



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 11:25 PM BST

PDB ID : 3OAX
Title : Crystal structure of bovine rhodopsin with beta-ionone
Authors : Makino, C.L.; Riley, C.K.; Looney, J.; Crouch, R.K.; Okada, T.
Deposited on : 2010-08-05
Resolution : 2.60 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 ⓘ 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 : 2.13.1
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

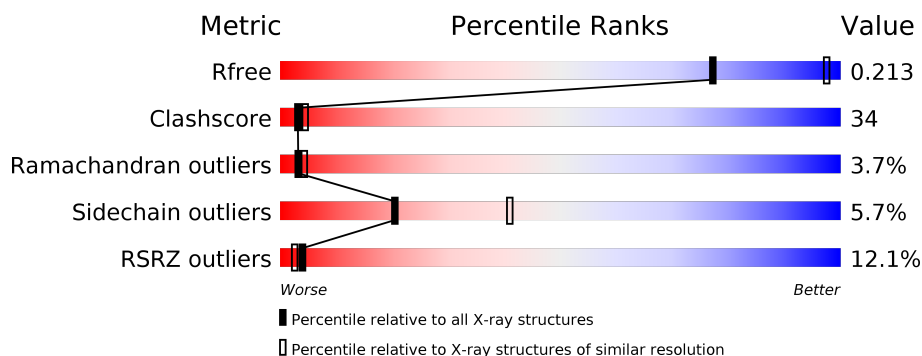
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	349	<div> <div>10%</div> <div>54%</div> <div>39%</div> <div>7%</div> </div>
1	B	349	<div> <div>14%</div> <div>51%</div> <div>43%</div> <div>5%</div> </div>
2	C	3	<div> <div>33%</div> <div>67%</div> </div>
3	D	2	<div> <div>50%</div> <div>50%</div> </div>
3	F	2	<div> <div>50%</div> <div>50%</div> </div>
4	E	4	<div> <div>25%</div> <div>25%</div> <div>50%</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
10	HTG	B	1506	-	-	-	X
11	ID3	B	6026	-	-	X	X
6	PLM	B	1322	-	-	-	X
6	PLM	B	1323	-	-	-	X
9	4E6	B	1407	-	-	-	X

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 6015 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
1	A	349	Total	C	N	O	S	0	0	0
			2749	1818	424	481	26			
1	B	349	Total	C	N	O	S	0	0	0
			2749	1818	424	481	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	acetylation	UNP P02699
B	0	ACE	-	acetylation	UNP P02699

- Molecule 2 is an oligosaccharide called 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
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



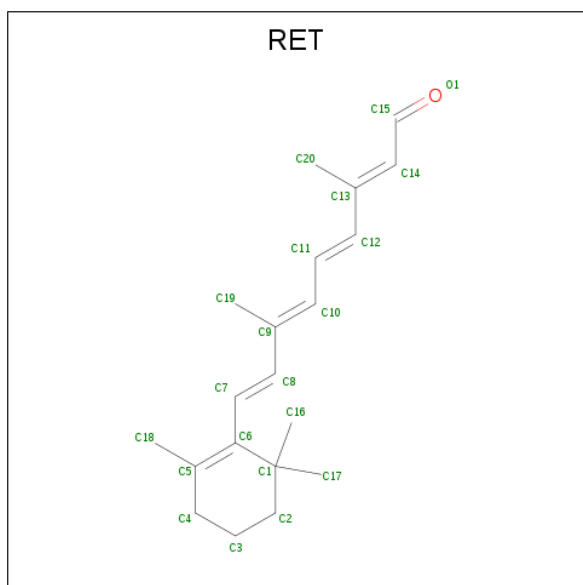
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called alpha-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.



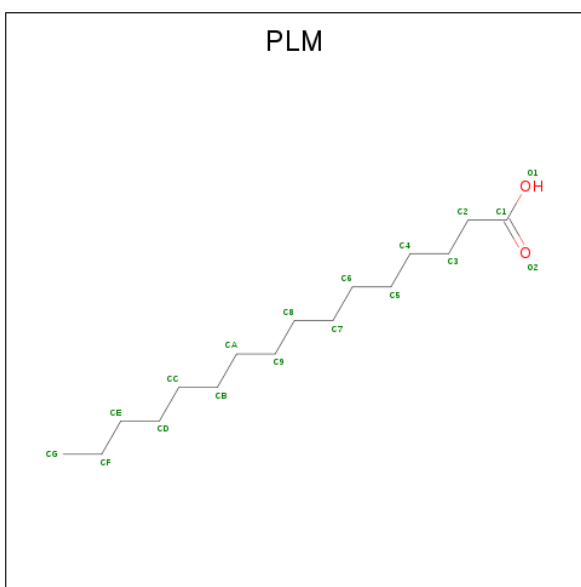
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



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

- Molecule 6 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



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

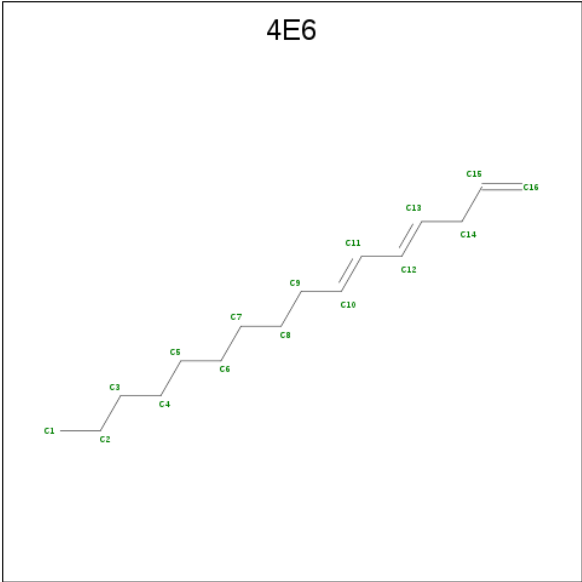
- Molecule 7 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

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

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

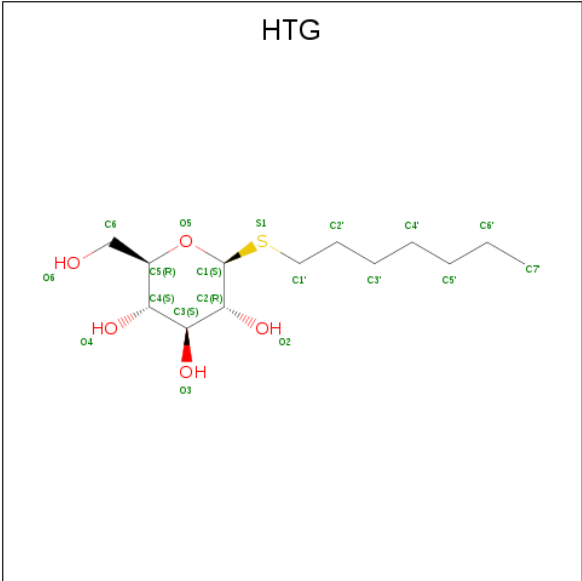
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	3	Total	Zn	0	0
			3	3		
8	A	4	Total	Zn	0	0
			4	4		

- Molecule 9 is (4E,6E)-hexadeca-1,4,6-triene (three-letter code: 4E6) (formula: C₁₆H₂₈).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	C	0	0
			16	16		
9	B	1	Total	C	0	0
			16	16		

- Molecule 10 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



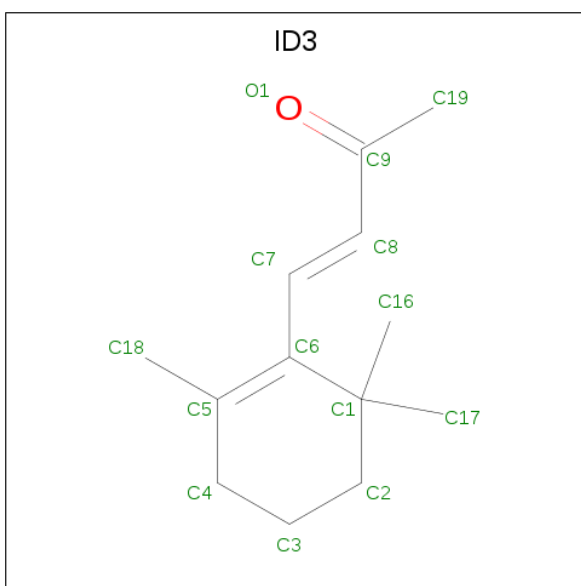
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	O	S	0	0
			19	13	5	1		

Continued on next page...

Continued from previous page...

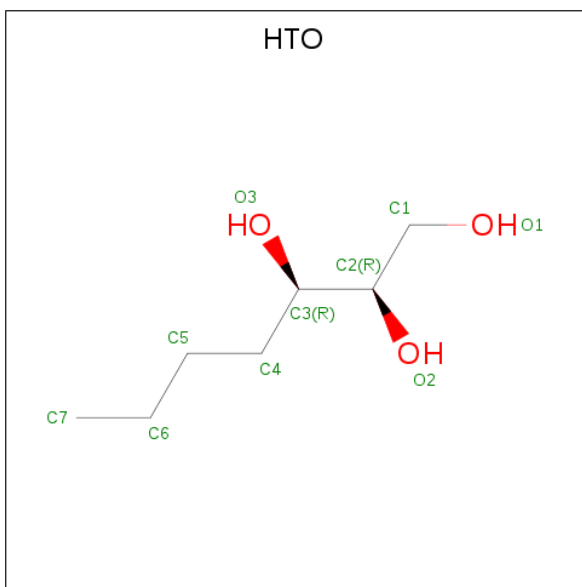
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	O	S	0	0
			19	13	5	1		
10	B	1	Total	C	O	S	0	0
			19	13	5	1		
10	B	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 11 is (3E)-4-(2,6,6-trimethylcyclohex-1-en-1-yl)but-3-en-2-one (three-letter code: ID3) (formula: C₁₃H₂₀O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	O		0	0
			14	13	1			
11	B	1	Total	C	O		0	0
			14	13	1			

- Molecule 12 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C₇H₁₆O₃).



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

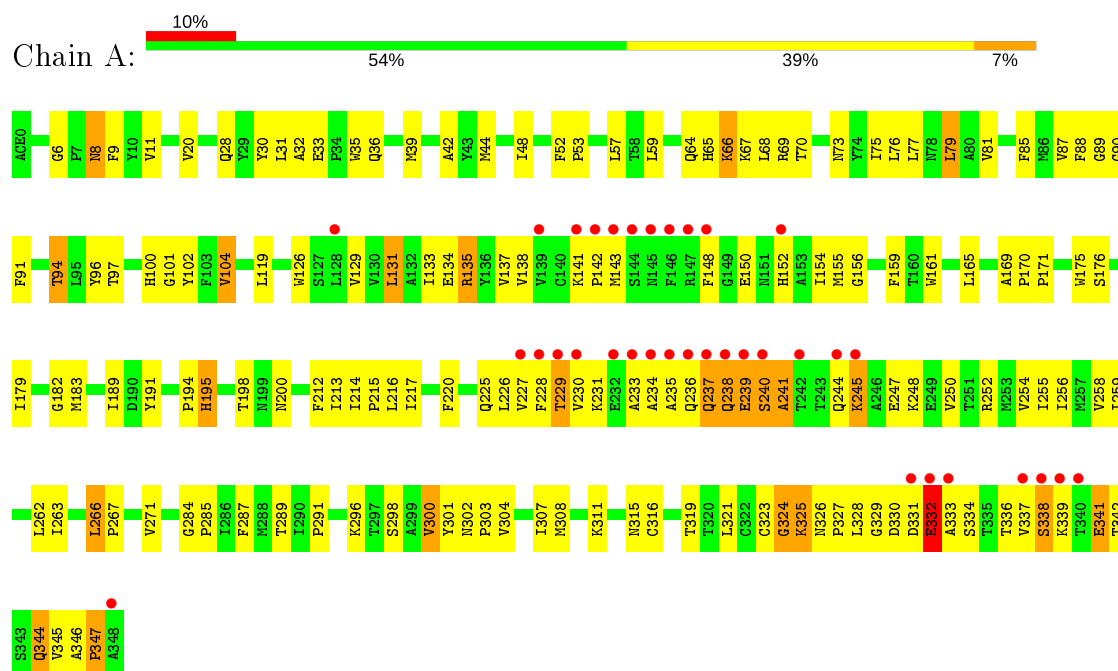
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	57	Total	O	0	0
			57	57		
13	B	48	Total	O	0	0
			48	48		

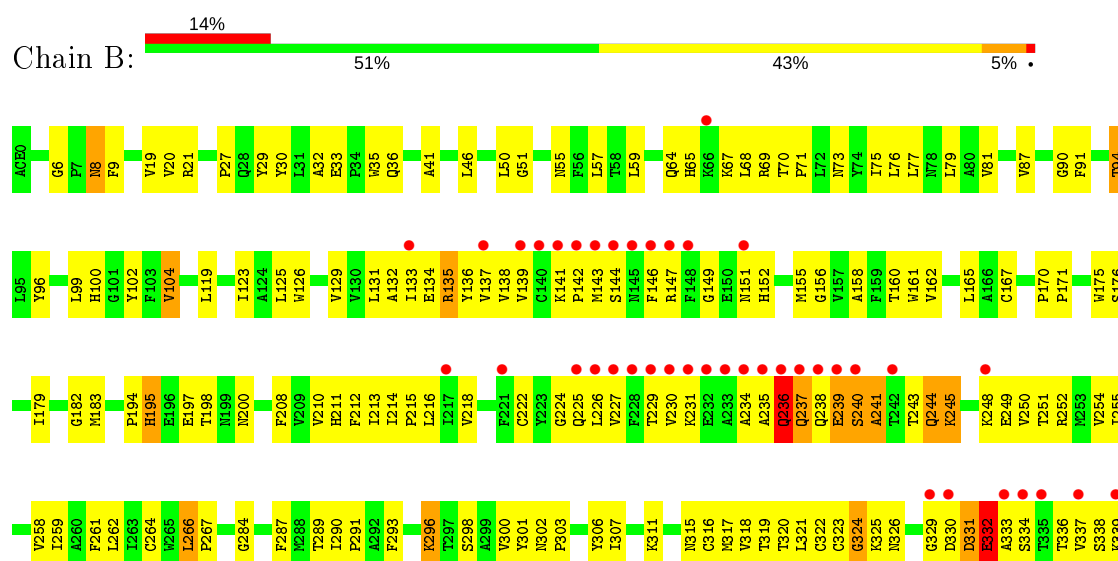
3 Residue-property plots

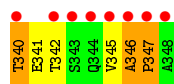
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Rhodopsin



• Molecule 1: Rhodopsin





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



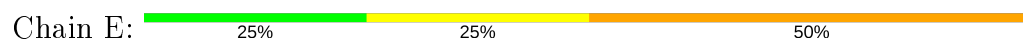
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 4: alpha-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



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	96.99 Å 96.99 Å 149.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 48.49 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.60) 93.6 (48.49-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.61 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.262 0.218 , 0.213	Depositor DCC
R_{free} test set	1996 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6015	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: HTG, ZN, BMA, NAG, ACE, HTO, ID3, RET, PLM, HG, 4E6, 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	0.51	0/2831	0.58	1/3859 (0.0%)
1	B	0.49	0/2831	0.57	1/3859 (0.0%)
All	All	0.50	0/5662	0.57	2/7718 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	LYS	CD-CE-NZ	5.79	125.03	111.70
1	B	296	LYS	CD-CE-NZ	5.48	124.31	111.70

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	2749	0	2706	183	0
1	B	2749	0	2708	215	0
2	C	39	0	34	1	0
3	D	28	0	25	0	0
3	F	28	0	25	0	0
4	E	50	0	43	2	0
5	A	20	0	27	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	20	0	27	0	0
6	A	34	0	62	0	0
6	B	34	0	62	2	0
7	A	3	0	0	0	0
7	B	3	0	0	1	0
8	A	4	0	0	0	0
8	B	3	0	0	0	0
9	A	16	0	27	1	0
9	B	16	0	27	0	0
10	A	38	0	52	1	0
10	B	38	0	52	3	0
11	A	14	0	20	5	0
11	B	14	0	20	9	0
12	B	10	0	16	1	0
13	A	57	0	0	2	0
13	B	48	0	0	3	0
All	All	6015	0	5933	397	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 34.

The worst 5 of 397 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:65:HIS:HB3	1:A:337:VAL:HG22	1.28	1.15
1:B:346:ALA:H	1:B:347:PRO:HD3	1.02	1.07
1:A:345:VAL:HG12	1:A:347:PRO:HD3	1.32	1.06
1:A:67:LYS:HB2	1:A:337:VAL:HB	1.36	1.06
1:A:341:GLU:HG3	1:A:342:THR:H	1.23	1.00

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	347/349 (99%)	302 (87%)	34 (10%)	11 (3%)	4	6
1	B	347/349 (99%)	300 (86%)	32 (9%)	15 (4%)	2	3
All	All	694/698 (99%)	602 (87%)	66 (10%)	26 (4%)	3	4

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	THR
1	A	238	GLN
1	A	241	ALA
1	A	325	LYS
1	B	240	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	296/296 (100%)	276 (93%)	20 (7%)	16	32
1	B	296/296 (100%)	282 (95%)	14 (5%)	26	50
All	All	592/592 (100%)	558 (94%)	34 (6%)	20	41

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	VAL
1	A	344	GLN
1	B	264	CYS
1	A	336	THR
1	A	119	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
1	B	8	ASN
1	B	237	GLN
1	A	302	ASN
1	B	244	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.59	0	17,19,21	0.73	0
2	NAG	C	2	2	14,14,15	0.62	0	17,19,21	0.80	0
2	BMA	C	3	2	11,11,12	0.51	0	15,15,17	0.43	0
3	NAG	D	1	1,3	14,14,15	0.53	0	17,19,21	0.69	0
3	NAG	D	2	3	14,14,15	0.48	0	17,19,21	0.72	1 (5%)
4	NAG	E	1	1,4	14,14,15	0.66	0	17,19,21	0.73	0
4	NAG	E	2	4	14,14,15	0.56	0	17,19,21	0.70	1 (5%)
4	BMA	E	3	4	11,11,12	0.63	0	15,15,17	0.45	0
4	MAN	E	4	4	11,11,12	0.69	0	15,15,17	0.66	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.55	0	17,19,21	0.55	0
3	NAG	F	2	3	14,14,15	0.58	0	17,19,21	0.72	1 (5%)

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	BMA	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	-	4/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
4	BMA	E	3	4	-	1/2/19/22	0/1/1/1
4	MAN	E	4	4	-	2/2/19/22	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.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	NAG	C2-N2-C7	-2.15	119.84	122.90
3	D	2	NAG	C2-N2-C7	-2.13	119.86	122.90
3	F	2	NAG	C2-N2-C7	-2.12	119.88	122.90
4	E	4	MAN	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 3 short contacts:

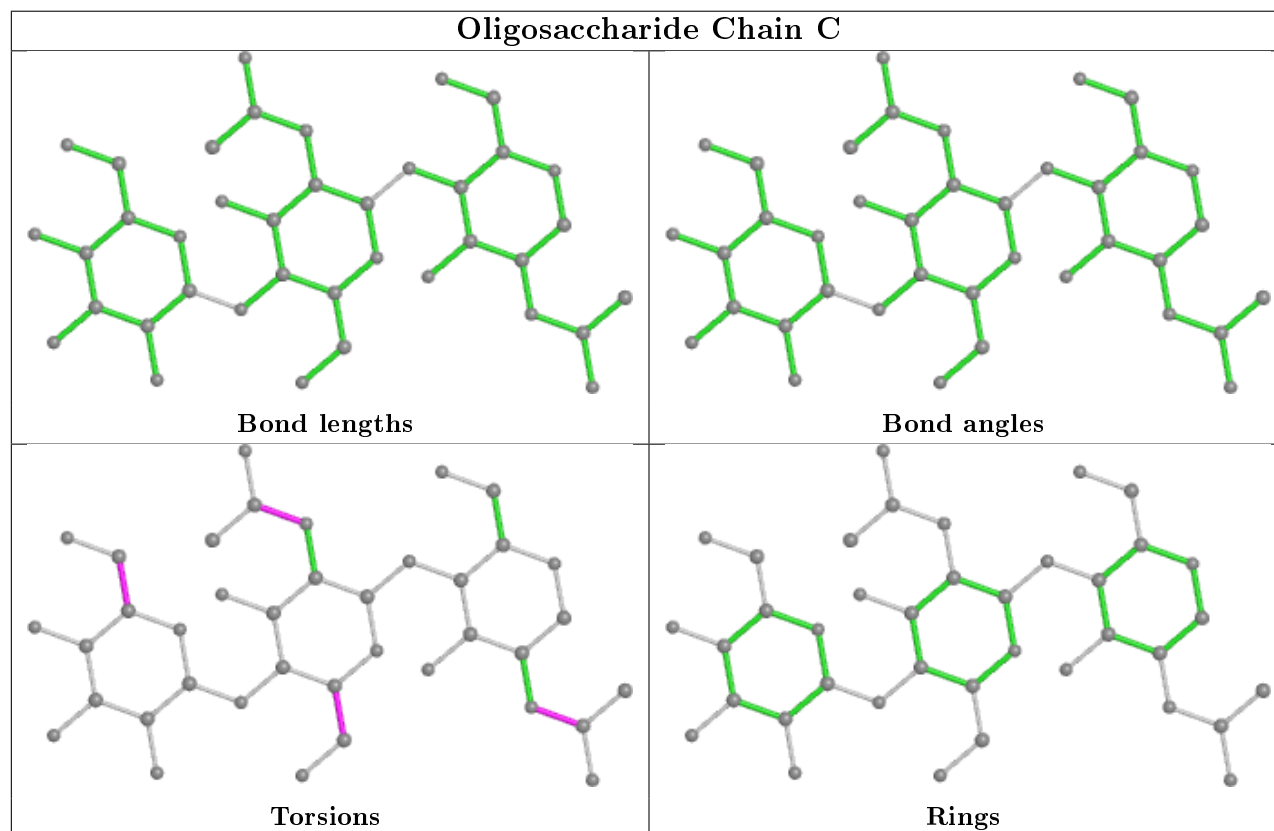
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	4	MAN	1	0

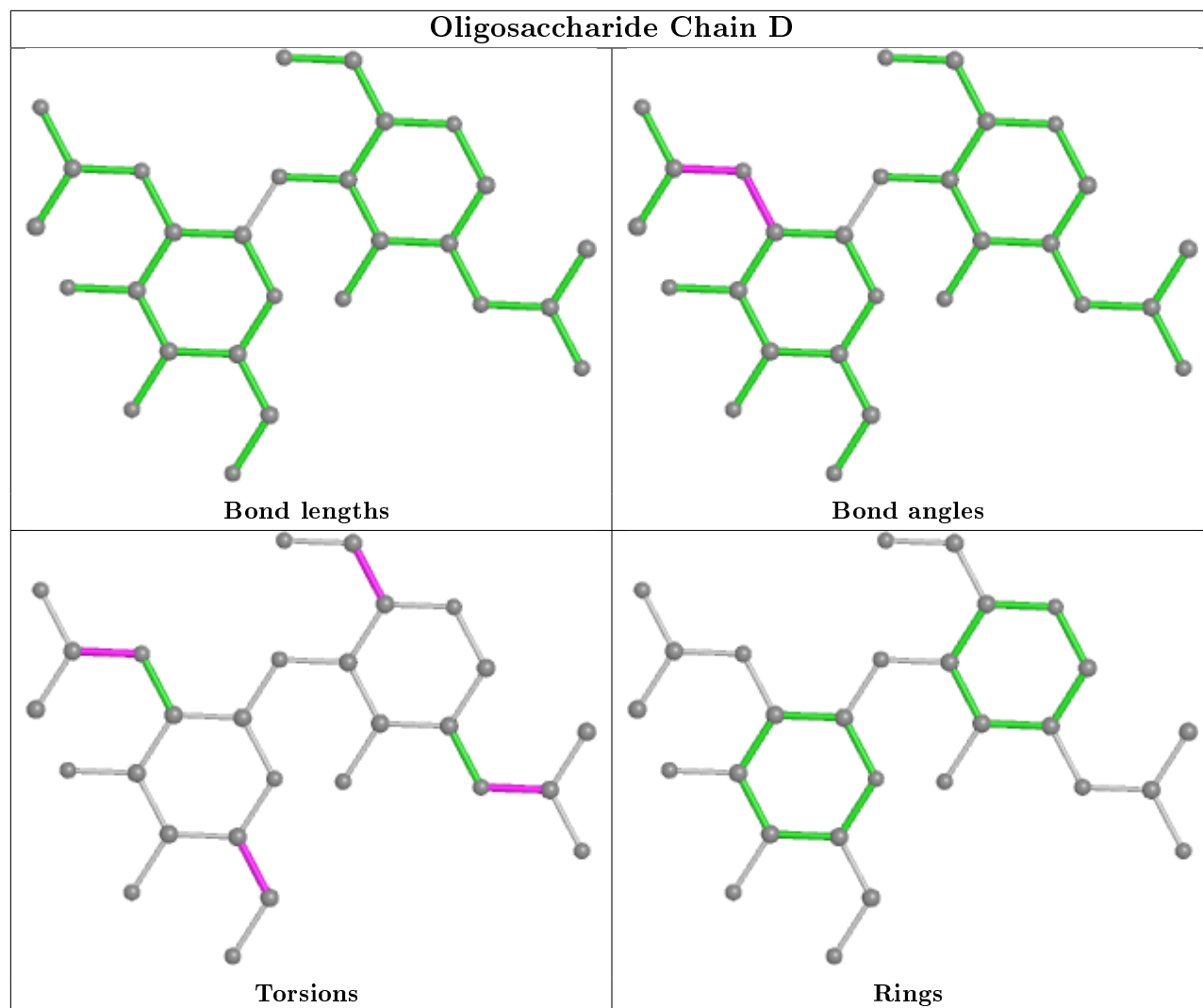
Continued on next page...

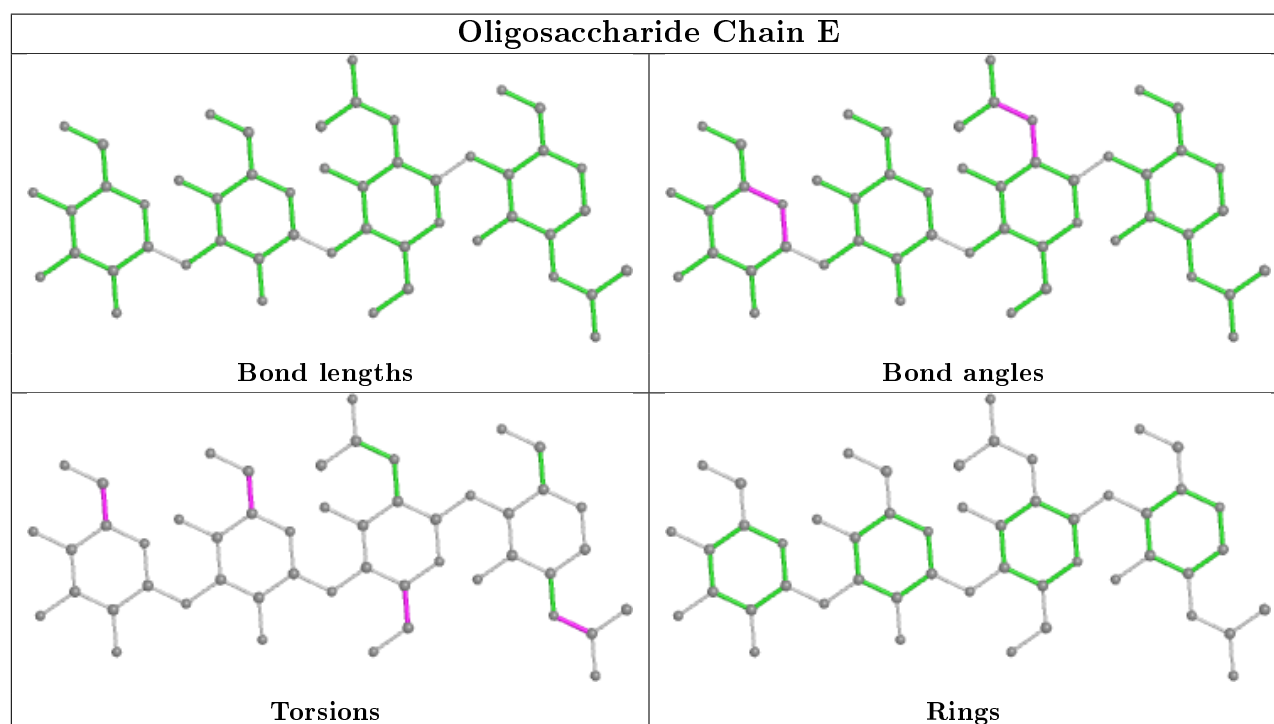
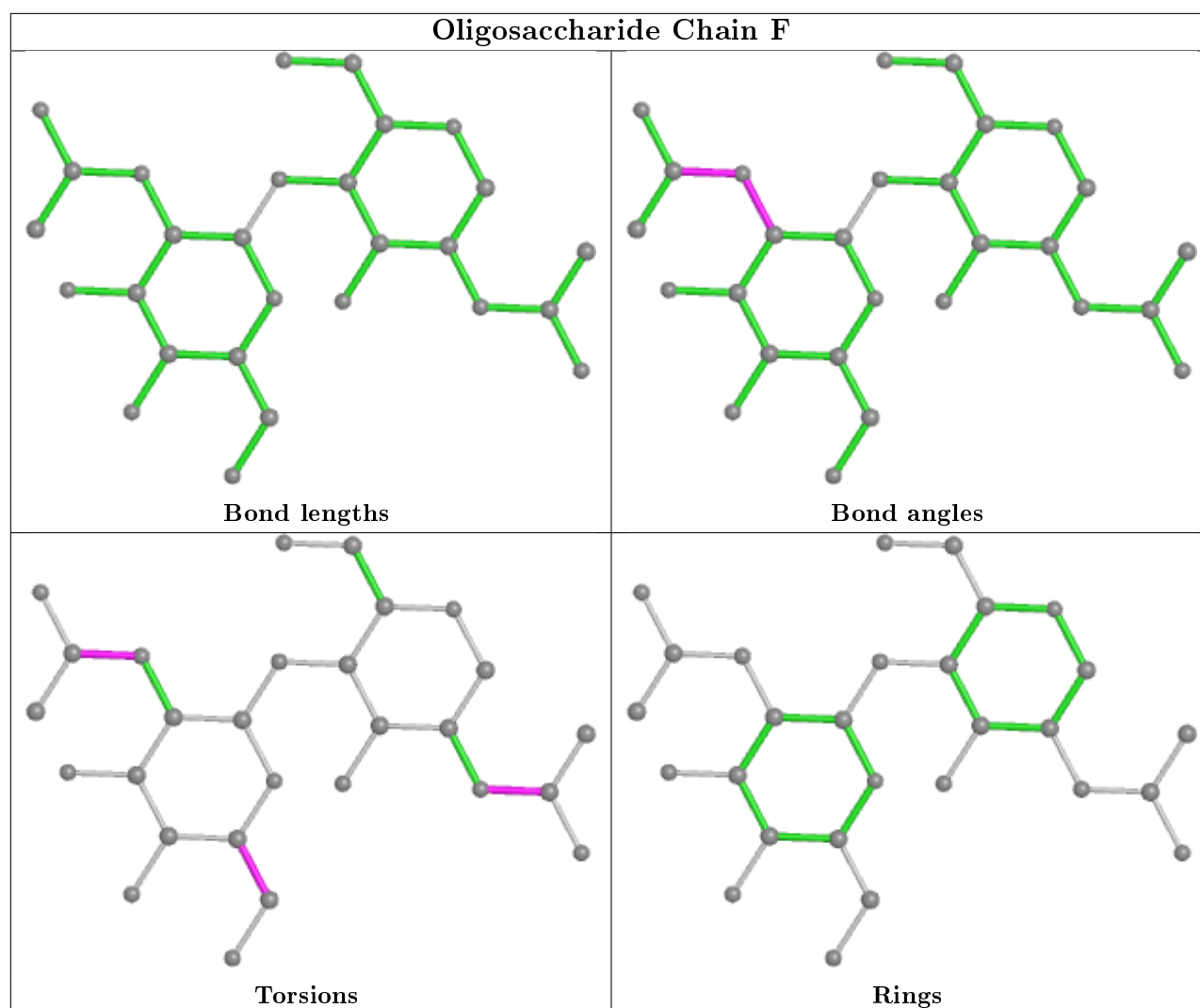
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0
4	E	3	BMA	1	0
4	E	2	NAG	1	0
2	C	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.







5.6 Ligand geometry

Of 28 ligands modelled in this entry, 13 are monoatomic - leaving 15 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
11	ID3	B	6026	-	14,14,14	2.41	4 (28%)	20,20,20	1.50	3 (15%)
5	RET	A	1296	1	20,20,21	2.08	4 (20%)	27,27,28	1.67	8 (29%)
10	HTG	B	1506	-	19,19,19	2.70	7 (36%)	23,24,24	2.54	4 (17%)
10	HTG	A	1507	-	19,19,19	2.83	7 (36%)	23,24,24	1.99	1 (4%)
5	RET	B	1296	1	20,20,21	2.10	3 (15%)	27,27,28	1.69	9 (33%)
6	PLM	A	1323	1	16,16,17	0.35	0	15,15,17	0.57	0
12	HTO	B	1401	-	9,9,9	1.83	2 (22%)	10,10,10	0.94	1 (10%)
11	ID3	A	6025	-	14,14,14	2.69	6 (42%)	20,20,20	1.72	5 (25%)
6	PLM	B	1322	1	16,16,17	0.37	0	15,15,17	0.52	0
9	4E6	A	1410	-	15,15,15	2.04	1 (6%)	13,14,14	2.99	5 (38%)
10	HTG	A	1508	-	19,19,19	2.46	7 (36%)	23,24,24	2.01	1 (4%)
6	PLM	A	1322	1	16,16,17	0.33	0	15,15,17	0.59	0
6	PLM	B	1323	1	16,16,17	0.42	0	15,15,17	0.51	0
9	4E6	B	1407	-	15,15,15	1.98	1 (6%)	13,14,14	2.83	6 (46%)
10	HTG	B	1509	-	19,19,19	2.79	7 (36%)	23,24,24	2.27	3 (13%)

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
11	ID3	B	6026	-	-	0/5/22/22	0/1/1/1
5	RET	A	1296	1	-	1/13/30/31	0/1/1/1
10	HTG	B	1506	-	-	2/10/30/30	0/1/1/1
10	HTG	A	1507	-	-	3/10/30/30	0/1/1/1
5	RET	B	1296	1	-	1/13/30/31	0/1/1/1
6	PLM	A	1323	1	-	9/13/14/15	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	HTO	B	1401	-	-	2/10/10/10	-
11	ID3	A	6025	-	-	0/5/22/22	0/1/1/1
6	PLM	B	1322	1	-	10/13/14/15	-
9	4E6	A	1410	-	-	3/13/13/13	-
10	HTG	A	1508	-	-	7/10/30/30	0/1/1/1
6	PLM	A	1322	1	-	8/13/14/15	-
6	PLM	B	1323	1	-	9/13/14/15	-
9	4E6	B	1407	-	-	3/13/13/13	-
10	HTG	B	1509	-	-	5/10/30/30	0/1/1/1

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1507	HTG	O5-C1	8.20	1.55	1.42
10	B	1509	HTG	O5-C1	8.06	1.54	1.42
10	B	1506	HTG	O5-C1	8.02	1.54	1.42
9	A	1410	4E6	C12-C11	-7.16	1.23	1.44
10	A	1508	HTG	O5-C1	7.13	1.53	1.42

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	1506	HTG	C1'-S1-C1	10.96	120.58	100.09
10	B	1509	HTG	C1'-S1-C1	9.89	118.59	100.09
10	A	1508	HTG	C1'-S1-C1	8.80	116.56	100.09
10	A	1507	HTG	C1'-S1-C1	8.50	115.98	100.09
9	A	1410	4E6	C8-C9-C10	7.48	155.32	112.43

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

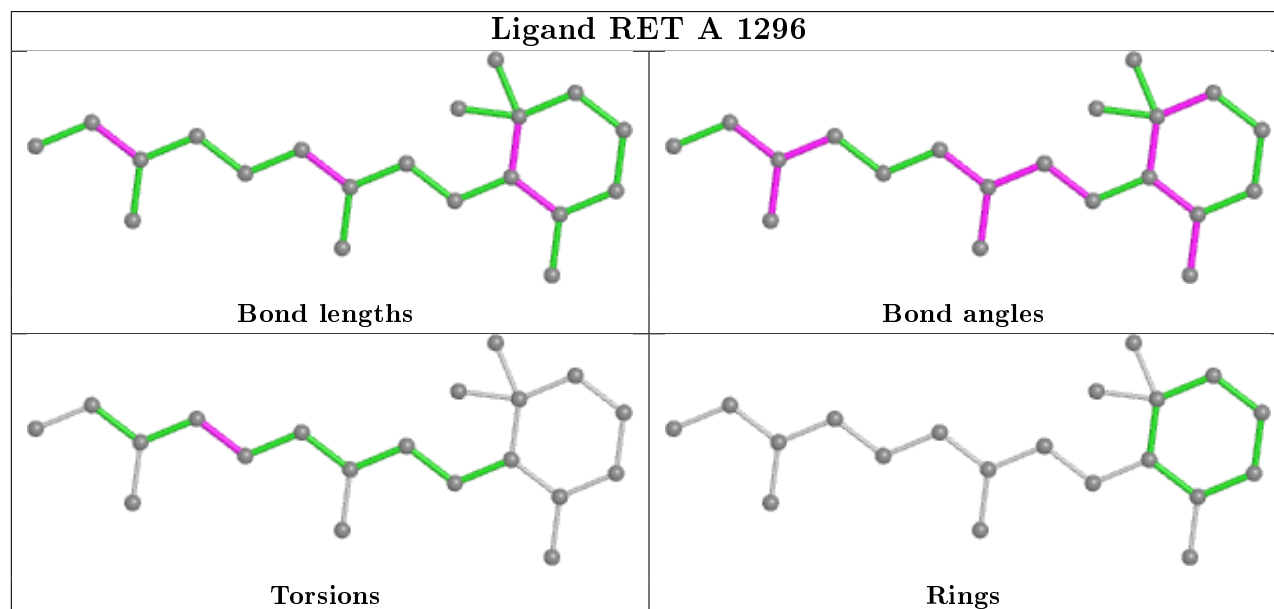
Mol	Chain	Res	Type	Atoms
5	B	1296	RET	C10-C11-C12-C13
5	A	1296	RET	C10-C11-C12-C13
10	A	1508	HTG	C2'-C1'-S1-C1
6	A	1322	PLM	C1-C2-C3-C4
10	B	1509	HTG	O5-C5-C6-O6

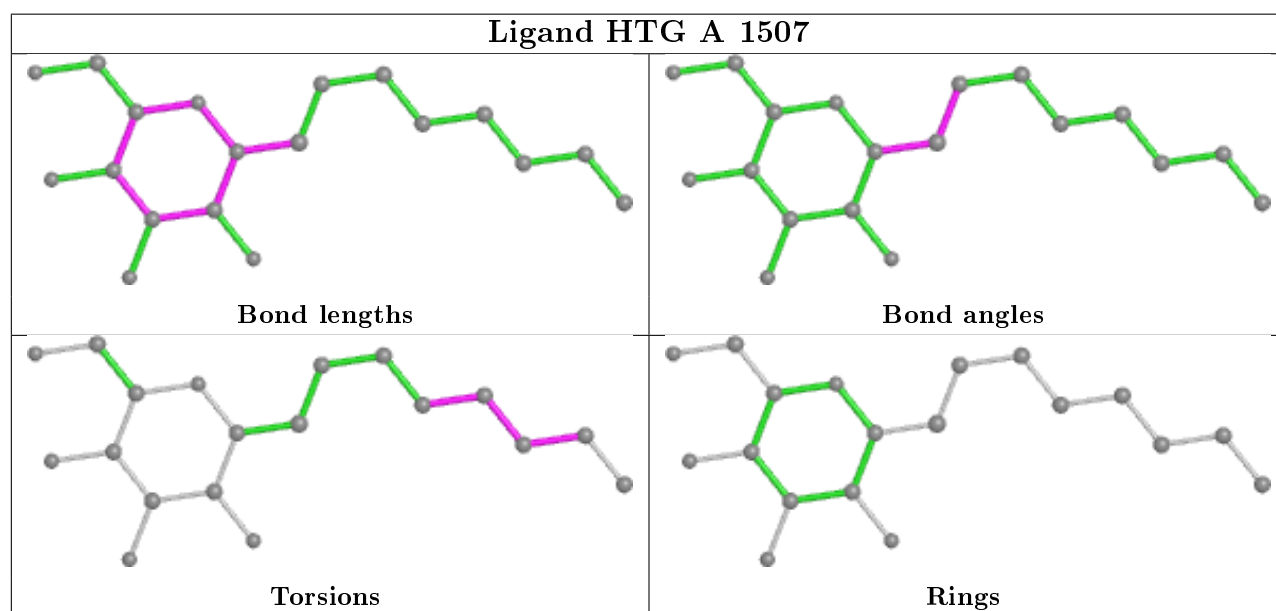
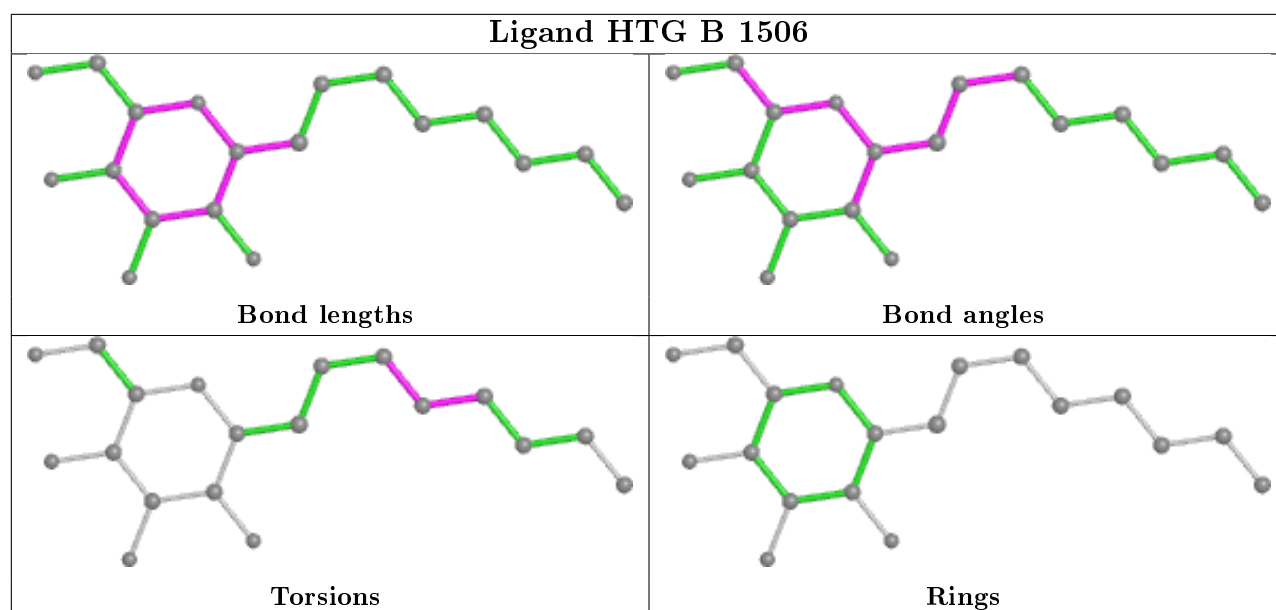
There are no ring outliers.

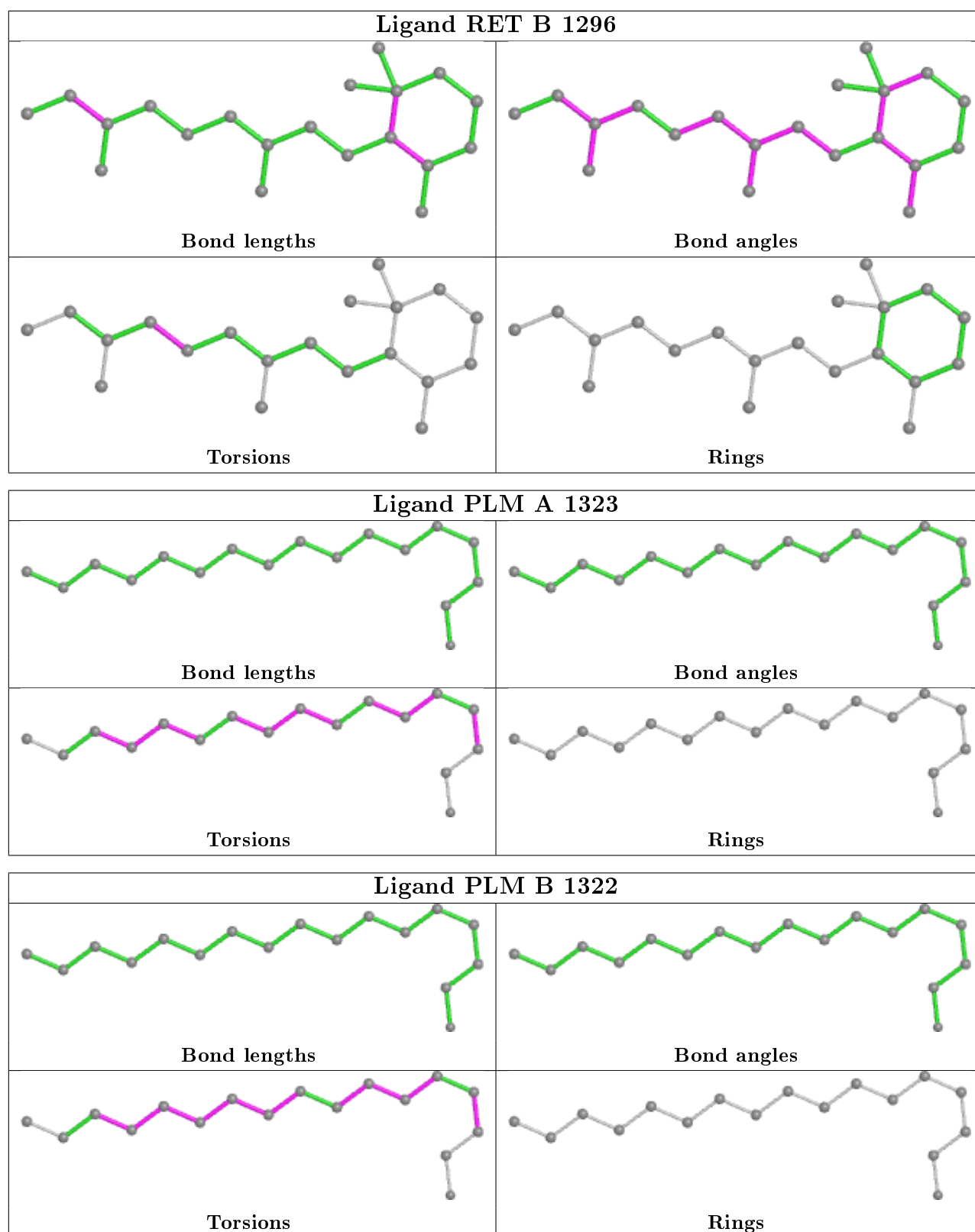
9 monomers are involved in 21 short contacts:

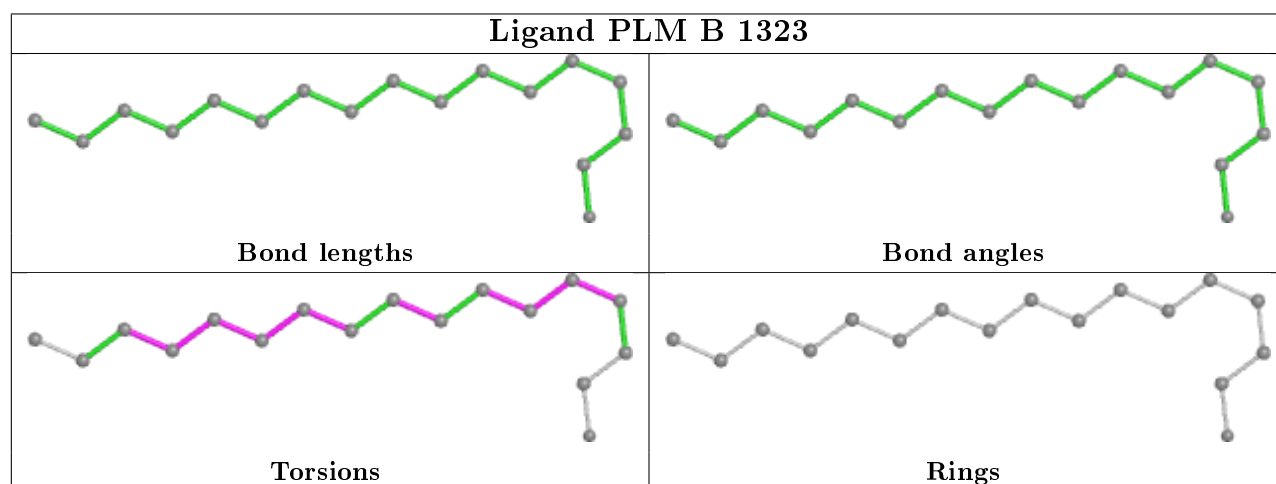
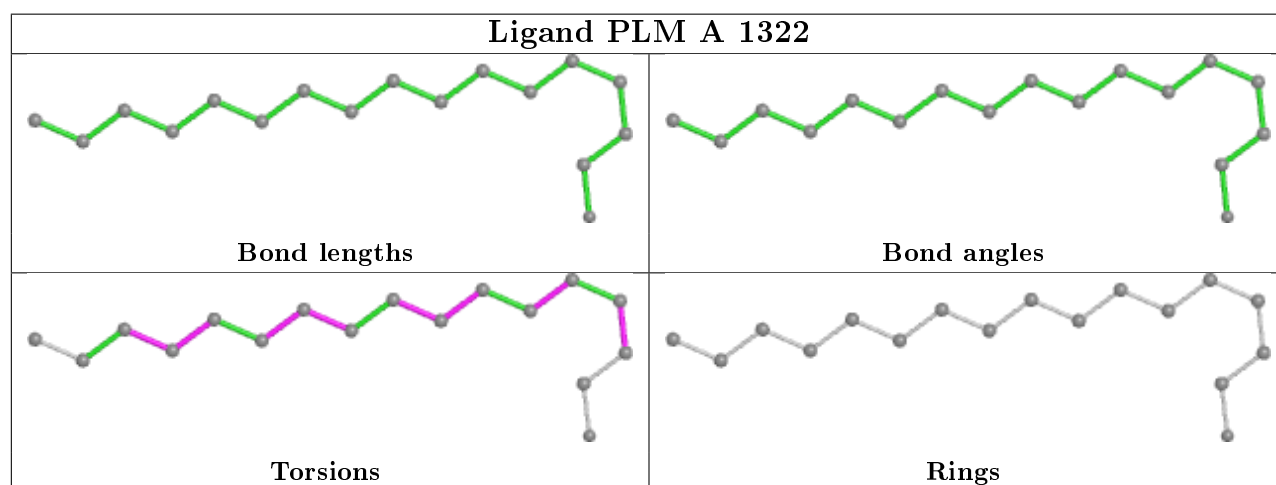
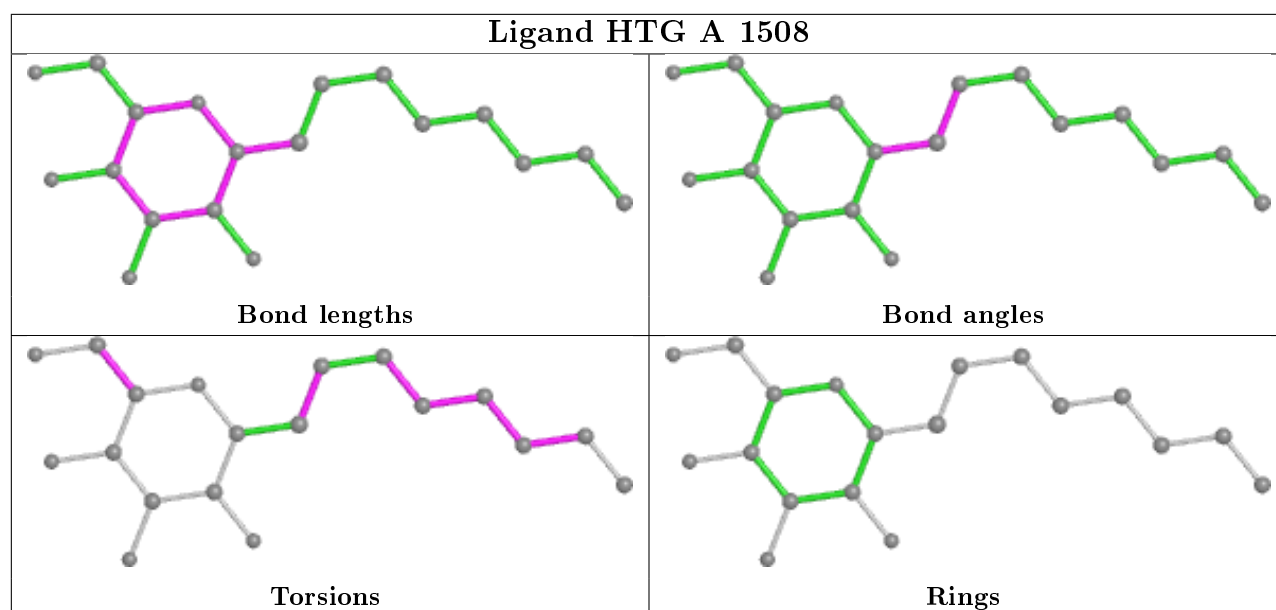
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	6026	ID3	9	0
5	A	1296	RET	1	0
10	B	1506	HTG	2	0
12	B	1401	HTO	1	0
11	A	6025	ID3	5	0
9	A	1410	4E6	1	0
10	A	1508	HTG	1	0
6	B	1323	PLM	2	0
10	B	1509	HTG	1	0

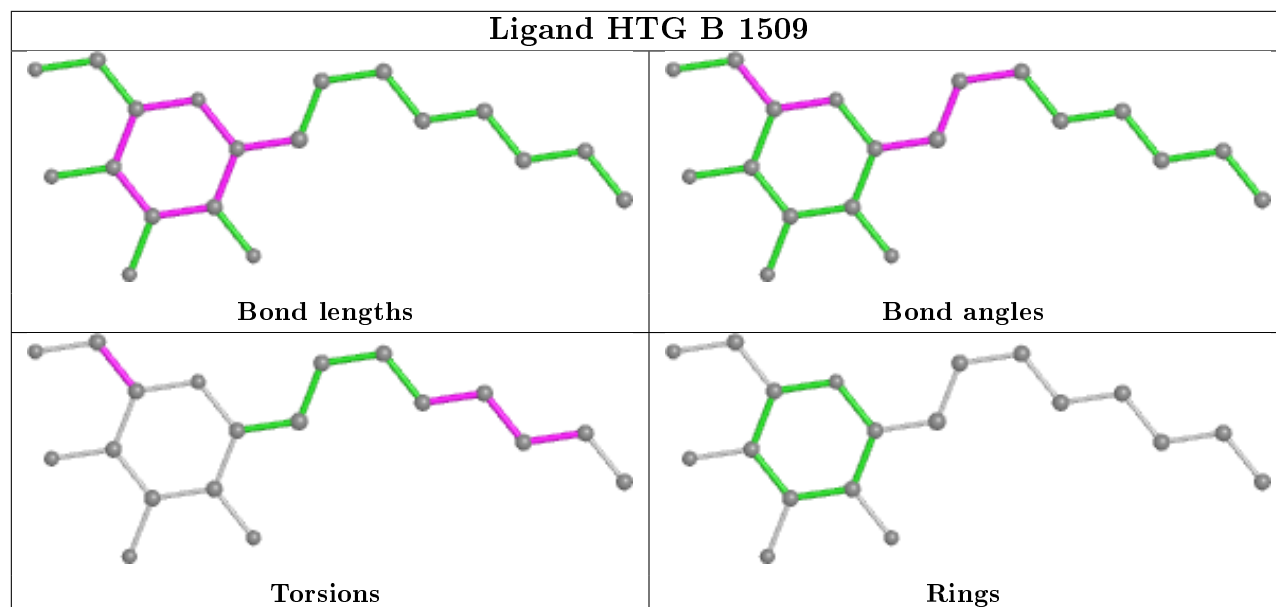
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	348/349 (99%)	0.27	35 (10%) 7 4	42, 56, 138, 155	0
1	B	348/349 (99%)	0.64	49 (14%) 2 1	41, 62, 156, 161	0
All	All	696/698 (99%)	0.45	84 (12%) 4 2	41, 58, 151, 161	0

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	GLN	14.4
1	B	348	ALA	12.4
1	A	237	GLN	11.2
1	A	235	ALA	11.1
1	B	343	SER	10.8

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](#)

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.

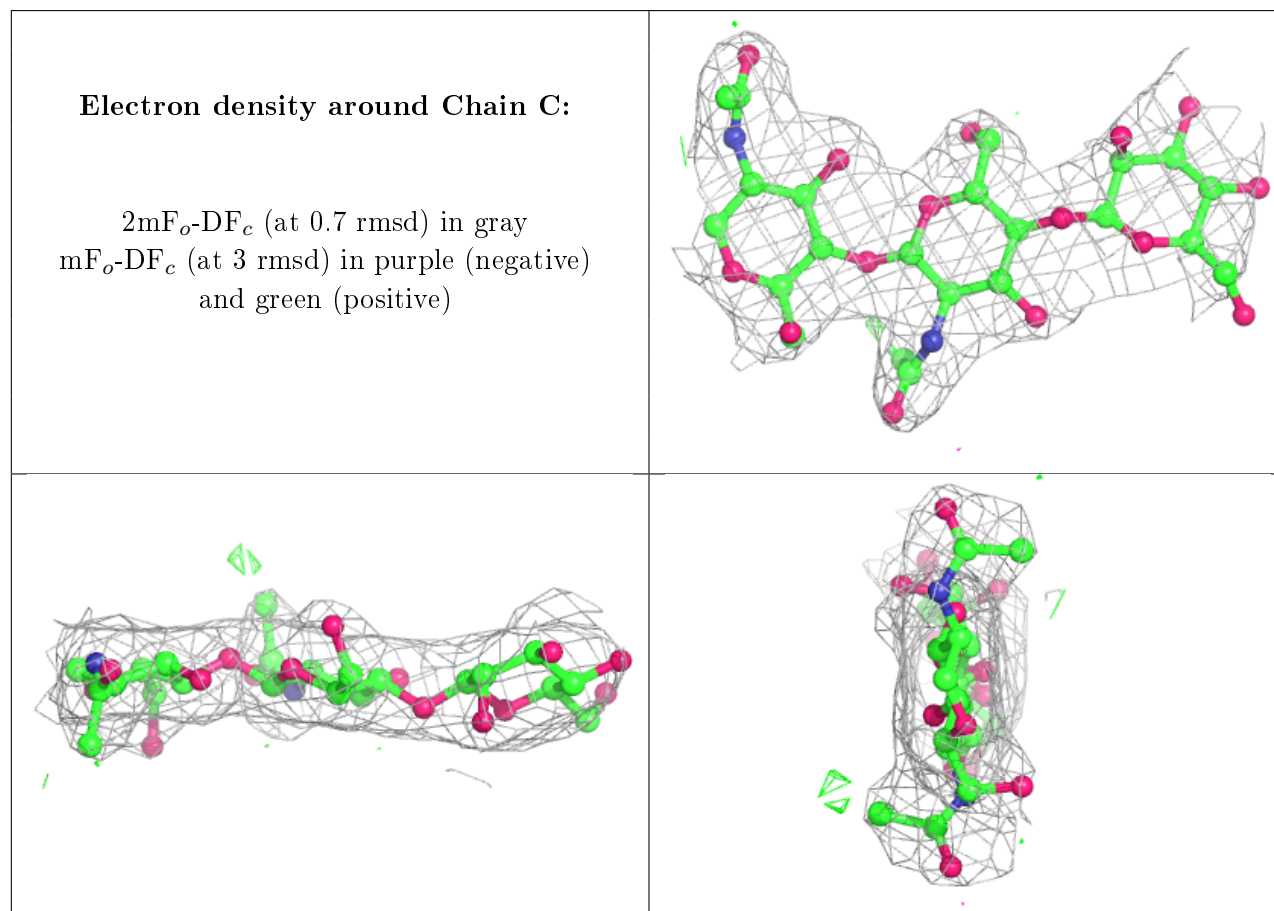
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	E	3	11/12	0.81	0.19	99,105,106,109	0
4	MAN	E	4	11/12	0.83	0.18	111,113,113,114	0
2	BMA	C	3	11/12	0.85	0.19	99,103,106,106	0
3	NAG	D	2	14/15	0.85	0.34	85,91,95,96	0
3	NAG	F	2	14/15	0.90	0.23	81,86,87,88	0

Continued on next page...

Continued from previous page...

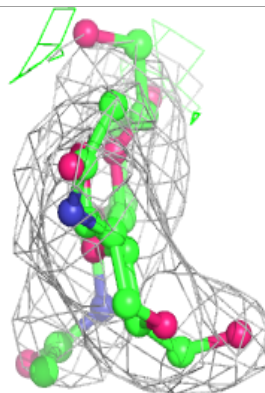
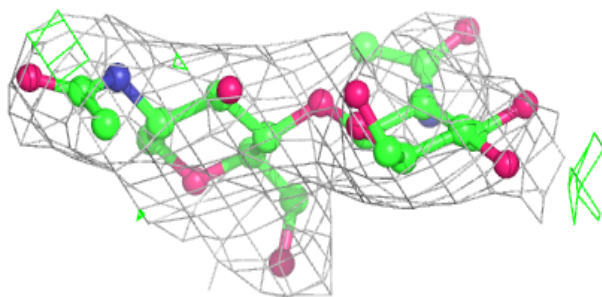
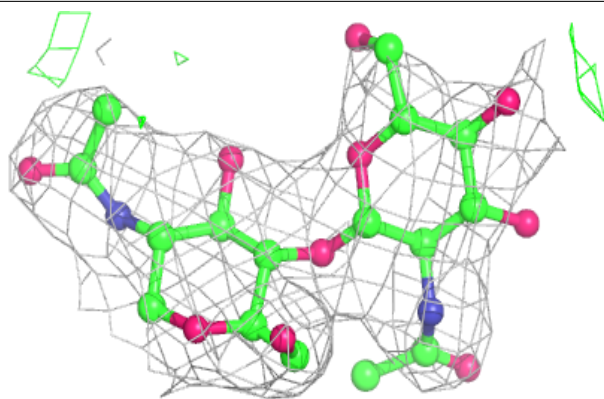
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	C	2	14/15	0.94	0.13	76,80,86,92	0
4	NAG	E	2	14/15	0.94	0.12	72,78,84,92	0
3	NAG	F	1	14/15	0.94	0.15	63,66,69,75	0
3	NAG	D	1	14/15	0.95	0.14	63,68,72,78	0
2	NAG	C	1	14/15	0.96	0.15	59,62,67,70	0
4	NAG	E	1	14/15	0.96	0.12	59,63,65,68	0

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.

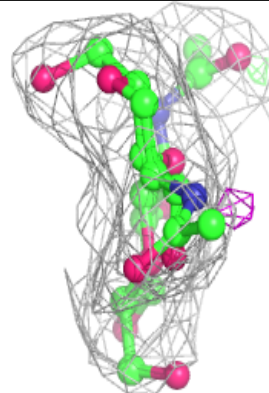
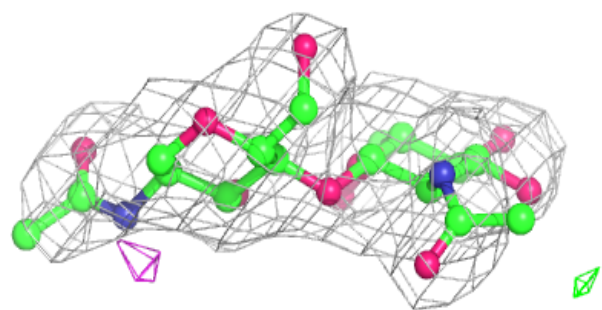
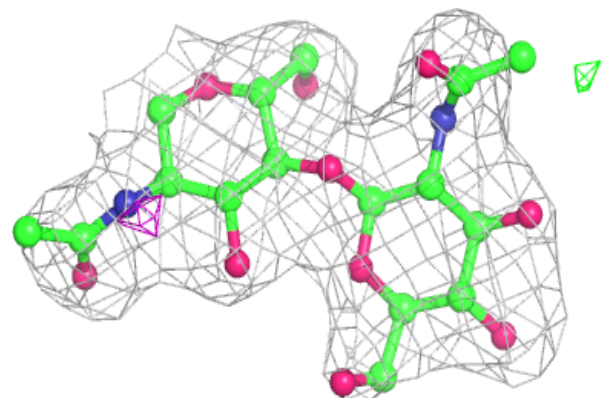


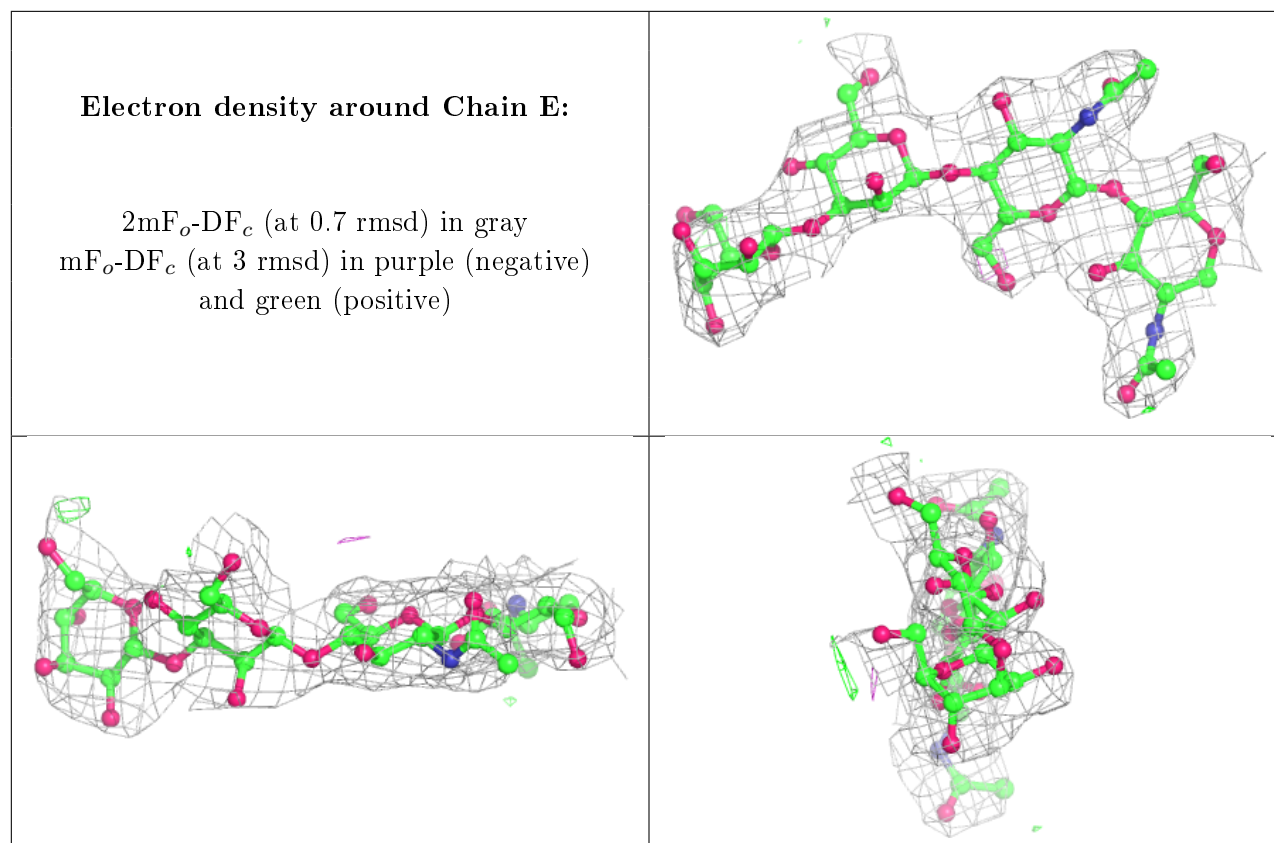
Electron density around Chain D:

$2mF_o-DF_c$ (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)





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.

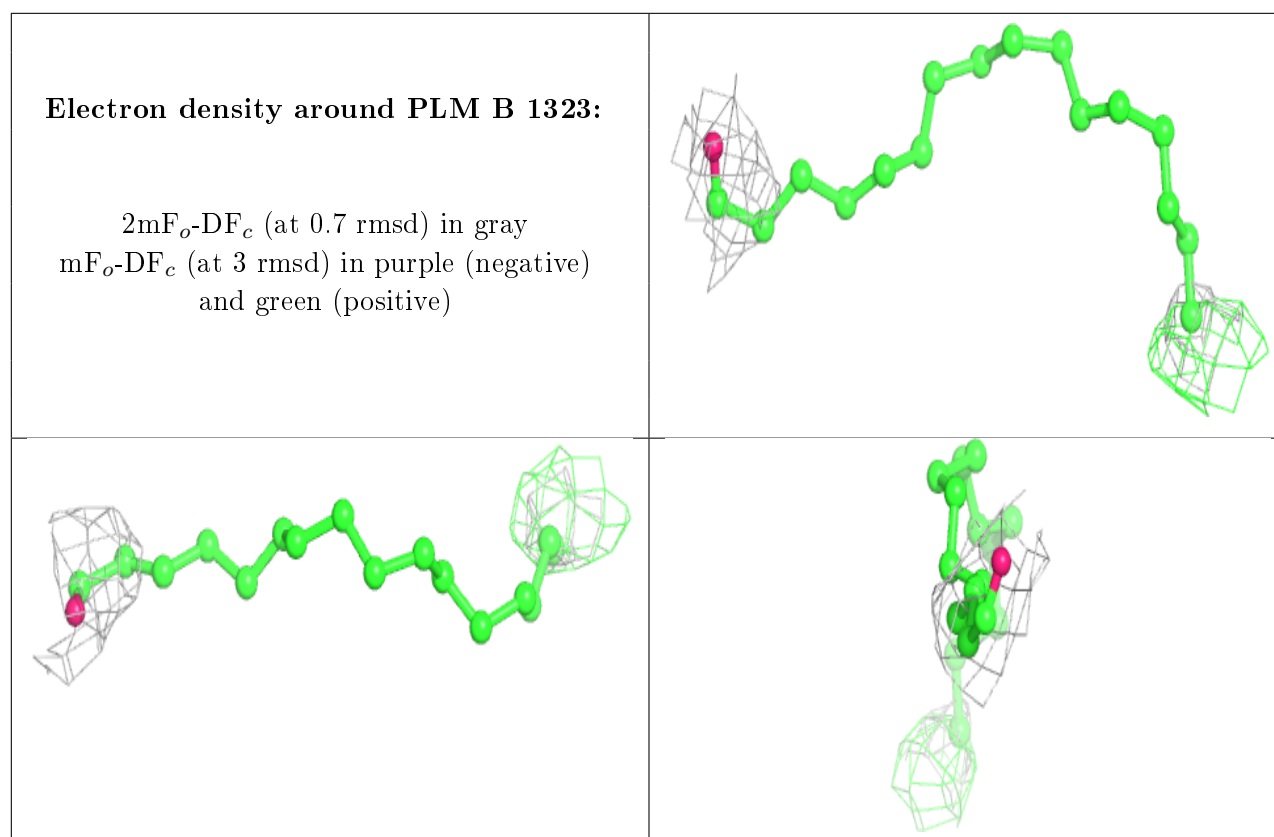
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PLM	B	1323	17/18	0.52	0.76	115,121,122,122	0
11	ID3	B	6026	14/14	0.62	0.42	69,75,76,78	0
9	4E6	A	1410	16/16	0.69	0.40	81,83,85,85	0
9	4E6	B	1407	16/16	0.69	0.43	83,91,97,97	0
11	ID3	A	6025	14/14	0.71	0.26	64,70,72,72	0
6	PLM	A	1323	17/18	0.75	0.38	100,108,113,113	0
10	HTG	B	1506	19/19	0.76	0.42	97,104,107,107	0
6	PLM	B	1322	17/18	0.79	0.41	102,104,106,106	0
6	PLM	A	1322	17/18	0.80	0.49	88,92,102,103	0
10	HTG	A	1507	19/19	0.82	0.35	95,102,105,105	0
10	HTG	B	1509	19/19	0.82	0.28	101,102,105,105	0
12	HTO	B	1401	10/10	0.86	0.36	63,67,68,72	0
10	HTG	A	1508	19/19	0.89	0.24	61,76,81,84	0
8	ZN	B	963	1/1	0.90	0.16	136,136,136,136	1

Continued on next page...

Continued from previous page...

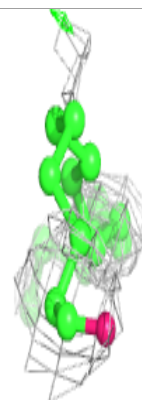
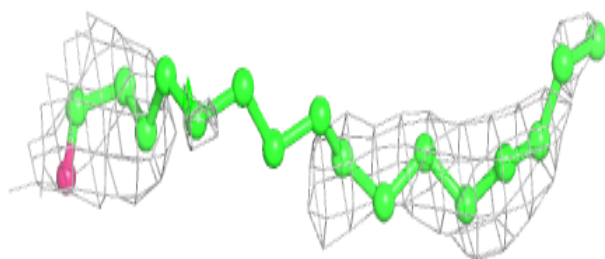
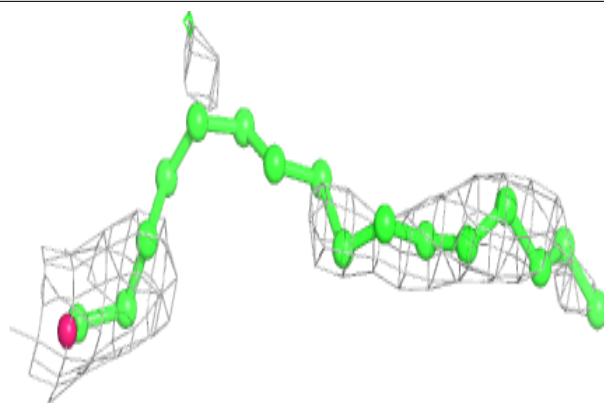
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	ZN	A	2011	1/1	0.90	0.20	59,59,59,59	1
7	HG	B	906	1/1	0.94	0.10	121,121,121,121	1
8	ZN	B	958	1/1	0.94	0.16	41,41,41,41	1
8	ZN	A	959	1/1	0.95	0.25	96,96,96,96	1
5	RET	B	1296	20/21	0.95	0.22	43,49,51,51	0
8	ZN	A	957	1/1	0.96	0.18	53,53,53,53	1
5	RET	A	1296	20/21	0.96	0.19	43,45,48,49	0
8	ZN	B	956	1/1	0.97	0.29	70,70,70,70	1
7	HG	B	904	1/1	0.97	0.12	98,98,98,98	1
8	ZN	A	962	1/1	0.97	0.22	120,120,120,120	1
7	HG	A	905	1/1	0.98	0.14	81,81,81,81	1
7	HG	A	903	1/1	0.99	0.12	82,82,82,82	1
7	HG	B	902	1/1	0.99	0.15	79,79,79,79	1
7	HG	A	901	1/1	0.99	0.17	73,73,73,73	1

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.

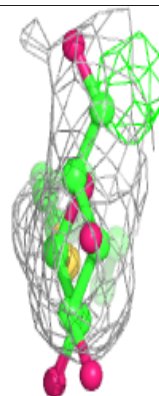
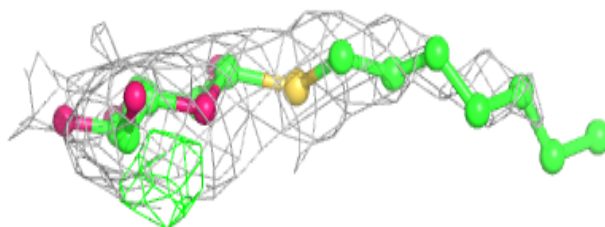
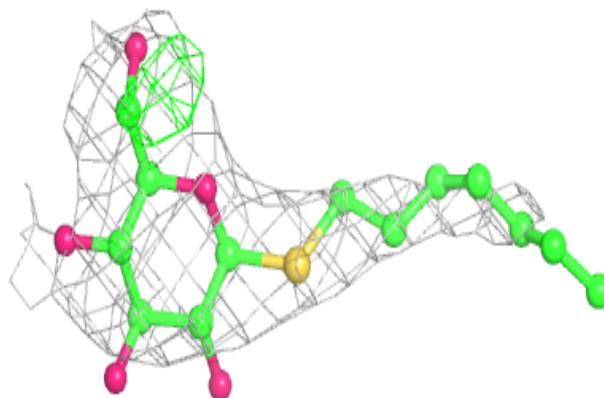


Electron density around PLM A 1323:

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

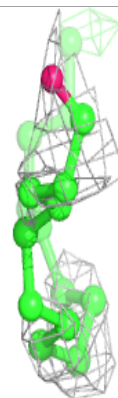
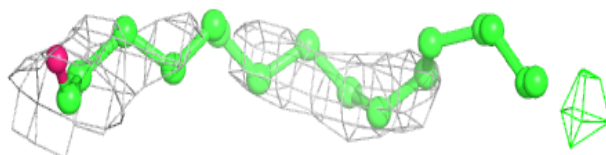
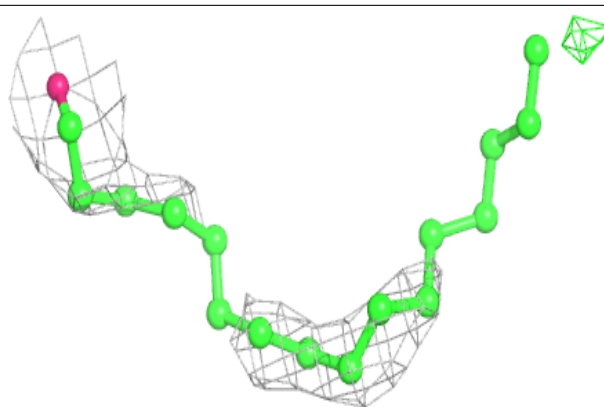
**Electron density around HTG B 1506:**

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

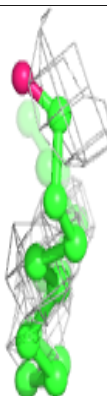
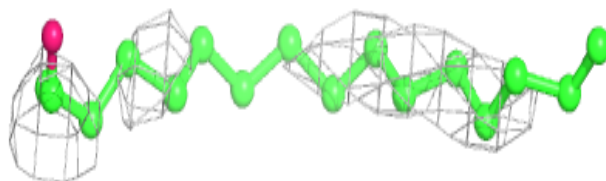
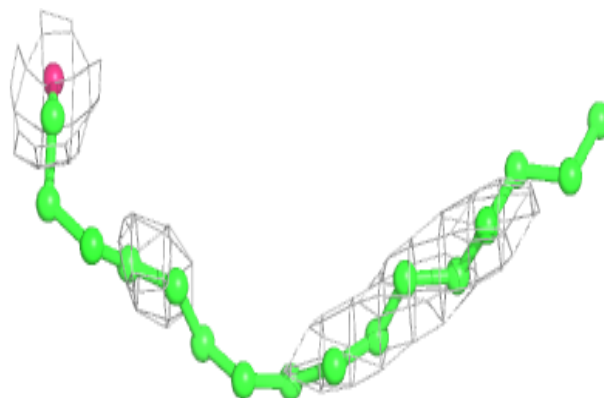


Electron density around PLM B 1322:

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

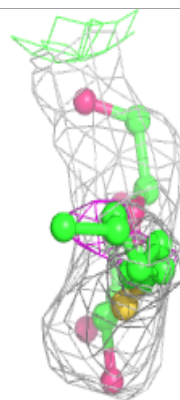
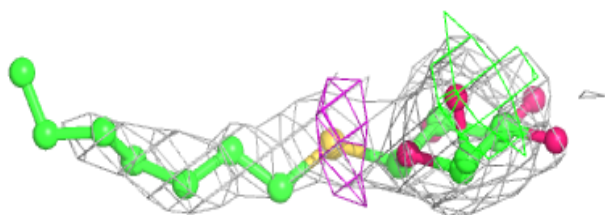
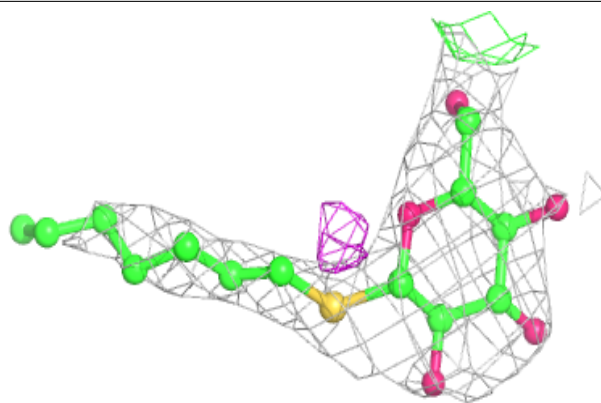
**Electron density around PLM A 1322:**

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

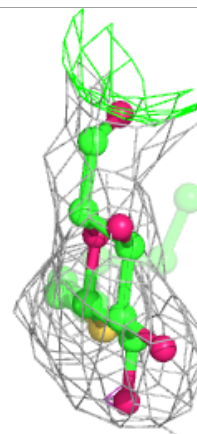
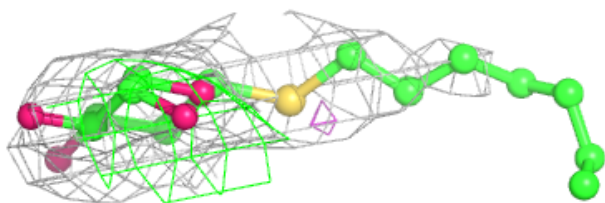
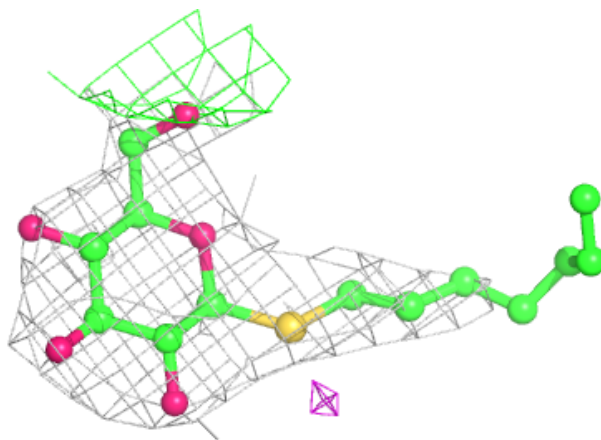


Electron density around HTG A 1507:

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

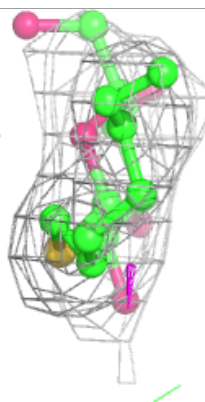
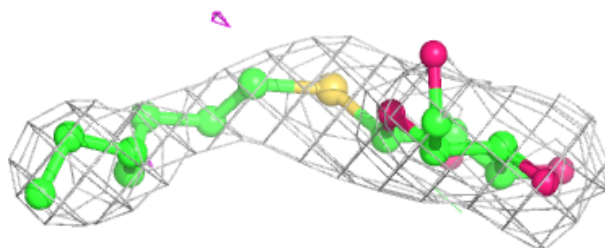
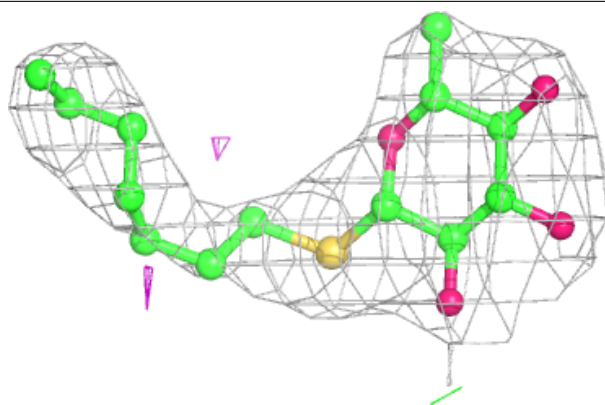
**Electron density around HTG B 1509:**

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

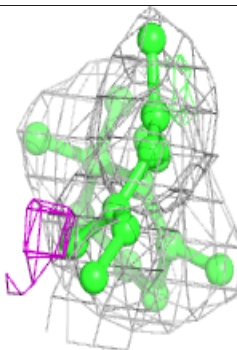
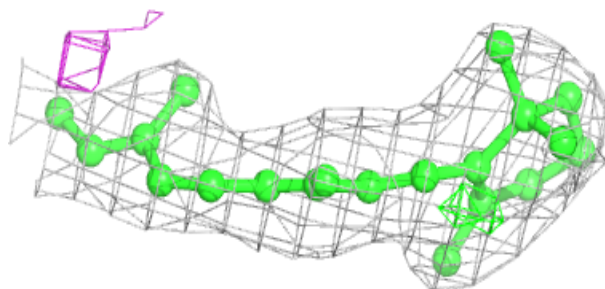
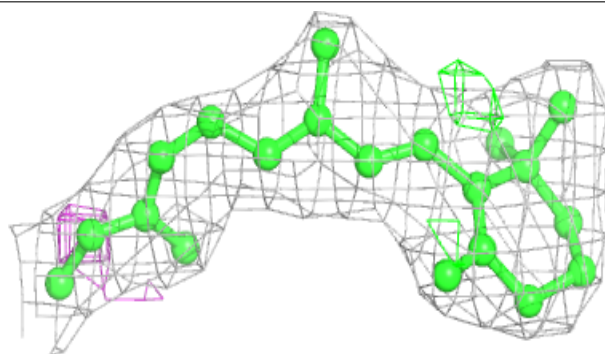


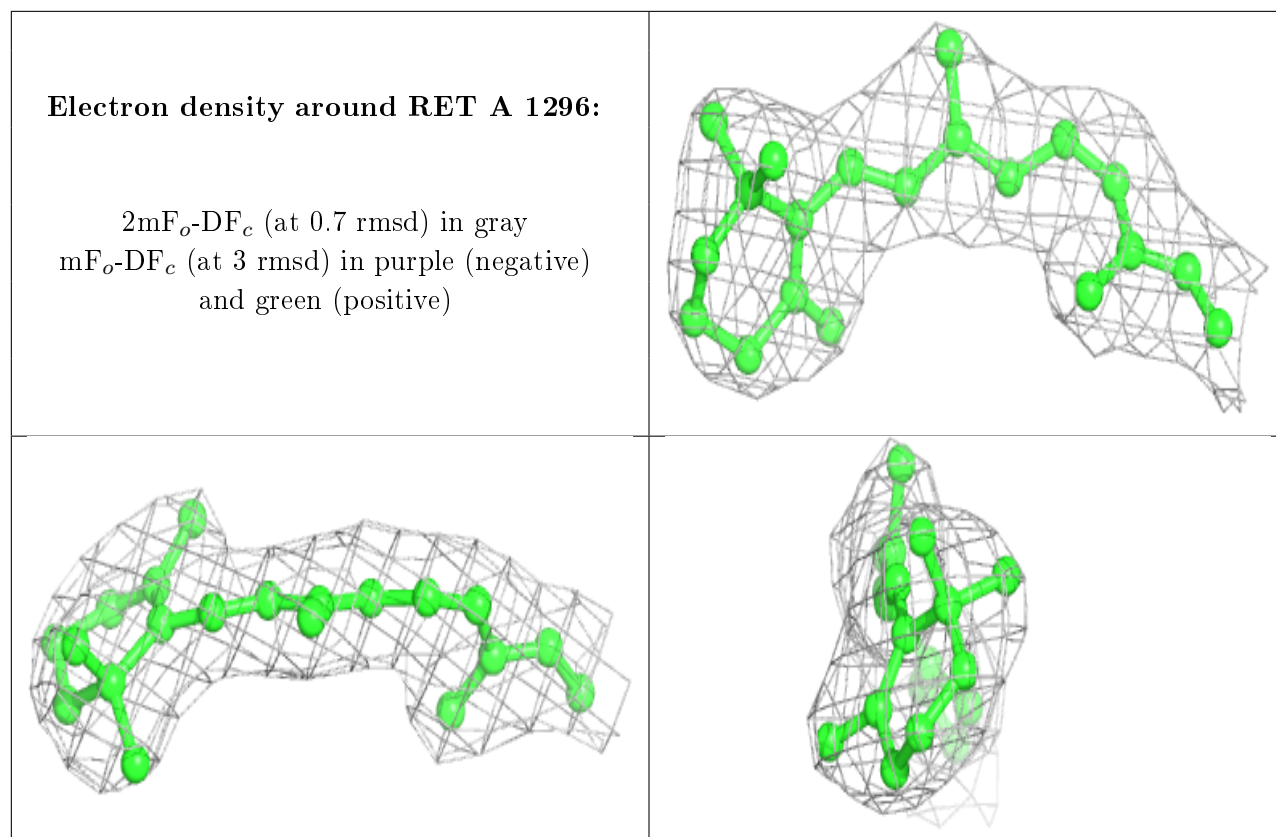
Electron density around HTG A 1508:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.