



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:36 pm BST

PDB ID : 6BW6
Title : Human GPT (DPAGT1) H129 variant in complex with tunicamycin
Authors : Yoo, J.; Kuk, A.C.Y.; Mashalidis, E.H.; Lee, S.-Y.
Deposited on : 2017-12-14
Resolution : 2.95 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

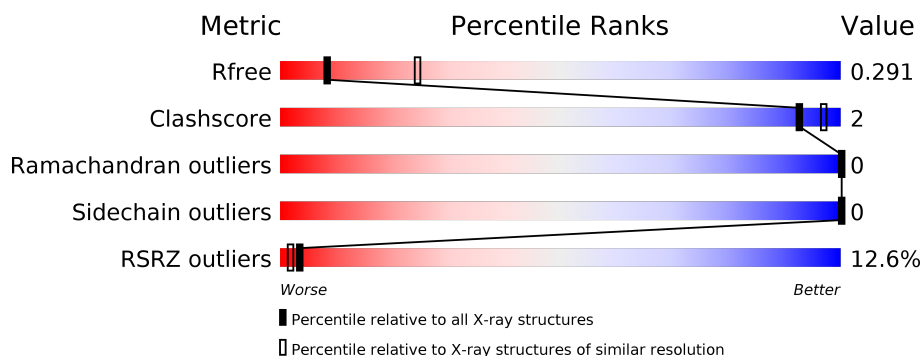
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	417	<div> <div>12%</div> <div> <div></div> <div>82%</div> <div>6%</div> <div>12%</div> </div> </div>
1	B	417	<div> <div>10%</div> <div> <div></div> <div>87%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	417	<div> <div>10%</div> <div> <div></div> <div>84%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	417	<div> <div>12%</div> <div> <div></div> <div>85%</div> <div>•</div> <div>12%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23372 atoms, of which 11728 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 UDP-N-acetylglucosamine--dolichyl-phosphate N-acetylglucosaminephosphotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	368	Total	C	H	N	O	S	0	0	0
			5574	1876	2777	430	471	20			
1	B	374	Total	C	H	N	O	S	0	0	0
			5769	1917	2901	455	475	21			
1	C	365	Total	C	H	N	O	S	0	0	0
			5607	1876	2806	438	467	20			
1	D	369	Total	C	H	N	O	S	0	0	0
			5638	1885	2824	441	468	20			

There are 40 discrepancies between the modelled and reference sequences:

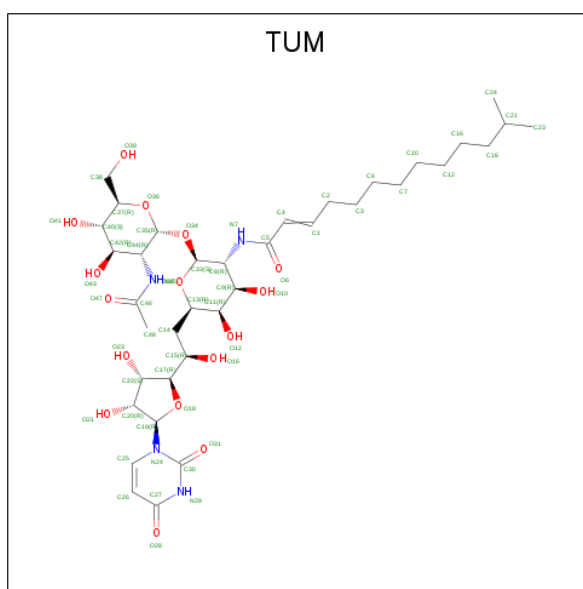
Chain	Residue	Modelled	Actual	Comment	Reference
A	129	HIS	PRO	variant	UNP Q9H3H5
A	409	THR	-	expression tag	UNP Q9H3H5
A	410	ASN	-	expression tag	UNP Q9H3H5
A	411	SER	-	expression tag	UNP Q9H3H5
A	412	LEU	-	expression tag	UNP Q9H3H5
A	413	GLU	-	expression tag	UNP Q9H3H5
A	414	VAL	-	expression tag	UNP Q9H3H5
A	415	LEU	-	expression tag	UNP Q9H3H5
A	416	PHE	-	expression tag	UNP Q9H3H5
A	417	GLN	-	expression tag	UNP Q9H3H5
B	129	HIS	PRO	variant	UNP Q9H3H5
B	409	THR	-	expression tag	UNP Q9H3H5
B	410	ASN	-	expression tag	UNP Q9H3H5
B	411	SER	-	expression tag	UNP Q9H3H5
B	412	LEU	-	expression tag	UNP Q9H3H5
B	413	GLU	-	expression tag	UNP Q9H3H5
B	414	VAL	-	expression tag	UNP Q9H3H5
B	415	LEU	-	expression tag	UNP Q9H3H5
B	416	PHE	-	expression tag	UNP Q9H3H5
B	417	GLN	-	expression tag	UNP Q9H3H5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	129	HIS	PRO	variant	UNP Q9H3H5
C	409	THR	-	expression tag	UNP Q9H3H5
C	410	ASN	-	expression tag	UNP Q9H3H5
C	411	SER	-	expression tag	UNP Q9H3H5
C	412	LEU	-	expression tag	UNP Q9H3H5
C	413	GLU	-	expression tag	UNP Q9H3H5
C	414	VAL	-	expression tag	UNP Q9H3H5
C	415	LEU	-	expression tag	UNP Q9H3H5
C	416	PHE	-	expression tag	UNP Q9H3H5
C	417	GLN	-	expression tag	UNP Q9H3H5
D	129	HIS	PRO	variant	UNP Q9H3H5
D	409	THR	-	expression tag	UNP Q9H3H5
D	410	ASN	-	expression tag	UNP Q9H3H5
D	411	SER	-	expression tag	UNP Q9H3H5
D	412	LEU	-	expression tag	UNP Q9H3H5
D	413	GLU	-	expression tag	UNP Q9H3H5
D	414	VAL	-	expression tag	UNP Q9H3H5
D	415	LEU	-	expression tag	UNP Q9H3H5
D	416	PHE	-	expression tag	UNP Q9H3H5
D	417	GLN	-	expression tag	UNP Q9H3H5

- Molecule 2 is Tunicamycin (three-letter code: TUM) (formula: $C_{37}H_{60}N_4O_{16}$) (labeled as "Ligand of Interest" by author).



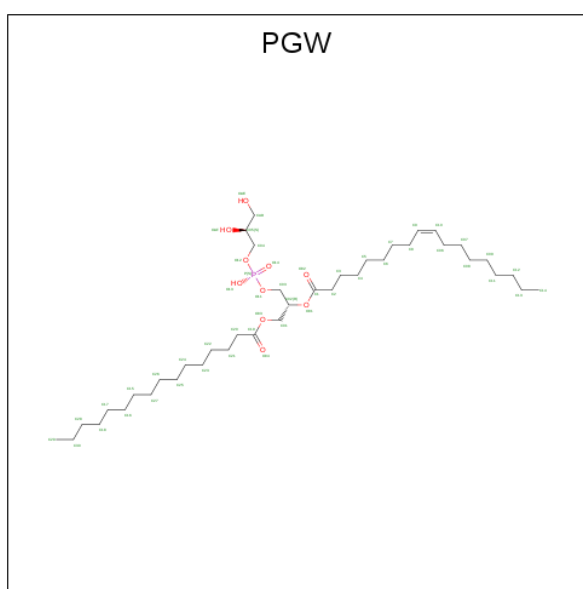
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			117	37	60	4	16		

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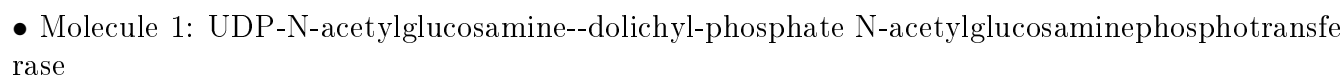
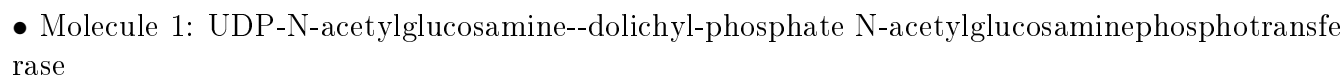
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	0	0
			117	37	60	4	16		
2	C	1	Total	C	H	N	O	0	0
			117	37	60	4	16		
2	D	1	Total	C	H	N	O	0	0
			117	37	60	4	16		

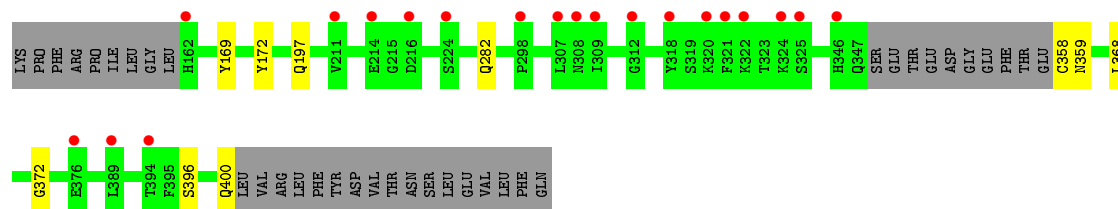
- Molecule 3 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: C₄₀H₇₇O₁₀P).



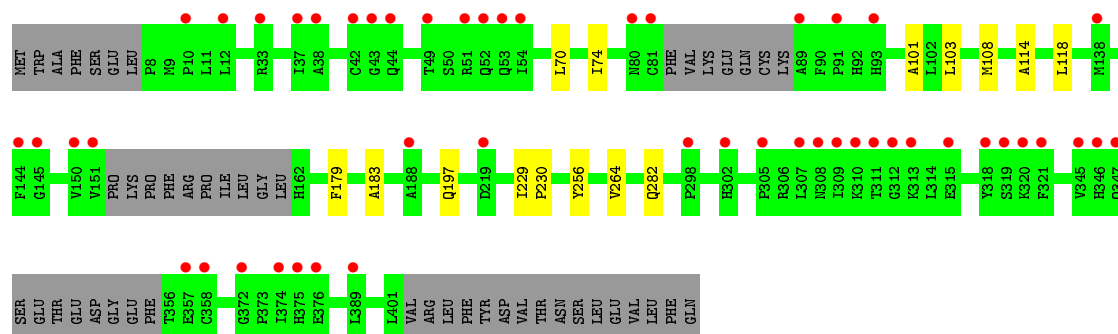
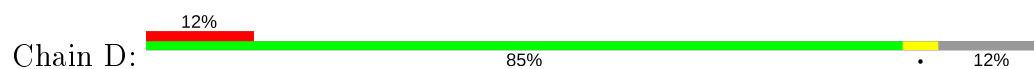
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	P	0	0
			79	24	45	9	1		
3	B	1	Total	C	H	O	P	0	0
			79	24	45	9	1		
3	C	1	Total	C	H	O	P	0	0
			79	24	45	9	1		
3	C	1	Total	C	H	O	P	0	0
			79	24	45	9	1		

- Molecule 1: UDP-N-acetylglucosamine--dolichyl-phosphate N-acetylglucosaminephosphotransferase





- Molecule 1: UDP-N-acetylglucosamine--dolichyl-phosphate N-acetylglucosaminophosphotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	210.62Å 105.36Å 148.08Å 90.00° 103.49° 90.00°	Depositor
Resolution (Å)	94.51 – 2.95 94.51 – 2.95	Depositor EDS
% Data completeness (in resolution range)	55.3 (94.51-2.95) 51.5 (94.51-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.260 , 0.291 0.259 , 0.291	Depositor DCC
R_{free} test set	1832 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	23372	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: PGW, TUM

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	0.27	0/2870	0.41	0/3923
1	B	0.27	0/2940	0.41	0/4009
1	C	0.26	0/2874	0.41	0/3922
1	D	0.27	0/2886	0.41	0/3939
All	All	0.27	0/11570	0.41	0/15793

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	2797	2777	2777	13	0
1	B	2868	2901	2901	7	0
1	C	2801	2806	2806	8	0
1	D	2814	2824	2824	8	0
2	A	57	60	0	1	0
2	B	57	60	0	0	0
2	C	57	60	0	0	0
2	D	57	60	0	0	0
3	A	34	45	45	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	34	45	45	0	0
3	C	68	90	90	0	0
All	All	11644	11728	11488	35	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (35) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:CYS:SG	1:C:359:ASN:N	2.76	0.58
1:C:396:SER:O	1:C:400:GLN:N	2.38	0.56
1:B:108:MET:HG3	1:B:256:TYR:HB3	1.88	0.55
1:B:191:ASN:ND2	1:B:376:GLU:OE2	2.42	0.53
1:C:115:ASP:O	1:C:119:ASN:N	2.39	0.51
1:A:57:SER:OG	1:A:116:ASP:OD2	2.29	0.50
1:A:185:ASN:ND2	2:A:501:TUM:O6	2.45	0.49
1:A:114:ALA:O	1:A:118:LEU:HG	2.12	0.49
1:D:197:GLN:OE1	1:D:282:GLN:NE2	2.46	0.49
1:A:58:GLN:HG3	1:A:248:VAL:HB	1.96	0.48
1:A:120:LEU:O	1:A:125:LYS:NZ	2.46	0.48
1:C:368:LEU:O	1:C:372:GLY:N	2.47	0.47
1:D:114:ALA:O	1:D:118:LEU:HG	2.14	0.47
1:B:197:GLN:OE1	1:B:282:GLN:NE2	2.41	0.47
1:A:368:LEU:O	1:A:372:GLY:N	2.47	0.47
1:D:101:ALA:HB1	1:D:264:VAL:HG11	1.98	0.46
1:B:377:ARG:NH2	1:B:378:ASN:OD1	2.49	0.46
1:C:197:GLN:OE1	1:C:282:GLN:NE2	2.43	0.46
1:C:169:TYR:O	1:C:172:TYR:HB3	2.16	0.46
1:A:140:TYR:O	1:A:145:GLY:N	2.49	0.45
1:B:93:HIS:O	1:B:96:VAL:HG12	2.16	0.45
1:D:229:ILE:HB	1:D:230:PRO:HD3	1.99	0.45
1:C:103:LEU:HA	1:D:103:LEU:HD13	1.99	0.45
1:D:70:LEU:O	1:D:74:ILE:HG13	2.17	0.45
1:D:108:MET:HG3	1:D:256:TYR:HB3	2.00	0.43
1:A:229:ILE:HB	1:A:230:PRO:HD3	2.01	0.42
1:D:179:PHE:O	1:D:183:ALA:N	2.45	0.42
1:A:60:VAL:HG13	1:A:61:ILE:N	2.35	0.42
1:A:122:TRP:O	1:A:126:LEU:HG	2.20	0.41
1:A:219:ASP:HA	1:A:222:VAL:HG12	2.03	0.41
1:A:108:MET:HG2	1:A:260:MET:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:MET:HG2	1:B:260:MET:HB2	2.03	0.41
1:A:169:TYR:O	1:A:172:TYR:HB3	2.21	0.40
1:B:74:ILE:N	1:B:75:PRO:CD	2.85	0.40
1:C:93:HIS:O	1:C:96:VAL:HG12	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	360/417 (86%)	352 (98%)	8 (2%)	0	100	100
1	B	366/417 (88%)	355 (97%)	11 (3%)	0	100	100
1	C	357/417 (86%)	342 (96%)	15 (4%)	0	100	100
1	D	361/417 (87%)	354 (98%)	7 (2%)	0	100	100
All	All	1444/1668 (87%)	1403 (97%)	41 (3%)	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	296/370 (80%)	296 (100%)	0	100	100
1	B	307/370 (83%)	307 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	298/370 (80%)	298 (100%)	0	100	100
1	D	298/370 (80%)	298 (100%)	0	100	100
All	All	1199/1480 (81%)	1199 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some 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 carbohydrates 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	TUM	A	501	-	56,60,60	1.76	11 (19%)	71,84,84	1.27	7 (9%)
2	TUM	D	501	-	56,60,60	1.76	11 (19%)	71,84,84	1.46	8 (11%)
3	PGW	B	501	-	33,33,50	0.88	2 (6%)	35,38,56	0.80	1 (2%)
3	PGW	C	502	-	33,33,50	0.88	2 (6%)	35,38,56	0.80	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TUM	C	501	-	56,60,60	1.75	11 (19%)	71,84,84	1.33	9 (12%)
3	PGW	A	502	-	33,33,50	0.88	2 (6%)	35,38,56	0.81	1 (2%)
3	PGW	C	503	-	33,33,50	0.88	2 (6%)	35,38,56	0.84	1 (2%)
2	TUM	B	502	-	56,60,60	1.76	11 (19%)	71,84,84	1.31	8 (11%)

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	TUM	A	501	-	-	3/37/95/95	0/4/4/4
2	TUM	D	501	-	-	10/37/95/95	0/4/4/4
3	PGW	B	501	-	-	15/37/37/55	-
3	PGW	C	502	-	-	20/37/37/55	-
2	TUM	C	501	-	-	11/37/95/95	0/4/4/4
3	PGW	A	502	-	-	13/37/37/55	-
3	PGW	C	503	-	-	12/37/37/55	-
2	TUM	B	502	-	-	10/37/95/95	0/4/4/4

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	TUM	O18-C19	6.75	1.50	1.41
2	B	502	TUM	O18-C19	6.61	1.50	1.41
2	C	501	TUM	O18-C19	6.60	1.50	1.41
2	D	501	TUM	O18-C19	6.52	1.50	1.41
2	B	502	TUM	C5-N7	5.39	1.47	1.34
2	D	501	TUM	C5-N7	5.38	1.47	1.34
2	C	501	TUM	C5-N7	5.35	1.47	1.34
2	A	501	TUM	C5-N7	5.31	1.47	1.34
2	A	501	TUM	O18-C17	4.03	1.50	1.44
2	C	501	TUM	O18-C17	3.83	1.49	1.44
2	B	502	TUM	O18-C17	3.78	1.49	1.44
2	D	501	TUM	O18-C17	3.77	1.49	1.44
2	B	502	TUM	C20-C19	-3.34	1.48	1.53
2	D	501	TUM	C20-C19	-3.32	1.48	1.53
2	C	501	TUM	C20-C19	-3.13	1.49	1.53
2	C	501	TUM	C46-N45	3.06	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	TUM	C46-N45	3.05	1.44	1.34
2	B	502	TUM	C46-N45	3.01	1.44	1.34
2	D	501	TUM	C46-N45	3.00	1.44	1.34
2	D	501	TUM	C25-N24	-2.97	1.32	1.35
2	A	501	TUM	C20-C19	-2.95	1.49	1.53
2	D	501	TUM	O6-C5	-2.92	1.18	1.24
2	B	502	TUM	C4-C5	2.92	1.54	1.48
2	C	501	TUM	O6-C5	-2.92	1.18	1.24
2	B	502	TUM	O6-C5	-2.84	1.19	1.24
2	A	501	TUM	O6-C5	-2.84	1.19	1.24
2	A	501	TUM	C4-C5	2.81	1.54	1.48
2	C	501	TUM	C4-C5	2.78	1.54	1.48
2	D	501	TUM	C4-C5	2.74	1.54	1.48
2	B	502	TUM	C25-N24	-2.66	1.32	1.35
2	C	501	TUM	C25-N24	-2.63	1.32	1.35
2	A	501	TUM	C25-N24	-2.61	1.32	1.35
2	C	501	TUM	C22-C20	-2.58	1.46	1.53
3	B	501	PGW	O01-C02	-2.55	1.40	1.46
3	C	502	PGW	O01-C02	-2.54	1.40	1.46
2	B	502	TUM	C22-C20	-2.53	1.46	1.53
3	C	503	PGW	O01-C02	-2.53	1.40	1.46
2	A	501	TUM	C22-C20	-2.52	1.46	1.53
2	D	501	TUM	C22-C20	-2.45	1.46	1.53
3	A	502	PGW	O01-C02	-2.43	1.40	1.46
2	B	502	TUM	O28-C27	-2.35	1.18	1.24
2	C	501	TUM	O28-C27	-2.30	1.18	1.24
3	A	502	PGW	O01-C1	2.26	1.40	1.34
2	D	501	TUM	O28-C27	-2.25	1.18	1.24
2	A	501	TUM	O28-C27	-2.24	1.18	1.24
2	C	501	TUM	O47-C46	-2.23	1.18	1.23
2	B	502	TUM	O47-C46	-2.22	1.18	1.23
2	D	501	TUM	O47-C46	-2.20	1.18	1.23
2	A	501	TUM	O47-C46	-2.18	1.18	1.23
3	C	503	PGW	O01-C1	2.14	1.40	1.34
3	C	502	PGW	O01-C1	2.11	1.40	1.34
3	B	501	PGW	O01-C1	2.10	1.40	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	TUM	C33-O32-C13	4.60	122.72	113.69
2	D	501	TUM	C22-C20-C19	4.26	107.40	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	TUM	C22-C20-C19	4.24	107.36	100.98
2	C	501	TUM	C22-C20-C19	4.19	107.28	100.98
2	B	502	TUM	C22-C20-C19	4.13	107.19	100.98
2	D	501	TUM	O32-C13-C11	3.99	116.94	109.69
2	A	501	TUM	C15-C17-C22	-3.81	110.76	115.86
3	C	503	PGW	O01-C1-C2	3.65	119.36	111.50
3	A	502	PGW	O01-C1-C2	3.63	119.31	111.50
2	B	502	TUM	C15-C17-C22	-3.43	111.28	115.86
3	B	501	PGW	O01-C1-C2	3.34	118.69	111.50
2	D	501	TUM	C15-C17-C22	-3.15	111.65	115.86
3	C	502	PGW	O01-C1-C2	3.11	118.20	111.50
2	D	501	TUM	C9-C8-N7	3.05	116.37	110.62
2	C	501	TUM	C15-C17-C22	-2.94	111.93	115.86
2	C	501	TUM	O32-C33-C8	-2.89	104.94	110.58
2	A	501	TUM	C33-O32-C13	2.72	119.02	113.69
2	D	501	TUM	C20-C22-C17	2.71	106.36	102.45
2	B	502	TUM	C2-C1-C4	-2.67	120.13	125.85
2	D	501	TUM	C2-C1-C4	-2.64	120.19	125.85
2	B	502	TUM	C33-O32-C13	2.63	118.84	113.69
2	A	501	TUM	C2-C1-C4	-2.61	120.26	125.85
2	C	501	TUM	C20-C22-C17	2.60	106.21	102.45
2	B	502	TUM	C14-C13-C11	-2.58	109.22	113.47
2	A	501	TUM	C20-C22-C17	2.49	106.05	102.45
2	C	501	TUM	C2-C1-C4	-2.44	120.62	125.85
2	B	502	TUM	C20-C22-C17	2.38	105.89	102.45
2	C	501	TUM	C11-C9-C8	-2.31	106.96	110.34
2	B	502	TUM	O32-C13-C11	2.27	113.82	109.69
2	C	501	TUM	C14-C13-C11	-2.25	109.77	113.47
2	A	501	TUM	C48-C46-N45	2.25	119.90	116.10
2	A	501	TUM	O32-C13-C11	2.24	113.76	109.69
2	C	501	TUM	C33-O32-C13	2.24	118.08	113.69
2	B	502	TUM	C11-C9-C8	-2.09	107.29	110.34
2	D	501	TUM	C48-C46-N45	2.05	119.56	116.10
2	C	501	TUM	C48-C46-N45	2.01	119.50	116.10

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	TUM	C9-C8-N7-C5
2	D	501	TUM	C9-C8-N7-C5
2	D	501	TUM	O16-C15-C17-O18

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Mol	Chain	Res	Type	Atoms
3	B	501	PGW	C03-O11-P-O13
3	B	501	PGW	C04-O12-P-O11
3	B	501	PGW	O12-C04-C05-CAD
3	C	502	PGW	C03-O11-P-O14
3	C	502	PGW	C04-O12-P-O11
3	C	502	PGW	C04-O12-P-O14
2	C	501	TUM	C33-C8-N7-C5
2	C	501	TUM	O16-C15-C17-O18
3	A	502	PGW	O12-C04-C05-CAD
3	C	503	PGW	C03-O11-P-O12
3	C	503	PGW	C03-O11-P-O14
2	B	502	TUM	C33-C8-N7-C5
2	B	502	TUM	C14-C15-C17-O18
2	B	502	TUM	O16-C15-C17-O18
3	B	501	PGW	C05-C04-O12-P
3	B	501	PGW	O12-C04-C05-OAF
3	A	502	PGW	C05-C04-O12-P
3	C	502	PGW	C1-C2-C3-C4
2	D	501	TUM	C1-C4-C5-O6
2	D	501	TUM	C1-C4-C5-N7
3	C	502	PGW	O12-C04-C05-OAF
3	A	502	PGW	O12-C04-C05-OAF
3	C	503	PGW	O12-C04-C05-OAF
3	C	502	PGW	C03-O11-P-O12
3	C	502	PGW	O12-C04-C05-CAD
3	C	503	PGW	O12-C04-C05-CAD
3	B	501	PGW	C5-C6-C7-C8
3	C	503	PGW	C1-C2-C3-C4
3	B	501	PGW	C1-C2-C3-C4
3	A	502	PGW	C3-C4-C5-C6
3	B	501	PGW	C06-C07-C08-C09
2	D	501	TUM	O16-C15-C17-C22
2	C	501	TUM	O16-C15-C17-C22
2	B	502	TUM	O16-C15-C17-C22
2	D	501	TUM	C14-C15-C17-O18
2	C	501	TUM	C14-C15-C17-O18
3	B	501	PGW	C2-C1-O01-C02
2	D	501	TUM	C14-C15-C17-C22
2	C	501	TUM	C14-C15-C17-C22
2	B	502	TUM	C14-C15-C17-C22
3	C	502	PGW	C6-C7-C8-C9
3	A	502	PGW	C06-C07-C08-C09

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Mol	Chain	Res	Type	Atoms
3	C	502	PGW	C4-C5-C6-C7
3	C	502	PGW	C06-C07-C08-C09
3	C	503	PGW	C06-C07-C08-C09
3	B	501	PGW	O02-C1-O01-C02
2	D	501	TUM	O36-C37-C38-O39
3	A	502	PGW	C5-C6-C7-C8
2	C	501	TUM	C12-C10-C7-C6
2	B	502	TUM	O36-C37-C38-O39
3	C	503	PGW	C01-C02-C03-O11
2	A	501	TUM	O36-C37-C38-O39
3	C	503	PGW	C6-C7-C8-C9
2	B	502	TUM	C1-C2-C3-C6
2	C	501	TUM	O36-C37-C38-O39
2	D	501	TUM	C12-C10-C7-C6
3	C	502	PGW	C01-C02-C03-O11
3	A	502	PGW	C6-C7-C8-C9
3	B	501	PGW	C03-O11-P-O12
3	C	502	PGW	O01-C02-C03-O11
2	D	501	TUM	C1-C2-C3-C6
3	C	502	PGW	C09-C11-C12-C13
3	B	501	PGW	O03-C01-C02-O01
3	A	502	PGW	C04-O12-P-O11
3	B	501	PGW	C03-O11-P-O14
3	C	502	PGW	C03-O11-P-O13
3	C	503	PGW	O01-C02-C03-O11
3	A	502	PGW	C2-C3-C4-C5
2	C	501	TUM	C2-C3-C6-C7
3	A	502	PGW	C08-C09-C11-C12
3	B	501	PGW	C09-C11-C12-C13
3	C	502	PGW	C2-C3-C4-C5
3	C	503	PGW	C04-O12-P-O11
3	C	502	PGW	C08-C09-C11-C12
2	B	502	TUM	C12-C10-C7-C6
3	A	502	PGW	C10-C06-C07-C08
3	C	502	PGW	C01-C02-O01-C1
3	C	503	PGW	C7-C8-C9-C10
2	B	502	TUM	C9-C8-N7-C5
3	C	503	PGW	C4-C5-C6-C7
2	B	502	TUM	C4-C1-C2-C3
3	C	502	PGW	C03-C02-O01-C1
2	C	501	TUM	C4-C1-C2-C3
3	A	502	PGW	O01-C02-C03-O11

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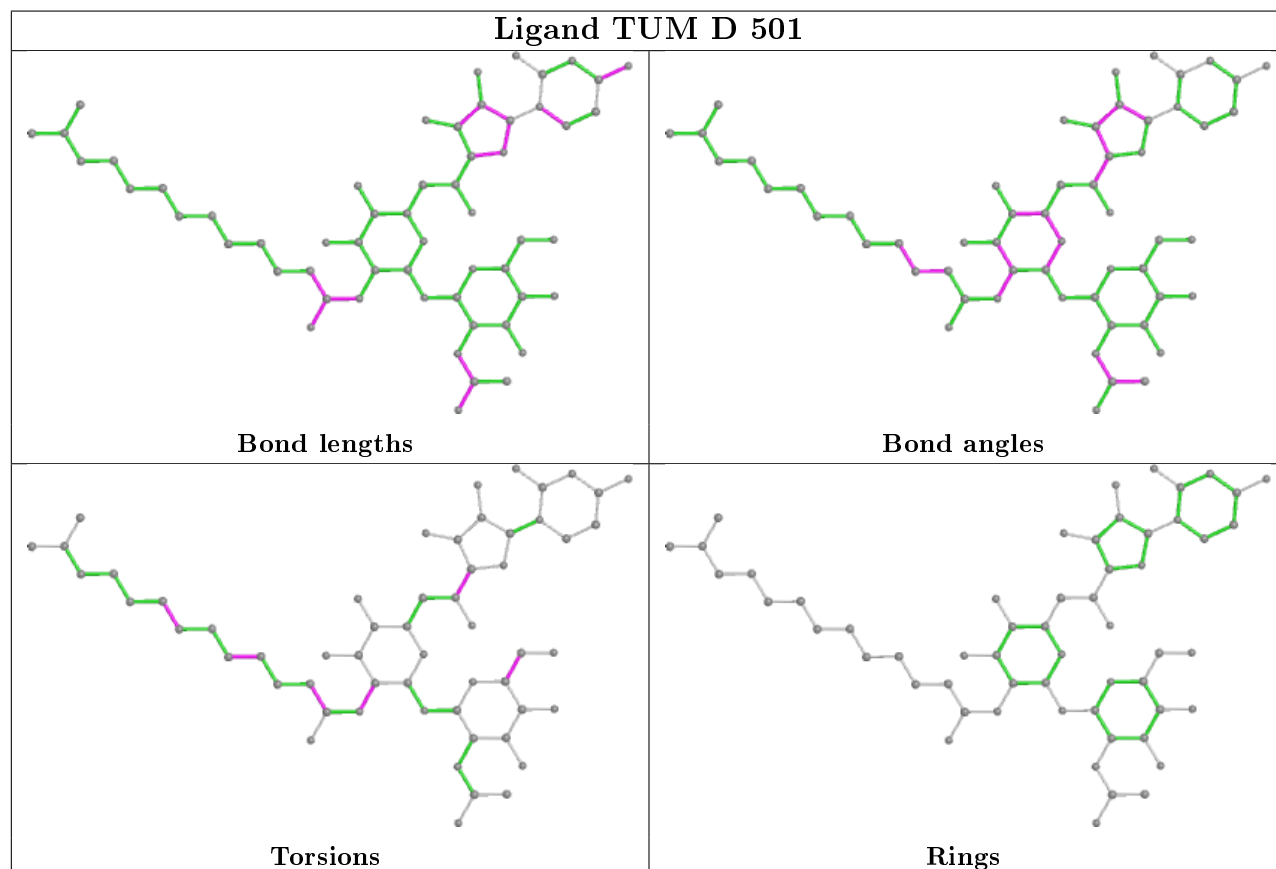
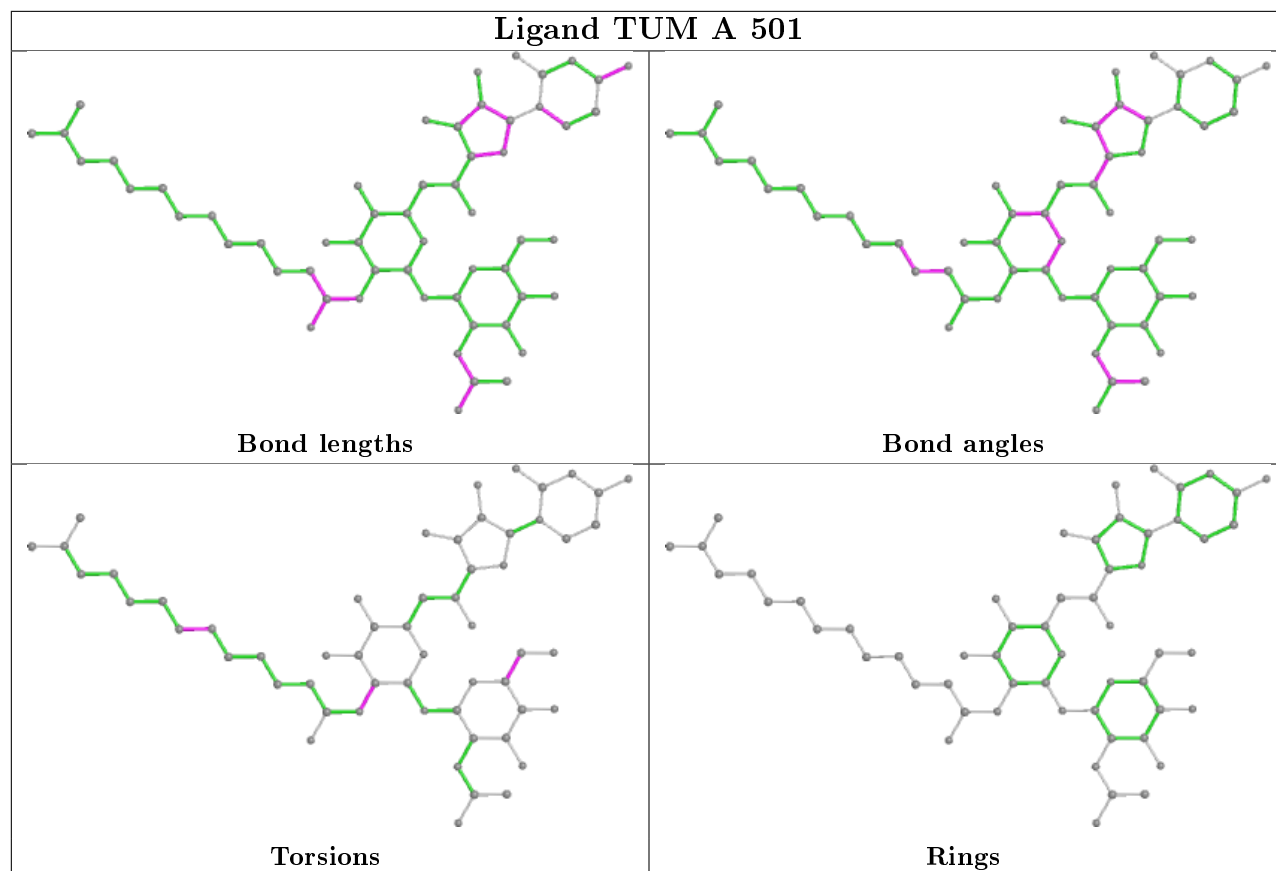
Mol	Chain	Res	Type	Atoms
3	C	502	PGW	C7-C8-C9-C10
2	C	501	TUM	O36-C35-O34-C33
3	A	502	PGW	C7-C8-C9-C10
2	C	501	TUM	C9-C8-N7-C5
3	C	502	PGW	O02-C1-O01-C02
2	A	501	TUM	C3-C6-C7-C10
3	B	501	PGW	C4-C5-C6-C7

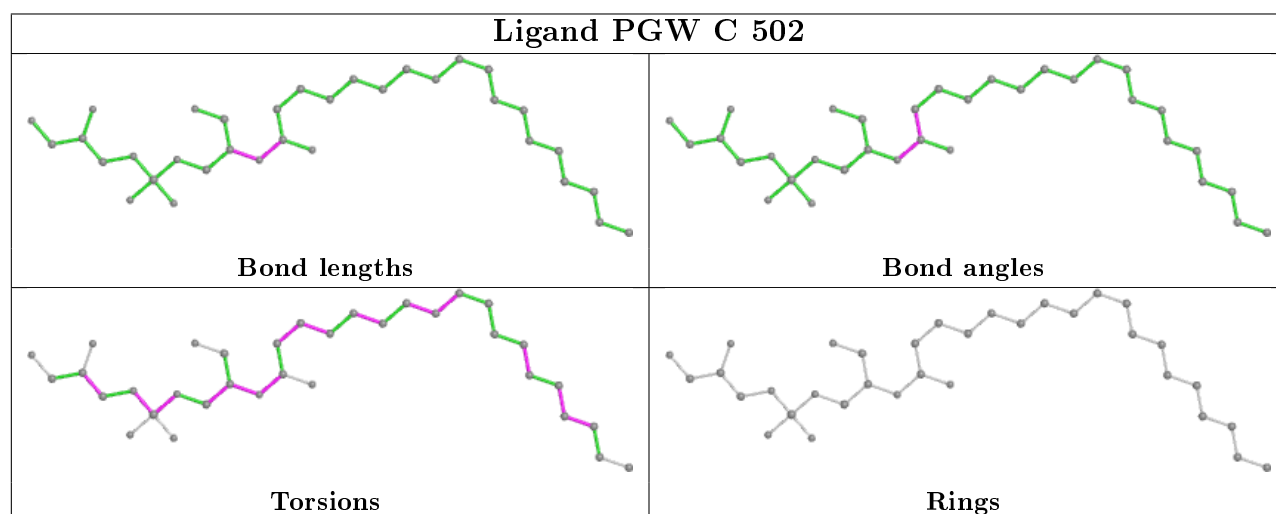
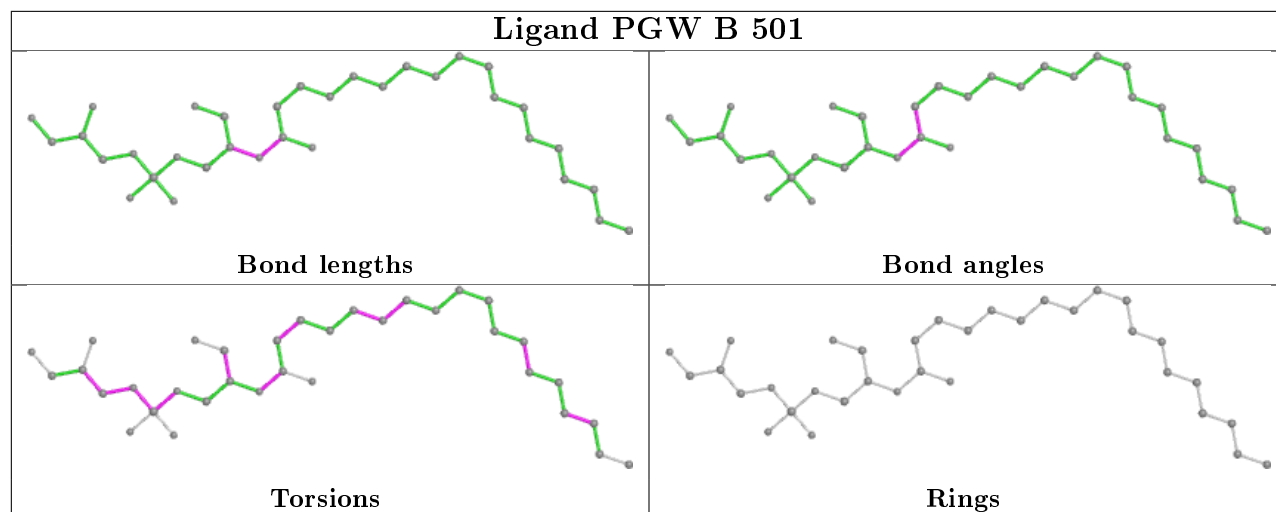
There are no ring outliers.

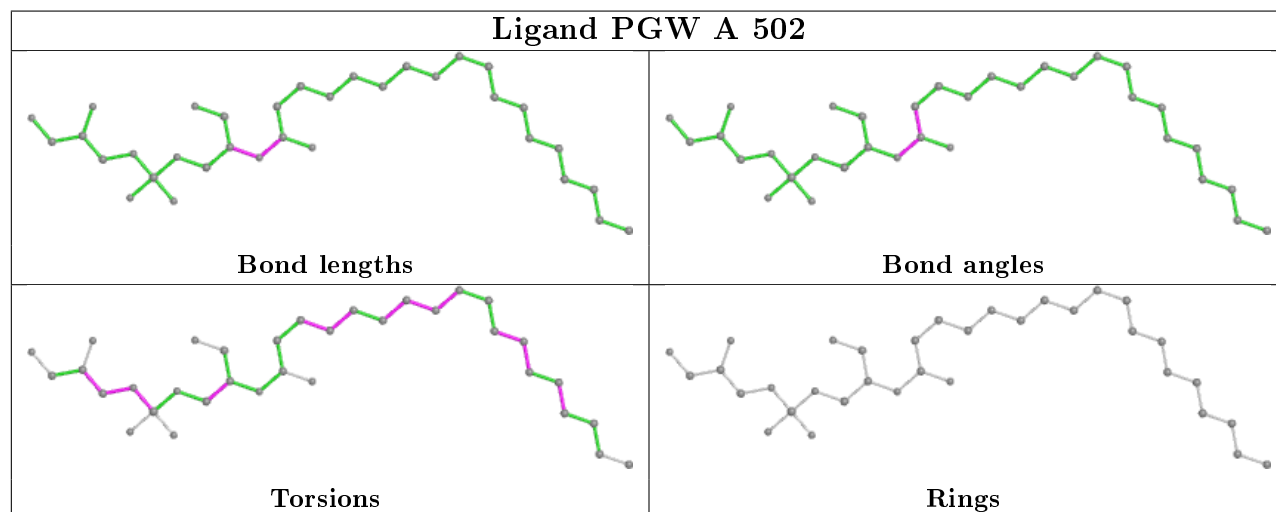
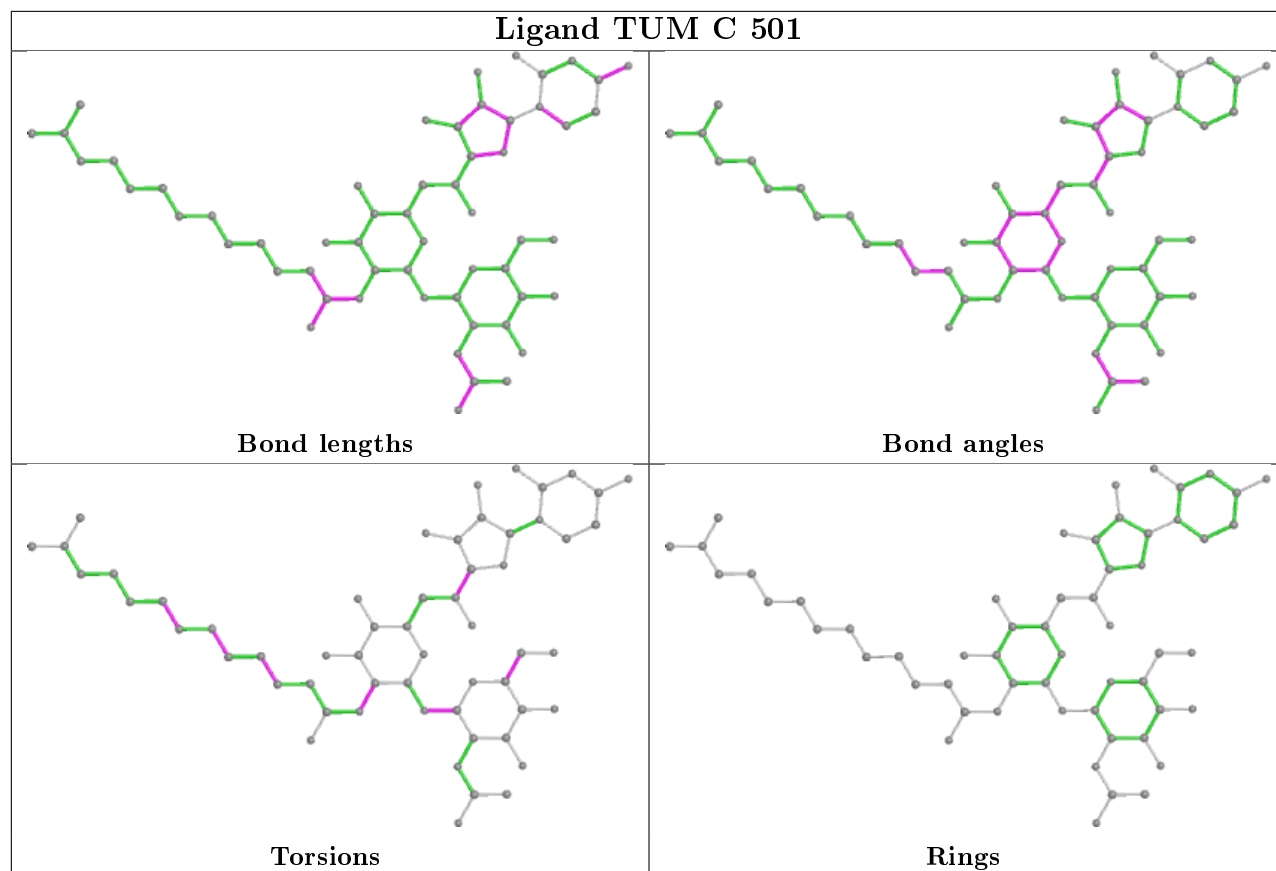
1 monomer is involved in 1 short contact:

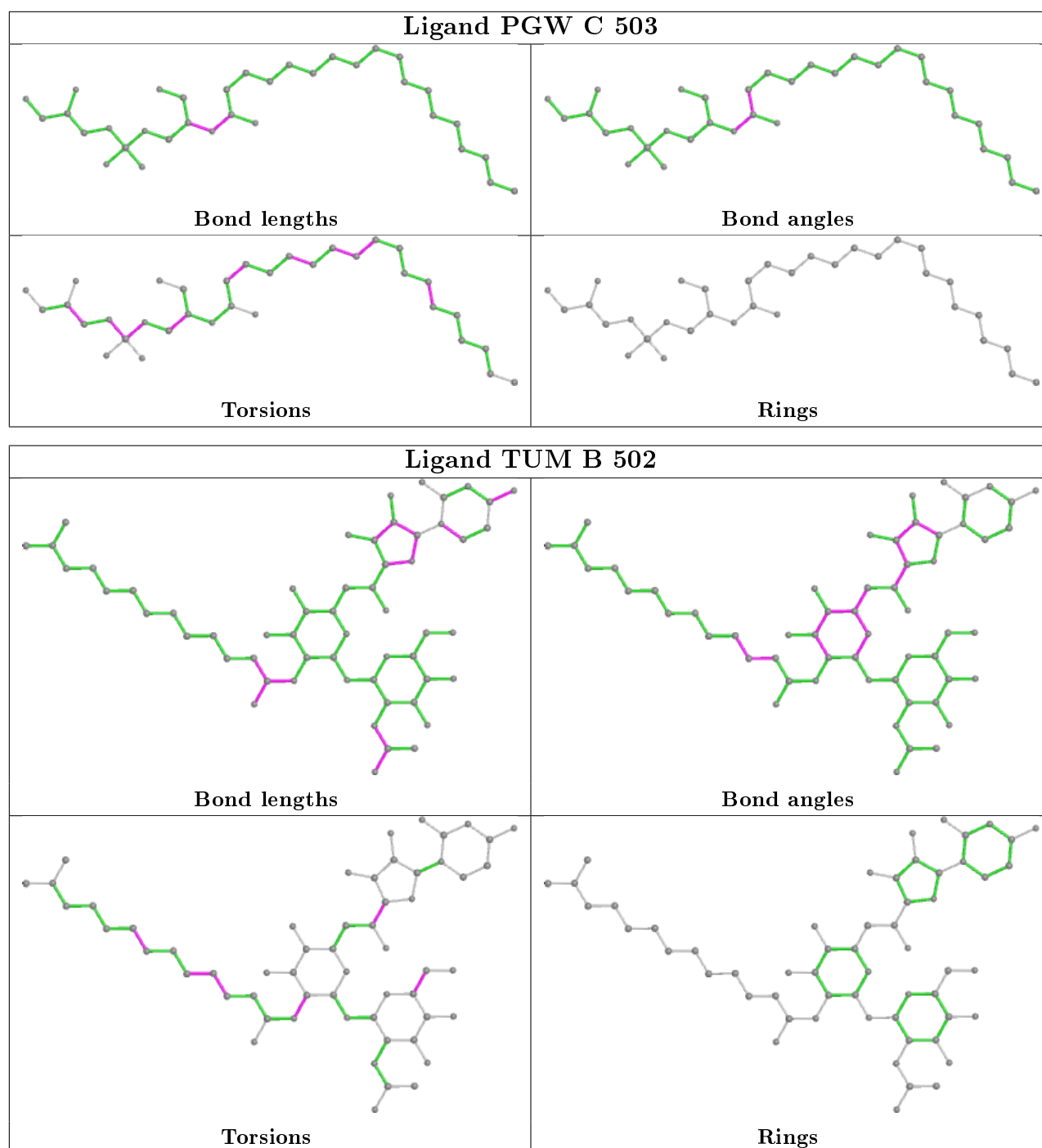
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	TUM	1	0

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 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	368/417 (88%)	0.87	52 (14%) 2 1	11, 54, 87, 108	0
1	B	374/417 (89%)	0.67	41 (10%) 5 3	8, 28, 67, 79	0
1	C	365/417 (87%)	0.79	43 (11%) 4 2	10, 42, 84, 101	0
1	D	369/417 (88%)	0.70	50 (13%) 3 1	8, 35, 73, 90	0
All	All	1476/1668 (88%)	0.76	186 (12%) 3 2	8, 39, 79, 108	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	GLN	9.9
1	D	309	ILE	8.6
1	C	51	ARG	8.2
1	C	52	GLN	7.8
1	C	81	CYS	7.5
1	C	53	GLN	7.3
1	A	51	ARG	7.0
1	A	81	CYS	6.9
1	B	53	GLN	6.6
1	A	44	GLN	6.5
1	D	81	CYS	6.5
1	D	318	TYR	6.2
1	B	357	GLU	6.0
1	A	52	GLN	5.9
1	B	81	CYS	5.8
1	A	53	GLN	5.8
1	D	53	GLN	5.8
1	D	311	THR	5.7
1	B	51	ARG	5.6
1	A	216	ASP	5.6
1	C	49	THR	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	51	ARG	5.3
1	A	49	THR	5.3
1	C	325	SER	5.3
1	D	151	VAL	5.3
1	D	308	ASN	5.1
1	B	321	PHE	5.1
1	A	50	SER	5.1
1	A	309	ILE	5.1
1	C	8	PRO	5.1
1	D	52	GLN	4.9
1	C	44	GLN	4.9
1	C	162	HIS	4.8
1	C	309	ILE	4.7
1	B	355	PHE	4.7
1	C	9	MET	4.7
1	D	313	LYS	4.5
1	C	312	GLY	4.4
1	C	10	PRO	4.3
1	D	49	THR	4.3
1	A	8	PRO	4.3
1	B	44	GLN	4.2
1	B	306	ARG	4.2
1	B	151	VAL	4.1
1	B	356	THR	4.1
1	C	37	ILE	4.1
1	A	214	GLU	4.1
1	D	357	GLU	4.0
1	D	42	CYS	3.9
1	A	54	ILE	3.9
1	A	294	LEU	3.9
1	C	394	THR	3.8
1	C	89	ALA	3.8
1	C	42	CYS	3.8
1	A	277	LEU	3.8
1	C	54	ILE	3.7
1	D	44	GLN	3.6
1	D	320	LYS	3.6
1	A	307	LEU	3.6
1	D	346	HIS	3.6
1	C	320	LYS	3.6
1	C	144	PHE	3.5
1	B	87	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	307	LEU	3.4
1	B	89	ALA	3.4
1	B	309	ILE	3.4
1	D	150	VAL	3.4
1	A	372	GLY	3.3
1	C	50	SER	3.3
1	B	326	LEU	3.3
1	C	321	PHE	3.3
1	A	9	MET	3.3
1	A	245	PRO	3.3
1	A	308	ASN	3.3
1	B	49	THR	3.2
1	D	345	VAL	3.2
1	C	33	ARG	3.2
1	C	145	GLY	3.2
1	B	150	VAL	3.2
1	D	358	CYS	3.1
1	A	33	ARG	3.1
1	D	347	GLN	3.1
1	D	307	LEU	3.1
1	B	37	ILE	3.1
1	D	315	GLU	3.1
1	D	372	GLY	3.1
1	C	80	ASN	3.0
1	B	345	VAL	3.0
1	D	305	PRO	3.0
1	B	311	THR	3.0
1	A	213	LEU	3.0
1	C	307	LEU	3.0
1	D	298	PRO	3.0
1	A	45	ASP	3.0
1	C	150	VAL	3.0
1	C	39	ALA	2.9
1	D	89	ALA	2.9
1	A	89	ALA	2.9
1	D	302	HIS	2.9
1	A	162	HIS	2.9
1	A	80	ASN	2.9
1	B	298	PRO	2.9
1	D	310	LYS	2.9
1	D	321	PHE	2.9
1	C	298	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	12	LEU	2.8
1	B	318	TYR	2.8
1	B	74	ILE	2.8
1	D	12	LEU	2.8
1	B	54	ILE	2.7
1	B	41	LEU	2.7
1	D	54	ILE	2.7
1	D	219	ASP	2.7
1	A	226	TYR	2.7
1	A	312	GLY	2.7
1	A	43	GLY	2.6
1	D	37	ILE	2.6
1	C	216	ASP	2.6
1	C	48	LYS	2.6
1	D	33	ARG	2.6
1	D	319	SER	2.6
1	D	38	ALA	2.6
1	D	80	ASN	2.6
1	D	389	LEU	2.5
1	A	46	LEU	2.5
1	C	318	TYR	2.5
1	A	72	CYS	2.5
1	B	373	PRO	2.5
1	A	318	TYR	2.4
1	C	346	HIS	2.4
1	A	360	ASN	2.4
1	A	37	ILE	2.4
1	A	90	PHE	2.4
1	B	162	HIS	2.4
1	C	322	LYS	2.4
1	C	324	LYS	2.4
1	D	144	PHE	2.4
1	A	244	TYR	2.4
1	A	42	CYS	2.4
1	B	170	TYR	2.4
1	B	374	ILE	2.4
1	C	211	VAL	2.3
1	D	43	GLY	2.3
1	A	223	PHE	2.3
1	A	286	PHE	2.3
1	D	312	GLY	2.3
1	B	358	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	213	LEU	2.3
1	B	88	LYS	2.3
1	A	207	VAL	2.3
1	D	375	HIS	2.3
1	B	308	ASN	2.2
1	B	320	LYS	2.2
1	D	10	PRO	2.2
1	C	376	GLU	2.2
1	C	308	ASN	2.2
1	D	91	PRO	2.2
1	C	224	SER	2.2
1	A	198	SER	2.2
1	D	374	ILE	2.2
1	D	188	ALA	2.2
1	B	334	LEU	2.1
1	B	346	HIS	2.1
1	C	214	GLU	2.1
1	A	243	TRP	2.1
1	D	376	GLU	2.1
1	A	17	VAL	2.1
1	B	43	GLY	2.1
1	D	93	HIS	2.1
1	A	183	ALA	2.1
1	A	200	VAL	2.1
1	A	219	ASP	2.1
1	D	145	GLY	2.1
1	A	310	LYS	2.1
1	C	389	LEU	2.0
1	B	38	ALA	2.0
1	A	11	LEU	2.0
1	A	302	HIS	2.0
1	A	215	GLY	2.0
1	A	291	PRO	2.0
1	A	138	MET	2.0
1	D	138	MET	2.0
1	A	376	GLU	2.0
1	B	325	SER	2.0
1	C	138	MET	2.0
1	B	80	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

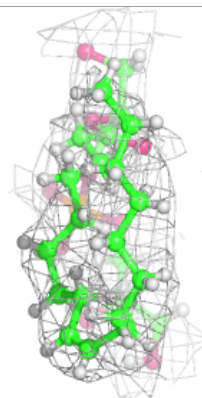
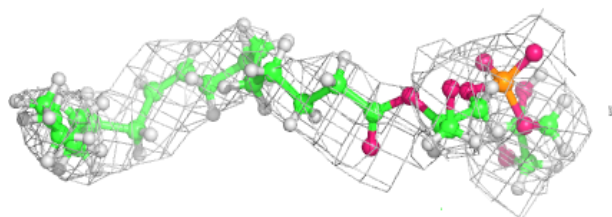
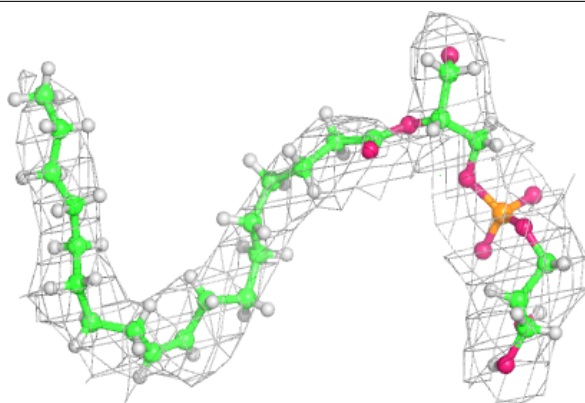
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PGW	A	502	34/51	0.87	0.24	18,64,92,110	0
3	PGW	C	503	34/51	0.89	0.23	9,43,91,119	0
3	PGW	B	501	34/51	0.90	0.20	14,41,80,87	0
3	PGW	C	502	34/51	0.90	0.27	9,40,93,100	0
2	TUM	A	501	57/57	0.93	0.21	28,49,69,81	0
2	TUM	B	502	57/57	0.93	0.25	45,57,75,84	0
2	TUM	C	501	57/57	0.94	0.23	27,45,69,83	0
2	TUM	D	501	57/57	0.94	0.23	15,34,58,69	0

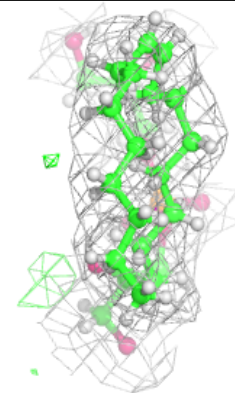
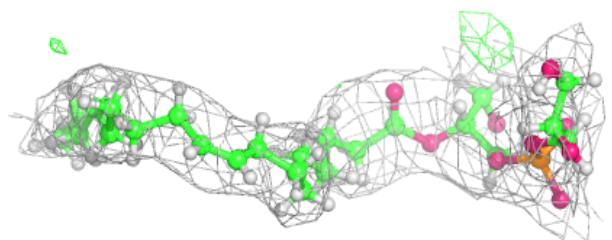
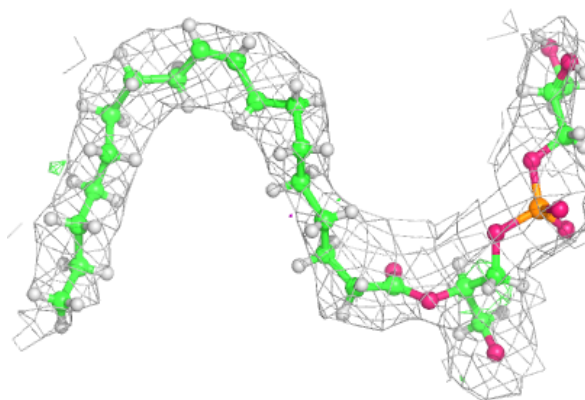
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PGW A 502:

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

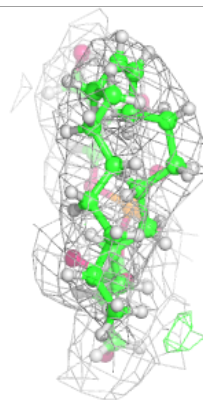
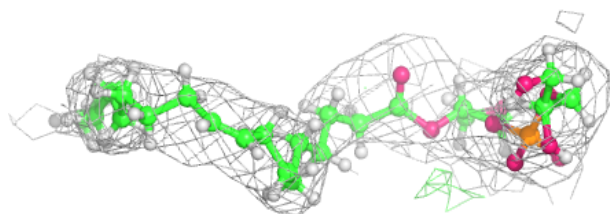
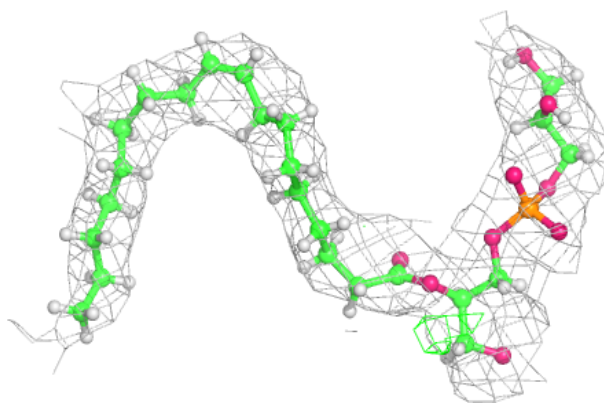
**Electron density around PGW C 503:**

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

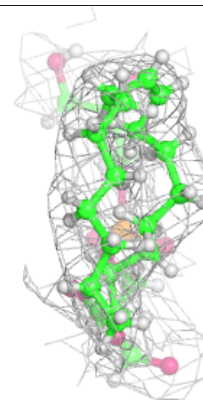
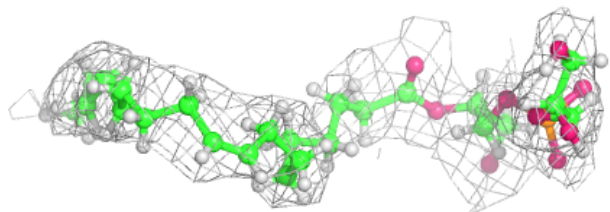
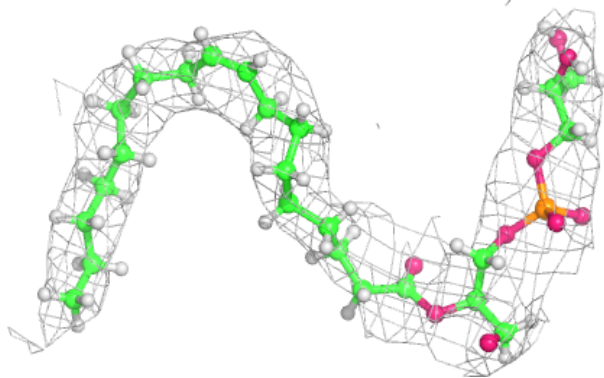


Electron density around PGW B 501:

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

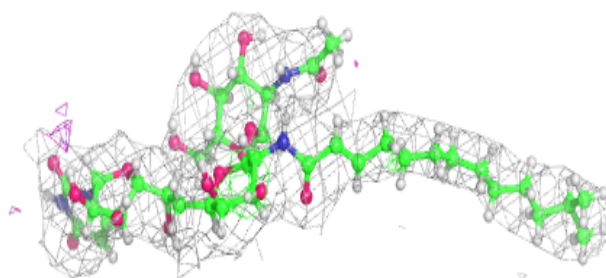
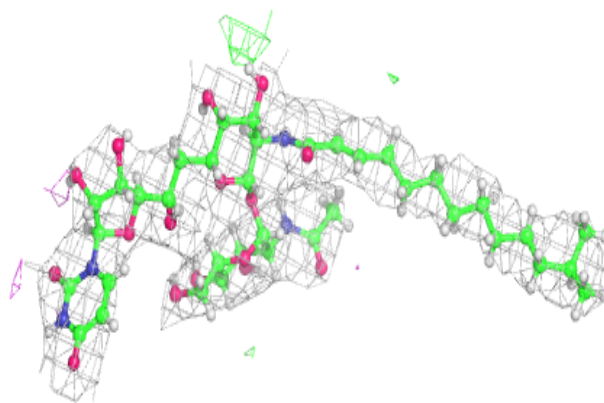
**Electron density around PGW C 502:**

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

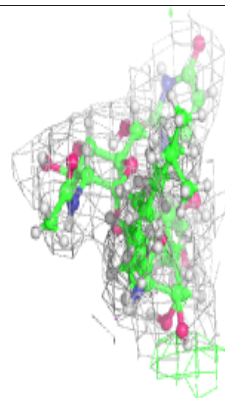
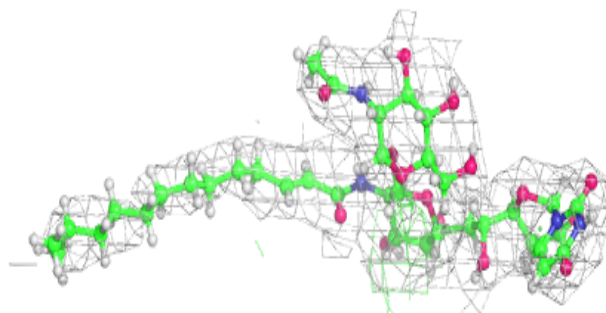
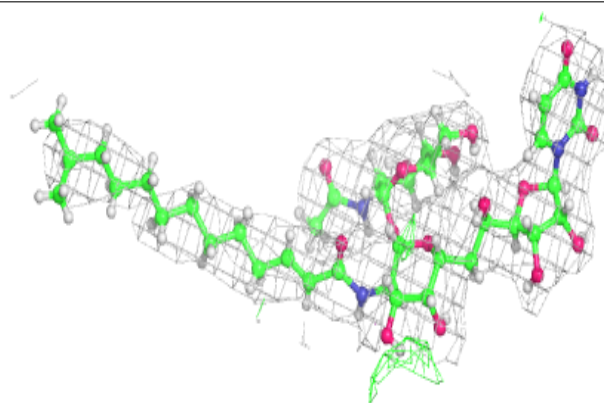


Electron density around TUM A 501:

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

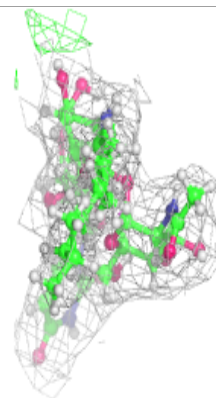
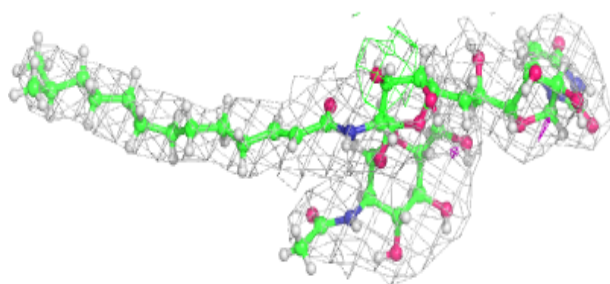
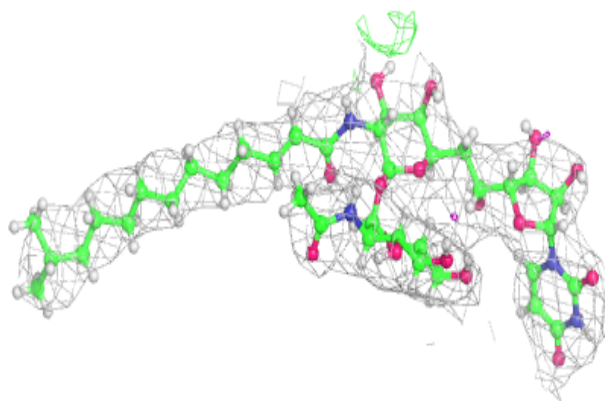
**Electron density around TUM B 502:**

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

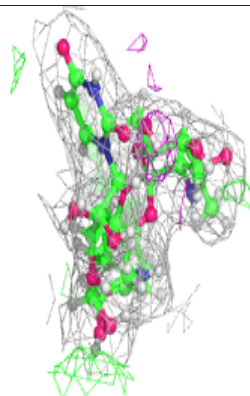
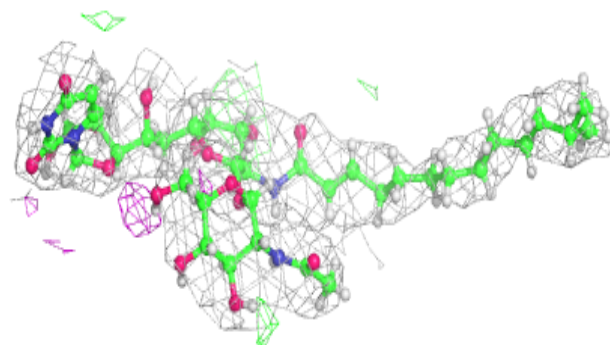
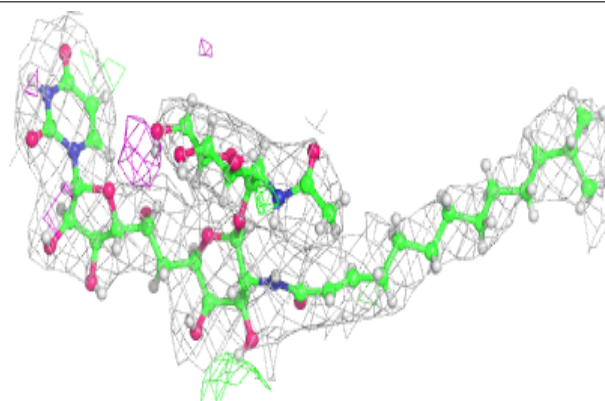


Electron density around TUM C 501:

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

**Electron density around TUM D 501:**

$2mF_o-DF_c$ (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.