wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2020 – 05:51 PM BST

PDB ID	:	2HPY
Title	:	Crystallographic model of lumirhodopsin
Authors	:	Nakamichi, H.; Okada, T.
Deposited on	:	2006-07-18
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (i)) were used in the production of this report:

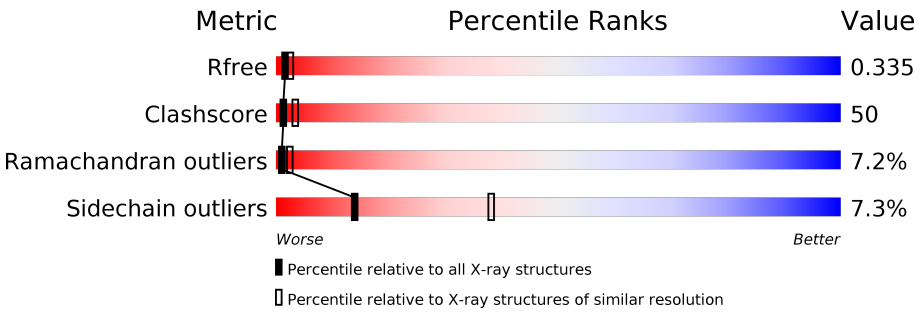
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	349	38% 53% 9%
1	B	349	34% 55% 10% •
2	C	3	33% 33% 33%
3	D	2	100%
3	F	2	50% 50%
4	E	4	50% 50%

2 Entry composition (i)

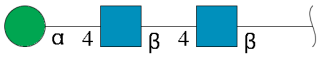
There are 11 unique types of molecules in this entry. The entry contains 5948 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	349	2749	1818	424	481	26	0	0	0
1	B	349	2749	1818	424	481	26	0	0	0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	39	22	2	15	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	2	28	16	2	10	0	0	0
3	F	2	28	16	2	10	0	0	0

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	4	50	28	2	20	0	0	0

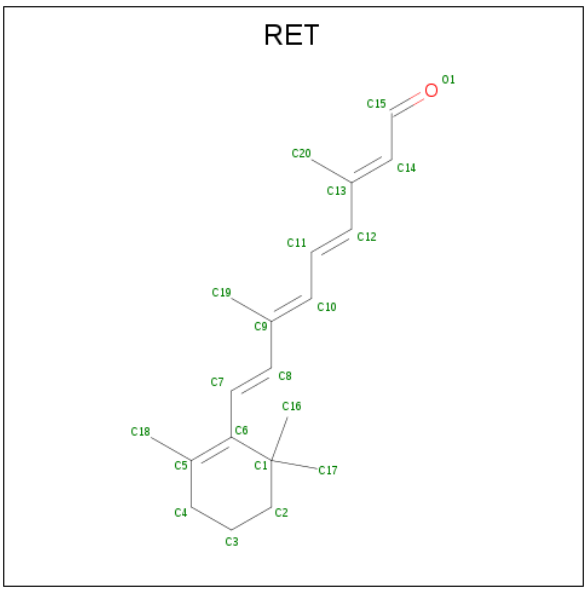
- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Hg		
5	B	3	3	3	0	0
5	A	3	Total	Hg	0	0
			3	3		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

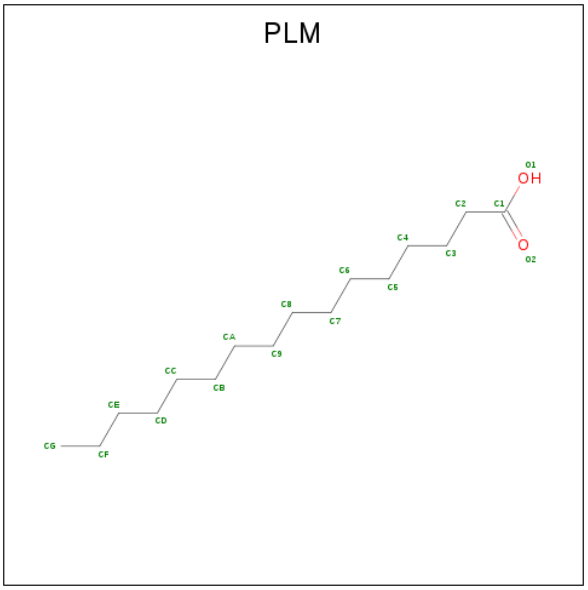
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	B	3	3	3	0	0
6	A	4	Total	Zn	0	0
			4	4		

- Molecule 7 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



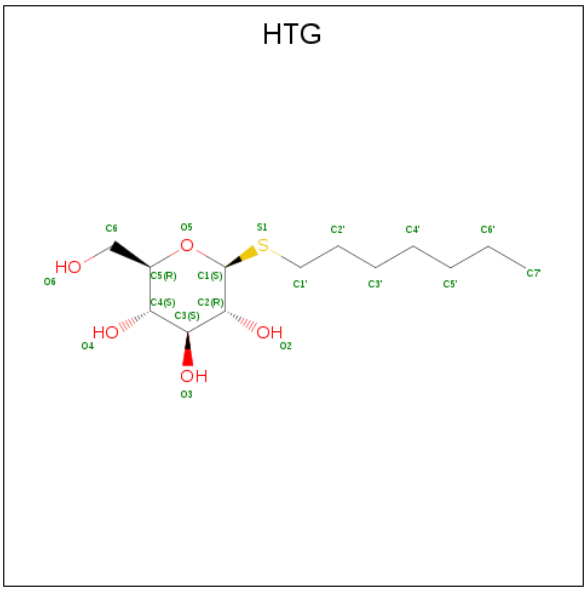
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 20 20	0	0
7	B	1	Total C 20 20	0	0

- Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



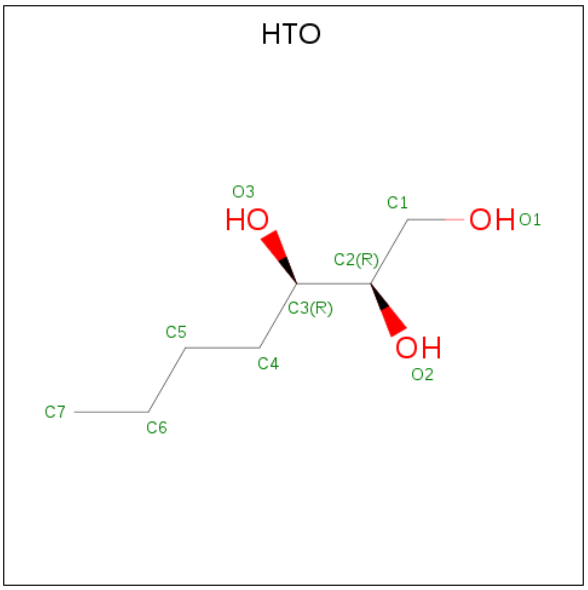
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 17 16 1	0	0
8	A	1	Total C O 17 16 1	0	0
8	A	1	Total C 16 16	0	0
8	B	1	Total C O 17 16 1	0	0
8	B	1	Total C O 17 16 1	0	0
8	B	1	Total C 16 16	0	0

- Molecule 9 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
9	A	1	19	13	5	1	0	0
			Total	C	O	S		
9	A	1	19	13	5	1	0	0
			Total	C	O	S		
9	B	1	19	13	5	1	0	0
			Total	C	O	S		
9	B	1	19	13	5	1	0	0

- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	B	1	10	7	3	0	0

- Molecule 11 is water.

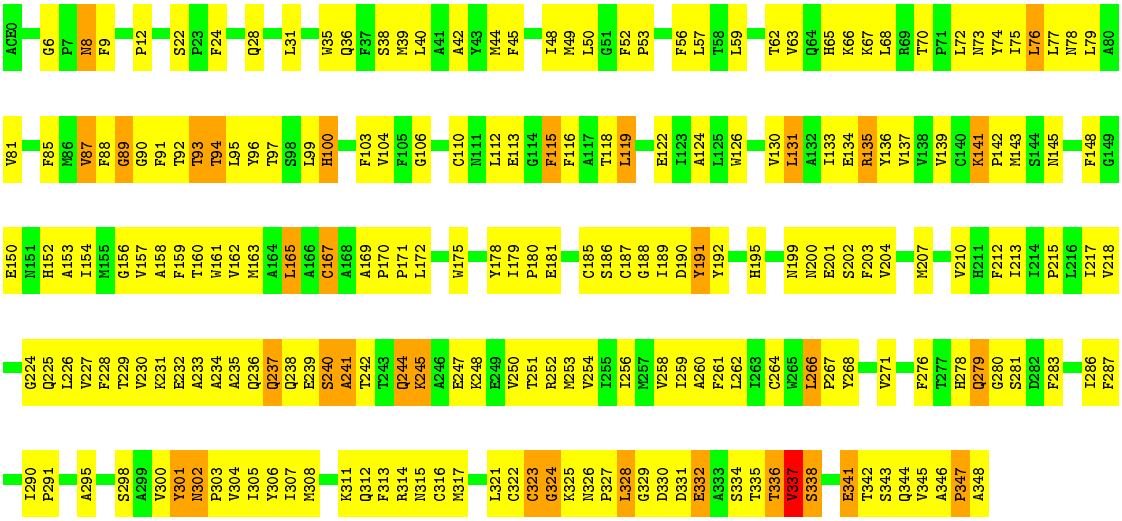
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	37	37	37	0	0
			Total	O		
11	B	29	29	29	0	0

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. 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. 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.

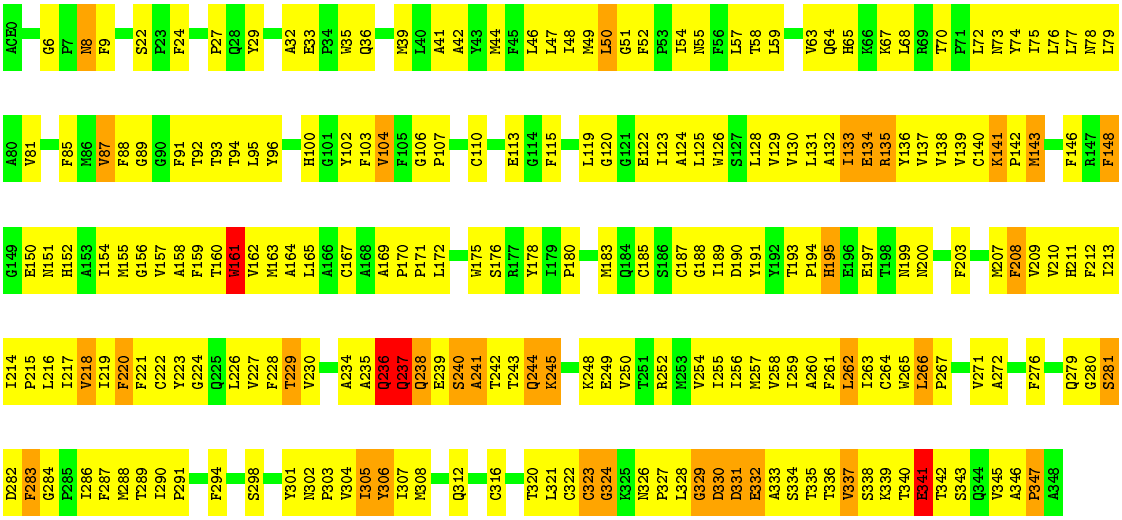
- Molecule 1: Rhodopsin

Chain A: 38% 53% 9%

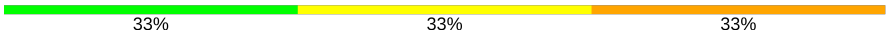


- Molecule 1: Rhodopsin

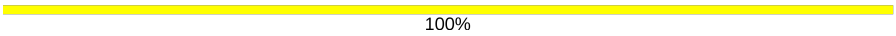
Chain B: 34% 55% 10%



• Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 4: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	96.72Å 96.72Å 150.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 35.05 – 2.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 87.3 (35.05-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.238 0.346 , 0.335	Depositor DCC
R_{free} test set	1531 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	64.8	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.15 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.138 for h,-k,-l	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	5948	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: HTG, ZN, BMA, NAG, ACE, HTO, RET, PLM, HG, MAN

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	0.65	0/2831	0.70	0/3859
1	B	0.65	0/2831	0.68	0/3859
All	All	0.65	0/5662	0.69	0/7718

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	306	TYR	Sidechain

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	2749	0	2709	257	1
1	B	2749	0	2709	327	0
2	C	39	0	34	1	0
3	D	28	0	25	0	0
3	F	28	0	25	1	0
4	E	50	0	43	0	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	4	0	0	0	0
6	B	3	0	0	0	0
7	A	20	0	27	2	0
7	B	20	0	27	2	0
8	A	50	0	89	7	0
8	B	50	0	89	4	0
9	A	38	0	52	3	0
9	B	38	0	52	4	1
10	B	10	0	16	1	0
11	A	37	0	0	6	0
11	B	29	0	0	10	0
All	All	5948	0	5897	584	1

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 50.

The worst 5 of 584 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:298:SER:HA	1:A:301:TYR:CE2	1.82	1.15
1:B:298:SER:HA	1:B:301:TYR:CE2	1.81	1.15
1:A:67:LYS:HB2	1:A:337:VAL:HB	1.38	1.02
1:B:64:GLN:HG3	1:B:339:LYS:HE2	1.39	1.02
1:A:345:VAL:HG12	1:A:347:PRO:HD3	1.45	0.98

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLN:NE2	9:B:1509:HTG:O6[4_564]	2.19	0.01

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	347/349 (99%)	264 (76%)	57 (16%)	26 (8%)	1 2
1	B	347/349 (99%)	254 (73%)	69 (20%)	24 (7%)	1 3
All	All	694/698 (99%)	518 (75%)	126 (18%)	50 (7%)	1 2

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	SER
1	A	241	ALA
1	A	323	CYS
1	A	328	LEU
1	A	341	GLU

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	296/296 (100%)	276 (93%)	20 (7%)	16 42
1	B	296/296 (100%)	273 (92%)	23 (8%)	12 35
All	All	592/592 (100%)	549 (93%)	43 (7%)	14 38

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	SER

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Mol	Chain	Res	Type
1	B	134	GLU
1	B	283	PHE
1	B	8	ASN
1	B	50	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	ASN
1	B	8	ASN
1	B	237	GLN
1	A	312	GLN
1	B	151	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)

11 monosaccharides 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	NAG	C	1	1,2	14,14,15	0.63	0	17,19,21	0.84	0
2	NAG	C	2	2	14,14,15	0.77	0	17,19,21	0.90	1 (5%)
2	MAN	C	3	2	11,11,12	0.80	0	15,15,17	0.79	0
3	NAG	D	1	1,3	14,14,15	0.54	0	17,19,21	0.80	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	D	2	3	14,14,15	0.62	0	17,19,21	0.96	1 (5%)
4	NAG	E	1	1,4	14,14,15	0.60	0	17,19,21	0.64	0
4	NAG	E	2	4	14,14,15	0.64	0	17,19,21	0.92	1 (5%)
4	BMA	E	3	4	11,11,12	0.82	0	15,15,17	0.67	0
4	BMA	E	4	4	11,11,12	0.83	0	15,15,17	0.85	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.65	0	17,19,21	0.81	1 (5%)
3	NAG	F	2	3	14,14,15	0.64	0	17,19,21	0.66	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	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	MAN	C	3	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
4	BMA	E	4	4	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2	NAG	C2-N2-C7	-3.02	118.61	122.90
4	E	2	NAG	C2-N2-C7	-2.65	119.13	122.90
3	D	1	NAG	C2-N2-C7	-2.61	119.18	122.90
4	E	4	BMA	C1-O5-C5	2.29	115.30	112.19
2	C	2	NAG	C8-C7-N2	2.20	119.83	116.10

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2

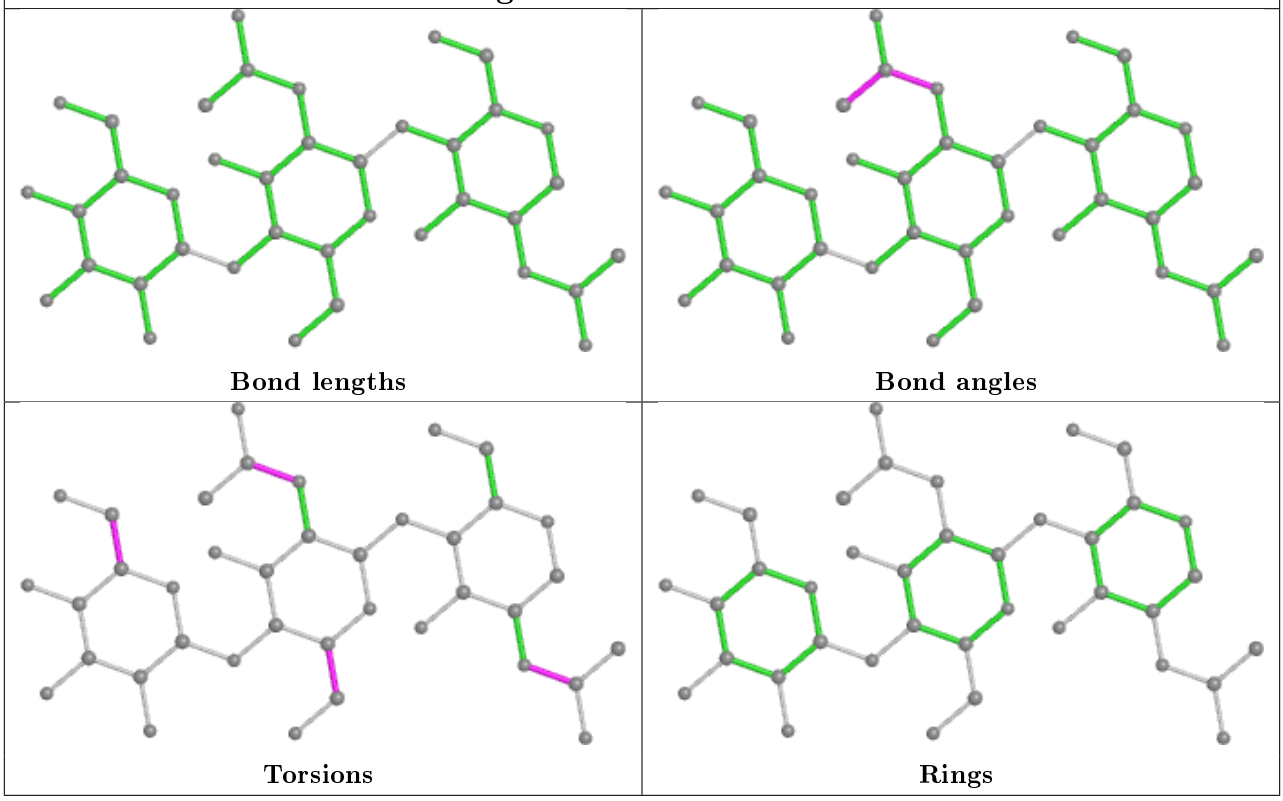
There are no ring outliers.

3 monomers are involved in 2 short contacts:

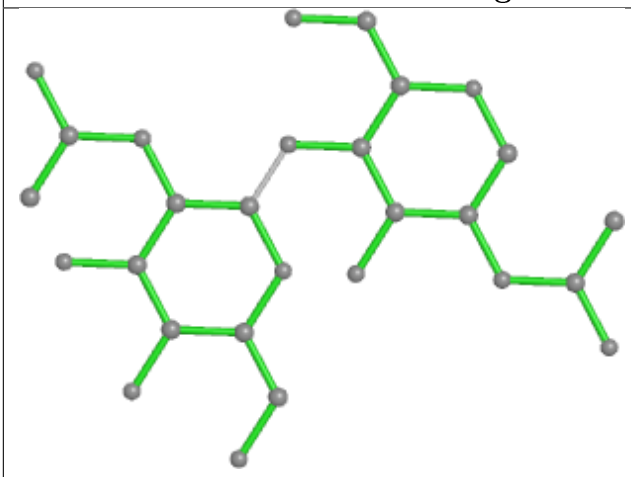
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
2	C	2	NAG	1	0
3	F	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

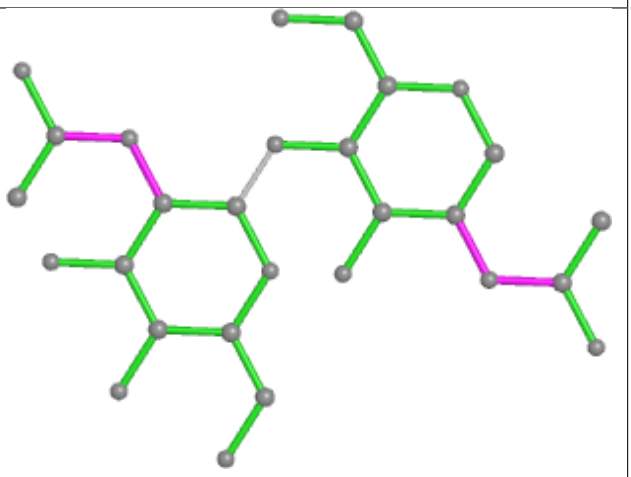
Oligosaccharide Chain C



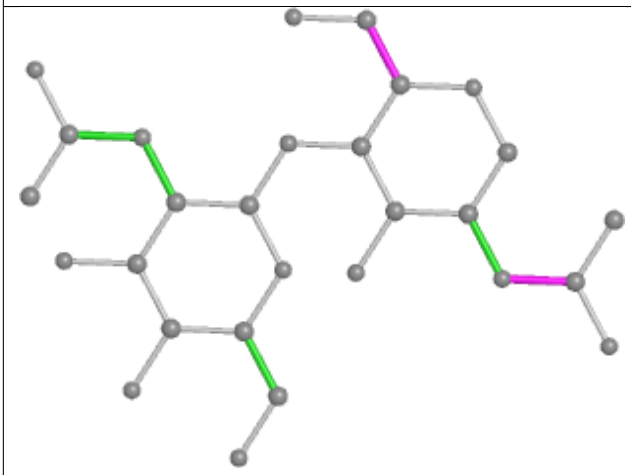
Oligosaccharide Chain D



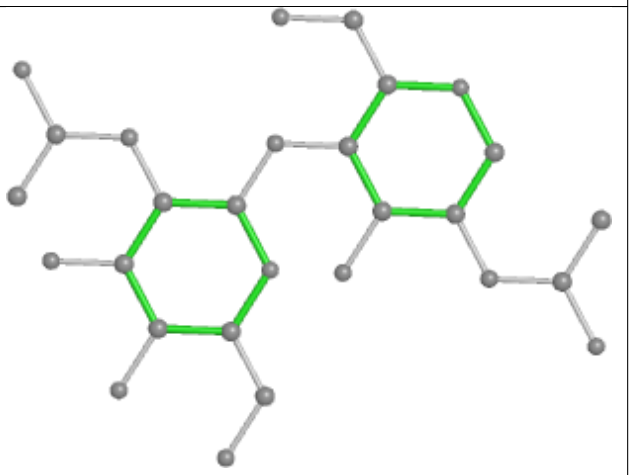
Bond lengths



Bond angles

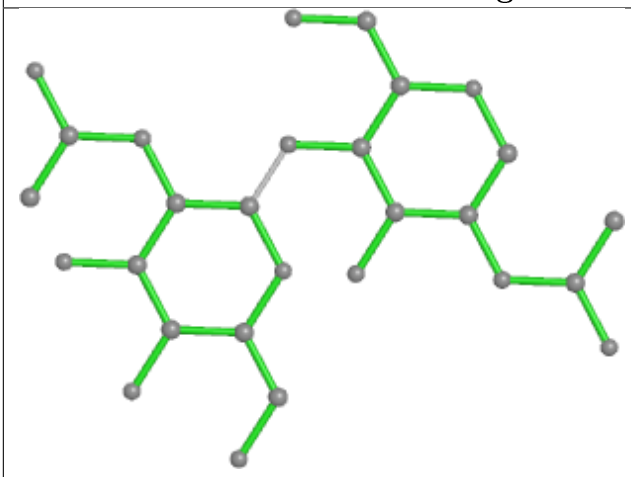


Torsions

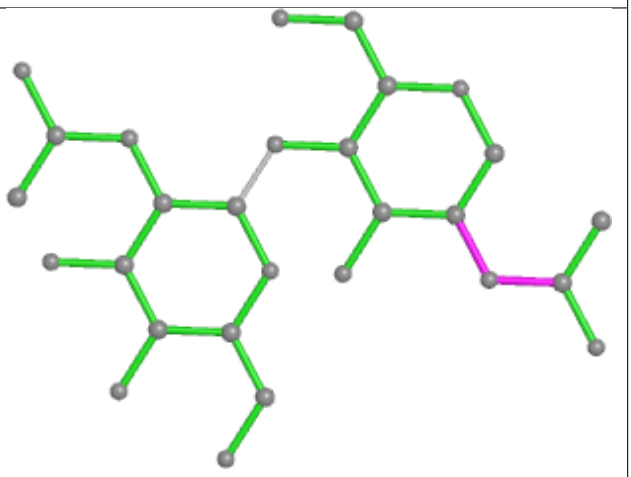


Rings

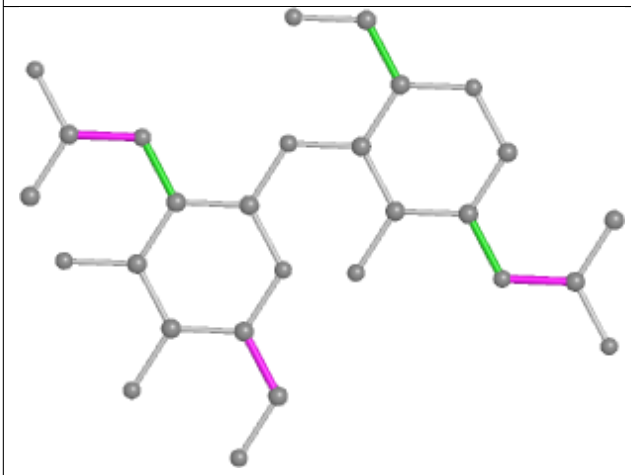
Oligosaccharide Chain F



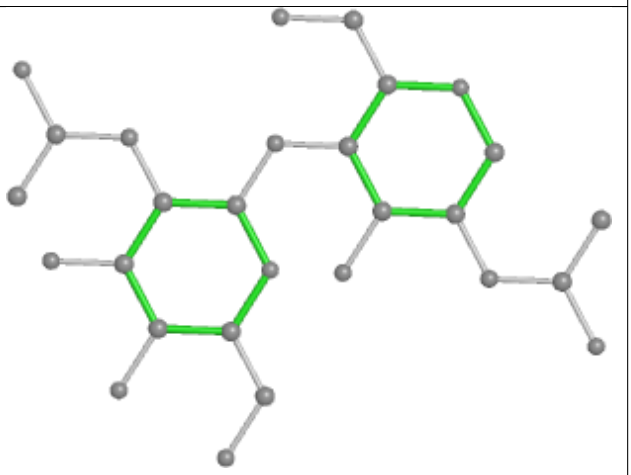
Bond lengths



Bond angles

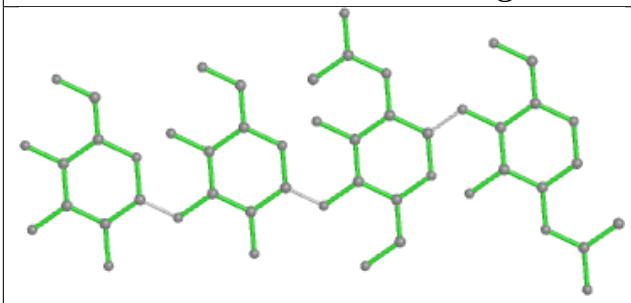


Torsions

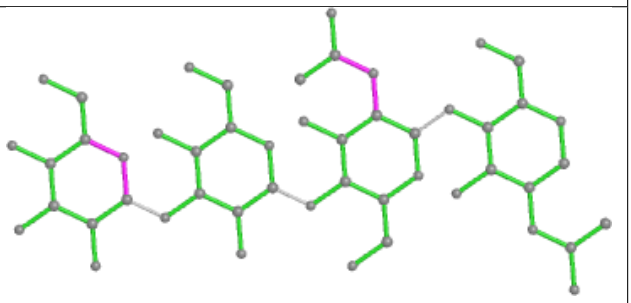


Rings

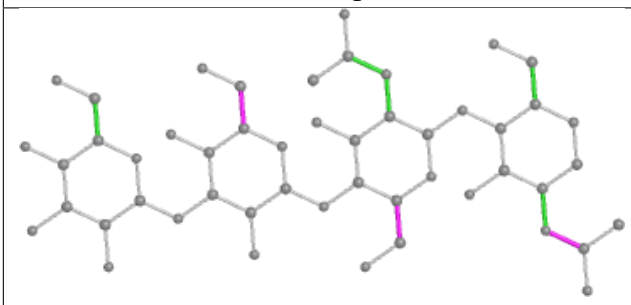
Oligosaccharide Chain E



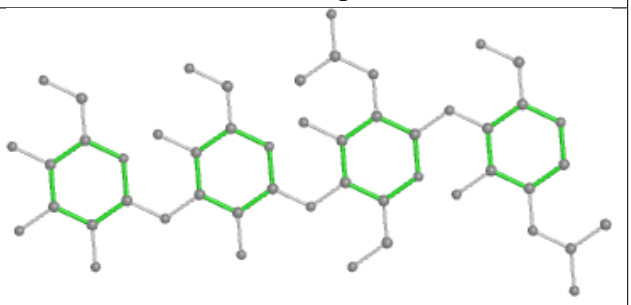
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 13 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
9	HTG	B	1506	-	19,19,19	3.12	8 (42%)	23,24,24	2.01	3 (13%)
7	RET	A	1296	1	20,20,21	2.45	3 (15%)	27,27,28	1.99	7 (25%)
8	PLM	B	1323	1	16,16,17	0.99	1 (6%)	15,15,17	0.44	0
10	HTO	B	1401	-	9,9,9	1.74	2 (22%)	10,10,10	1.14	1 (10%)
8	PLM	A	1323	1	16,16,17	0.98	1 (6%)	15,15,17	0.52	0
9	HTG	A	1507	-	19,19,19	3.32	8 (42%)	23,24,24	2.28	2 (8%)
7	RET	B	1296	1	20,20,21	2.19	4 (20%)	27,27,28	1.87	7 (25%)
8	PLM	A	1410	-	15,15,17	1.82	3 (20%)	14,14,17	3.38	6 (42%)
8	PLM	B	1322	1	16,16,17	1.02	1 (6%)	15,15,17	0.43	0
8	PLM	A	1322	1	16,16,17	0.98	1 (6%)	15,15,17	0.60	0
9	HTG	A	1508	-	19,19,19	2.53	8 (42%)	23,24,24	2.64	2 (8%)
8	PLM	B	1407	-	15,15,17	1.77	3 (20%)	14,14,17	3.37	7 (50%)
9	HTG	B	1509	-	19,19,19	2.83	8 (42%)	23,24,24	2.27	2 (8%)

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
9	HTG	B	1506	-	-	2/10/30/30	0/1/1/1
7	RET	A	1296	1	-	4/13/30/31	0/1/1/1
8	PLM	B	1323	1	-	9/14/14/15	-
10	HTO	B	1401	-	-	1/10/10/10	-
8	PLM	A	1323	1	-	10/14/14/15	-
9	HTG	A	1507	-	-	5/10/30/30	0/1/1/1
7	RET	B	1296	1	-	5/13/30/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PLM	A	1410	-	-	5/13/13/15	-
8	PLM	B	1322	1	-	11/14/14/15	-
8	PLM	A	1322	1	-	11/14/14/15	-
9	HTG	A	1508	-	-	4/10/30/30	0/1/1/1
8	PLM	B	1407	-	-	5/13/13/15	-
9	HTG	B	1509	-	-	5/10/30/30	0/1/1/1

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1507	HTG	O5-C1	9.50	1.57	1.42
9	B	1506	HTG	O5-C1	9.07	1.56	1.42
9	B	1509	HTG	O5-C1	8.06	1.54	1.42
7	A	1296	RET	C1-C6	7.30	1.63	1.53
9	A	1508	HTG	O5-C1	7.13	1.53	1.42

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1508	HTG	C1'-S1-C1	11.87	122.30	100.09
9	B	1509	HTG	C1'-S1-C1	9.91	118.62	100.09
9	A	1507	HTG	C1'-S1-C1	9.83	118.47	100.09
9	B	1506	HTG	C1'-S1-C1	8.44	115.88	100.09
8	A	1410	PLM	CD-CC-CB	8.29	156.51	114.42

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1296	RET	C1-C6-C7-C8
7	A	1296	RET	C5-C6-C7-C8
7	B	1296	RET	C5-C6-C7-C8
8	B	1407	PLM	CA-CB-CC-CD
9	B	1509	HTG	O5-C5-C6-O6

There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1506	HTG	1	0

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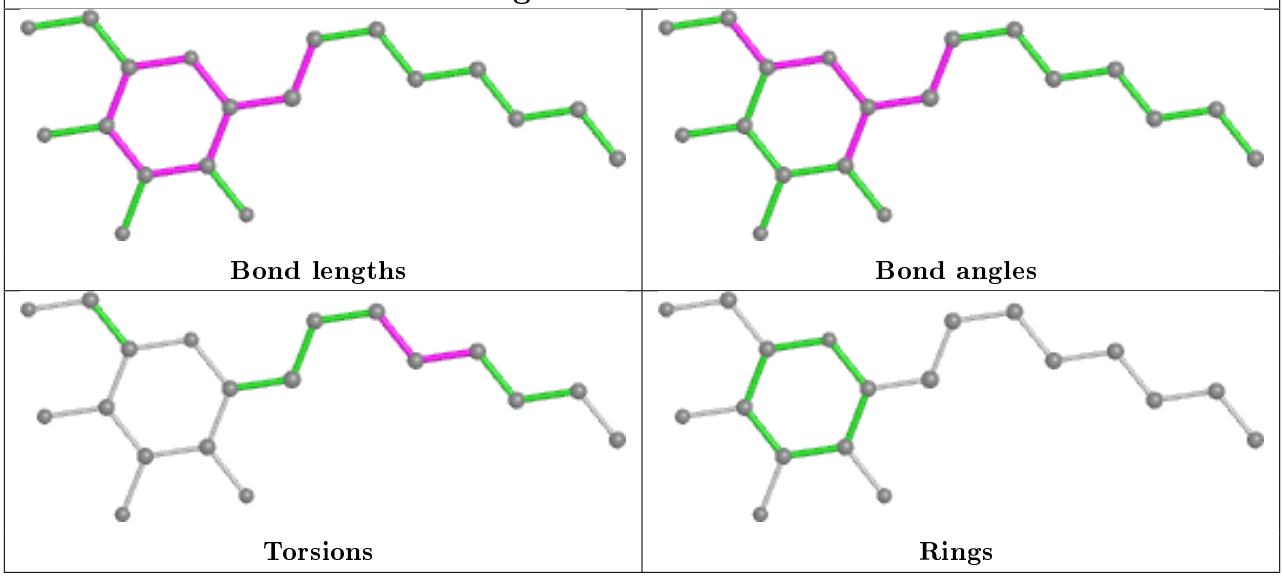
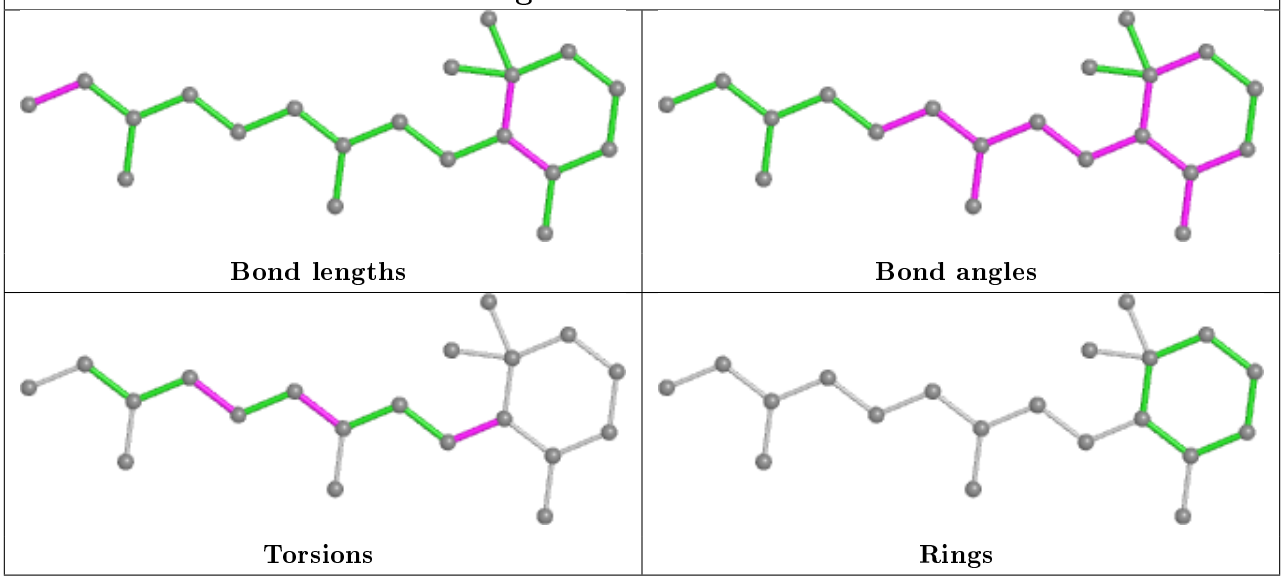
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1296	RET	2	0
8	B	1323	PLM	2	0
10	B	1401	HTO	1	0
9	A	1507	HTG	2	0
7	B	1296	RET	2	0
8	A	1410	PLM	1	0
8	B	1322	PLM	2	0
8	A	1322	PLM	6	0
9	A	1508	HTG	1	0
8	B	1407	PLM	1	0
9	B	1509	HTG	3	1

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.

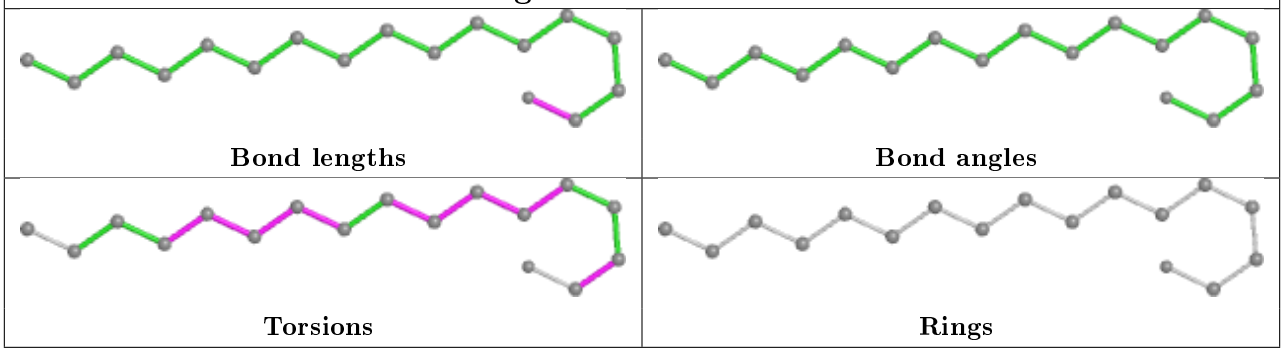
Ligand HTG B 1506



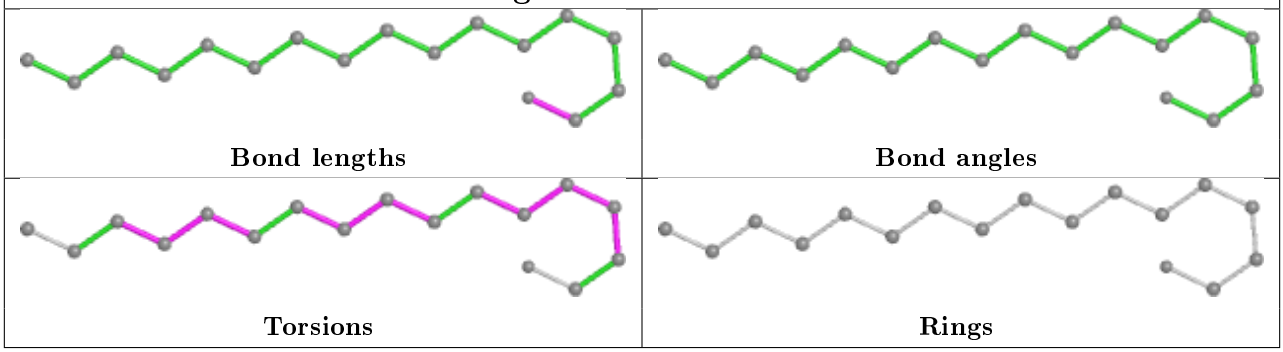
Ligand RET A 1296



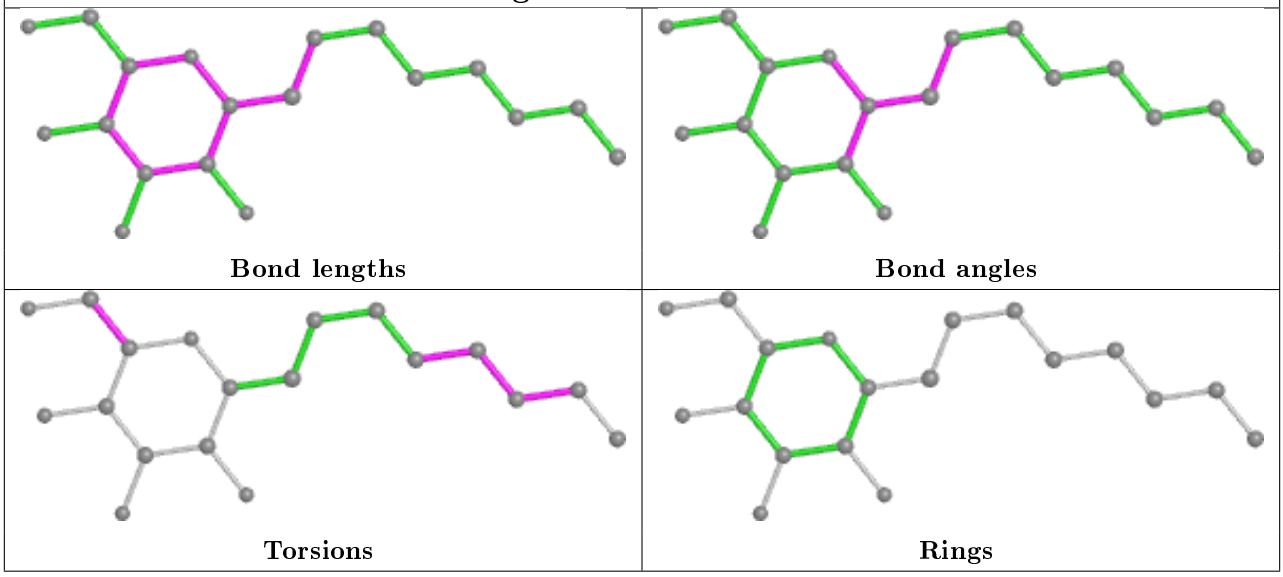
Ligand PLM B 1323



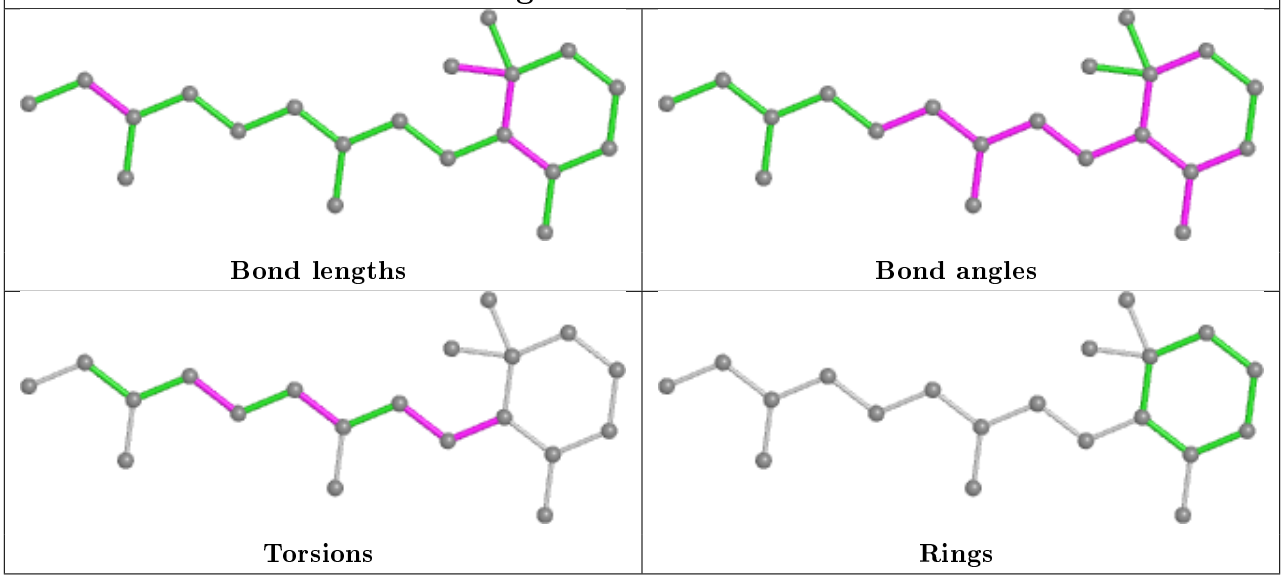
Ligand PLM A 1323



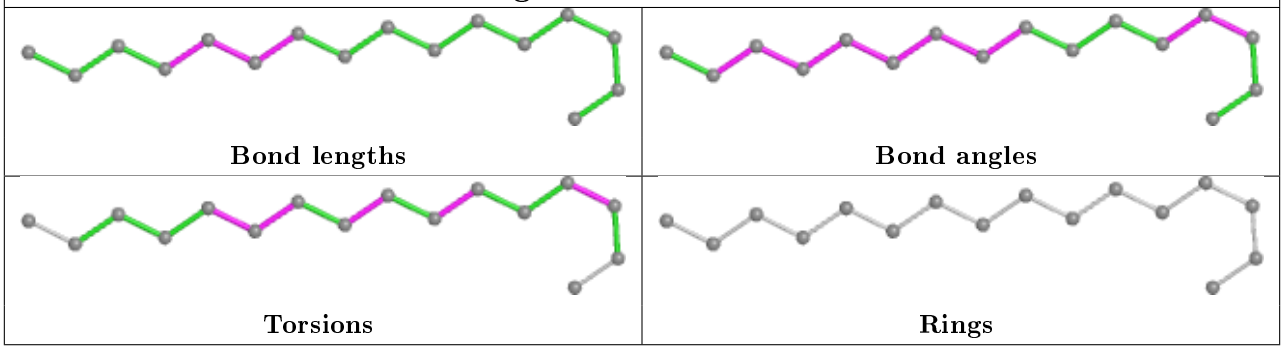
Ligand HTG A 1507



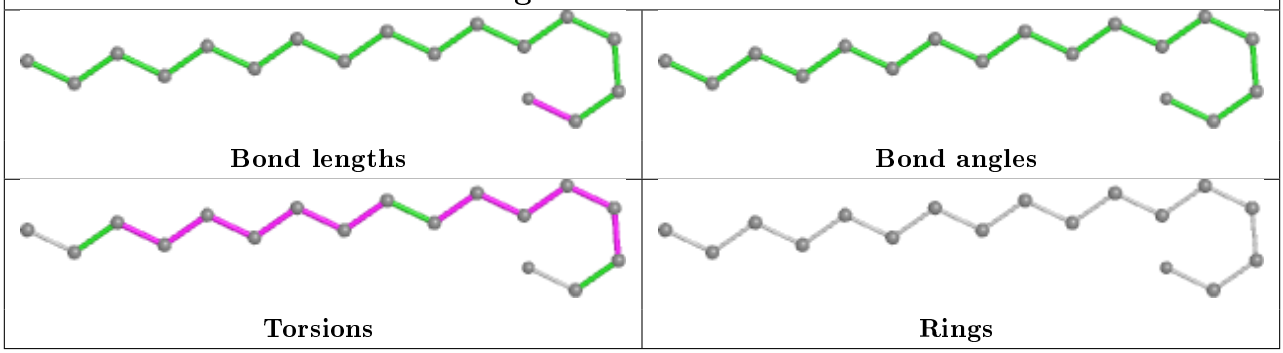
Ligand RET B 1296



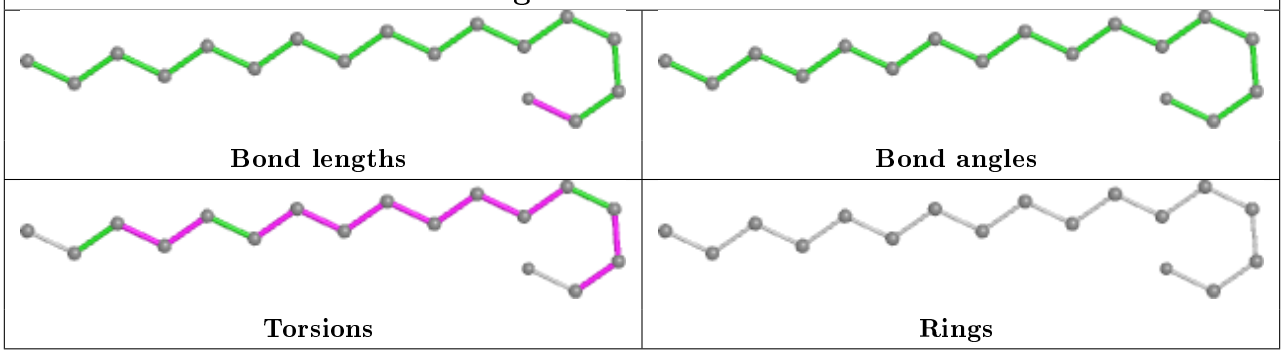
Ligand PLM A 1410



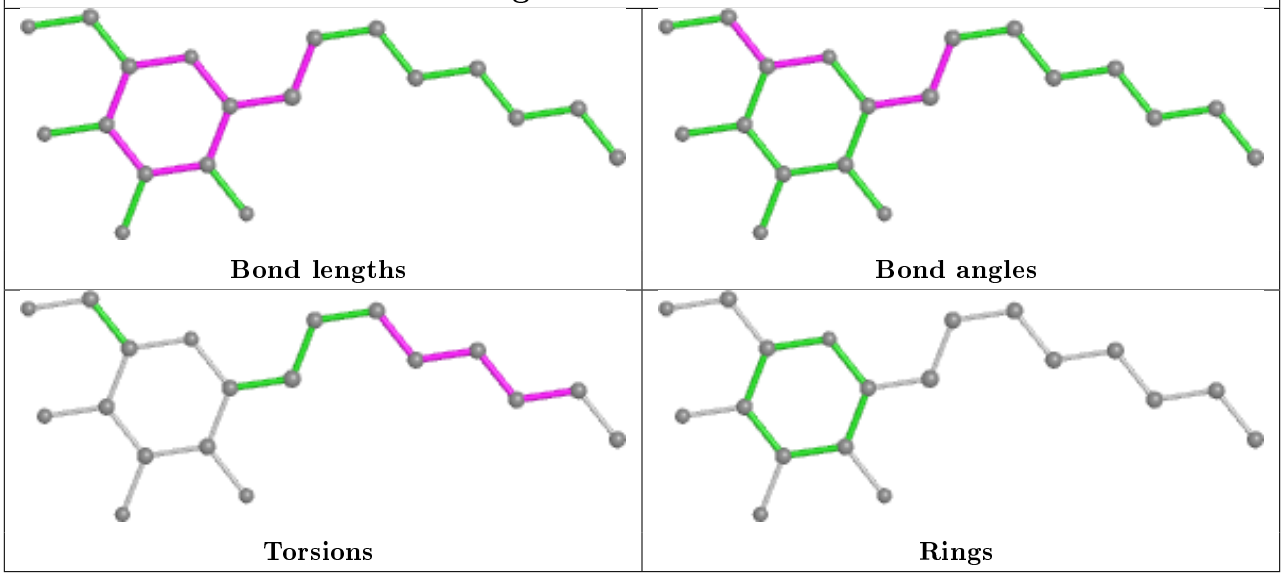
Ligand PLM B 1322



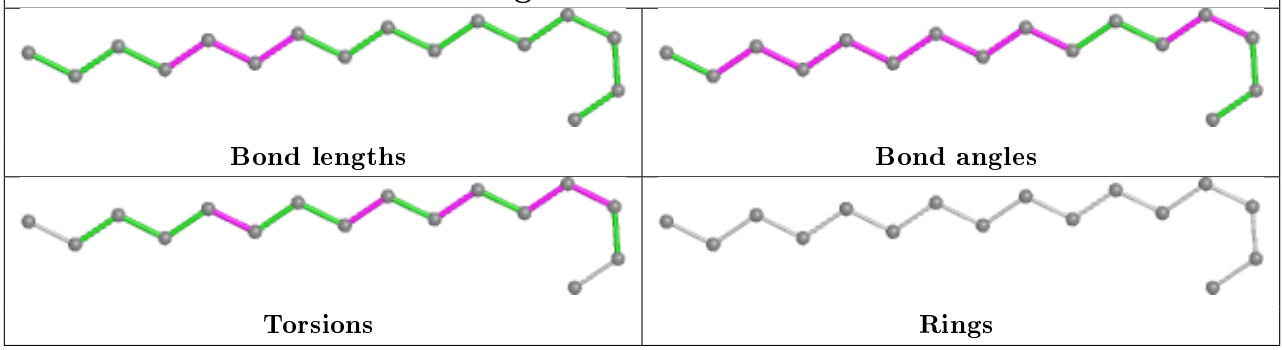
Ligand PLM A 1322

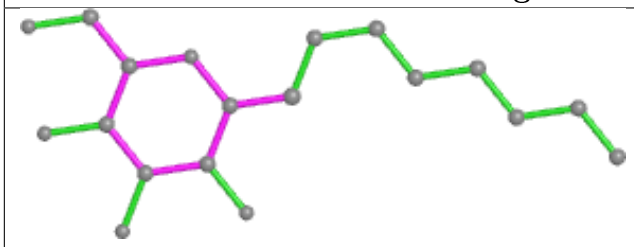
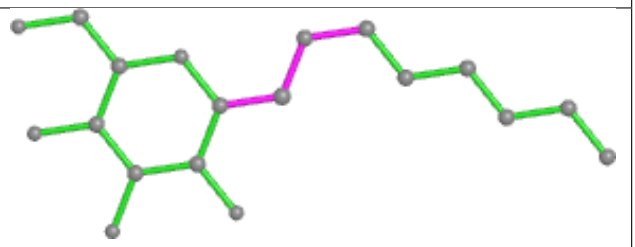
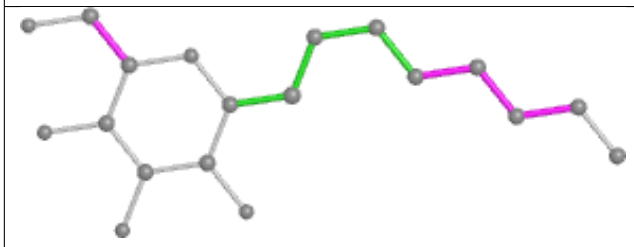
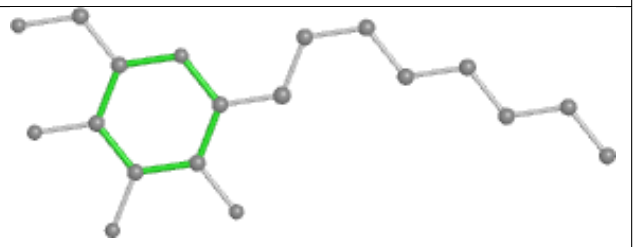


Ligand HTG A 1508



Ligand PLM B 1407



Ligand HTG B 1509	
 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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

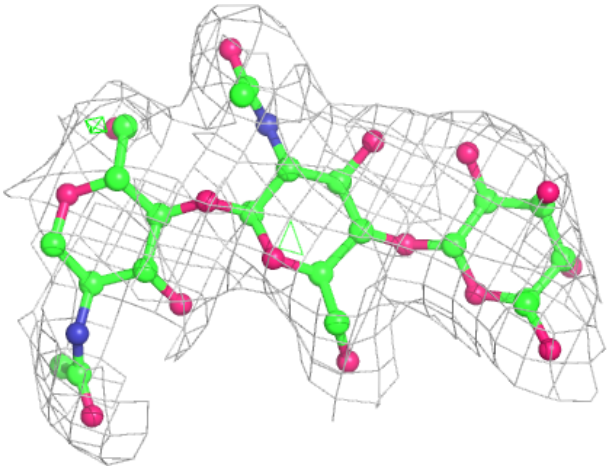
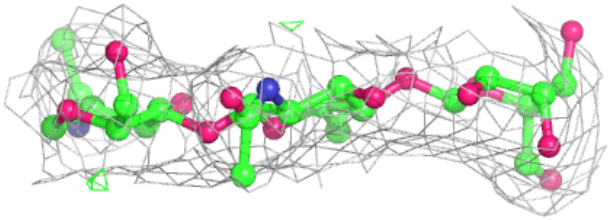
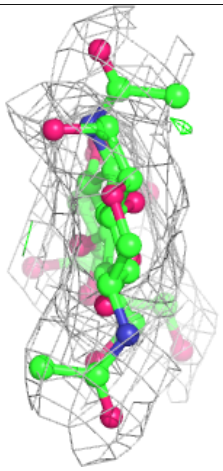
6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

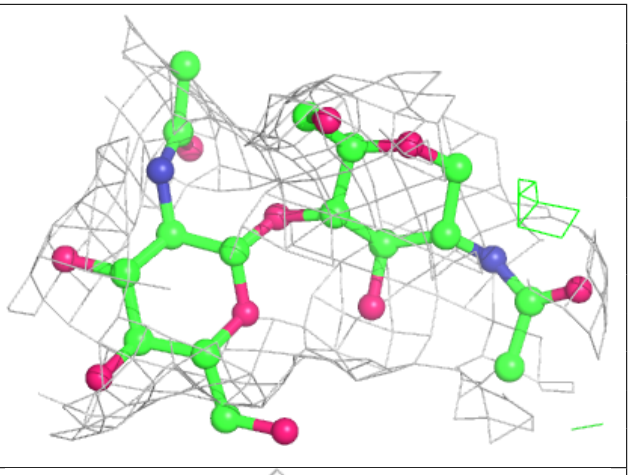
Unable to reproduce the depositors R factor - this section is therefore empty.

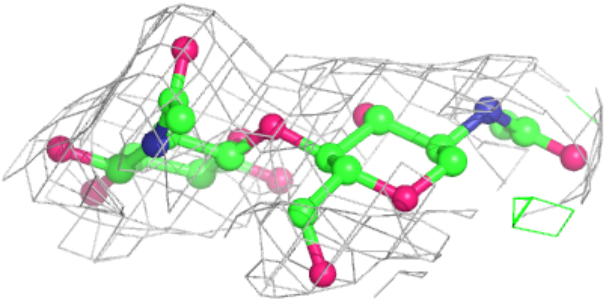
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

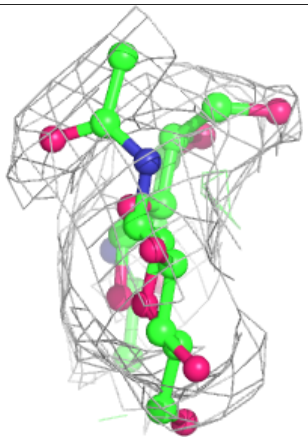
Electron density around Chain C: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around Chain D:

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

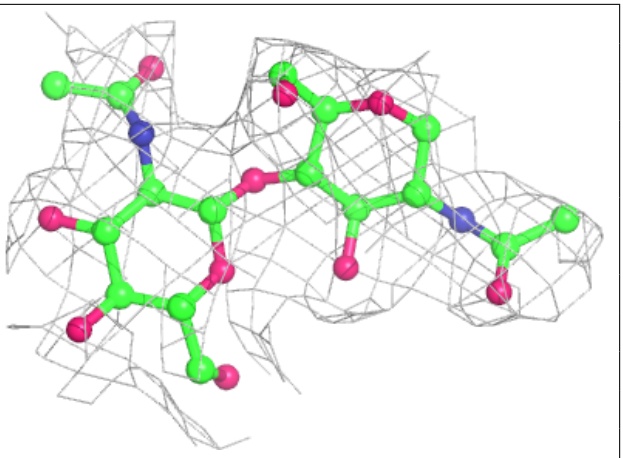


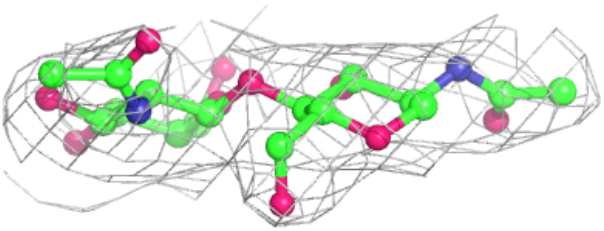


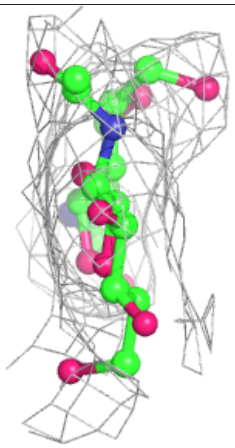


Electron density around Chain F:

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

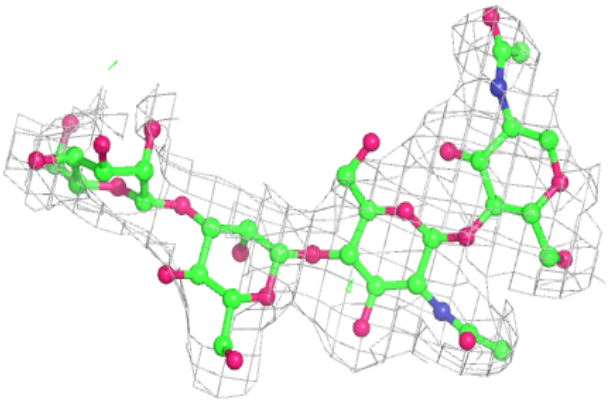


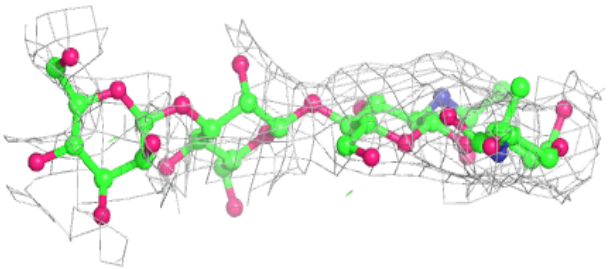


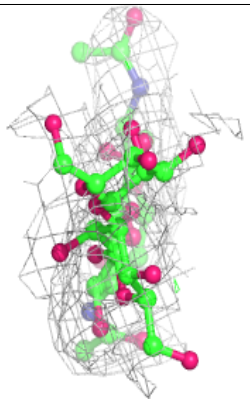


Electron density around Chain E:

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







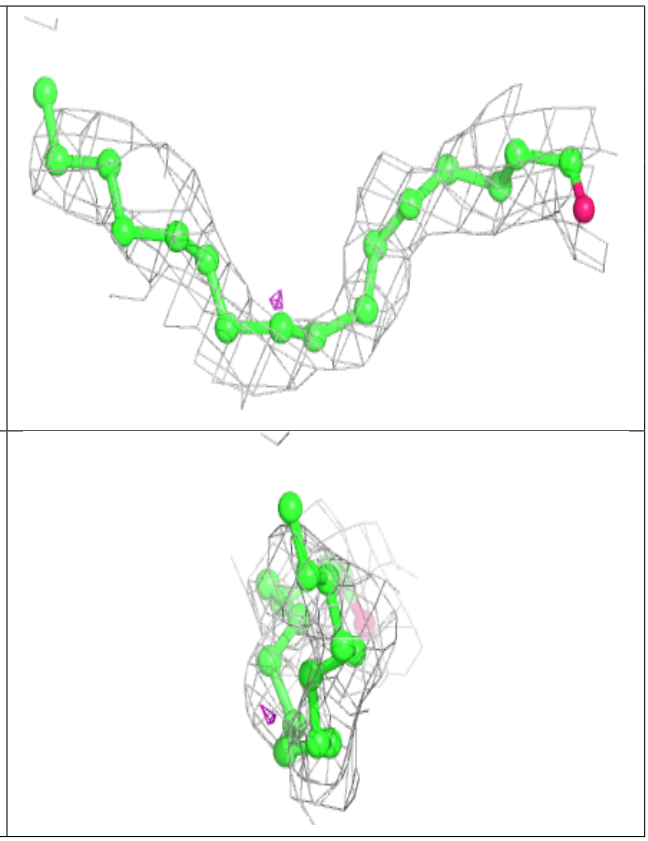
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

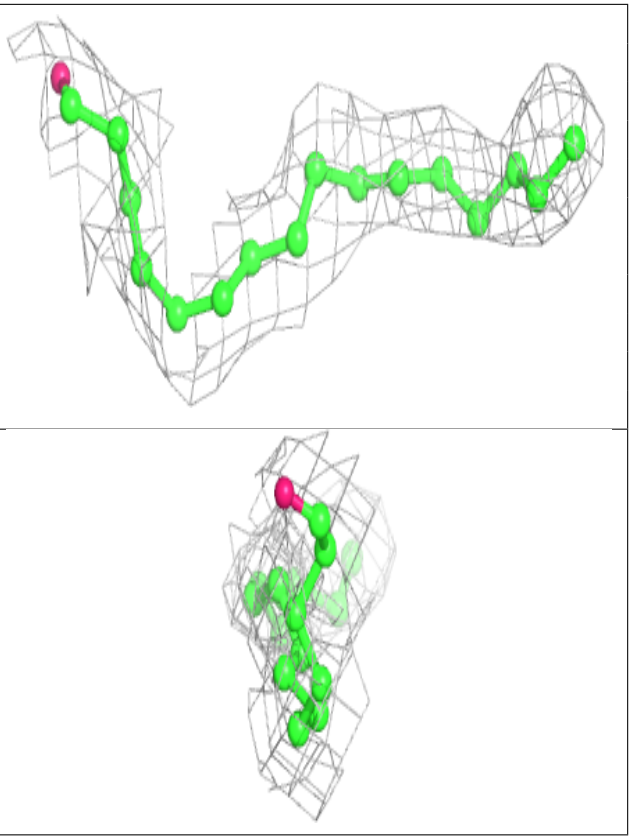
Electron density around PLM B 1323:

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



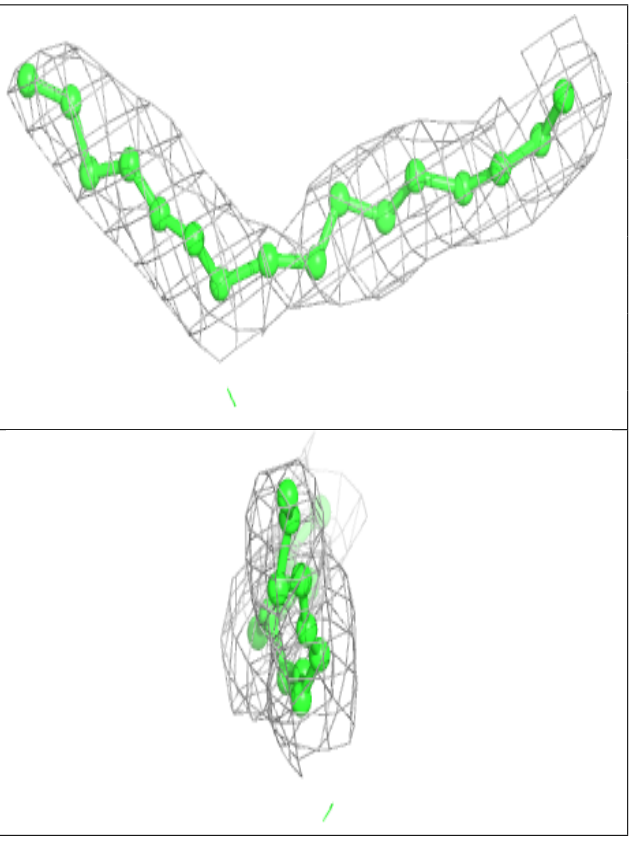
Electron density around PLM A 1323:

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



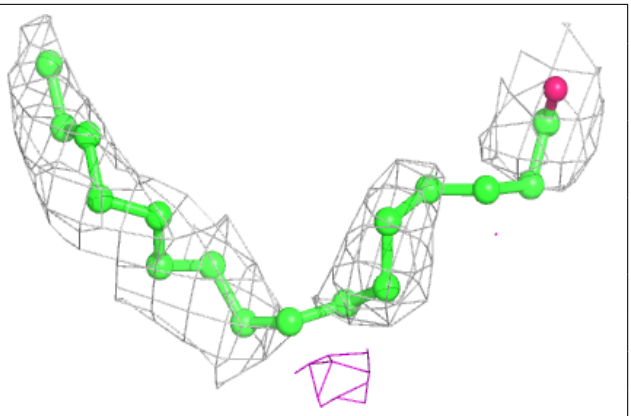
Electron density around PLM A 1410:

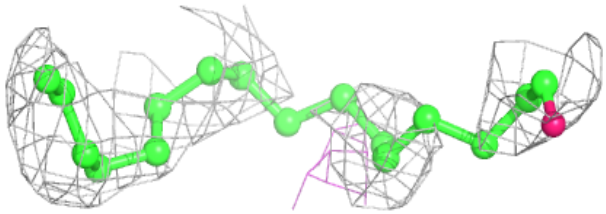
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PLM B 1322:

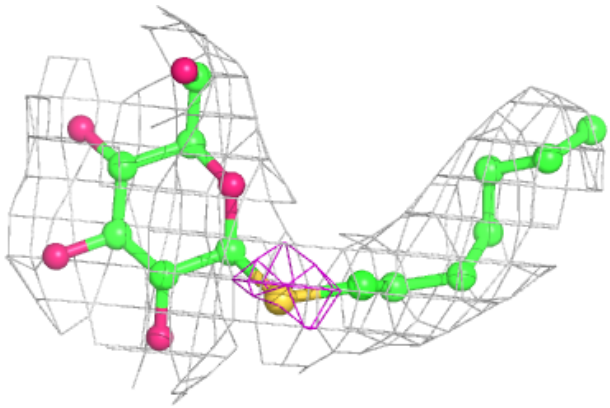
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

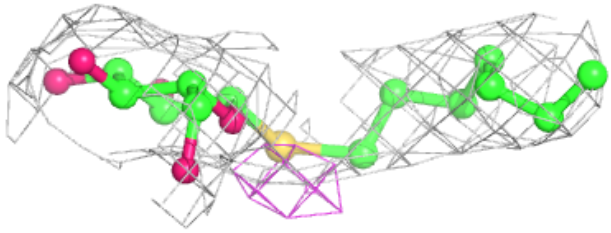


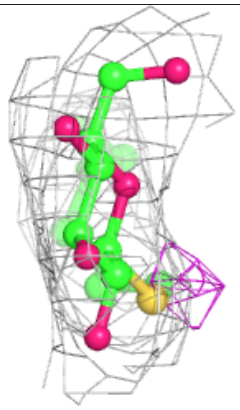


Electron density around HTG A 1508:

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

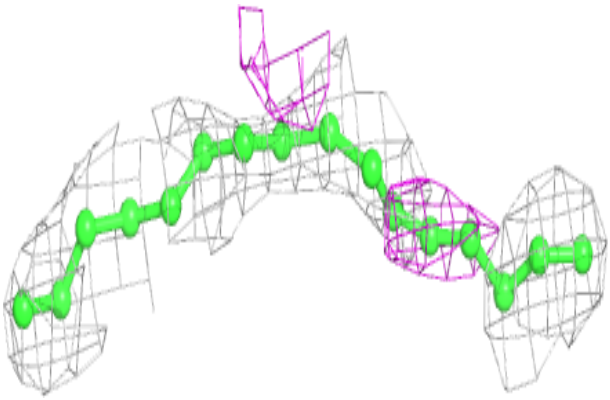


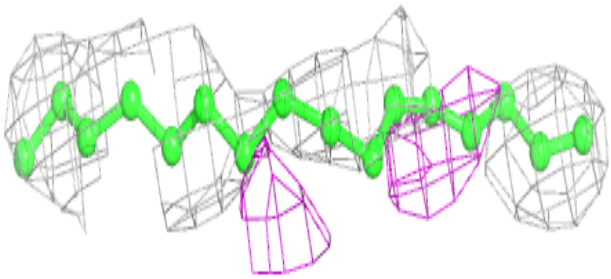


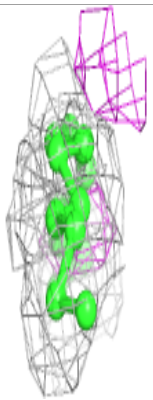


Electron density around PLM B 1407:

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

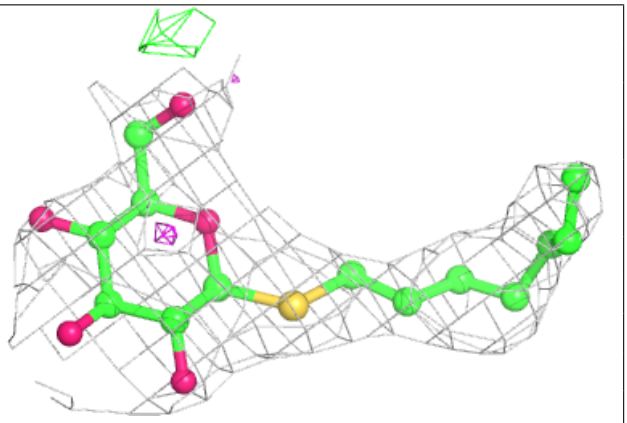


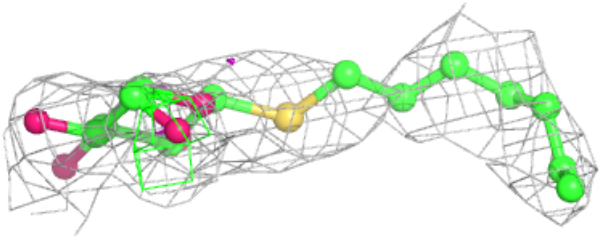


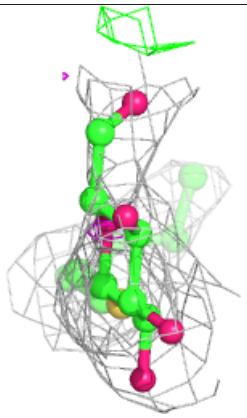


Electron density around HTG B 1509:

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

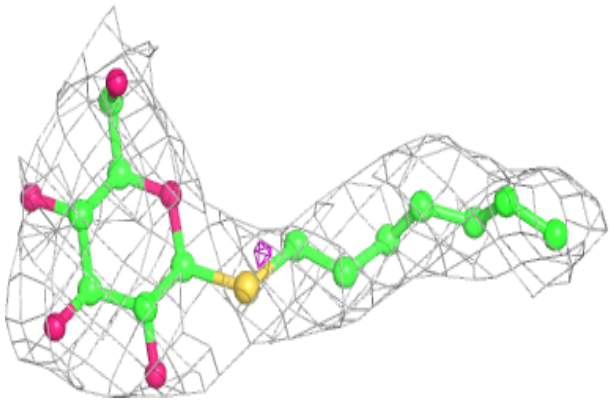


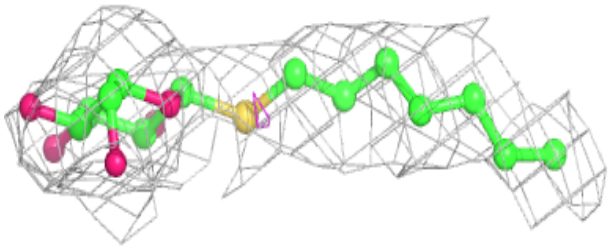


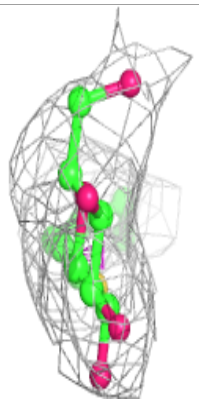


Electron density around HTG B 1506:

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

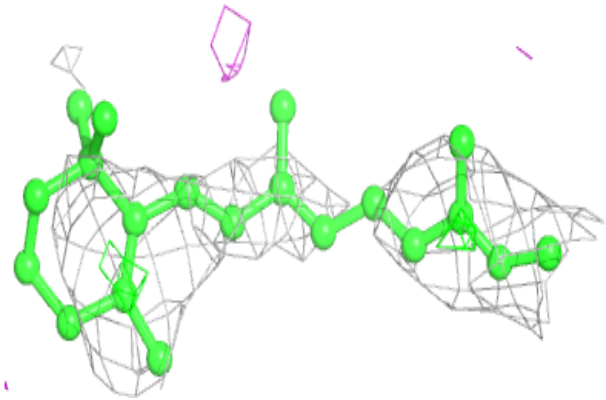


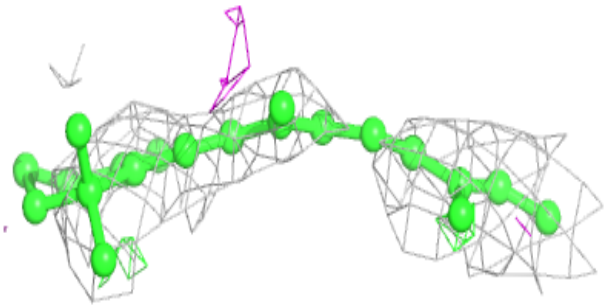


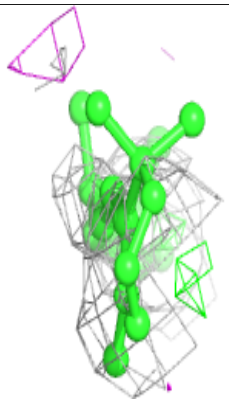


Electron density around RET A 1296:

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

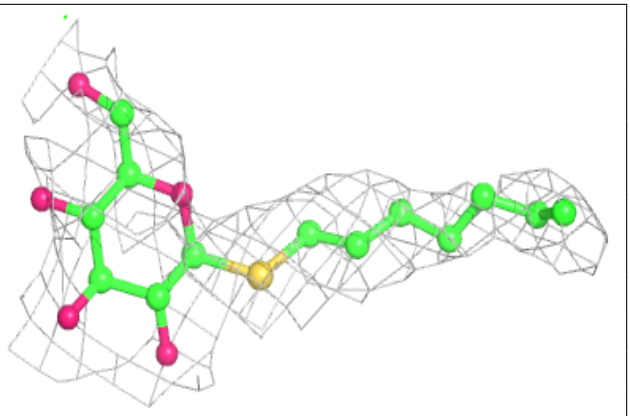


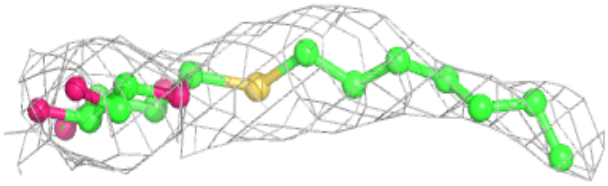


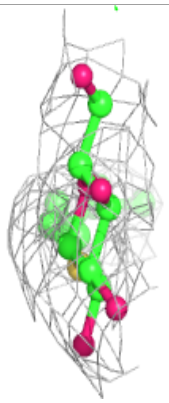


Electron density around HTG A 1507:

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

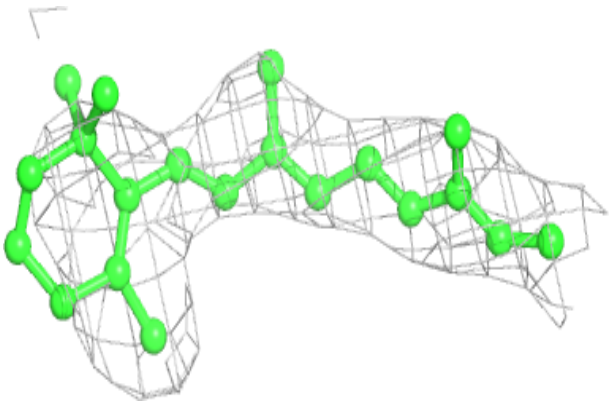


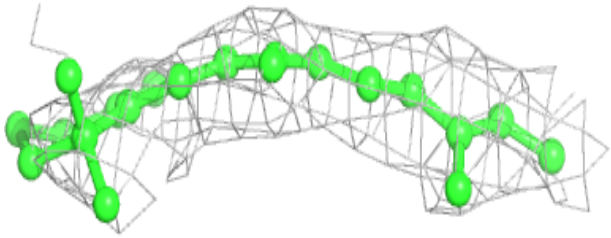


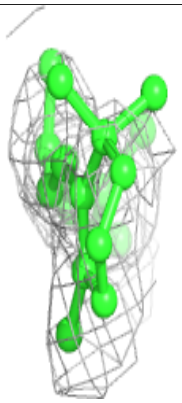


Electron density around RET B 1296:

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

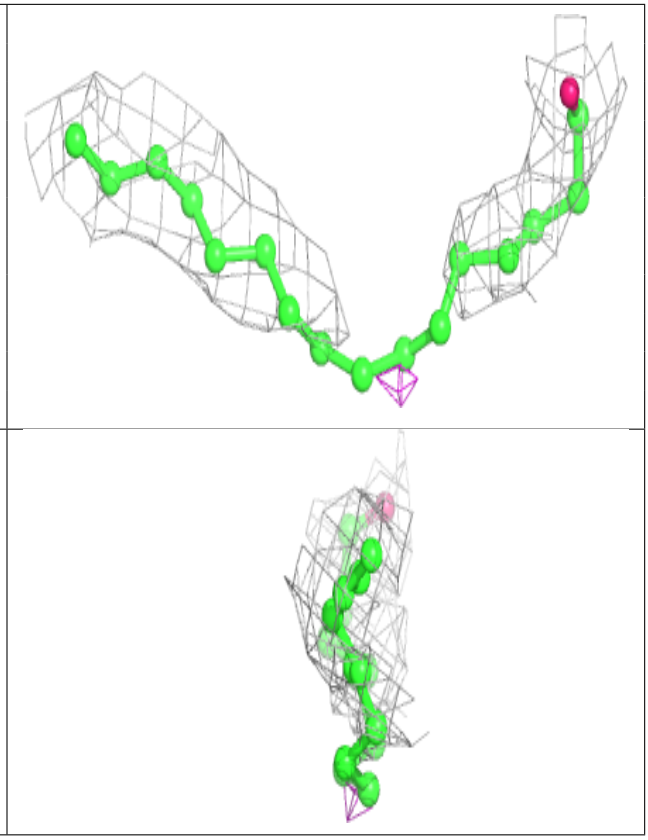






Electron density around PLM A 1322:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.