wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 04:35 AM EDT

PDB ID	:	6PW0
Title	:	Cytochrome C oxidase delta 6 mutant
Authors	:	Liu, J.; Ferguson-Miller, S.
Deposited on	:	2019-07-21
Resolution	:	2.50 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:

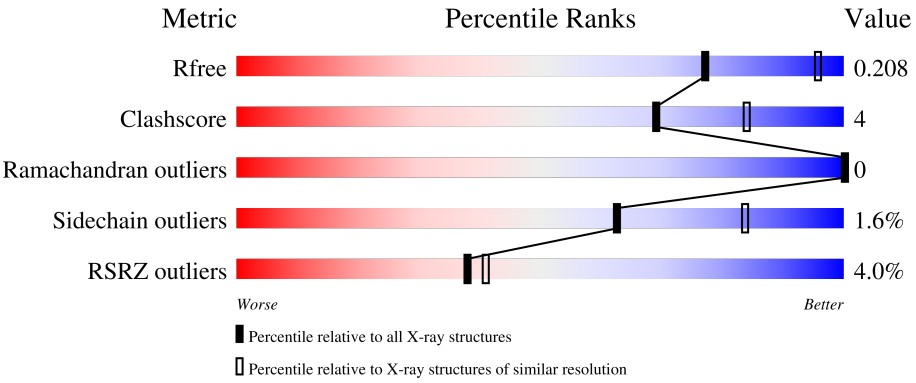
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	560	2% 87% 8% .
1	C	560	8% 85% 10% 5%
2	B	262	% 90% 7% . .
2	D	262	2% 90% 7% .
3	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	F	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	HEA	A	602	X	-	-	-
5	HEA	A	603	X	-	-	-
5	HEA	C	602	X	-	-	-
5	HEA	C	603	X	-	-	-
7	TRD	A	610	-	-	-	X
7	TRD	A	613	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 13540 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	2785	655	689	31			
1	C	531	Total	C	N	O	S	0	0	0
			4118	2761	645	682	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
			2018	1316	333	363	6			
2	D	256	Total	C	N	O	S	0	0	0
			1999	1305	326	362	6			

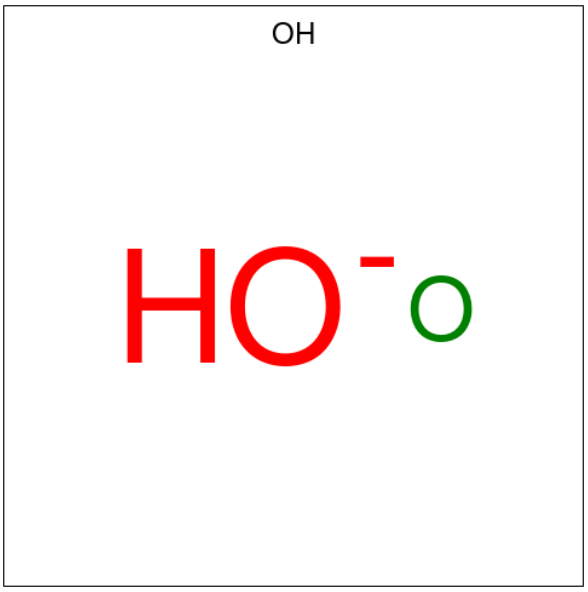
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	282	HIS	-	expression tag	UNP Q3J5G0
B	283	HIS	-	expression tag	UNP Q3J5G0
B	284	HIS	-	expression tag	UNP Q3J5G0
B	285	HIS	-	expression tag	UNP Q3J5G0
B	286	HIS	-	expression tag	UNP Q3J5G0
B	287	HIS	-	expression tag	UNP Q3J5G0
D	282	HIS	-	expression tag	UNP Q3J5G0
D	283	HIS	-	expression tag	UNP Q3J5G0
D	284	HIS	-	expression tag	UNP Q3J5G0
D	285	HIS	-	expression tag	UNP Q3J5G0
D	286	HIS	-	expression tag	UNP Q3J5G0
D	287	HIS	-	expression tag	UNP Q3J5G0

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

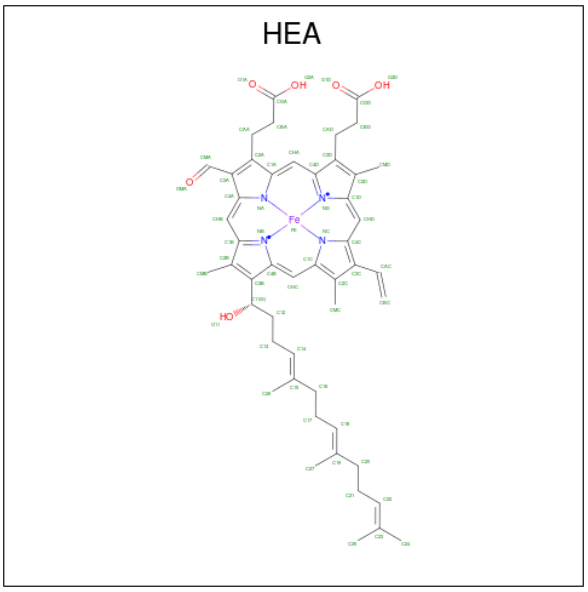
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	E	2	Total C O 23 12 11	0	0	0
3	F	2	Total C O 23 12 11	0	0	0

- Molecule 4 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



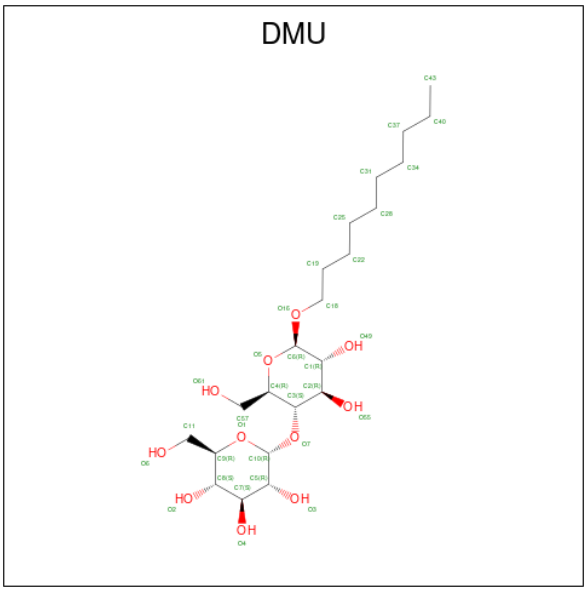
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	C	1	Total O 1 1	0	0

- Molecule 5 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



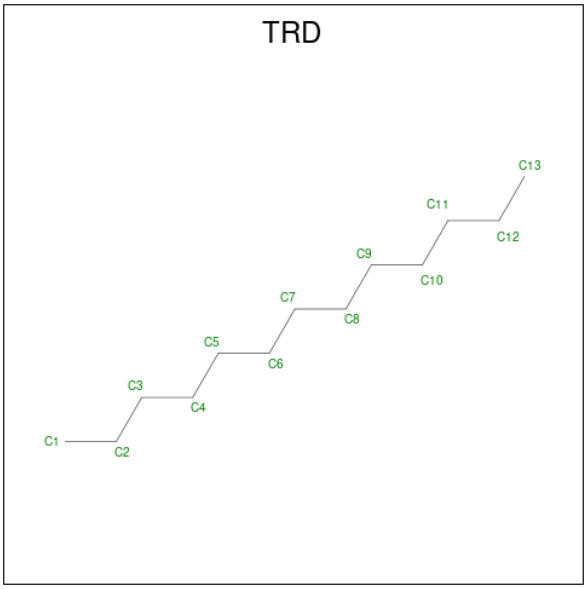
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	C	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	C	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 6 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 33 22 11	0	0
6	A	1	Total C O 33 22 11	0	0
6	A	1	Total C O 33 22 11	0	0
6	A	1	Total C O 33 22 11	0	0
6	A	1	Total C O 33 22 11	0	0
6	B	1	Total C O 30 19 11	0	0
6	C	1	Total C O 23 12 11	0	0
6	C	1	Total C O 33 22 11	0	0
6	D	1	Total C O 23 12 11	0	0

- Molecule 7 is TRIDECANE (three-letter code: TRD) (formula: $C_{13}H_{28}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 13 13	0	0
7	A	1	Total C 13 13	0	0
7	A	1	Total C 13 13	0	0

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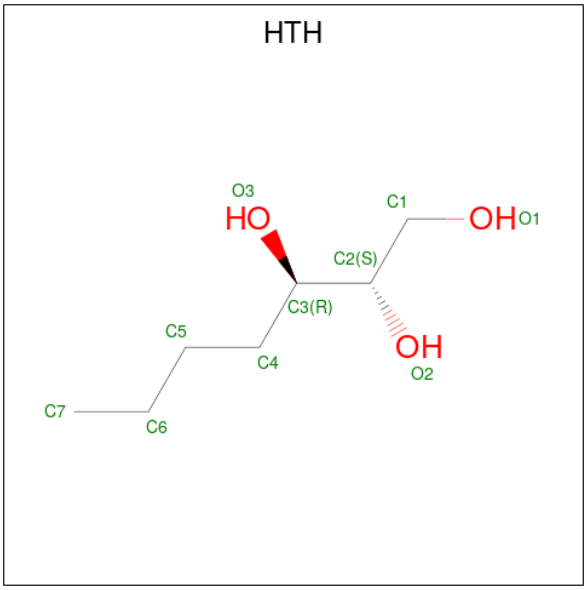
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 13 13	0	0
7	A	1	Total C 7 7	0	0
7	A	1	Total C 13 13	0	0
7	A	1	Total C 13 13	0	0
7	B	1	Total C 13 13	0	0
7	B	1	Total C 13 13	0	0
7	B	1	Total C 13 13	0	0
7	C	1	Total C 13 13	0	0
7	C	1	Total C 13 13	0	0
7	C	1	Total C 13 13	0	0
7	D	1	Total C 13 13	0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

- Molecule 8 is (2S,3R)-heptane-1,2,3-triol (three-letter code: HTH) (formula: $C_7H_{16}O_3$).



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

- Molecule 9 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

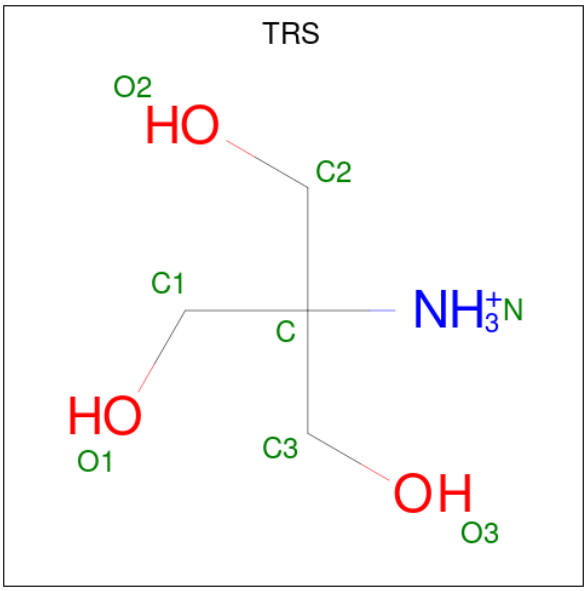
- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 12 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	2	Total Cd 2 2	0	0
12	D	2	Total Cd 2 2	0	0

- Molecule 13 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
13	B	1	Total C N O 8 4 1 3	0	0

- Molecule 14 is water.

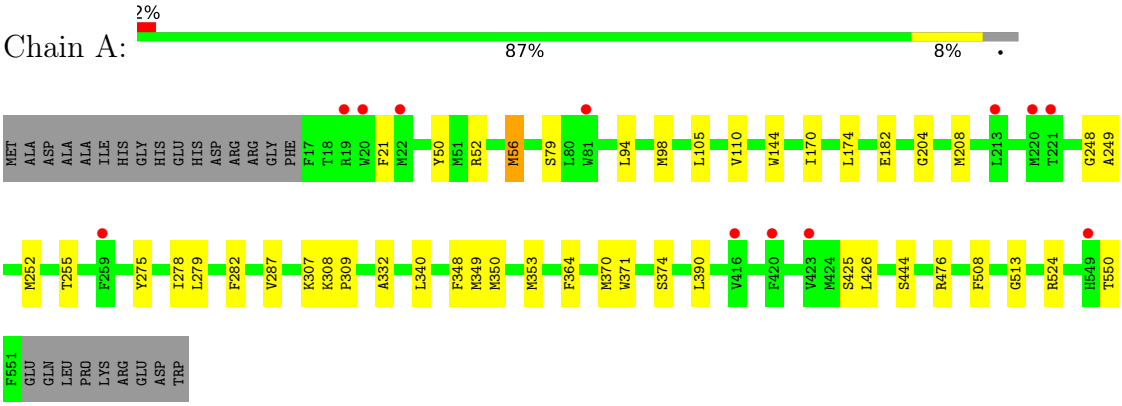
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	139	Total O 139 139	0	0
14	B	129	Total O 129 129	0	0
14	C	86	Total O 86 86	0	0
14	D	102	Total O 102 102	0	0

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.

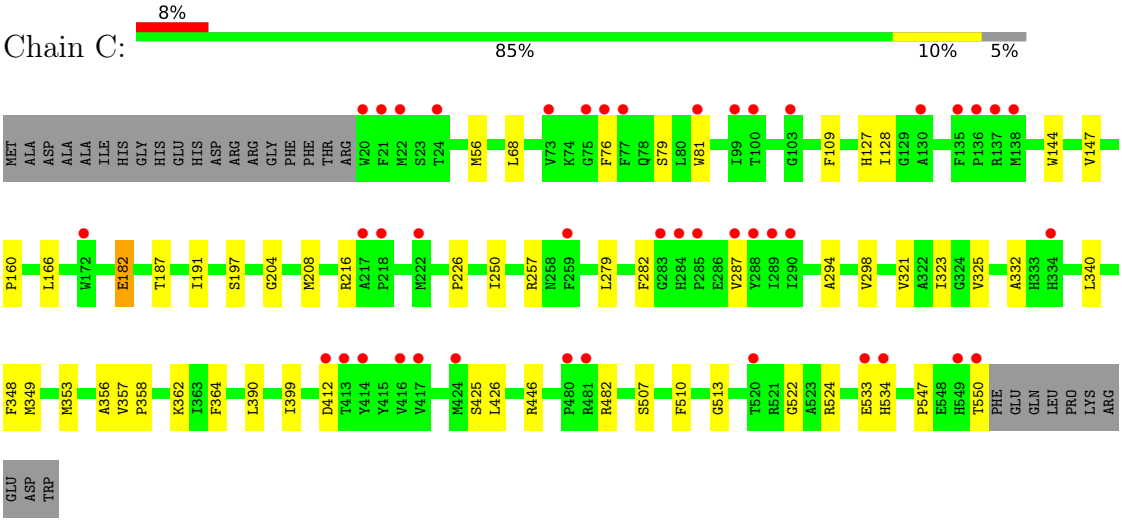
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



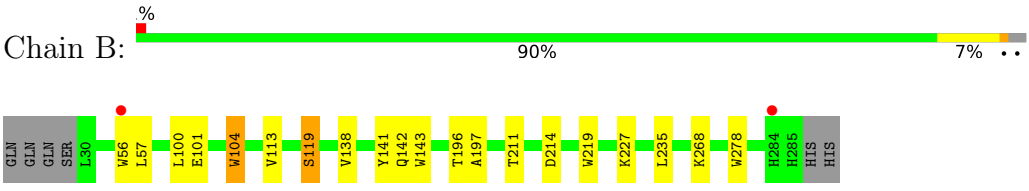
• Molecule 1: Cytochrome c oxidase subunit 1

Chain C:



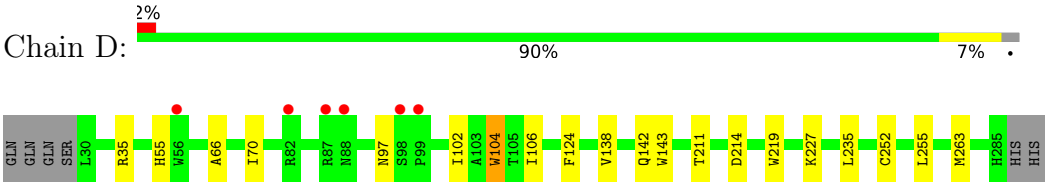
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



• Molecule 2: Cytochrome c oxidase subunit 2

Chain D:

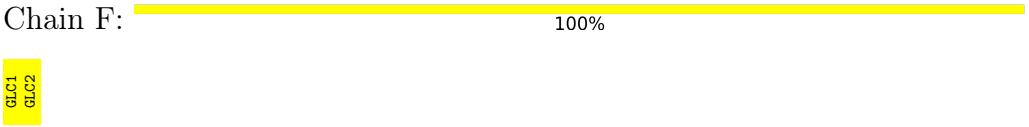


• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:

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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	124.91Å 131.48Å 176.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.84 – 2.50 42.84 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.7 (42.84-2.50) 84.4 (42.84-2.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.14_3260, PHENIX 1.14_3260	Depositor
R, R_{free}	0.173 , 0.208 0.173 , 0.208	Depositor DCC
R_{free} test set	2984 reflections (2.54%)	wwPDB-VP
Wilson B-factor (Å^2)	40.6	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 65.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13540	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: HEA, CU, CA, GLC, TRD, OH, CD, TRS, HTH, DMU, MG

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	0.38	0/4312	0.51	0/5889
1	C	0.34	0/4270	0.49	1/5836 (0.0%)
2	B	0.37	0/2080	0.54	0/2848
2	D	0.34	0/2060	0.50	0/2824
All	All	0.36	0/12722	0.51	1/17397 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	524	ARG	NE-CZ-NH2	-8.06	116.27	120.30

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	4055	31	0
1	C	4118	0	4009	33	0
2	B	2018	0	1969	16	0
2	D	1999	0	1936	10	0
3	E	23	0	21	0	0
3	F	23	0	21	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	1	0
4	C	1	0	0	1	0
5	A	120	0	108	6	0
5	C	120	0	108	4	0
6	A	165	0	210	5	0
6	B	30	0	33	2	0
6	C	56	0	63	2	0
6	D	23	0	21	1	0
7	A	85	0	181	4	0
7	B	39	0	84	7	0
7	C	39	0	84	5	0
7	D	22	0	45	0	0
8	A	10	0	16	2	0
8	B	10	0	16	0	0
9	A	1	0	0	0	0
9	B	2	0	0	0	0
9	C	1	0	0	0	0
9	D	2	0	0	0	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
11	A	1	0	0	0	0
11	C	1	0	0	0	0
12	B	2	0	0	0	0
12	D	2	0	0	0	0
13	B	8	0	12	0	0
14	A	139	0	0	3	0
14	B	129	0	0	0	0
14	C	86	0	0	3	0
14	D	102	0	0	0	0
All	All	13540	0	12992	97	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 97 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)
4:C:601:OH:O	14:C:701:HOH:O	1.95	0.85
4:A:601:OH:O	14:A:701:HOH:O	1.98	0.82
1:A:275:TYR:OH	1:A:279:LEU:HD13	1.84	0.78
1:A:476:ARG:HH21	7:B:304:TRD:H31	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:THR:OG1	14:A:702:HOH:O	2.06	0.73

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	533/560 (95%)	519 (97%)	14 (3%)	0	100	100
1	C	529/560 (94%)	517 (98%)	12 (2%)	0	100	100
2	B	254/262 (97%)	242 (95%)	12 (5%)	0	100	100
2	D	254/262 (97%)	242 (95%)	12 (5%)	0	100	100
All	All	1570/1644 (96%)	1520 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	424/455 (93%)	419 (99%)	5 (1%)	71	88
1	C	419/455 (92%)	413 (99%)	6 (1%)	67	86
2	B	213/221 (96%)	209 (98%)	4 (2%)	57	80
2	D	209/221 (95%)	204 (98%)	5 (2%)	49	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1265/1352 (94%)	1245 (98%)	20 (2%)	62 84

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	507	SER
2	D	104	TRP
2	D	227	LYS
2	D	214	ASP
2	B	119	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
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)

4 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	0.54	0	17,17,17	0.47	0
3	GLC	E	2	3	11,11,12	0.62	0	15,15,17	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GLC	F	1	3	12,12,12	0.56	0	17,17,17	0.72	0
3	GLC	F	2	3	11,11,12	0.57	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	-	1/2/22/22	0/1/1/1
3	GLC	F	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(^{o})	Ideal(^{o})
3	F	2	GLC	C1-O5-C5	2.78	115.95	112.19
3	F	2	GLC	O5-C5-C6	2.40	110.96	107.20
3	E	2	GLC	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

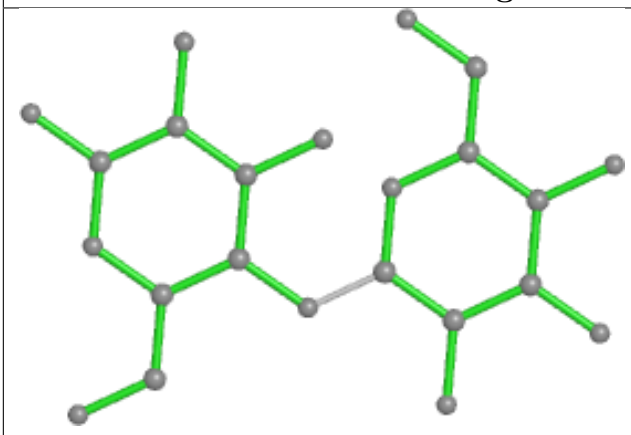
There are no ring outliers.

1 monomer is involved in 2 short contacts:

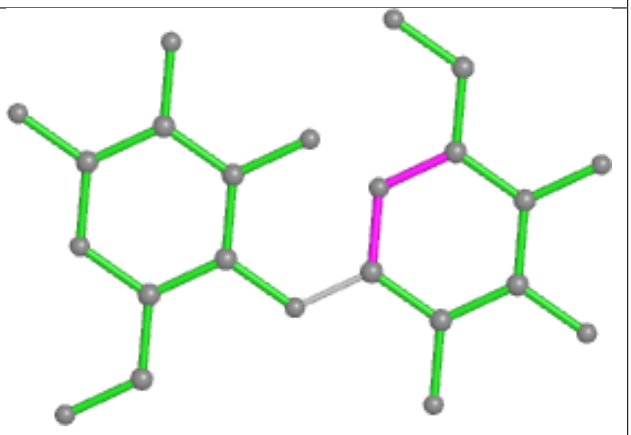
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	GLC	2	0

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

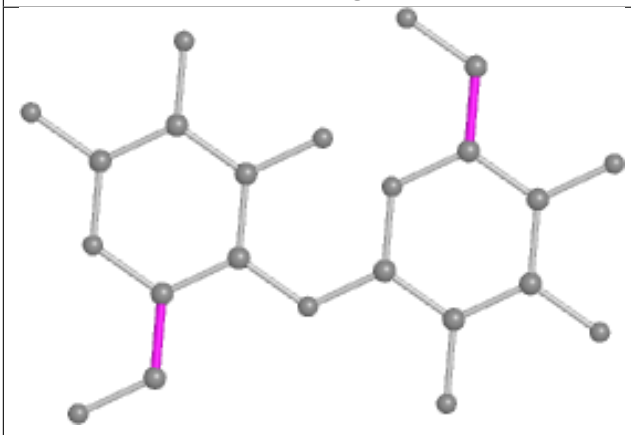
Oligosaccharide Chain E



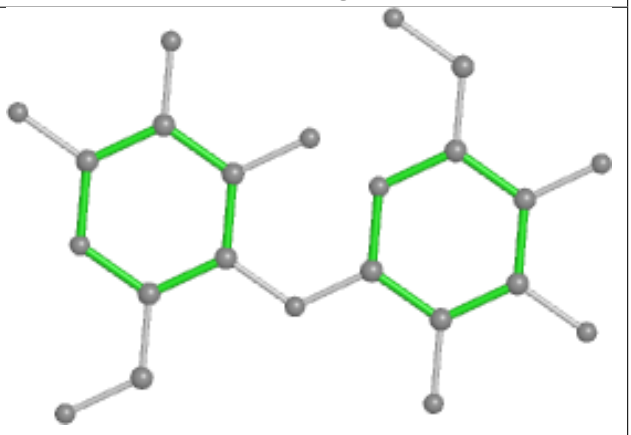
Bond lengths



Bond angles

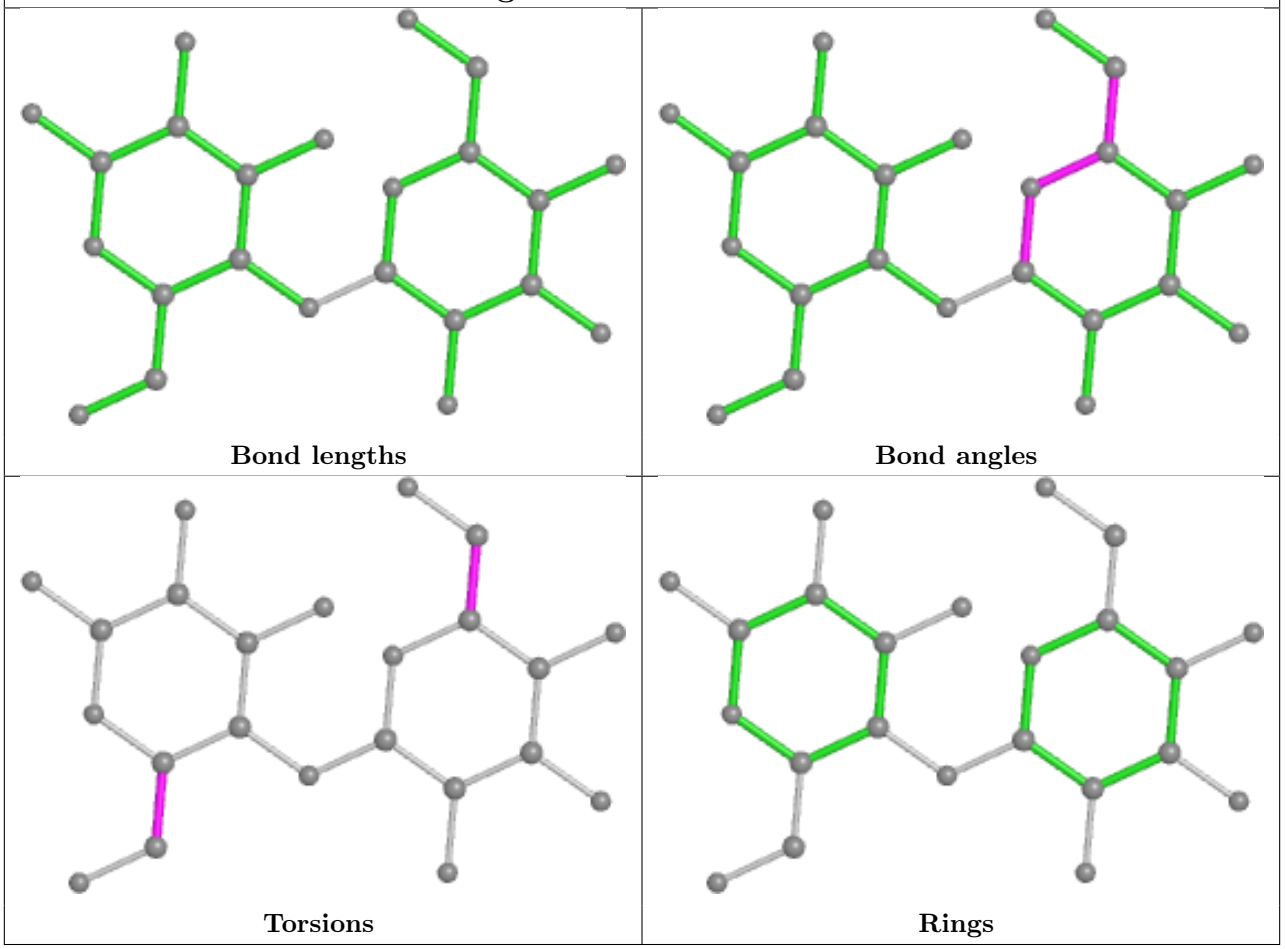


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 47 ligands modelled in this entry, 2 are modelled with single atom and 14 are monoatomic - leaving 31 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	$\#\|Z\| > 2$
6	DMU	C	604	-	24,24,34	2.09	14 (58%)	35,35,45	0.99	2 (5%)
6	DMU	B	301	-	31,31,34	2.01	13 (41%)	42,42,45	1.04	2 (4%)
6	DMU	A	604	-	34,34,34	1.96	12 (35%)	45,45,45	1.19	4 (8%)
6	DMU	A	607	-	34,34,34	1.93	12 (35%)	45,45,45	1.21	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	TRD	C	608	-	12,12,12	0.13	0	11,11,11	0.78	0
7	TRD	B	304	-	12,12,12	0.16	0	11,11,11	0.73	0
5	HEA	A	603	14,1	57,67,67	2.11	17 (29%)	61,103,103	2.36	22 (36%)
7	TRD	C	606	-	12,12,12	0.14	0	11,11,11	0.79	0
8	HTH	B	306	-	9,9,9	0.33	0	10,10,10	1.23	2 (20%)
6	DMU	D	301	-	24,24,34	2.08	12 (50%)	35,35,45	1.39	6 (17%)
7	TRD	A	611	-	12,12,12	0.18	0	11,11,11	0.72	0
5	HEA	A	602	1	57,67,67	2.09	15 (26%)	61,103,103	2.44	24 (39%)
8	HTH	A	616	-	9,9,9	0.52	0	10,10,10	1.38	1 (10%)
5	HEA	C	602	1	57,67,67	2.16	17 (29%)	61,103,103	2.35	23 (37%)
5	HEA	C	603	14,1	57,67,67	2.11	17 (29%)	61,103,103	2.40	23 (37%)
7	TRD	A	614	-	12,12,12	0.13	0	11,11,11	0.78	0
13	TRS	B	311	-	7,7,7	0.36	0	9,9,9	1.10	0
7	TRD	D	302	-	12,12,12	0.12	0	11,11,11	0.90	0
7	TRD	A	615	-	12,12,12	0.17	0	11,11,11	0.71	0
6	DMU	A	605	-	34,34,34	1.94	12 (35%)	45,45,45	1.18	5 (11%)
6	DMU	A	606	-	34,34,34	1.93	12 (35%)	45,45,45	1.46	9 (20%)
7	TRD	C	607	-	12,12,12	0.14	0	11,11,11	0.74	0
7	TRD	A	613	-	6,6,12	0.18	0	5,5,11	0.48	0
7	TRD	A	612	-	12,12,12	0.17	0	11,11,11	0.75	0
7	TRD	B	302	-	12,12,12	0.16	0	11,11,11	0.66	0
7	TRD	A	609	-	12,12,12	0.12	0	11,11,11	0.78	0
7	TRD	A	610	-	12,12,12	0.14	0	11,11,11	0.82	0
7	TRD	D	303	-	8,8,12	0.12	0	7,7,11	0.84	0
6	DMU	A	608	-	34,34,34	1.89	9 (26%)	45,45,45	1.24	4 (8%)
6	DMU	C	605	-	34,34,34	2.00	14 (41%)	45,45,45	1.43	6 (13%)
7	TRD	B	303	-	12,12,12	0.20	0	11,11,11	0.46	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
6	DMU	C	604	-	-	4/8/48/59	0/2/2/2
6	DMU	B	301	-	-	10/16/56/59	0/2/2/2
6	DMU	A	604	-	-	11/19/59/59	0/2/2/2
6	DMU	A	607	-	-	8/19/59/59	0/2/2/2
7	TRD	C	608	-	-	0/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TRD	B	304	-	-	6/10/10/10	-
5	HEA	A	603	14,1	2/2/7/16	4/32/76/76	-
7	TRD	C	606	-	-	4/10/10/10	-
8	HTH	B	306	-	-	6/10/10/10	-
6	DMU	D	301	-	-	4/8/48/59	0/2/2/2
7	TRD	A	611	-	-	2/10/10/10	-
5	HEA	A	602	1	2/2/7/16	5/32/76/76	-
8	HTH	A	616	-	-	5/10/10/10	-
5	HEA	C	602	1	2/2/7/16	5/32/76/76	-
5	HEA	C	603	14,1	2/2/7/16	6/32/76/76	-
7	TRD	A	614	-	-	6/10/10/10	-
13	TRS	B	311	-	-	6/9/9/9	-
7	TRD	D	302	-	-	5/10/10/10	-
7	TRD	A	615	-	-	6/10/10/10	-
6	DMU	A	605	-	-	11/19/59/59	0/2/2/2
6	DMU	A	606	-	-	5/19/59/59	0/2/2/2
7	TRD	C	607	-	-	1/10/10/10	-
7	TRD	A	613	-	-	2/4/4/10	-
7	TRD	A	612	-	-	3/10/10/10	-
7	TRD	B	302	-	-	7/10/10/10	-
7	TRD	A	609	-	-	0/10/10/10	-
7	TRD	A	610	-	-	1/10/10/10	-
7	TRD	D	303	-	-	4/6/6/10	-
6	DMU	A	608	-	-	7/19/59/59	0/2/2/2
6	DMU	C	605	-	-	10/19/59/59	0/2/2/2
7	TRD	B	303	-	-	6/10/10/10	-

The worst 5 of 176 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEA	C3B-C2B	5.83	1.47	1.34
5	C	602	HEA	C3B-C2B	5.79	1.47	1.34
5	C	602	HEA	C3C-C2C	5.68	1.48	1.40
5	C	603	HEA	C3B-C2B	5.58	1.47	1.34
5	C	602	HEA	C3D-C2D	5.34	1.48	1.36

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	603	HEA	C3D-C4D-ND	6.60	116.75	110.36
5	A	602	HEA	C3D-C4D-ND	6.32	116.48	110.36
5	A	603	HEA	C3D-C4D-ND	6.19	116.35	110.36
5	C	602	HEA	C3D-C4D-ND	6.04	116.20	110.36
5	A	603	HEA	C2B-C1B-NB	6.01	117.08	109.88

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	602	HEA	ND
5	A	602	HEA	NB
5	A	603	HEA	ND
5	A	603	HEA	NB
5	C	602	HEA	ND

5 of 160 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	HEA	C19-C20-C21-C22
5	C	602	HEA	C19-C20-C21-C22
6	A	605	DMU	C19-C18-O16-C6
6	A	607	DMU	C1-C6-O16-C18
6	A	607	DMU	O5-C6-O16-C18

There are no ring outliers.

20 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	301	DMU	2	0
6	A	604	DMU	1	0
7	C	608	TRD	2	0
7	B	304	TRD	1	0
5	A	603	HEA	3	0
7	C	606	TRD	1	0
6	D	301	DMU	1	0
5	A	602	HEA	3	0
8	A	616	HTH	2	0
5	C	602	HEA	2	0
5	C	603	HEA	2	0
7	A	614	TRD	2	0
6	A	605	DMU	3	0
7	C	607	TRD	2	0
7	B	302	TRD	1	0

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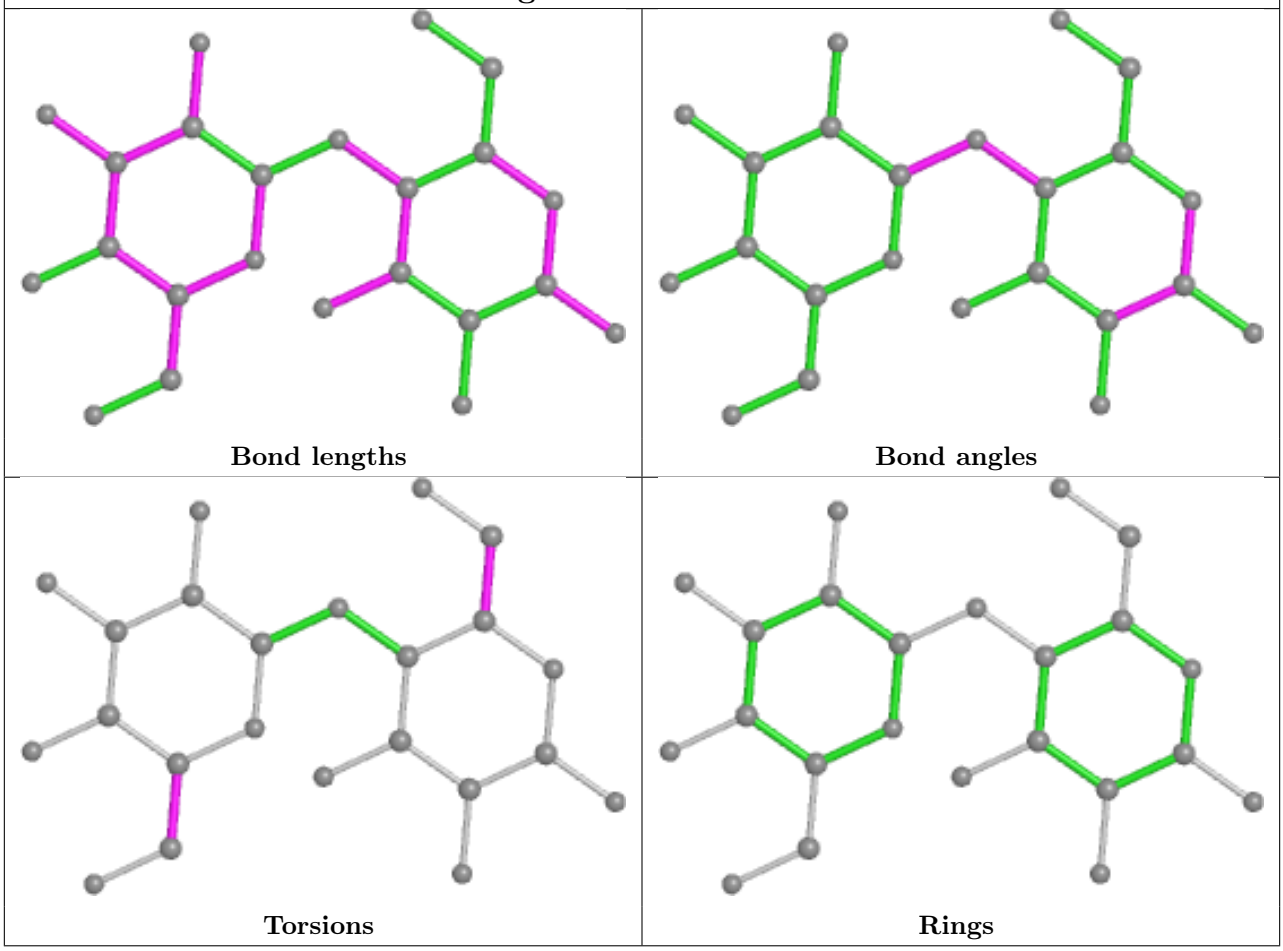
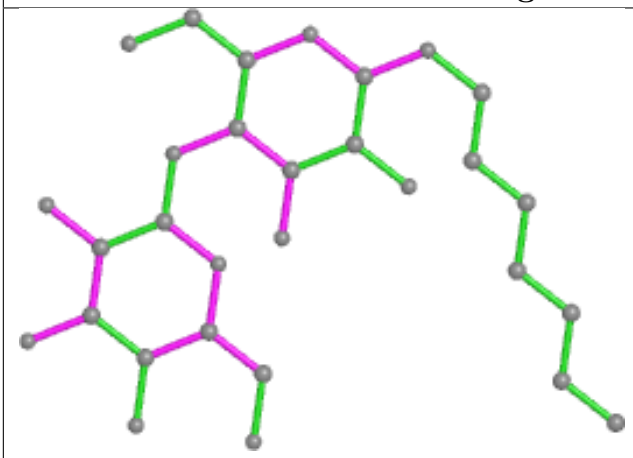
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	609	TRD	1	0
7	A	610	TRD	1	0
6	A	608	DMU	1	0
6	C	605	DMU	2	0
7	B	303	TRD	5	0

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.

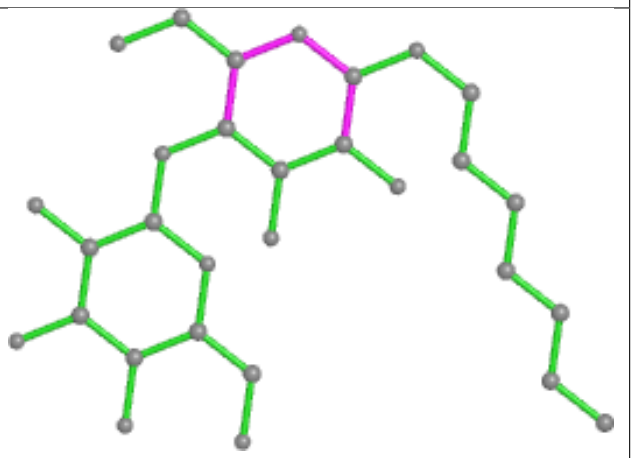
Ligand DMU C 604



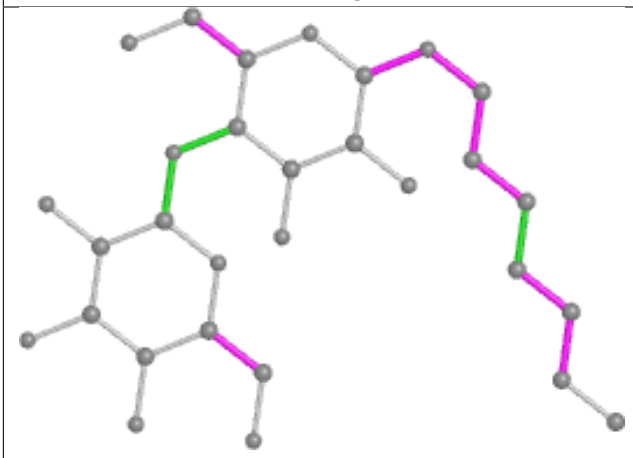
Ligand DMU B 301



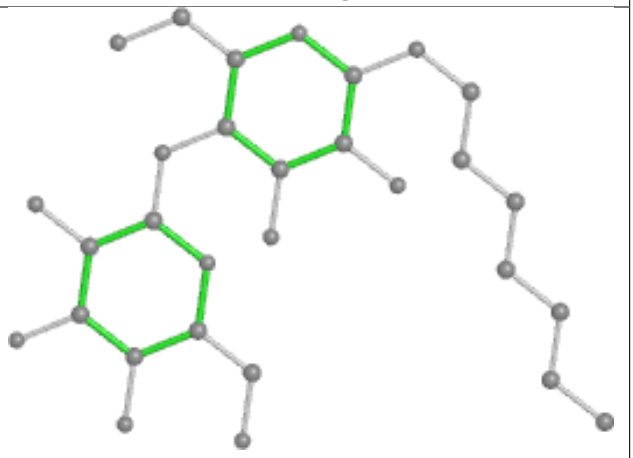
Bond lengths



Bond angles

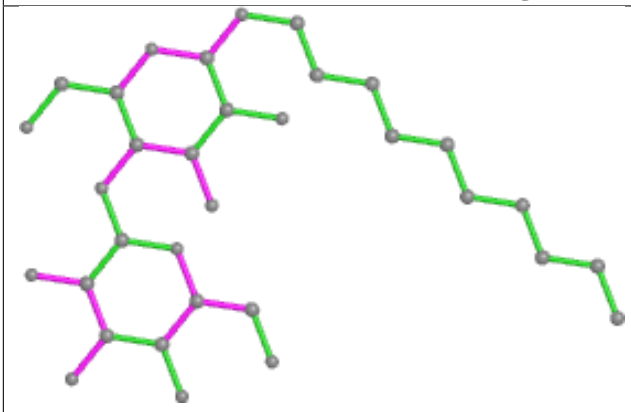


Torsions

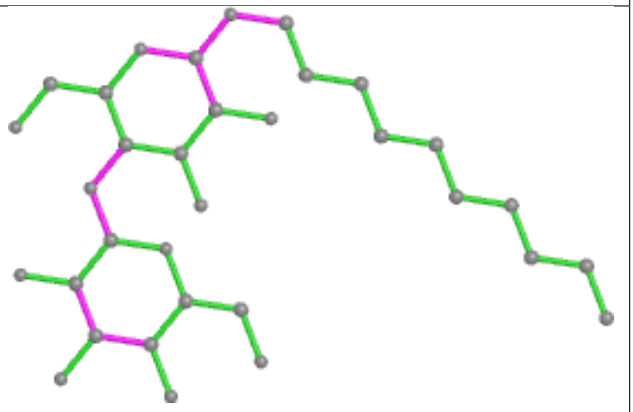


Rings

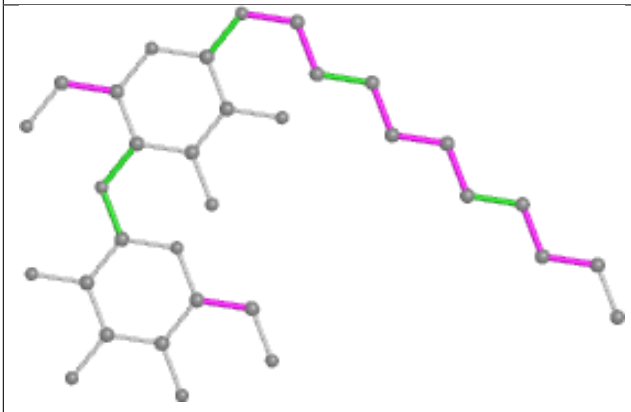
Ligand DMU A 604



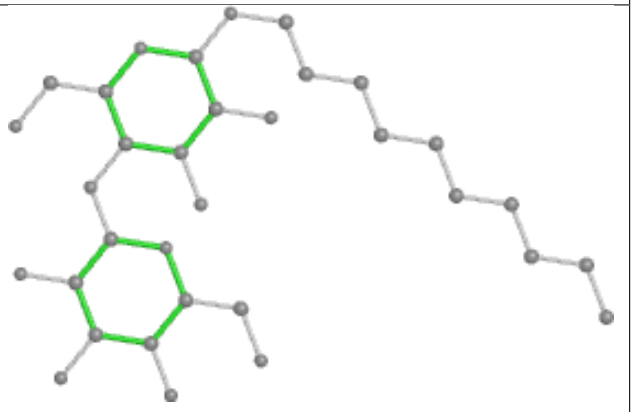
Bond lengths



Bond angles

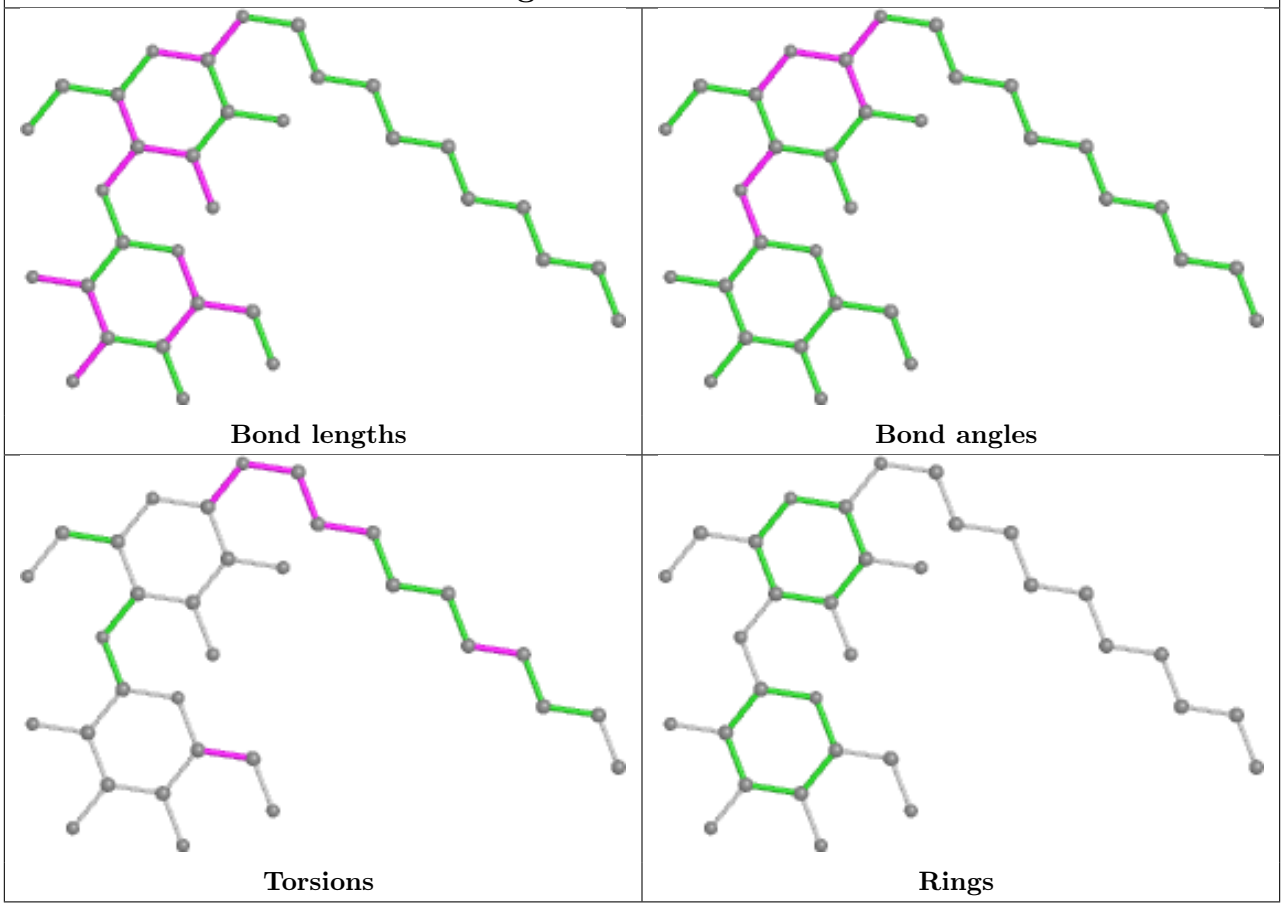


Torsions

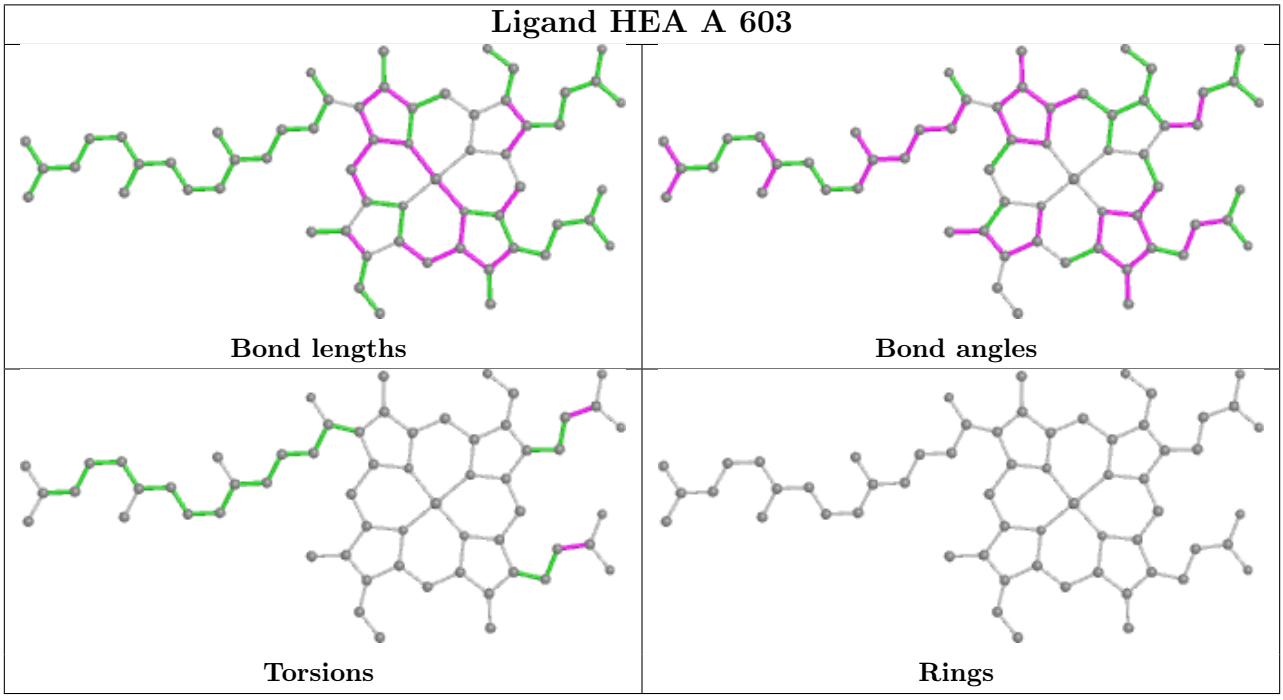


Rings

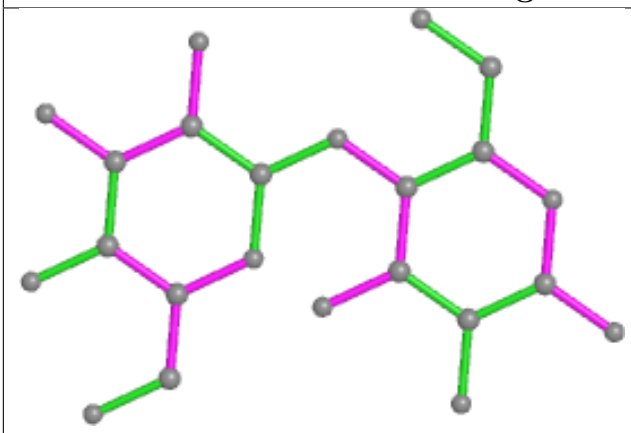
Ligand DMU A 607



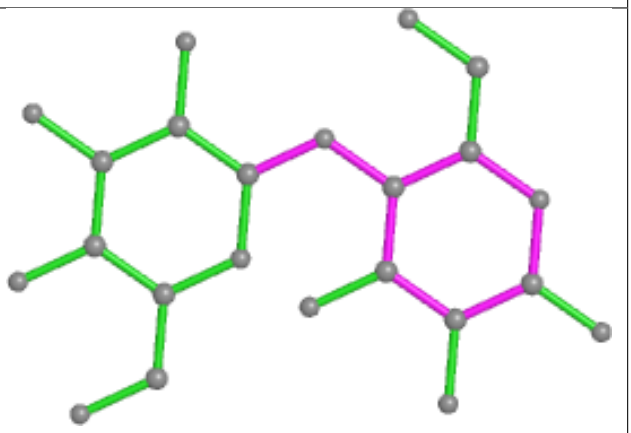
Ligand HEA A 603



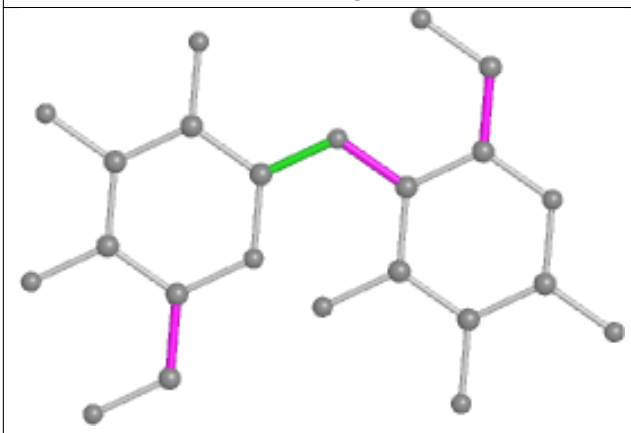
Ligand DMU D 301



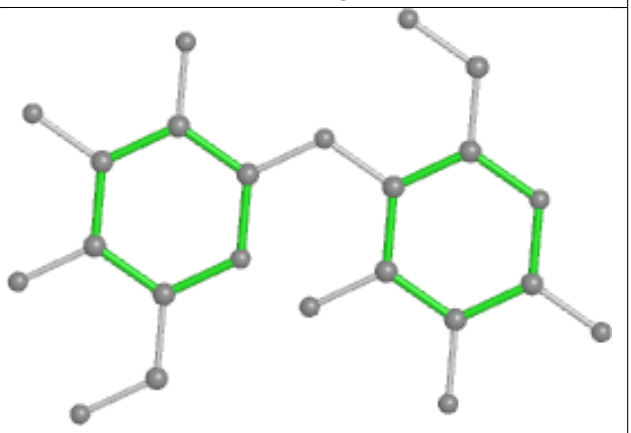
Bond lengths



Bond angles

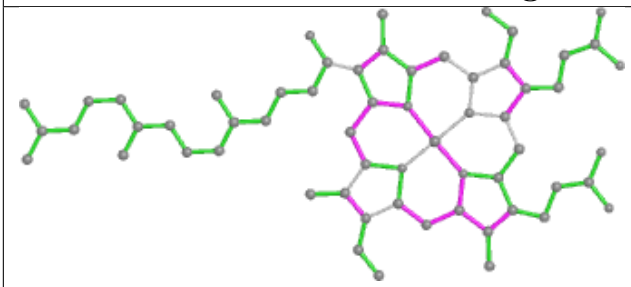


Torsions

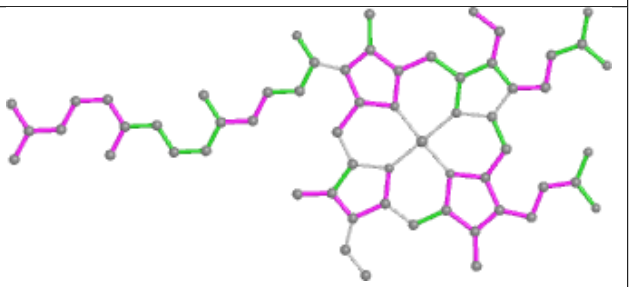


Rings

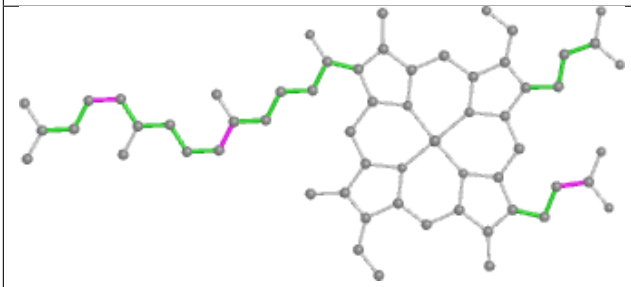
Ligand HEA A 602



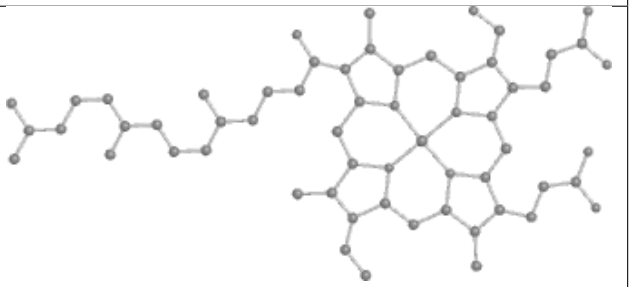
Bond lengths



Bond angles

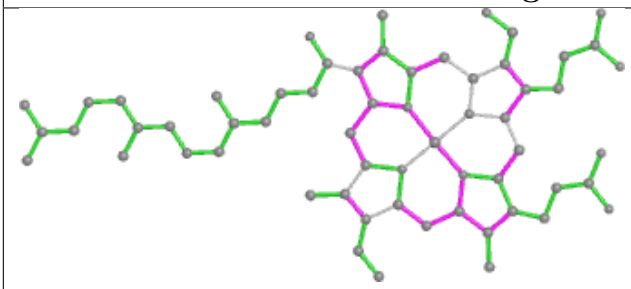


Torsions

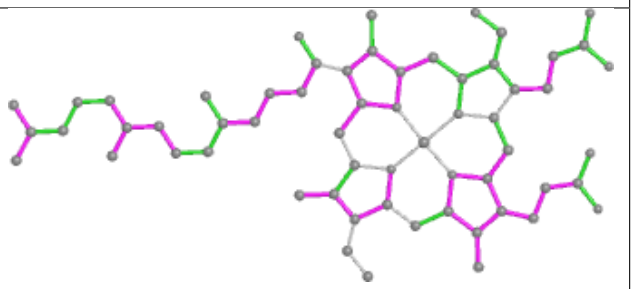


Rings

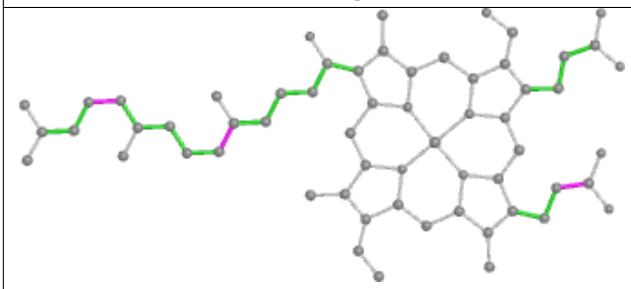
Ligand HEA C 602



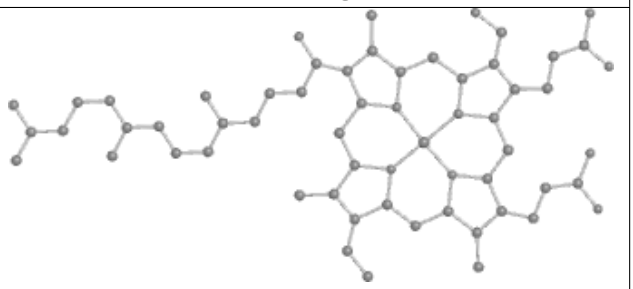
Bond lengths



Bond angles

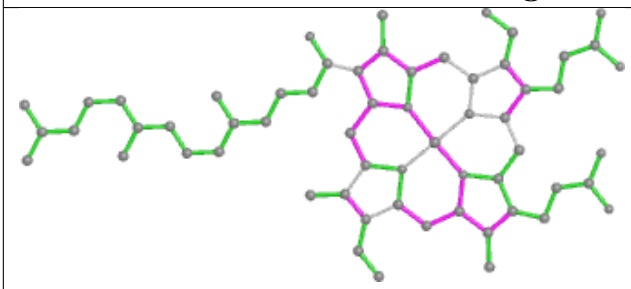


Torsions

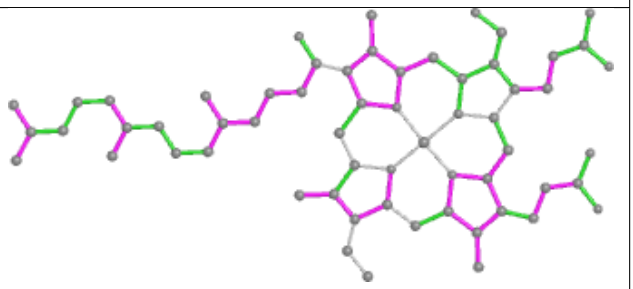


Rings

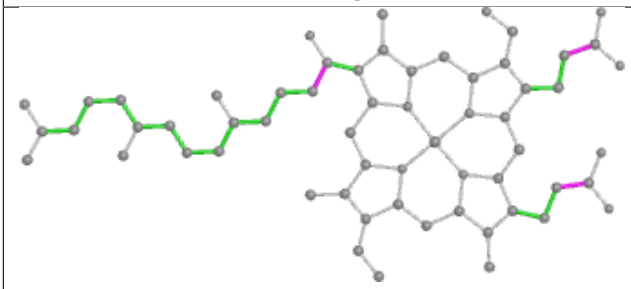
Ligand HEA C 603



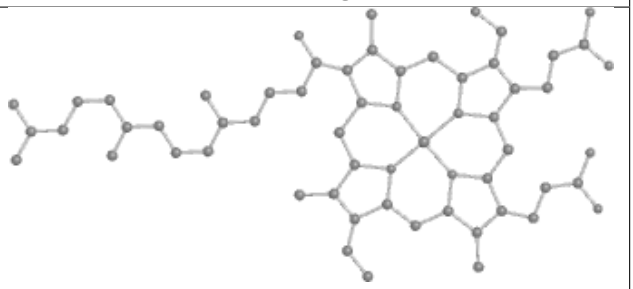
Bond lengths



Bond angles

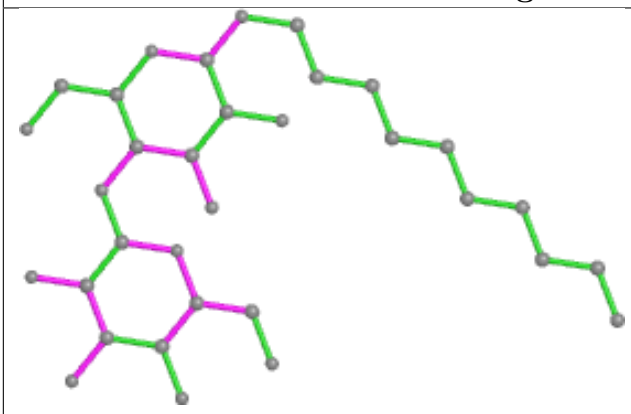


Torsions

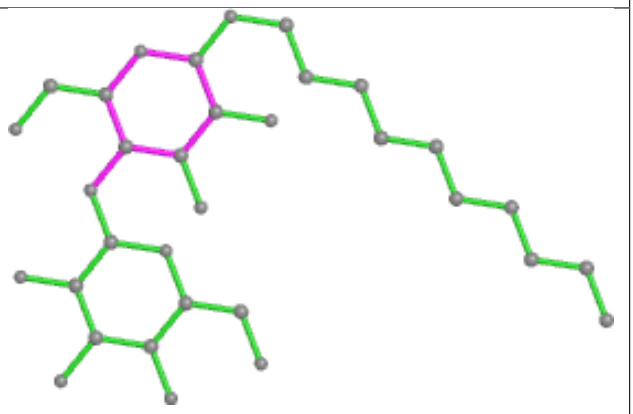


Rings

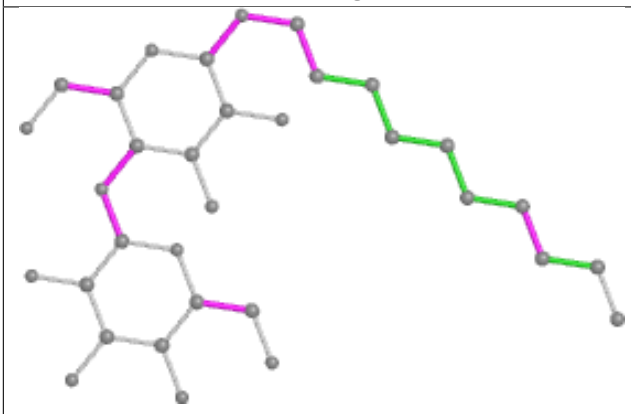
Ligand DMU A 605



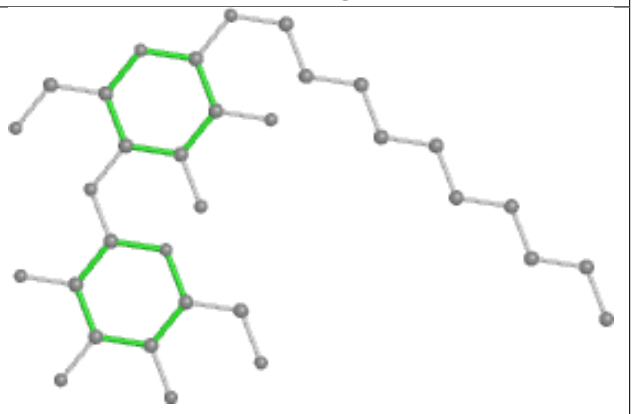
Bond lengths



Bond angles

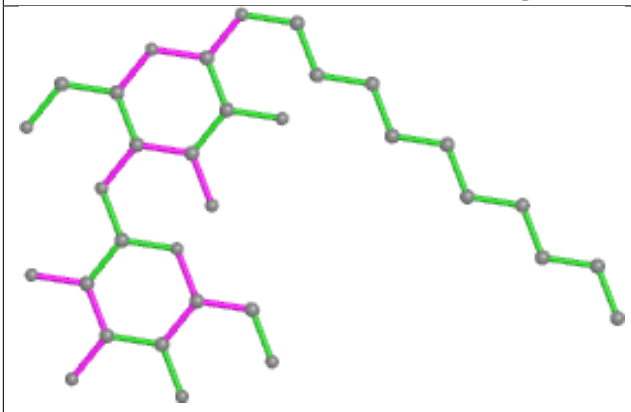


Torsions

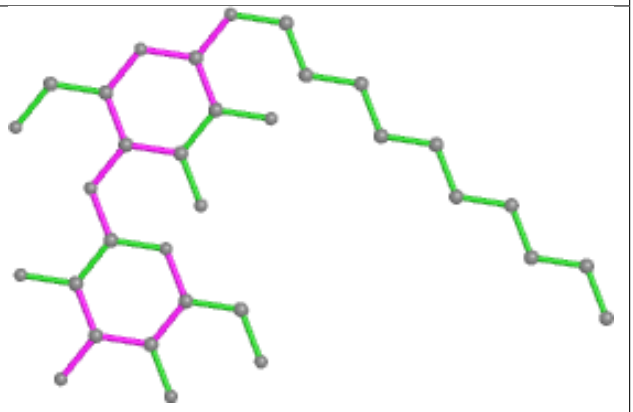


Rings

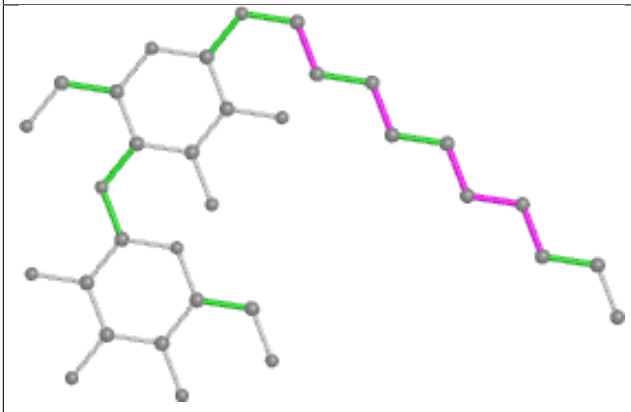
Ligand DMU A 606



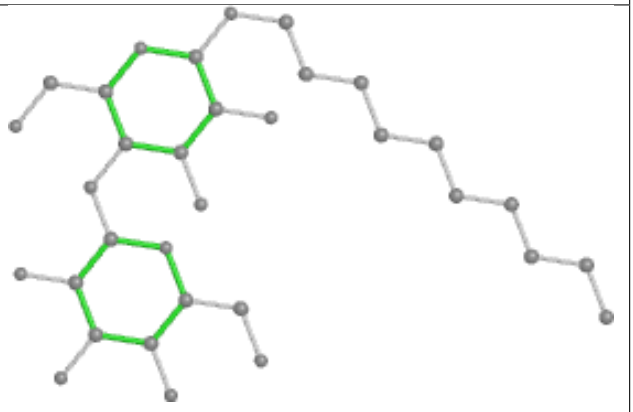
Bond lengths



Bond angles

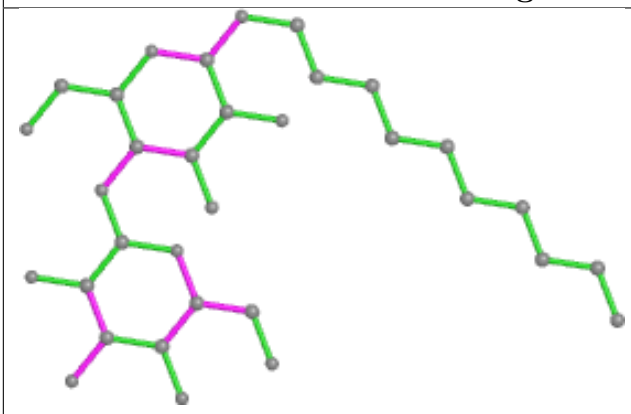


Torsions

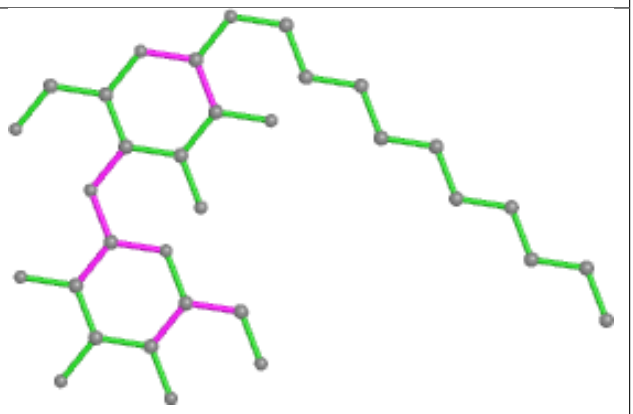


Rings

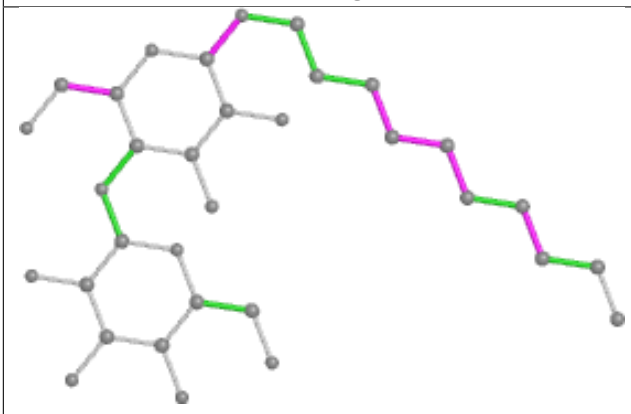
Ligand DMU A 608



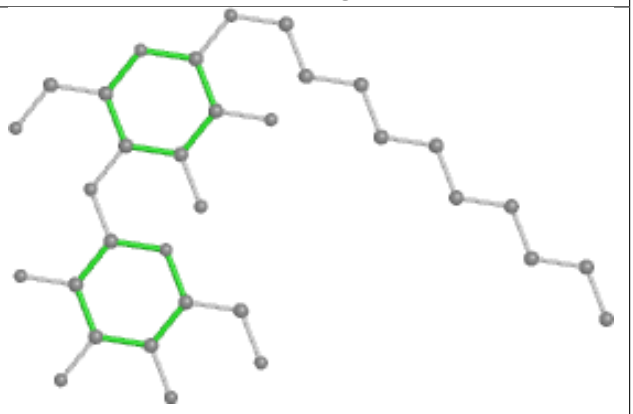
Bond lengths



Bond angles

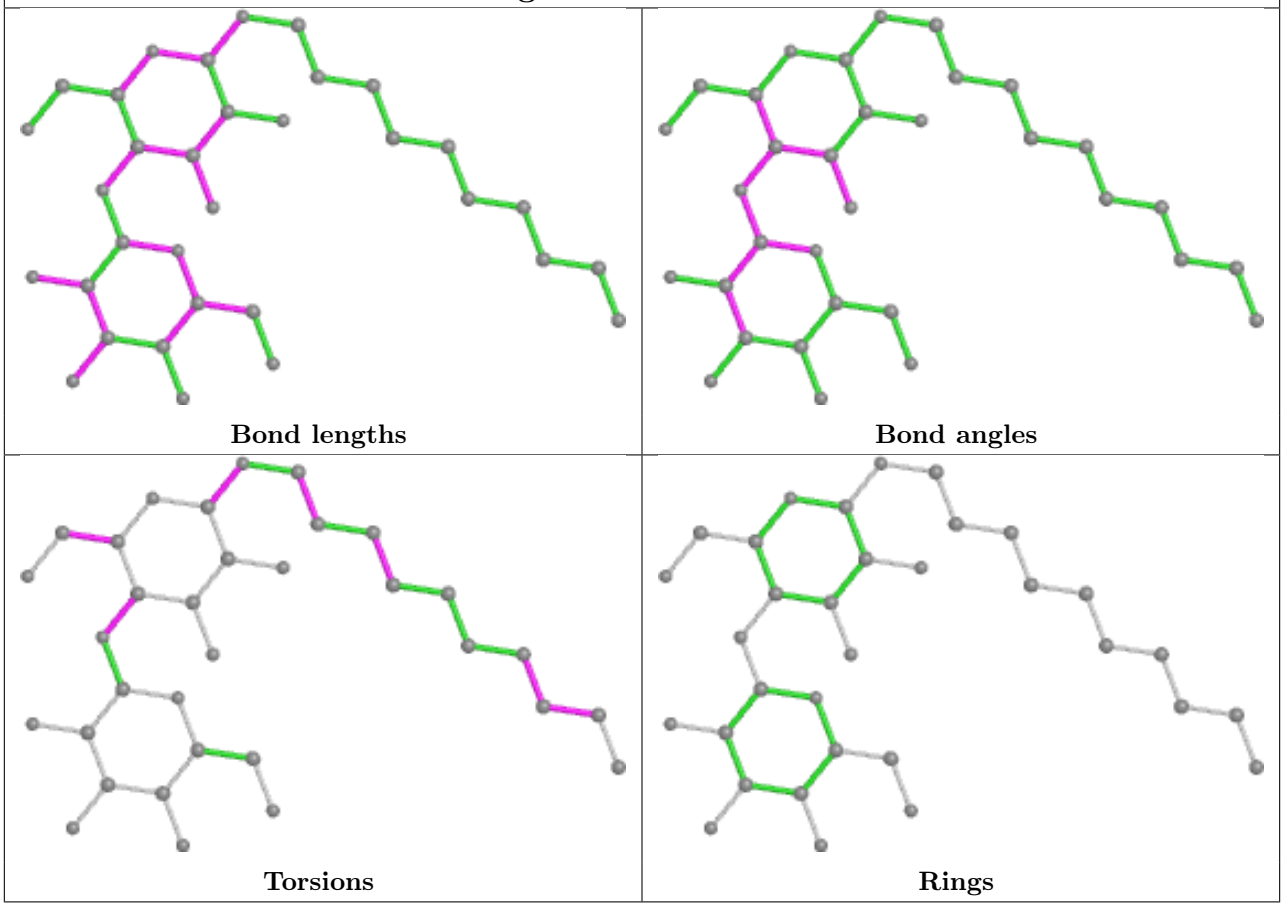


Torsions



Rings

Ligand DMU C 605



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	535/560 (95%)	-0.33	12 (2%)	62	65	30, 42, 66, 99	0
1	C	531/560 (94%)	0.15	43 (8%)	12	12	39, 56, 80, 110	0
2	B	256/262 (97%)	-0.62	2 (0%)	86	87	31, 46, 63, 73	0
2	D	256/262 (97%)	-0.47	6 (2%)	60	63	37, 50, 71, 87	0
All	All	1578/1644 (95%)	-0.24	63 (3%)	38	41	30, 48, 74, 110	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	TRP	5.0
1	C	222	MET	4.7
1	C	259	PHE	4.7
1	C	218	PRO	4.2
1	C	217	ALA	3.9

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	F	2	11/12	0.76	0.39	106,117,124,135	0
3	GLC	F	1	12/12	0.82	0.32	85,97,108,111	0

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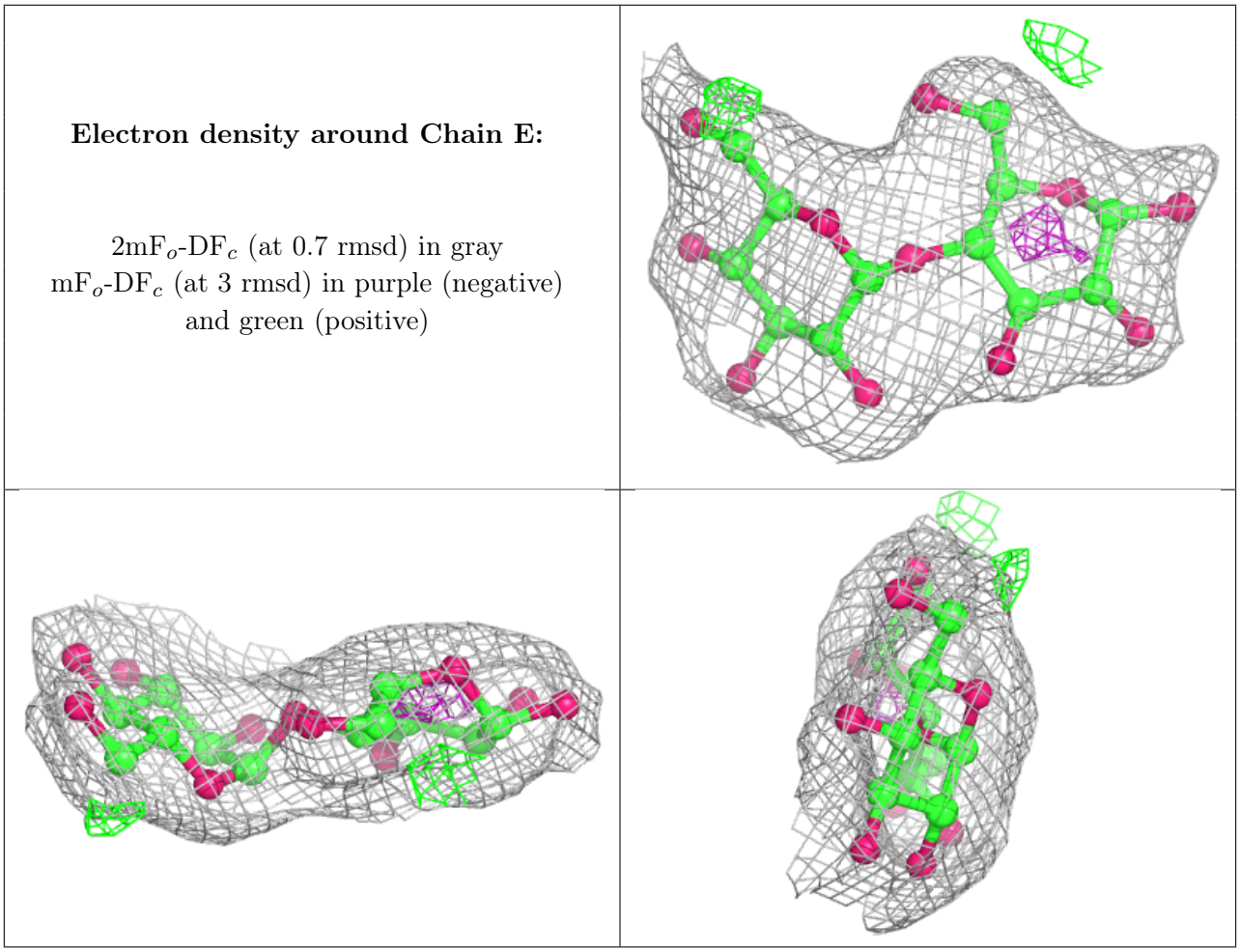
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	E	1	12/12	0.84	0.28	76,89,98,98	0
3	GLC	E	2	11/12	0.91	0.23	74,78,81,89	0

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.

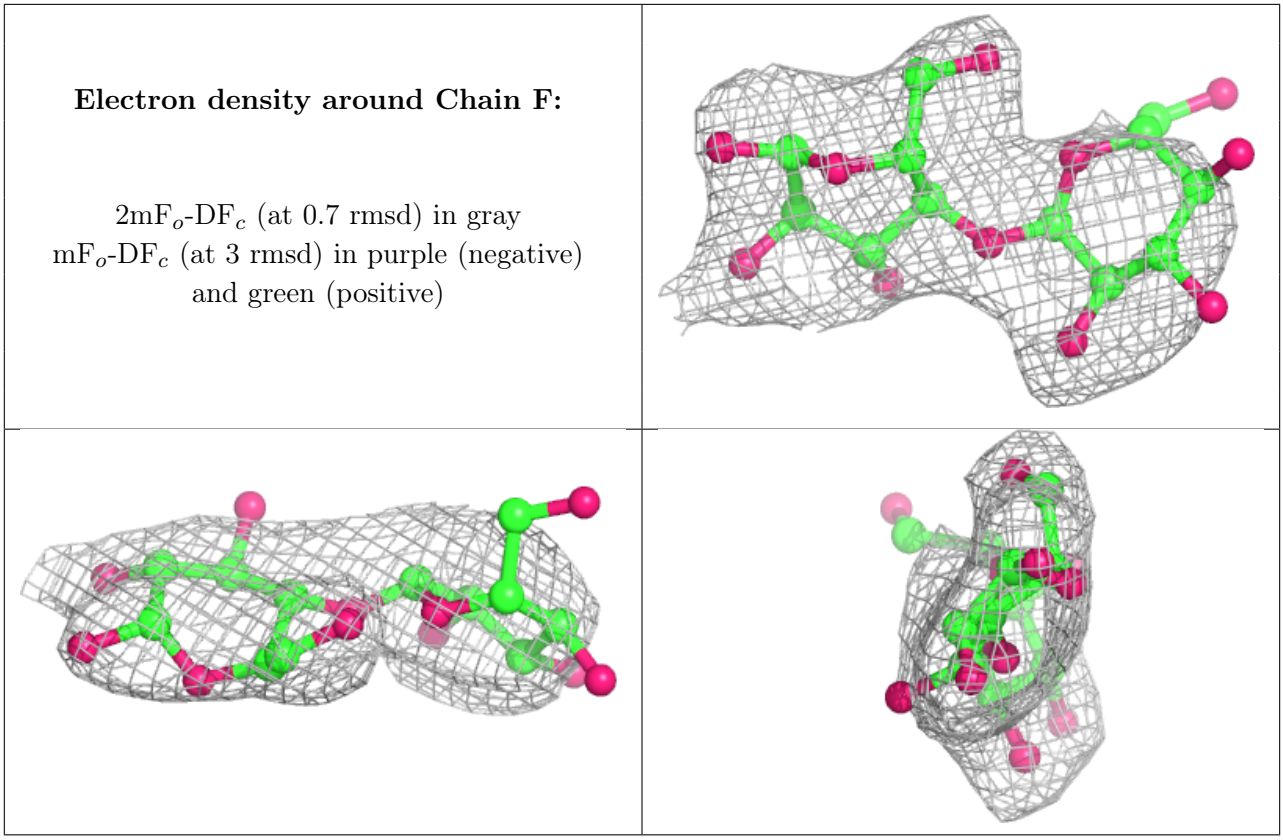
Electron density around Chain E:

$2mF_o$-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)



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^{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
7	TRD	C	607	13/13	0.55	0.36	68,74,86,87	0
7	TRD	B	302	13/13	0.68	0.36	61,73,81,81	0
7	TRD	A	610	13/13	0.70	0.41	55,67,75,80	0
7	TRD	C	608	13/13	0.75	0.37	74,77,95,97	0
7	TRD	A	613	7/13	0.77	0.40	52,60,66,69	0
6	DMU	A	606	33/33	0.77	0.30	50,63,72,79	33
7	TRD	A	609	13/13	0.78	0.36	59,67,80,81	0
13	TRS	B	311	8/8	0.78	0.13	53,71,79,80	0
6	DMU	A	605	33/33	0.79	0.34	40,61,75,75	33
6	DMU	A	604	33/33	0.79	0.28	38,84,122,125	0
7	TRD	A	612	13/13	0.79	0.20	49,60,66,66	0
8	HTH	A	616	10/10	0.79	0.37	56,69,80,87	0
6	DMU	C	604	23/33	0.79	0.36	83,89,98,101	23
7	TRD	B	303	13/13	0.80	0.36	38,58,71,72	0

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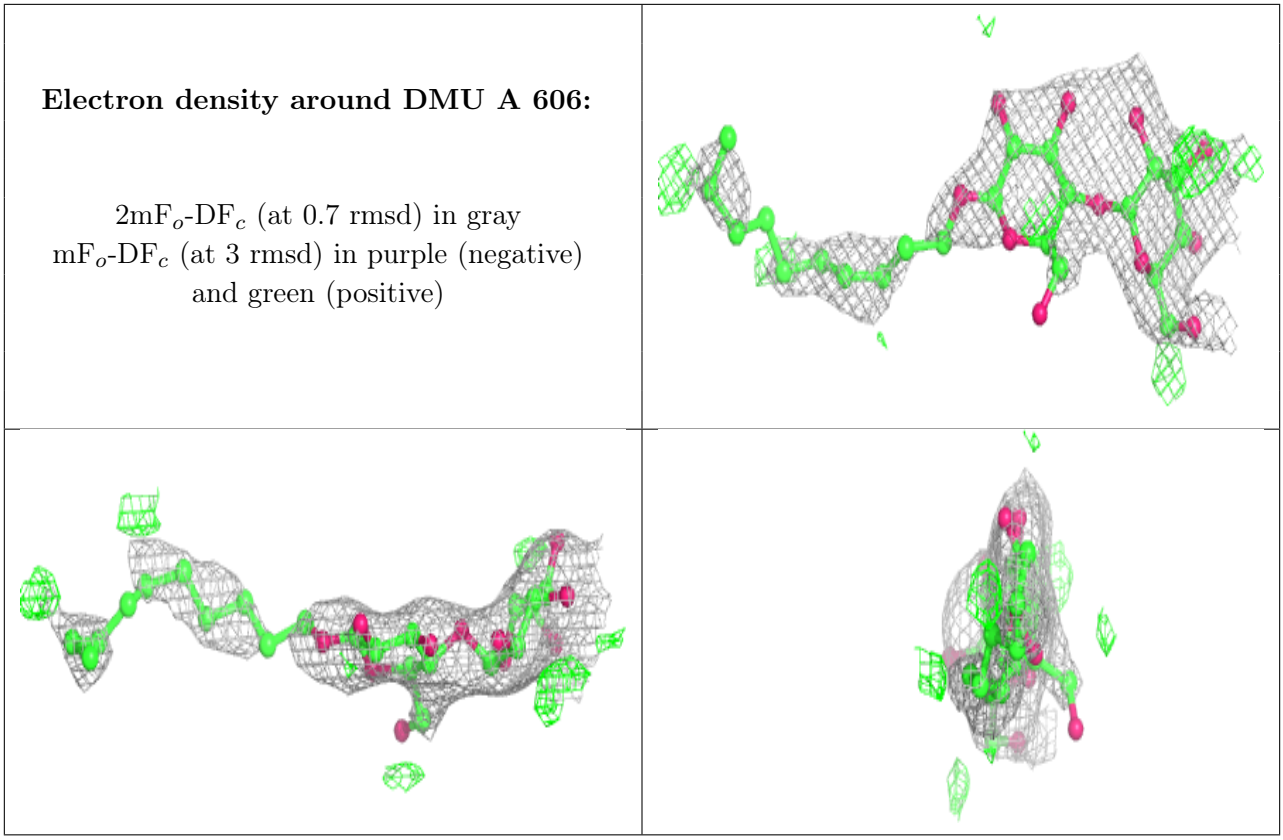
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	DMU	D	301	23/33	0.81	0.30	66,80,91,102	23
7	TRD	A	611	13/13	0.82	0.20	46,59,76,77	0
6	DMU	C	605	33/33	0.83	0.23	57,82,92,93	33
7	TRD	A	614	13/13	0.83	0.44	60,70,84,86	0
6	DMU	B	301	30/33	0.84	0.35	52,79,88,89	0
7	TRD	C	606	13/13	0.84	0.21	57,64,73,74	0
7	TRD	A	615	13/13	0.86	0.25	50,56,75,75	0
8	HTH	B	306	10/10	0.88	0.29	48,60,71,73	0
7	TRD	D	303	9/13	0.88	0.17	59,63,68,70	0
7	TRD	B	304	13/13	0.89	0.23	43,48,56,68	0
7	TRD	D	302	13/13	0.92	0.20	45,52,55,56	0
6	DMU	A	607	33/33	0.93	0.26	51,66,80,83	0
12	CD	D	308	1/1	0.95	0.06	84,84,84,84	1
4	OH	C	601	1/1	0.95	0.23	48,48,48,48	0
5	HEA	A	603	60/60	0.96	0.25	29,37,46,48	0
6	DMU	A	608	33/33	0.97	0.10	35,46,58,60	0
5	HEA	C	602	60/60	0.97	0.26	35,44,63,75	0
5	HEA	C	603	60/60	0.97	0.23	37,44,50,52	0
12	CD	B	310	1/1	0.98	0.05	69,69,69,69	1
5	HEA	A	602	60/60	0.98	0.22	27,32,40,59	0
11	CA	C	611	1/1	0.98	0.06	50,50,50,50	0
11	CA	A	619	1/1	0.99	0.09	35,35,35,35	0
9	CU	B	307	1/1	0.99	0.13	37,37,37,37	0
9	CU	C	609	1/1	0.99	0.16	44,44,44,44	0
10	MG	A	618	1/1	0.99	0.24	19,19,19,19	0
10	MG	C	610	1/1	0.99	0.23	24,24,24,24	0
9	CU	A	617	1/1	1.00	0.15	38,38,38,38	0
9	CU	D	305	1/1	1.00	0.15	40,40,40,40	0
12	CD	B	309	1/1	1.00	0.11	49,49,49,49	0
9	CU	D	306	1/1	1.00	0.11	38,38,38,38	0
12	CD	D	307	1/1	1.00	0.11	49,49,49,49	0
4	OH	A	601	1/1	1.00	0.20	40,40,40,40	0
9	CU	B	308	1/1	1.00	0.12	33,33,33,33	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.

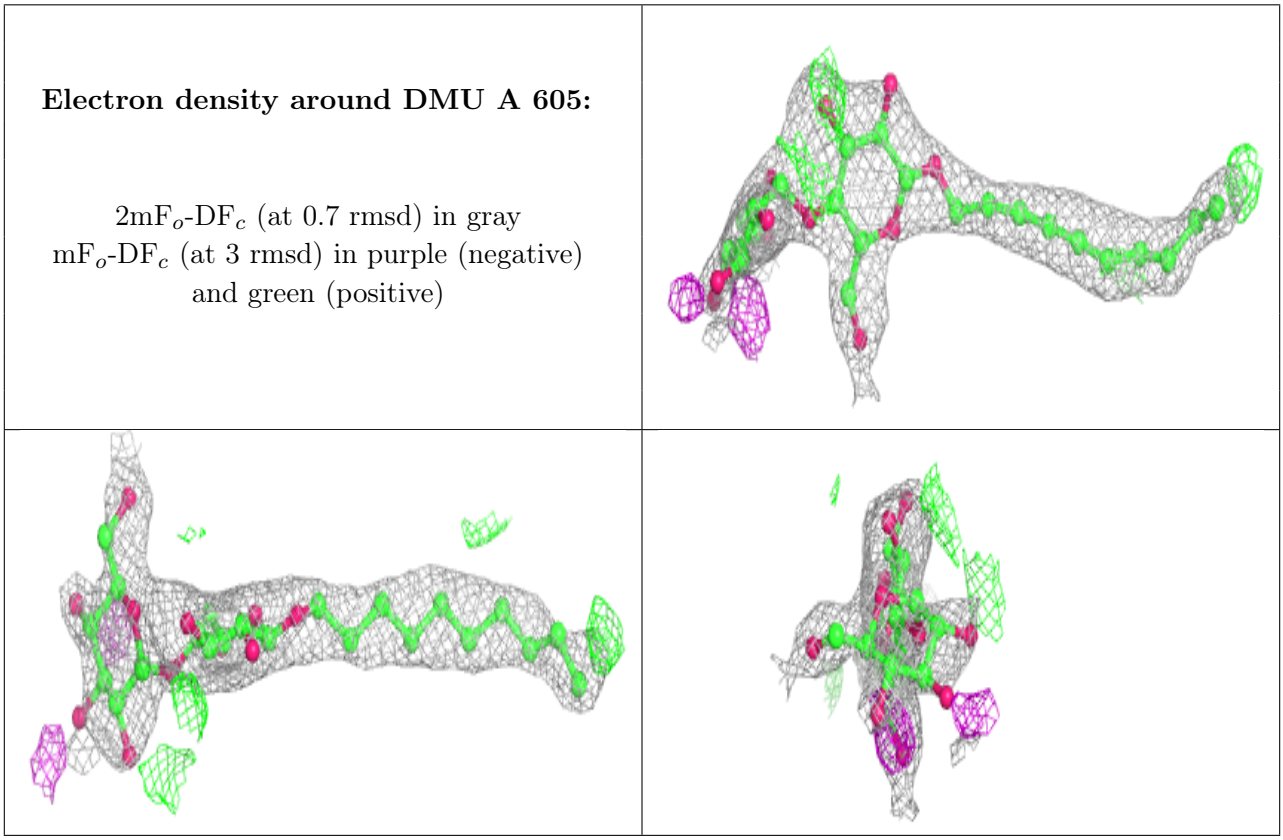
Electron density around DMU A 606:

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



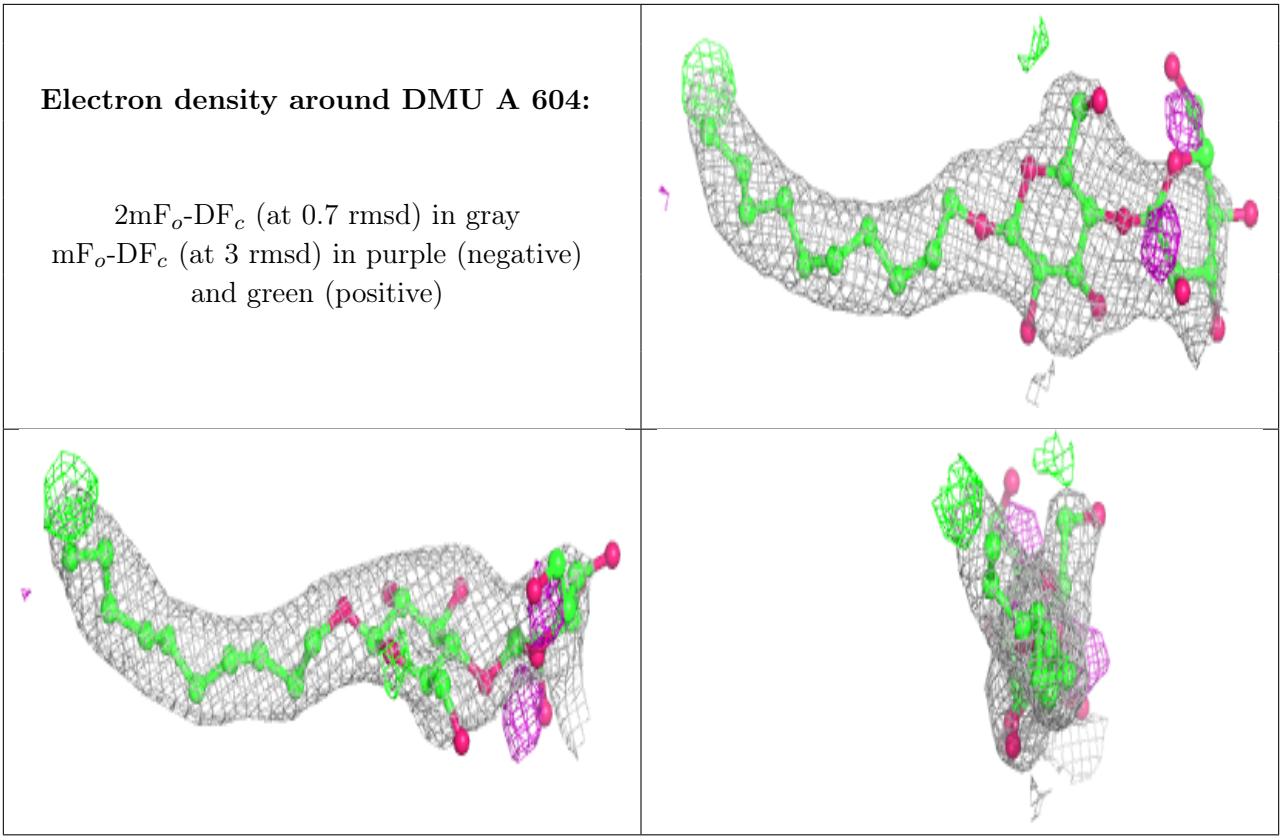
Electron density around DMU A 605:

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



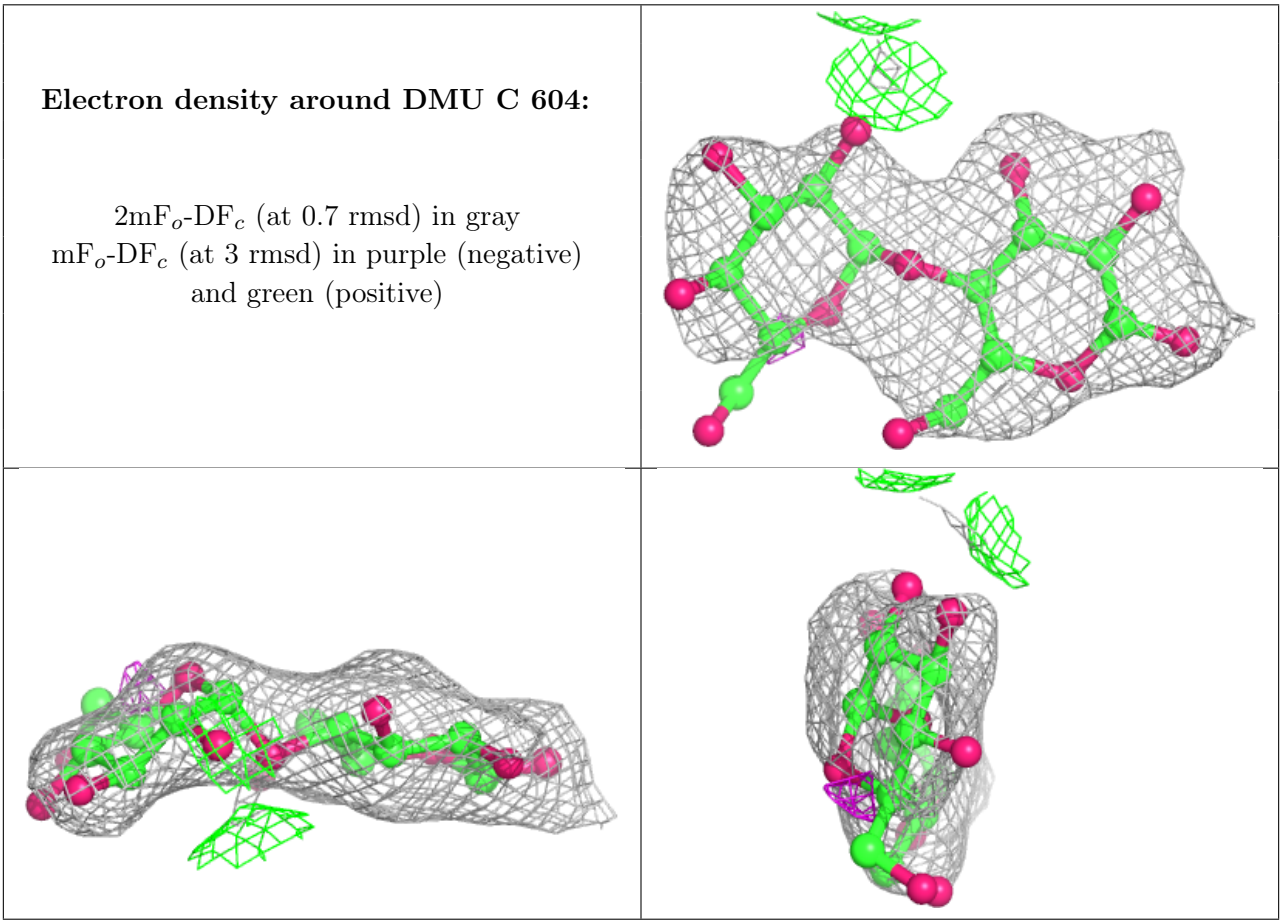
Electron density around DMU A 604:

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



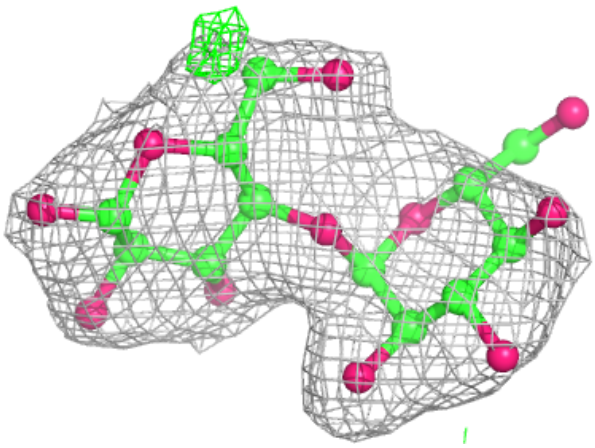
Electron density around DMU C 604:

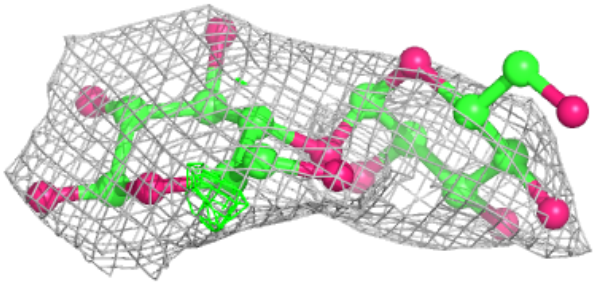
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

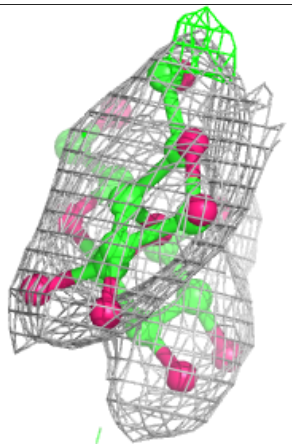


Electron density around DMU D 301:

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

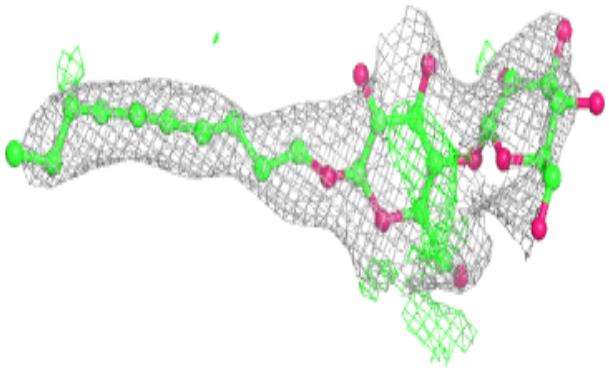


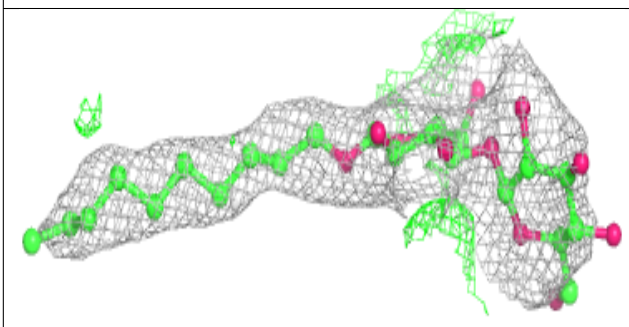


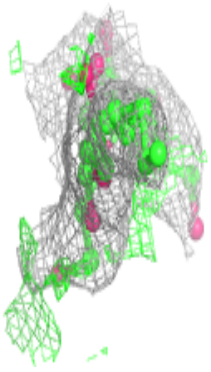


Electron density around DMU C 605:

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

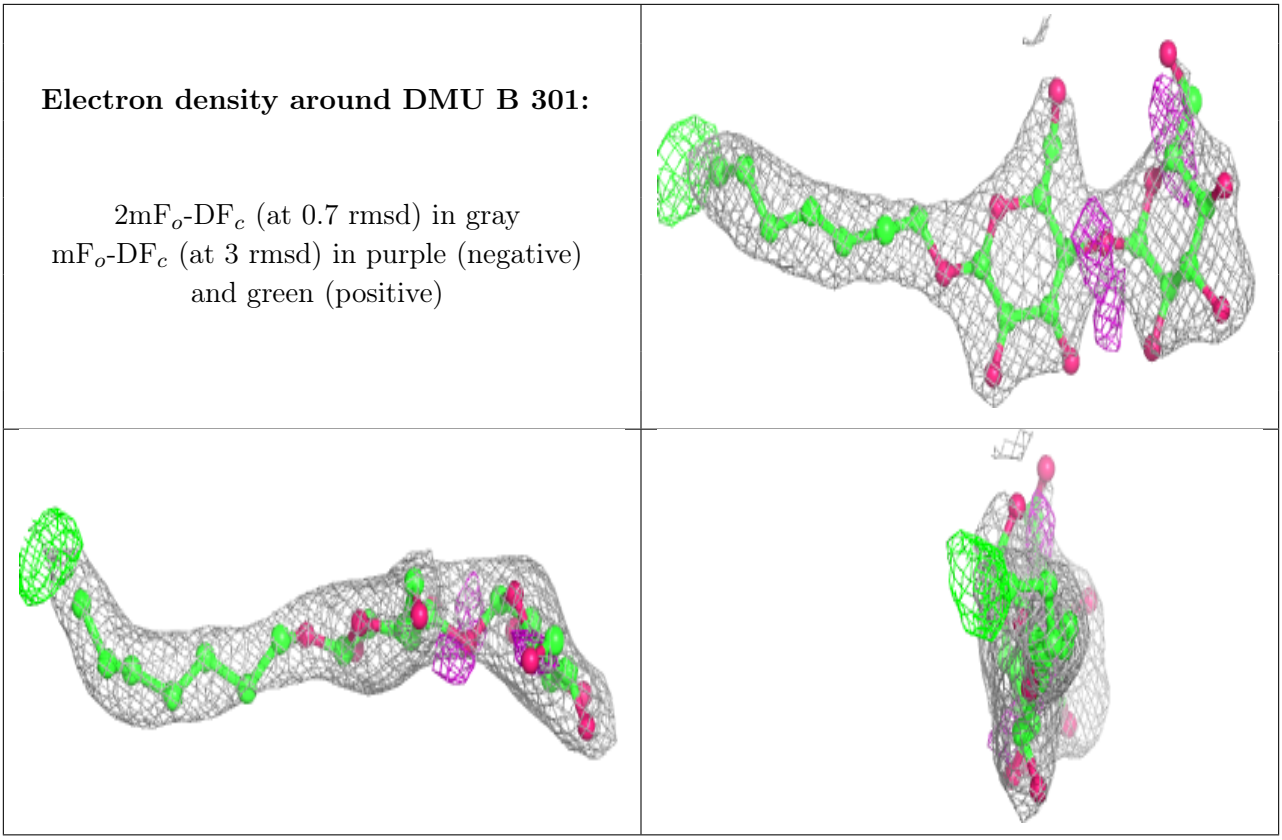






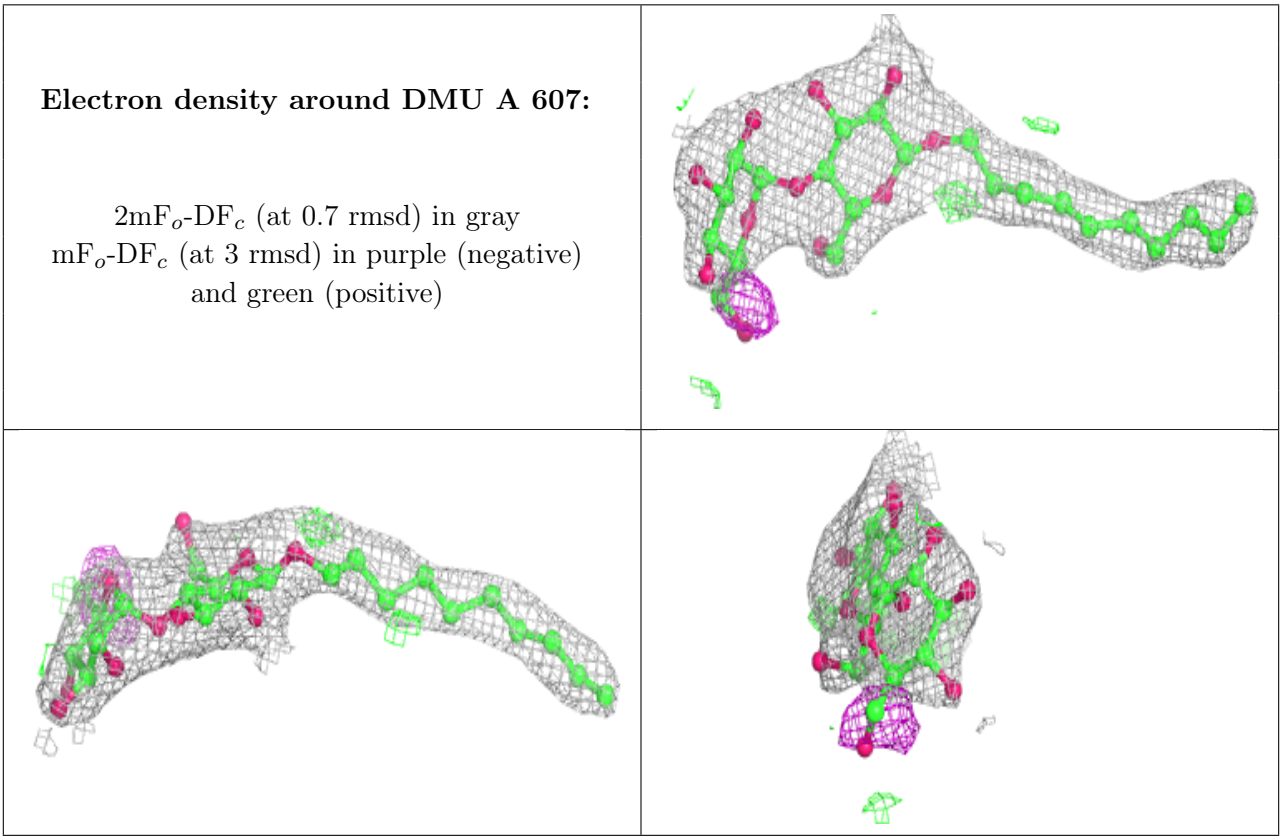
Electron density around DMU B 301:

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



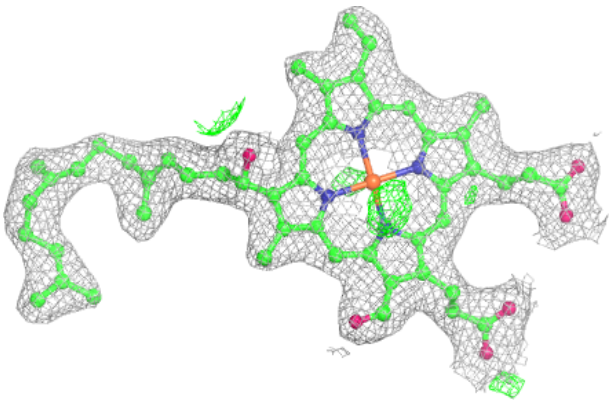
Electron density around DMU A 607:

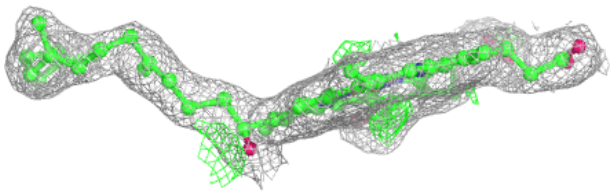
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

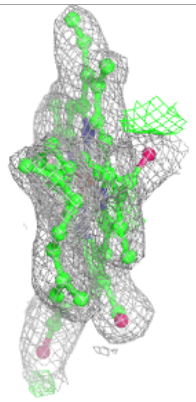


Electron density around HEA A 603:

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

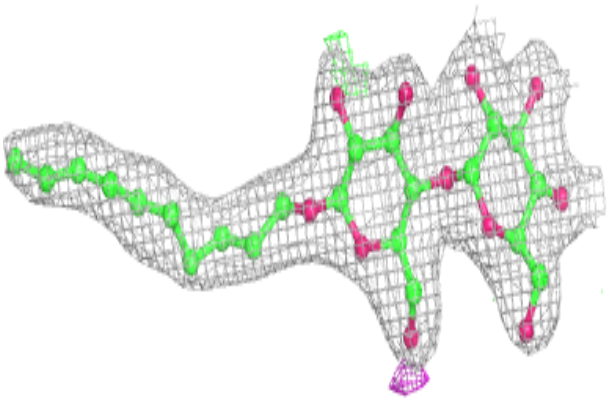


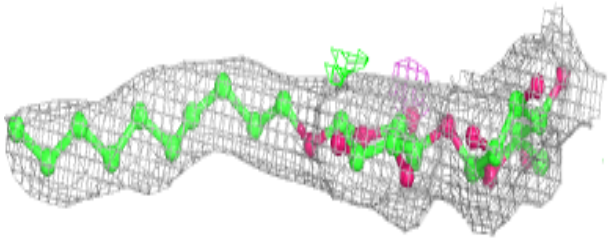


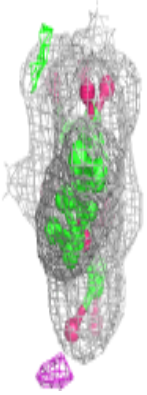


Electron density around DMU A 608:

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

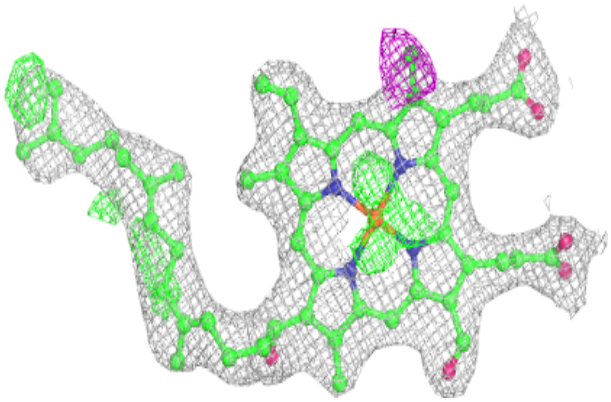


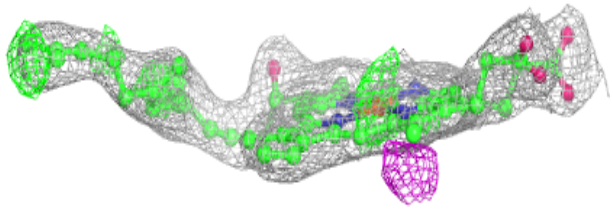


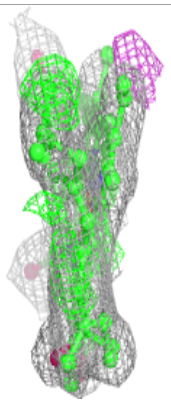


Electron density around HEA C 602:

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

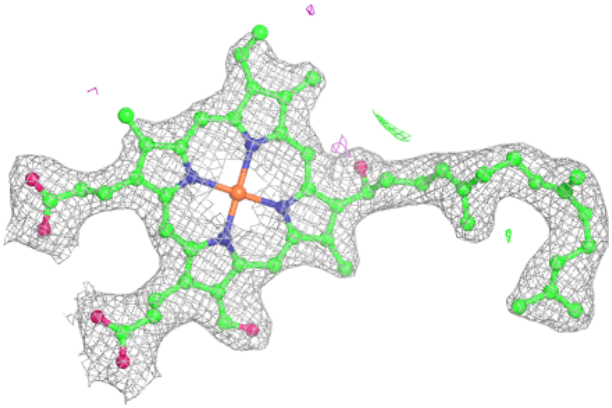


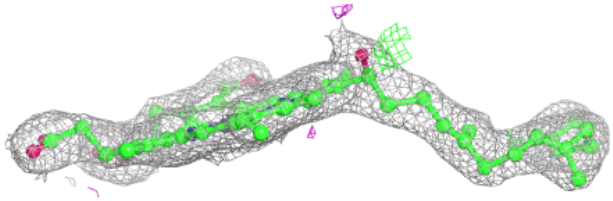


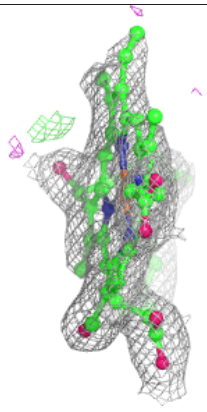


Electron density around HEA C 603:

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

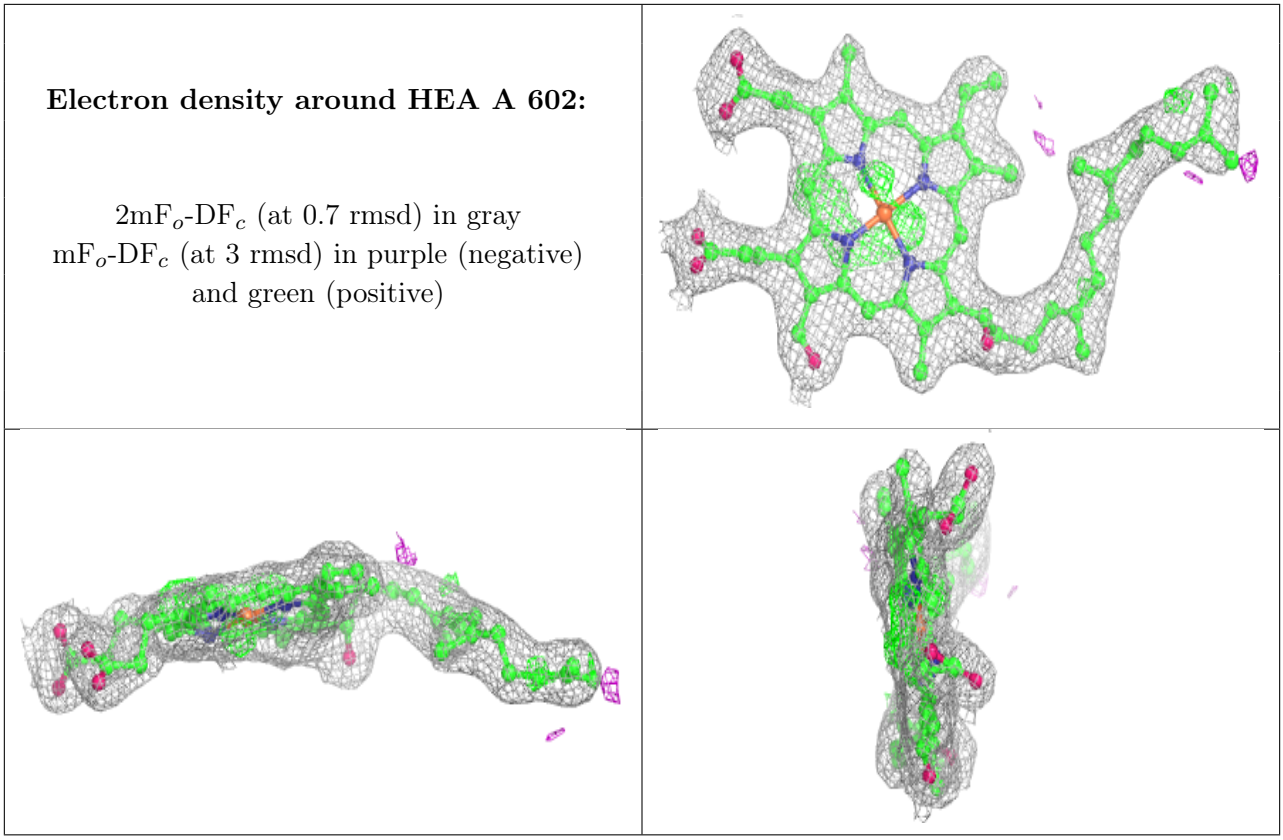






Electron density around HEA A 602:

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



6.5 Other polymers (i)

There are no such residues in this entry.