



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 12:28 AM BST

PDB ID : 6CI0  
Title : Catalytic core subunits (I and II) of cytochrome C oxidase from Rhodobacter sphaeroides with E101A (II) mutation  
Authors : Liu, J.; Hiser, C.; Ferguson-Miller, S.  
Deposited on : 2018-02-23  
Resolution : 2.40 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 : 2.13.1  
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

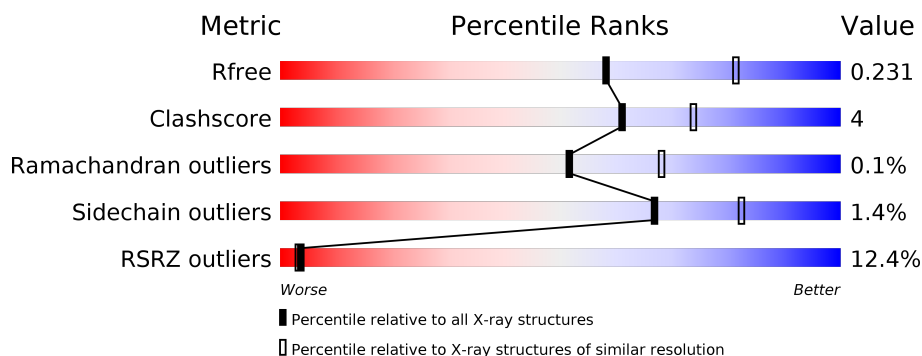
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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.



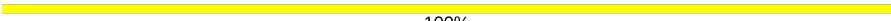
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	535	<div> <div>8%</div> <div>92%</div> <div>8%</div> </div>
1	C	535	<div> <div>24%</div> <div>85%</div> <div>13%</div> <div>••</div> </div>
2	B	257	<div> <div>3%</div> <div>91%</div> <div>7%</div> <div>•</div> </div>
2	D	257	<div> <div>8%</div> <div>95%</div> <div>5%</div> </div>
3	E	2	<div> <div>100%</div> </div>
3	F	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	2	 100%

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
5	TRD	A	607	-	-	-	X
5	TRD	B	302	-	-	-	X
5	TRD	C	601	-	-	-	X
9	HEA	A	617	X	-	-	-
9	HEA	A	618	X	-	-	-
9	HEA	C	605	X	-	-	-
9	HEA	C	606	X	-	-	-

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 13231 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4160	2787	651	691	31			
1	C	531	Total	C	N	O	S	0	0	0
			4094	2742	641	681	30			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			2013	1314	331	362	6			
2	D	257	Total	C	N	O	S	0	0	0
			1995	1303	324	362	6			

There are 10 discrepancies between the modelled and reference sequences:

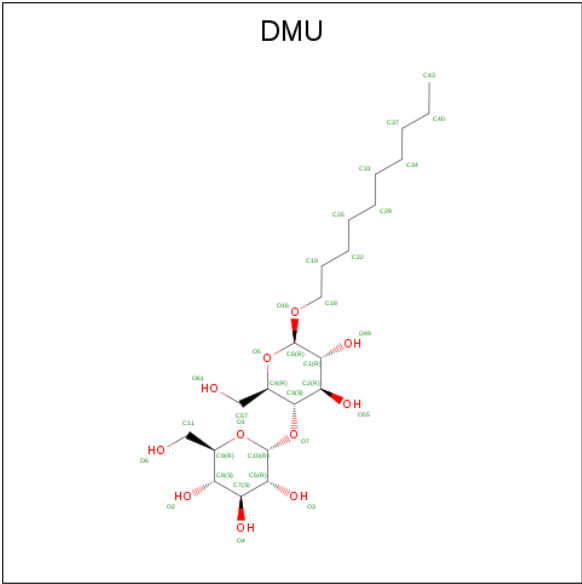
Chain	Residue	Modelled	Actual	Comment	Reference
B	101	ALA	GLU	engineered mutation	UNP Q03736
B	282	HIS	-	expression tag	UNP Q03736
B	283	HIS	-	expression tag	UNP Q03736
B	284	HIS	-	expression tag	UNP Q03736
B	285	HIS	-	expression tag	UNP Q03736
D	101	ALA	GLU	engineered mutation	UNP Q03736
D	282	HIS	-	expression tag	UNP Q03736
D	283	HIS	-	expression tag	UNP Q03736
D	284	HIS	-	expression tag	UNP Q03736
D	285	HIS	-	expression tag	UNP Q03736

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



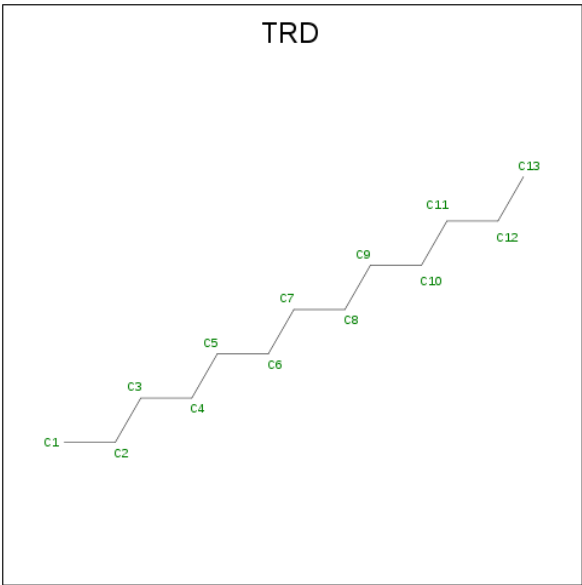
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	E	2	Total	C	O	0	0	0
			23	12	11			
3	F	2	Total	C	O	0	0	0
			23	12	11			
3	G	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			33	22	11		
4	A	1	Total	C	O	0	0
			33	22	11		
4	A	1	Total	C	O	0	0
			33	22	11		
4	A	1	Total	C	O	0	0
			33	22	11		
4	A	1	Total	C	O	0	0
			33	22	11		
4	D	1	Total	C	O	0	0
			30	19	11		

- Molecule 5 is TRIDECANE (three-letter code: TRD) (formula: C<sub>13</sub>H<sub>28</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 13 13	0	0
5	A	1	Total C 13 13	0	0
5	A	1	Total C 13 13	0	0
5	A	1	Total C 13 13	0	0
5	A	1	Total C 7 7	0	0
5	A	1	Total C 13 13	0	0
5	A	1	Total C 13 13	0	0
5	A	1	Total C 13 13	0	0
5	B	1	Total C 13 13	0	0
5	B	1	Total C 13 13	0	0
5	B	1	Total C 13 13	0	0
5	C	1	Total C 13 13	0	0
5	D	1	Total C 13 13	0	0
5	D	1	Total C 9 9	0	0

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Cu	0	0
			2	2		
6	A	1	Total	Cu	0	0
			1	1		
6	D	2	Total	Cu	0	0
			2	2		
6	C	1	Total	Cu	0	0
			1	1		

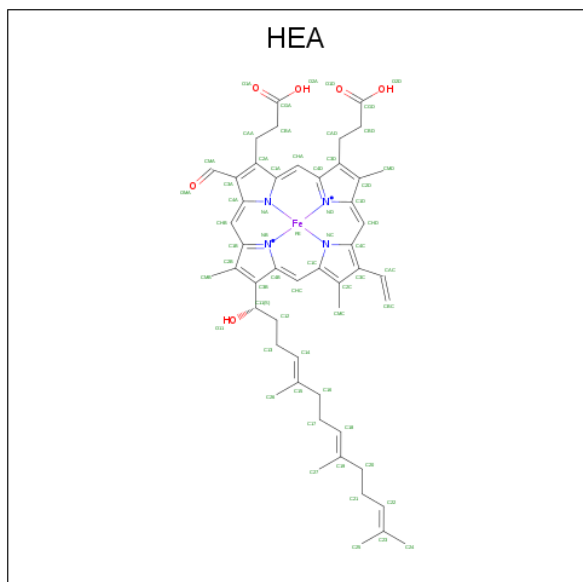
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		
8	C	1	Total	Ca	0	0
			1	1		

- Molecule 9 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).

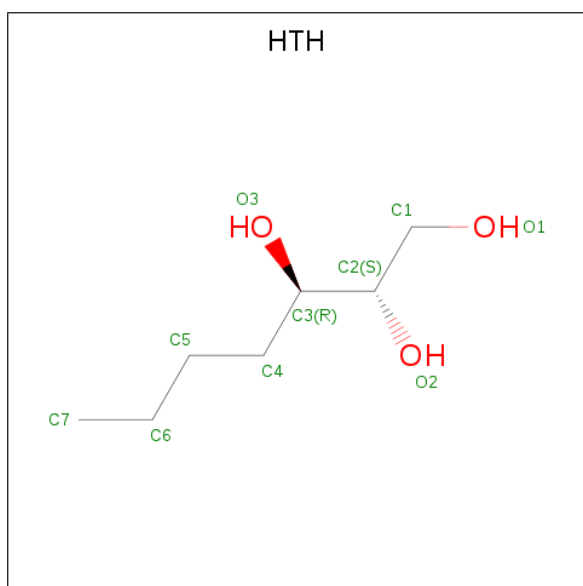


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	
9	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	
9	C	1	Total	C	Fe	N	O	
			60	49	1	4	6	
9	C	1	Total	C	Fe	N	O	
			60	49	1	4	6	

- Molecule 10 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Cd	0	0
			1	1		
10	D	1	Total	Cd	0	0
			1	1		

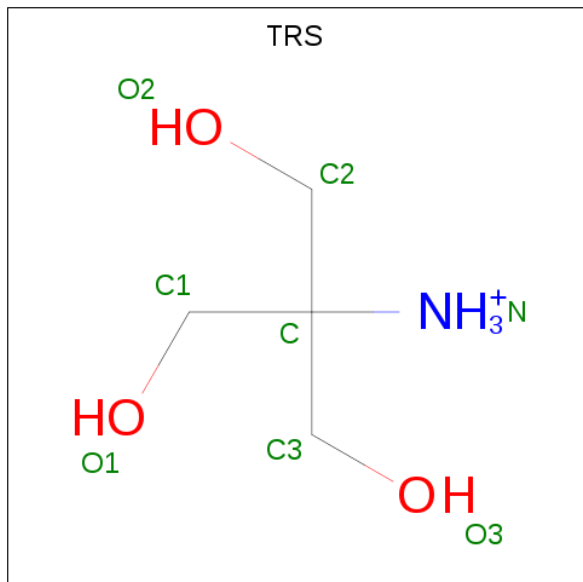
- Molecule 11 is (2S,3R)-heptane-1,2,3-triol (three-letter code: HTH) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).



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



- Molecule 12 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 13 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total	K	0	0
			1	1		

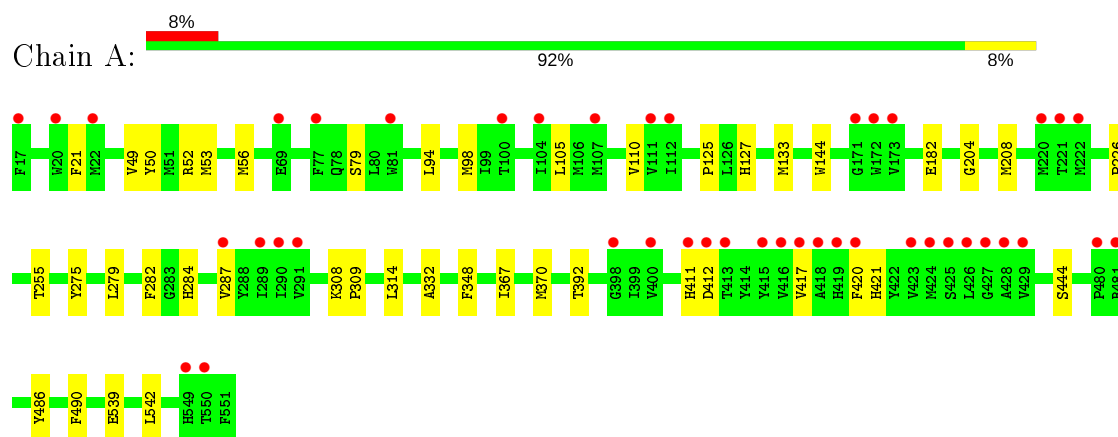
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	94	Total	O	0	0
			94	94		
14	B	69	Total	O	0	0
			69	69		
14	C	37	Total	O	0	0
			37	37		
14	D	42	Total	O	0	0
			42	42		

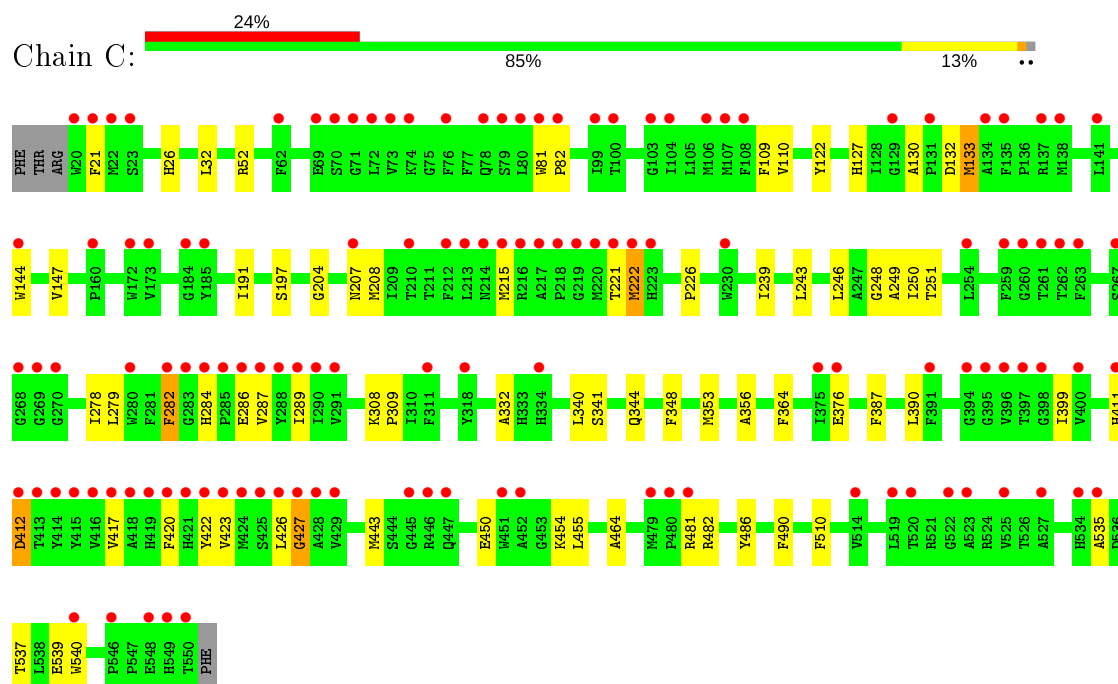
### 3 Residue-property plots [i](#)

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

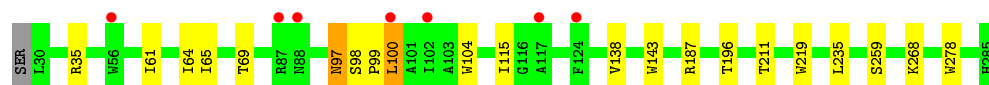
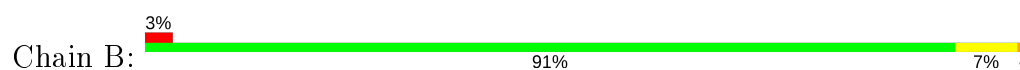
#### • Molecule 1: Cytochrome c oxidase subunit 1



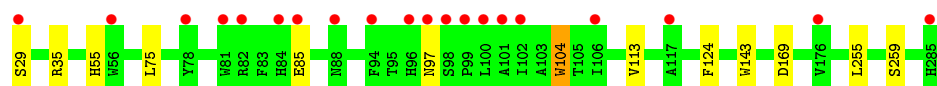
#### • Molecule 1: Cytochrome c oxidase subunit 1



#### • Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.92Å 130.97Å 177.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.09 – 2.40 43.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.09-2.40) 90.9 (43.80-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.89 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.199 , 0.234 0.199 , 0.231	Depositor DCC
$R_{free}$ test set	3901 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.6	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 67.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13231	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, GLC, TRD, CD, HEA, TRS, HTH, CA, CU, DMU

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	0.33	0/4312	0.44	0/5892
1	C	0.30	0/4244	0.44	0/5804
2	B	0.29	0/2074	0.46	0/2839
2	D	0.27	0/2056	0.45	0/2820
All	All	0.31	0/12686	0.45	0/17355

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4160	0	4054	30	0
1	C	4094	0	3968	58	0
2	B	2013	0	1972	13	0
2	D	1995	0	1929	9	0
3	E	23	0	21	0	0
3	F	23	0	21	1	0
3	G	23	0	21	1	0
4	A	165	0	210	4	0
4	D	30	0	33	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	98	0	209	4	0
5	B	39	0	84	3	0
5	C	13	0	28	0	0
5	D	22	0	45	2	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	A	120	0	108	9	0
9	C	120	0	108	7	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
11	B	30	0	48	1	0
12	B	8	0	11	0	0
13	B	1	0	0	0	0
14	A	94	0	0	0	0
14	B	69	0	0	0	0
14	C	37	0	0	1	0
14	D	42	0	0	0	0
All	All	13231	0	12870	115	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 4.

All (115) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:VAL:HG22	9:C:606:HEA:HAC	1.51	0.93
1:A:125:PRO:HG3	1:A:133:MET:HE2	1.51	0.91
1:A:287:VAL:HG13	9:A:618:HEA:C3C	2.01	0.90
9:C:605:HEA:HMC1	9:C:605:HEA:HBC1	1.56	0.86
9:A:617:HEA:HMC1	9:A:617:HEA:HBC1	1.58	0.86
1:C:133:MET:HB3	1:C:207:ASN:HD21	1.41	0.85
1:A:125:PRO:HG3	1:A:133:MET:CE	2.10	0.81
1:C:133:MET:HG2	1:C:207:ASN:ND2	1.95	0.81
1:C:287:VAL:HG22	9:C:606:HEA:CAC	2.13	0.78
2:B:64:ILE:HD11	2:B:115:ILE:HD11	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:HIS:O	1:C:287:VAL:HG12	1.89	0.73
1:C:287:VAL:HG21	9:C:606:HEA:CHD	2.19	0.73
4:A:604:DMU:H2	5:A:607:TRD:H121	1.75	0.69
1:C:133:MET:CB	1:C:207:ASN:HD21	2.08	0.66
1:C:81:TRP:CD2	1:C:82:PRO:HD2	2.32	0.65
2:B:278:TRP:HE1	5:B:302:TRD:H42	1.62	0.64
1:C:133:MET:CG	1:C:207:ASN:ND2	2.61	0.64
1:C:133:MET:HB3	1:C:207:ASN:ND2	2.13	0.63
1:A:255:THR:HG21	5:A:612:TRD:H22	1.80	0.63
2:B:196:THR:HB	5:B:302:TRD:H31	1.80	0.62
1:C:127:HIS:NE2	1:C:539:GLU:OE2	2.32	0.62
1:A:287:VAL:HG13	9:A:618:HEA:CAC	2.29	0.62
1:C:426:LEU:HD21	1:C:464:ALA:HB1	1.82	0.62
1:C:21:PHE:HA	1:C:32:LEU:HD11	1.82	0.60
1:A:314:LEU:HB2	11:B:310:HTH:H7A	1.83	0.60
1:C:287:VAL:CG2	9:C:606:HEA:HAC	2.29	0.59
1:A:287:VAL:CG1	9:A:618:HEA:C3C	2.78	0.59
1:C:411:HIS:NE2	1:C:412:ASP:OD1	2.36	0.58
1:C:387:PHE:HD2	1:C:427:GLY:O	1.86	0.57
9:A:618:HEA:HBC1	9:A:618:HEA:HMC1	1.86	0.56
1:C:450:GLU:OE1	1:C:454:LYS:NZ	2.37	0.56
2:B:268:LYS:HD2	5:B:302:TRD:H71	1.88	0.56
1:C:411:HIS:NE2	14:C:701:HOH:O	2.33	0.55
1:C:133:MET:CB	1:C:207:ASN:ND2	2.70	0.54
1:C:364:PHE:HB3	2:D:104:TRP:CE3	2.42	0.54
1:A:444:SER:HB3	4:A:601:DMU:H8	1.89	0.54
1:A:204:GLY:O	1:A:208:MET:HG2	2.09	0.53
2:B:211:THR:HB	2:B:235:LEU:HD12	1.91	0.53
1:C:133:MET:HG2	1:C:207:ASN:CG	2.28	0.53
1:A:275:TYR:OH	1:A:279:LEU:HD13	2.09	0.52
1:C:26:HIS:HD2	1:C:132:ASP:HA	1.74	0.52
1:C:282:PHE:CE1	1:C:286:GLU:HB2	2.44	0.52
1:C:422:TYR:HA	1:C:426:LEU:HB2	1.92	0.52
1:A:411:HIS:NE2	1:A:412:ASP:OD2	2.44	0.51
1:C:387:PHE:CD2	1:C:427:GLY:O	2.63	0.51
1:C:127:HIS:HB3	1:C:226:PRO:HG2	1.94	0.50
1:C:239:ILE:HA	1:C:243:LEU:HD13	1.94	0.50
1:A:539:GLU:HA	1:A:542:LEU:HD12	1.94	0.49
1:C:356:ALA:HB2	1:C:399:ILE:HD11	1.95	0.49
1:A:367:ILE:HA	1:A:370:MET:HE2	1.95	0.48
1:C:537:THR:OG1	1:C:539:GLU:OE1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:HIS:HB3	1:A:226:PRO:HG2	1.97	0.47
1:A:332:ALA:HB3	1:A:348:PHE:CG	2.49	0.47
1:A:392:THR:HG22	2:B:69:THR:HG22	1.96	0.47
1:C:332:ALA:HB3	1:C:348:PHE:CG	2.49	0.47
1:A:56:MET:HE1	4:A:604:DMU:H7	1.96	0.47
1:C:81:TRP:CE3	1:C:82:PRO:HD2	2.50	0.47
1:C:353:MET:HE3	5:D:303:TRD:H42	1.96	0.47
1:C:286:GLU:HA	1:C:289:ILE:HD12	1.97	0.47
1:A:308:LYS:HG3	1:A:309:PRO:HD2	1.96	0.46
2:B:100:LEU:HD12	2:B:100:LEU:O	2.14	0.46
1:C:204:GLY:O	1:C:208:MET:HG2	2.15	0.46
1:C:191:ILE:HG23	1:C:250:ILE:HB	1.96	0.46
1:A:21:PHE:HB3	1:A:144:TRP:HZ2	1.80	0.46
5:A:612:TRD:H42	5:A:612:TRD:H71	1.68	0.46
1:A:50:TYR:OH	1:A:79:SER:HB3	2.15	0.46
2:D:124:PHE:HB3	3:F:2:GLC:H3	1.98	0.46
2:B:138:VAL:HG11	2:B:219:TRP:CD1	2.51	0.46
1:C:221:THR:OG1	1:C:222:MET:N	2.50	0.45
1:C:486:TYR:CD1	1:C:490:PHE:HB2	2.52	0.44
9:C:605:HEA:CMC	9:C:605:HEA:HBC1	2.35	0.44
1:C:110:VAL:HG11	9:C:605:HEA:H271	1.99	0.44
1:C:248:GLY:O	1:C:251:THR:HG22	2.17	0.44
1:A:417:VAL:HG13	1:A:421:HIS:CE1	2.52	0.44
1:C:144:TRP:HA	1:C:147:VAL:HG12	2.00	0.44
1:C:390:LEU:HD13	1:C:426:LEU:HB3	2.00	0.44
2:D:113:VAL:HA	5:D:303:TRD:H52	2.00	0.44
1:C:390:LEU:HD13	1:C:426:LEU:HD13	2.00	0.44
1:A:486:TYR:CD1	1:A:490:PHE:HB2	2.53	0.43
1:C:249:ALA:HB2	1:C:278:ILE:HG22	2.00	0.43
1:C:109:PHE:CE1	1:C:197:SER:HB2	2.53	0.43
1:C:122:TYR:CZ	1:C:443:MET:HG2	2.54	0.43
1:C:246:LEU:HD22	1:C:282:PHE:CZ	2.53	0.43
1:C:417:VAL:HA	1:C:420:PHE:CE2	2.54	0.43
4:A:604:DMU:H10	5:A:606:TRD:H52	2.00	0.43
1:C:341:SER:OG	1:C:344:GLN:HG3	2.18	0.43
9:A:618:HEA:CBC	9:A:618:HEA:HMC1	2.47	0.43
1:A:105:LEU:O	1:A:110:VAL:HG23	2.19	0.43
1:A:284:HIS:O	1:A:287:VAL:HB	2.19	0.43
2:D:75:LEU:HA	2:D:75:LEU:HD12	1.89	0.43
1:C:482:ARG:HD3	2:D:255:LEU:HB2	2.02	0.42
1:A:49:VAL:HG12	1:A:53:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:ALA:HB1	1:C:540:TRP:CD1	2.55	0.42
2:D:143:TRP:CG	2:D:259:SER:HB2	2.55	0.42
1:A:94:LEU:O	1:A:98:MET:HG2	2.19	0.42
2:B:97:ASN:ND2	4:D:301:DMU:H29	2.34	0.42
1:C:332:ALA:HB1	1:C:340:LEU:HD11	2.00	0.42
1:C:130:ALA:HB2	1:C:215:MET:O	2.20	0.42
2:B:98:SER:N	2:B:99:PRO:HD2	2.35	0.41
9:A:618:HEA:CMC	9:A:618:HEA:HBC1	2.50	0.41
1:A:420:PHE:CD2	9:A:618:HEA:HAD1	2.55	0.41
2:B:98:SER:OG	2:B:99:PRO:HD3	2.20	0.41
1:C:376:GLU:HG2	2:D:85:GLU:OE1	2.20	0.41
2:B:143:TRP:CG	2:B:259:SER:HB2	2.55	0.41
1:C:539:GLU:OE1	1:C:539:GLU:N	2.49	0.41
2:D:169:ASP:N	2:D:169:ASP:OD1	2.54	0.41
2:B:61:ILE:O	2:B:65:ILE:HG12	2.21	0.40
1:C:308:LYS:HG3	1:C:309:PRO:HD2	2.03	0.40
1:A:21:PHE:HB3	1:A:144:TRP:CZ2	2.55	0.40
1:C:455:LEU:HD23	1:C:510:PHE:CZ	2.56	0.40
1:A:417:VAL:HG13	1:A:421:HIS:HE1	1.87	0.40
1:A:287:VAL:CG1	9:A:618:HEA:C4C	2.99	0.40
1:C:420:PHE:HA	1:C:423:VAL:HG22	2.03	0.40
1:C:412:ASP:HA	1:C:481:ARG:HD3	2.04	0.40
2:D:97:ASN:ND2	3:G:1:GLC:H62	2.36	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	533/535 (100%)	518 (97%)	15 (3%)	0	100	100
1	C	529/535 (99%)	514 (97%)	14 (3%)	1 (0%)	47	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	254/257 (99%)	246 (97%)	7 (3%)	1 (0%)	34	48
2	D	255/257 (99%)	246 (96%)	9 (4%)	0	100	100
All	All	1571/1584 (99%)	1524 (97%)	45 (3%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	97	ASN
1	C	427	GLY

### 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	424/435 (98%)	421 (99%)	3 (1%)	84	92
1	C	414/435 (95%)	408 (99%)	6 (1%)	67	82
2	B	212/215 (99%)	208 (98%)	4 (2%)	57	75
2	D	208/215 (97%)	204 (98%)	4 (2%)	57	75
All	All	1258/1300 (97%)	1241 (99%)	17 (1%)	67	82

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	182	GLU
1	A	282	PHE
2	B	35	ARG
2	B	100	LEU
2	B	104	TRP
2	B	187	ARG
1	C	52	ARG
1	C	133	MET
1	C	222	MET

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Mol	Chain	Res	Type
1	C	279	LEU
1	C	282	PHE
1	C	412	ASP
2	D	29	SER
2	D	35	ARG
2	D	55	HIS
2	D	104	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	207	ASN
1	C	214	ASN

### 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 ⓘ

6 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	$\# Z  > 2$
3	GLC	E	1	3	12,12,12	0.51	0	17,17,17	0.45	0
3	GLC	E	2	3	11,11,12	0.60	0	15,15,17	0.63	0
3	GLC	F	1	3	12,12,12	0.51	0	17,17,17	0.47	0
3	GLC	F	2	3	11,11,12	0.57	0	15,15,17	0.84	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GLC	G	1	3	12,12,12	0.54	0	17,17,17	0.50	0
3	GLC	G	2	3	11,11,12	0.56	0	15,15,17	1.01	2 (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
3	GLC	E	1	3	-	1/2/22/22	0/1/1/1
3	GLC	E	2	3	-	1/2/19/22	0/1/1/1
3	GLC	F	1	3	-	0/2/22/22	0/1/1/1
3	GLC	F	2	3	-	1/2/19/22	0/1/1/1
3	GLC	G	1	3	-	1/2/22/22	0/1/1/1
3	GLC	G	2	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	GLC	C1-O5-C5	2.74	115.91	112.19
3	F	2	GLC	C1-O5-C5	2.54	115.63	112.19
3	G	2	GLC	O5-C5-C6	2.48	111.09	107.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

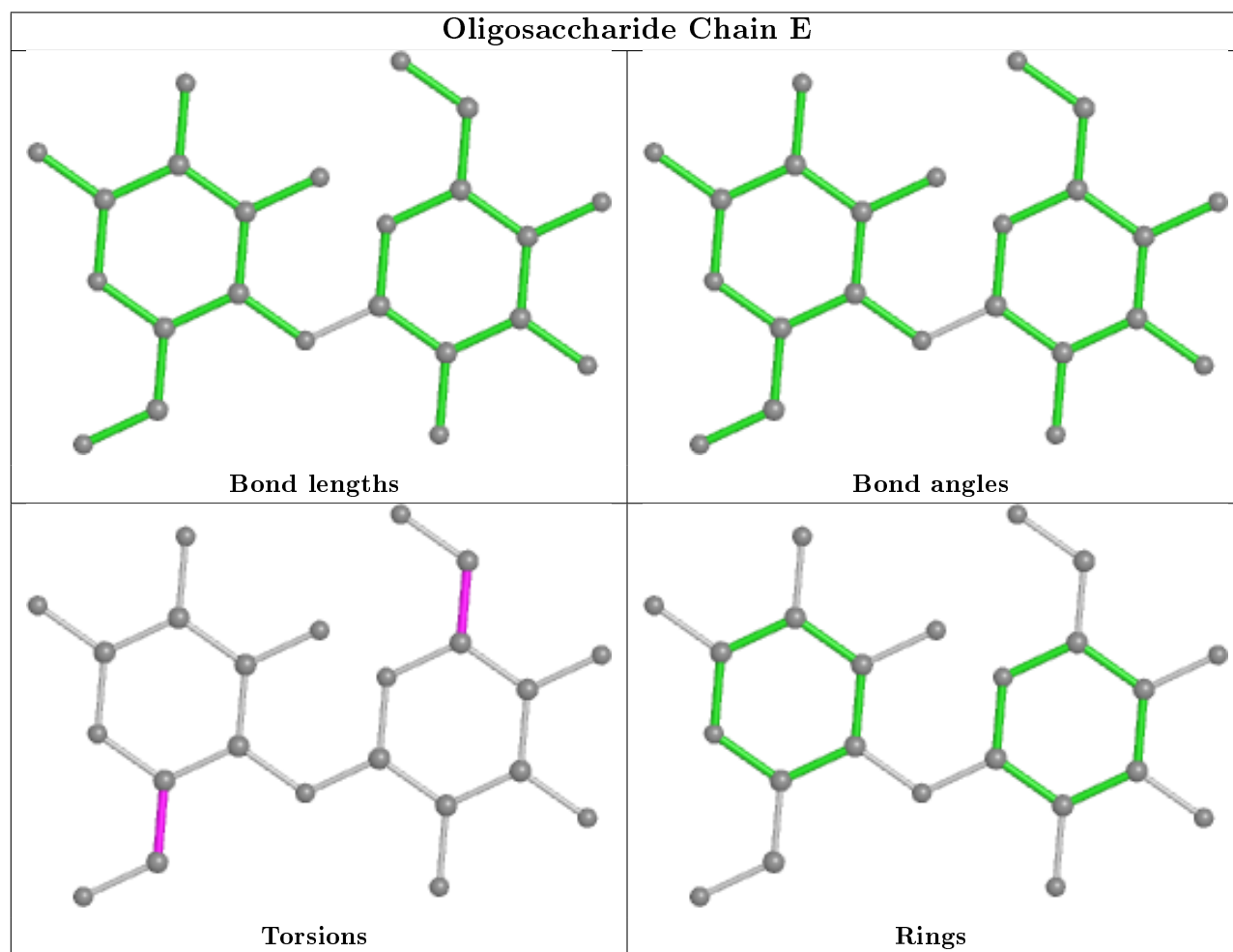
Mol	Chain	Res	Type	Atoms
3	F	2	GLC	O5-C5-C6-O6
3	E	2	GLC	O5-C5-C6-O6
3	E	1	GLC	O5-C5-C6-O6
3	G	2	GLC	O5-C5-C6-O6
3	G	1	GLC	O5-C5-C6-O6

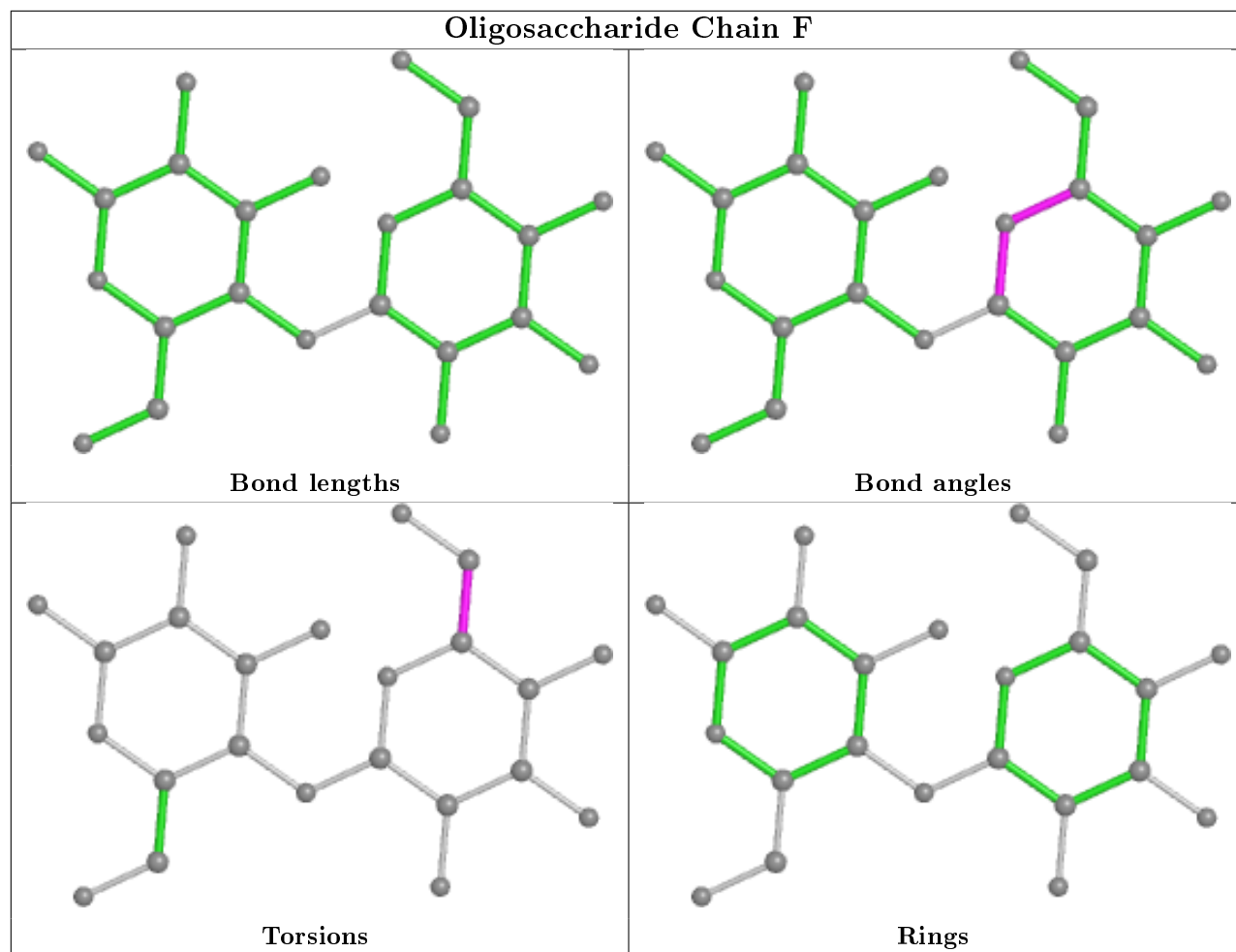
There are no ring outliers.

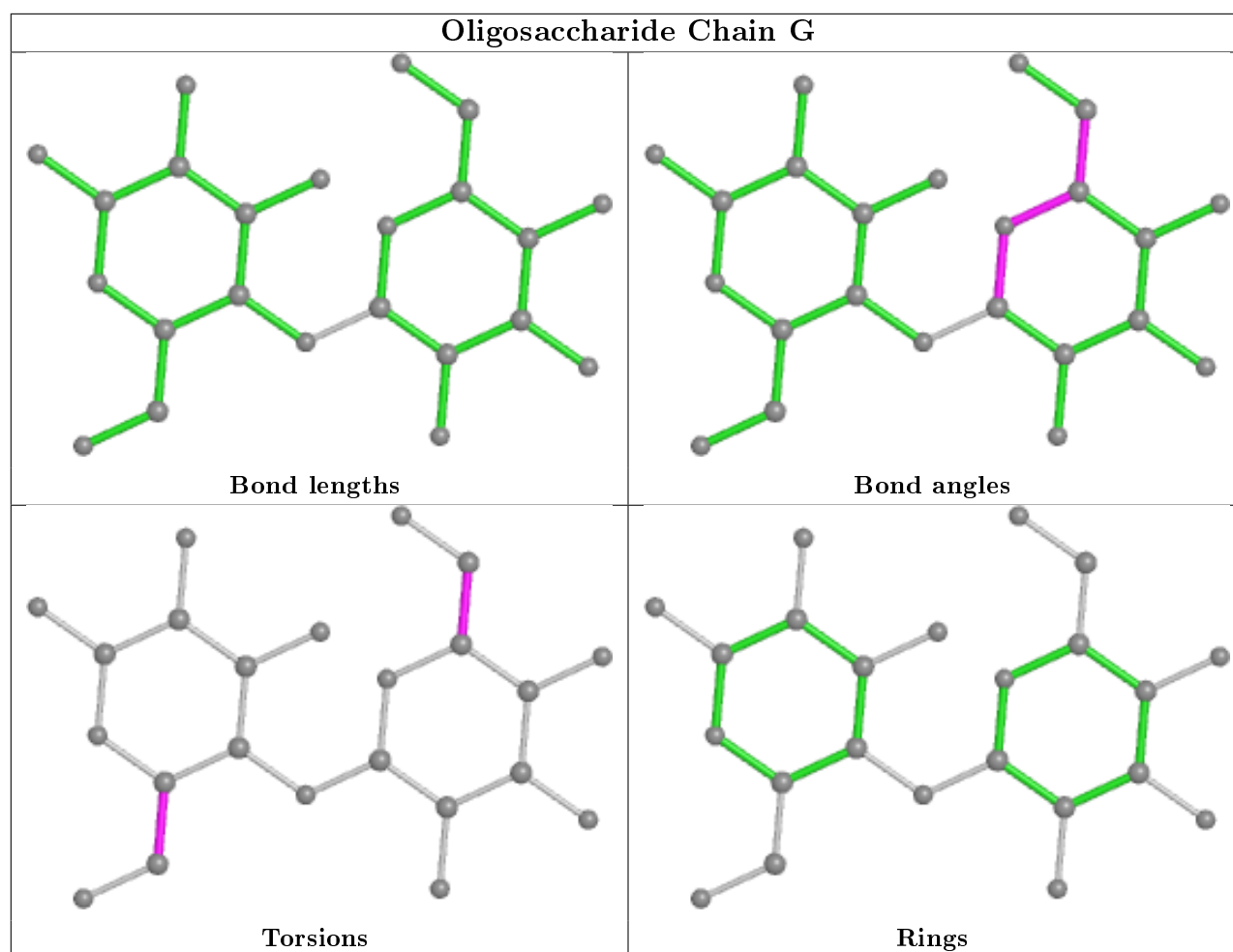
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	GLC	1	0
3	G	1	GLC	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 [i](#)

Of 41 ligands modelled in this entry, 13 are monoatomic - leaving 28 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	$\# Z  > 2$
5	TRD	D	302	-	12,12,12	0.11	0	11,11,11	0.81	0
5	TRD	B	302	-	12,12,12	0.16	0	11,11,11	0.56	0
5	TRD	A	610	-	6,6,12	0.16	0	5,5,11	0.53	0
5	TRD	B	303	-	12,12,12	0.12	0	11,11,11	0.81	0
11	HTH	B	308	-	9,9,9	0.44	0	10,10,10	1.28	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DMU	A	603	-	34,34,34	1.92	12 (35%)	45,45,45	1.21	5 (11%)
5	TRD	A	607	-	12,12,12	0.12	0	11,11,11	0.85	0
9	HEA	C	605	1	44,67,67	1.74	6 (13%)	37,103,103	2.53	15 (40%)
4	DMU	A	602	-	34,34,34	1.91	11 (32%)	45,45,45	1.03	3 (6%)
12	TRS	B	311	13	7,7,7	0.49	0	9,9,9	0.62	0
4	DMU	A	601	-	34,34,34	1.96	12 (35%)	45,45,45	1.06	1 (2%)
9	HEA	C	606	1,14	44,67,67	1.84	11 (25%)	37,103,103	2.38	12 (32%)
9	HEA	A	618	1,14	44,67,67	1.66	4 (9%)	37,103,103	2.23	9 (24%)
11	HTH	B	310	-	9,9,9	0.52	0	10,10,10	1.16	1 (10%)
4	DMU	A	604	-	34,34,34	1.95	13 (38%)	45,45,45	1.14	4 (8%)
5	TRD	C	601	-	12,12,12	0.19	0	11,11,11	0.53	0
9	HEA	A	617	1	44,67,67	1.72	5 (11%)	37,103,103	2.49	15 (40%)
5	TRD	A	606	-	12,12,12	0.11	0	11,11,11	0.80	0
11	HTH	B	309	-	9,9,9	0.55	0	10,10,10	1.27	1 (10%)
5	TRD	A	611	-	12,12,12	0.10	0	11,11,11	0.85	0
4	DMU	D	301	-	31,31,34	2.02	13 (41%)	42,42,45	1.07	2 (4%)
5	TRD	B	301	-	12,12,12	0.11	0	11,11,11	0.82	0
4	DMU	A	605	-	34,34,34	1.90	12 (35%)	45,45,45	1.29	6 (13%)
5	TRD	A	608	-	12,12,12	0.12	0	11,11,11	0.78	0
5	TRD	D	303	-	8,8,12	0.12	0	7,7,11	0.75	0
5	TRD	A	609	-	12,12,12	0.12	0	11,11,11	0.77	0
5	TRD	A	613	-	12,12,12	0.12	0	11,11,11	0.79	0
5	TRD	A	612	-	12,12,12	0.10	0	11,11,11	0.83	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
5	TRD	D	302	-	-	3/10/10/10	-
5	TRD	B	302	-	-	4/10/10/10	-
5	TRD	A	610	-	-	1/4/4/10	-
5	TRD	B	303	-	-	4/10/10/10	-
11	HTH	B	308	-	-	7/10/10/10	-
4	DMU	A	603	-	-	8/19/59/59	0/2/2/2
5	TRD	A	607	-	-	0/10/10/10	-
9	HEA	C	605	1	2/2/7/16	3/24/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMU	A	602	-	-	3/19/59/59	0/2/2/2
12	TRS	B	311	13	-	4/9/9/9	-
4	DMU	A	601	-	-	9/19/59/59	0/2/2/2
9	HEA	C	606	1,14	2/2/7/16	3/24/76/76	-
9	HEA	A	618	1,14	3/3/7/16	2/24/76/76	-
11	HTH	B	310	-	-	7/10/10/10	-
4	DMU	A	604	-	-	10/19/59/59	0/2/2/2
5	TRD	C	601	-	-	4/10/10/10	-
9	HEA	A	617	1	3/3/7/16	3/24/76/76	-
5	TRD	A	606	-	-	0/10/10/10	-
11	HTH	B	309	-	-	7/10/10/10	-
5	TRD	A	611	-	-	3/10/10/10	-
4	DMU	D	301	-	-	7/16/56/59	0/2/2/2
5	TRD	B	301	-	-	2/10/10/10	-
4	DMU	A	605	-	-	6/19/59/59	0/2/2/2
5	TRD	A	608	-	-	1/10/10/10	-
5	TRD	D	303	-	-	4/6/6/10	-
5	TRD	A	609	-	-	3/10/10/10	-
5	TRD	A	613	-	-	5/10/10/10	-
5	TRD	A	612	-	-	4/10/10/10	-

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	605	HEA	C3B-C11	-8.19	1.46	1.52
9	A	617	HEA	C3B-C11	-7.80	1.46	1.52
9	A	618	HEA	C3B-C11	-7.14	1.47	1.52
9	C	606	HEA	C3B-C11	-5.47	1.48	1.52
9	C	606	HEA	C3A-C2A	5.43	1.47	1.40
9	C	606	HEA	C3C-C2C	4.89	1.47	1.40
4	A	602	DMU	O16-C6	-4.60	1.32	1.40
4	A	601	DMU	O16-C6	-4.51	1.32	1.40
4	A	603	DMU	O16-C6	-4.34	1.32	1.40
4	A	604	DMU	O16-C6	-4.34	1.32	1.40
4	A	605	DMU	O16-C6	-4.25	1.32	1.40
4	D	301	DMU	O16-C6	-4.24	1.32	1.40
4	A	604	DMU	O1-C9	3.73	1.53	1.44
4	D	301	DMU	C11-C9	-3.70	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	DMU	C11-C9	-3.67	1.39	1.51
4	A	605	DMU	C11-C9	-3.66	1.39	1.51
4	A	601	DMU	O1-C9	3.66	1.53	1.44
4	A	601	DMU	C11-C9	-3.65	1.39	1.51
4	A	604	DMU	C11-C9	-3.65	1.39	1.51
4	A	603	DMU	C11-C9	-3.64	1.39	1.51
9	A	618	HEA	C3A-C2A	3.62	1.45	1.40
4	D	301	DMU	O1-C9	3.59	1.53	1.44
4	A	603	DMU	O1-C9	3.56	1.53	1.44
4	A	605	DMU	O1-C9	3.50	1.52	1.44
4	A	602	DMU	O1-C9	3.40	1.52	1.44
9	C	605	HEA	C3A-C2A	3.39	1.45	1.40
9	C	606	HEA	C3D-C2D	3.30	1.47	1.37
4	A	601	DMU	O5-C6	3.26	1.50	1.41
4	A	603	DMU	O5-C6	3.22	1.50	1.41
4	A	605	DMU	O5-C6	3.21	1.50	1.41
4	D	301	DMU	O5-C6	3.21	1.50	1.41
4	A	604	DMU	O5-C6	3.17	1.49	1.41
4	A	602	DMU	O5-C6	3.10	1.49	1.41
9	C	606	HEA	C1D-C2D	3.09	1.49	1.42
9	C	606	HEA	C4B-C3B	2.97	1.49	1.42
4	A	604	DMU	C7-C5	-2.83	1.45	1.52
4	A	604	DMU	O7-C3	2.82	1.51	1.43
9	C	605	HEA	C3C-C2C	2.80	1.44	1.40
4	A	602	DMU	O4-C7	2.76	1.49	1.43
4	D	301	DMU	O7-C3	2.74	1.51	1.43
9	C	606	HEA	C1A-C2A	2.72	1.48	1.42
4	A	602	DMU	C2-C3	-2.70	1.45	1.52
4	A	602	DMU	O7-C3	2.68	1.50	1.43
4	A	601	DMU	C7-C5	-2.68	1.45	1.52
4	A	603	DMU	C7-C5	-2.67	1.45	1.52
4	D	301	DMU	C7-C5	-2.67	1.45	1.52
4	A	601	DMU	C2-C3	-2.67	1.45	1.52
4	A	603	DMU	C2-C3	-2.67	1.45	1.52
4	A	601	DMU	O4-C7	2.67	1.49	1.43
4	A	601	DMU	O7-C3	2.66	1.50	1.43
4	A	604	DMU	O4-C7	2.66	1.49	1.43
4	A	603	DMU	O7-C3	2.63	1.50	1.43
4	A	605	DMU	O7-C3	2.62	1.50	1.43
4	D	301	DMU	O4-C7	2.61	1.49	1.43
4	D	301	DMU	C2-C3	-2.58	1.45	1.52
4	A	605	DMU	C7-C5	-2.58	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	DMU	C7-C5	-2.55	1.45	1.52
4	A	605	DMU	C2-C3	-2.51	1.45	1.52
9	A	617	HEA	C1B-NB	-2.45	1.31	1.36
4	A	604	DMU	C2-C3	-2.45	1.45	1.52
4	A	605	DMU	O4-C7	2.43	1.48	1.43
4	A	601	DMU	C8-C9	2.43	1.58	1.53
9	C	605	HEA	C3D-C2D	2.39	1.44	1.37
4	A	604	DMU	O1-C10	2.39	1.47	1.41
9	C	606	HEA	C4C-CHD	2.39	1.47	1.41
4	A	603	DMU	O4-C7	2.37	1.48	1.43
9	C	605	HEA	C1B-NB	-2.30	1.31	1.36
4	A	605	DMU	O5-C4	2.24	1.49	1.44
9	C	606	HEA	C1C-CHC	2.23	1.47	1.41
4	A	602	DMU	C8-C9	2.23	1.57	1.53
4	D	301	DMU	O55-C2	2.23	1.48	1.43
9	A	617	HEA	C3C-C2C	2.23	1.43	1.40
4	A	604	DMU	O55-C2	2.22	1.48	1.43
4	A	605	DMU	O55-C2	2.21	1.48	1.43
9	C	605	HEA	C4C-NC	-2.20	1.31	1.36
9	A	617	HEA	C3A-C2A	2.20	1.43	1.40
9	C	606	HEA	C1B-CHB	2.19	1.47	1.41
4	A	605	DMU	C8-C9	2.18	1.57	1.53
9	A	617	HEA	C4C-NC	-2.18	1.31	1.36
4	A	601	DMU	O55-C2	2.17	1.48	1.43
4	D	301	DMU	C8-C9	2.17	1.57	1.53
4	A	602	DMU	O55-C2	2.16	1.48	1.43
4	A	603	DMU	O3-C5	2.15	1.48	1.43
4	A	601	DMU	O5-C4	2.15	1.49	1.44
4	A	603	DMU	O55-C2	2.14	1.48	1.43
9	C	606	HEA	C4D-CHA	2.13	1.46	1.41
4	A	604	DMU	C8-C9	2.12	1.57	1.53
4	A	601	DMU	O3-C5	2.11	1.47	1.43
4	A	603	DMU	O1-C10	2.10	1.47	1.41
4	A	603	DMU	O5-C4	2.09	1.49	1.44
4	A	604	DMU	O3-C5	2.09	1.47	1.43
4	D	301	DMU	O3-C5	2.09	1.47	1.43
4	D	301	DMU	O5-C4	2.09	1.49	1.44
9	A	618	HEA	C3C-C2C	2.09	1.43	1.40
4	A	605	DMU	O3-C5	2.08	1.47	1.43
9	A	618	HEA	C4B-C3B	2.05	1.47	1.42
4	A	602	DMU	O3-C5	2.03	1.47	1.43
4	D	301	DMU	O1-C10	2.02	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	DMU	O5-C4	2.02	1.49	1.44

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	618	HEA	C4B-C3B-C2B	-7.75	101.45	106.87
9	C	605	HEA	C4B-C3B-C2B	-7.34	101.74	106.87
9	A	617	HEA	C1B-C2B-C3B	-6.82	102.25	107.00
9	A	617	HEA	C4B-C3B-C2B	-6.72	102.17	106.87
9	C	605	HEA	C1B-C2B-C3B	-6.66	102.36	107.00
9	C	606	HEA	C4B-C3B-C2B	-6.40	102.40	106.87
9	C	606	HEA	C1B-C2B-C3B	-6.33	102.59	107.00
9	A	618	HEA	C1B-C2B-C3B	-5.08	103.46	107.00
9	C	606	HEA	CBA-CAA-C2A	-4.72	103.78	112.48
9	C	605	HEA	C3C-C4C-NC	4.33	114.81	109.21
9	A	617	HEA	C3C-C4C-NC	4.14	114.56	109.21
9	C	606	HEA	CAD-CBD-CGD	-3.93	106.08	112.67
9	C	606	HEA	C3C-C4C-NC	3.89	114.24	109.21
9	A	617	HEA	C13-C14-C15	-3.88	118.32	127.66
9	A	618	HEA	C3C-C4C-NC	3.68	113.96	109.21
9	C	605	HEA	CBA-CAA-C2A	-3.46	106.09	112.48
9	C	605	HEA	CMC-C2C-C3C	3.43	131.09	124.68
9	C	605	HEA	C13-C12-C11	-3.41	109.22	114.35
9	A	618	HEA	C3A-C4A-NA	-3.40	104.53	110.94
9	C	605	HEA	C27-C19-C20	3.38	120.95	115.27
9	C	605	HEA	C13-C14-C15	-3.33	119.65	127.66
11	B	309	HTH	C5-C4-C3	-3.28	108.79	114.18
4	A	603	DMU	C10-O7-C3	-3.27	109.88	117.96
9	A	618	HEA	CMC-C2C-C3C	3.21	130.69	124.68
9	A	618	HEA	CBA-CAA-C2A	-3.21	106.56	112.48
9	C	606	HEA	CMC-C2C-C3C	3.18	130.63	124.68
4	A	605	DMU	O5-C4-C3	3.17	116.44	109.75
4	A	601	DMU	C10-O7-C3	-3.12	110.23	117.96
9	A	617	HEA	CBA-CAA-C2A	-3.12	106.73	112.48
4	A	602	DMU	C10-O7-C3	-3.07	110.37	117.96
9	A	618	HEA	C27-C19-C20	3.05	120.41	115.27
9	A	617	HEA	C13-C12-C11	-3.03	109.80	114.35
9	C	605	HEA	C17-C18-C19	-3.01	120.41	127.66
9	A	617	HEA	C17-C18-C19	-2.95	120.56	127.66
9	C	606	HEA	C26-C15-C16	2.92	120.19	115.27
9	A	617	HEA	C27-C19-C20	2.91	120.16	115.27
9	A	618	HEA	C13-C14-C15	-2.89	120.71	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	310	HTH	C5-C4-C3	-2.87	109.47	114.18
9	C	606	HEA	C13-C14-C15	-2.84	120.82	127.66
11	B	308	HTH	C5-C4-C3	-2.83	109.53	114.18
9	C	605	HEA	CAD-CBD-CGD	-2.83	107.93	112.67
9	C	606	HEA	C27-C19-C20	2.82	120.02	115.27
9	A	618	HEA	CAD-CBD-CGD	-2.79	107.99	112.67
9	C	606	HEA	C13-C12-C11	-2.73	110.25	114.35
4	A	605	DMU	C10-O7-C3	-2.72	111.22	117.96
9	A	617	HEA	O11-C11-C3B	-2.71	104.20	112.00
4	A	605	DMU	O5-C6-C1	-2.66	104.72	110.35
9	A	617	HEA	CMC-C2C-C3C	2.64	129.62	124.68
4	A	604	DMU	O1-C10-C5	2.64	115.94	110.35
9	C	605	HEA	CMB-C2B-C3B	2.61	129.79	124.69
4	A	602	DMU	O1-C9-C8	-2.61	104.96	109.69
4	D	301	DMU	C10-O7-C3	-2.60	111.53	117.96
9	A	617	HEA	C20-C21-C22	-2.60	103.35	111.88
4	A	605	DMU	O16-C6-C1	2.59	112.35	108.30
4	A	605	DMU	C2-C3-C4	2.57	116.81	110.93
4	A	604	DMU	O5-C6-C1	-2.56	104.93	110.35
9	A	617	HEA	CMB-C2B-C3B	2.46	129.50	124.69
4	A	603	DMU	O5-C4-C3	2.30	114.59	109.75
9	C	606	HEA	C17-C18-C19	-2.29	122.16	127.66
4	A	604	DMU	O5-C4-C3	2.27	114.53	109.75
9	C	605	HEA	O11-C11-C3B	-2.25	105.53	112.00
4	A	605	DMU	C1-C2-C3	2.24	114.80	109.68
4	A	603	DMU	O1-C9-C8	-2.23	105.65	109.69
4	D	301	DMU	C1-C2-C3	2.21	114.73	109.68
4	A	602	DMU	O5-C6-C1	-2.21	105.67	110.35
9	C	605	HEA	C16-C17-C18	-2.17	104.74	111.88
4	A	603	DMU	O16-C6-C1	2.15	111.66	108.30
4	A	604	DMU	C1-C2-C3	2.14	114.56	109.68
9	C	606	HEA	C25-C23-C24	2.12	119.29	114.60
9	C	605	HEA	C27-C19-C18	-2.07	118.37	123.68
9	A	617	HEA	C25-C23-C24	2.05	119.12	114.60
9	C	605	HEA	C25-C23-C24	2.04	119.12	114.60
4	A	603	DMU	O1-C9-C11	2.04	111.50	106.44
9	A	617	HEA	C26-C15-C16	2.03	118.69	115.27
9	A	617	HEA	C25-C23-C22	-2.01	116.85	122.65

All (10) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
9	C	605	HEA	ND
9	C	605	HEA	NB
9	C	606	HEA	ND
9	C	606	HEA	NB
9	A	618	HEA	ND
9	A	618	HEA	NA
9	A	618	HEA	NB
9	A	617	HEA	ND
9	A	617	HEA	NA
9	A	617	HEA	NB

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	308	HTH	O1-C1-C2-C3
11	B	308	HTH	C1-C2-C3-O3
11	B	308	HTH	O2-C2-C3-C4
9	C	605	HEA	C19-C20-C21-C22
12	B	311	TRS	C1-C-C3-O3
12	B	311	TRS	C2-C-C3-O3
9	C	606	HEA	C3B-C11-C12-C13
9	C	606	HEA	O11-C11-C12-C13
9	A	618	HEA	C3B-C11-C12-C13
9	A	618	HEA	O11-C11-C12-C13
11	B	310	HTH	O1-C1-C2-O2
11	B	310	HTH	O1-C1-C2-C3
11	B	310	HTH	C1-C2-C3-O3
11	B	310	HTH	C1-C2-C3-C4
11	B	310	HTH	O2-C2-C3-O3
11	B	310	HTH	O2-C2-C3-C4
4	A	604	DMU	C19-C18-O16-C6
9	A	617	HEA	C19-C20-C21-C22
11	B	309	HTH	C1-C2-C3-O3
11	B	309	HTH	C1-C2-C3-C4
11	B	309	HTH	O2-C2-C3-O3
11	B	309	HTH	O2-C2-C3-C4
4	D	301	DMU	C19-C18-O16-C6
4	A	604	DMU	O1-C10-O7-C3
11	B	308	HTH	O1-C1-C2-O2
4	D	301	DMU	O5-C4-C57-O61
4	A	603	DMU	O5-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
4	A	603	DMU	O6-C11-C9-O1
4	D	301	DMU	C3-C4-C57-O61
4	D	301	DMU	O5-C6-O16-C18
4	A	604	DMU	C3-C4-C57-O61
4	A	603	DMU	O6-C11-C9-C8
5	B	302	TRD	C4-C5-C6-C7
4	A	604	DMU	O16-C18-C19-C22
4	A	604	DMU	O5-C4-C57-O61
4	A	603	DMU	C3-C4-C57-O61
5	A	611	TRD	C11-C10-C9-C8
5	B	303	TRD	C11-C10-C9-C8
5	B	303	TRD	C9-C10-C11-C12
5	A	611	TRD	C7-C8-C9-C10
4	A	601	DMU	C19-C22-C25-C28
4	A	605	DMU	C25-C28-C31-C34
4	A	601	DMU	O16-C18-C19-C22
4	A	605	DMU	O16-C18-C19-C22
5	A	609	TRD	C9-C10-C11-C12
4	A	601	DMU	C22-C25-C28-C31
4	A	601	DMU	C19-C18-O16-C6
5	A	612	TRD	C6-C7-C8-C9
5	D	303	TRD	C3-C4-C5-C6
5	A	612	TRD	C7-C8-C9-C10
5	A	613	TRD	C9-C10-C11-C12
11	B	309	HTH	O1-C1-C2-O2
4	A	601	DMU	C31-C34-C37-C40
4	A	604	DMU	C31-C34-C37-C40
4	A	601	DMU	O5-C4-C57-O61
4	A	605	DMU	C19-C22-C25-C28
5	B	301	TRD	C11-C10-C9-C8
4	A	602	DMU	C3-C4-C57-O61
11	B	308	HTH	O3-C3-C4-C5
4	A	604	DMU	O6-C11-C9-C8
5	A	613	TRD	C1-C2-C3-C4
5	A	613	TRD	C7-C8-C9-C10
4	D	301	DMU	C22-C25-C28-C31
5	A	609	TRD	C10-C11-C12-C13
4	D	301	DMU	O16-C18-C19-C22
5	B	302	TRD	C6-C7-C8-C9
11	B	308	HTH	O2-C2-C3-O3
5	A	613	TRD	C6-C7-C8-C9
4	A	603	DMU	C19-C18-O16-C6

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Mol	Chain	Res	Type	Atoms
5	A	611	TRD	C9-C10-C11-C12
5	A	612	TRD	C11-C10-C9-C8
11	B	309	HTH	O1-C1-C2-C3
4	A	605	DMU	C34-C37-C40-C43
4	A	605	DMU	O5-C4-C57-O61
5	C	601	TRD	C9-C10-C11-C12
9	C	605	HEA	C26-C15-C16-C17
4	A	604	DMU	O6-C11-C9-O1
4	A	603	DMU	C18-C19-C22-C25
11	B	308	HTH	C2-C3-C4-C5
12	B	311	TRS	N-C-C3-O3
5	B	302	TRD	C5-C6-C7-C8
9	C	605	HEA	C14-C15-C16-C17
5	B	303	TRD	C4-C5-C6-C7
5	B	301	TRD	C6-C7-C8-C9
4	A	601	DMU	C28-C31-C34-C37
5	A	610	TRD	C1-C2-C3-C4
9	A	617	HEA	C26-C15-C16-C17
4	A	601	DMU	C18-C19-C22-C25
4	A	603	DMU	C19-C22-C25-C28
4	A	602	DMU	C25-C28-C31-C34
5	D	303	TRD	C6-C7-C8-C9
5	B	302	TRD	C9-C10-C11-C12
5	C	601	TRD	C2-C3-C4-C5
4	A	602	DMU	O5-C4-C57-O61
12	B	311	TRS	C1-C-C2-O2
5	A	613	TRD	C11-C10-C9-C8
5	D	302	TRD	C4-C5-C6-C7
11	B	309	HTH	C3-C4-C5-C6
4	A	601	DMU	C34-C37-C40-C43
4	A	604	DMU	O5-C6-O16-C18
4	D	301	DMU	C18-C19-C22-C25
9	A	617	HEA	C14-C15-C16-C17
5	D	303	TRD	C5-C6-C7-C8
5	A	608	TRD	C3-C4-C5-C6
5	D	302	TRD	C3-C4-C5-C6
5	A	609	TRD	C4-C5-C6-C7
5	D	302	TRD	C6-C7-C8-C9
4	A	604	DMU	C2-C3-O7-C10
5	C	601	TRD	C5-C6-C7-C8
11	B	310	HTH	C3-C4-C5-C6
4	A	605	DMU	C28-C31-C34-C37

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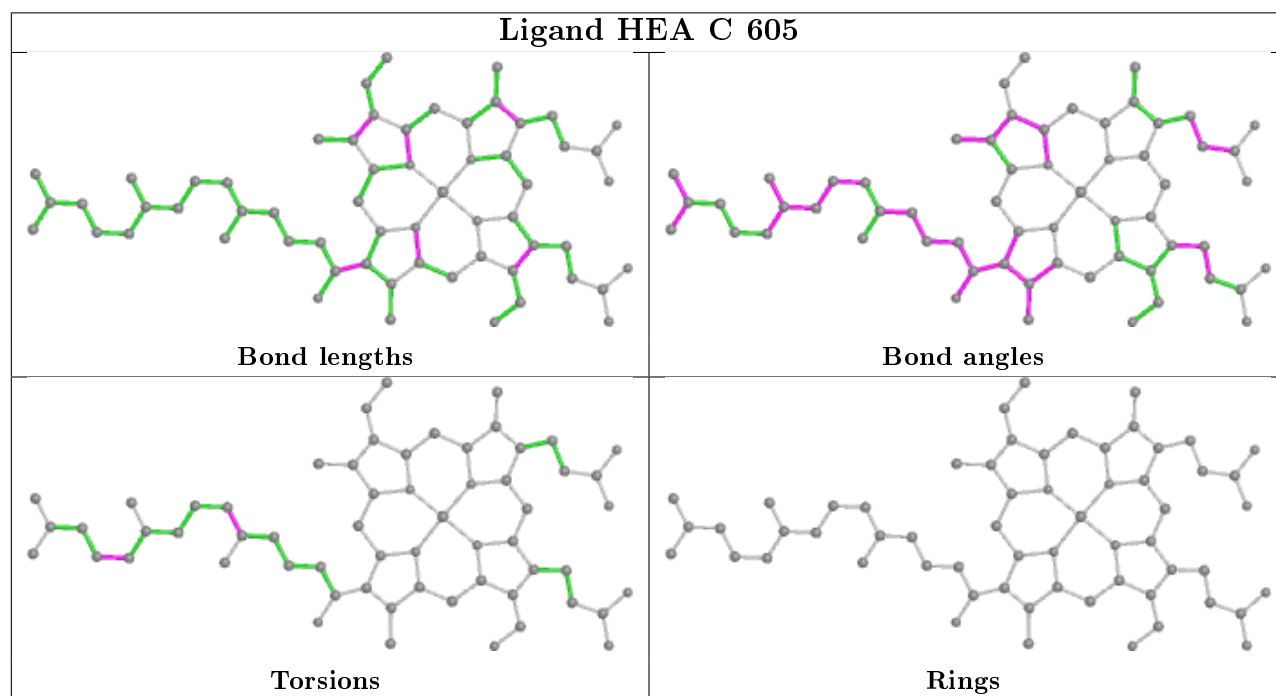
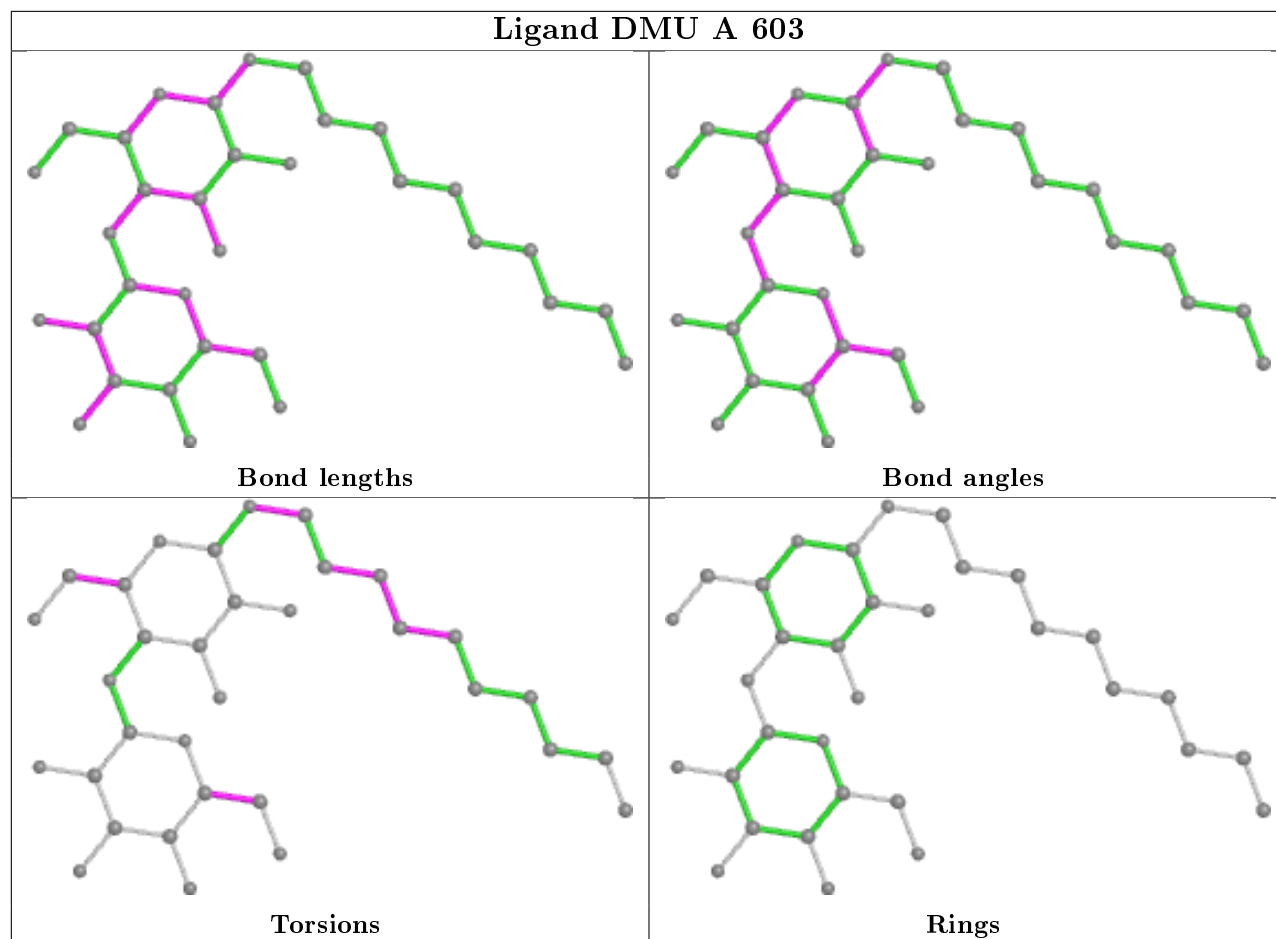
Mol	Chain	Res	Type	Atoms
5	B	303	TRD	C10-C11-C12-C13
5	A	612	TRD	C4-C5-C6-C7
4	A	603	DMU	C22-C25-C28-C31
5	C	601	TRD	C7-C8-C9-C10
9	C	606	HEA	C26-C15-C16-C17
5	D	303	TRD	C4-C5-C6-C7

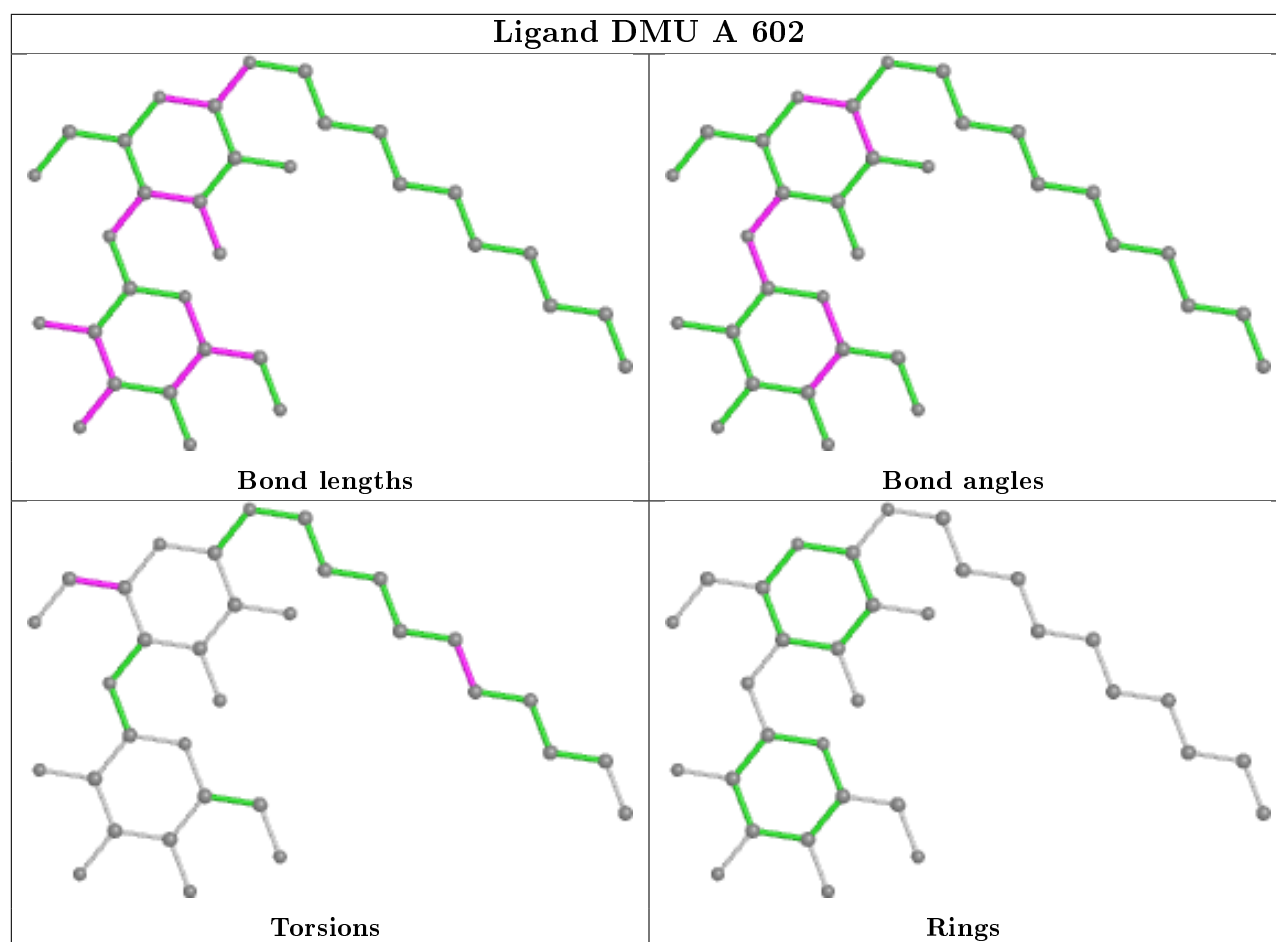
There are no ring outliers.

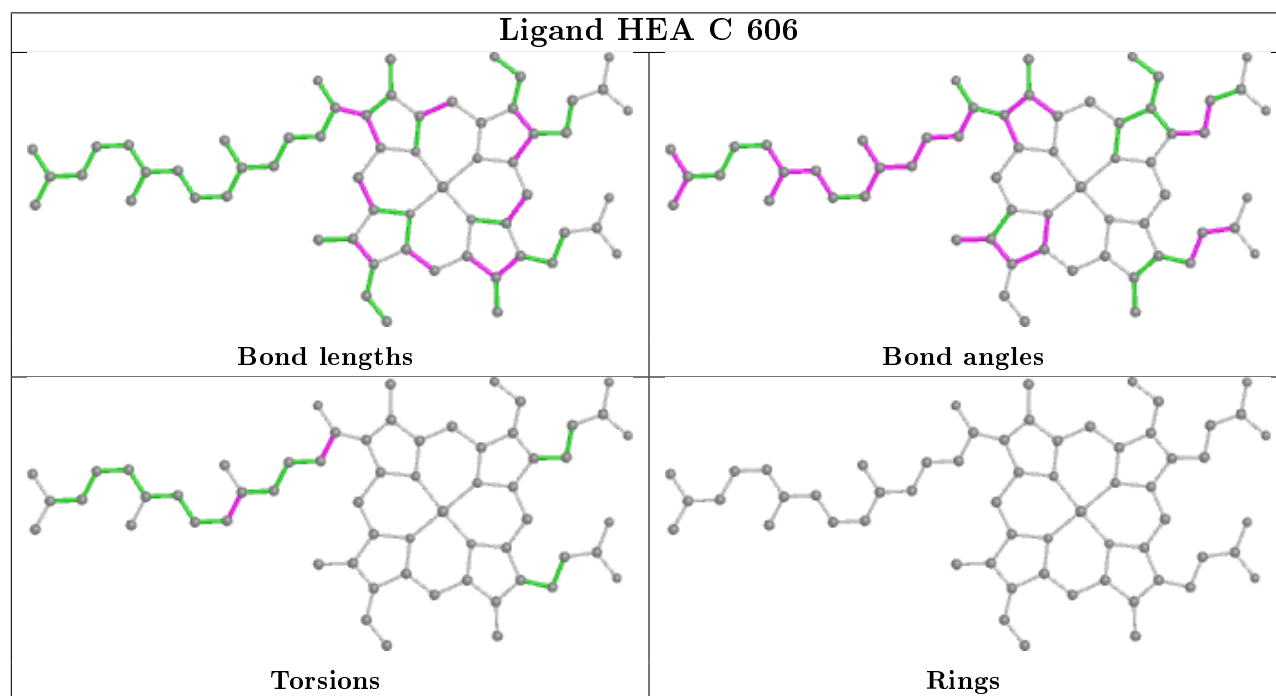
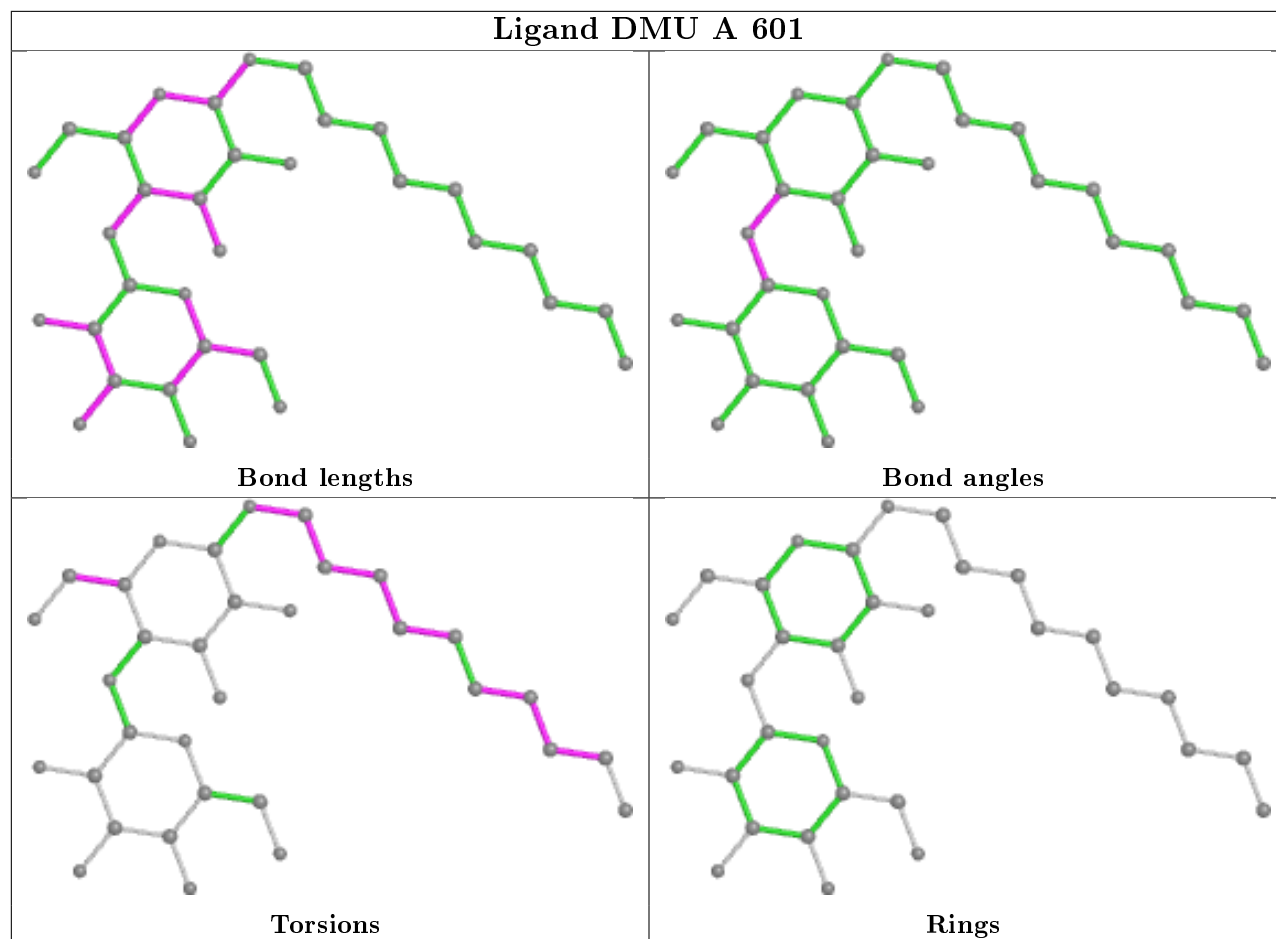
13 monomers are involved in 29 short contacts:

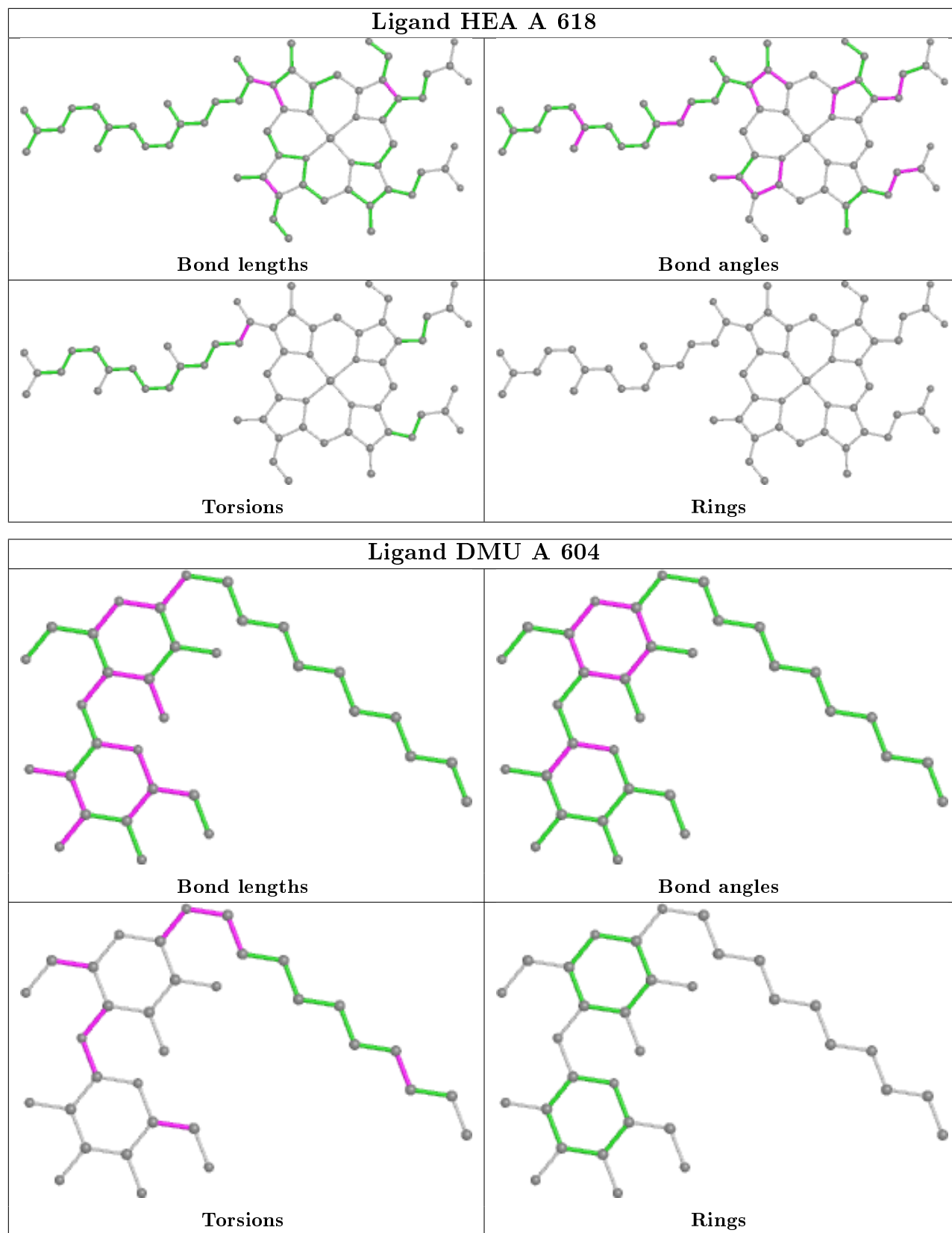
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	302	TRD	3	0
5	A	607	TRD	1	0
9	C	605	HEA	3	0
4	A	601	DMU	1	0
9	C	606	HEA	4	0
9	A	618	HEA	8	0
11	B	310	HTH	1	0
4	A	604	DMU	3	0
9	A	617	HEA	1	0
5	A	606	TRD	1	0
4	D	301	DMU	1	0
5	D	303	TRD	2	0
5	A	612	TRD	2	0

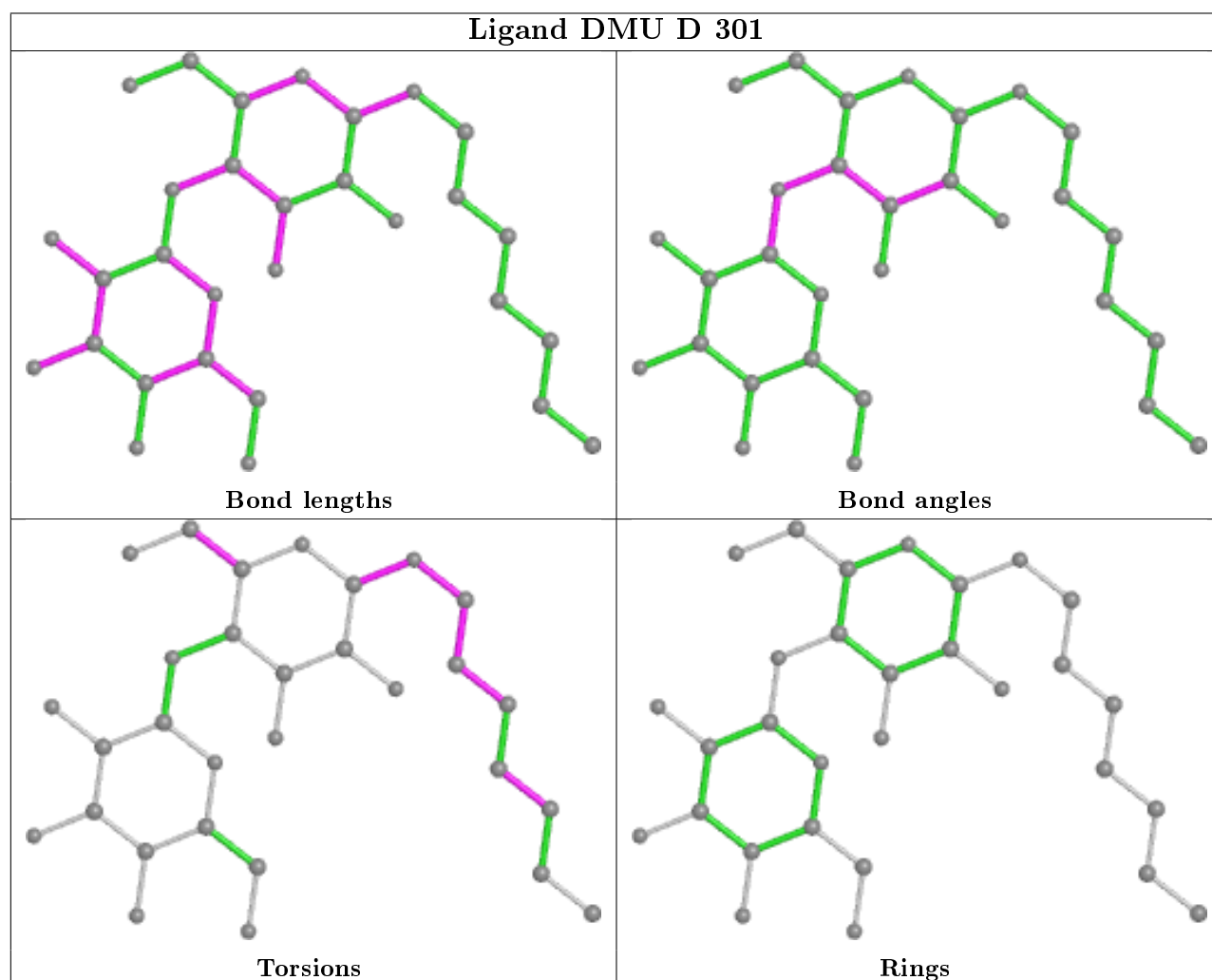
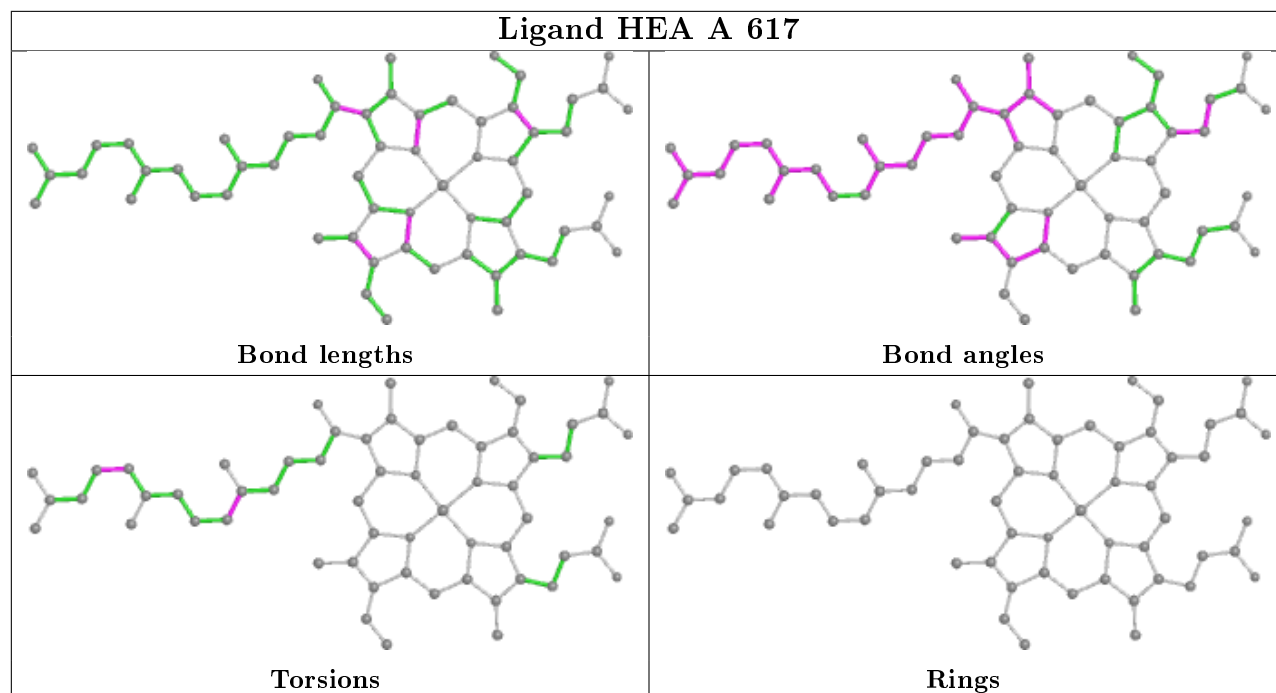
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

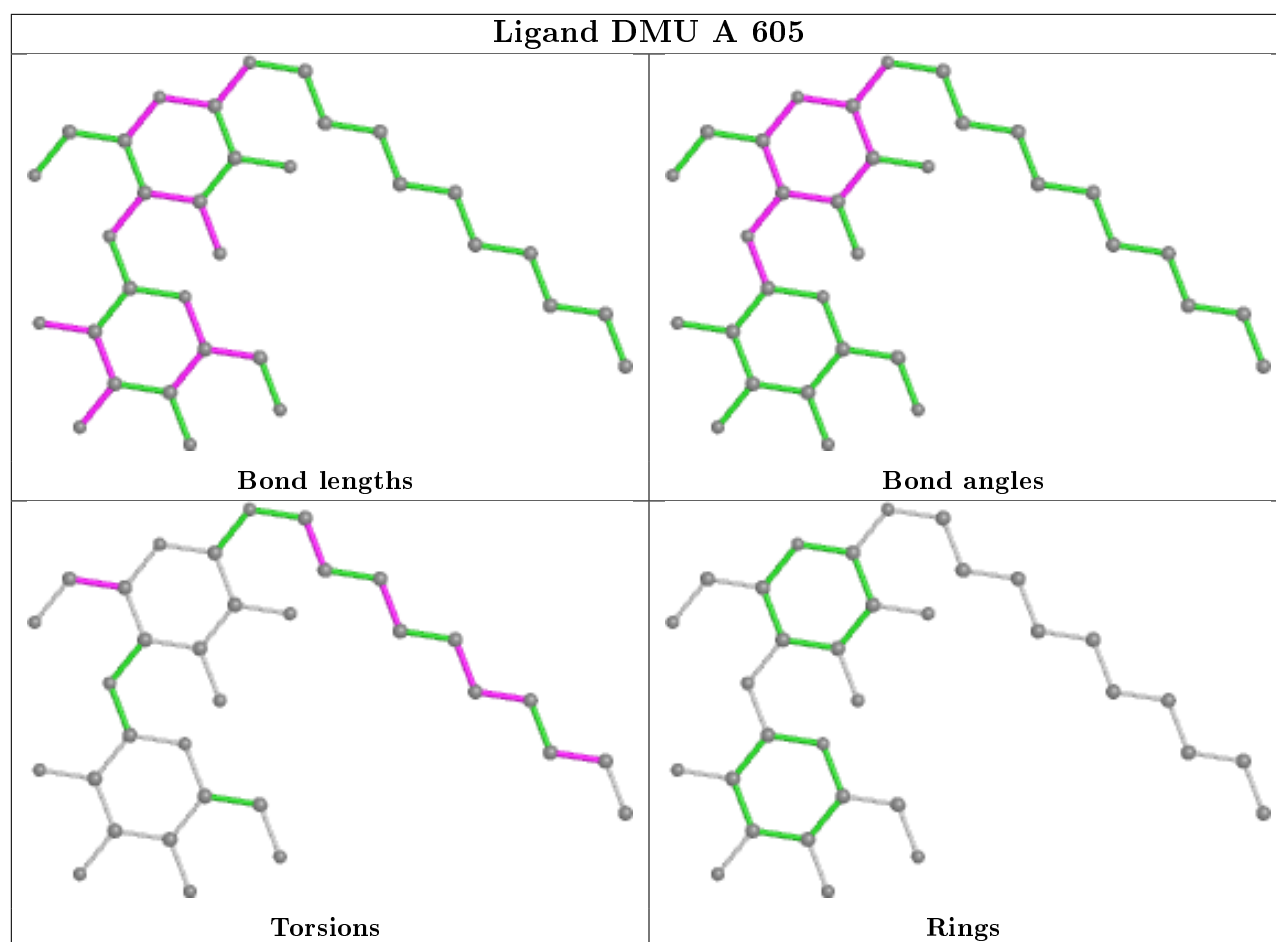












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	535/535 (100%)	0.21	43 (8%) 12 11	37, 54, 83, 115	0
1	C	531/535 (99%)	0.99	126 (23%) 0 0	51, 77, 108, 130	0
2	B	256/257 (99%)	-0.08	7 (2%) 54 52	39, 58, 81, 89	0
2	D	257/257 (100%)	0.19	20 (7%) 13 11	45, 66, 96, 116	0
All	All	1579/1584 (99%)	0.42	196 (12%) 4 3	37, 64, 99, 130	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	287	VAL	6.5
1	C	217	ALA	6.2
1	C	172	TRP	6.2
1	C	218	PRO	6.2
1	C	520	THR	5.7
1	C	21	PHE	5.5
1	C	290	ILE	5.4
2	D	99	PRO	5.4
1	C	550	THR	5.3
1	C	259	PHE	5.3
1	C	23	SER	5.2
1	C	173	VAL	5.1
1	C	213	LEU	5.1
1	C	222	MET	4.9
1	C	549	HIS	4.8
2	D	98	SER	4.8
1	C	268	GLY	4.8
2	D	82	ARG	4.7
1	C	522	GLY	4.7
1	A	172	TRP	4.5
1	C	135	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	287	VAL	4.4
1	C	73	VAL	4.3
1	C	452	ALA	4.3
2	D	81	TRP	4.3
1	C	184	GLY	4.3
1	C	81	TRP	4.3
1	C	414	TYR	4.2
1	C	289	ILE	4.2
1	A	416	VAL	4.2
1	C	74	LYS	4.2
2	D	96	HIS	4.1
2	D	29	SER	4.1
1	C	223	HIS	4.1
1	C	445	GLY	4.1
1	C	527	ALA	4.0
1	C	107	MET	4.0
1	C	71	GLY	4.0
1	C	72	LEU	3.9
2	B	56	TRP	3.9
1	C	185	TYR	3.9
1	C	451	TRP	3.9
1	C	424	MET	3.9
1	C	219	GLY	3.8
1	C	103	GLY	3.8
1	C	423	VAL	3.7
1	C	288	TYR	3.7
2	D	56	TRP	3.7
1	C	426	LEU	3.6
1	C	210	THR	3.6
1	C	260	GLY	3.6
1	A	81	TRP	3.6
1	A	398	GLY	3.6
1	A	20	TRP	3.6
1	C	421	HIS	3.5
1	C	525	VAL	3.5
2	D	97	ASN	3.5
1	C	160	PRO	3.5
1	A	173	VAL	3.5
2	D	78	TYR	3.4
1	C	134	ALA	3.4
1	C	481	ARG	3.4
1	C	425	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	290	ILE	3.4
1	C	76	PHE	3.4
1	C	446	ARG	3.4
1	C	221	THR	3.4
1	A	417	VAL	3.3
2	D	100	LEU	3.3
1	C	262	THR	3.3
1	A	107	MET	3.3
1	C	514	VAL	3.3
1	C	548	GLU	3.2
1	A	424	MET	3.2
1	C	82	PRO	3.2
1	C	108	PHE	3.2
1	C	523	ALA	3.1
2	B	117	ALA	3.1
1	C	106	MET	3.1
1	C	22	MET	3.1
1	C	427	GLY	3.1
1	C	413	THR	3.1
1	A	428	ALA	3.1
1	C	428	ALA	3.1
1	C	129	GLY	3.1
1	C	261	THR	3.1
1	A	549	HIS	3.1
1	A	427	GLY	3.0
1	C	534	HIS	3.0
1	C	400	VAL	3.0
1	C	104	ILE	2.9
1	C	417	VAL	2.9
1	C	318	TYR	2.9
1	A	425	SER	2.9
2	D	101	ALA	2.8
2	B	87	ARG	2.8
2	B	102	ILE	2.8
1	A	423	VAL	2.8
1	C	397	THR	2.8
1	C	422	TYR	2.8
1	A	413	THR	2.8
2	D	85	GLU	2.7
1	A	420	PHE	2.7
1	C	519	LEU	2.7
1	C	70	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	286	GLU	2.7
1	A	481	ARG	2.7
2	B	100	LEU	2.7
1	C	20	TRP	2.7
1	A	426	LEU	2.7
1	C	376	GLU	2.7
1	C	207	ASN	2.7
2	D	88	ASN	2.6
1	C	214	ASN	2.6
1	C	480	PRO	2.6
1	A	291	VAL	2.6
1	C	280	TRP	2.6
1	C	216	ARG	2.6
1	A	550	THR	2.6
1	A	412	ASP	2.6
1	A	221	THR	2.5
1	A	112	ILE	2.5
1	C	420	PHE	2.5
1	C	447	GLN	2.5
1	A	418	ALA	2.5
1	C	418	ALA	2.5
1	C	291	VAL	2.4
1	C	415	TYR	2.4
1	C	283	GLY	2.4
1	A	289	ILE	2.4
2	B	124	PHE	2.4
2	D	102	ILE	2.4
1	C	220	MET	2.4
1	C	100	THR	2.4
1	A	111	VAL	2.4
1	C	131	PRO	2.4
2	D	117	ALA	2.4
2	D	106	ILE	2.4
1	C	230	TRP	2.4
1	A	400	VAL	2.4
1	C	282	PHE	2.4
1	A	480	PRO	2.4
1	C	479	MET	2.4
1	C	212	PHE	2.4
1	C	263	PHE	2.4
1	C	269	GLY	2.3
1	C	334	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	88	ASN	2.3
1	C	396	VAL	2.3
2	D	285	HIS	2.3
1	C	429	VAL	2.3
1	A	415	TYR	2.3
1	C	137	ARG	2.3
1	C	540	TRP	2.3
1	C	416	VAL	2.3
1	C	144	TRP	2.3
2	D	94	PHE	2.3
1	A	411	HIS	2.3
1	C	138	MET	2.3
2	D	84	HIS	2.3
1	C	394	GLY	2.2
2	D	176	VAL	2.2
1	A	17	PHE	2.2
1	C	419	HIS	2.2
1	C	80	LEU	2.2
1	A	222	MET	2.2
1	A	429	VAL	2.2
1	C	411	HIS	2.2
1	A	77	PHE	2.2
1	A	100	THR	2.2
1	C	412	ASP	2.2
1	A	22	MET	2.2
1	A	104	ILE	2.2
1	C	391	PHE	2.2
1	C	398	GLY	2.2
1	C	78	GLN	2.2
1	A	220	MET	2.1
1	C	99	ILE	2.1
1	C	375	ILE	2.1
1	A	419	HIS	2.1
1	C	215	MET	2.1
1	C	285	PRO	2.1
1	A	69	GLU	2.1
1	C	69	GLU	2.1
1	C	311	PHE	2.1
1	C	62	PHE	2.1
1	C	141	LEU	2.1
1	C	535	ALA	2.0
1	C	79	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	254	LEU	2.0
1	C	270	GLY	2.0
1	C	395	GLY	2.0
1	C	284	HIS	2.0
1	C	267	SER	2.0
1	A	171	GLY	2.0
1	C	546	PRO	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](#)

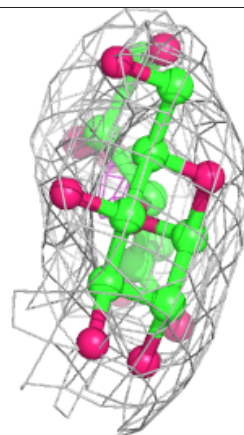
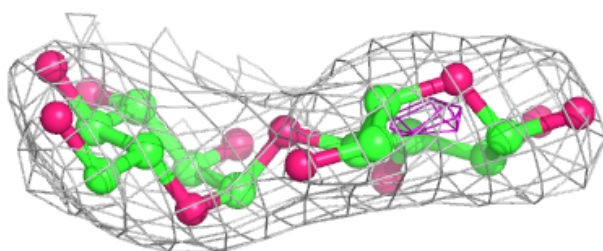
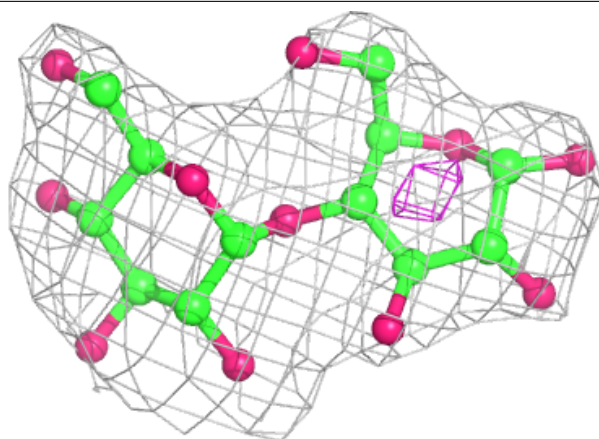
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	GLC	G	1	12/12	0.78	0.33	116,126,136,136	0
3	GLC	F	2	11/12	0.85	0.35	96,105,110,112	0
3	GLC	F	1	12/12	0.85	0.32	110,114,120,121	0
3	GLC	G	2	11/12	0.86	0.33	130,136,140,142	0
3	GLC	E	2	11/12	0.88	0.33	87,98,107,107	0
3	GLC	E	1	12/12	0.88	0.39	97,111,118,119	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.

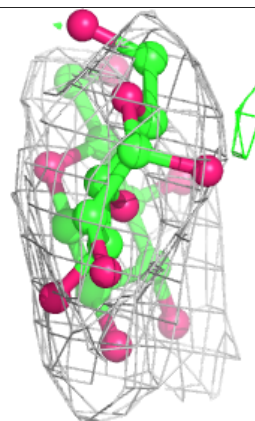
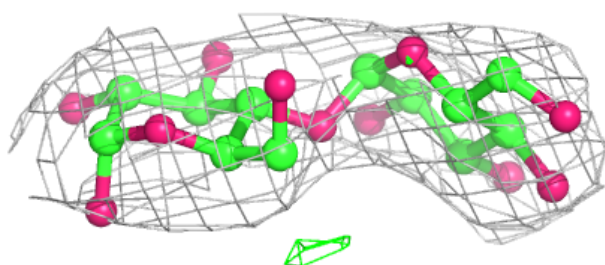
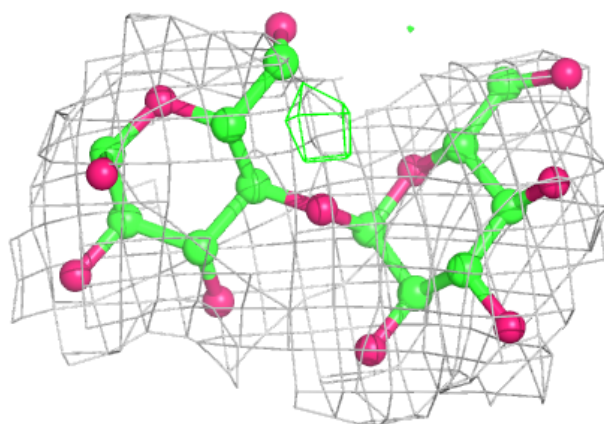
**Electron density around Chain E:**

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

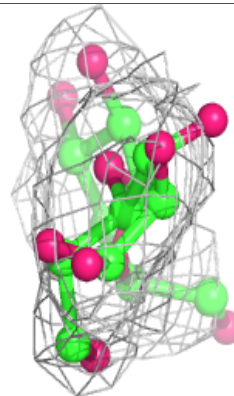
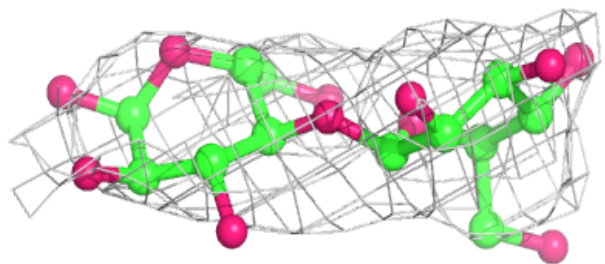
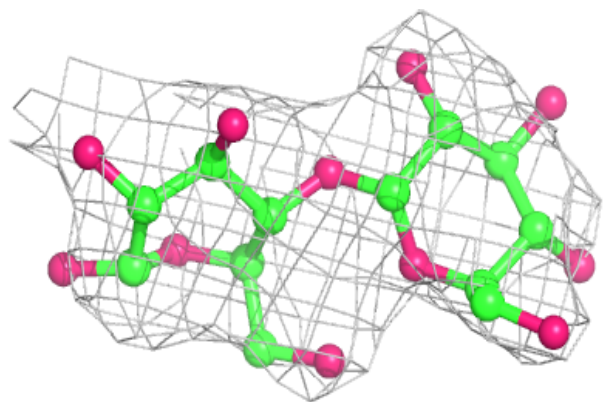


**Electron density around Chain F:**

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

**Electron density around Chain G:**

$2mF_o - DF_c$  (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, 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
5	TRD	C	601	13/13	0.24	0.62	88,112,125,125	0
5	TRD	A	607	13/13	0.63	0.43	65,77,84,91	0
11	HTH	B	310	10/10	0.65	0.24	77,105,110,114	0
5	TRD	A	608	13/13	0.68	0.23	63,70,88,93	0
5	TRD	A	610	7/13	0.70	0.25	58,69,74,78	0
5	TRD	B	301	13/13	0.71	0.37	74,86,93,99	0
5	TRD	B	303	13/13	0.72	0.35	55,65,78,79	0
5	TRD	B	302	13/13	0.72	0.44	52,68,83,84	0
5	TRD	D	302	13/13	0.75	0.29	61,72,85,87	0
5	TRD	A	609	13/13	0.75	0.32	64,74,83,91	0
4	DMU	A	601	33/33	0.76	0.25	53,88,122,126	0
4	DMU	A	604	33/33	0.78	0.26	46,68,79,83	33
5	TRD	A	611	13/13	0.80	0.34	67,77,88,91	0
4	DMU	A	605	33/33	0.81	0.33	56,67,74,79	33
11	HTH	B	309	10/10	0.82	0.49	76,85,99,104	0
12	TRS	B	311	8/8	0.82	0.11	63,91,103,104	0
5	TRD	A	612	13/13	0.82	0.41	68,80,93,97	0
5	TRD	A	606	13/13	0.83	0.23	72,76,88,90	0
5	TRD	A	613	13/13	0.83	0.21	62,69,82,87	0
11	HTH	B	308	10/10	0.83	0.75	56,66,77,78	10
4	DMU	D	301	30/33	0.86	0.32	67,100,113,115	0
13	K	B	312	1/1	0.89	0.09	123,123,123,123	0
5	TRD	D	303	9/13	0.92	0.36	83,84,84,88	0
4	DMU	A	603	33/33	0.93	0.19	58,73,86,96	0
9	HEA	C	606	60/60	0.95	0.28	50,63,75,81	0
4	DMU	A	602	33/33	0.96	0.13	41,54,69,71	0
8	CA	C	603	1/1	0.96	0.07	69,69,69,69	0
9	HEA	C	605	60/60	0.96	0.28	47,63,80,92	0
9	HEA	A	618	60/60	0.97	0.25	38,47,61,65	0
9	HEA	A	617	60/60	0.98	0.27	34,42,56,73	0
6	CU	C	604	1/1	0.98	0.19	62,62,62,62	0
7	MG	C	602	1/1	0.98	0.33	46,46,46,46	0
10	CD	D	306	1/1	0.99	0.13	62,62,62,62	0
6	CU	A	614	1/1	0.99	0.21	51,51,51,51	0
8	CA	A	616	1/1	0.99	0.13	44,44,44,44	0
7	MG	A	615	1/1	0.99	0.29	37,37,37,37	0
10	CD	B	305	1/1	0.99	0.15	63,63,63,63	0

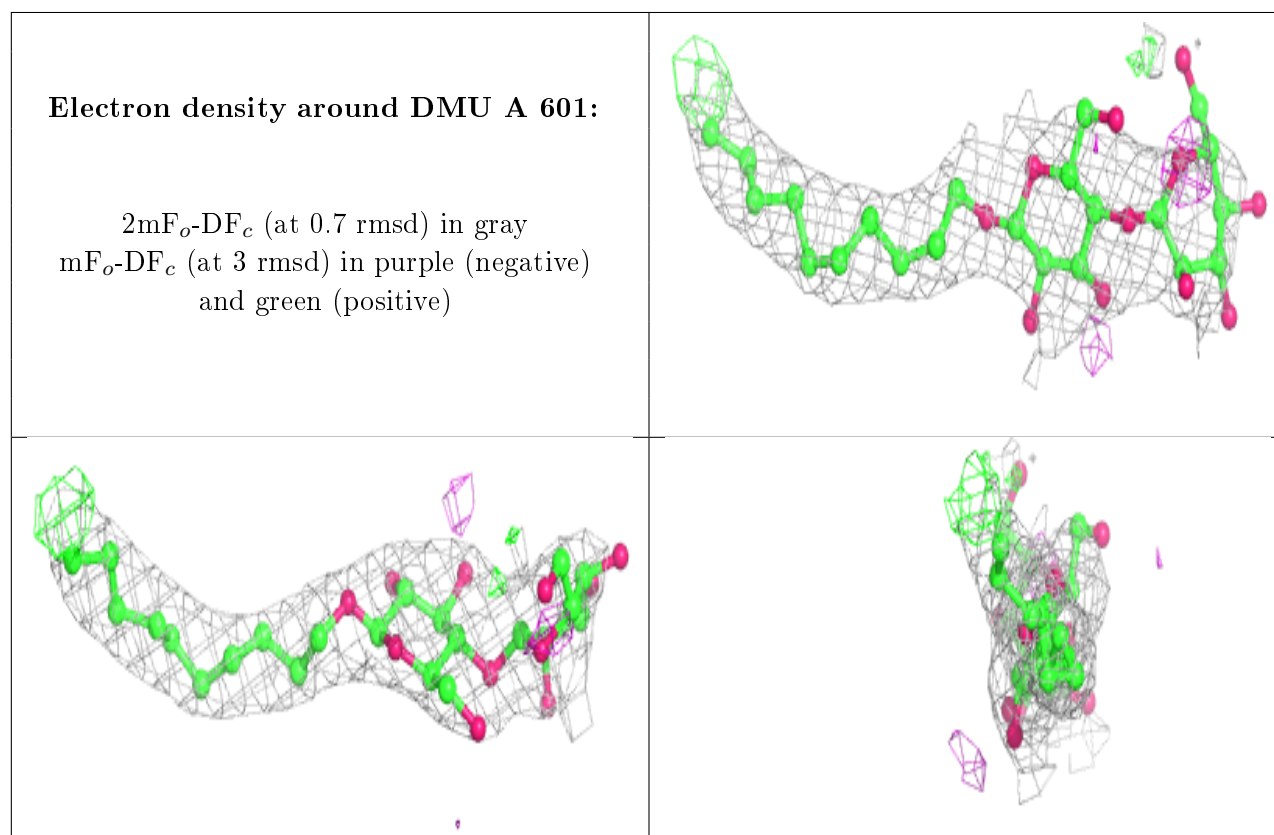
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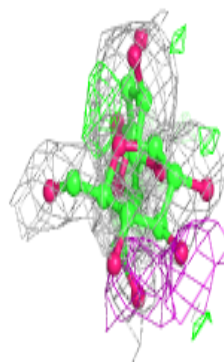
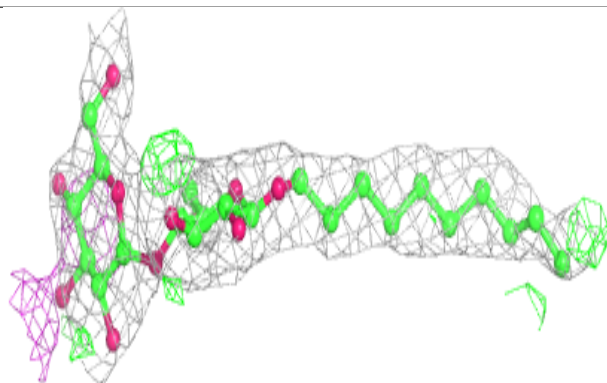
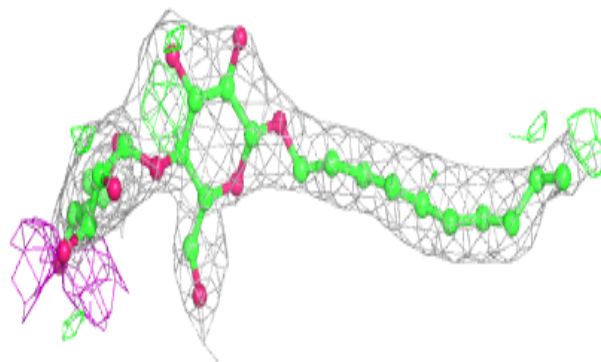
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CU	D	307	1/1	0.99	0.14	51,51,51,51	0
6	CU	D	308	1/1	1.00	0.16	53,53,53,53	0
6	CU	B	307	1/1	1.00	0.15	41,41,41,41	0
6	CU	B	306	1/1	1.00	0.16	42,42,42,42	0

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.

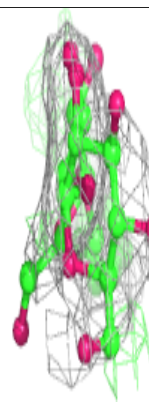
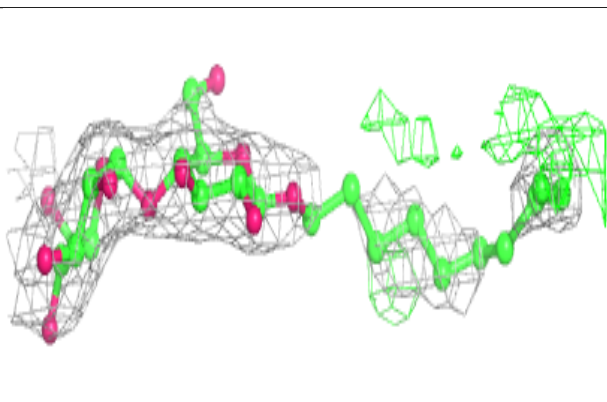
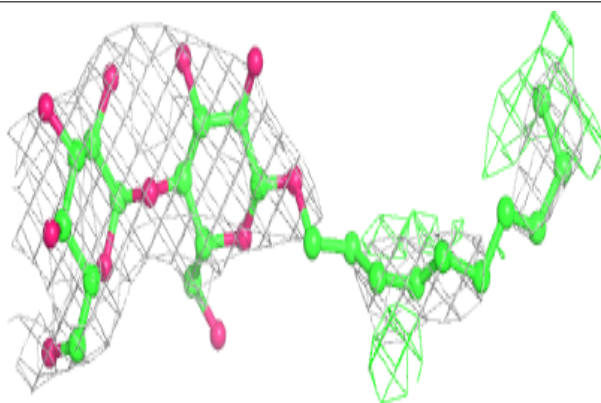


**Electron density around DMU A 604:**

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

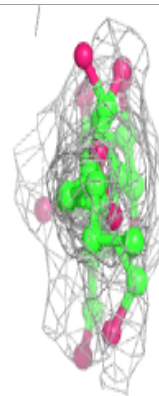
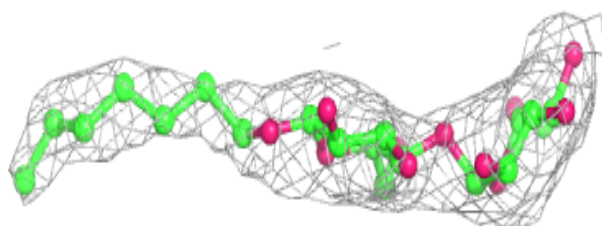
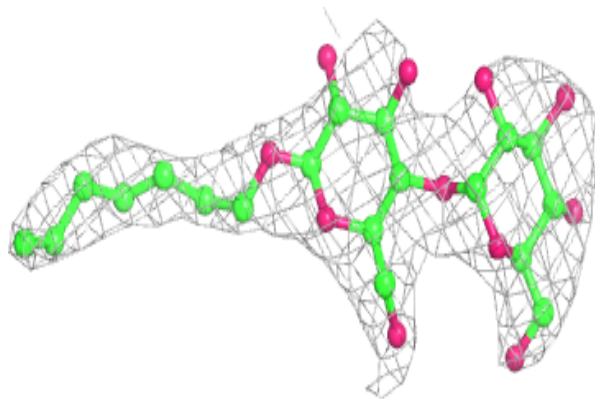
**Electron density around DMU A 605:**

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

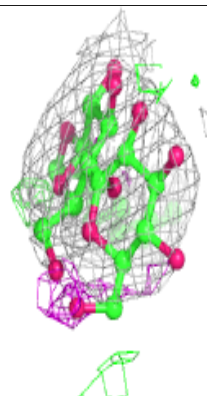
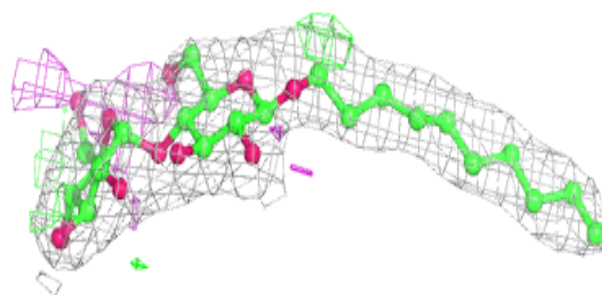
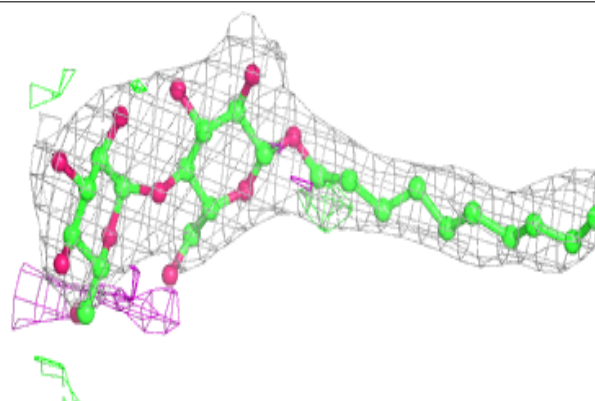


**Electron density around DMU D 301:**

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

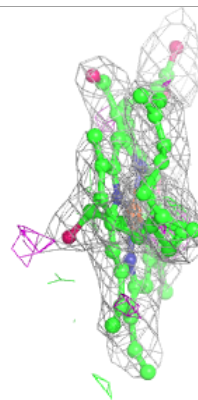
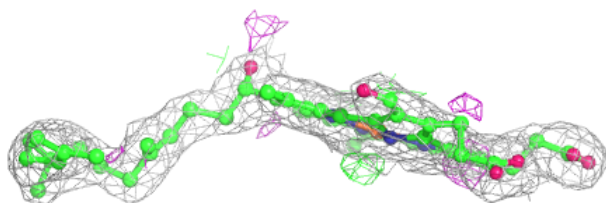
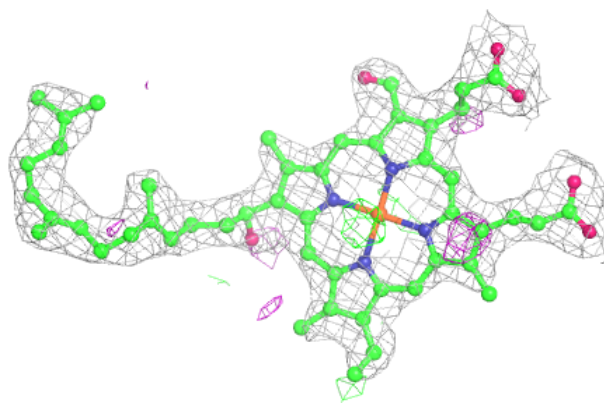
**Electron density around DMU A 603:**

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

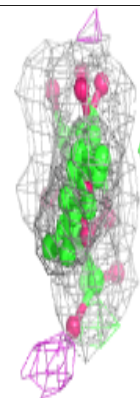
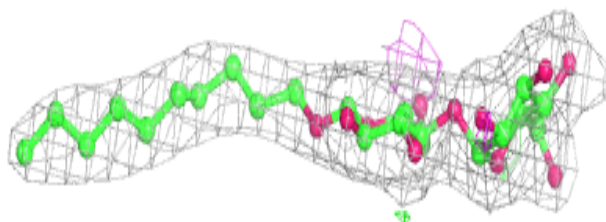
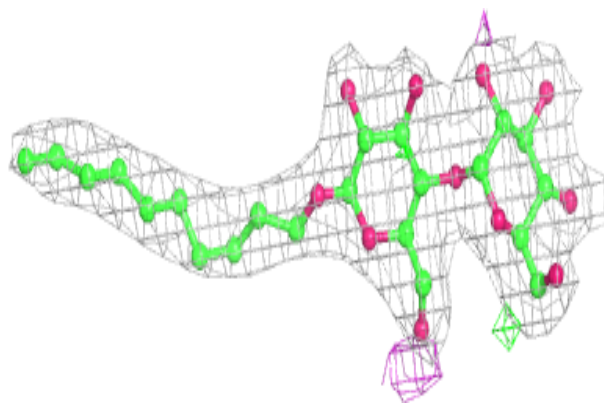


**Electron density around HEA C 606:**

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

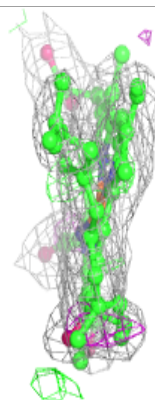
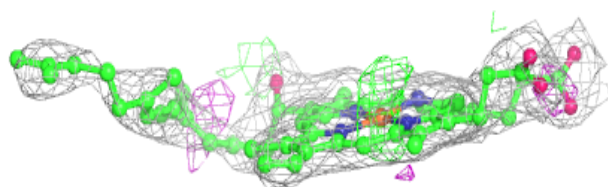
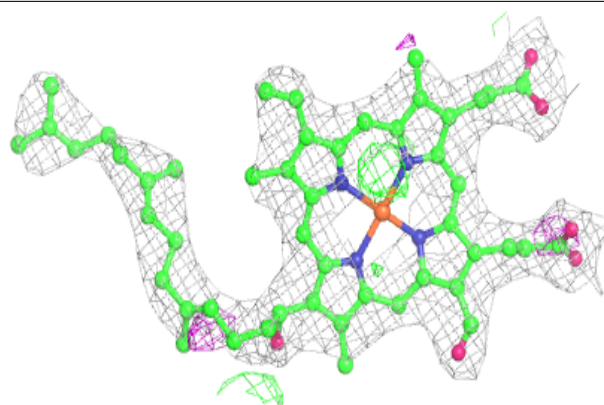
**Electron density around DMU A 602:**

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

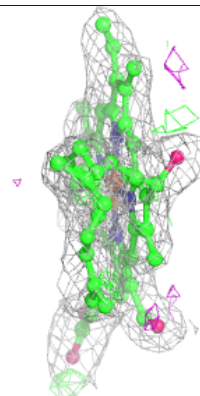
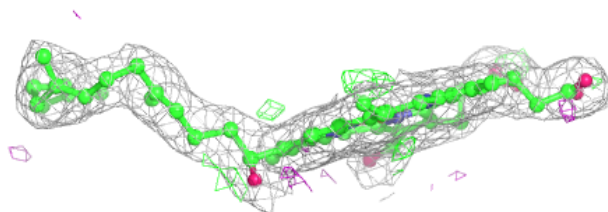
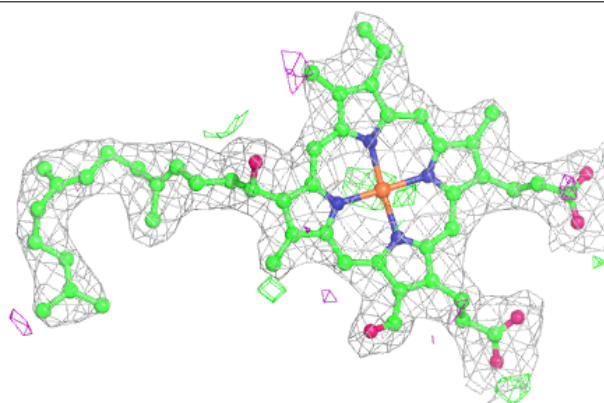


**Electron density around HEA C 605:**

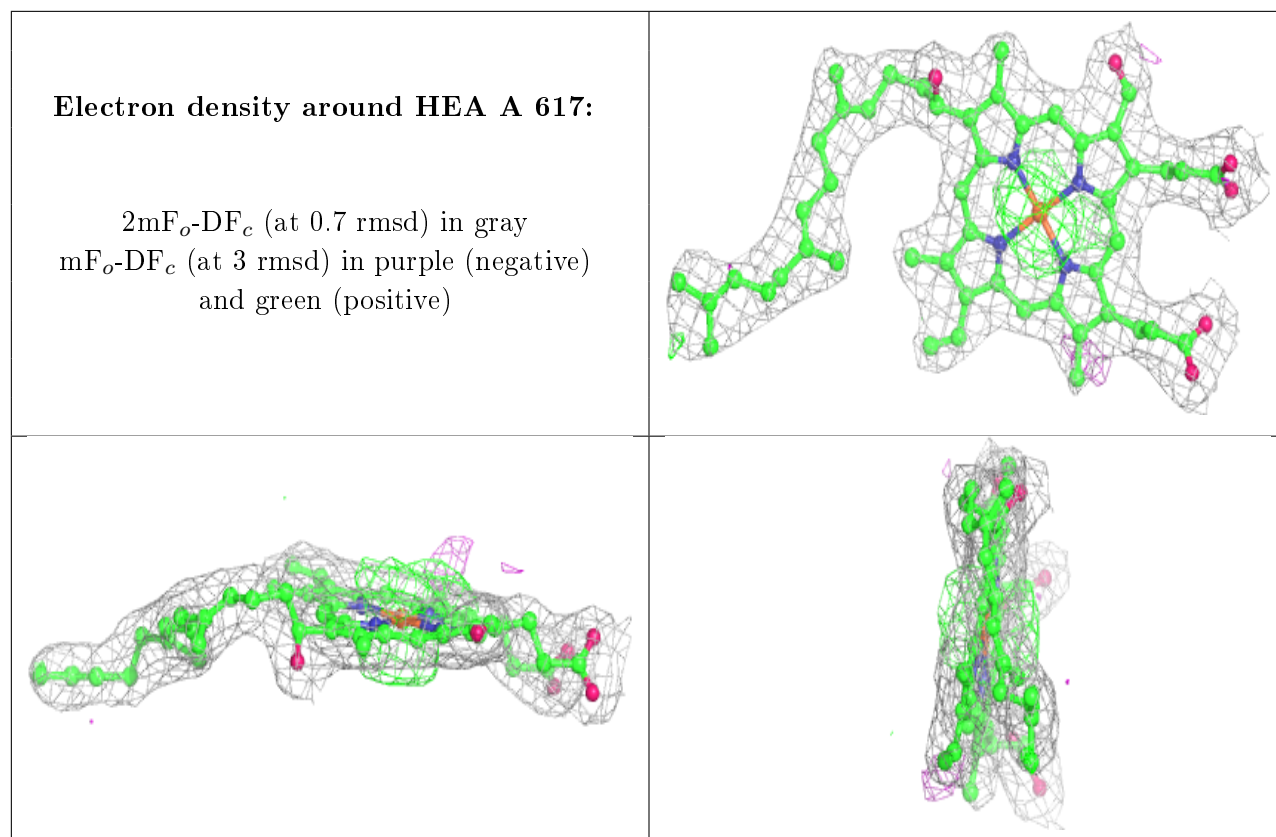
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around HEA A 618:**

$2mF_o-DF_c$  (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.