



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:08 am BST

PDB ID : 5L26  
Title : Structure of CNTnw in an inward-facing substrate-bound state  
Authors : Hirschi, M.; Johnson, Z.L.; Lee, S.-Y.  
Deposited on : 2016-07-31  
Resolution : 3.40 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](mailto: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.

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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

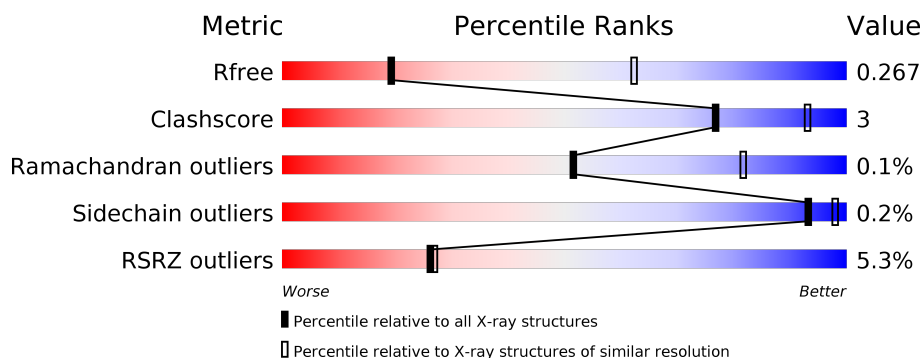
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	431	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div></div> </div> <div></div> </div>
1	B	431	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div></div> </div> <div></div> </div>
1	C	431	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>6%</div> </div> <div></div> </div>

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
2	6ZL	A	501	-	-	-	X
2	6ZL	A	502	-	-	-	X
2	6ZL	A	503	-	-	-	X
2	6ZL	A	504	-	-	-	X
2	6ZL	C	502	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8985 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.

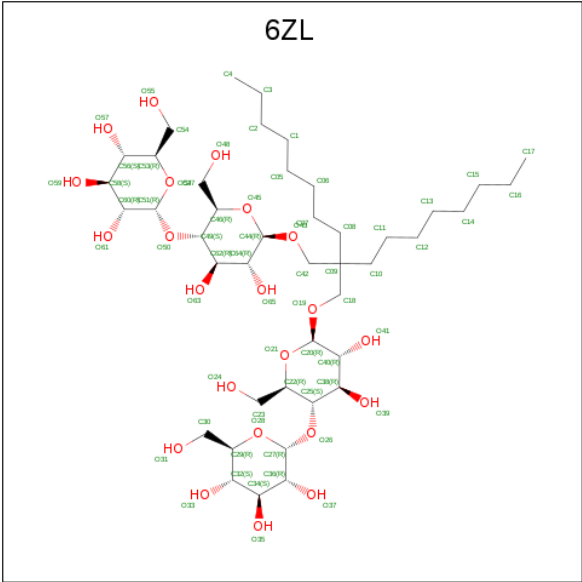
- Molecule 1 is a protein called Nucleoside permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			2947	1931	479	520	17			
1	B	415	Total	C	N	O	S	0	0	0
			2881	1895	466	505	15			
1	C	406	Total	C	N	O	S	0	0	0
			2823	1853	450	505	15			

There are 18 discrepancies between the modelled and reference sequences:

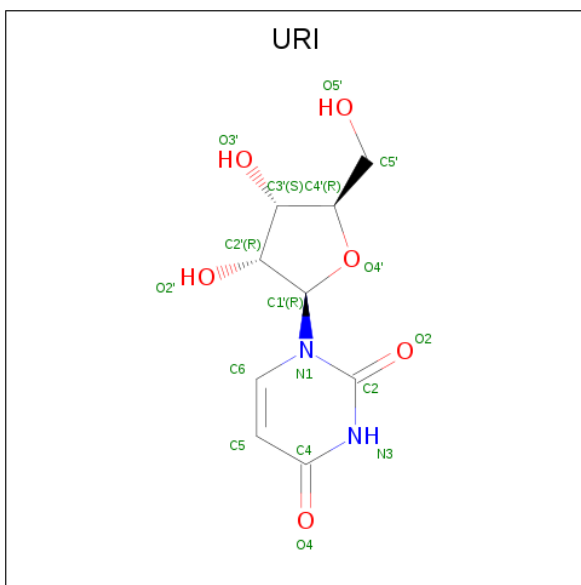
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP G4CRQ5
A	-4	PRO	-	expression tag	UNP G4CRQ5
A	-3	ALA	-	expression tag	UNP G4CRQ5
A	-2	VAL	-	expression tag	UNP G4CRQ5
A	-1	PRO	-	expression tag	UNP G4CRQ5
A	0	ARG	-	expression tag	UNP G4CRQ5
B	-5	GLY	-	expression tag	UNP G4CRQ5
B	-4	PRO	-	expression tag	UNP G4CRQ5
B	-3	ALA	-	expression tag	UNP G4CRQ5
B	-2	VAL	-	expression tag	UNP G4CRQ5
B	-1	PRO	-	expression tag	UNP G4CRQ5
B	0	ARG	-	expression tag	UNP G4CRQ5
C	-5	GLY	-	expression tag	UNP G4CRQ5
C	-4	PRO	-	expression tag	UNP G4CRQ5
C	-3	ALA	-	expression tag	UNP G4CRQ5
C	-2	VAL	-	expression tag	UNP G4CRQ5
C	-1	PRO	-	expression tag	UNP G4CRQ5
C	0	ARG	-	expression tag	UNP G4CRQ5

- Molecule 2 is 2-{{(4-O-alpha-D-glucopyranosyl-beta-D-glucopyranosyl)oxy}methyl}-2-octyld ecyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (three-letter code: 6ZL) (formula: C<sub>43</sub>H<sub>80</sub>O<sub>22</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 9	0	0
2	A	1	Total C O 31 20 11	0	0
2	A	1	Total C O 23 17 6	0	0
2	A	1	Total C O 54 37 17	0	0
2	B	1	Total C O 24 13 11	0	0
2	B	1	Total C O 40 24 16	0	0
2	B	1	Total C O 33 22 11	0	0
2	C	1	Total C O 33 22 11	0	0
2	C	1	Total C O 30 24 6	0	0

- Molecule 3 is URIDINE (three-letter code: URI) (formula: C<sub>9</sub>H<sub>12</sub>N<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	2	6		
3	B	1	Total	C	N	O	0	0
			17	9	2	6		
3	C	1	Total	C	N	O	0	0
			17	9	2	6		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	A	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		

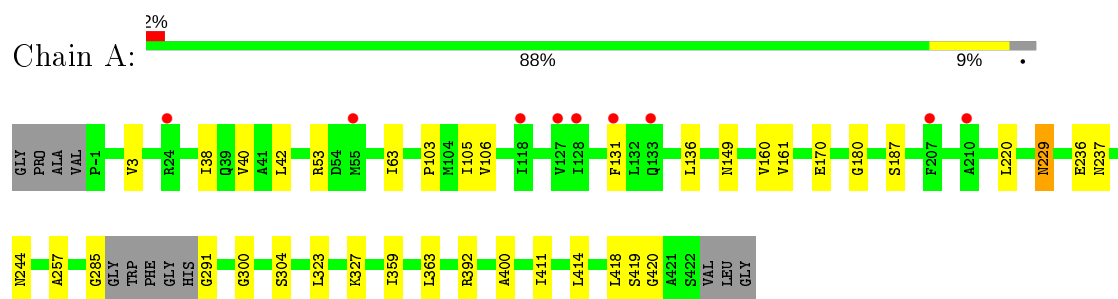
- Molecule 5 is water.

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

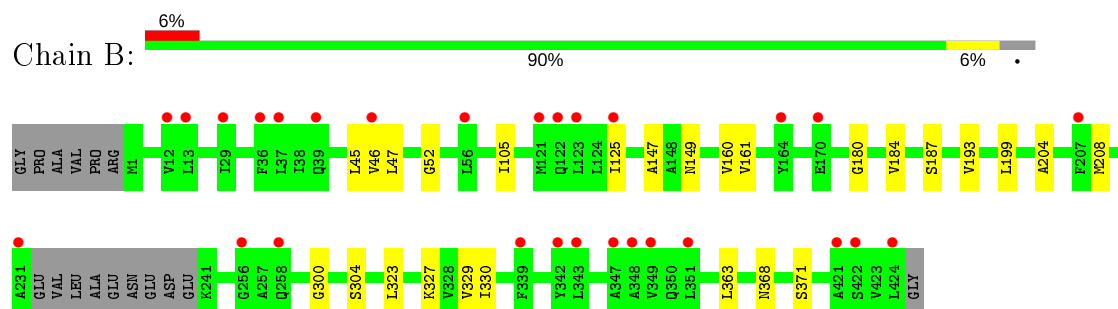
### 3 Residue-property plots [i](#)

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.

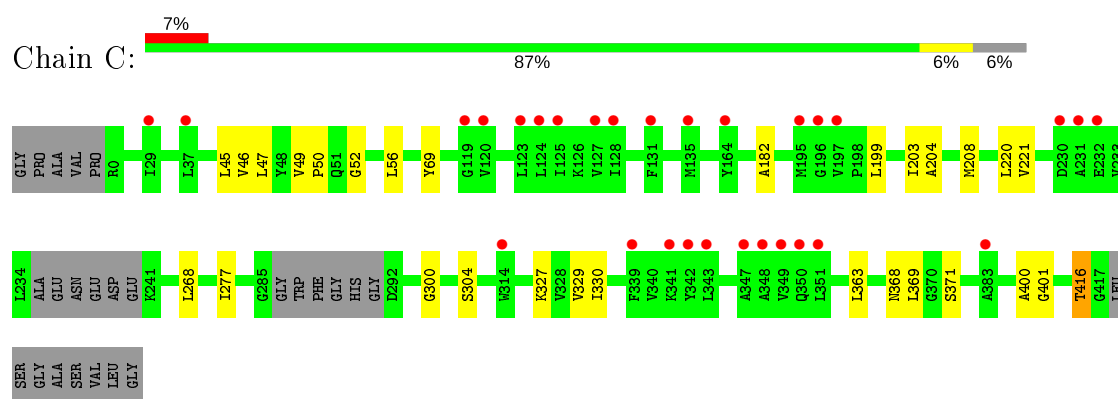
#### • Molecule 1: Nucleoside permease



#### • Molecule 1: Nucleoside permease



#### • Molecule 1: Nucleoside permease



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.22Å 115.22Å 264.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.05 – 3.40 55.05 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (55.05-3.40) 99.7 (55.05-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.242 , 0.266 0.244 , 0.267	Depositor DCC
$R_{free}$ test set	1925 reflections (7.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	101.7	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 38.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	8985	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, URI, 6ZL

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	0.23	0/2995	0.42	1/4081 (0.0%)
1	B	0.21	0/2930	0.38	0/3999
1	C	0.21	0/2869	0.38	0/3917
All	All	0.22	0/8794	0.40	1/11997 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	SER	N-CA-C	6.70	129.09	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	GLU	Peptide
1	A	237	ASN	Peptide
1	C	416	THR	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2947	0	3019	21	0
1	B	2881	0	2930	13	0
1	C	2823	0	2848	18	0
2	A	117	0	0	5	0
2	B	97	0	0	1	0
2	C	63	0	0	4	0
3	A	17	0	12	0	0
3	B	17	0	12	0	0
3	C	17	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
All	All	8985	0	8833	54	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 3.

All (54) 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:42:LEU:HD11	2:A:502:6ZL:C2	2.08	0.83
1:C:69:TYR:HE2	2:C:501:6ZL:O41	1.66	0.79
1:A:63:ILE:HD11	2:A:504:6ZL:C17	2.21	0.70
1:A:327:LYS:HD2	1:A:363:LEU:HA	1.81	0.62
1:C:327:LYS:HD2	1:C:363:LEU:HA	1.81	0.62
1:B:327:LYS:HD2	1:B:363:LEU:HA	1.81	0.61
1:B:329:VAL:HG23	1:B:330:ILE:HG12	1.83	0.61
1:C:300:GLY:O	1:C:304:SER:OG	2.15	0.61
1:C:329:VAL:HG23	1:C:330:ILE:HG12	1.82	0.61
1:C:204:ALA:HB1	1:C:208:MET:HE3	1.82	0.59
1:B:105:ILE:HA	1:B:187:SER:HB2	1.85	0.58
1:B:46:VAL:HG23	1:B:47:LEU:HG	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLY:O	1:A:291:GLY:N	2.39	0.56
1:A:53:ARG:NH2	1:A:418:LEU:HD11	2.20	0.56
2:A:503:6ZL:C3	1:C:277:ILE:HD11	2.37	0.55
1:C:46:VAL:HB	1:C:56:LEU:HD22	1.89	0.54
2:C:502:6ZL:C07	2:C:502:6ZL:C12	2.86	0.54
2:C:502:6ZL:C07	2:C:502:6ZL:C11	2.86	0.54
1:B:160:VAL:HG23	1:B:161:VAL:HG13	1.90	0.53
1:C:69:TYR:CE2	2:C:501:6ZL:O41	2.55	0.53
2:B:501:6ZL:O37	2:B:501:6ZL:O24	2.27	0.52
1:A:103:PRO:HB3	1:C:268:LEU:HD11	1.92	0.51
1:C:46:VAL:HG23	1:C:47:LEU:HG	1.93	0.51
1:C:416:THR:O	1:C:416:THR:HG23	2.12	0.50
2:A:504:6ZL:C27	2:A:504:6ZL:C23	2.91	0.49
1:B:204:ALA:HB1	1:B:208:MET:HE3	1.94	0.48
1:B:300:GLY:O	1:B:304:SER:OG	2.20	0.48
1:A:170:GLU:OE2	1:A:392:ARG:NH2	2.48	0.47
1:B:125:ILE:HG23	1:B:147:ALA:HB3	1.96	0.47
1:A:105:ILE:HA	1:A:187:SER:HB2	1.96	0.46
1:A:160:VAL:HG23	1:A:161:VAL:HG13	1.97	0.46
1:B:149:ASN:OD1	1:B:180:GLY:HA2	2.15	0.46
1:A:418:LEU:HD12	1:A:420:GLY:H	1.79	0.46
1:B:45:LEU:O	1:B:52:GLY:HA3	2.15	0.46
1:A:300:GLY:O	1:A:304:SER:OG	2.24	0.46
1:C:182:ALA:HB2	1:C:401:GLY:HA2	1.98	0.45
1:B:323:LEU:HB3	1:B:363:LEU:HD21	1.98	0.45
1:A:106:VAL:HG22	1:A:257:ALA:HA	1.98	0.45
1:A:323:LEU:HD23	1:A:359:ILE:HG21	1.98	0.45
1:A:220:LEU:HD12	1:A:400:ALA:HB2	1.99	0.45
1:A:38:ILE:HD12	1:A:136:LEU:HD21	1.98	0.44
1:C:368:ASN:OD1	1:C:371:SER:N	2.50	0.44
1:C:45:LEU:O	1:C:52:GLY:HA3	2.18	0.44
1:A:40:VAL:HA	1:A:411:ILE:HD13	2.01	0.43
1:A:244:ASN:ND2	1:C:369:LEU:HB3	2.34	0.43
1:A:3:VAL:HG12	1:A:414:LEU:HD11	2.02	0.42
1:C:49:VAL:HA	1:C:50:PRO:HD3	1.91	0.42
1:C:220:LEU:HD12	1:C:400:ALA:HB2	2.01	0.41
1:B:368:ASN:OD1	1:B:371:SER:N	2.54	0.41
1:A:149:ASN:OD1	1:A:180:GLY:HA2	2.21	0.41
1:A:229:ASN:OD1	1:A:229:ASN:N	2.48	0.41
1:B:193:VAL:HG21	1:B:199:LEU:HD13	2.02	0.41
1:C:199:LEU:O	1:C:203:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:CD2	2:A:502:6ZL:C06	3.04	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	415/431 (96%)	404 (97%)	11 (3%)	0	100	100
1	B	411/431 (95%)	399 (97%)	11 (3%)	1 (0%)	47	78
1	C	400/431 (93%)	389 (97%)	11 (3%)	0	100	100
All	All	1226/1293 (95%)	1192 (97%)	33 (3%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	286/322 (89%)	285 (100%)	1 (0%)	92	97
1	B	273/322 (85%)	273 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	269/322 (84%)	268 (100%)	1 (0%)	91	95
All	All	828/966 (86%)	826 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	C	221	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	326	GLN
1	A	405	ASN
1	B	405	ASN
1	C	405	ASN

### 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](#)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	6ZL	A	502	-	32,32,68	0.65	0	43,43,94	0.73	1 (2%)
3	URI	B	504	-	14,18,18	1.10	1 (7%)	14,26,26	1.16	1 (7%)
2	6ZL	C	502	-	30,30,68	0.63	0	35,36,94	0.82	1 (2%)
3	URI	C	503	-	14,18,18	1.09	1 (7%)	14,26,26	1.16	1 (7%)
2	6ZL	A	503	-	23,23,68	0.65	0	28,28,94	0.84	1 (3%)
2	6ZL	B	503	-	34,34,68	0.67	0	45,45,94	0.95	2 (4%)
2	6ZL	A	504	-	56,56,68	0.69	0	74,76,94	0.87	2 (2%)
3	URI	A	505	-	14,18,18	1.10	1 (7%)	14,26,26	1.17	1 (7%)
2	6ZL	B	502	-	42,42,68	0.72	0	57,59,94	0.72	0
2	6ZL	C	501	-	34,34,68	0.64	0	45,45,94	0.73	1 (2%)
2	6ZL	B	501	-	25,25,68	0.73	0	36,36,94	0.88	1 (2%)
2	6ZL	A	501	-	8,8,68	0.80	0	7,7,94	0.33	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	6ZL	A	502	-	-	9/17/57/126	0/2/2/4
3	URI	B	504	-	-	0/4/22/22	0/2/2/2
2	6ZL	C	502	-	-	11/23/43/126	0/1/1/4
3	URI	C	503	-	-	0/4/22/22	0/2/2/2
2	6ZL	A	503	-	-	10/15/35/126	0/1/1/4
2	6ZL	B	503	-	-	8/19/59/126	0/2/2/4
2	6ZL	A	504	-	-	12/40/100/126	0/3/3/4
3	URI	A	505	-	-	0/4/22/22	0/2/2/2
2	6ZL	B	502	-	-	12/22/79/126	0/3/3/4
2	6ZL	C	501	-	-	17/19/59/126	0/2/2/4
2	6ZL	B	501	-	-	6/10/50/126	0/2/2/4
2	6ZL	A	501	-	-	2/6/6/126	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	504	URI	C4-N3	3.14	1.38	1.33
3	A	505	URI	C4-N3	3.12	1.38	1.33
3	C	503	URI	C4-N3	3.08	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	505	URI	C5-C4-N3	-3.97	114.58	123.31
3	C	503	URI	C5-C4-N3	-3.95	114.61	123.31
3	B	504	URI	C5-C4-N3	-3.94	114.64	123.31
2	B	501	6ZL	C18-O19-C20	3.07	118.01	113.27
2	A	503	6ZL	C18-O19-C20	2.52	118.02	113.84
2	A	502	6ZL	C18-O19-C20	2.51	118.00	113.84
2	C	501	6ZL	C18-O19-C20	2.50	117.99	113.84
2	A	504	6ZL	C11-C10-C09	-2.39	109.48	117.16
2	A	504	6ZL	C07-C08-C09	-2.38	109.51	117.16
2	B	503	6ZL	C18-O19-C20	2.30	117.65	113.84
2	B	503	6ZL	C27-O26-C25	2.29	123.62	117.96
2	C	502	6ZL	C18-O19-C20	2.18	118.01	113.74

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	6ZL	C09-C18-O19-C20
2	A	502	6ZL	O21-C20-O19-C18
2	C	502	6ZL	O21-C20-O19-C18
2	C	502	6ZL	C40-C20-O19-C18
2	A	503	6ZL	C09-C18-O19-C20
2	A	503	6ZL	O21-C20-O19-C18
2	A	504	6ZL	O21-C20-O19-C18
2	A	504	6ZL	C40-C20-O19-C18
2	A	504	6ZL	O45-C44-O43-C42
2	B	502	6ZL	C42-C09-C18-O19
2	B	501	6ZL	O21-C20-O19-C18
2	B	501	6ZL	C40-C20-O19-C18
2	B	502	6ZL	O52-C51-O50-C49
2	B	502	6ZL	C60-C51-O50-C49
2	B	503	6ZL	C38-C25-O26-C27
2	B	503	6ZL	C36-C27-O26-C25
2	B	501	6ZL	O28-C27-O26-C25
2	B	502	6ZL	O45-C46-C47-O48

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Mol	Chain	Res	Type	Atoms
2	B	501	6ZL	O28-C29-C30-O31
2	A	503	6ZL	O21-C22-C23-O24
2	B	501	6ZL	C36-C27-O26-C25
2	B	502	6ZL	C46-C49-O50-C51
2	A	502	6ZL	C38-C25-O26-C27
2	B	502	6ZL	C49-C46-C47-O48
2	B	501	6ZL	C32-C29-C30-O31
2	B	503	6ZL	O28-C29-C30-O31
2	B	502	6ZL	O52-C53-C54-O55
2	C	501	6ZL	O21-C20-O19-C18
2	C	501	6ZL	C32-C29-C30-O31
2	B	502	6ZL	C56-C53-C54-O55
2	A	503	6ZL	C25-C22-C23-O24
2	A	503	6ZL	C40-C20-O19-C18
2	B	502	6ZL	C64-C44-O43-C42
2	C	501	6ZL	C40-C20-O19-C18
2	C	501	6ZL	C25-C22-C23-O24
2	C	501	6ZL	O28-C29-C30-O31
2	C	502	6ZL	O21-C22-C23-O24
2	C	501	6ZL	C22-C25-O26-C27
2	C	502	6ZL	C10-C09-C18-O19
2	B	503	6ZL	C32-C29-C30-O31
2	B	502	6ZL	O45-C44-O43-C42
2	C	502	6ZL	C25-C22-C23-O24
2	C	501	6ZL	O21-C22-C23-O24
2	C	502	6ZL	C09-C10-C11-C12
2	C	501	6ZL	C05-C06-C07-C08
2	A	502	6ZL	C08-C09-C18-O19
2	C	502	6ZL	C1-C05-C06-C07
2	A	502	6ZL	C40-C20-O19-C18
2	C	501	6ZL	C38-C25-O26-C27
2	A	502	6ZL	C05-C06-C07-C08
2	B	502	6ZL	C62-C49-O50-C51
2	A	504	6ZL	C05-C06-C07-C08
2	A	504	6ZL	C10-C11-C12-C13
2	C	502	6ZL	C08-C09-C18-O19
2	C	501	6ZL	C07-C08-C09-C18
2	A	503	6ZL	C05-C06-C07-C08
2	A	502	6ZL	O28-C29-C30-O31
2	A	503	6ZL	C38-C25-O26-C27
2	B	503	6ZL	C1-C05-C06-C07
2	A	502	6ZL	C22-C25-O26-C27

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Mol	Chain	Res	Type	Atoms
2	A	504	6ZL	C64-C44-O43-C42
2	A	502	6ZL	C07-C08-C09-C18
2	C	501	6ZL	O28-C27-O26-C25
2	C	501	6ZL	C08-C09-C18-O19
2	A	501	6ZL	C13-C14-C15-C16
2	A	504	6ZL	C08-C09-C18-O19
2	A	504	6ZL	C14-C15-C16-C17
2	B	502	6ZL	C08-C09-C18-O19
2	A	504	6ZL	C38-C25-O26-C27
2	C	501	6ZL	C36-C27-O26-C25
2	C	502	6ZL	C1-C2-C3-C4
2	A	504	6ZL	C22-C25-O26-C27
2	A	503	6ZL	C1-C2-C3-C4
2	A	504	6ZL	C1-C2-C3-C4
2	C	502	6ZL	C05-C1-C2-C3
2	A	503	6ZL	C1-C05-C06-C07
2	C	501	6ZL	C05-C1-C2-C3
2	B	503	6ZL	O28-C27-O26-C25
2	C	501	6ZL	C1-C05-C06-C07
2	B	503	6ZL	C06-C05-C1-C2
2	A	503	6ZL	C06-C05-C1-C2
2	A	501	6ZL	C14-C15-C16-C17
2	C	502	6ZL	C06-C05-C1-C2
2	A	504	6ZL	C10-C09-C18-O19
2	B	503	6ZL	C22-C25-O26-C27
2	C	501	6ZL	C1-C2-C3-C4
2	C	501	6ZL	C09-C18-O19-C20

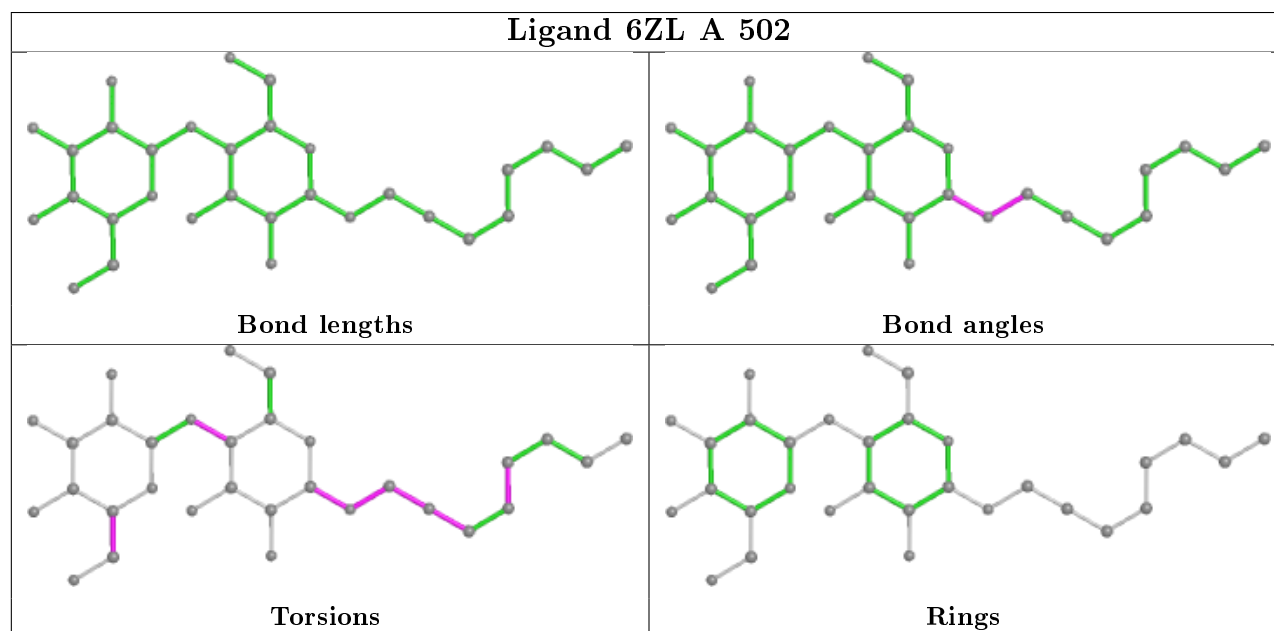
There are no ring outliers.

6 monomers are involved in 10 short contacts:

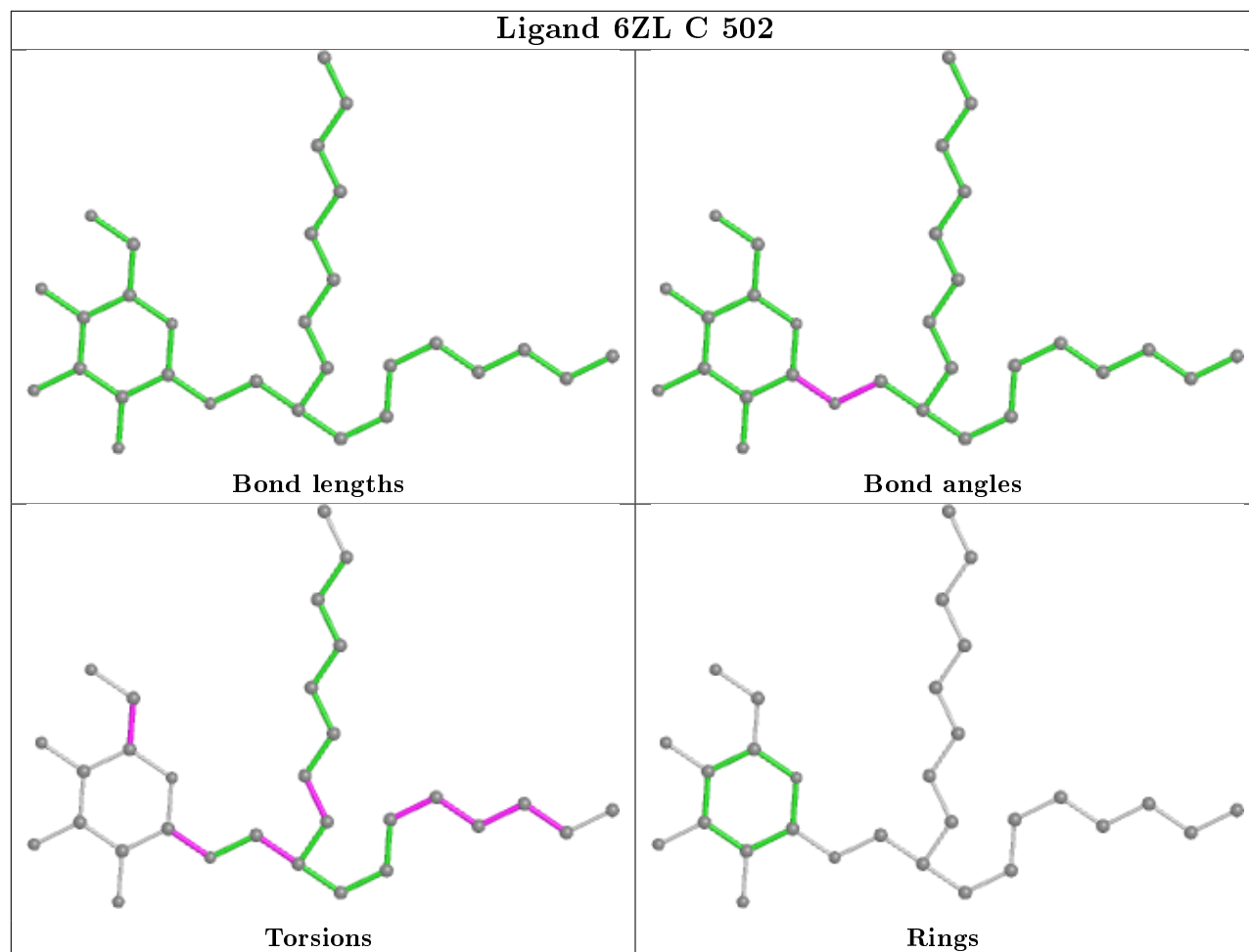
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	6ZL	2	0
2	C	502	6ZL	2	0
2	A	503	6ZL	1	0
2	A	504	6ZL	2	0
2	C	501	6ZL	2	0
2	B	501	6ZL	1	0

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

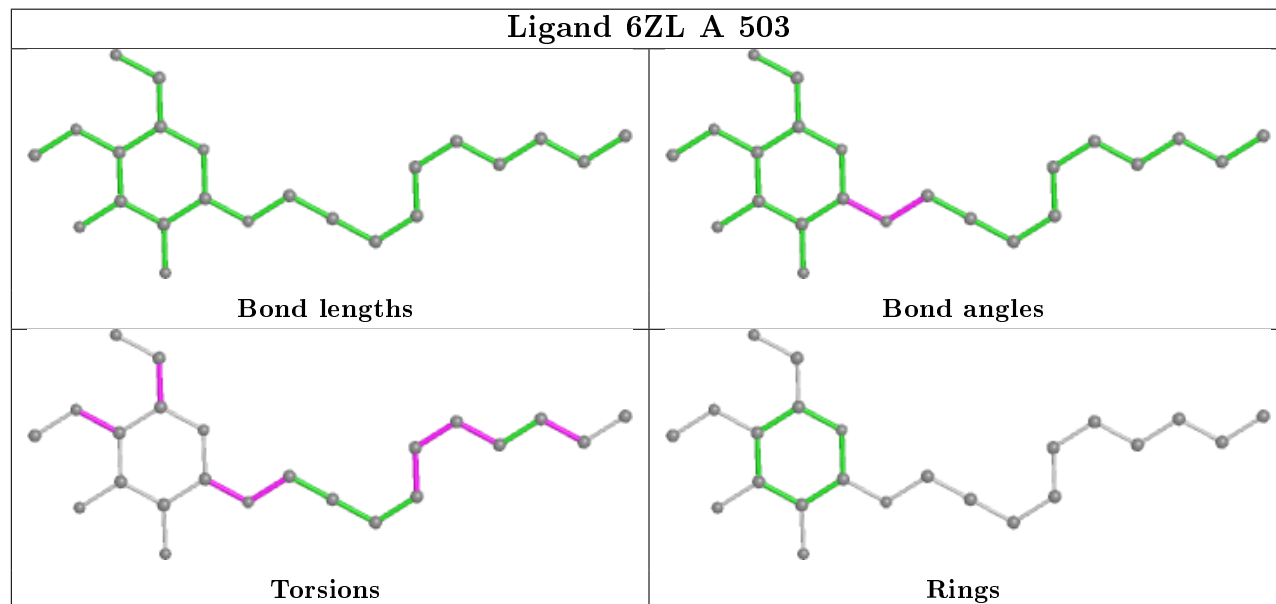
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

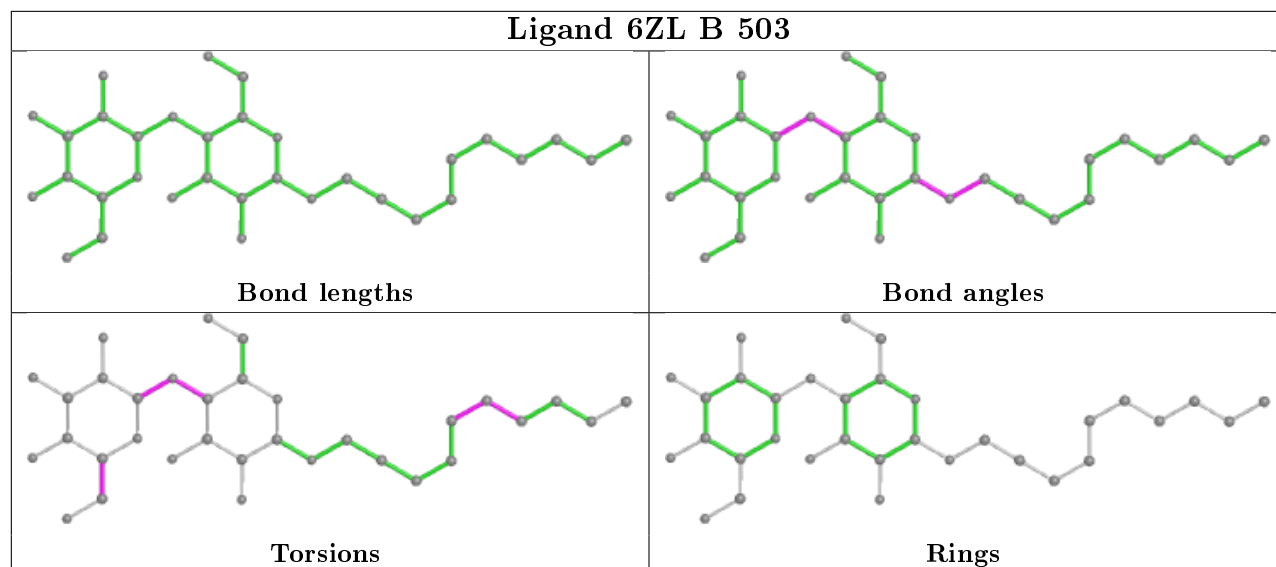
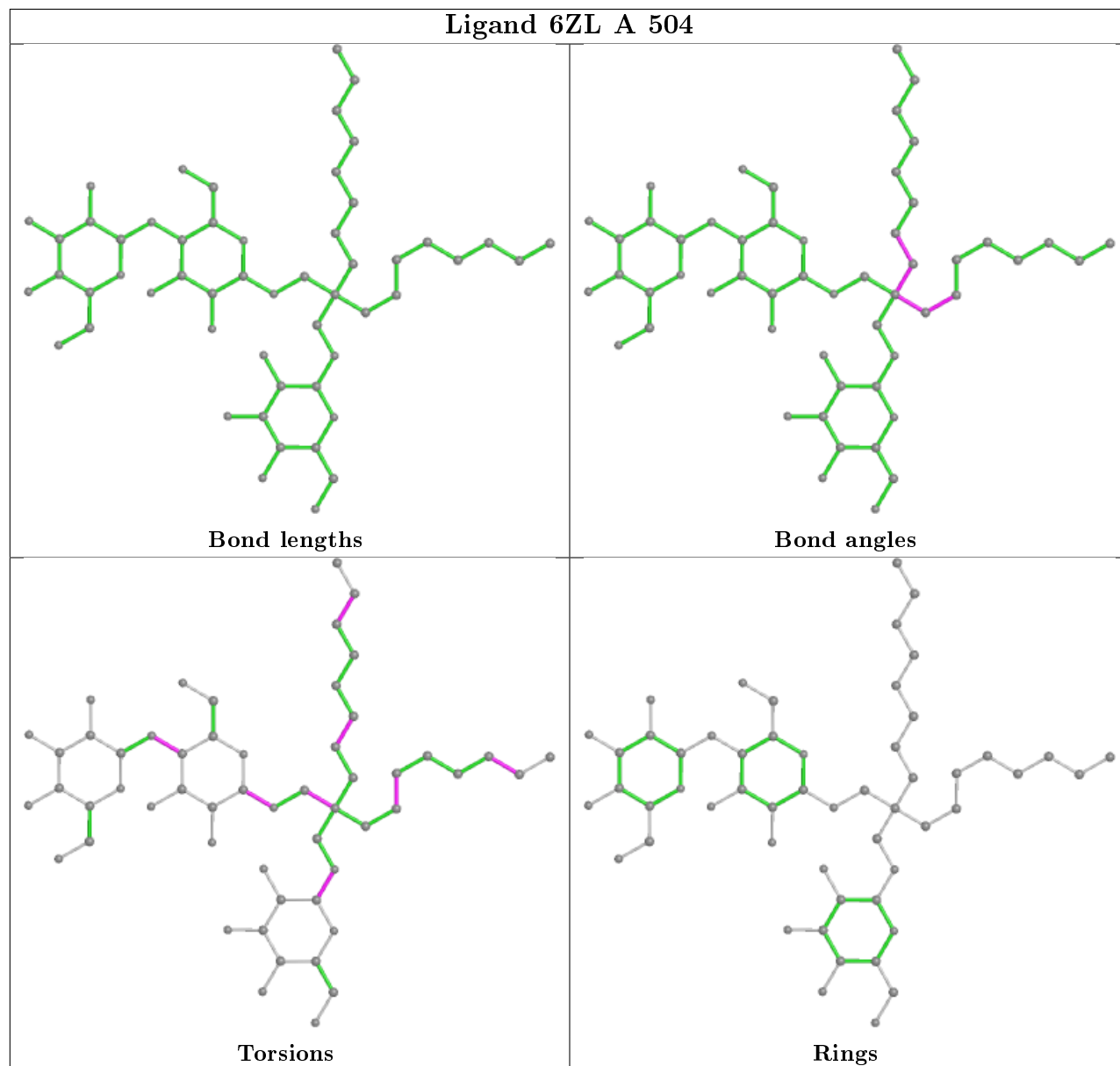


## Ligand 6ZL C 502

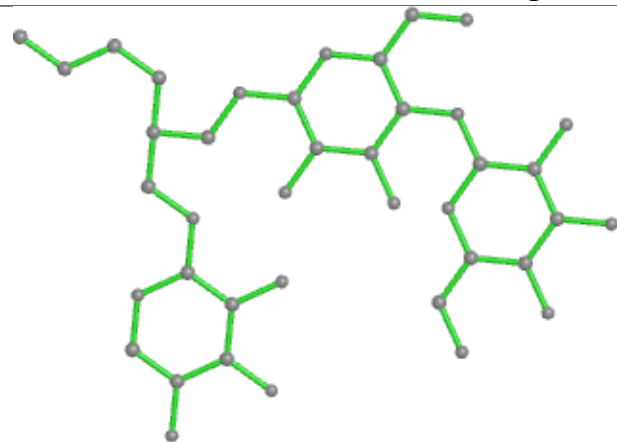


## Ligand 6ZL A 503

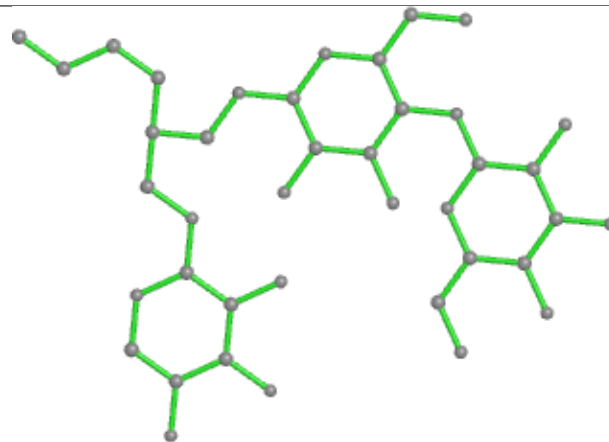


**Ligand 6ZL B 503****Ligand 6ZL A 504**

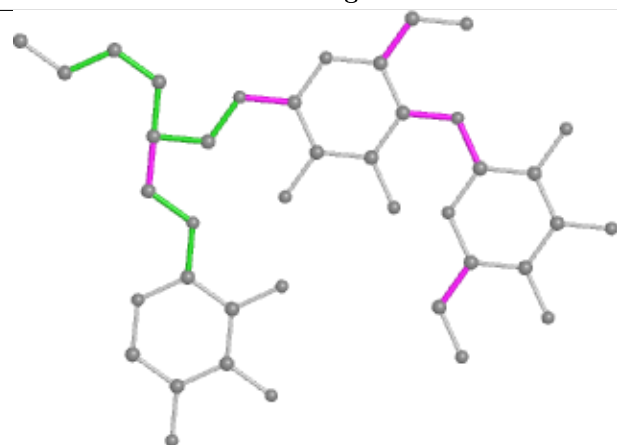
## Ligand 6ZL B 502



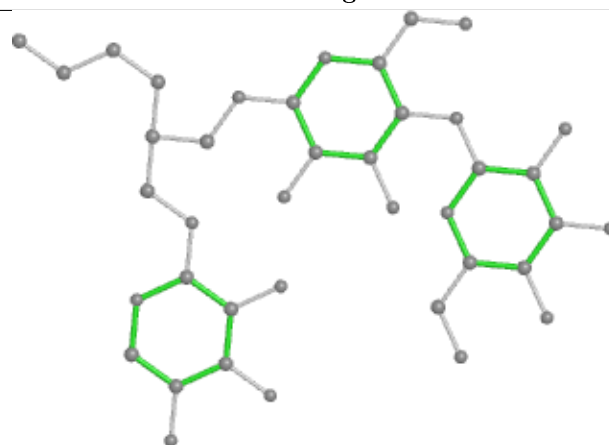
Bond lengths



Bond angles

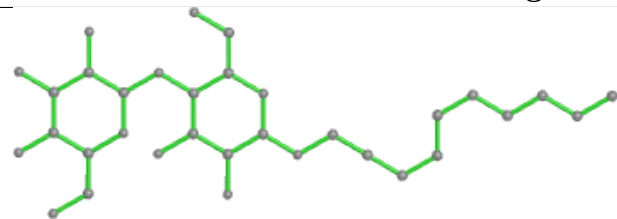


Torsions

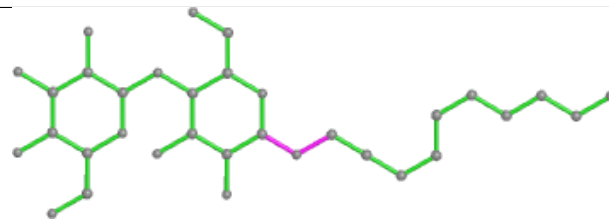


Rings

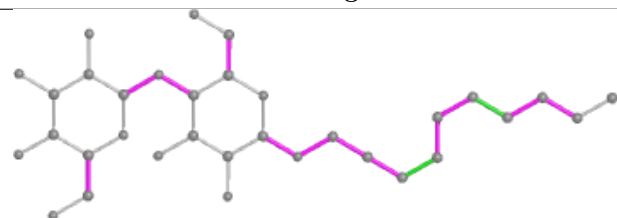
## Ligand 6ZL C 501



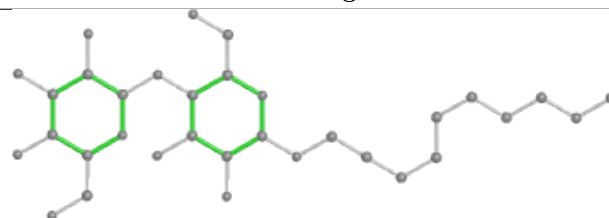
Bond lengths



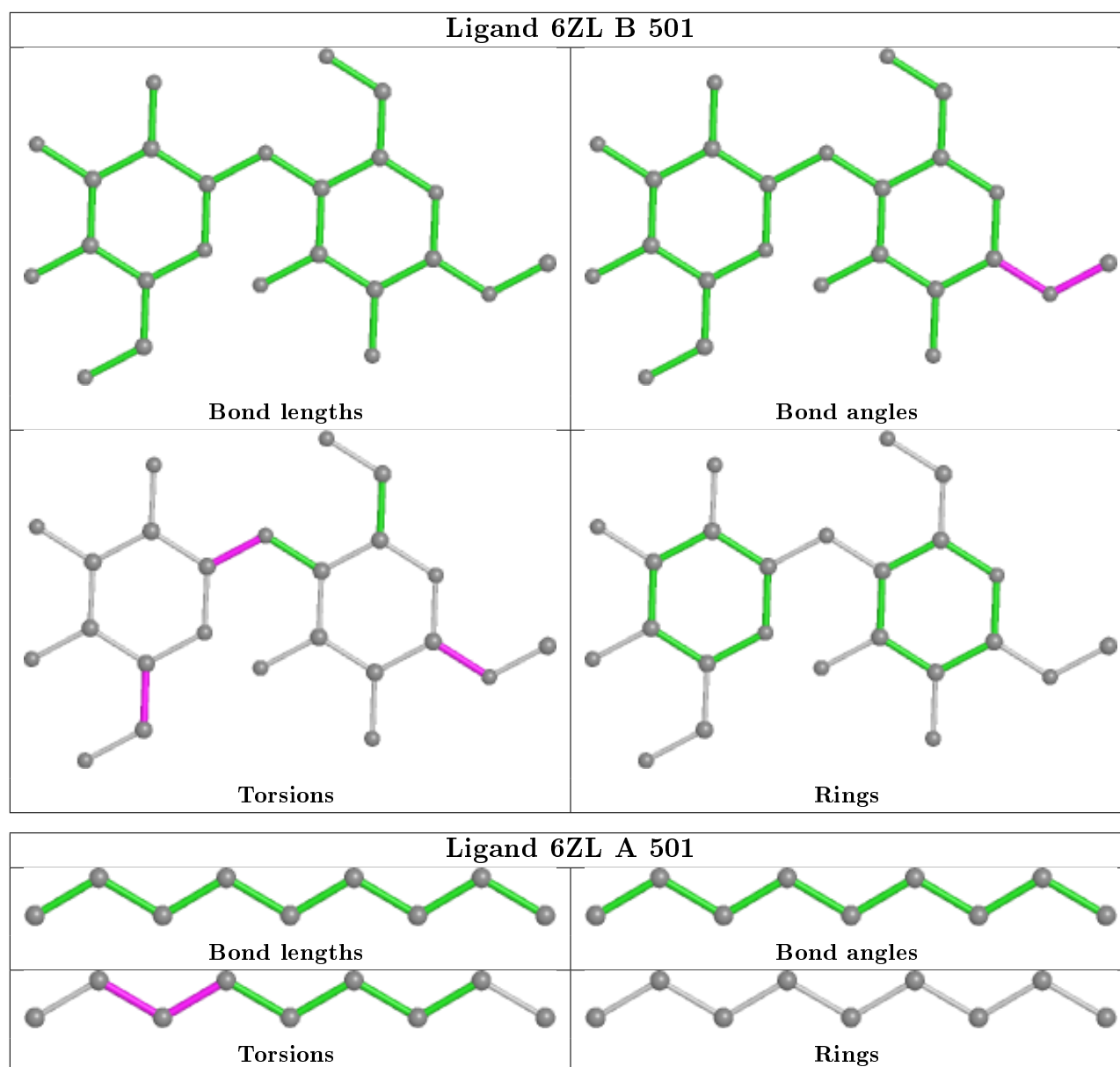
Bond angles



Torsions



Rings



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	419/431 (97%)	-0.12	9 (2%) 63 62	57, 79, 107, 136	0
1	B	415/431 (96%)	0.14	28 (6%) 17 19	61, 90, 125, 161	0
1	C	406/431 (94%)	0.15	29 (7%) 16 18	58, 88, 116, 141	0
All	All	1240/1293 (95%)	0.06	66 (5%) 26 27	57, 85, 117, 161	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	231	ALA	7.4
1	C	349	VAL	7.0
1	C	348	ALA	6.3
1	C	196	GLY	5.8
1	B	421	ALA	5.8
1	B	342	TYR	5.2
1	C	342	TYR	4.3
1	B	422	SER	4.3
1	B	13	LEU	4.3
1	B	349	VAL	4.0
1	B	343	LEU	4.0
1	C	351	LEU	4.0
1	B	348	ALA	3.9
1	B	123	LEU	3.9
1	C	350	GLN	3.9
1	A	55	MET	3.6
1	B	125	ILE	3.6
1	C	195	MET	3.5
1	B	121	MET	3.4
1	C	232	GLU	3.3
1	B	37	LEU	3.3
1	C	343	LEU	3.2
1	C	124	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	197	VAL	3.0
1	B	351	LEU	3.0
1	C	131	PHE	3.0
1	C	230	ASP	3.0
1	B	164	TYR	3.0
1	C	347	ALA	2.9
1	B	46	VAL	2.8
1	B	36	PHE	2.8
1	C	127	VAL	2.7
1	A	131	PHE	2.7
1	B	39	GLN	2.7
1	B	424	LEU	2.6
1	C	29	ILE	2.6
1	B	122	GLN	2.6
1	C	128	ILE	2.6
1	C	314	TRP	2.6
1	C	231	ALA	2.6
1	C	135	MET	2.6
1	C	339	PHE	2.5
1	C	119	GLY	2.5
1	A	127	VAL	2.5
1	C	164	TYR	2.5
1	C	120	VAL	2.5
1	A	207	PHE	2.4
1	B	170	GLU	2.4
1	A	128	ILE	2.4
1	B	207	PHE	2.3
1	B	339	PHE	2.3
1	C	341	LYS	2.3
1	B	256	GLY	2.3
1	A	133	GLN	2.3
1	C	123	LEU	2.3
1	C	125	ILE	2.2
1	B	56	LEU	2.2
1	A	118	ILE	2.2
1	B	29	ILE	2.2
1	C	383	ALA	2.2
1	C	37	LEU	2.2
1	B	258	GLN	2.1
1	B	347	ALA	2.1
1	A	24	ARG	2.1
1	A	210	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	12	VAL	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

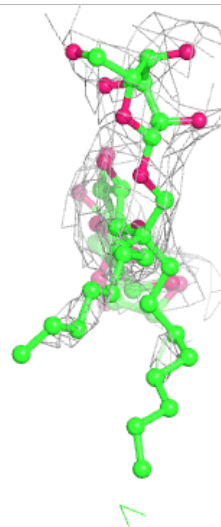
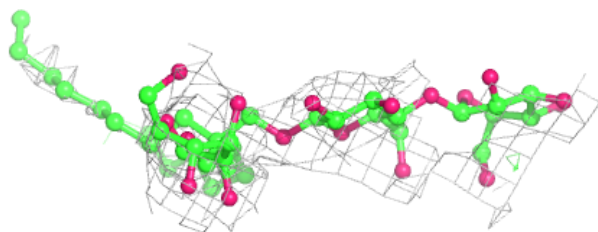
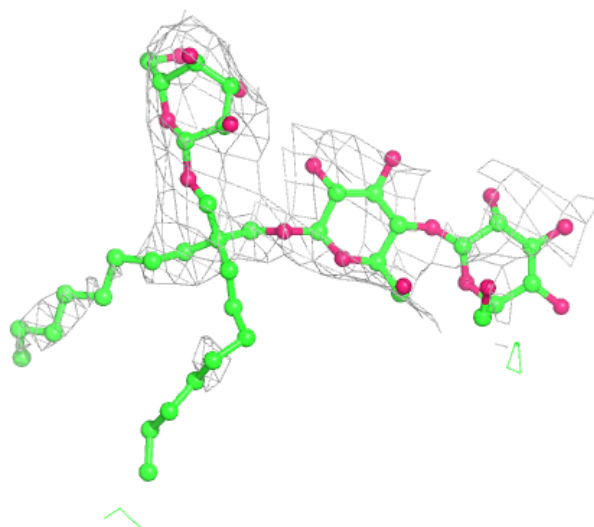
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NA	C	504	1/1	0.56	0.11	69,69,69,69	0
2	6ZL	A	504	54/65	0.66	0.41	70,153,162,165	0
2	6ZL	A	502	31/65	0.66	0.66	64,124,153,160	0
2	6ZL	A	503	23/65	0.68	0.71	78,108,123,130	0
2	6ZL	A	501	9/65	0.74	0.60	65,84,86,92	0
2	6ZL	B	501	24/65	0.77	0.21	117,133,140,145	0
2	6ZL	B	502	40/65	0.77	0.38	91,152,163,165	0
4	NA	A	506	1/1	0.77	0.11	67,67,67,67	0
2	6ZL	C	502	30/65	0.80	0.52	59,114,148,151	0
4	NA	B	505	1/1	0.80	0.07	81,81,81,81	0
2	6ZL	B	503	33/65	0.82	0.32	71,116,130,134	0
2	6ZL	C	501	33/65	0.83	0.34	72,124,152,154	0
3	URI	B	504	17/17	0.92	0.25	64,71,84,88	0
3	URI	A	505	17/17	0.93	0.31	56,66,76,78	0
3	URI	C	503	17/17	0.95	0.33	66,73,85,91	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.

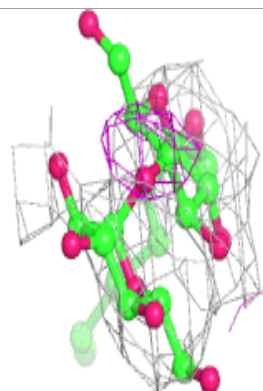
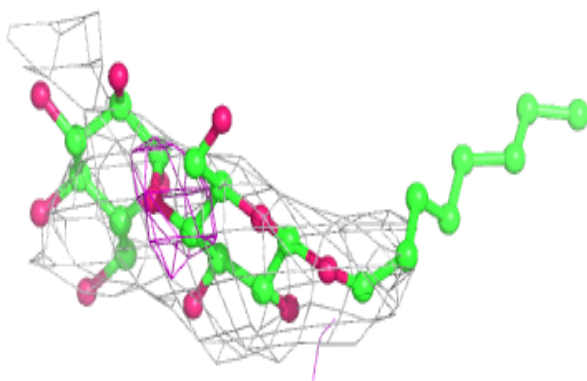
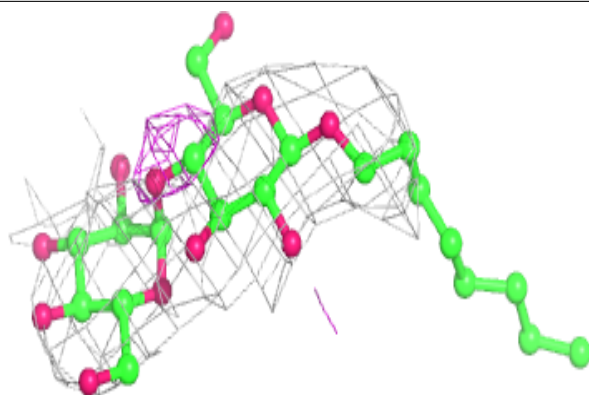
**Electron density around 6ZL A 504:**

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

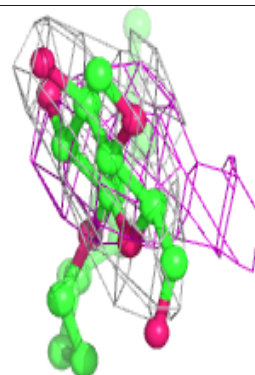
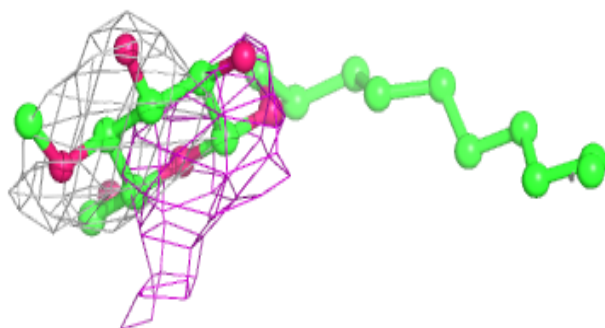
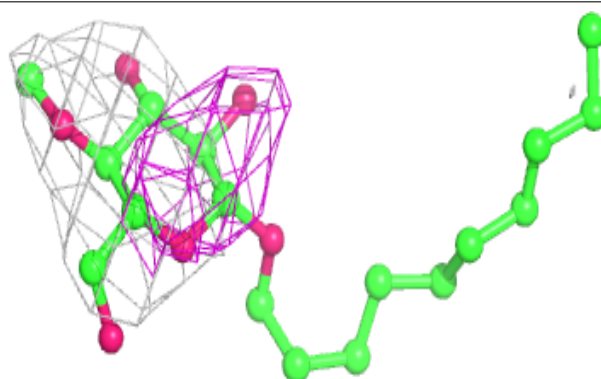


**Electron density around 6ZL A 502:**

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

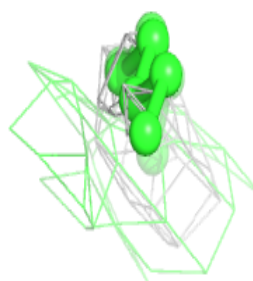
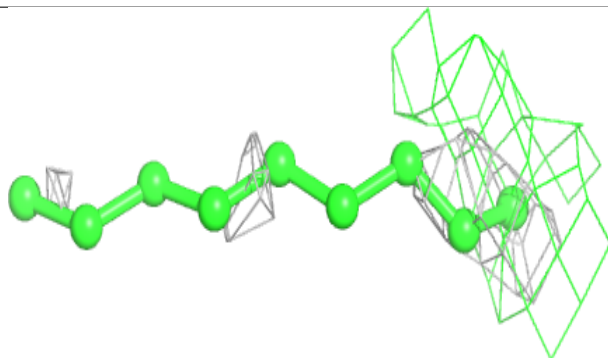
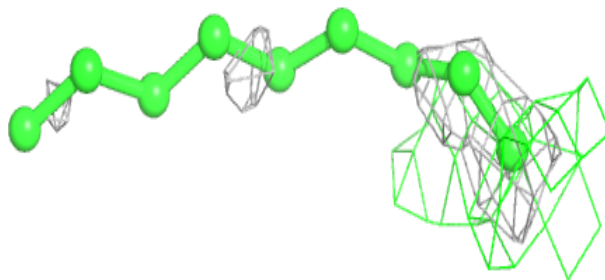
**Electron density around 6ZL A 503:**

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

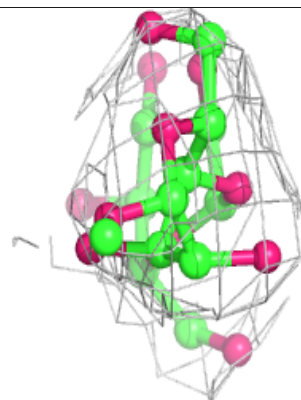
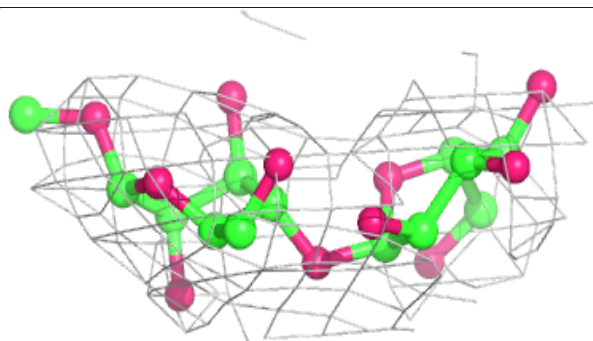
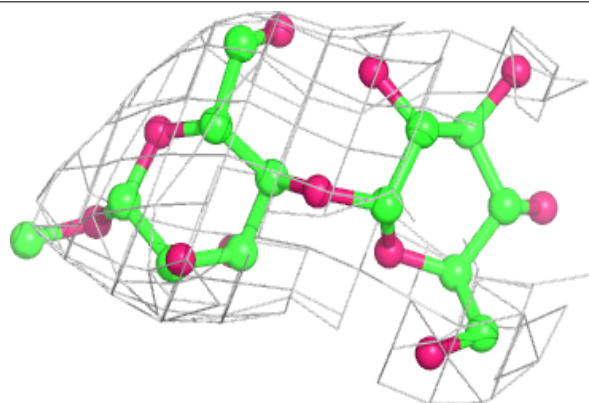


**Electron density around 6ZL A 501:**

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

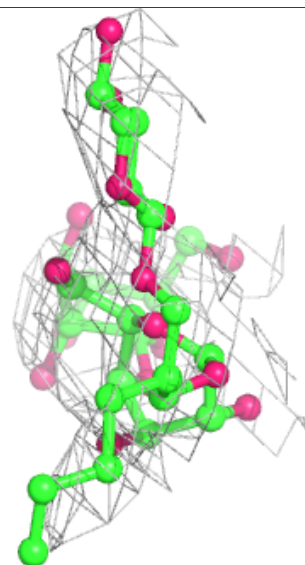
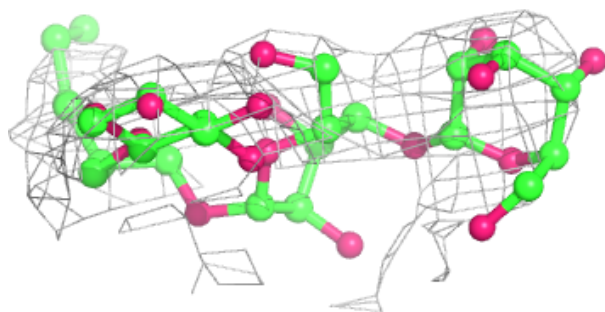
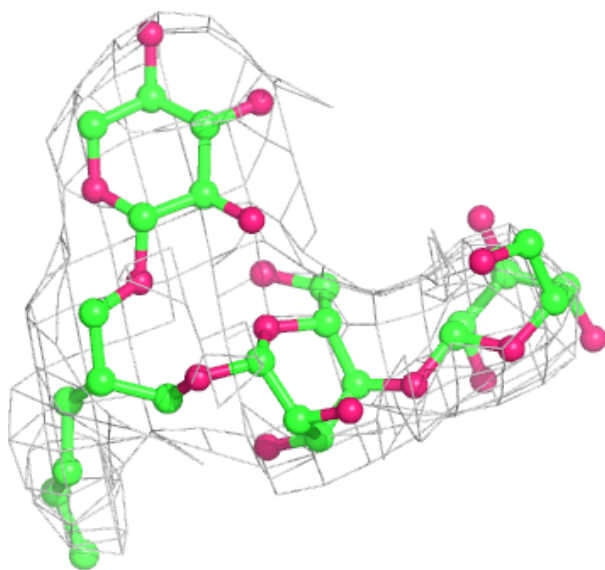
**Electron density around 6ZL B 501:**

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



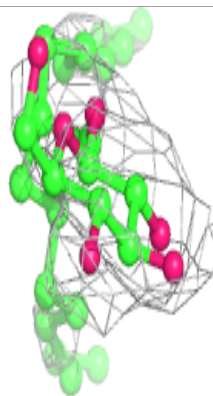
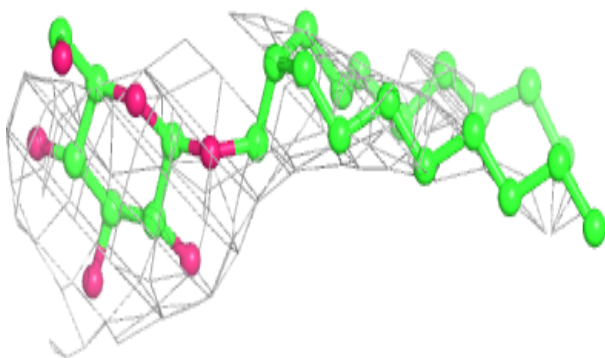
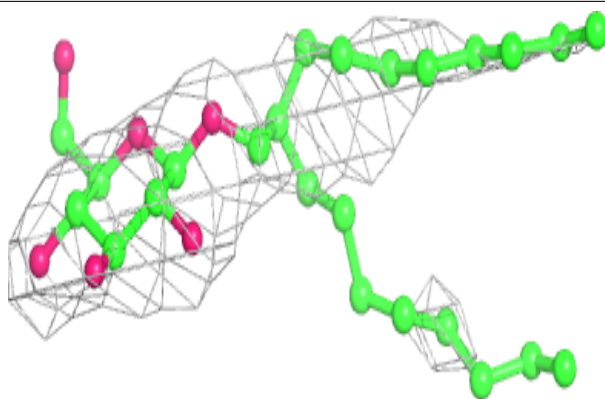
**Electron density around 6ZL B 502:**

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

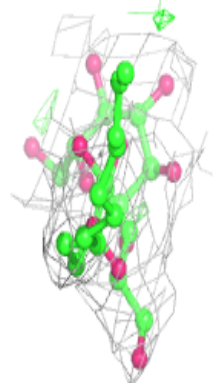
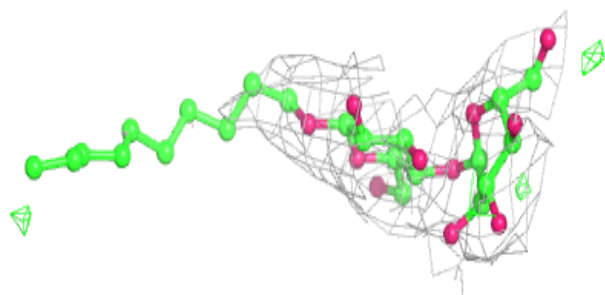
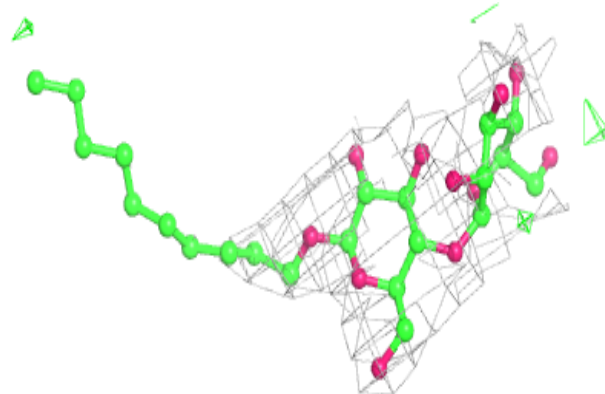


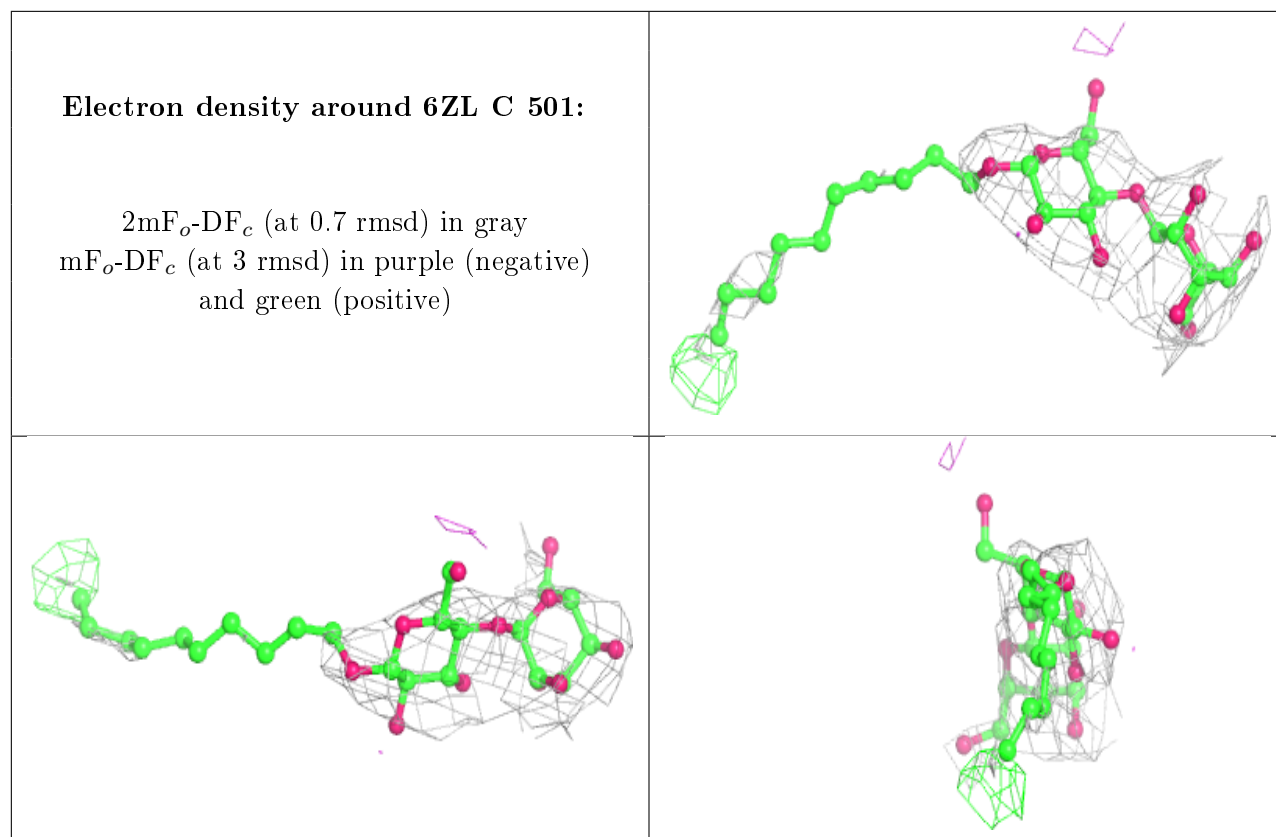
**Electron density around 6ZL C 502:**

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

**Electron density around 6ZL B 503:**

$2mF_o-DF_c$  (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.