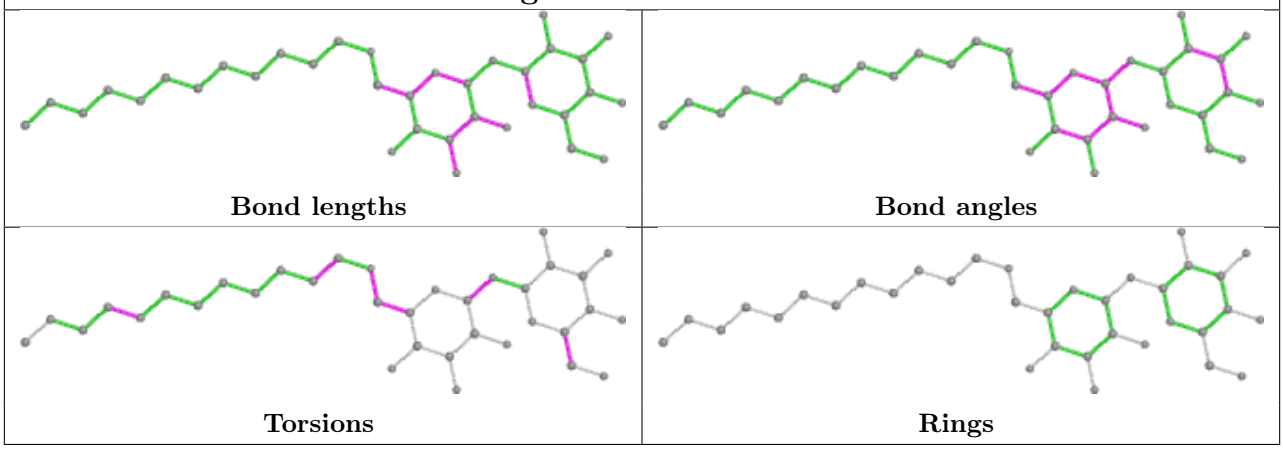
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

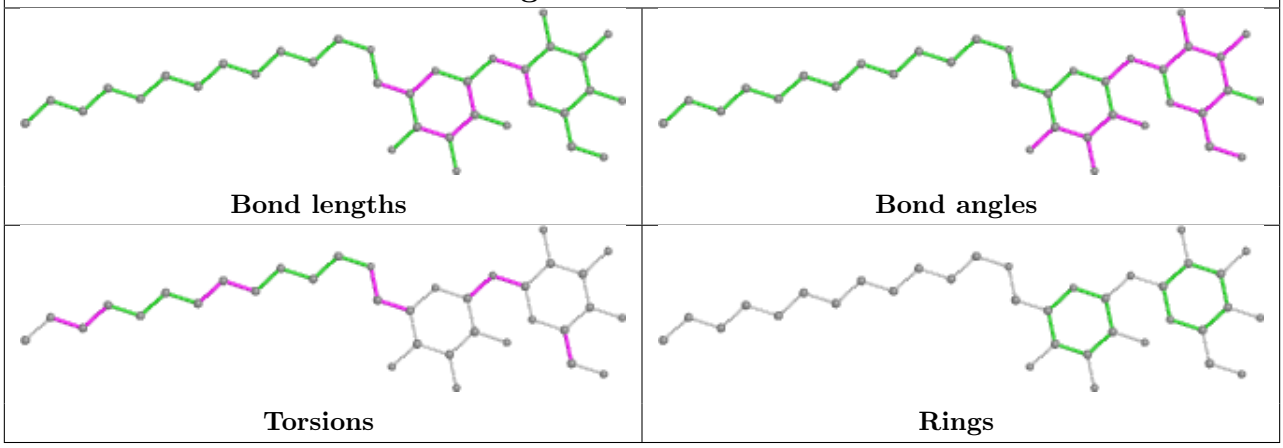
Ligand FFU A 1001



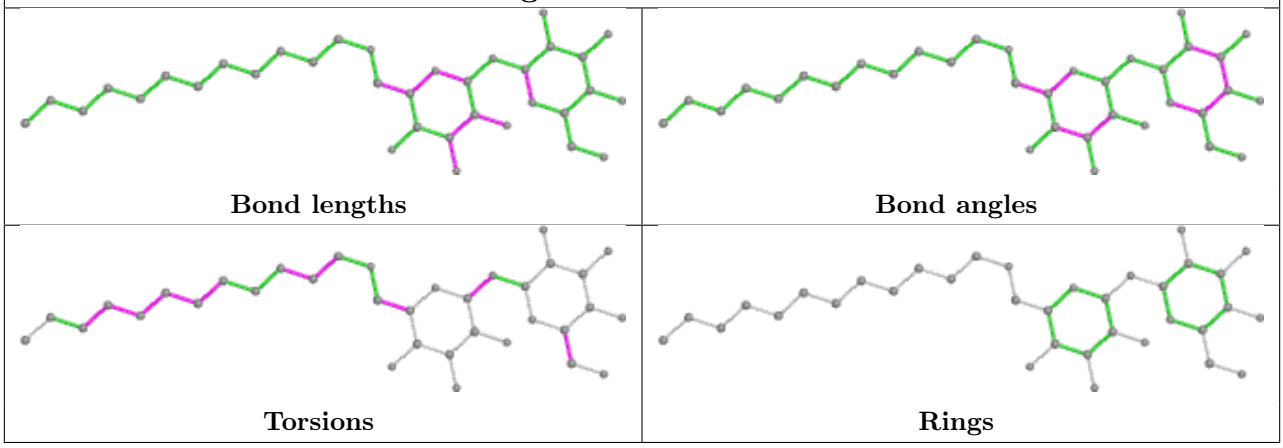
Ligand L6T A 1002



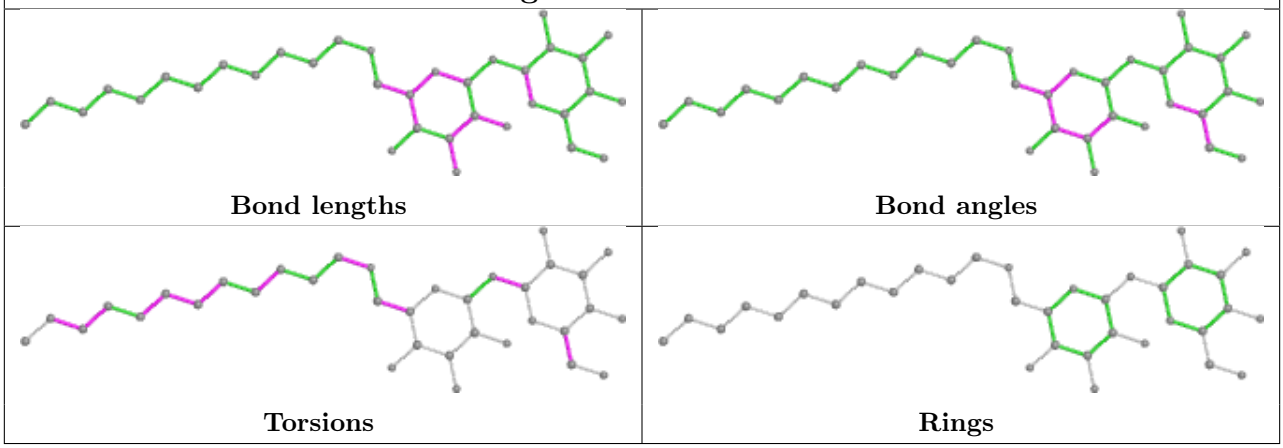
Ligand L6T A 1003



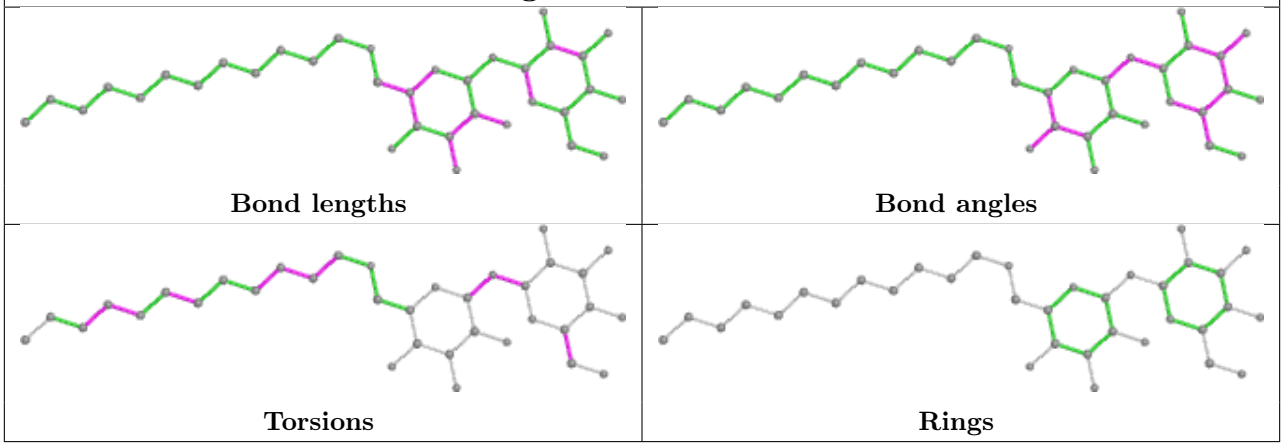
Ligand L6T A 1006



Ligand L6T A 1004



Ligand L6T A 1005



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	900/934 (96%)	-0.20	27 (3%) 50 27	64, 96, 152, 208	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	GLN	6.8
1	A	742	MET	5.0
1	A	739	PRO	4.5
1	A	737	TRP	4.3
1	A	740	ARG	4.2
1	A	741	TRP	4.2
1	A	347	ALA	3.7
1	A	492	ASN	3.6
1	A	1	MET	3.3
1	A	489	ASP	3.3
1	A	235	PHE	3.0
1	A	745	VAL	3.0
1	A	403	ALA	3.0
1	A	490	PRO	2.9
1	A	494	PRO	2.7
1	A	929	HIS	2.7
1	A	744	ARG	2.7
1	A	344	ARG	2.7
1	A	491	ASP	2.7
1	A	421	GLN	2.7
1	A	14	TYR	2.6
1	A	92	GLU	2.5
1	A	423	SER	2.3
1	A	392	ARG	2.3
1	A	391	GLY	2.2
1	A	773	TYR	2.0
1	A	389	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

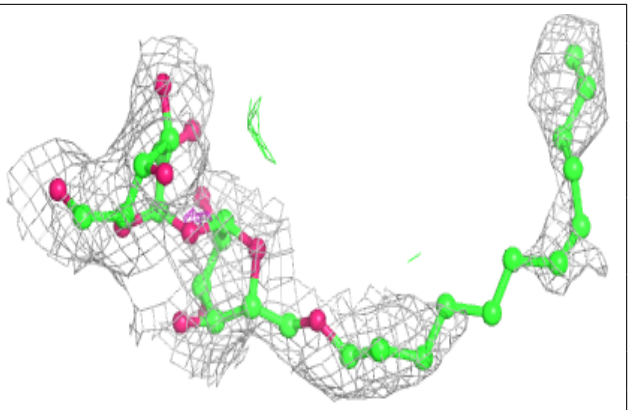
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

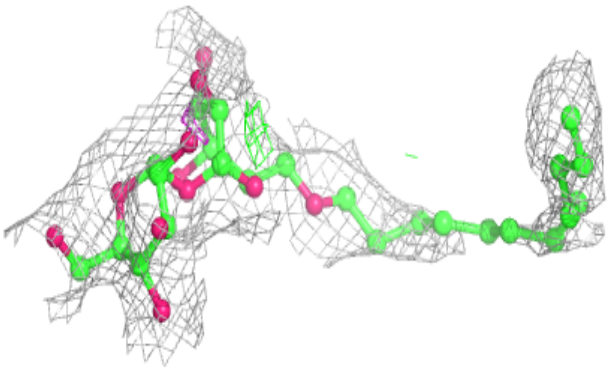
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	L6T	A	1005	35/35	0.73	0.31	74,137,162,166	0
3	L6T	A	1006	35/35	0.73	0.54	96,142,161,163	0
3	L6T	A	1002	35/35	0.81	0.43	98,141,169,187	0
3	L6T	A	1004	35/35	0.84	0.42	68,140,173,183	0
4	MHA	A	1008	13/13	0.85	0.47	85,102,135,139	0
3	L6T	A	1003	35/35	0.87	0.33	68,102,126,132	0
4	MHA	A	1007	13/13	0.91	0.21	85,95,105,111	0
2	FFU	A	1001	22/22	0.93	0.35	85,105,114,129	0

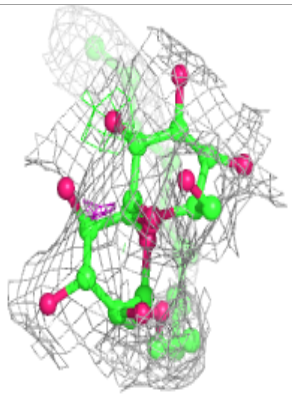
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

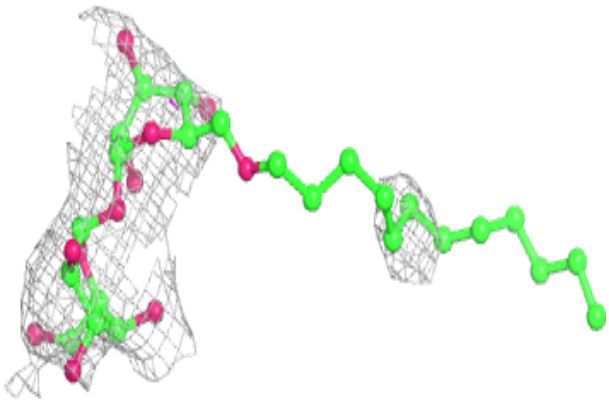


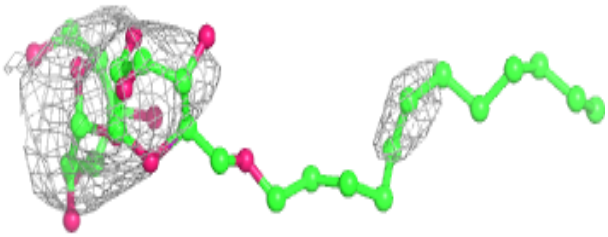


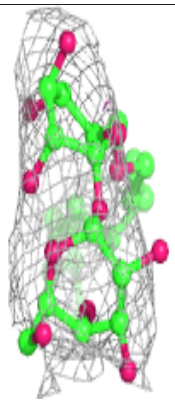


Electron density around L6T A 1006:

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

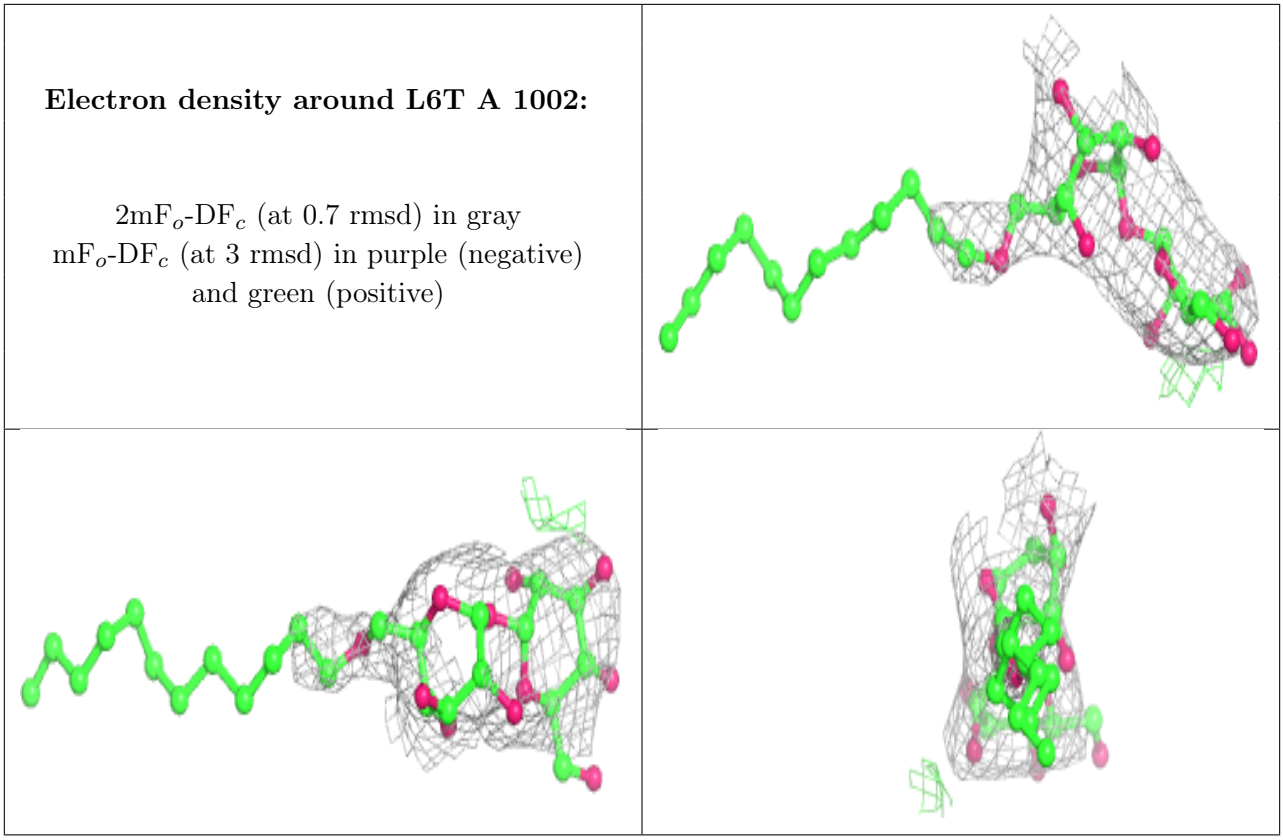






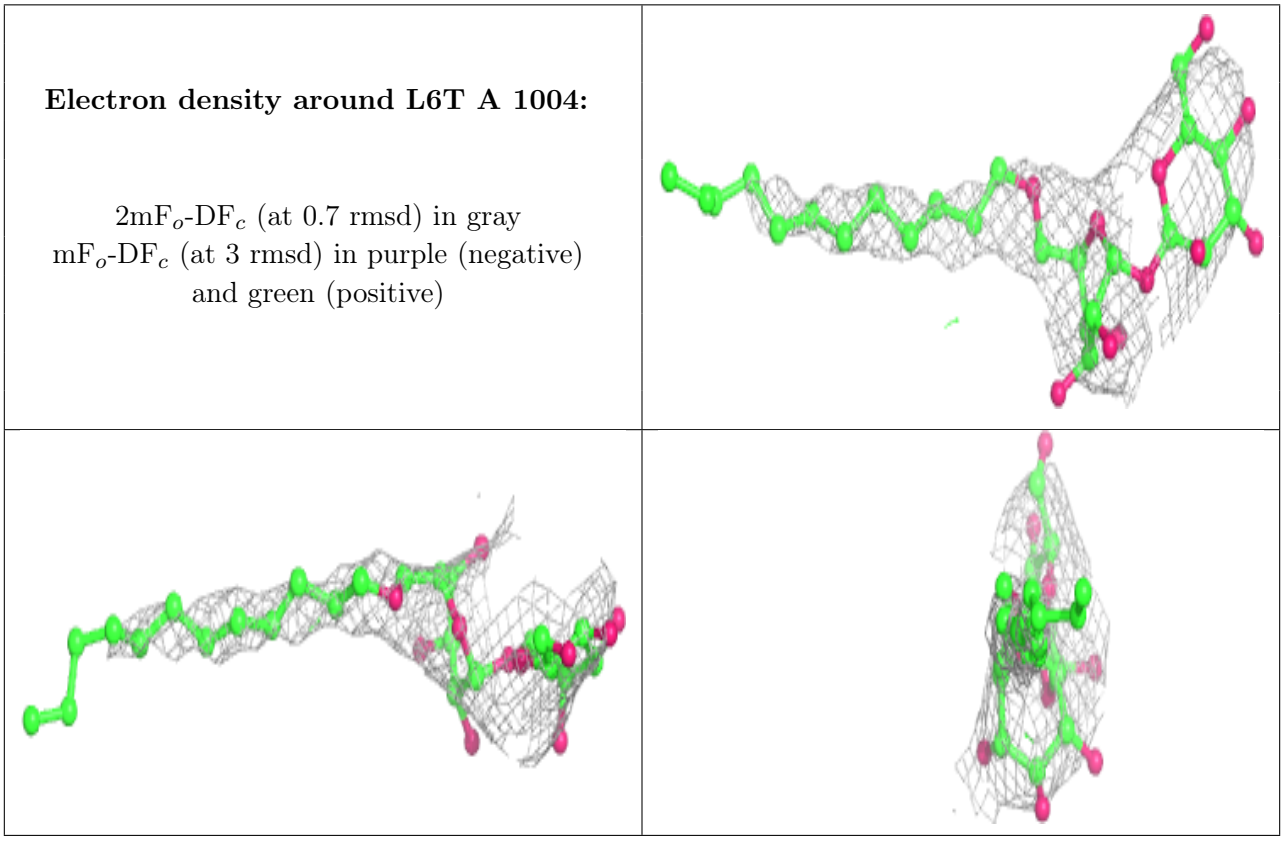
Electron density around L6T A 1002:

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



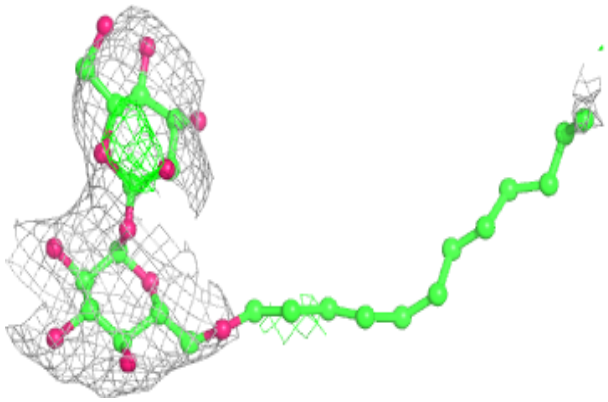
Electron density around L6T A 1004:

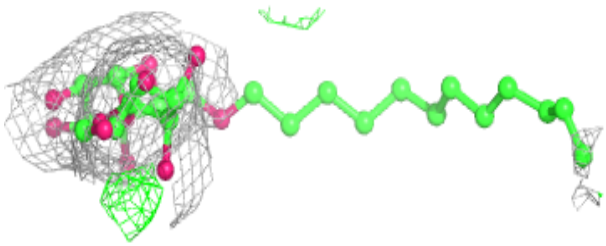
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

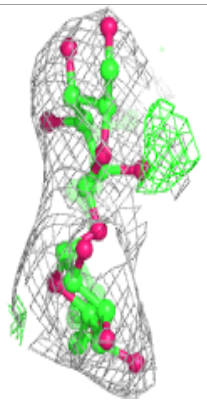


Electron density around L6T A 1003:

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

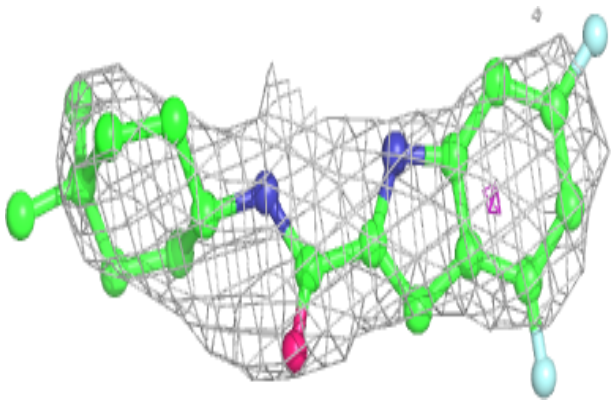


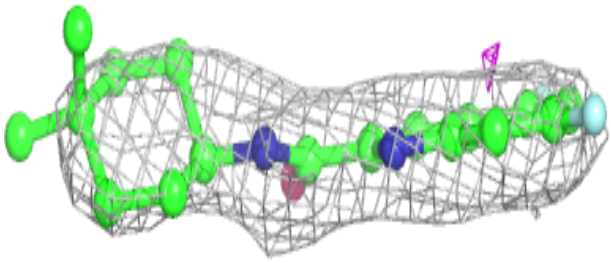


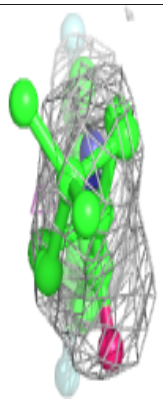


Electron density around FFU A 1001:

$2mF_o$-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.