wwPDB X-ray Structure Validation Summary Report (i)

Sep 28, 2024 – 08:57 AM EDT

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

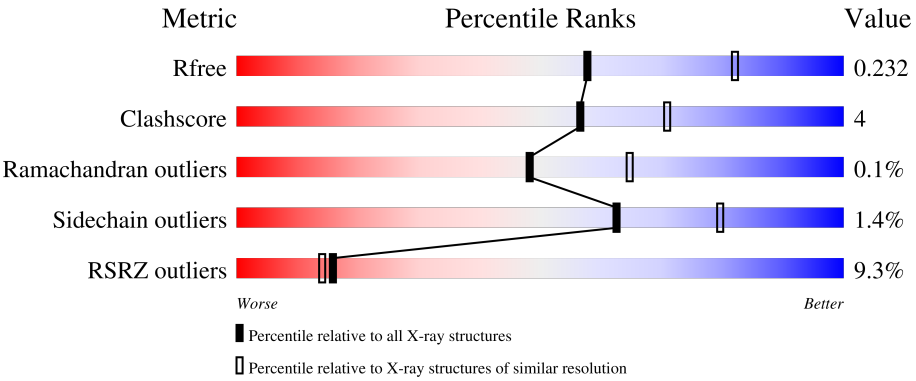
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	3% 92% 8%
1	C	535	19% 85% 13%
2	B	257	4% 91% 7%
2	D	257	7% 95% 5%
3	E	2	100%

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Mol	Chain	Length	Quality of chain
3	F	2	50% 50%
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	C	601	-	-	-	X

2 Entry composition (i)

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			

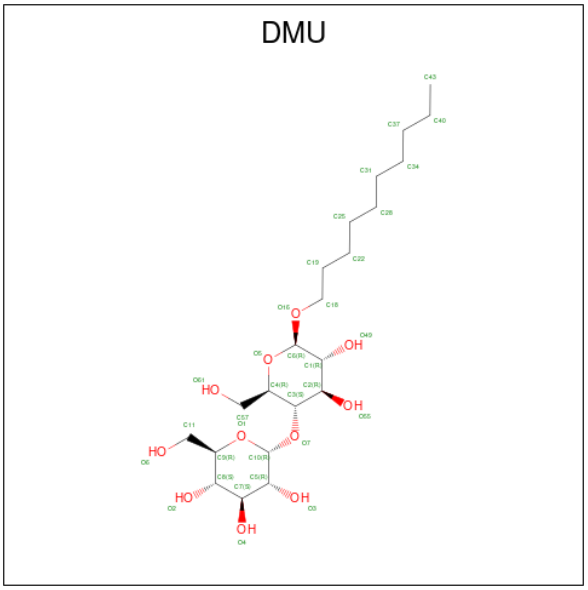
There are 10 discrepancies between the modelled and reference sequences:

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.

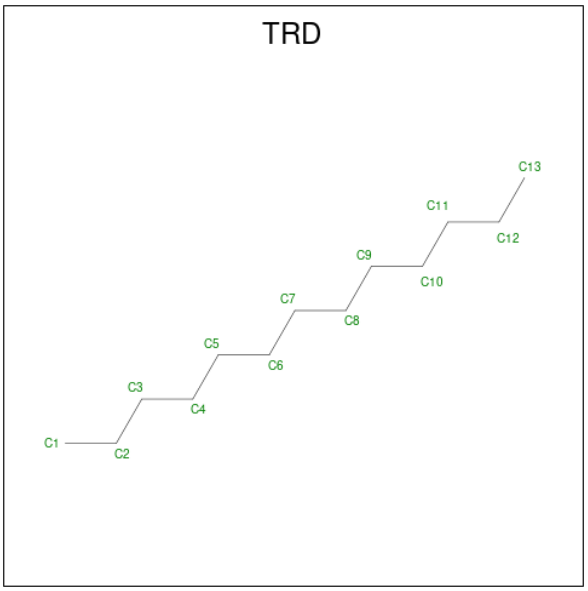
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	E	2	Total C O 23 12 11	0	0	0
3	F	2	Total C O 23 12 11	0	0	0
3	G	2	Total C O 23 12 11	0	0	0

- Molecule 4 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

- Molecule 5 is TRIDECANE (three-letter code: TRD) (formula: $C_{13}H_{28}$).



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	A	1	Total Cu 1 1	0	0
6	B	2	Total Cu 2 2	0	0
6	C	1	Total Cu 1 1	0	0
6	D	2	Total Cu 2 2	0	0

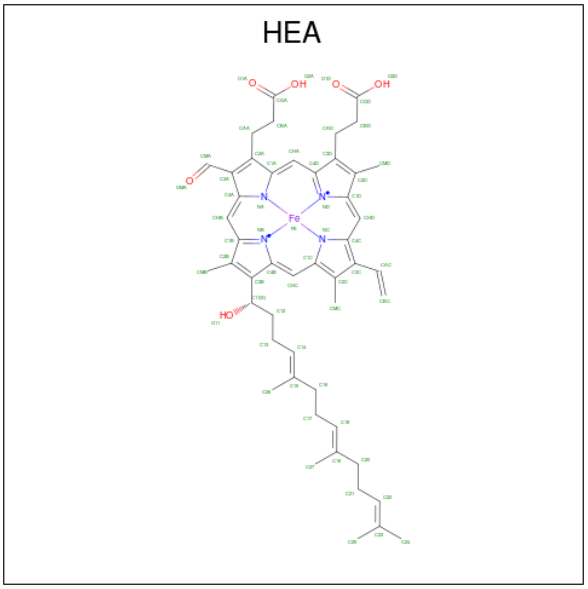
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 9 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

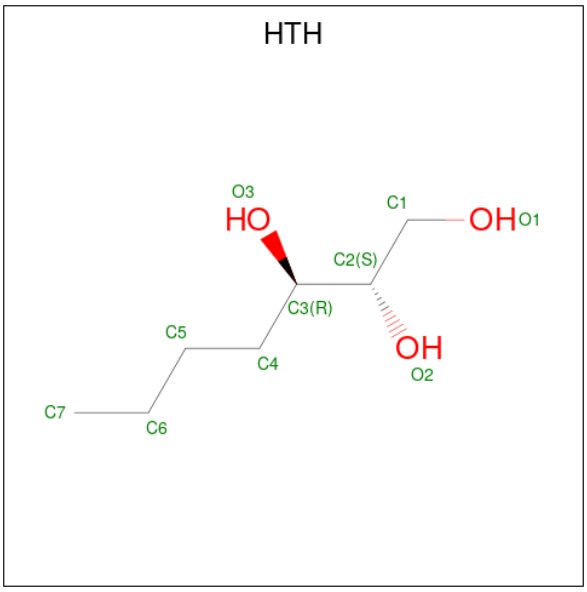


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
9	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
9	C	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
9	C	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

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

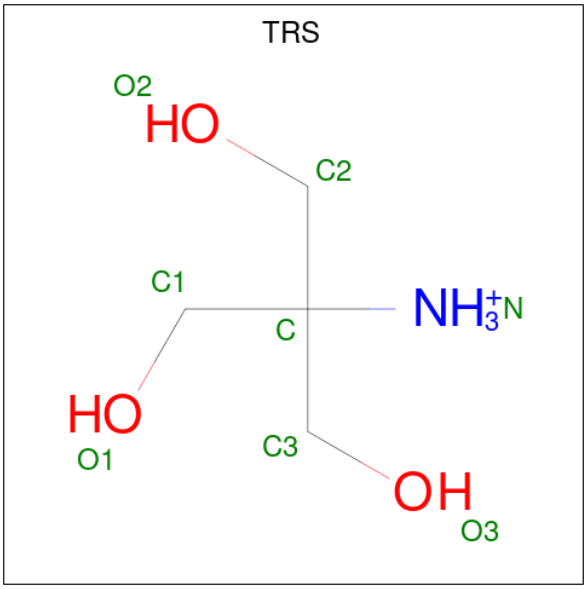
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Cd	0	0
			1	1		
10	D	1	Total	Cd	0	0
			1	1		

- Molecule 11 is (2S,3R)-heptane-1,2,3-triol (three-letter code: HTH) (formula: $C_7H_{16}O_3$).



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 8 4 1 3	0	0

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

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

- Molecule 14 is water.

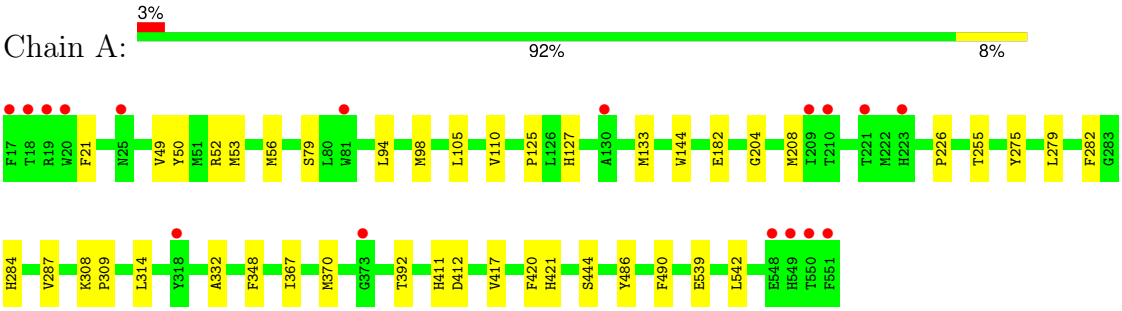
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	94	Total O 94 94	0	0
14	B	69	Total O 69 69	0	0
14	C	37	Total O 37 37	0	0
14	D	42	Total O 42 42	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

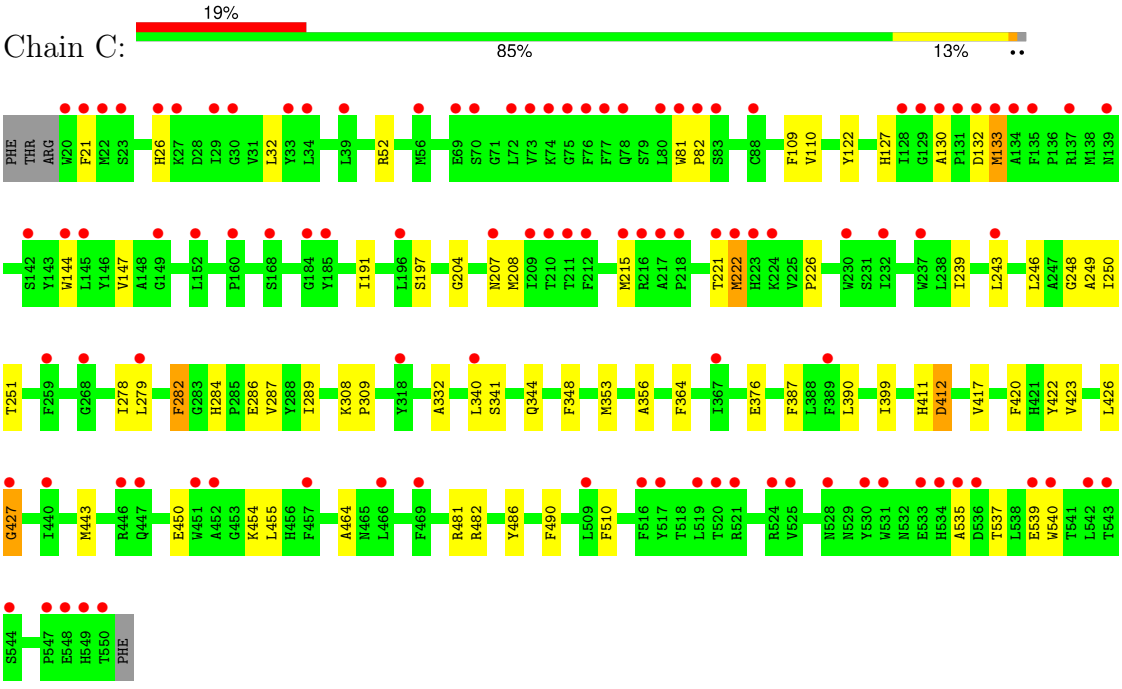
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



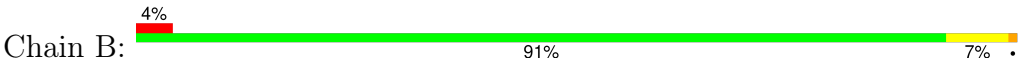
• Molecule 1: Cytochrome c oxidase subunit 1

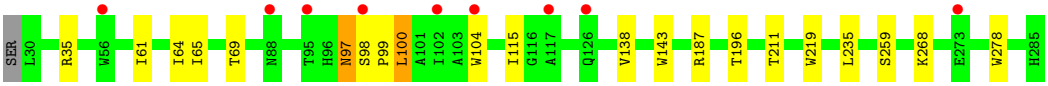
Chain C:



• Molecule 2: Cytochrome c oxidase subunit 2

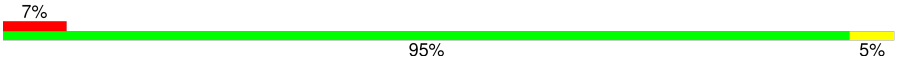
Chain B:

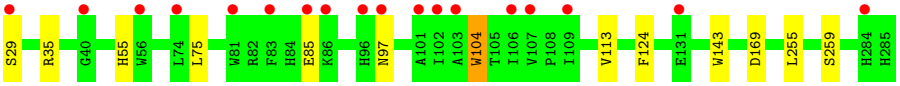




- Molecule 2: Cytochrome c oxidase subunit 2

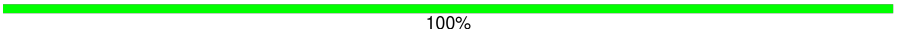
Chain D:





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

Chain E:

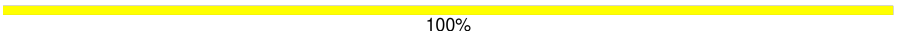


- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:

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

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	124.92Å 130.97Å 177.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.09 – 2.40 42.09 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.09-2.40) 92.5 (42.09-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.89 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.199 , 0.234 0.200 , 0.232	Depositor DCC
R_{free} test set	3467 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

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.

The worst 5 of 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

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%)	44	59
2	B	254/257 (99%)	246 (97%)	7 (3%)	1 (0%)	30	44
2	D	255/257 (99%)	246 (96%)	9 (4%)	0	100	100
All	All	1571/1584 (99%)	1524 (97%)	45 (3%)	2 (0%)	48	65

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	424/435 (98%)	421 (99%)	3 (1%)	81	91
1	C	414/435 (95%)	408 (99%)	6 (1%)	62	79
2	B	212/215 (99%)	208 (98%)	4 (2%)	52	72
2	D	208/215 (97%)	204 (98%)	4 (2%)	52	72
All	All	1258/1300 (97%)	1241 (99%)	17 (1%)	62	79

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	35	ARG
2	D	104	TRP
1	C	52	ARG
1	C	133	MET
1	C	222	MET

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	0.50	0	17,17,17	0.45	0
3	GLC	E	2	3	11,11,12	0.58	0	15,15,17	0.56	0
3	GLC	F	1	3	12,12,12	0.50	0	17,17,17	0.47	0
3	GLC	F	2	3	11,11,12	0.55	0	15,15,17	0.82	1 (6%)
3	GLC	G	1	3	12,12,12	0.53	0	17,17,17	0.51	0
3	GLC	G	2	3	11,11,12	0.54	0	15,15,17	0.91	1 (6%)

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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	2	GLC	C1-O5-C5	2.78	115.91	112.19
3	F	2	GLC	C1-O5-C5	2.57	115.63	112.19

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

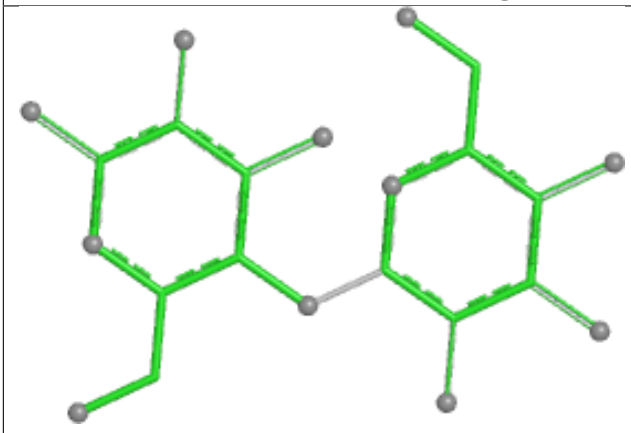
There are no ring outliers.

2 monomers are involved in 2 short contacts:

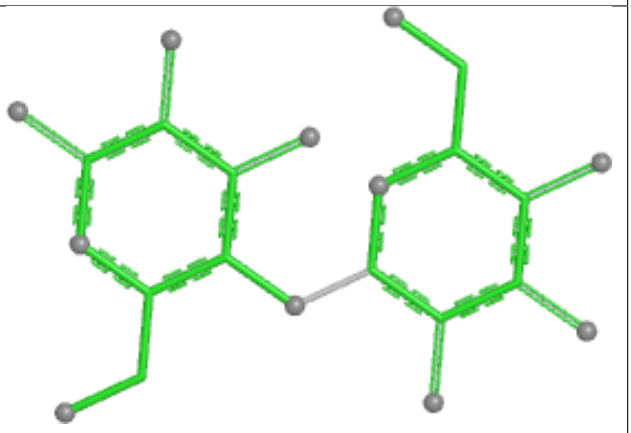
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	GLC	1	0
3	F	2	GLC	1	0

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

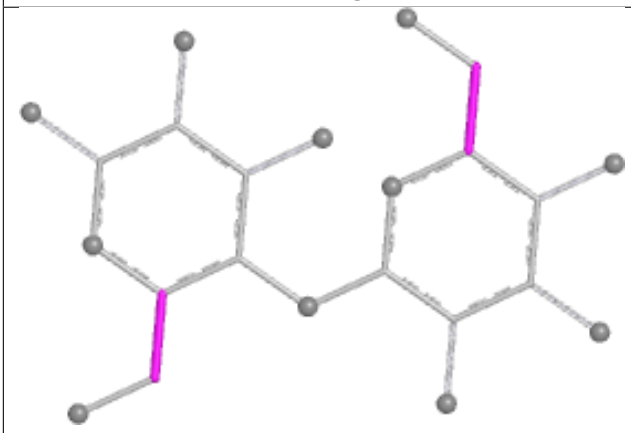
Oligosaccharide Chain E



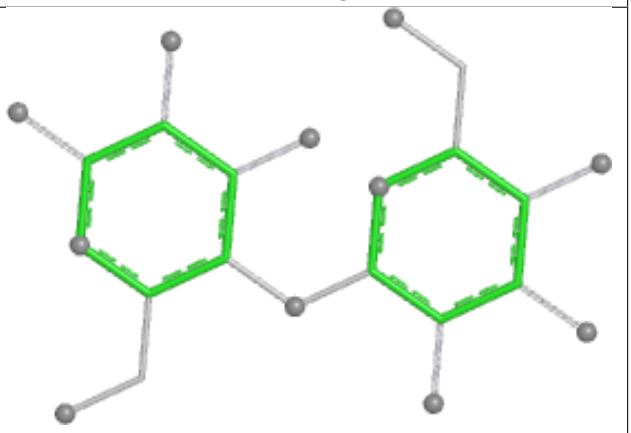
Bond lengths



Bond angles

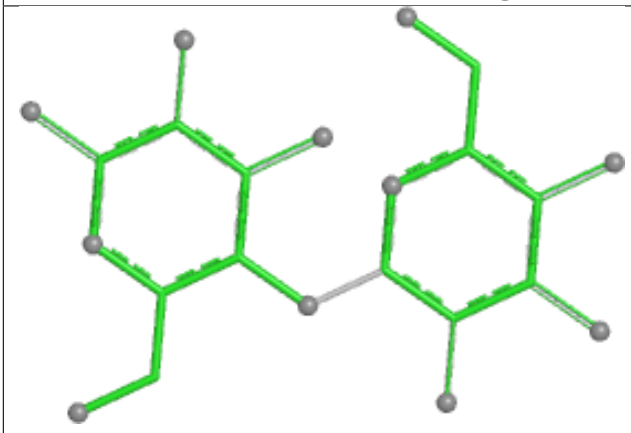


Torsions

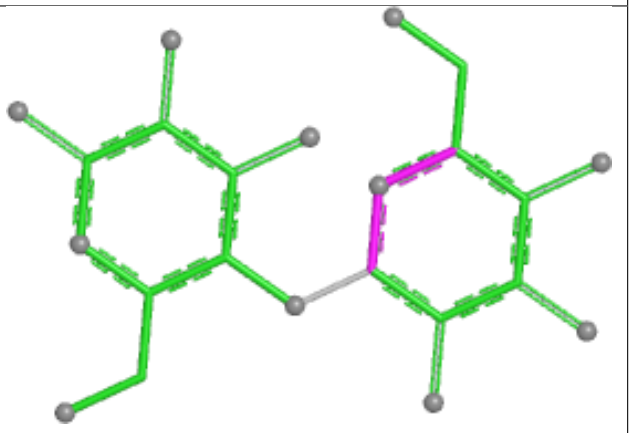


Rings

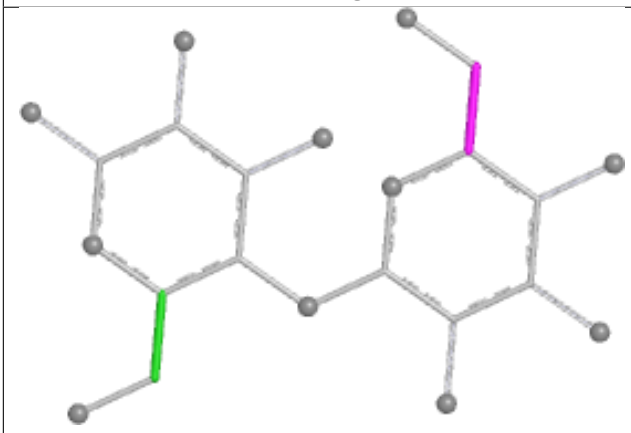
Oligosaccharide Chain F



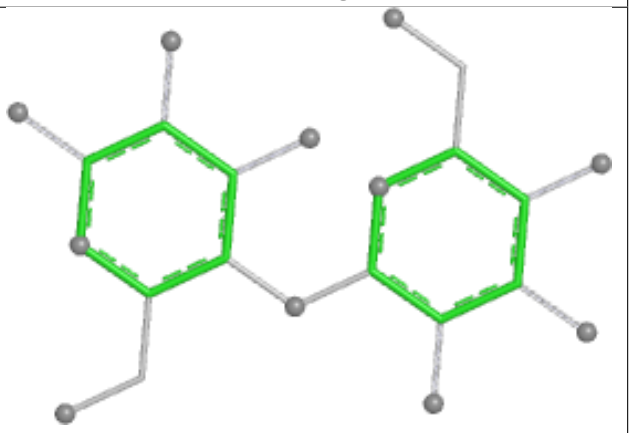
Bond lengths



Bond angles

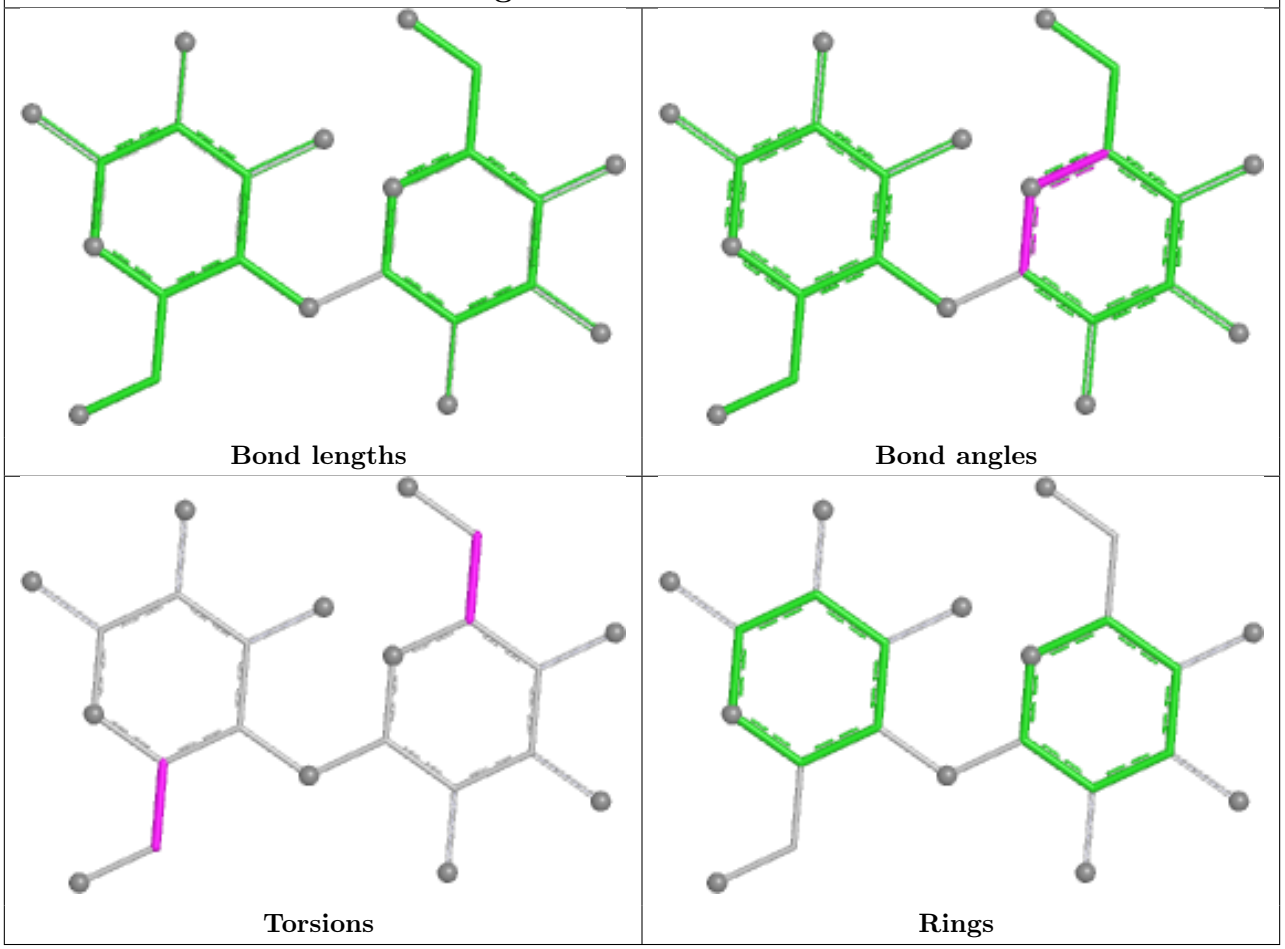


Torsions



Rings

Oligosaccharide Chain G



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	$\#\|Z\| > 2$
4	DMU	A	605	-	34,34,34	1.89	11 (32%)	45,45,45	1.32	6 (13%)
9	HEA	C	605	1	58,67,67	1.98	15 (25%)	63,103,103	2.65	27 (42%)
5	TRD	A	610	-	6,6,12	0.15	0	5,5,11	0.55	0
12	TRS	B	311	13	7,7,7	0.51	0	9,9,9	0.66	0
5	TRD	B	301	-	12,12,12	0.09	0	11,11,11	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	DMU	A	603	-	34,34,34	1.91	12 (35%)	45,45,45	1.24	5 (11%)
4	DMU	A	602	-	34,34,34	1.91	10 (29%)	45,45,45	1.06	3 (6%)
5	TRD	A	606	-	12,12,12	0.10	0	11,11,11	0.81	0
5	TRD	A	611	-	12,12,12	0.09	0	11,11,11	0.86	0
4	DMU	A	601	-	34,34,34	1.95	12 (35%)	45,45,45	1.08	1 (2%)
4	DMU	D	301	-	31,31,34	2.01	12 (38%)	42,42,45	1.09	2 (4%)
5	TRD	A	612	-	12,12,12	0.09	0	11,11,11	0.83	0
9	HEA	C	606	1,14	58,67,67	2.24	21 (36%)	63,103,103	2.41	26 (41%)
5	TRD	C	601	-	12,12,12	0.18	0	11,11,11	0.54	0
5	TRD	B	303	-	12,12,12	0.10	0	11,11,11	0.81	0
5	TRD	D	302	-	12,12,12	0.10	0	11,11,11	0.82	0
5	TRD	A	609	-	12,12,12	0.10	0	11,11,11	0.77	0
9	HEA	A	618	1,14	58,67,67	1.97	15 (25%)	63,103,103	2.50	26 (41%)
9	HEA	A	617	1	58,67,67	2.04	15 (25%)	63,103,103	2.85	30 (47%)
5	TRD	A	607	-	12,12,12	0.10	0	11,11,11	0.85	0
5	TRD	A	613	-	12,12,12	0.10	0	11,11,11	0.79	0
11	HTH	B	309	-	9,9,9	0.56	0	10,10,10	1.28	1 (10%)
11	HTH	B	308	-	9,9,9	0.45	0	10,10,10	1.31	1 (10%)
5	TRD	A	608	-	12,12,12	0.11	0	11,11,11	0.78	0
11	HTH	B	310	-	9,9,9	0.52	0	10,10,10	1.17	1 (10%)
5	TRD	B	302	-	12,12,12	0.14	0	11,11,11	0.57	0
4	DMU	A	604	-	34,34,34	1.95	11 (32%)	45,45,45	1.16	5 (11%)
5	TRD	D	303	-	8,8,12	0.10	0	7,7,11	0.77	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
4	DMU	A	605	-	-	6/19/59/59	0/2/2/2
9	HEA	C	605	1	-	6/32/76/76	-
5	TRD	A	610	-	-	1/4/4/10	-
12	TRS	B	311	13	-	6/9/9/9	-
5	TRD	B	301	-	-	2/10/10/10	-
4	DMU	A	603	-	-	8/19/59/59	0/2/2/2
4	DMU	A	602	-	-	3/19/59/59	0/2/2/2
5	TRD	A	606	-	-	0/10/10/10	-
5	TRD	A	611	-	-	3/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMU	A	601	-	-	9/19/59/59	0/2/2/2
4	DMU	D	301	-	-	8/16/56/59	0/2/2/2
5	TRD	A	612	-	-	4/10/10/10	-
9	HEA	C	606	1,14	-	7/32/76/76	-
5	TRD	C	601	-	-	4/10/10/10	-
5	TRD	B	303	-	-	4/10/10/10	-
5	TRD	D	302	-	-	3/10/10/10	-
5	TRD	A	609	-	-	3/10/10/10	-
9	HEA	A	618	1,14	-	6/32/76/76	-
9	HEA	A	617	1	-	7/32/76/76	-
5	TRD	A	607	-	-	0/10/10/10	-
5	TRD	A	613	-	-	5/10/10/10	-
11	HTH	B	309	-	-	7/10/10/10	-
11	HTH	B	308	-	-	7/10/10/10	-
5	TRD	A	608	-	-	1/10/10/10	-
11	HTH	B	310	-	-	7/10/10/10	-
5	TRD	B	302	-	-	5/10/10/10	-
4	DMU	A	604	-	-	11/19/59/59	0/2/2/2
5	TRD	D	303	-	-	3/6/6/10	-

The worst 5 of 134 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	606	HEA	C3A-C2A	5.56	1.47	1.40
9	C	606	HEA	CHD-C1D	5.40	1.47	1.34
9	C	606	HEA	C3B-C2B	5.31	1.46	1.34
9	C	606	HEA	CHC-C4B	5.23	1.47	1.34
9	C	606	HEA	C3A-C4A	5.22	1.49	1.41

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	617	HEA	C3D-C4D-ND	9.24	119.28	110.35
9	C	605	HEA	C3D-C4D-ND	7.56	117.66	110.35
9	A	618	HEA	C3D-C4D-ND	7.43	117.53	110.35
9	C	605	HEA	C3B-C4B-NB	6.45	117.26	109.84
9	C	606	HEA	C3D-C4D-ND	6.31	116.45	110.35

There are no chirality outliers.

5 of 136 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604	DMU	C19-C18-O16-C6
9	A	617	HEA	C19-C20-C21-C22
11	B	308	HTH	O1-C1-C2-C3
11	B	308	HTH	C1-C2-C3-O3
11	B	308	HTH	O2-C2-C3-C4

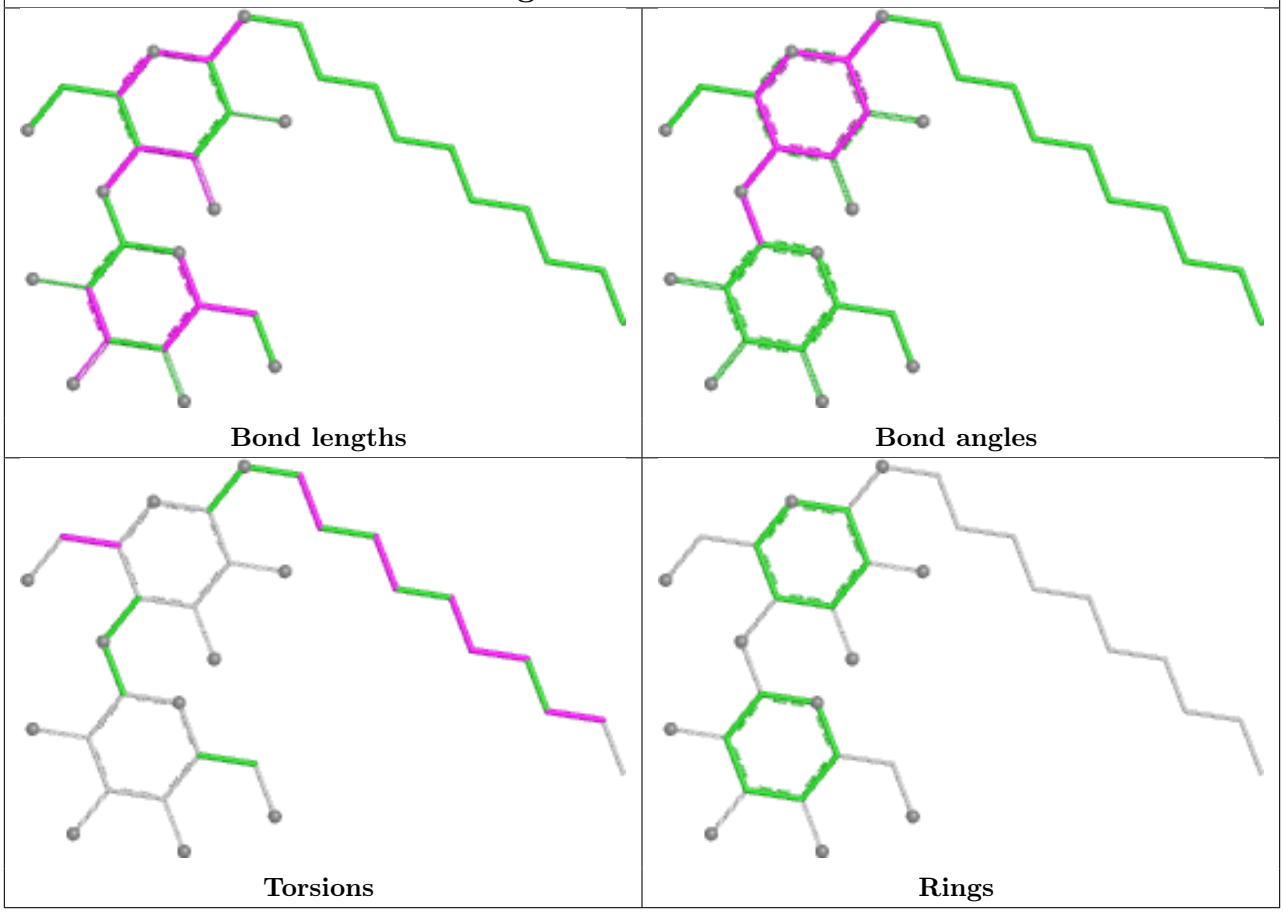
There are no ring outliers.

13 monomers are involved in 29 short contacts:

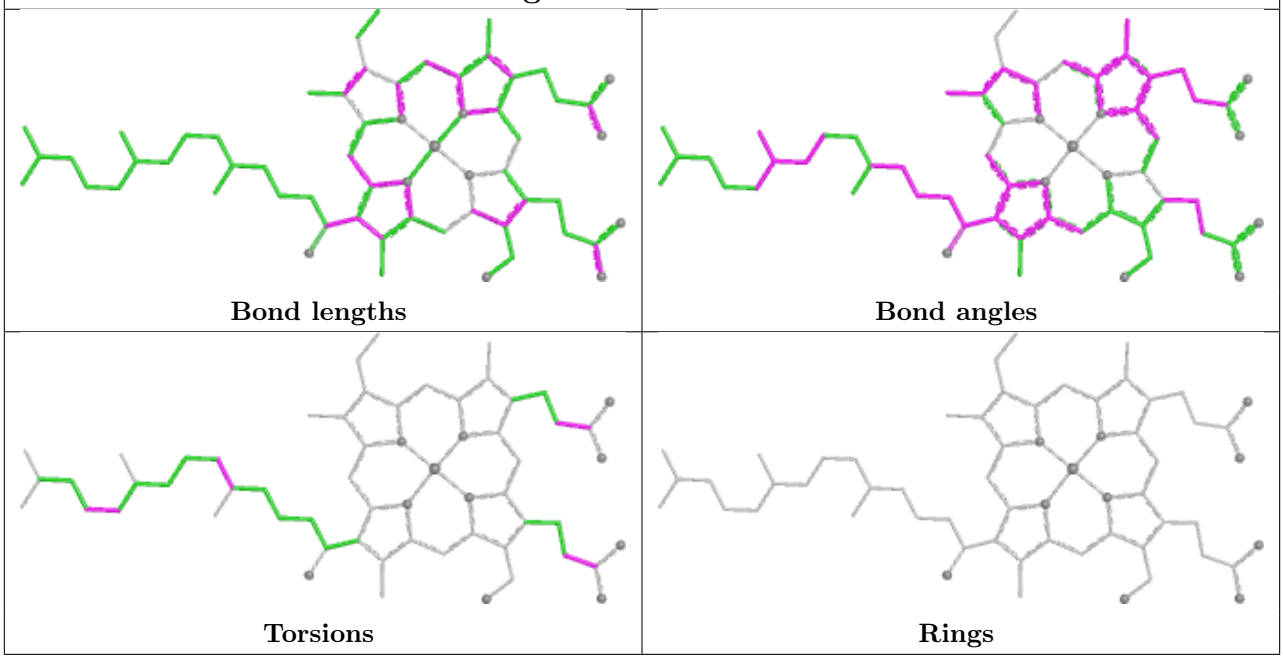
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	605	HEA	3	0
5	A	606	TRD	1	0
4	A	601	DMU	1	0
4	D	301	DMU	1	0
5	A	612	TRD	2	0
9	C	606	HEA	4	0
9	A	618	HEA	8	0
9	A	617	HEA	1	0
5	A	607	TRD	1	0
11	B	310	HTH	1	0
5	B	302	TRD	3	0
4	A	604	DMU	3	0
5	D	303	TRD	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

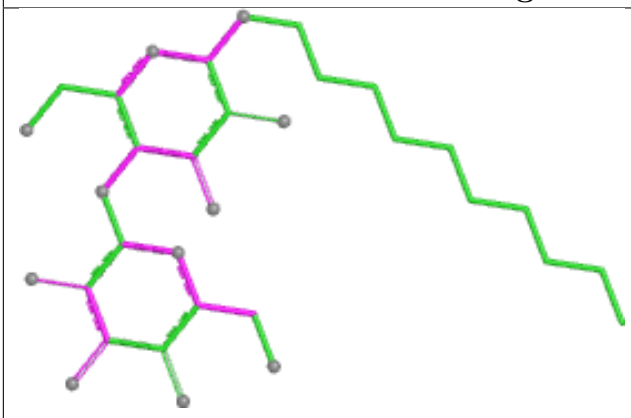
Ligand DMU A 605



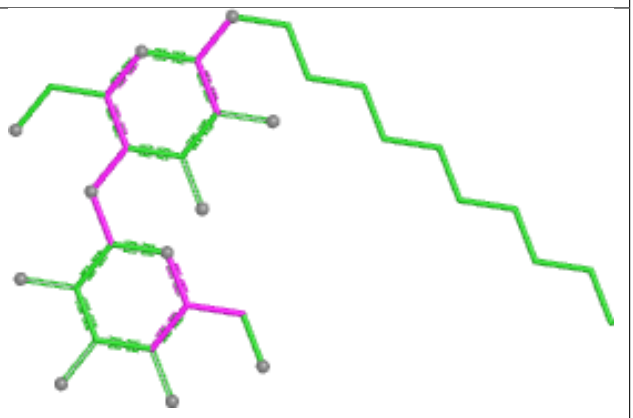
Ligand HEA C 605



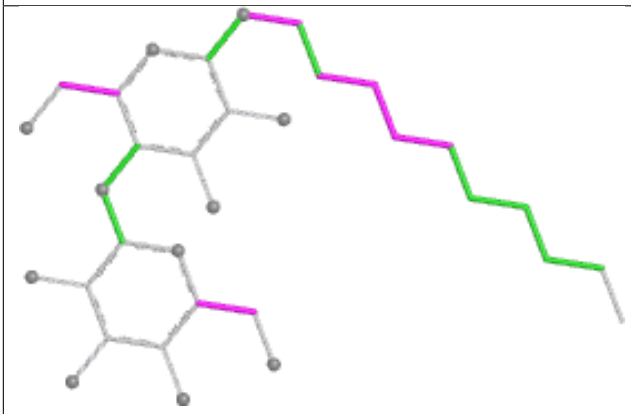
Ligand DMU A 603



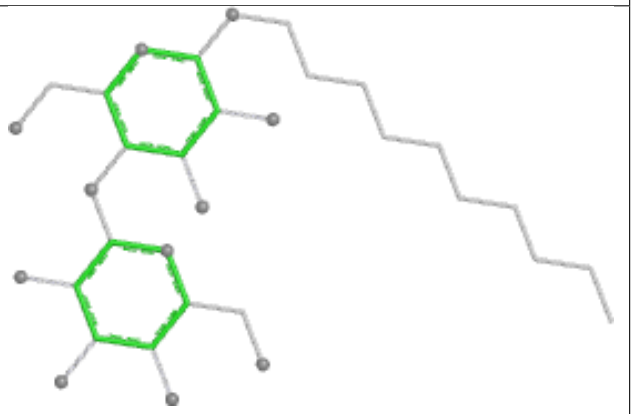
Bond lengths



Bond angles

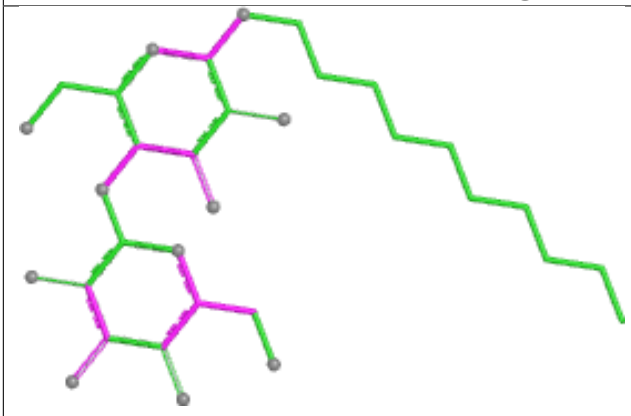


Torsions

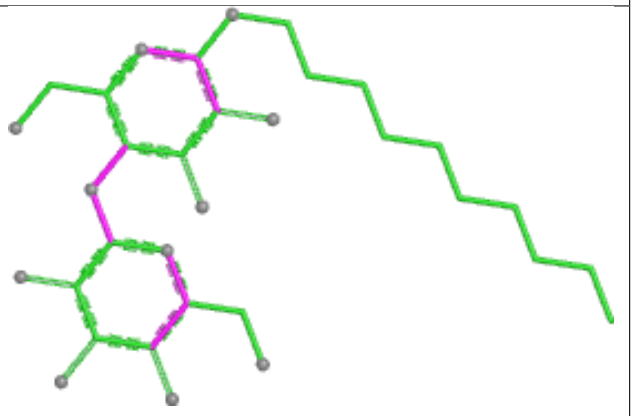


Rings

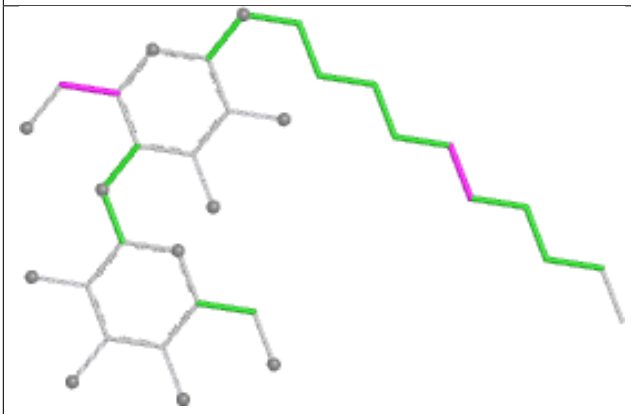
Ligand DMU A 602



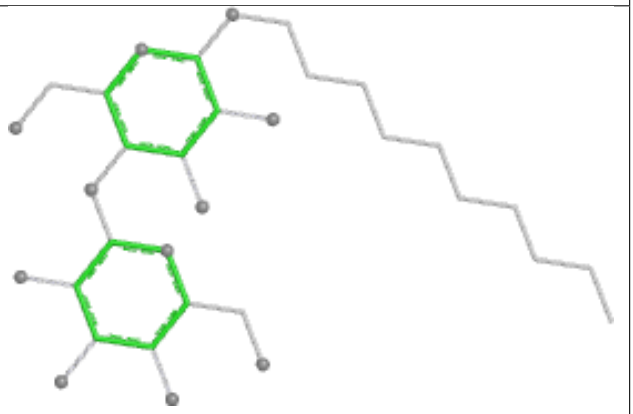
Bond lengths



Bond angles

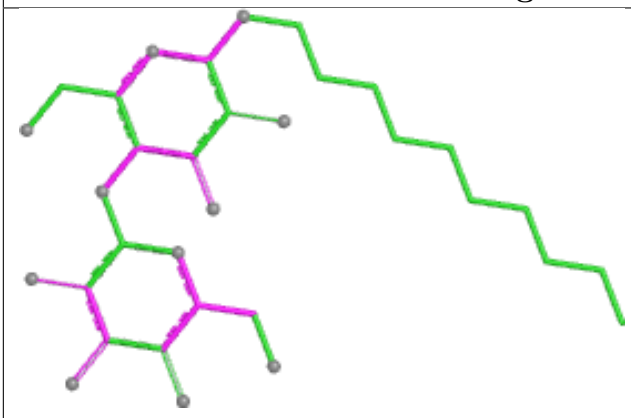


Torsions

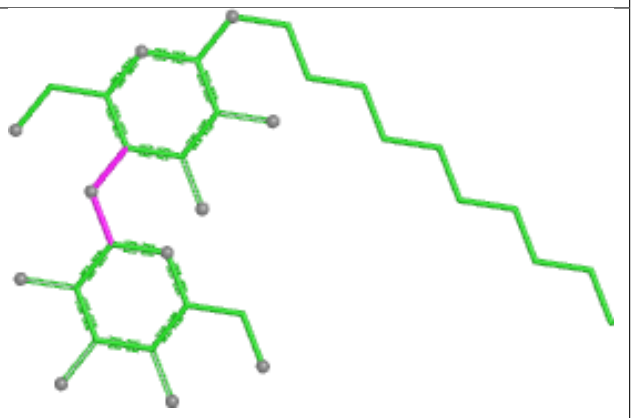


Rings

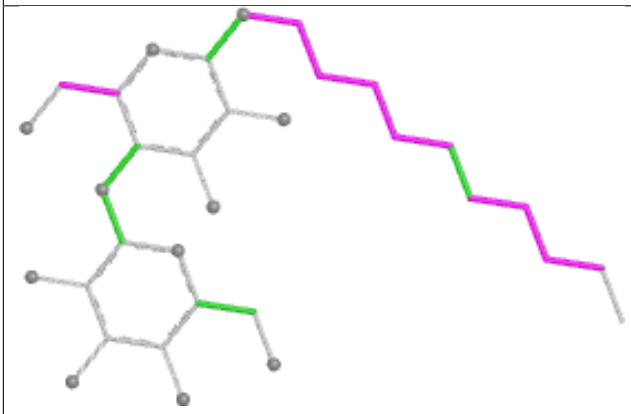
Ligand DMU A 601



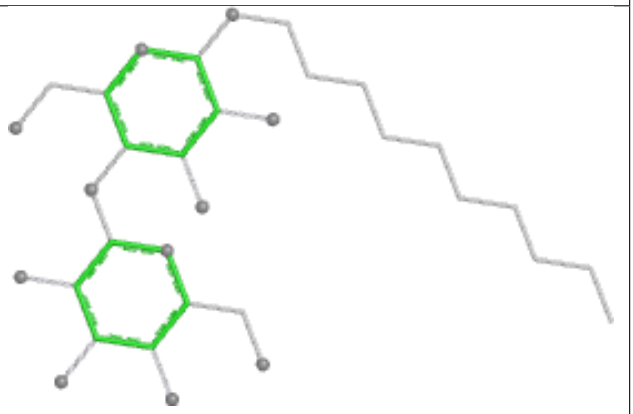
Bond lengths



Bond angles

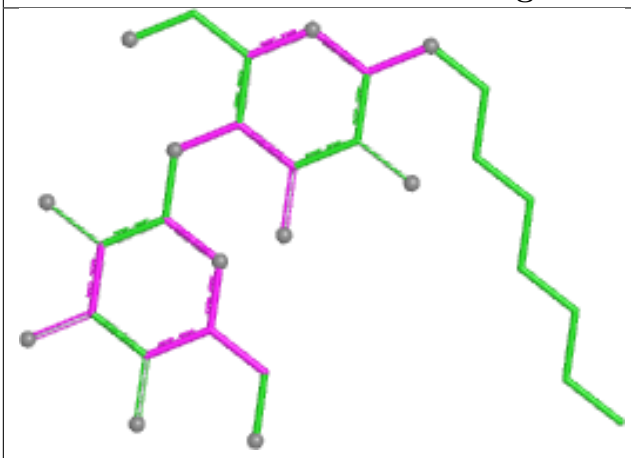


Torsions

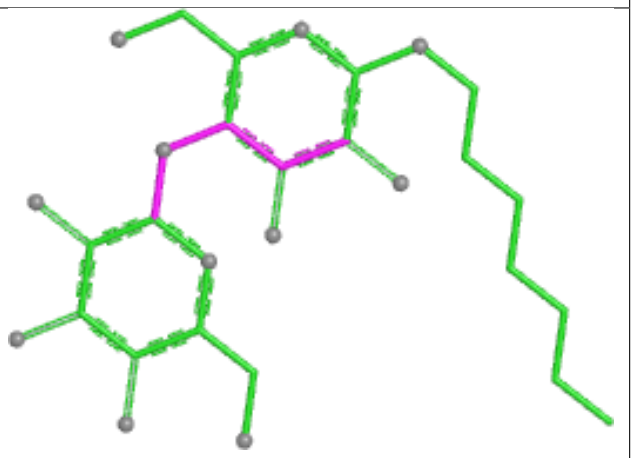


Rings

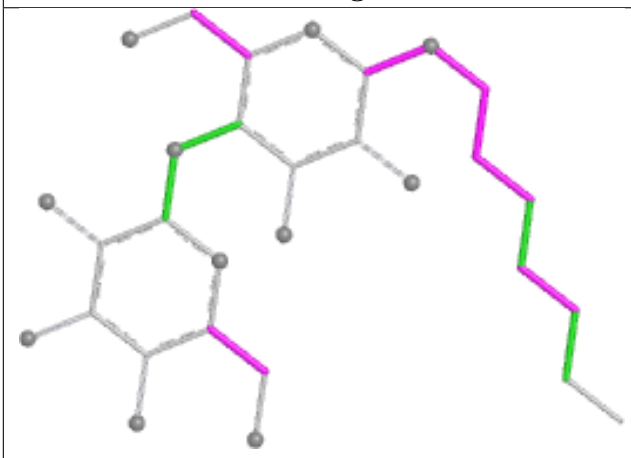
Ligand DMU D 301



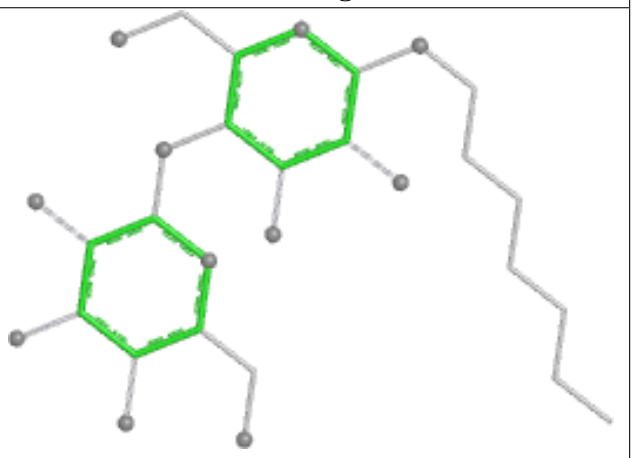
Bond lengths



Bond angles

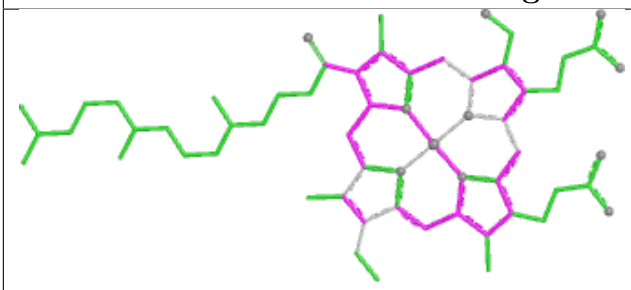


Torsions

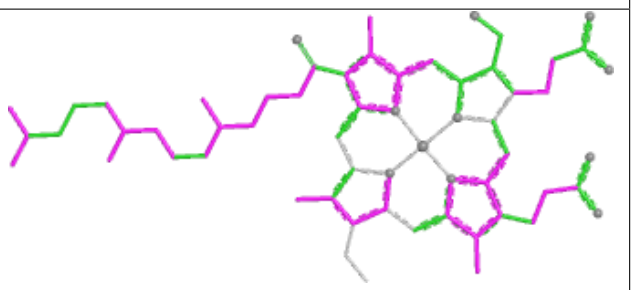


Rings

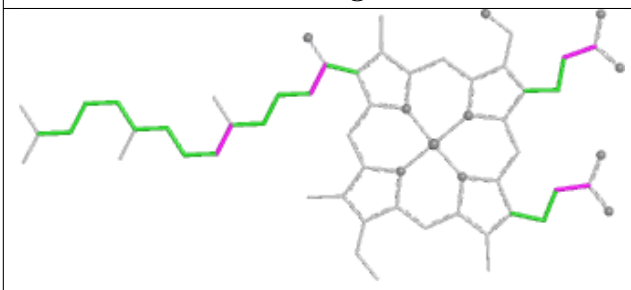
Ligand HEA C 606



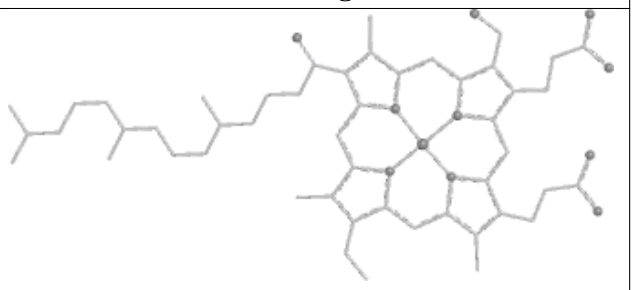
Bond lengths



Bond angles

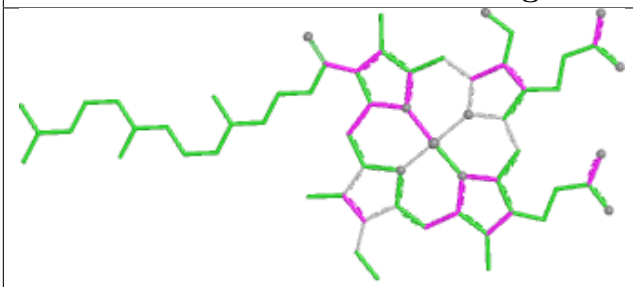


Torsions

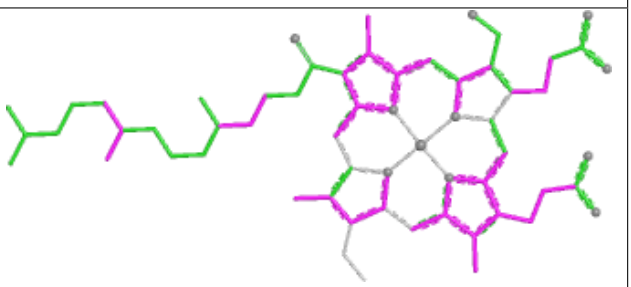


Rings

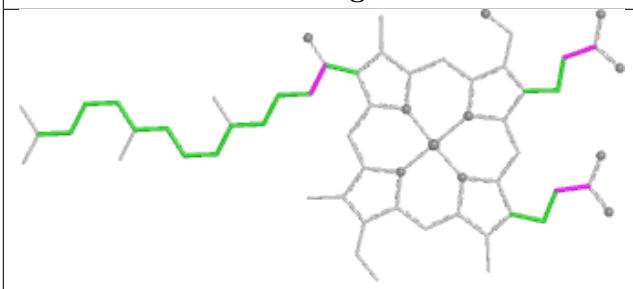
Ligand HEA A 618



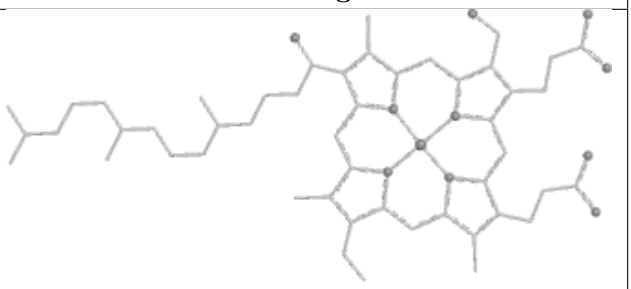
Bond lengths



Bond angles

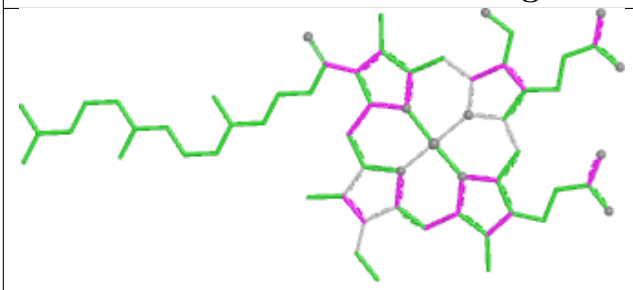


Torsions

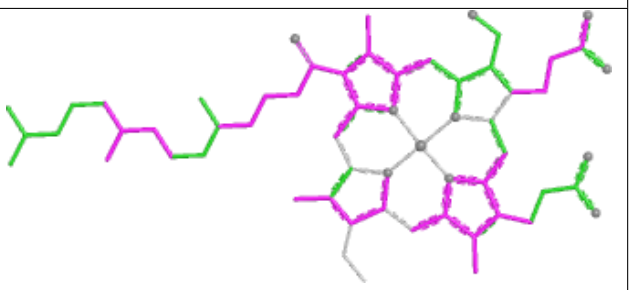


Rings

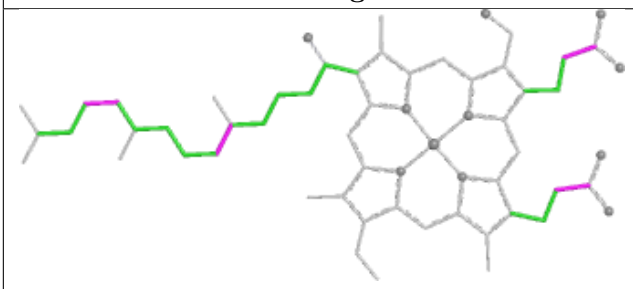
Ligand HEA A 617



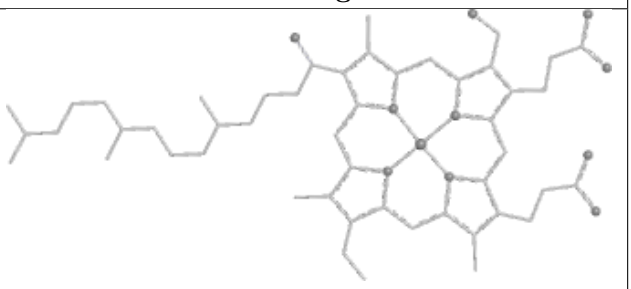
Bond lengths



Bond angles

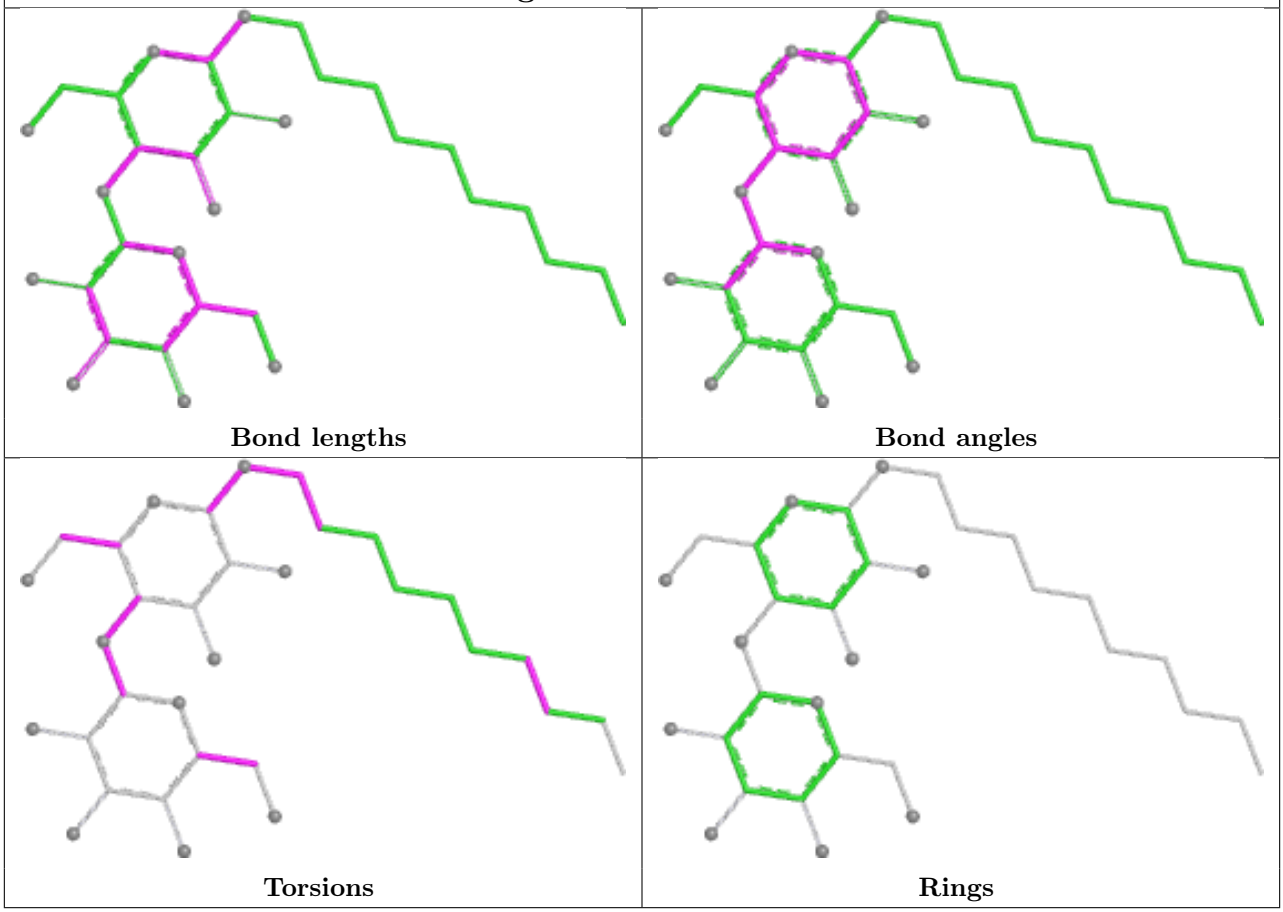


Torsions



Rings

Ligand DMU A 604



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^{th} 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	535/535 (100%)	0.22	17 (3%) 50 47	37, 54, 83, 115	0
1	C	531/535 (99%)	1.15	103 (19%) 4 3	51, 77, 108, 130	0
2	B	256/257 (99%)	0.23	9 (3%) 47 44	38, 58, 81, 89	0
2	D	257/257 (100%)	0.53	18 (7%) 24 22	45, 66, 96, 116	0
All	All	1579/1584 (99%)	0.59	147 (9%) 16 14	37, 64, 99, 130	0

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	TRP	6.2
1	C	548	GLU	6.2
1	C	549	HIS	5.3
1	C	69	GLU	4.8
1	C	517	TYR	4.7

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

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

6.3 Carbohydrates

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	G	2	11/12	0.70	0.14	130,136,140,142	0
3	GLC	G	1	12/12	0.73	0.14	116,126,136,136	0

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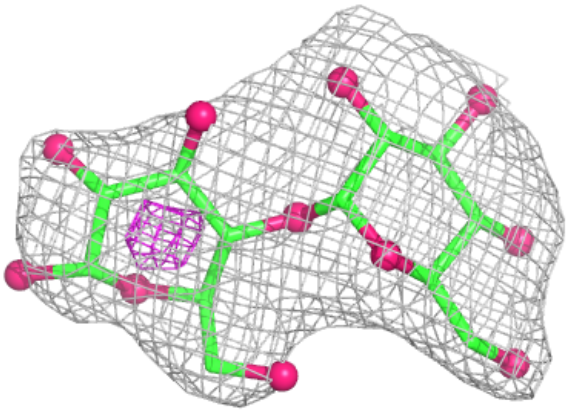
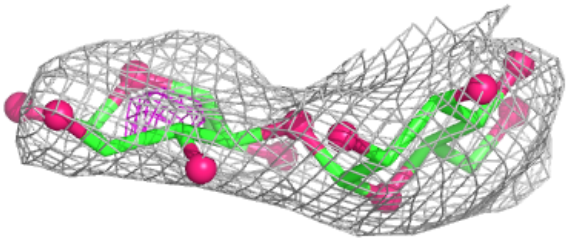
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	F	2	11/12	0.76	0.16	96,105,110,112	0
3	GLC	F	1	12/12	0.77	0.12	110,114,120,121	0
3	GLC	E	1	12/12	0.80	0.15	97,111,118,119	0
3	GLC	E	2	11/12	0.83	0.13	87,98,107,107	0

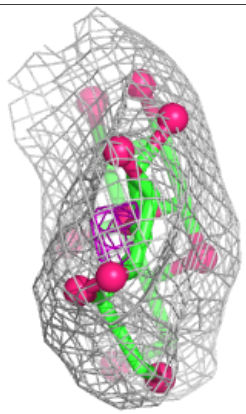
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

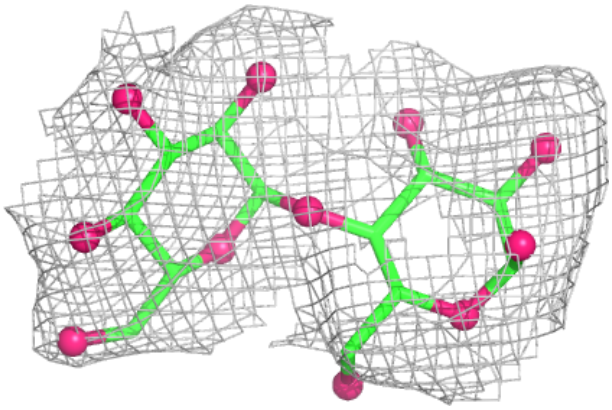


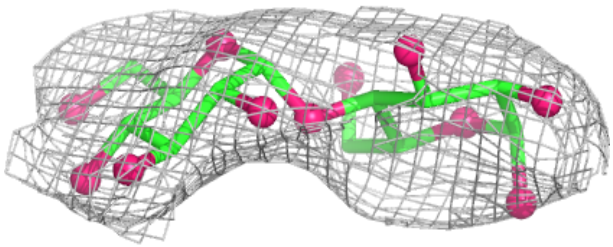


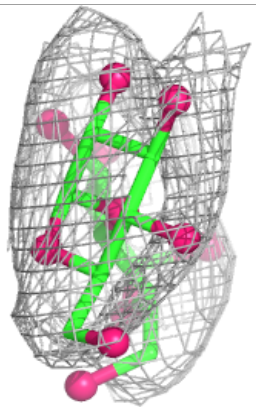


Electron density around Chain F:

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

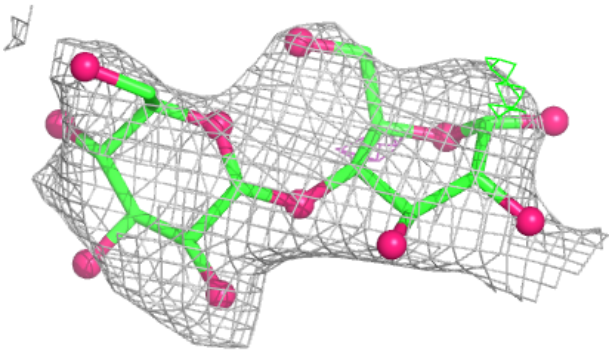


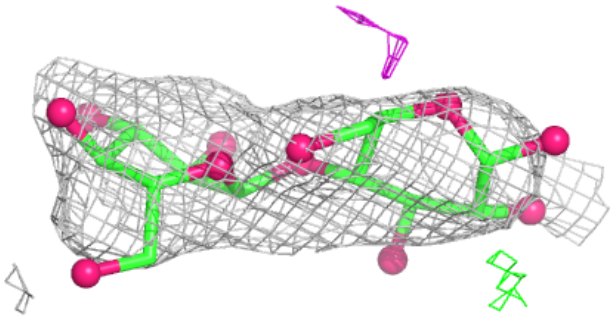


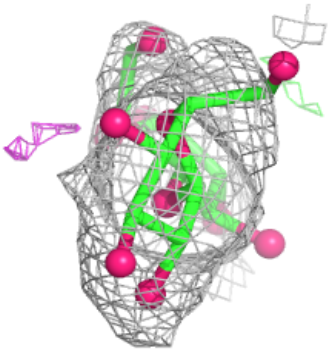


Electron density around Chain G:

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







6.4 Ligands (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^{th} 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
5	TRD	C	601	13/13	0.54	0.42	88,112,125,125	0
11	HTH	B	310	10/10	0.58	0.27	77,105,110,114	0
5	TRD	B	302	13/13	0.64	0.26	52,68,83,84	0
5	TRD	A	607	13/13	0.66	0.29	65,77,84,91	0
5	TRD	A	609	13/13	0.68	0.30	64,74,83,91	0
5	TRD	A	611	13/13	0.72	0.30	67,77,88,91	0
5	TRD	A	608	13/13	0.74	0.28	63,70,88,93	0
5	TRD	A	613	13/13	0.75	0.22	62,69,82,87	0
5	TRD	B	301	13/13	0.76	0.26	74,86,93,99	0
5	TRD	D	302	13/13	0.78	0.25	61,72,85,87	0
5	TRD	A	606	13/13	0.78	0.21	72,76,88,90	0
5	TRD	B	303	13/13	0.80	0.26	55,65,78,79	0
11	HTH	B	309	10/10	0.81	0.22	76,85,99,104	0
12	TRS	B	311	8/8	0.81	0.15	63,91,103,104	0
4	DMU	A	604	33/33	0.82	0.17	46,68,79,83	33
5	TRD	A	610	7/13	0.82	0.26	58,69,74,78	0
4	DMU	A	601	33/33	0.83	0.15	53,88,122,126	0
13	K	B	312	1/1	0.83	0.15	123,123,123,123	0
4	DMU	A	605	33/33	0.84	0.20	56,67,74,79	33
5	TRD	A	612	13/13	0.84	0.22	68,80,93,97	0
4	DMU	D	301	30/33	0.85	0.14	67,100,113,115	0
4	DMU	A	603	33/33	0.87	0.13	58,73,86,96	0
5	TRD	D	303	9/13	0.90	0.20	83,84,84,88	0
11	HTH	B	308	10/10	0.91	0.22	56,66,77,78	10
4	DMU	A	602	33/33	0.95	0.09	41,54,69,71	0
9	HEA	C	606	60/60	0.96	0.12	50,63,75,81	0
9	HEA	A	618	60/60	0.97	0.08	38,47,61,65	0
9	HEA	C	605	60/60	0.97	0.11	47,63,80,92	0
9	HEA	A	617	60/60	0.98	0.08	34,42,56,73	0
7	MG	C	602	1/1	0.99	0.09	46,46,46,46	0
10	CD	B	305	1/1	0.99	0.07	63,63,63,63	0
10	CD	D	306	1/1	0.99	0.06	62,62,62,62	0
8	CA	A	616	1/1	0.99	0.05	44,44,44,44	0
8	CA	C	603	1/1	0.99	0.03	69,69,69,69	0
6	CU	A	614	1/1	0.99	0.05	51,51,51,51	0
6	CU	C	604	1/1	0.99	0.03	62,62,62,62	0
7	MG	A	615	1/1	0.99	0.09	37,37,37,37	0

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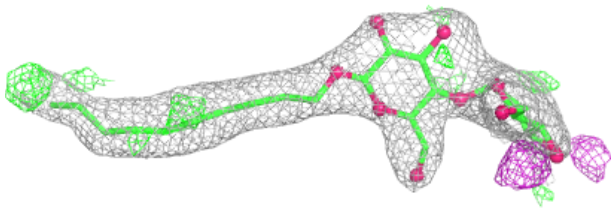
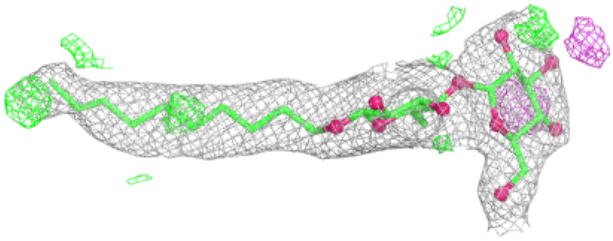
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CU	D	308	1/1	1.00	0.03	53,53,53,53	0
6	CU	B	307	1/1	1.00	0.02	41,41,41,41	0
6	CU	B	306	1/1	1.00	0.02	42,42,42,42	0
6	CU	D	307	1/1	1.00	0.04	51,51,51,51	0

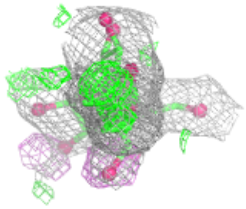
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

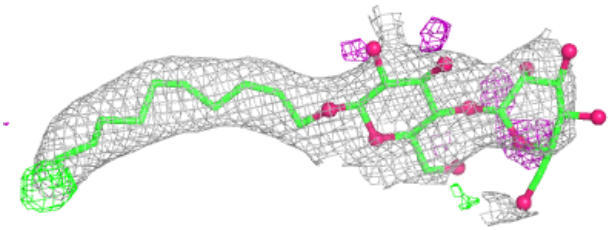


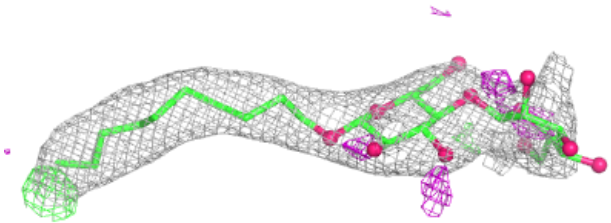


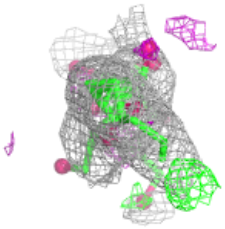


Electron density around DMU A 601:

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

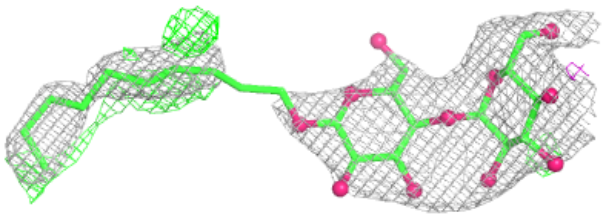


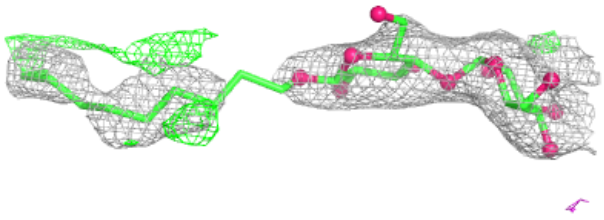


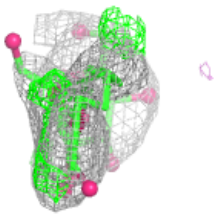


Electron density around DMU A 605:

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

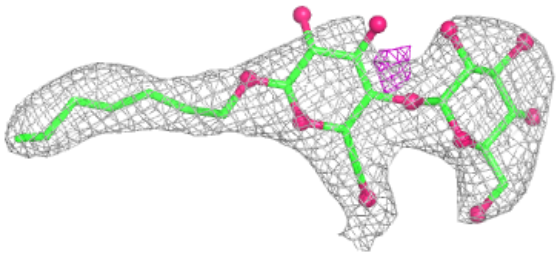


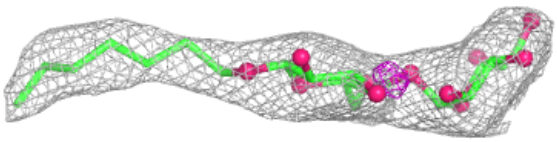


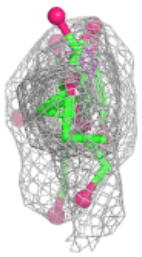


Electron density around DMU D 301:

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

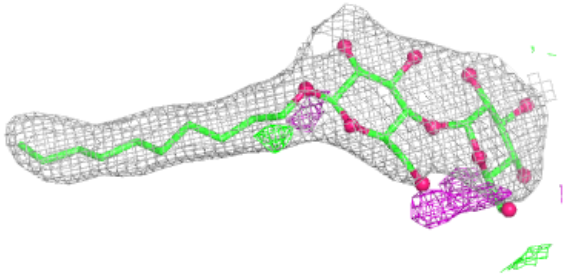


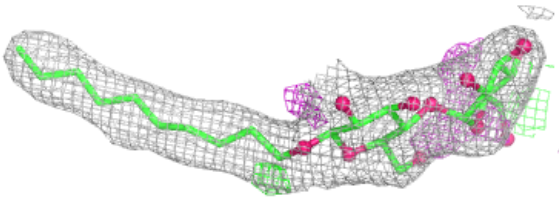


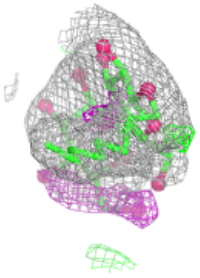


Electron density around DMU A 603:

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

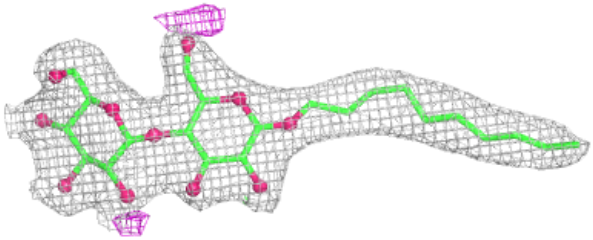


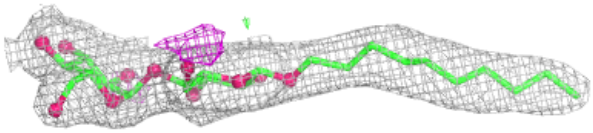




Electron density around DMU A 602:

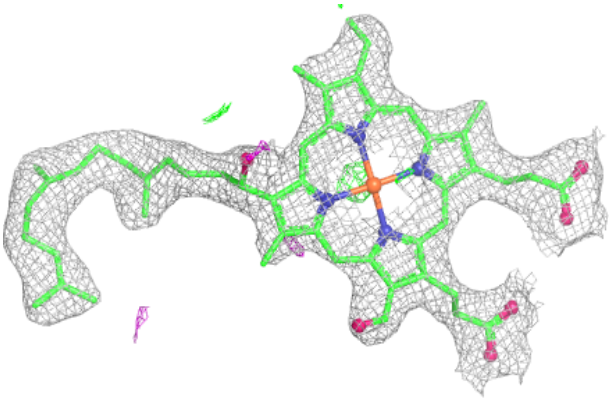
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

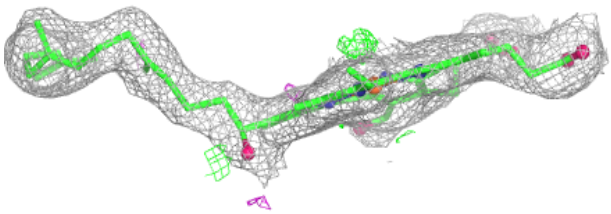


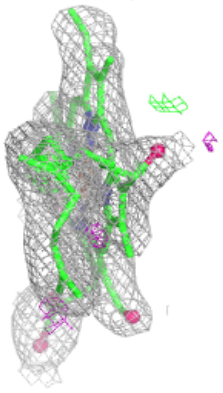


Electron density around HEA C 606:

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

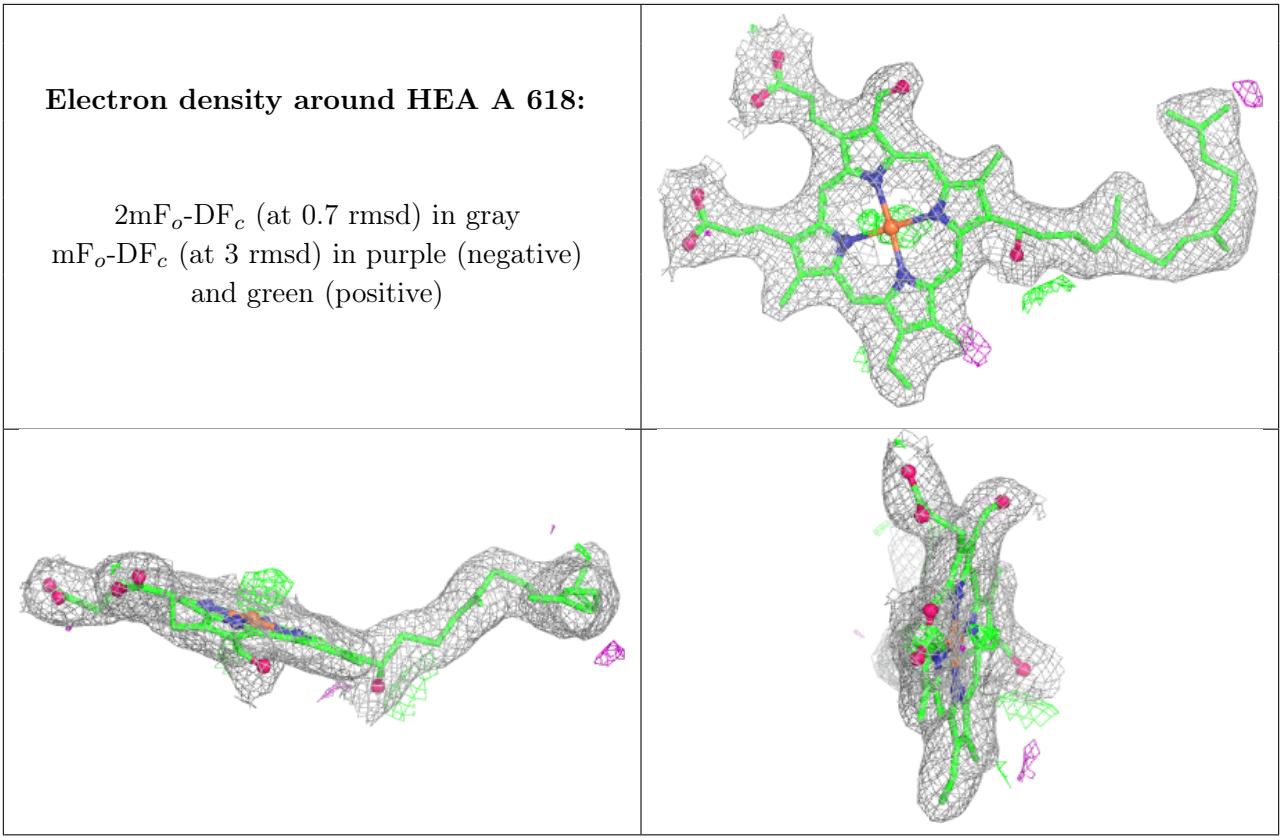






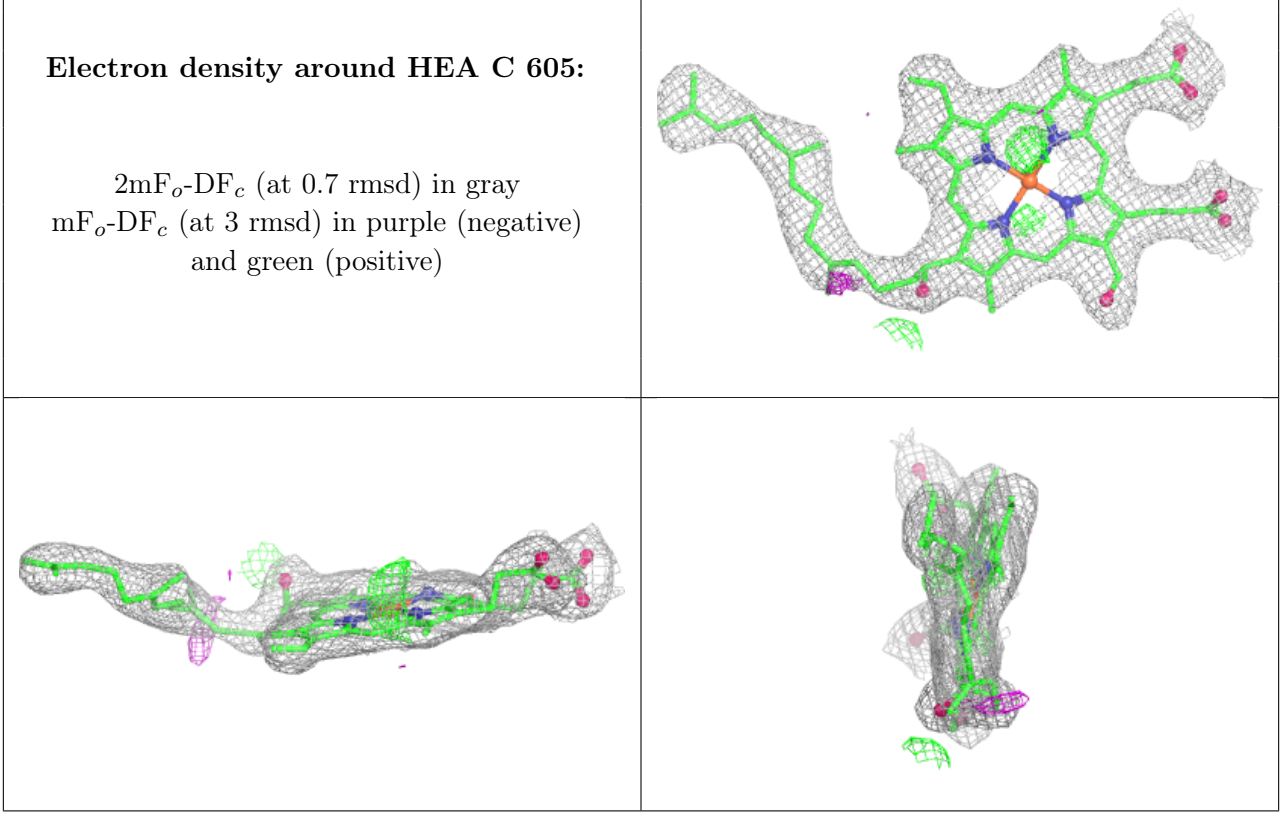
Electron density around HEA A 618:

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



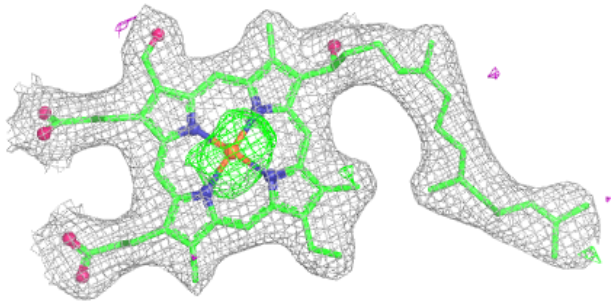
Electron density around HEA C 605:

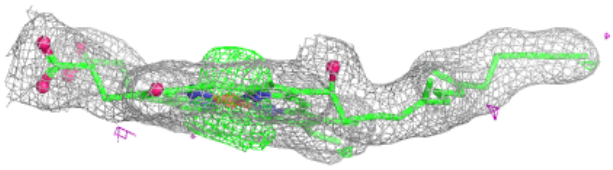
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

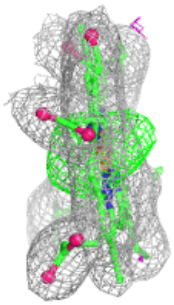


Electron density around HEA A 617:

$2mF_o$-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.