Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 08:57 PM EDT

PDB ID	:	6PW1
Title	:	Cytochrome c Oxidase delta 16
Authors	:	Liu, J.; Ferguson-Miller, S.
Deposited on	:	2019-07-21
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
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:

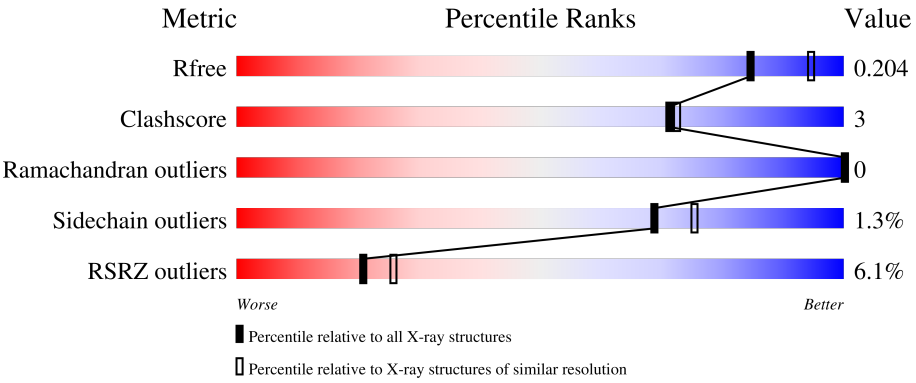
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	534	5% 92% 8%
1	C	534	10% 90% 10%
2	B	257	2% 94% 5%
2	D	257	4% 95% 5%
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
4	TRD	A	605	-	-	-	X
4	TRD	A	607	-	-	-	X
6	HEA	A	615	X	-	-	-
6	HEA	A	616	X	-	-	-
6	HEA	C	604	X	-	-	-
6	HEA	C	605	X	-	-	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 13526 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	534	Total	C	N	O	S	0	0	0
			4154	2780	650	694	30			
1	C	533	Total	C	N	O	S	0	0	0
			4164	2788	655	691	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	1	0	0
			2022	1319	333	364	6			
2	D	256	Total	C	N	O	S	0	0	0
			2003	1308	326	363	6			

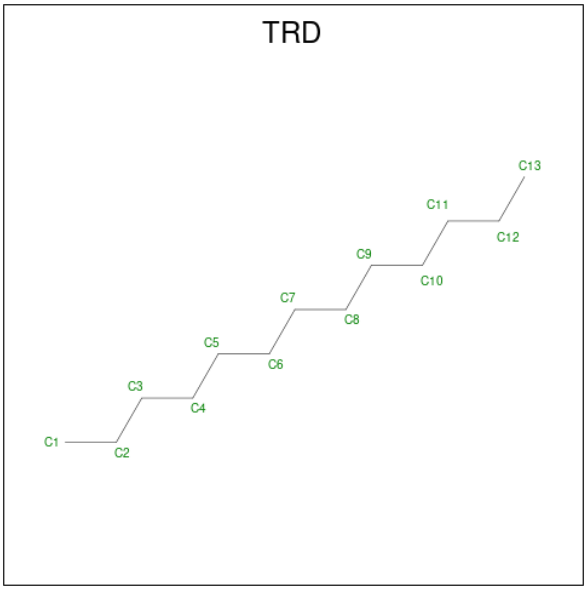
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	29	ALA	-	expression tag	UNP Q3J5G0
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
D	29	ALA	-	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

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



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

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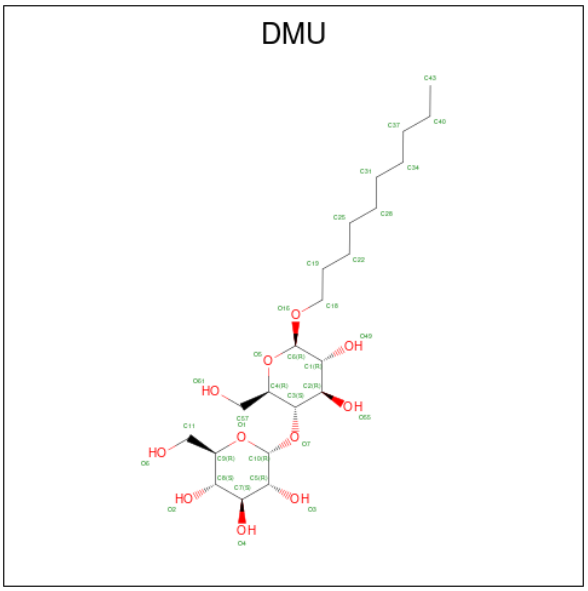
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C 13 13	0	0
4	C	1	Total C 13 13	0	0
4	C	1	Total C 13 13	0	0
4	D	1	Total C 9 9	0	0

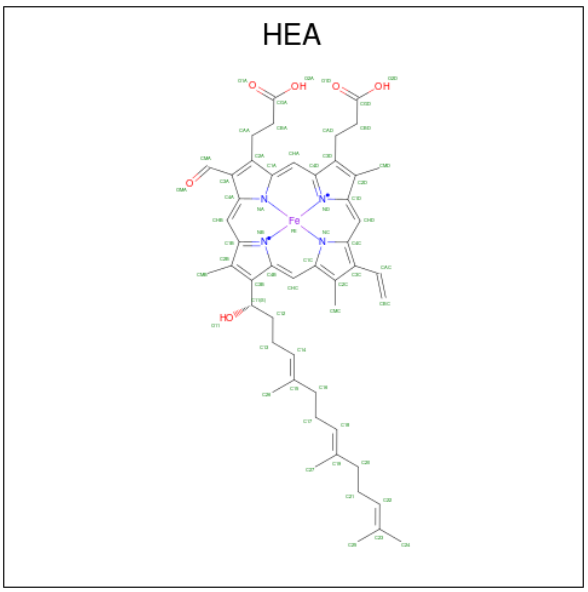
- Molecule 5 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 33 22 11	0	0
5	A	1	Total C O 33 22 11	0	0
5	A	1	Total C O 33 22 11	0	0
5	A	1	Total C O 33 22 11	0	0
5	B	1	Total C O 30 19 11	0	0
5	C	1	Total C O 23 17 6	0	0

- Molecule 6 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Lig-

and of Interest" by depositor).



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

- Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		

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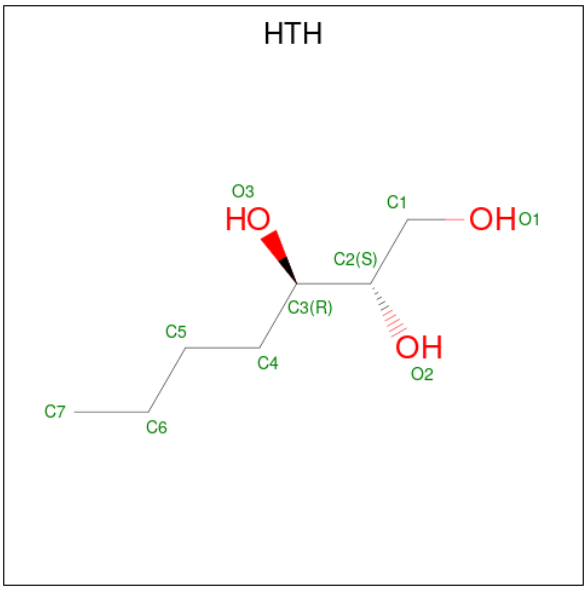
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Mg 1 1	0	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

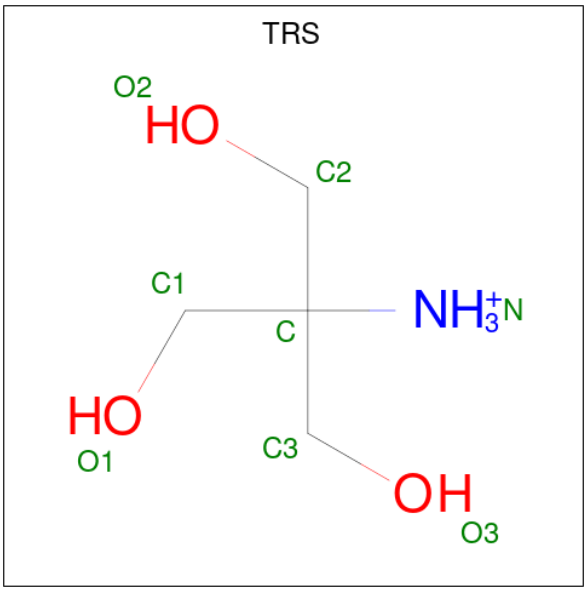
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Ca 1 1	0	0
9	C	1	Total Ca 1 1	0	0

- Molecule 10 is (2S,3R)-heptane-1,2,3-triol (three-letter code: HTH) (formula: $C_7H_{16}O_3$).



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

- Molecule 11 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
11	B	1	Total C N O 8 4 1 3	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 water.

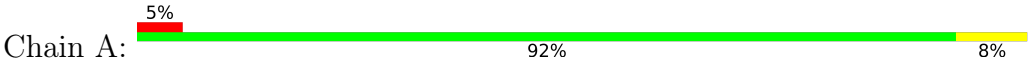
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	150	Total O 150 150	0	0
13	B	124	Total O 124 124	0	0
13	C	102	Total O 102 102	0	0
13	D	122	Total O 122 122	0	0

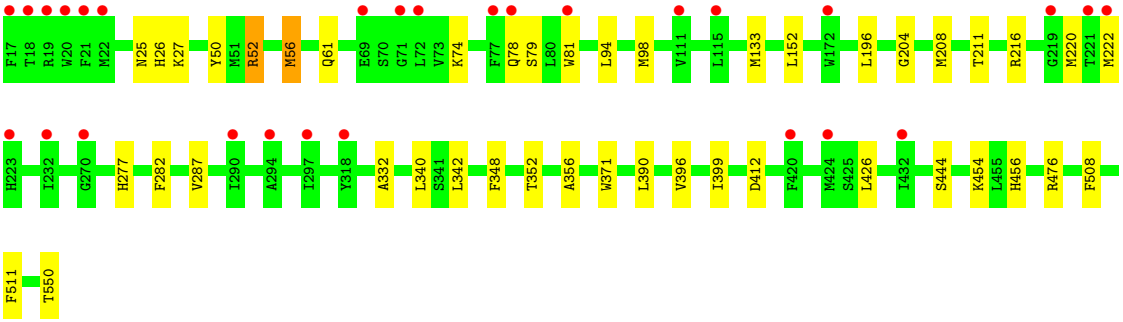
3 Residue-property plots (i)

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

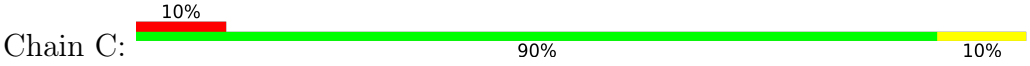
Chain A:

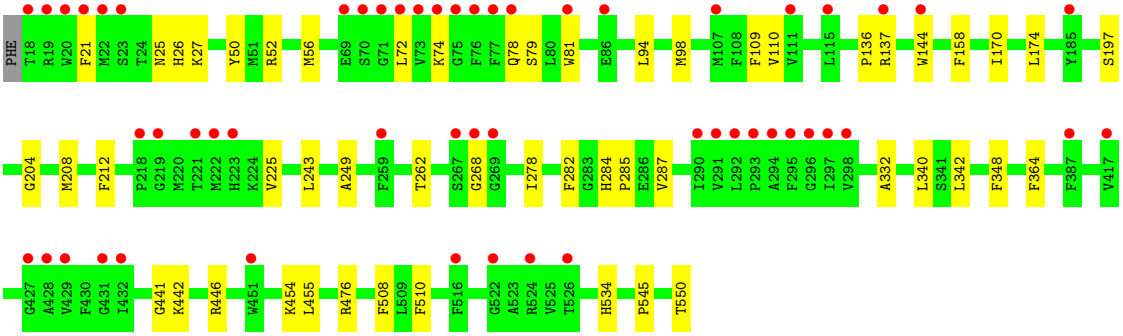




• Molecule 1: Cytochrome c oxidase subunit 1

Chain C:



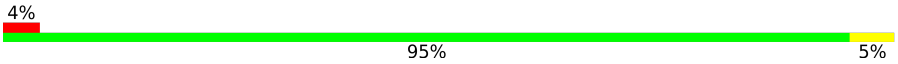


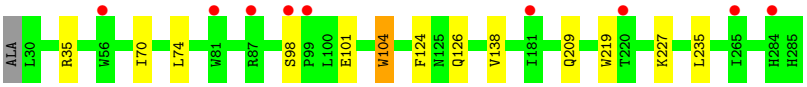
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:

• Molecule 2: Cytochrome c oxidase subunit 2

Chain D:



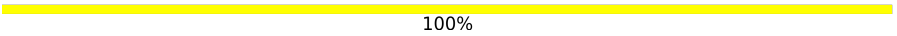


• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

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	123.31Å 130.00Å 177.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.96 – 2.10 35.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.96-2.10) 93.9 (35.85-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.180 , 0.204 0.180 , 0.204	Depositor DCC
R_{free} test set	5009 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 68.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13526	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: CA, MG, HTH, CU, TRD, HEA, TRS, CD, GLC, DMU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.42	0/4306	0.55	0/5883
1	C	0.37	0/4318	0.53	0/5899
2	B	0.41	0/2084	0.53	0/2852
2	D	0.37	0/2064	0.51	0/2828
All	All	0.40	0/12772	0.53	0/17462

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	4154	0	4045	37	0
1	C	4164	0	4062	36	0
2	B	2022	0	1978	8	0
2	D	2003	0	1945	6	0
3	E	23	0	21	0	0
3	F	23	0	21	0	0
4	A	124	0	265	6	0
4	B	13	0	28	0	0
4	C	26	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	9	0	17	0	0
5	A	132	0	168	5	0
5	B	30	0	33	3	0
5	C	23	0	31	0	0
6	A	120	0	108	8	0
6	C	120	0	108	6	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	2	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	A	10	0	16	1	0
10	B	10	0	16	0	0
11	B	8	0	12	0	0
12	B	2	0	0	0	0
12	D	2	0	0	0	0
13	A	150	0	0	1	0
13	B	124	0	0	0	0
13	C	102	0	0	2	0
13	D	122	0	0	0	0
All	All	13526	0	12930	90	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 3.

All (90) 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:170:ILE:HD11	1:C:174:LEU:HD22	1.56	0.86
1:A:27:LYS:NZ	1:A:550:THR:HG22	1.98	0.78
1:A:27:LYS:HZ2	1:A:550:THR:HG22	1.47	0.78
6:A:615:HEA:HBC1	6:A:615:HEA:HMC1	1.68	0.75
6:C:604:HEA:HMC1	6:C:604:HEA:HBC1	1.72	0.72
1:C:170:ILE:CD1	1:C:174:LEU:HD22	2.21	0.70
1:C:27:LYS:HZ2	1:C:550:THR:HG22	1.59	0.67
5:A:614:DMU:O49	13:A:701:HOH:O	1.81	0.65
1:A:74:LYS:O	1:A:78:GLN:HG3	1.98	0.63
1:A:25:ASN:HD21	1:A:550:THR:CG2	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:PHE:HB3	1:C:144:TRP:HZ2	1.65	0.61
1:A:56:MET:HE1	5:A:614:DMU:H10	1.83	0.61
1:A:61:GLN:HG2	5:A:614:DMU:H32	1.82	0.60
1:C:74:LYS:O	1:C:78:GLN:HG3	2.01	0.60
1:A:454:LYS:HD3	4:A:604:TRD:H91	1.85	0.59
1:C:508:PHE:HB2	6:C:604:HEA:H261	1.86	0.58
1:A:287:VAL:HB	6:A:616:HEA:CAC	2.34	0.58
1:C:27:LYS:NZ	1:C:550:THR:HG22	2.20	0.57
1:A:390:LEU:HD13	1:A:426:LEU:HD12	1.86	0.57
1:C:136:PRO:HD2	1:C:137:ARG:HH12	1.71	0.56
1:C:287:VAL:HB	6:C:605:HEA:CAC	2.37	0.54
2:B:96:HIS:O	5:B:302:DMU:O61	2.23	0.52
1:A:52:ARG:NH2	6:A:615:HEA:OMA	2.42	0.52
1:C:50:TYR:OH	1:C:79:SER:HB3	2.09	0.52
6:C:605:HEA:HMC1	6:C:605:HEA:HBC1	1.91	0.52
6:A:616:HEA:HMC1	6:A:616:HEA:HBC1	1.93	0.51
1:A:508:PHE:HB2	6:A:615:HEA:H261	1.92	0.50
1:C:25:ASN:HD21	1:C:550:THR:CG2	2.24	0.50
1:C:26:HIS:CD2	1:C:550:THR:HG21	2.47	0.50
1:C:170:ILE:HD11	1:C:174:LEU:CD2	2.34	0.50
1:A:356:ALA:HB2	1:A:399:ILE:HD11	1.94	0.49
1:C:332:ALA:HB1	1:C:340:LEU:HD11	1.94	0.49
1:C:364:PHE:HB3	2:D:104:TRP:CE3	2.48	0.49
1:C:204:GLY:O	1:C:208:MET:HG2	2.13	0.49
1:A:94:LEU:O	1:A:98:MET:HG2	2.12	0.48
1:C:110:VAL:HG11	6:C:604:HEA:H271	1.94	0.48
1:C:476:ARG:HH21	4:C:601:TRD:H122	1.77	0.48
1:A:26:HIS:CD2	1:A:550:THR:HG21	2.48	0.48
1:C:534:HIS:HD2	13:C:801:HOH:O	1.95	0.48
1:C:109:PHE:CE1	1:C:197:SER:HB2	2.50	0.47
1:C:342:LEU:HD21	2:D:124:PHE:CD2	2.49	0.46
1:A:352:THR:HG22	6:A:616:HEA:HMB2	1.97	0.46
1:A:204:GLY:O	1:A:208:MET:HG2	2.15	0.46
1:C:26:HIS:NE2	1:C:550:THR:HG21	2.30	0.46
1:A:25:ASN:HD21	1:A:550:THR:HG23	1.79	0.46
1:A:456:HIS:CE1	1:A:511:PHE:HB2	2.51	0.46
2:D:209:GLN:HB3	2:D:235:LEU:HD11	1.96	0.46
1:A:332:ALA:HB1	1:A:340:LEU:HD11	1.98	0.46
2:B:138:VAL:HG11	2:B:219:TRP:CD1	2.51	0.46
1:A:277:HIS:HB3	4:A:606:TRD:H81	1.99	0.45
1:A:476:ARG:HH21	4:A:609:TRD:H31	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LEU:HD21	2:B:124:PHE:CD2	2.52	0.44
1:A:371:TRP:CD1	5:B:302:DMU:H9	2.52	0.44
1:C:442:LYS:O	1:C:545:PRO:HA	2.18	0.44
1:A:133:MET:HE3	1:A:211:THR:HG21	2.00	0.44
1:A:287:VAL:HB	6:A:616:HEA:C3C	2.48	0.43
5:A:614:DMU:H36	5:A:614:DMU:H2	1.33	0.43
1:C:262:THR:OG1	1:C:268:GLY:HA3	2.18	0.43
1:C:72:LEU:HD21	1:C:158:PHE:CE1	2.53	0.43
1:C:170:ILE:CD1	1:C:174:LEU:CD2	2.93	0.43
2:D:101:GLU:HA	2:D:104:TRP:CD1	2.53	0.43
10:A:620:HTH:H3	2:B:113:VAL:HA	2.01	0.43
1:C:455:LEU:HD23	1:C:510:PHE:CZ	2.54	0.43
2:D:70:ILE:O	2:D:74:LEU:HG	2.18	0.43
1:C:332:ALA:HB3	1:C:348:PHE:CD2	2.54	0.43
1:C:212:PHE:CE2	1:C:225:VAL:HG11	2.54	0.43
1:A:27:LYS:HZ3	1:A:550:THR:HG22	1.81	0.43
1:A:332:ALA:HB3	1:A:348:PHE:CD2	2.54	0.42
4:A:607:TRD:H71	4:A:607:TRD:H42	1.61	0.42
2:B:97:ASN:ND2	5:B:302:DMU:H29	2.34	0.42
1:C:249:ALA:HB2	1:C:278:ILE:HG22	2.02	0.42
2:B:211:THR:HB	2:B:235:LEU:HD12	2.00	0.42
1:C:454:LYS:HE3	13:C:779:HOH:O	2.18	0.42
1:A:50:TYR:OH	1:A:79:SER:HB3	2.20	0.42
2:D:138:VAL:HG11	2:D:219:TRP:CD1	2.55	0.42
1:A:352:THR:CG2	6:A:616:HEA:HMB2	2.50	0.42
1:A:216:ARG:HD2	1:A:220:MET:O	2.20	0.41
1:C:441:GLY:HA2	1:C:446:ARG:O	2.19	0.41
1:A:396:VAL:HB	2:B:65:ILE:HB	2.02	0.41
1:A:444:SER:HB3	5:A:611:DMU:H8	2.01	0.41
1:C:94:LEU:O	1:C:98:MET:HG2	2.20	0.41
1:C:287:VAL:HB	6:C:605:HEA:C3C	2.50	0.41
1:A:216:ARG:CZ	1:A:222:MET:HG3	2.51	0.41
1:C:243:LEU:HD13	1:C:243:LEU:HA	1.90	0.40
1:A:81:TRP:CZ2	4:A:601:TRD:H62	2.56	0.40
1:A:454:LYS:HD2	4:A:604:TRD:H133	2.04	0.40
1:C:284:HIS:HB3	1:C:285:PRO:HD3	2.04	0.40
1:A:56:MET:HE3	1:A:56:MET:HB3	1.87	0.40
1:A:152:LEU:HD12	1:A:196:LEU:HD12	2.02	0.40
2:B:66:ALA:O	2:B:70:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	532/534 (100%)	520 (98%)	12 (2%)	0	100	100
1	C	531/534 (99%)	521 (98%)	10 (2%)	0	100	100
2	B	254/257 (99%)	246 (97%)	8 (3%)	0	100	100
2	D	254/257 (99%)	246 (97%)	8 (3%)	0	100	100
All	All	1571/1582 (99%)	1533 (98%)	38 (2%)	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	425/434 (98%)	421 (99%)	4 (1%)	78	84
1	C	426/434 (98%)	422 (99%)	4 (1%)	78	84
2	B	214/215 (100%)	211 (99%)	3 (1%)	67	73
2	D	210/215 (98%)	205 (98%)	5 (2%)	49	53
All	All	1275/1298 (98%)	1259 (99%)	16 (1%)	69	75

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	56	MET

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Mol	Chain	Res	Type
1	A	282	PHE
1	A	412	ASP
2	B	35	ARG
2	B	104	TRP
2	B	126	GLN
1	C	52	ARG
1	C	56	MET
1	C	81	TRP
1	C	282	PHE
2	D	35	ARG
2	D	98	SER
2	D	104	TRP
2	D	126	GLN
2	D	227	LYS

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	78	GLN

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	0.50	0	17,17,17	0.49	0
3	GLC	E	2	3	11,11,12	0.58	0	15,15,17	1.24	1 (6%)
3	GLC	F	1	3	12,12,12	0.50	0	17,17,17	1.25	2 (11%)
3	GLC	F	2	3	11,11,12	0.75	0	15,15,17	2.10	3 (20%)

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	-	2/2/22/22	0/1/1/1
3	GLC	F	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2	GLC	C1-C2-C3	5.81	116.81	109.67
3	E	2	GLC	C1-O5-C5	3.83	117.38	112.19
3	F	2	GLC	O5-C1-C2	3.64	116.40	110.77
3	F	1	GLC	C4-C3-C2	-2.88	105.80	110.82
3	F	1	GLC	O4-C4-C5	2.78	116.19	109.30
3	F	2	GLC	C3-C4-C5	-2.31	106.12	110.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1	GLC	O5-C5-C6-O6
3	F	1	GLC	C4-C5-C6-O6
3	E	2	GLC	O5-C5-C6-O6
3	E	1	GLC	O5-C5-C6-O6

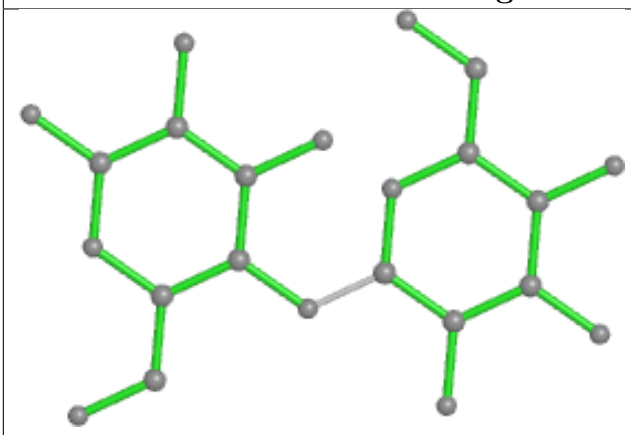
There are no ring outliers.

No monomer is involved in short contacts.

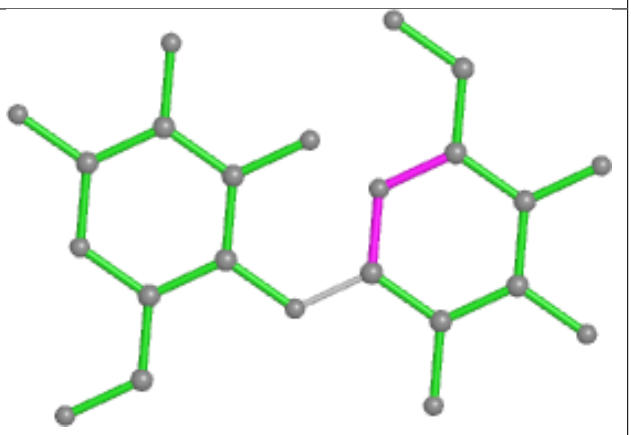
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

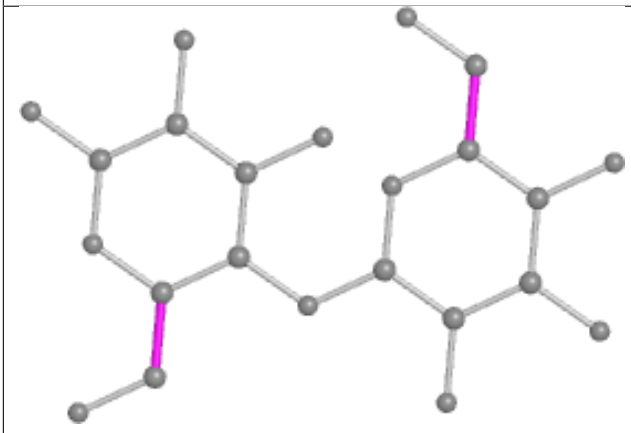
Oligosaccharide Chain E



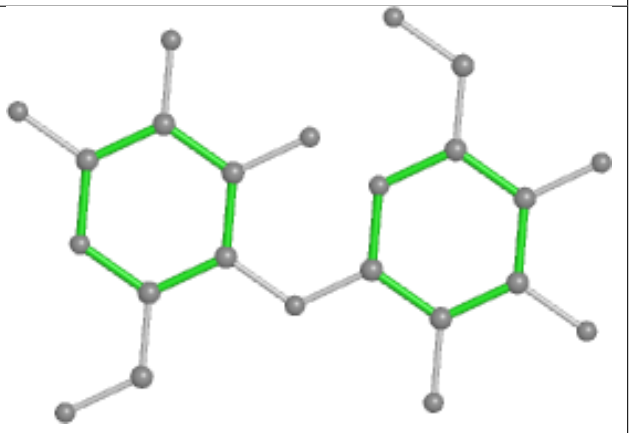
Bond lengths



Bond angles

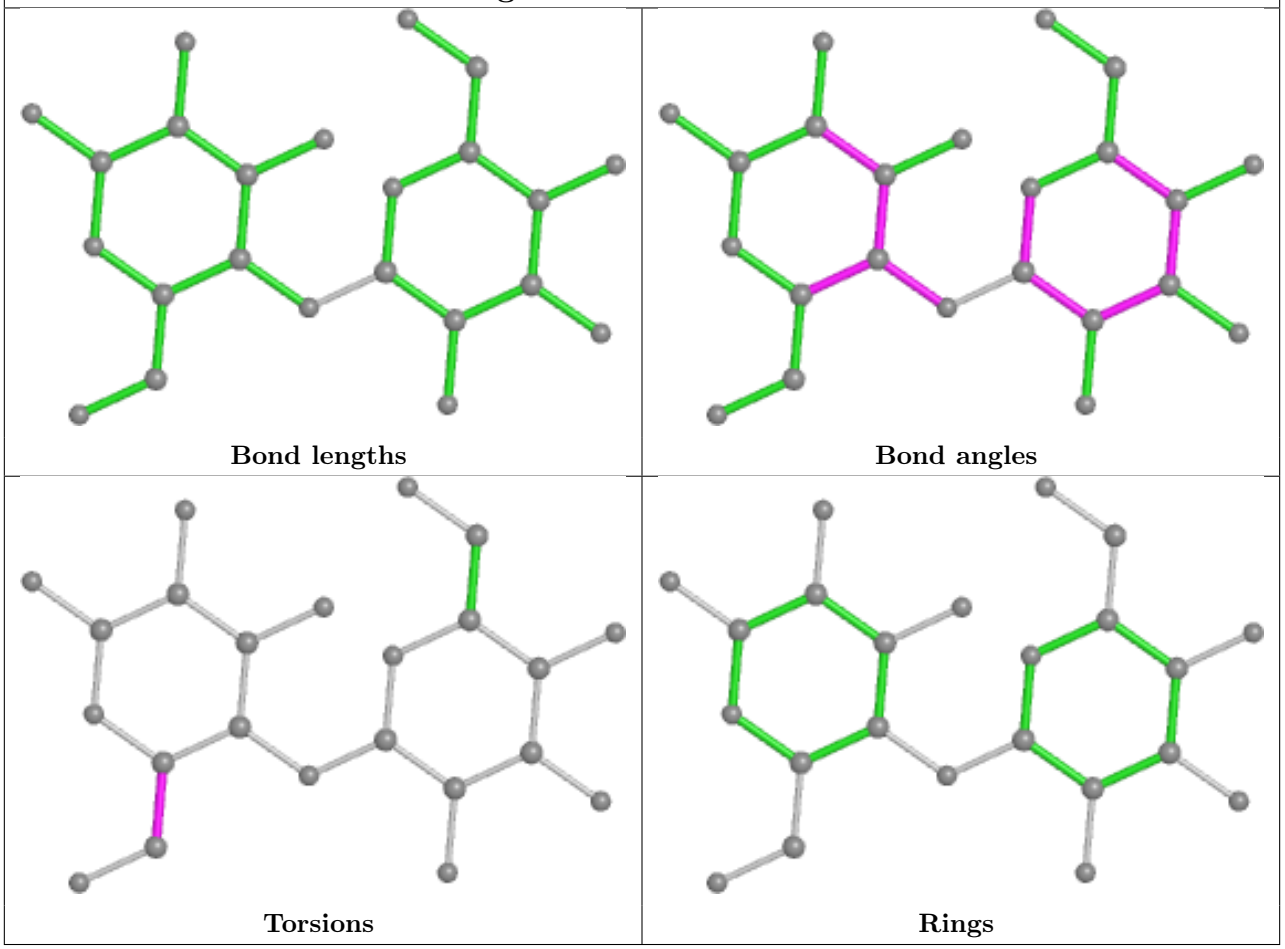


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 41 ligands modelled in this entry, 14 are monoatomic - leaving 27 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	TRD	A	608	-	12,12,12	0.16	0	11,11,11	0.71	0
4	TRD	A	605	-	6,6,12	0.18	0	5,5,11	0.53	0
4	TRD	A	610	-	12,12,12	0.17	0	11,11,11	0.73	0
4	TRD	B	301	-	12,12,12	0.16	0	11,11,11	0.76	0
5	DMU	A	612	-	34,34,34	1.78	9 (26%)	45,45,45	1.24	5 (11%)
4	TRD	A	606	-	12,12,12	0.13	0	11,11,11	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	TRD	A	604	-	12,12,12	0.18	0	11,11,11	0.63	0
4	TRD	A	602	-	12,12,12	0.18	0	11,11,11	0.81	0
6	HEA	C	605	1,13	57,67,67	2.08	15 (26%)	61,103,103	2.43	24 (39%)
5	DMU	A	611	-	34,34,34	1.95	13 (38%)	45,45,45	1.26	4 (8%)
10	HTH	B	309	-	9,9,9	0.57	0	10,10,10	1.12	1 (10%)
4	TRD	C	602	-	12,12,12	0.15	0	11,11,11	0.69	0
10	HTH	A	620	-	9,9,9	0.57	0	10,10,10	1.31	1 (10%)
4	TRD	A	609	-	12,12,12	0.14	0	11,11,11	0.81	0
5	DMU	C	603	-	23,23,34	1.81	6 (26%)	28,28,45	1.01	2 (7%)
4	TRD	D	301	-	8,8,12	0.13	0	7,7,11	0.80	0
4	TRD	A	601	-	12,12,12	0.16	0	11,11,11	0.64	0
11	TRS	B	304	-	7,7,7	0.33	0	9,9,9	1.12	1 (11%)
4	TRD	A	603	-	12,12,12	0.17	0	11,11,11	0.72	0
5	DMU	A	613	-	34,34,34	1.94	10 (29%)	45,45,45	1.39	6 (13%)
6	HEA	A	615	1	57,67,67	1.99	15 (26%)	61,103,103	2.39	21 (34%)
4	TRD	A	607	-	12,12,12	0.11	0	11,11,11	0.87	0
6	HEA	C	604	1	57,67,67	2.03	13 (22%)	61,103,103	2.33	22 (36%)
5	DMU	B	302	-	31,31,34	1.98	13 (41%)	42,42,45	1.24	4 (9%)
5	DMU	A	614	-	34,34,34	1.92	13 (38%)	45,45,45	1.88	11 (24%)
4	TRD	C	601	-	12,12,12	0.15	0	11,11,11	0.92	0
6	HEA	A	616	1,13	57,67,67	1.99	15 (26%)	61,103,103	2.36	22 (36%)

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	TRD	A	608	-	-	7/10/10/10	-
4	TRD	A	605	-	-	1/4/4/10	-
4	TRD	A	610	-	-	3/10/10/10	-
4	TRD	B	301	-	-	3/10/10/10	-
5	DMU	A	612	-	-	3/19/59/59	0/2/2/2
4	TRD	A	606	-	-	3/10/10/10	-
4	TRD	A	604	-	-	5/10/10/10	-
4	TRD	A	602	-	-	2/10/10/10	-
6	HEA	C	605	1,13	2/2/7/16	5/32/76/76	-
5	DMU	A	611	-	-	13/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HTH	B	309	-	-	5/10/10/10	-
4	TRD	C	602	-	-	2/10/10/10	-
10	HTH	A	620	-	-	7/10/10/10	-
4	TRD	A	609	-	-	3/10/10/10	-
5	DMU	C	603	-	-	5/15/35/59	0/1/1/2
4	TRD	D	301	-	-	1/6/6/10	-
4	TRD	A	601	-	-	0/10/10/10	-
11	TRS	B	304	-	-	8/9/9/9	-
4	TRD	A	603	-	-	4/10/10/10	-
5	DMU	A	613	-	-	6/19/59/59	0/2/2/2
6	HEA	A	615	1	2/2/7/16	5/32/76/76	-
4	TRD	A	607	-	-	4/10/10/10	-
6	HEA	C	604	1	2/2/7/16	4/32/76/76	-
5	DMU	B	302	-	-	8/16/56/59	0/2/2/2
6	HEA	A	616	1,13	2/2/7/16	4/32/76/76	-
4	TRD	C	601	-	-	3/10/10/10	-
5	DMU	A	614	-	-	8/19/59/59	0/2/2/2

All (122) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	604	HEA	C3B-C2B	5.61	1.47	1.34
6	C	604	HEA	C3C-C2C	5.18	1.47	1.40
6	C	605	HEA	C3B-C2B	5.13	1.46	1.34
6	A	616	HEA	C3B-C2B	5.12	1.46	1.34
6	C	604	HEA	CHD-C1D	5.03	1.47	1.35
6	A	615	HEA	C3B-C2B	5.00	1.46	1.34
6	C	605	HEA	C3C-C2C	4.97	1.47	1.40
6	A	615	HEA	C3C-C2C	4.95	1.47	1.40
6	C	605	HEA	CHD-C1D	4.89	1.47	1.35
6	A	616	HEA	C3C-C2C	4.85	1.47	1.40
6	A	615	HEA	CHC-C4B	4.83	1.47	1.35
6	C	605	HEA	C3A-C2A	4.79	1.47	1.40
6	A	616	HEA	CHD-C1D	4.78	1.47	1.35
6	A	616	HEA	C3A-C2A	4.73	1.46	1.40
6	C	605	HEA	CHC-C4B	4.71	1.47	1.35
6	C	604	HEA	C3D-C2D	4.68	1.46	1.36
6	A	615	HEA	C3D-C2D	4.65	1.46	1.36
6	C	604	HEA	CHC-C4B	4.60	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	616	HEA	CHC-C4B	4.59	1.46	1.35
6	C	605	HEA	C3D-C2D	4.58	1.46	1.36
6	A	616	HEA	C3D-C2D	4.52	1.46	1.36
6	C	604	HEA	C3A-C2A	4.51	1.46	1.40
6	A	615	HEA	CHD-C1D	4.43	1.46	1.35
5	C	603	DMU	O16-C6	-4.39	1.32	1.40
5	A	614	DMU	O16-C6	-4.38	1.32	1.40
6	A	615	HEA	C3A-C2A	4.10	1.46	1.40
5	A	612	DMU	O16-C6	-3.94	1.33	1.40
5	A	611	DMU	O1-C9	3.87	1.53	1.44
5	A	611	DMU	O16-C6	-3.84	1.33	1.40
5	A	613	DMU	O16-C6	-3.82	1.33	1.40
5	B	302	DMU	O16-C6	-3.76	1.33	1.40
5	A	614	DMU	C11-C9	-3.70	1.39	1.51
5	B	302	DMU	C11-C9	-3.62	1.39	1.51
5	A	613	DMU	C11-C9	-3.61	1.39	1.51
5	B	302	DMU	O1-C9	3.54	1.52	1.44
5	A	611	DMU	C11-C9	-3.52	1.40	1.51
5	A	614	DMU	O1-C9	3.49	1.52	1.44
5	A	613	DMU	O5-C6	3.48	1.50	1.41
5	A	613	DMU	O1-C9	3.43	1.52	1.44
5	C	603	DMU	O7-C3	3.40	1.51	1.42
5	A	612	DMU	O1-C9	3.33	1.52	1.44
5	A	612	DMU	C11-C9	-3.32	1.40	1.51
5	A	614	DMU	O5-C6	3.27	1.50	1.41
5	C	603	DMU	O5-C6	3.26	1.50	1.41
5	A	611	DMU	O5-C6	3.26	1.50	1.41
6	A	615	HEA	C4B-NB	-3.21	1.34	1.40
6	C	604	HEA	C4B-NB	-3.19	1.34	1.40
6	C	605	HEA	FE-NB	3.17	2.12	1.96
5	B	302	DMU	O5-C6	3.16	1.49	1.41
6	C	605	HEA	C1D-ND	-3.06	1.35	1.40
6	A	615	HEA	C1D-ND	-3.06	1.35	1.40
5	A	612	DMU	C8-C9	3.03	1.59	1.53
5	A	613	DMU	O7-C3	2.97	1.51	1.43
6	A	616	HEA	C2A-C1A	2.97	1.49	1.42
6	C	605	HEA	C2A-C1A	2.96	1.49	1.42
5	A	611	DMU	O7-C3	2.96	1.51	1.43
6	C	605	HEA	FE-ND	2.94	2.11	1.96
5	B	302	DMU	O7-C3	2.90	1.51	1.43
5	A	612	DMU	C2-C3	-2.90	1.44	1.52
6	A	616	HEA	C1D-ND	-2.82	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	612	DMU	O5-C6	2.80	1.49	1.41
5	B	302	DMU	C2-C3	-2.80	1.44	1.52
5	A	614	DMU	O7-C3	2.80	1.51	1.43
6	C	604	HEA	C1D-ND	-2.79	1.35	1.40
6	A	616	HEA	FE-ND	2.78	2.10	1.96
5	A	613	DMU	C2-C3	-2.78	1.44	1.52
6	C	605	HEA	C4B-NB	-2.77	1.35	1.40
6	A	615	HEA	C2A-C1A	2.73	1.48	1.42
6	C	605	HEA	C4B-C3B	2.72	1.49	1.44
5	A	614	DMU	O3-C5	2.71	1.49	1.43
5	A	611	DMU	O4-C7	2.71	1.49	1.43
6	C	604	HEA	C2A-C1A	2.67	1.48	1.42
6	C	604	HEA	FE-ND	2.66	2.10	1.96
6	A	616	HEA	FE-NB	2.65	2.10	1.96
6	A	615	HEA	FE-NB	2.63	2.09	1.96
5	A	613	DMU	O5-C4	2.63	1.50	1.44
5	A	613	DMU	O4-C7	2.63	1.49	1.43
5	B	302	DMU	C7-C5	-2.62	1.45	1.52
5	A	614	DMU	C7-C5	-2.61	1.45	1.52
6	C	604	HEA	FE-NB	2.59	2.09	1.96
5	A	611	DMU	C2-C3	-2.59	1.45	1.52
5	A	611	DMU	C8-C9	2.57	1.58	1.53
5	B	302	DMU	O4-C7	2.53	1.48	1.43
5	C	603	DMU	C2-C3	-2.52	1.45	1.52
5	A	612	DMU	O4-C7	2.52	1.48	1.43
5	A	611	DMU	C7-C5	-2.49	1.46	1.52
5	A	611	DMU	O5-C4	2.49	1.50	1.44
6	A	615	HEA	FE-ND	2.45	2.09	1.96
5	A	613	DMU	O55-C2	2.44	1.48	1.43
6	A	615	HEA	C1B-NB	-2.37	1.33	1.38
5	C	603	DMU	O5-C4	2.37	1.50	1.44
6	A	615	HEA	C4C-CHD	2.33	1.47	1.41
6	A	616	HEA	C4B-C3B	2.31	1.48	1.44
6	C	605	HEA	C4D-ND	-2.29	1.34	1.38
5	C	603	DMU	O55-C2	2.28	1.48	1.43
5	A	613	DMU	C7-C5	-2.25	1.46	1.52
6	C	605	HEA	C1C-CHC	2.24	1.47	1.41
6	C	604	HEA	C1C-CHC	2.24	1.47	1.41
5	A	614	DMU	C2-C3	-2.24	1.46	1.52
6	A	616	HEA	C1C-CHC	2.22	1.47	1.41
6	A	616	HEA	C4B-NB	-2.22	1.36	1.40
5	A	614	DMU	O55-C2	2.21	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	614	DMU	C8-C9	2.21	1.57	1.53
5	B	302	DMU	O55-C2	2.21	1.48	1.43
5	A	611	DMU	O3-C5	2.20	1.48	1.43
5	A	611	DMU	O55-C2	2.19	1.48	1.43
6	C	605	HEA	C4C-CHD	2.19	1.47	1.41
5	B	302	DMU	O5-C4	2.16	1.49	1.44
6	A	615	HEA	C1C-CHC	2.14	1.46	1.41
5	A	611	DMU	O1-C10	2.14	1.47	1.41
6	C	604	HEA	C4C-CHD	2.12	1.46	1.41
6	A	616	HEA	C4D-ND	-2.12	1.34	1.38
5	A	612	DMU	O7-C3	2.12	1.49	1.43
6	A	616	HEA	CHB-C1B	2.11	1.47	1.41
5	B	302	DMU	C8-C9	2.11	1.57	1.53
5	A	614	DMU	O1-C10	2.09	1.47	1.41
5	A	614	DMU	O5-C4	2.09	1.49	1.44
5	B	302	DMU	O1-C10	2.08	1.47	1.41
5	B	302	DMU	O3-C5	2.08	1.47	1.43
5	A	614	DMU	O4-C7	2.05	1.47	1.43
6	A	615	HEA	C1D-C2D	2.04	1.48	1.44
5	A	612	DMU	C7-C5	-2.01	1.47	1.52

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	605	HEA	C3D-C4D-ND	6.45	116.60	110.36
6	A	616	HEA	C3D-C4D-ND	6.24	116.40	110.36
6	A	615	HEA	C2B-C1B-NB	5.76	116.78	109.88
6	C	604	HEA	C2B-C1B-NB	5.63	116.63	109.88
6	A	615	HEA	C3D-C4D-ND	5.61	115.79	110.36
6	C	604	HEA	C3D-C4D-ND	5.57	115.75	110.36
5	A	614	DMU	C10-O7-C3	-5.51	104.32	117.96
6	C	605	HEA	C2B-C1B-NB	5.44	116.40	109.88
6	A	616	HEA	CAD-CBD-CGD	-5.43	101.92	113.60
6	A	616	HEA	C2D-C1D-ND	5.31	116.13	109.84
5	A	614	DMU	C1-C2-C3	5.17	121.47	109.68
6	C	604	HEA	C2D-C1D-ND	5.16	115.96	109.84
6	C	605	HEA	CBA-CAA-C2A	-5.14	103.94	112.60
6	C	605	HEA	C2D-C1D-ND	5.06	115.84	109.84
6	C	605	HEA	C3B-C4B-NB	4.99	115.75	109.84
6	A	616	HEA	CBA-CAA-C2A	-4.93	104.29	112.60
6	C	605	HEA	CAD-CBD-CGD	-4.93	103.00	113.60
6	A	616	HEA	C2B-C1B-NB	4.88	115.73	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	616	HEA	C3B-C4B-NB	4.77	115.49	109.84
6	A	615	HEA	C3B-C4B-NB	4.66	115.36	109.84
6	A	616	HEA	C1D-C2D-C3D	-4.64	102.08	106.96
6	A	615	HEA	C2D-C1D-ND	4.53	115.21	109.84
6	C	605	HEA	C1D-C2D-C3D	-4.50	102.22	106.96
6	C	604	HEA	C1B-C2B-C3B	-4.43	101.50	106.80
6	A	615	HEA	C1D-C2D-C3D	-4.41	102.32	106.96
6	C	604	HEA	C1D-C2D-C3D	-4.39	102.35	106.96
6	A	615	HEA	CBA-CAA-C2A	-4.31	105.34	112.60
6	C	604	HEA	C3B-C4B-NB	4.30	114.94	109.84
6	A	615	HEA	C13-C12-C11	-4.25	107.97	114.35
5	A	614	DMU	C6-C1-C2	4.20	118.75	110.00
6	A	615	HEA	CAD-CBD-CGD	-4.14	104.69	113.60
6	C	604	HEA	CBA-CAA-C2A	-4.12	105.66	112.60
6	A	615	HEA	C1B-C2B-C3B	-4.10	101.89	106.80
5	A	613	DMU	C10-C5-C7	4.02	118.38	110.00
6	C	604	HEA	C13-C12-C11	-3.89	108.51	114.35
6	C	605	HEA	C3C-C4C-NC	3.85	114.19	109.21
6	A	615	HEA	C3C-C4C-NC	3.82	114.15	109.21
5	A	614	DMU	C2-C3-C4	3.77	119.58	110.93
6	A	615	HEA	CHB-C1B-C2B	-3.73	119.16	124.98
6	C	604	HEA	C3C-C4C-NC	3.68	113.97	109.21
10	A	620	HTH	C5-C4-C3	-3.68	108.13	114.18
6	A	616	HEA	CHA-C4D-C3D	-3.61	119.53	124.84
6	A	616	HEA	C3C-C4C-NC	3.61	113.88	109.21
5	A	613	DMU	C8-C7-C5	3.61	117.12	110.82
6	C	605	HEA	C1B-C2B-C3B	-3.58	102.52	106.80
6	C	604	HEA	CMC-C2C-C3C	3.53	131.29	124.68
6	C	605	HEA	CMC-C2C-C3C	3.50	131.23	124.68
6	A	616	HEA	CMC-C2C-C3C	3.43	131.10	124.68
6	C	604	HEA	CHB-C1B-C2B	-3.34	119.76	124.98
6	C	604	HEA	CAD-CBD-CGD	-3.29	106.53	113.60
6	A	615	HEA	C13-C14-C15	-3.28	119.77	127.66
5	B	302	DMU	O5-C4-C3	3.22	116.53	109.75
6	A	615	HEA	CHA-C4D-C3D	-3.18	120.17	124.84
6	C	605	HEA	CMB-C2B-C1B	3.17	129.87	125.04
6	C	605	HEA	CHA-C4D-C3D	-3.16	120.19	124.84
5	A	611	DMU	O5-C6-C1	-3.16	103.66	110.35
5	A	611	DMU	C18-O16-C6	3.11	119.00	113.84
5	A	613	DMU	O16-C6-C1	3.09	113.12	108.30
5	A	612	DMU	C10-O7-C3	-2.98	110.60	117.96
6	A	616	HEA	C4B-C3B-C2B	-2.96	102.36	107.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	616	HEA	CHB-C1B-C2B	-2.94	120.39	124.98
5	A	611	DMU	O5-C4-C3	2.93	115.94	109.75
6	C	605	HEA	C4D-C3D-C2D	-2.93	102.62	106.90
6	A	615	HEA	CMC-C2C-C3C	2.89	130.09	124.68
5	A	612	DMU	O1-C9-C8	-2.88	104.47	109.69
5	C	603	DMU	O5-C4-C3	2.84	115.74	109.75
5	B	302	DMU	C10-O7-C3	-2.83	110.97	117.96
6	A	615	HEA	C27-C19-C20	2.83	120.02	115.27
6	A	616	HEA	C1B-C2B-C3B	-2.79	103.47	106.80
6	C	604	HEA	CMD-C2D-C1D	2.77	129.26	125.04
6	C	605	HEA	C4B-C3B-C2B	-2.75	102.72	107.41
6	A	616	HEA	C4D-C3D-C2D	-2.70	102.96	106.90
6	A	616	HEA	C27-C19-C20	2.68	119.78	115.27
6	C	604	HEA	C4D-C3D-C2D	-2.68	102.99	106.90
6	C	604	HEA	CHA-C4D-C3D	-2.64	120.96	124.84
6	A	616	HEA	C1D-ND-C4D	-2.61	102.37	105.07
5	B	302	DMU	O5-C6-C1	-2.61	104.83	110.35
6	A	615	HEA	CMD-C2D-C1D	2.60	129.00	125.04
6	C	604	HEA	C13-C14-C15	-2.60	121.40	127.66
5	A	611	DMU	C10-O7-C3	-2.60	111.53	117.96
5	B	302	DMU	C57-C4-C3	-2.56	105.86	113.33
6	A	615	HEA	C4D-C3D-C2D	-2.52	103.22	106.90
5	A	614	DMU	O1-C10-C5	2.48	115.61	110.35
6	A	615	HEA	C4B-C3B-C2B	-2.48	103.18	107.41
6	C	605	HEA	C27-C19-C20	2.47	119.42	115.27
5	A	614	DMU	O7-C10-C5	2.46	114.48	108.10
11	B	304	TRS	C1-C-N	2.46	115.31	107.98
6	C	605	HEA	C4B-NB-C1B	-2.43	102.57	105.07
5	A	613	DMU	O5-C4-C3	2.41	114.84	109.75
6	C	604	HEA	C17-C18-C19	-2.40	121.88	127.66
5	C	603	DMU	O5-C6-C1	-2.38	105.31	110.35
6	C	605	HEA	CMD-C2D-C1D	2.37	128.64	125.04
6	C	605	HEA	CHB-C1B-C2B	-2.35	121.30	124.98
6	C	605	HEA	C1D-ND-C4D	-2.34	102.66	105.07
5	A	613	DMU	O5-C6-C1	-2.31	105.47	110.35
5	A	614	DMU	O55-C2-C1	-2.29	105.06	110.35
5	A	612	DMU	O5-C6-C1	-2.27	105.55	110.35
5	A	612	DMU	O61-C57-C4	-2.27	103.52	111.29
6	C	604	HEA	C25-C23-C24	2.25	119.56	114.60
6	A	616	HEA	CMD-C2D-C1D	2.24	128.46	125.04
6	C	605	HEA	C26-C15-C16	2.24	119.04	115.27
6	A	616	HEA	CHD-C1D-C2D	-2.24	120.53	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	613	DMU	O4-C7-C8	-2.23	105.19	110.35
6	A	615	HEA	C4B-NB-C1B	-2.22	102.78	105.07
6	C	604	HEA	C4B-C3B-C2B	-2.20	103.65	107.41
5	A	614	DMU	O5-C4-C3	2.18	114.36	109.75
6	A	616	HEA	CMB-C2B-C1B	2.16	128.33	125.04
5	A	614	DMU	O1-C9-C11	2.12	111.70	106.44
6	C	605	HEA	C13-C14-C15	-2.12	122.56	127.66
10	B	309	HTH	C5-C4-C3	-2.10	110.72	114.18
6	C	604	HEA	C21-C22-C23	-2.10	120.58	127.75
6	A	615	HEA	C17-C18-C19	-2.09	122.63	127.66
5	A	614	DMU	O3-C5-C7	2.08	115.16	110.35
6	A	616	HEA	C4B-NB-C1B	-2.07	102.93	105.07
6	C	605	HEA	CHC-C4B-NB	-2.06	121.84	124.38
5	A	614	DMU	O49-C1-C2	-2.06	105.59	110.35
6	C	604	HEA	CHD-C1D-C2D	-2.05	121.04	126.72
6	C	604	HEA	C1D-ND-C4D	-2.05	102.95	105.07
6	A	616	HEA	O1A-CGA-CBA	-2.05	116.49	123.08
5	A	612	DMU	C11-C9-C8	2.04	117.77	113.00
6	A	616	HEA	C25-C23-C24	2.03	119.08	114.60
6	C	605	HEA	CHB-C1B-NB	-2.02	122.24	124.43
6	A	615	HEA	CAA-CBA-CGA	-2.01	108.11	113.76
6	C	605	HEA	CHD-C1D-C2D	-2.00	121.18	126.72

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	615	HEA	NB
6	A	615	HEA	ND
6	A	616	HEA	NB
6	A	616	HEA	ND
6	C	604	HEA	NB
6	C	604	HEA	ND
6	C	605	HEA	NB
6	C	605	HEA	ND

All (122) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	302	DMU	O5-C6-O16-C18
5	B	302	DMU	C19-C18-O16-C6
10	A	620	HTH	C1-C2-C3-O3
10	A	620	HTH	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
10	A	620	HTH	O2-C2-C3-O3
10	A	620	HTH	O2-C2-C3-C4
10	B	309	HTH	O1-C1-C2-O2
11	B	304	TRS	C1-C-C3-O3
11	B	304	TRS	C2-C-C3-O3
11	B	304	TRS	N-C-C3-O3
5	A	614	DMU	C2-C3-O7-C10
10	B	309	HTH	O1-C1-C2-C3
5	A	613	DMU	O5-C4-C57-O61
5	B	302	DMU	C3-C4-C57-O61
5	A	611	DMU	O5-C4-C57-O61
5	B	302	DMU	O5-C4-C57-O61
5	A	611	DMU	C3-C4-C57-O61
5	A	611	DMU	O6-C11-C9-O1
5	C	603	DMU	O16-C18-C19-C22
5	A	614	DMU	C4-C3-O7-C10
5	A	614	DMU	O16-C18-C19-C22
5	B	302	DMU	O16-C18-C19-C22
5	A	611	DMU	C31-C34-C37-C40
4	A	608	TRD	C6-C7-C8-C9
4	A	609	TRD	C11-C10-C9-C8
4	D	301	TRD	C3-C4-C5-C6
4	A	610	TRD	C6-C7-C8-C9
4	A	604	TRD	C4-C5-C6-C7
5	A	611	DMU	C25-C28-C31-C34
4	A	608	TRD	C7-C8-C9-C10
5	A	614	DMU	O6-C11-C9-O1
4	A	603	TRD	C3-C4-C5-C6
5	A	611	DMU	C22-C25-C28-C31
5	A	611	DMU	C19-C18-O16-C6
5	A	613	DMU	C19-C18-O16-C6
10	B	309	HTH	O3-C3-C4-C5
4	A	607	TRD	C7-C8-C9-C10
6	A	615	HEA	C14-C15-C16-C17
4	A	604	TRD	C9-C10-C11-C12
4	A	606	TRD	C9-C10-C11-C12
6	A	615	HEA	C26-C15-C16-C17
5	A	614	DMU	C34-C37-C40-C43
4	C	601	TRD	C3-C4-C5-C6
5	C	603	DMU	C3-C4-C57-O61
4	A	609	TRD	C4-C5-C6-C7
5	A	611	DMU	O16-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
4	A	607	TRD	C6-C7-C8-C9
11	B	304	TRS	C3-C-C1-O1
5	A	611	DMU	O6-C11-C9-C8
5	A	611	DMU	C19-C22-C25-C28
4	C	601	TRD	C11-C10-C9-C8
5	B	302	DMU	C18-C19-C22-C25
6	C	604	HEA	C26-C15-C16-C17
6	C	604	HEA	C14-C15-C16-C17
5	B	302	DMU	C22-C25-C28-C31
4	B	301	TRD	C1-C2-C3-C4
5	A	611	DMU	C34-C37-C40-C43
5	A	612	DMU	C31-C34-C37-C40
10	B	309	HTH	C2-C3-C4-C5
5	C	603	DMU	C25-C28-C31-C34
4	C	602	TRD	C7-C8-C9-C10
5	A	614	DMU	C19-C18-O16-C6
5	C	603	DMU	C19-C18-O16-C6
4	A	608	TRD	C10-C11-C12-C13
4	A	603	TRD	C11-C10-C9-C8
5	A	611	DMU	C18-C19-C22-C25
4	A	606	TRD	C11-C10-C9-C8
4	A	608	TRD	C3-C4-C5-C6
4	A	608	TRD	C11-C10-C9-C8
4	A	603	TRD	C10-C11-C12-C13
5	B	302	DMU	C25-C28-C31-C34
4	A	610	TRD	C11-C10-C9-C8
4	C	601	TRD	C1-C2-C3-C4
5	A	613	DMU	C25-C28-C31-C34
5	A	611	DMU	O5-C6-O16-C18
5	A	613	DMU	C3-C4-C57-O61
11	B	304	TRS	N-C-C1-O1
4	A	607	TRD	C3-C4-C5-C6
5	C	603	DMU	C19-C22-C25-C28
4	A	604	TRD	C6-C7-C8-C9
4	A	610	TRD	C7-C8-C9-C10
10	A	620	HTH	O3-C3-C4-C5
4	A	602	TRD	C9-C10-C11-C12
4	A	607	TRD	C9-C10-C11-C12
4	A	608	TRD	C9-C10-C11-C12
10	B	309	HTH	C4-C5-C6-C7
10	A	620	HTH	C4-C5-C6-C7
4	A	608	TRD	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	A	609	TRD	C3-C4-C5-C6
4	A	602	TRD	C11-C10-C9-C8
6	A	616	HEA	CAA-CBA-CGA-O1A
5	A	614	DMU	O6-C11-C9-C8
4	B	301	TRD	C7-C8-C9-C10
4	A	603	TRD	C1-C2-C3-C4
4	C	602	TRD	C6-C7-C8-C9
5	A	613	DMU	C28-C31-C34-C37
11	B	304	TRS	C2-C-C1-O1
11	B	304	TRS	C1-C-C2-O2
5	A	613	DMU	C22-C25-C28-C31
6	A	616	HEA	CAA-CBA-CGA-O2A
6	C	605	HEA	CAD-CBD-CGD-O2D
6	C	605	HEA	CAD-CBD-CGD-O1D
6	A	616	HEA	CAD-CBD-CGD-O1D
4	A	604	TRD	C1-C2-C3-C4
6	A	616	HEA	CAD-CBD-CGD-O2D
4	B	301	TRD	C5-C6-C7-C8
4	A	606	TRD	C7-C8-C9-C10
6	C	604	HEA	CAD-CBD-CGD-O2D
5	A	614	DMU	C18-C19-C22-C25
5	A	612	DMU	C3-C4-C57-O61
6	C	605	HEA	CAA-CBA-CGA-O1A
6	C	604	HEA	CAD-CBD-CGD-O1D
6	A	615	HEA	CAD-CBD-CGD-O1D
6	A	615	HEA	CAD-CBD-CGD-O2D
4	A	604	TRD	C10-C11-C12-C13
6	C	605	HEA	CAA-CBA-CGA-O2A
10	A	620	HTH	C2-C3-C4-C5
11	B	304	TRS	C3-C-C2-O2
6	A	615	HEA	CAA-CBA-CGA-O1A
4	A	605	TRD	C1-C2-C3-C4
5	A	612	DMU	C18-C19-C22-C25
6	C	605	HEA	C26-C15-C16-C17

There are no ring outliers.

14 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	606	TRD	1	0
4	A	604	TRD	2	0
6	C	605	HEA	3	0

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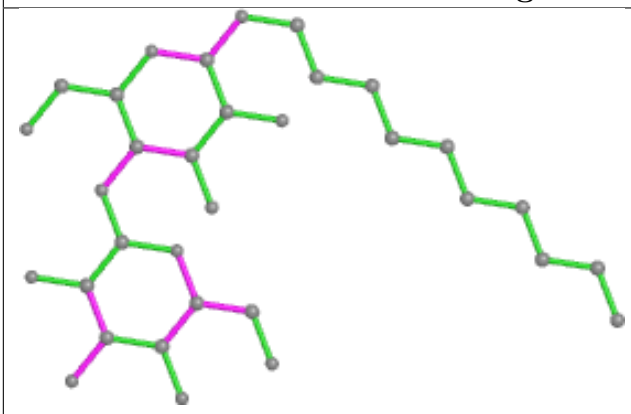
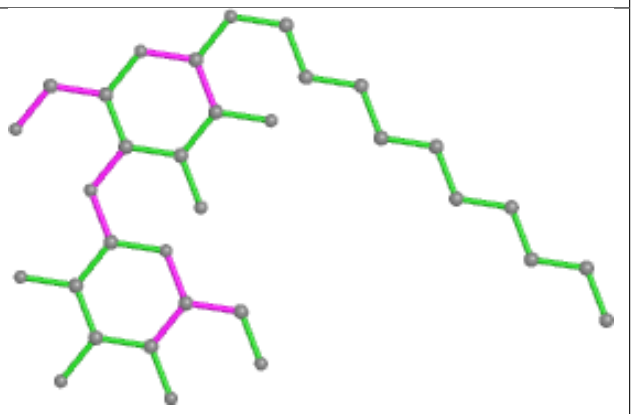
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	611	DMU	1	0
10	A	620	HTH	1	0
4	A	609	TRD	1	0
4	A	601	TRD	1	0
6	A	615	HEA	3	0
4	A	607	TRD	1	0
6	C	604	HEA	3	0
5	B	302	DMU	3	0
5	A	614	DMU	4	0
4	C	601	TRD	1	0
6	A	616	HEA	5	0

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.

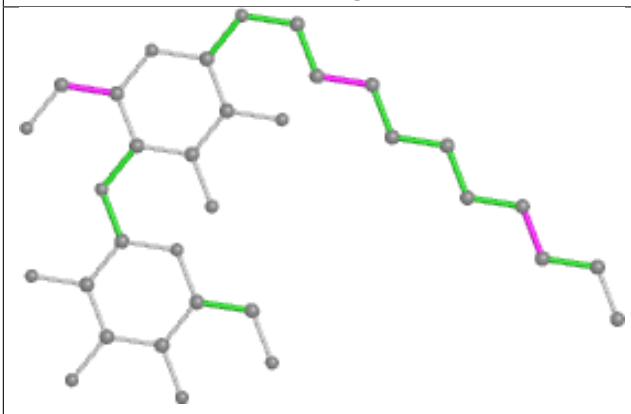
Ligand DMU A 612



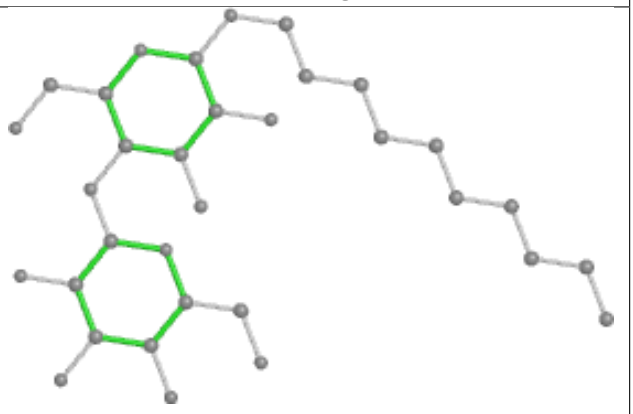
Bond lengths



Bond angles

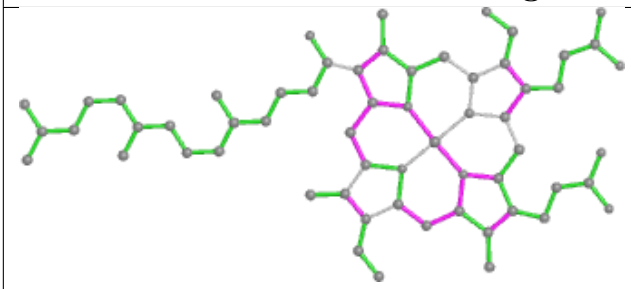


Torsions

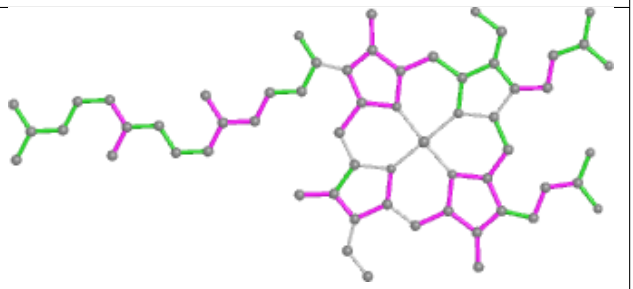


Rings

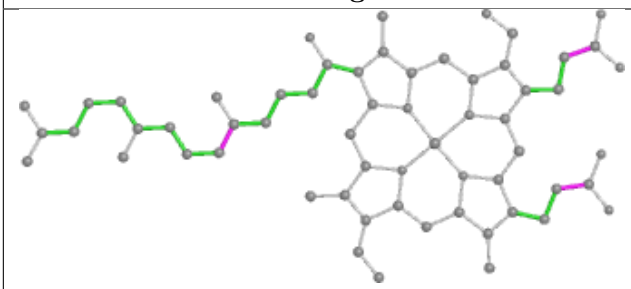
Ligand HEA C 605



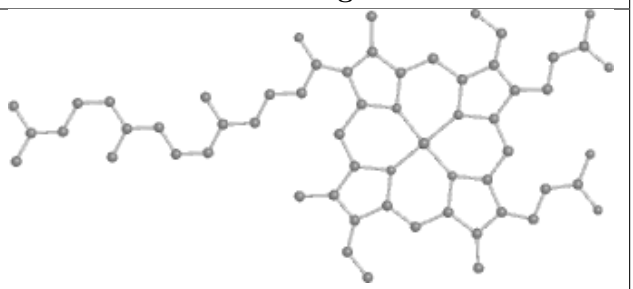
Bond lengths



Bond angles

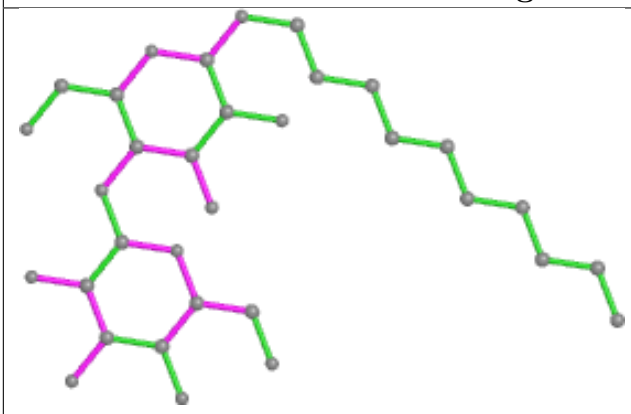


Torsions

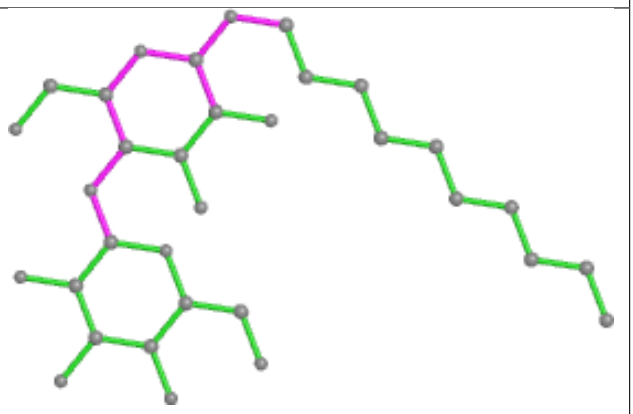


Rings

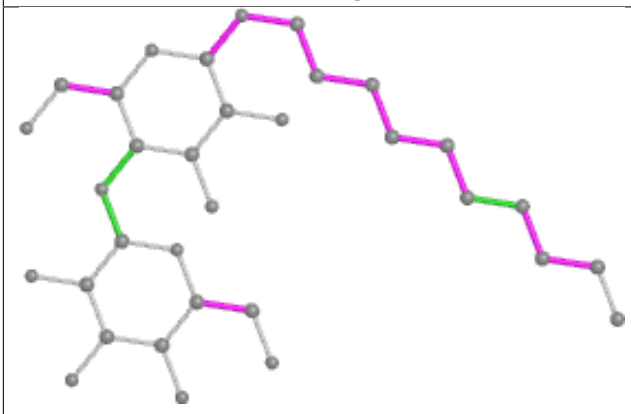
Ligand DMU A 611



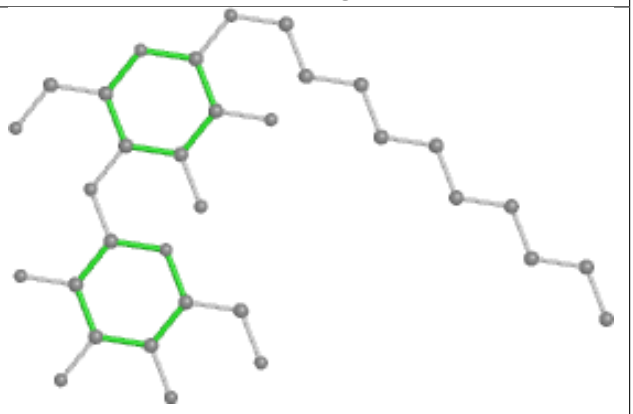
Bond lengths



Bond angles

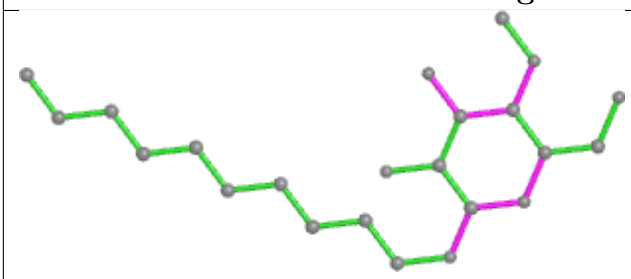


Torsions

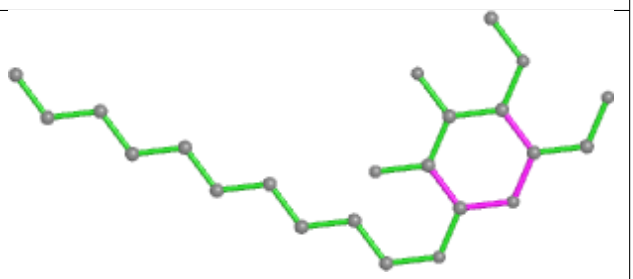


Rings

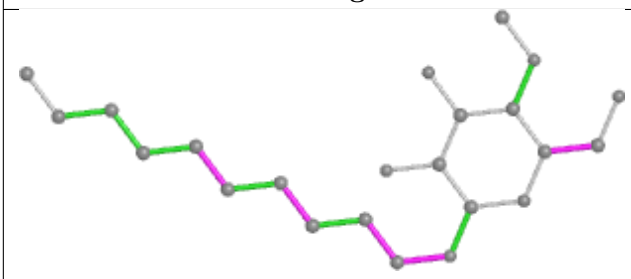
Ligand DMU C 603



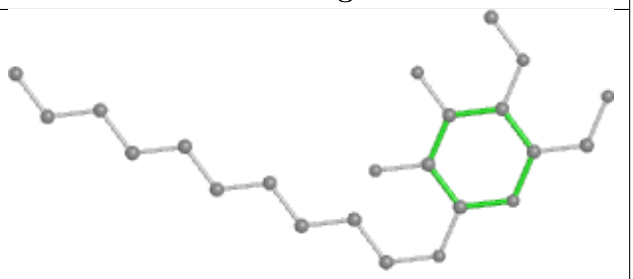
Bond lengths



Bond angles

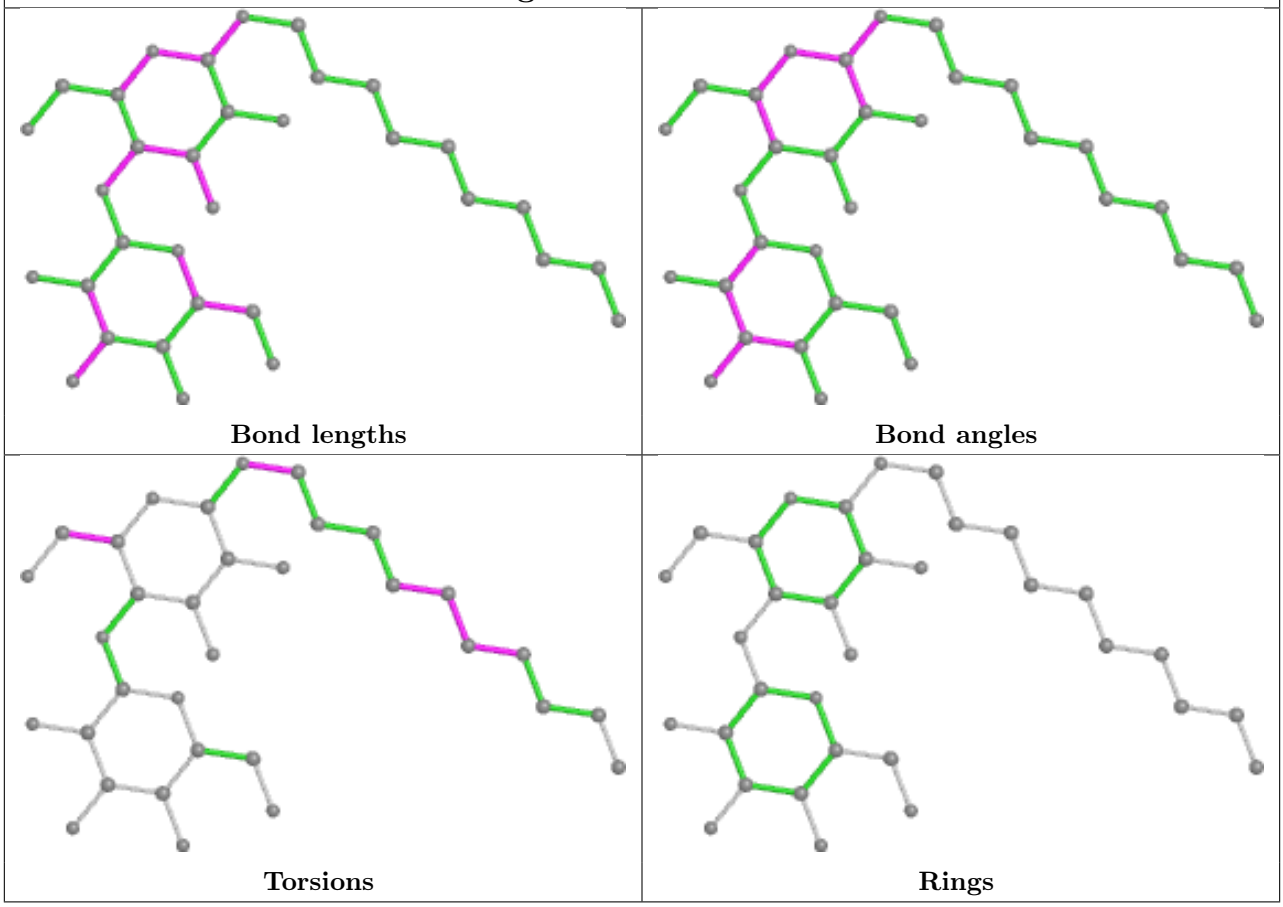


Torsions

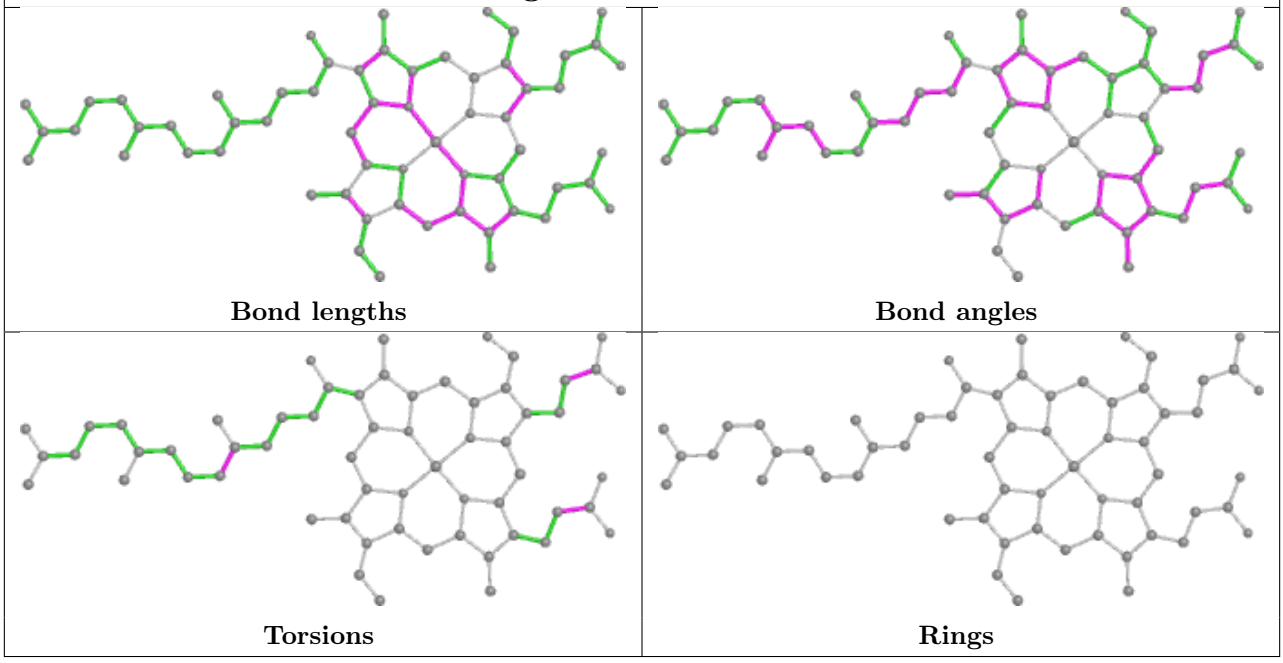


Rings

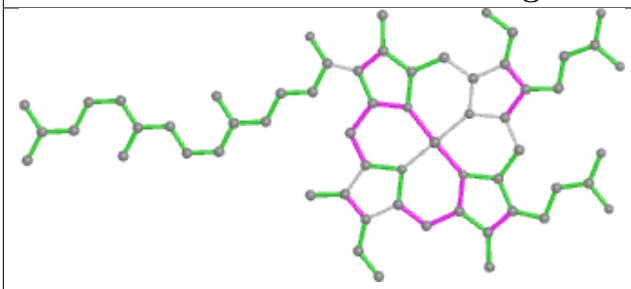
Ligand DMU A 613



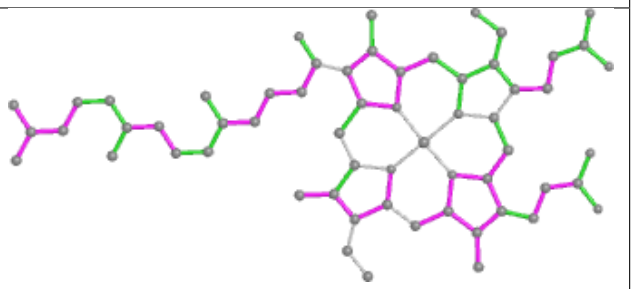
Ligand HEA A 615



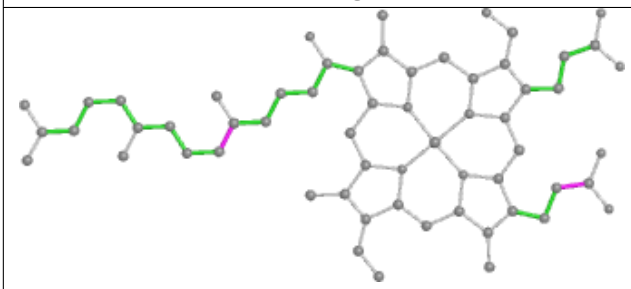
Ligand HEA C 604



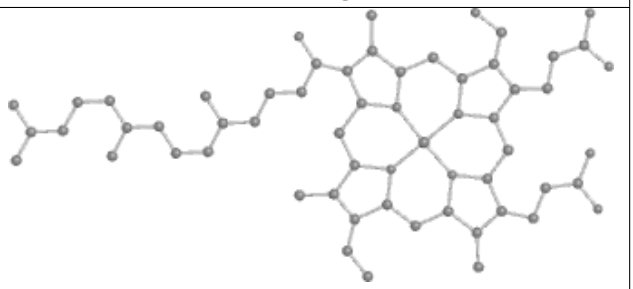
Bond lengths



Bond angles

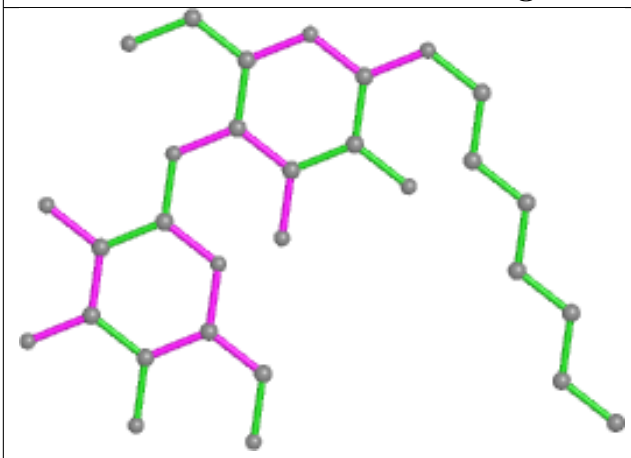


Torsions

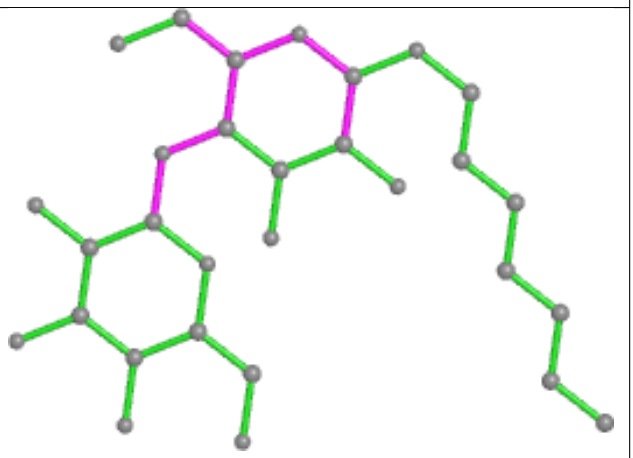


Rings

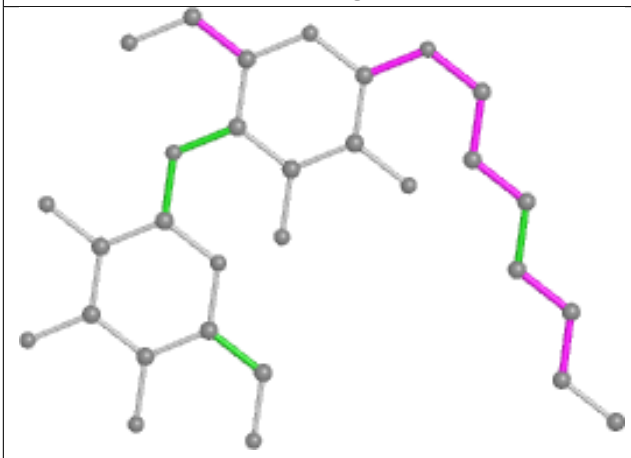
Ligand DMU B 302



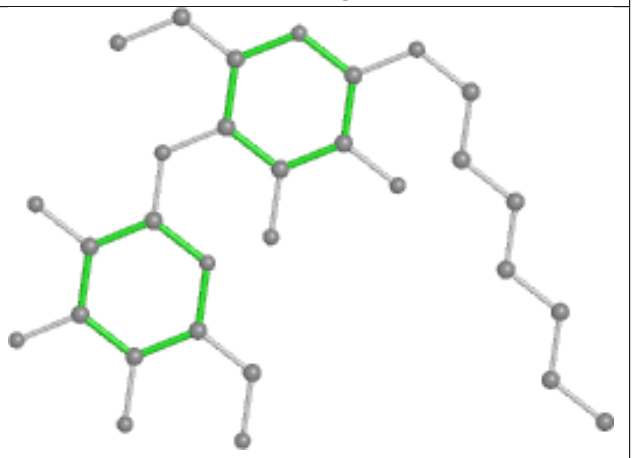
Bond lengths



Bond angles

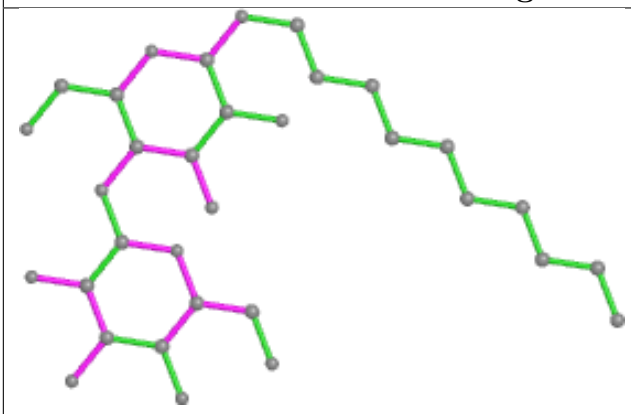


Torsions

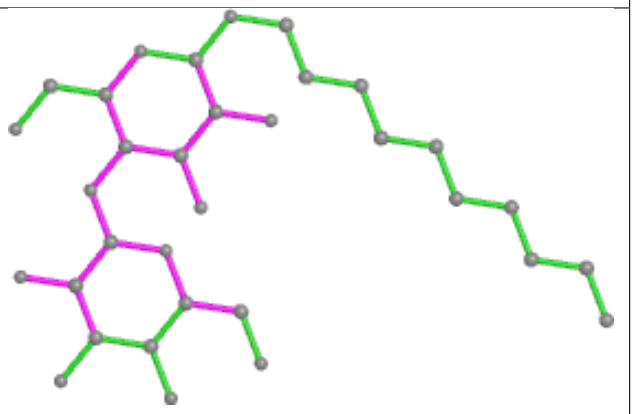


Rings

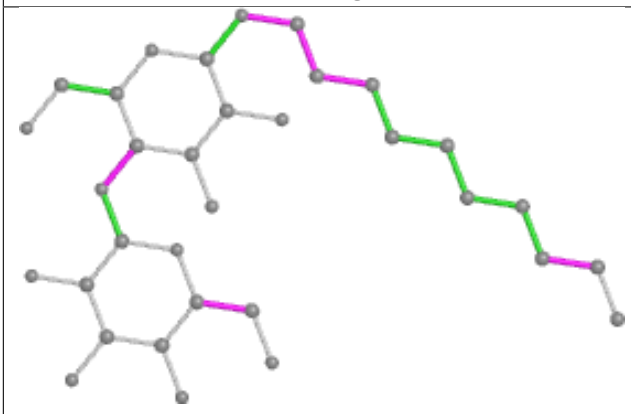
Ligand DMU A 614



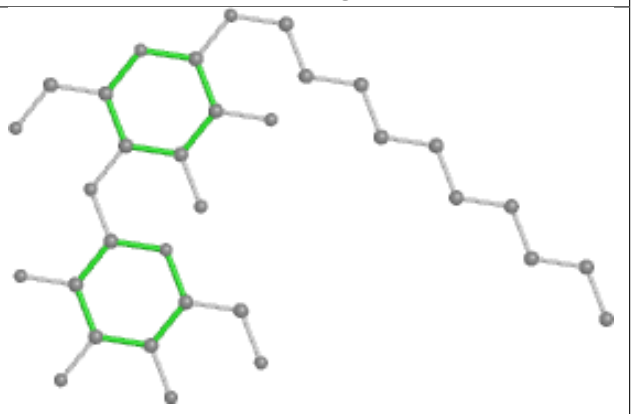
Bond lengths



Bond angles

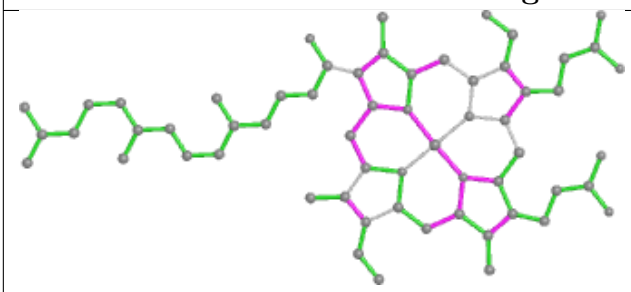


Torsions

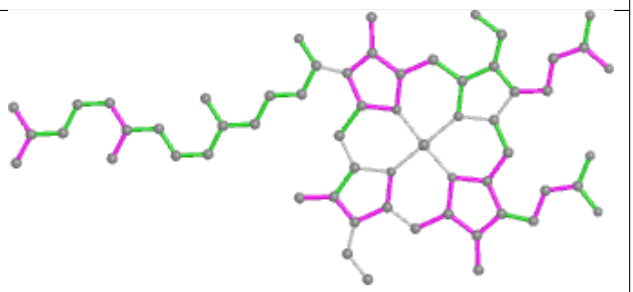


Rings

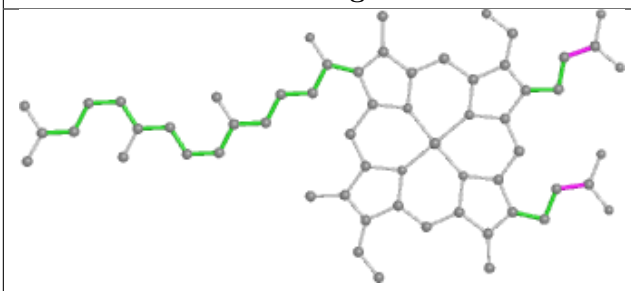
Ligand HEA A 616



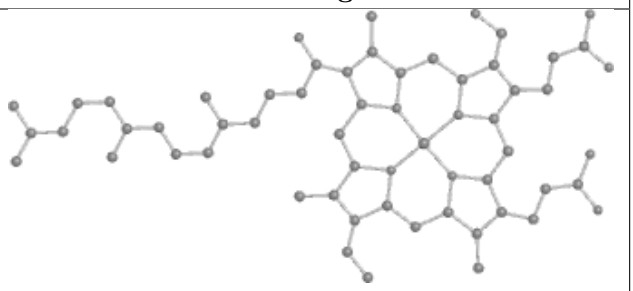
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	534/534 (100%)	-0.15	28 (5%) 27 32	24, 34, 55, 92	0
1	C	533/534 (99%)	0.11	54 (10%) 7 9	27, 41, 64, 88	0
2	B	256/257 (99%)	-0.35	5 (1%) 65 69	24, 37, 50, 60	1 (0%)
2	D	256/257 (99%)	-0.19	9 (3%) 44 50	28, 40, 57, 67	0
All	All	1579/1582 (99%)	-0.10	96 (6%) 21 26	24, 38, 58, 92	1 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	TRP	6.7
1	C	72	LEU	6.1
1	C	21	PHE	6.0
1	A	18	THR	5.4
1	A	17	PHE	5.1
1	A	20	TRP	5.0
1	C	19	ARG	4.9
2	D	284	HIS	4.8
1	A	221	THR	4.7
1	A	19	ARG	4.5
1	C	71	GLY	4.4
1	C	81	TRP	4.4
1	C	73	VAL	4.4
1	C	18	THR	4.2
1	C	70	SER	4.0
2	B	56	TRP	3.9
1	C	77	PHE	3.9
1	C	23	SER	3.8
1	C	297	ILE	3.7
1	C	428	ALA	3.6
1	C	290	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	81	TRP	3.6
1	C	294	ALA	3.6
1	A	77	PHE	3.5
1	C	431	GLY	3.5
1	C	387	PHE	3.5
1	A	21	PHE	3.5
1	A	22	MET	3.5
2	D	56	TRP	3.5
1	C	526	THR	3.4
1	C	69	GLU	3.4
1	C	115	LEU	3.4
1	C	291	VAL	3.3
1	A	72	LEU	3.3
1	C	429	VAL	3.3
1	C	219	GLY	3.2
1	A	222	MET	3.2
2	B	284	HIS	3.1
1	C	295	PHE	3.1
1	C	221	THR	3.1
1	C	298	VAL	3.1
2	D	99	PRO	3.0
1	C	75	GLY	3.0
1	A	69	GLU	3.0
1	A	71	GLY	2.9
1	A	223	HIS	2.9
2	D	81	TRP	2.8
1	C	111	VAL	2.8
1	C	432	ILE	2.8
1	C	259	PHE	2.7
1	C	292	LEU	2.7
1	C	76	PHE	2.7
1	C	293	PRO	2.7
1	C	524	ARG	2.7
1	C	74	LYS	2.7
1	C	144	TRP	2.6
1	C	451	TRP	2.6
1	C	427	GLY	2.5
1	C	218	PRO	2.5
1	A	318	TYR	2.5
1	C	296	GLY	2.5
1	A	290	ILE	2.4
1	A	115	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	269	GLY	2.4
1	A	172	TRP	2.4
1	A	111	VAL	2.4
1	C	268	GLY	2.4
1	A	420	PHE	2.4
1	C	22	MET	2.3
1	C	185	TYR	2.3
1	C	223	HIS	2.3
1	C	267	SER	2.3
1	A	432	ILE	2.3
1	C	516	PHE	2.3
1	C	86	GLU	2.3
1	C	417	VAL	2.3
1	A	219	GLY	2.3
1	C	78	GLN	2.2
1	C	222	MET	2.2
1	A	270	GLY	2.2
2	D	181	ILE	2.2
2	D	220	THR	2.2
2	D	98	SER	2.2
2	D	265	ILE	2.1
1	A	232	ILE	2.1
1	C	522	GLY	2.1
2	B	250	GLY	2.1
1	A	424	MET	2.1
2	B	285	HIS	2.1
1	C	107	MET	2.1
1	A	78	GLN	2.1
1	A	294	ALA	2.1
2	D	87	ARG	2.0
1	A	297	ILE	2.0
2	B	265	ILE	2.0
1	C	137	ARG	2.0

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

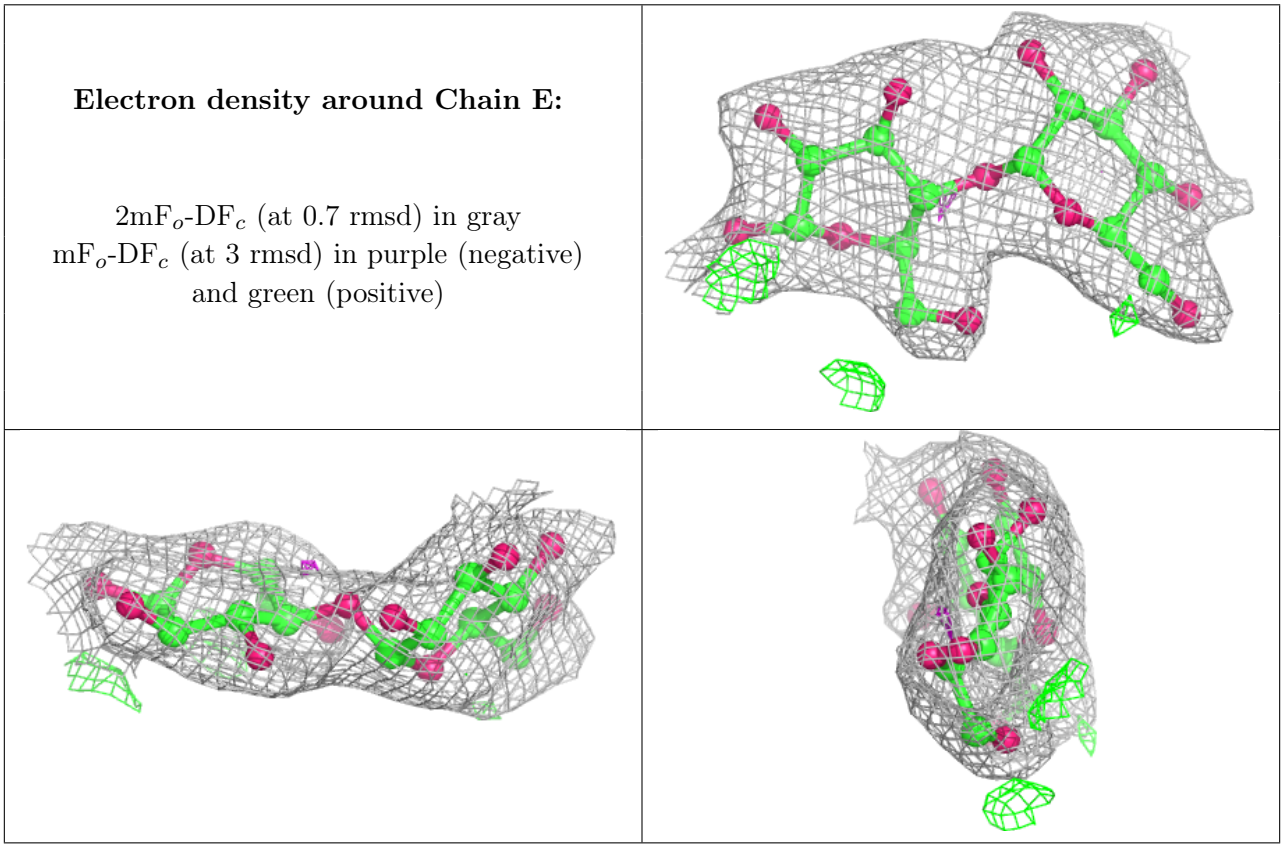
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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.

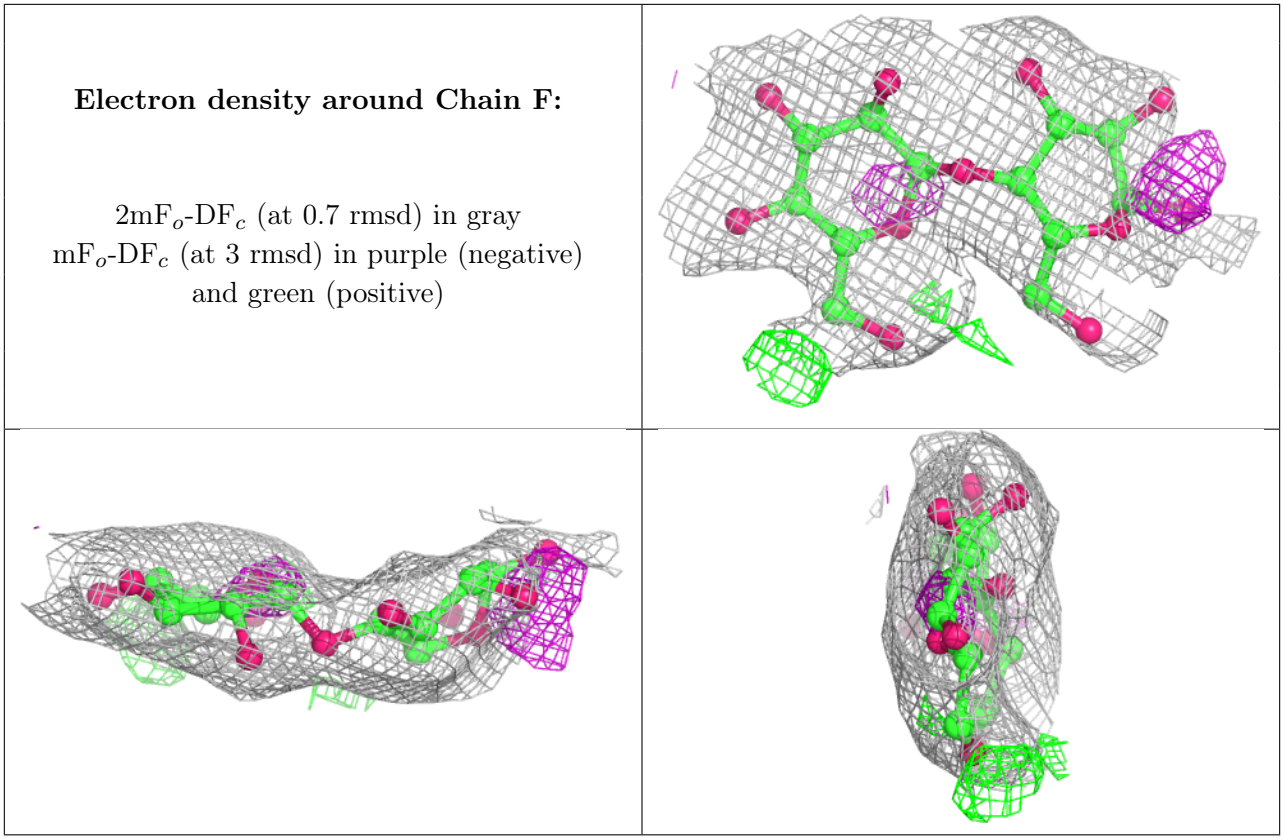
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	F	2	11/12	0.66	0.27	69,76,80,81	0
3	GLC	F	1	12/12	0.78	0.28	71,74,76,79	0
3	GLC	E	1	12/12	0.86	0.30	68,75,81,82	0
3	GLC	E	2	11/12	0.87	0.24	66,68,72,74	0

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 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
5	DMU	A	611	33/33	0.52	0.33	43,73,102,108	0
4	TRD	A	604	13/13	0.54	0.24	45,52,57,58	0
4	TRD	B	301	13/13	0.58	0.31	52,57,61,66	0
4	TRD	A	610	13/13	0.64	0.28	47,53,58,59	0
11	TRS	B	304	8/8	0.64	0.16	52,59,64,71	0
4	TRD	A	605	7/13	0.65	0.50	51,55,59,59	0
10	HTH	A	620	10/10	0.68	0.30	42,51,59,71	0
4	TRD	A	608	13/13	0.69	0.34	50,55,70,72	0
4	TRD	A	602	13/13	0.69	0.35	50,56,64,65	0
5	DMU	C	603	23/33	0.70	0.24	49,73,86,91	0
4	TRD	A	607	13/13	0.74	0.64	52,61,66,66	0
4	TRD	A	603	13/13	0.78	0.18	44,50,63,66	0
4	TRD	C	602	13/13	0.78	0.23	59,64,72,72	0
5	DMU	A	614	33/33	0.79	0.29	44,59,75,81	0

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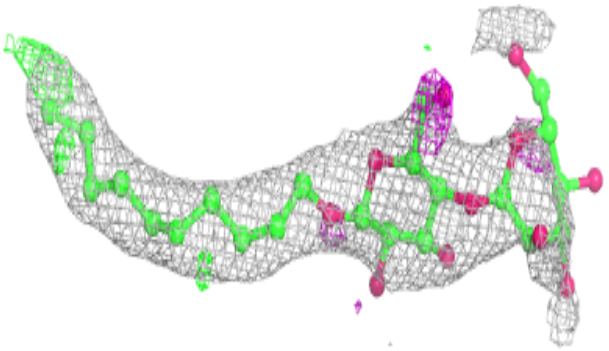
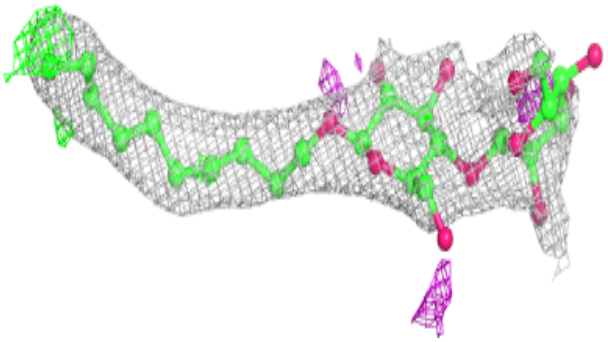
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TRD	A	601	13/13	0.83	0.15	51,55,68,68	0
5	DMU	A	613	33/33	0.85	0.25	47,61,67,70	0
4	TRD	A	606	13/13	0.86	0.21	46,52,63,64	0
5	DMU	B	302	30/33	0.87	0.19	46,57,62,67	0
4	TRD	A	609	13/13	0.88	0.17	37,43,49,54	0
10	HTH	B	309	10/10	0.89	0.18	39,48,51,60	10
4	TRD	C	601	13/13	0.92	0.10	41,45,46,52	0
4	TRD	D	301	9/13	0.94	0.09	48,50,53,55	0
5	DMU	A	612	33/33	0.95	0.09	26,35,48,52	0
6	HEA	C	604	60/60	0.96	0.19	24,30,38,45	0
12	CD	B	308	1/1	0.97	0.04	57,57,57,57	1
9	CA	C	608	1/1	0.98	0.06	33,33,33,33	0
6	HEA	A	616	60/60	0.98	0.14	23,27,36,39	0
6	HEA	A	615	60/60	0.98	0.19	20,25,30,33	0
6	HEA	C	605	60/60	0.98	0.14	26,31,40,43	0
8	MG	C	607	1/1	0.98	0.21	19,19,19,19	0
12	CD	D	306	1/1	0.98	0.04	62,62,62,62	1
7	CU	C	606	1/1	0.99	0.10	34,34,34,34	0
9	CA	A	619	1/1	0.99	0.08	28,28,28,28	0
7	CU	D	303	1/1	0.99	0.09	31,31,31,31	0
12	CD	D	305	1/1	0.99	0.07	39,39,39,39	0
8	MG	A	618	1/1	0.99	0.16	15,15,15,15	0
7	CU	B	305	1/1	1.00	0.07	25,25,25,25	0
12	CD	B	307	1/1	1.00	0.08	40,40,40,40	0
7	CU	D	304	1/1	1.00	0.08	31,31,31,31	0
7	CU	B	306	1/1	1.00	0.08	25,25,25,25	0
7	CU	A	617	1/1	1.00	0.09	30,30,30,30	0

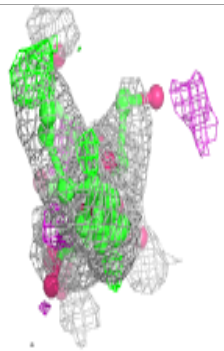
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU A 611:

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

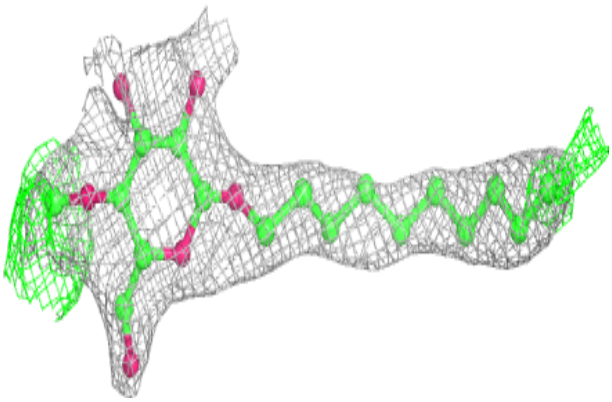


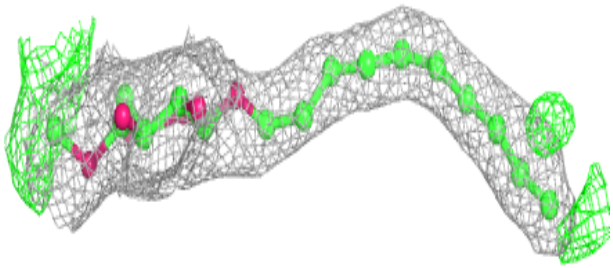


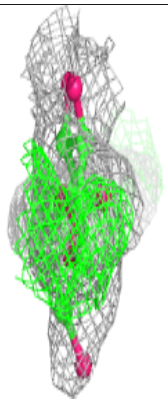


Electron density around DMU C 603:

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

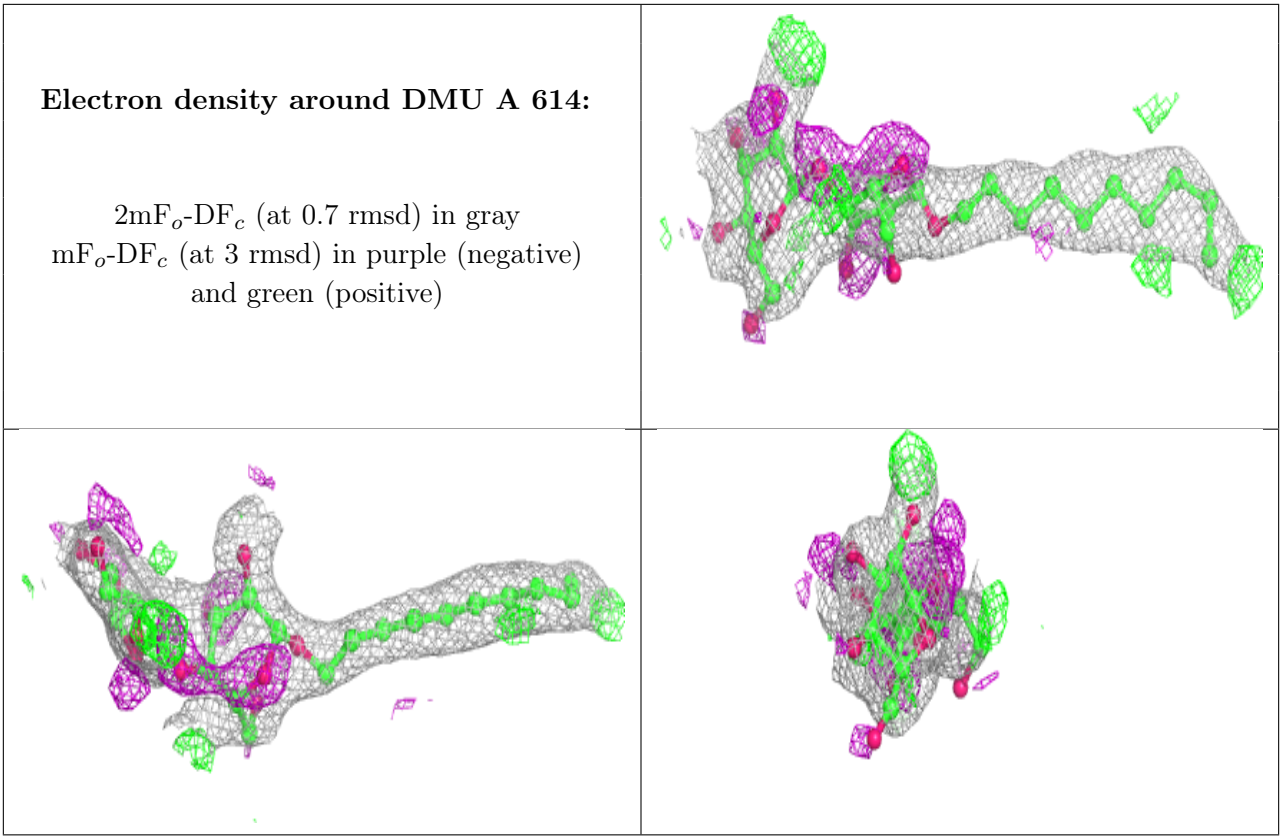






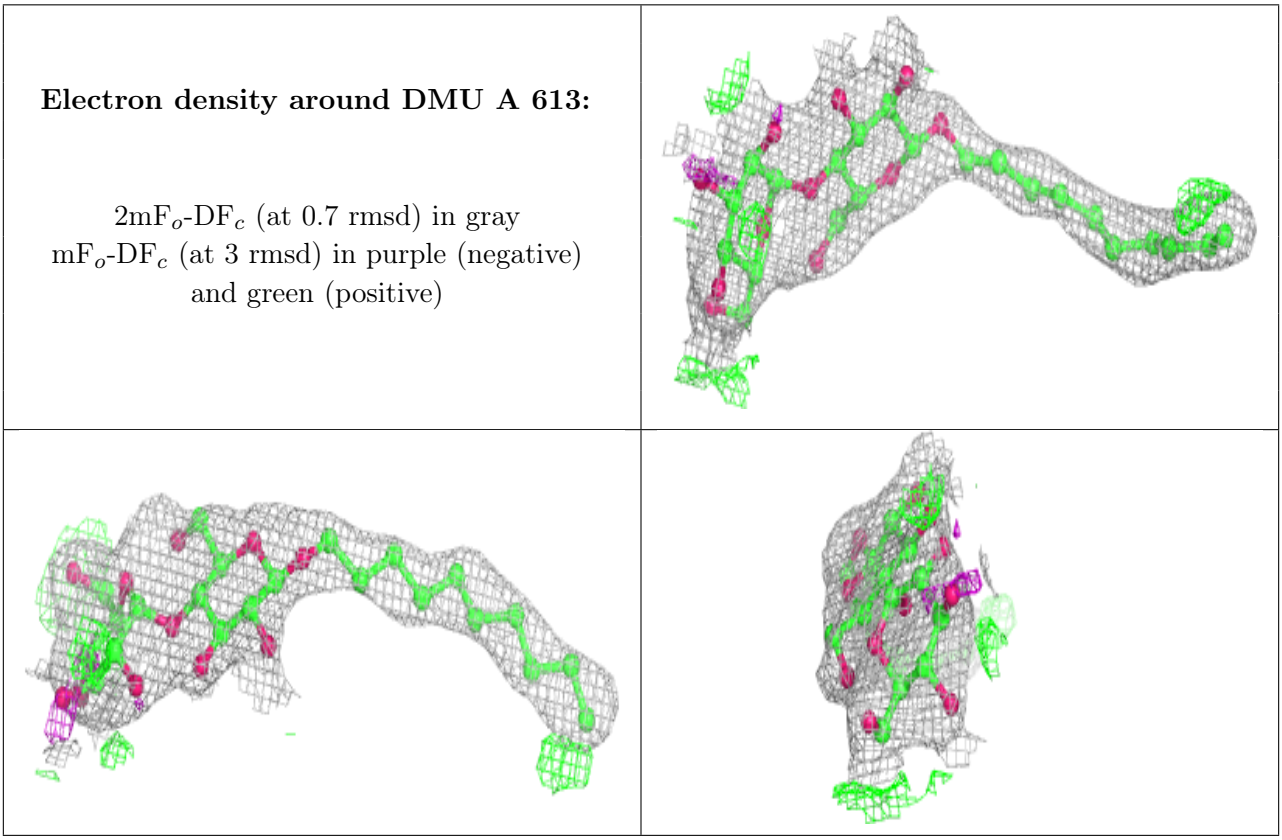
Electron density around DMU A 614:

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



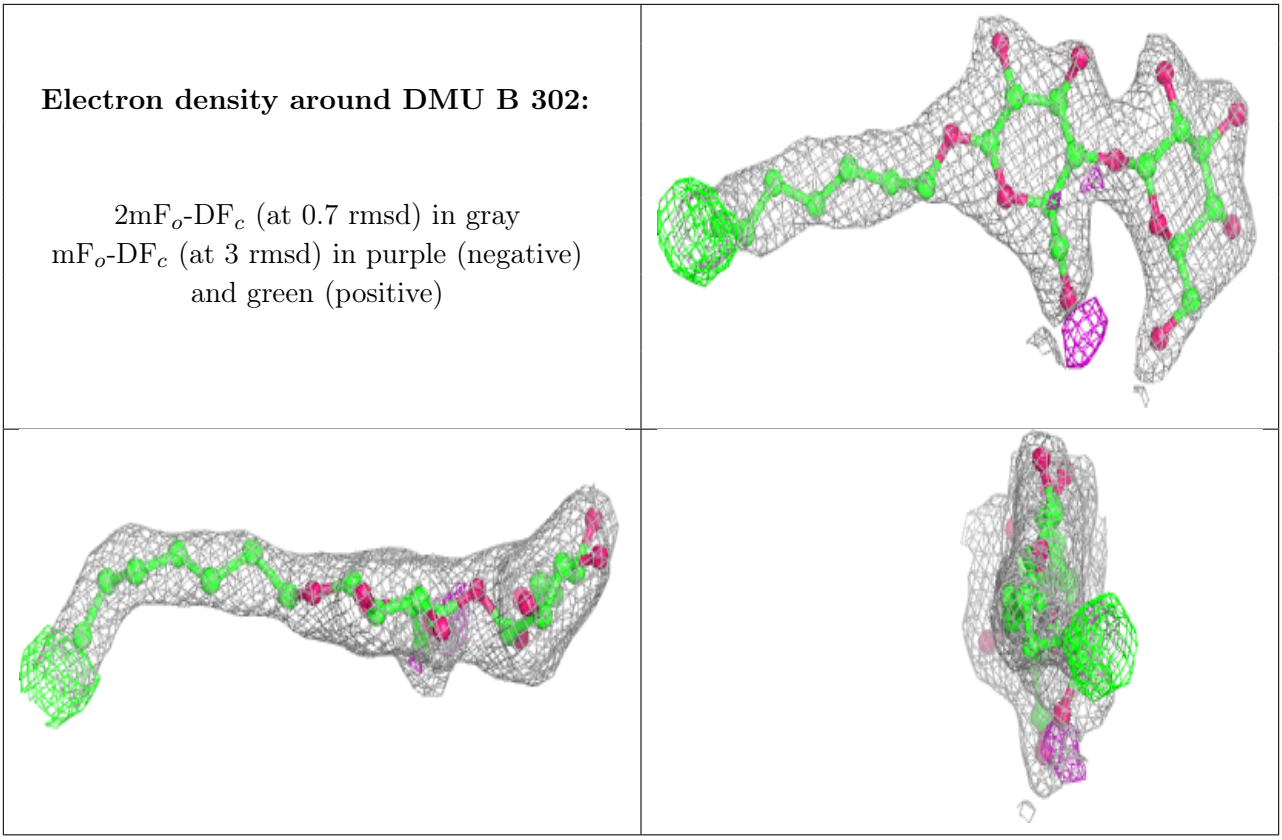
Electron density around DMU A 613:

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



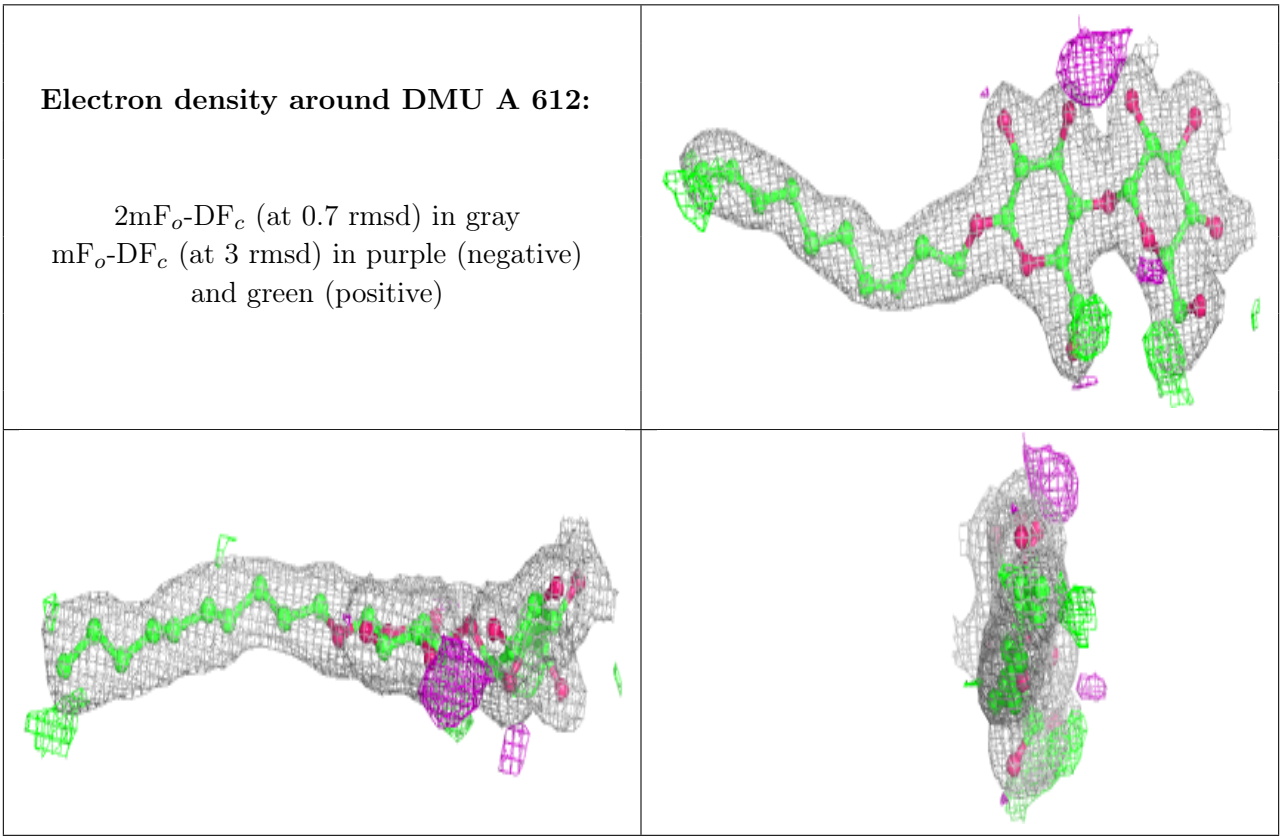
Electron density around DMU B 302:

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



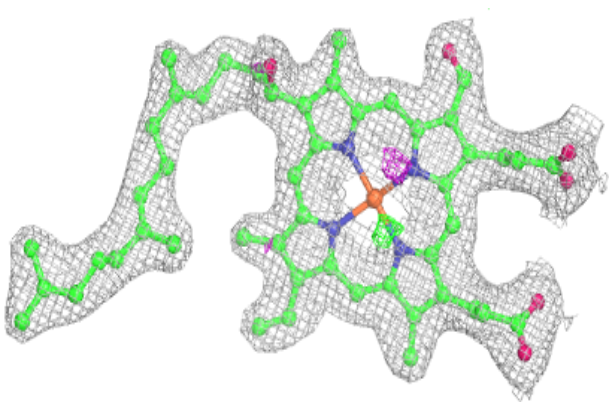
Electron density around DMU A 612:

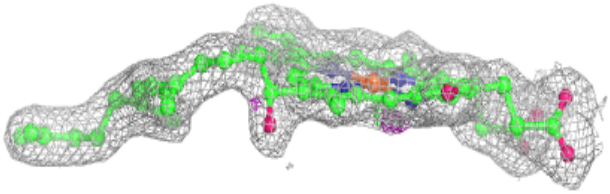
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

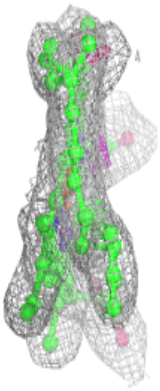


Electron density around HEA C 604:

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

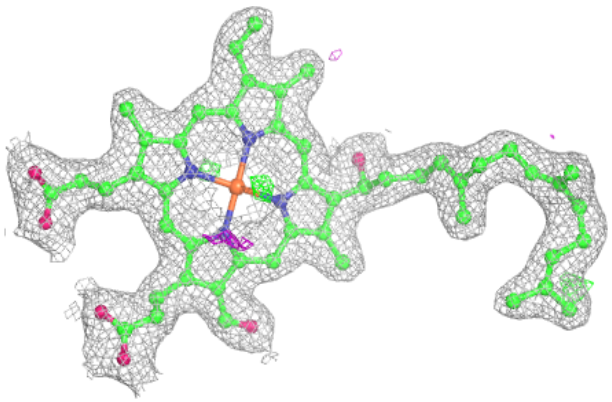


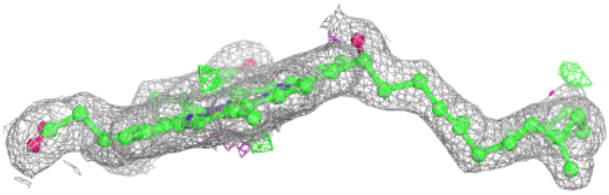




Electron density around HEA A 616:

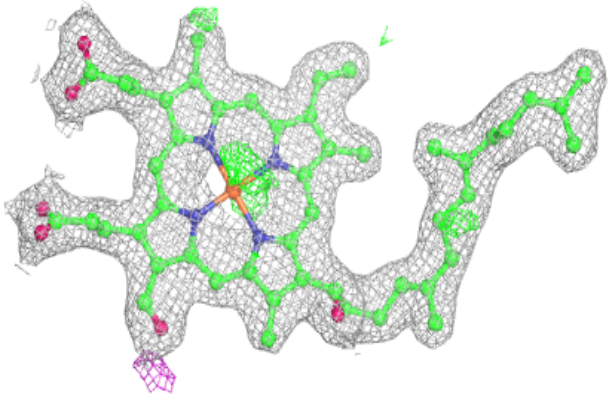
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

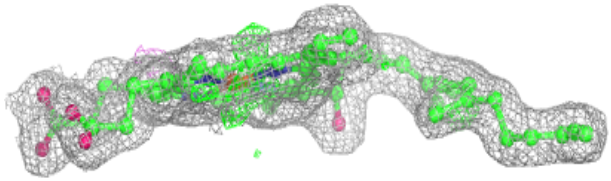


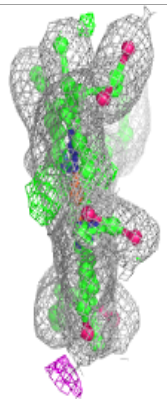


Electron density around HEA A 615:

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

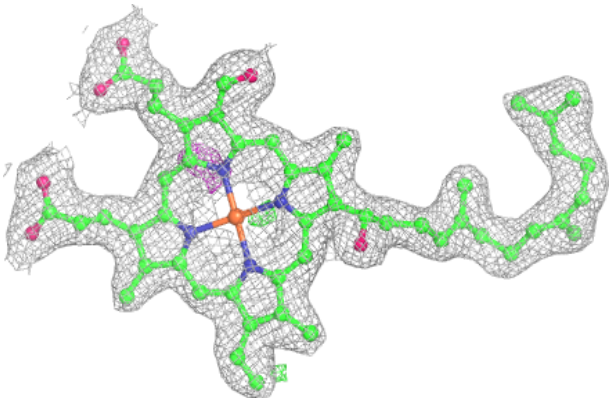


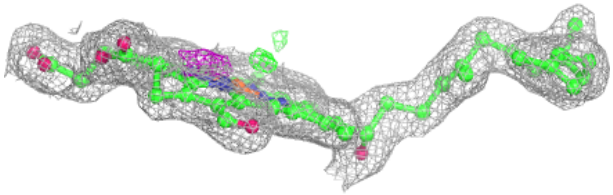


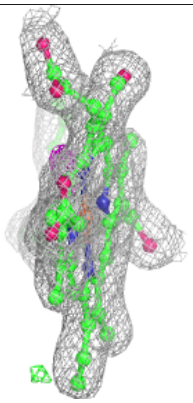


Electron density around HEA C 605:

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







6.5 Other polymers (i)

There are no such residues in this entry.