wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 02:39 PM EDT

PDB ID	:	3OMN / pdb_00003omn
Title	:	Catalytic core subunits (I and II) of cytochrome C oxidase from Rhodobacter sphaeroides with D132A mutation in the reduced state
Authors	:	Liu, J.; Qin, L.; Ferguson-Miller, S.
Deposited on	:	2010-08-27
Resolution	:	2.15 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:

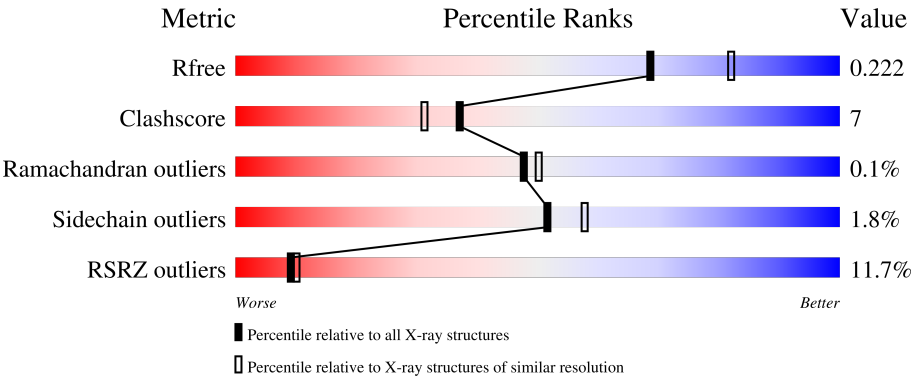
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	535	7% 88% 11%
1	C	535	20% 85% 13%
2	B	256	4% 95%
2	D	256	10% 93% 6%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 13755 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, aa3 type, subunit I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	13	0
			4274	2862	673	707	32			
1	C	531	Total	C	N	O	S	0	13	0
			4219	2826	663	698	32			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	ALA	ASP	engineered mutation	UNP Q3J5A7
C	132	ALA	ASP	engineered mutation	UNP Q3J5A7

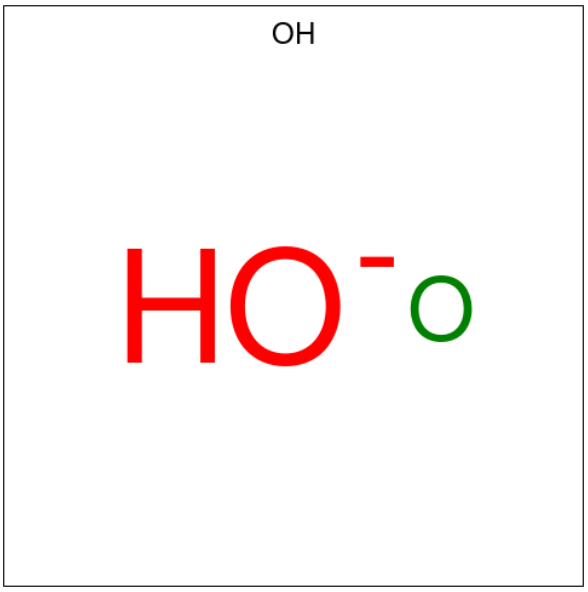
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			2021	1319	333	363	6			
2	D	256	Total	C	N	O	S	0	0	0
			2015	1316	330	363	6			

There are 8 discrepancies between the modelled and reference sequences:

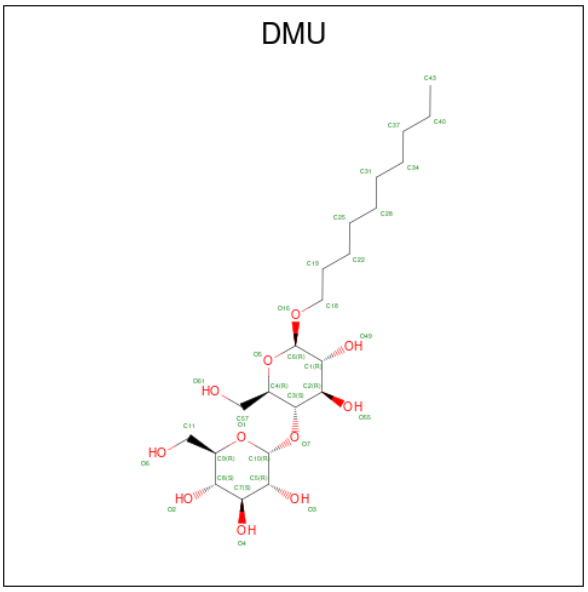
Chain	Residue	Modelled	Actual	Comment	Reference
B	282	HIS	-	expression tag	UNP Q3J5G0
B	283	HIS	-	expression tag	UNP Q3J5G0
B	284	HIS	-	expression tag	UNP Q3J5G0
B	285	HIS	-	expression tag	UNP Q3J5G0
D	282	HIS	-	expression tag	UNP Q3J5G0
D	283	HIS	-	expression tag	UNP Q3J5G0
D	284	HIS	-	expression tag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

- Molecule 3 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



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

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



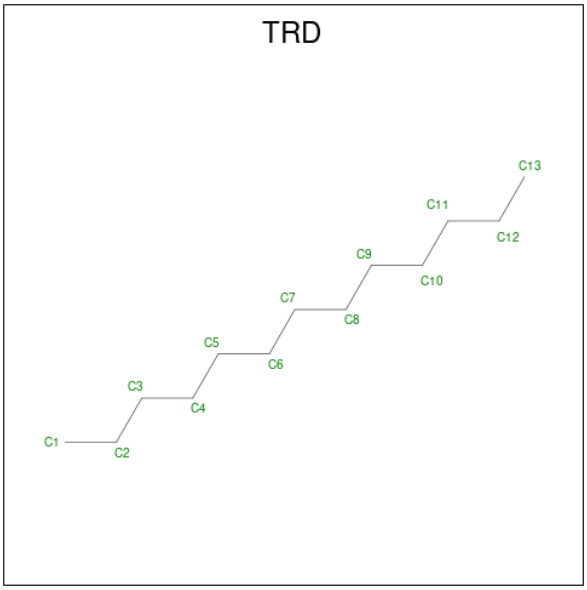
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 22 16 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 21 16 5	0	0
4	B	1	Total C O 33 22 11	0	0
4	B	1	Total C O 33 22 11	0	0
4	B	1	Total C O 33 22 11	0	0
4	B	1	Total C O 23 12 11	0	0
4	C	1	Total C O 23 12 11	0	0
4	C	1	Total C O 23 12 11	0	0
4	C	1	Total C O 33 22 11	0	0
4	D	1	Total C O 23 12 11	0	0
4	D	1	Total C O 23 12 11	0	0

- Molecule 5 is TRIDECANE (CCD ID: TRD) (formula: $C_{13}H_{28}$).



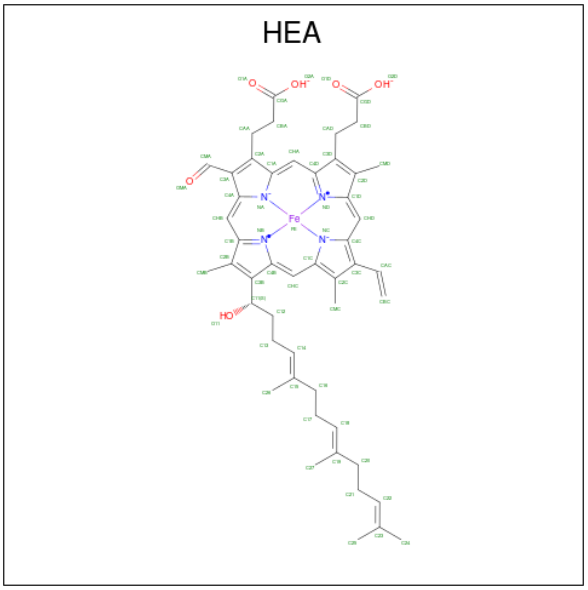
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 7 7	0	0
5	A	1	Total C 6 6	0	0
5	A	1	Total C 13 13	0	0
5	A	1	Total C 13 13	0	0
5	B	1	Total C 8 8	0	0
5	C	1	Total C 13 13	0	0
5	D	1	Total C 13 13	0	0
5	D	1	Total C 7 7	0	0

- Molecule 6 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C Fe N O 60 49 1 4 6	0	0
6	A	1	Total C Fe N O 120 98 2 8 12	0	1
6	C	1	Total C Fe N O 60 49 1 4 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	Fe	N	O	0	1
			120	98	2	8	12		

- Molecule 7 is COPPER (I) ION (CCD ID: CU1) (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 (CCD ID: MG) (formula: Mg).

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

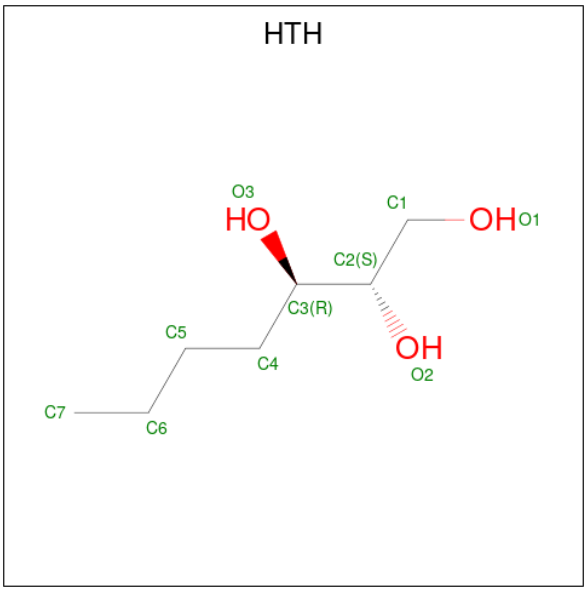
- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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



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

- Molecule 12 is CADMIUM ION (CCD ID: 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.

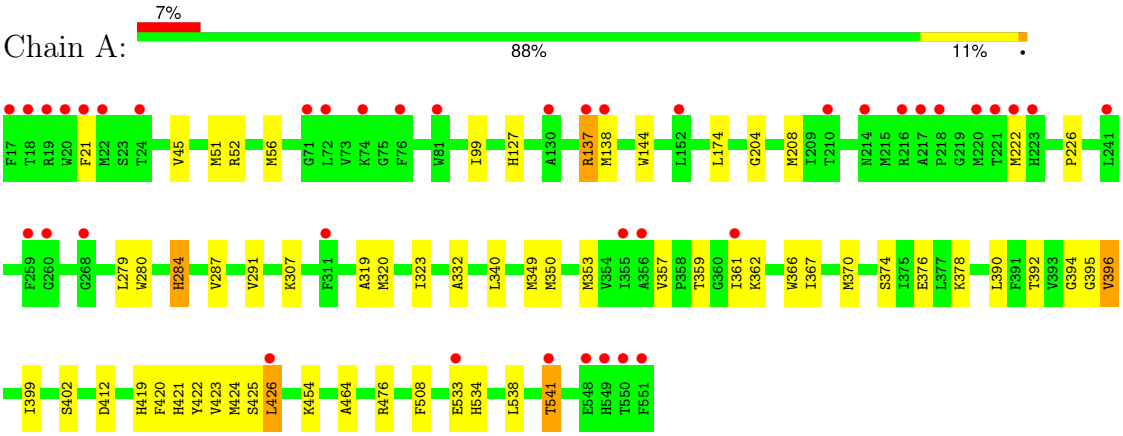
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	132	Total O 133 133	0	1
13	B	128	Total O 128 128	0	0
13	C	88	Total O 88 88	0	0
13	D	112	Total O 112 112	0	0

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.

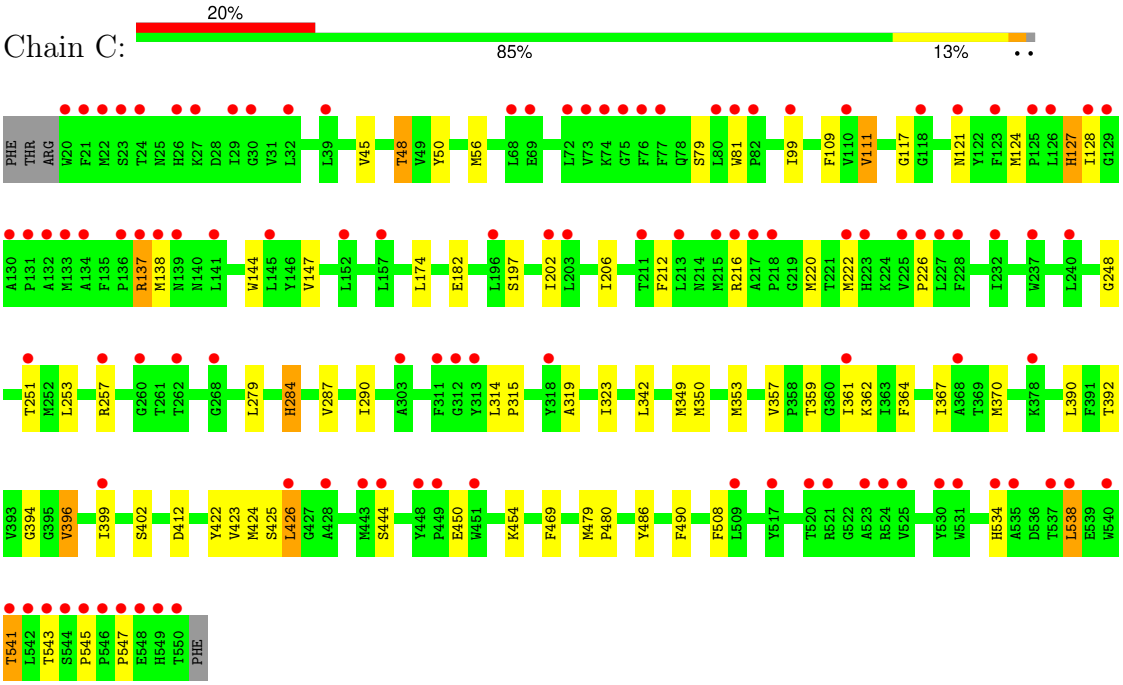
• Molecule 1: Cytochrome c oxidase, aa3 type, subunit I

Chain A:



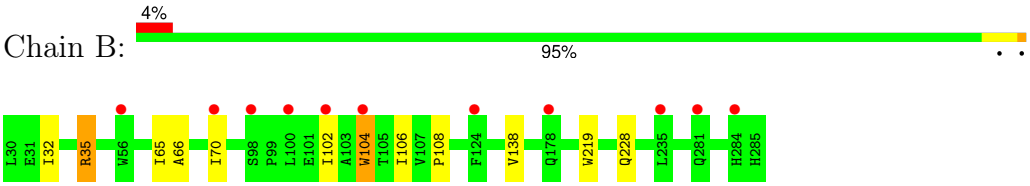
• Molecule 1: Cytochrome c oxidase, aa3 type, subunit I

Chain C:



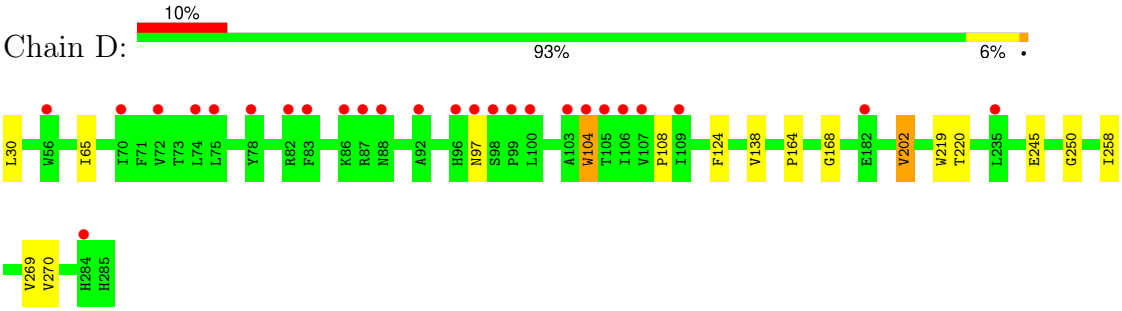
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



• Molecule 2: Cytochrome c oxidase subunit 2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	124.67Å 132.03Å 176.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.70 – 2.15 42.70 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.2 (42.70-2.15) 97.2 (42.70-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.16Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.219 0.200 , 0.222	Depositor DCC
R_{free} test set	4627 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.9	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	13755	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DMU, CL, CA, HTH, OH, CU1, HEA, CD, MG, TRD

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	0.66	1/4430 (0.0%)	0.88	3/6048 (0.0%)
1	C	0.57	1/4373 (0.0%)	0.90	4/5973 (0.1%)
2	B	0.62	0/2083	0.78	0/2852
2	D	0.57	0/2077	0.79	1/2845 (0.0%)
All	All	0.61	2/12963 (0.0%)	0.86	8/17718 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	534	HIS	ND1-CE1	5.35	1.37	1.32
1	C	127	HIS	ND1-CE1	5.29	1.37	1.32

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	284	HIS	N-CA-CB	7.32	117.35	110.39
1	C	127	HIS	CB-CG-CD2	-6.64	122.56	131.20
1	A	534	HIS	CB-CG-CD2	-6.54	122.70	131.20
1	C	127	HIS	CB-CG-ND1	5.70	131.25	122.70
1	A	534	HIS	CB-CG-ND1	5.64	131.16	122.70

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	4274	0	4182	71	0
1	C	4219	0	4120	88	0
2	B	2021	0	1978	11	0
2	D	2015	0	1967	15	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	43	0	61	2	0
4	B	122	0	147	0	0
4	C	79	0	84	2	0
4	D	46	0	42	1	0
5	A	46	0	90	2	0
5	B	8	0	12	0	0
5	C	13	0	28	1	0
5	D	20	0	41	0	0
6	A	180	0	162	20	0
6	C	180	0	162	21	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	1	0	0	0	0
10	C	1	0	0	0	0
11	B	10	0	16	0	0
12	B	2	0	0	0	0
12	D	2	0	0	0	0
13	A	133	0	0	1	0
13	B	128	0	0	2	0
13	C	88	0	0	1	0
13	D	112	0	0	1	0
All	All	13755	0	13092	186	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 7.

The worst 5 of 186 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:HG3	1:A:137:ARG:HH11	1.03	1.17
1:A:357:VAL:O	1:A:361[B]:ILE:HG12	1.52	1.07
1:C:422[A]:TYR:HA	1:C:426[A]:LEU:HG	1.41	1.00
1:C:422[A]:TYR:CD2	1:C:426[A]:LEU:HD12	1.97	0.99
1:C:137:ARG:HH11	1:C:137:ARG:HG3	1.30	0.93

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	546/535 (102%)	533 (98%)	13 (2%)	0	100	100
1	C	542/535 (101%)	526 (97%)	16 (3%)	0	100	100
2	B	254/256 (99%)	246 (97%)	8 (3%)	0	100	100
2	D	254/256 (99%)	248 (98%)	5 (2%)	1 (0%)	30	26
All	All	1596/1582 (101%)	1553 (97%)	42 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	97	ASN

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	437/434 (101%)	427 (98%)	10 (2%)	44 49
1	C	430/434 (99%)	419 (97%)	11 (3%)	40 43
2	B	214/215 (100%)	212 (99%)	2 (1%)	70 77
2	D	213/215 (99%)	211 (99%)	2 (1%)	70 77
All	All	1294/1298 (100%)	1269 (98%)	25 (2%)	51 56

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	111	VAL
1	C	279	LEU
2	D	202	VAL
1	C	174	LEU
1	C	396	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	96	HIS
2	D	251	GLN
2	B	251	GLN
1	C	25	ASN
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)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 45 ligands modelled in this entry, 2 are modelled with single atom and 16 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	$\#\|Z\| > 2$
5	TRD	A	3	-	12,12,12	0.28	0	11,11,11	0.51	0
4	DMU	C	9	-	24,24,34	0.57	0	35,35,45	0.88	2 (5%)
6	HEA	C	2[B]	13,1	67,67,67	1.67	8 (11%)	81,103,103	1.48	15 (18%)
6	HEA	C	1	1	67,67,67	1.42	8 (11%)	81,103,103	1.45	14 (17%)
6	HEA	C	2[A]	13,1	67,67,67	1.50	8 (11%)	81,103,103	1.36	11 (13%)
5	TRD	A	1013	-	6,6,12	0.25	0	5,5,11	0.47	0
5	TRD	A	1009	-	6,6,12	0.26	0	5,5,11	0.39	0
4	DMU	D	8	-	24,24,34	0.53	0	35,35,45	0.61	0
11	HTH	B	286	-	9,9,9	0.41	0	10,10,10	0.84	0
4	DMU	B	1	-	34,34,34	0.49	0	45,45,45	0.89	2 (4%)
4	DMU	C	10	-	34,34,34	0.59	0	45,45,45	0.80	1 (2%)
4	DMU	D	4	-	24,24,34	0.51	0	35,35,45	0.63	0
4	DMU	B	3	-	34,34,34	0.56	0	45,45,45	0.59	0
6	HEA	A	2[B]	13,1	67,67,67	1.72	8 (11%)	81,103,103	1.51	16 (19%)
4	DMU	B	2	-	34,34,34	0.53	0	45,45,45	0.77	1 (2%)
5	TRD	A	552	-	5,5,12	0.33	0	4,4,11	0.33	0
5	TRD	A	553	-	12,12,12	0.23	0	11,11,11	0.52	0
6	HEA	A	2[A]	13,1	67,67,67	1.56	7 (10%)	81,103,103	1.39	11 (13%)
5	TRD	B	4	-	7,7,12	0.25	0	6,6,11	0.41	0
5	TRD	D	14	-	6,6,12	0.25	0	5,5,11	0.37	0
4	DMU	C	5	-	24,24,34	0.51	0	35,35,45	0.61	0
5	TRD	C	552	-	12,12,12	0.23	0	11,11,11	0.56	0
5	TRD	D	3	-	12,12,12	0.18	0	11,11,11	0.66	0
4	DMU	B	6	-	24,24,34	0.54	0	35,35,45	0.68	0
6	HEA	A	1	1	67,67,67	1.42	8 (11%)	81,103,103	1.53	18 (22%)
4	DMU	A	7	-	21,21,34	0.60	0	24,25,45	1.09	2 (8%)
4	DMU	A	1005	-	22,22,34	0.56	0	27,27,45	0.93	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TRD	A	3	-	-	2/10/10/10	-
4	DMU	C	9	-	-	4/8/48/59	0/2/2/2
6	HEA	C	2[B]	13,1	-	12/36/76/76	-
6	HEA	C	1	1	-	5/36/76/76	-
6	HEA	C	2[A]	13,1	-	5/36/76/76	-
5	TRD	A	1013	-	-	1/4/4/10	-
5	TRD	A	1009	-	-	1/4/4/10	-
4	DMU	D	8	-	-	2/8/48/59	0/2/2/2
11	HTH	B	286	-	-	5/10/10/10	-
4	DMU	B	1	-	-	1/19/59/59	0/2/2/2
4	DMU	C	10	-	-	10/19/59/59	0/2/2/2
4	DMU	D	4	-	-	0/8/48/59	0/2/2/2
4	DMU	B	3	-	-	6/19/59/59	0/2/2/2
6	HEA	A	2[B]	13,1	-	12/36/76/76	-
4	DMU	B	2	-	-	8/19/59/59	0/2/2/2
5	TRD	A	552	-	-	0/3/3/10	-
5	TRD	A	553	-	-	6/10/10/10	-
6	HEA	A	2[A]	13,1	-	11/36/76/76	-
5	TRD	B	4	-	-	4/5/5/10	-
5	TRD	D	14	-	-	1/4/4/10	-
4	DMU	C	5	-	-	2/8/48/59	0/2/2/2
5	TRD	C	552	-	-	4/10/10/10	-
5	TRD	D	3	-	-	9/10/10/10	-
4	DMU	B	6	-	-	2/8/48/59	0/2/2/2
6	HEA	A	1	1	-	7/36/76/76	-
4	DMU	A	7	-	-	6/13/29/59	0/1/1/2
4	DMU	A	1005	-	-	3/13/33/59	0/1/1/2

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2[B]	HEA	FE-ND	8.70	2.21	1.94
6	A	2[A]	HEA	FE-NB	6.99	2.16	1.94
6	C	2[B]	HEA	FE-NB	6.61	2.15	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1	HEA	FE-NA	6.55	2.16	1.95
6	A	2[B]	HEA	FE-NA	5.47	2.13	1.95

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	2[B]	HEA	C3C-C4C-NC	-4.41	106.08	109.80
6	C	1	HEA	C2A-C1A-NA	-4.18	106.29	110.32
6	C	2[B]	HEA	C3C-C4C-NC	-3.64	106.73	109.80
6	A	2[A]	HEA	CAD-CBD-CGD	-3.61	104.10	113.67
6	A	1	HEA	C4B-NB-C1B	3.51	109.36	105.21

There are no chirality outliers.

5 of 129 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	7	DMU	C1-C6-O16-C18
4	B	2	DMU	C19-C18-O16-C6
6	A	2[A]	HEA	C2A-C3A-CMA-OMA
6	A	2[B]	HEA	C2D-C3D-CAD-CBD
6	A	2[B]	HEA	C19-C20-C21-C22

There are no ring outliers.

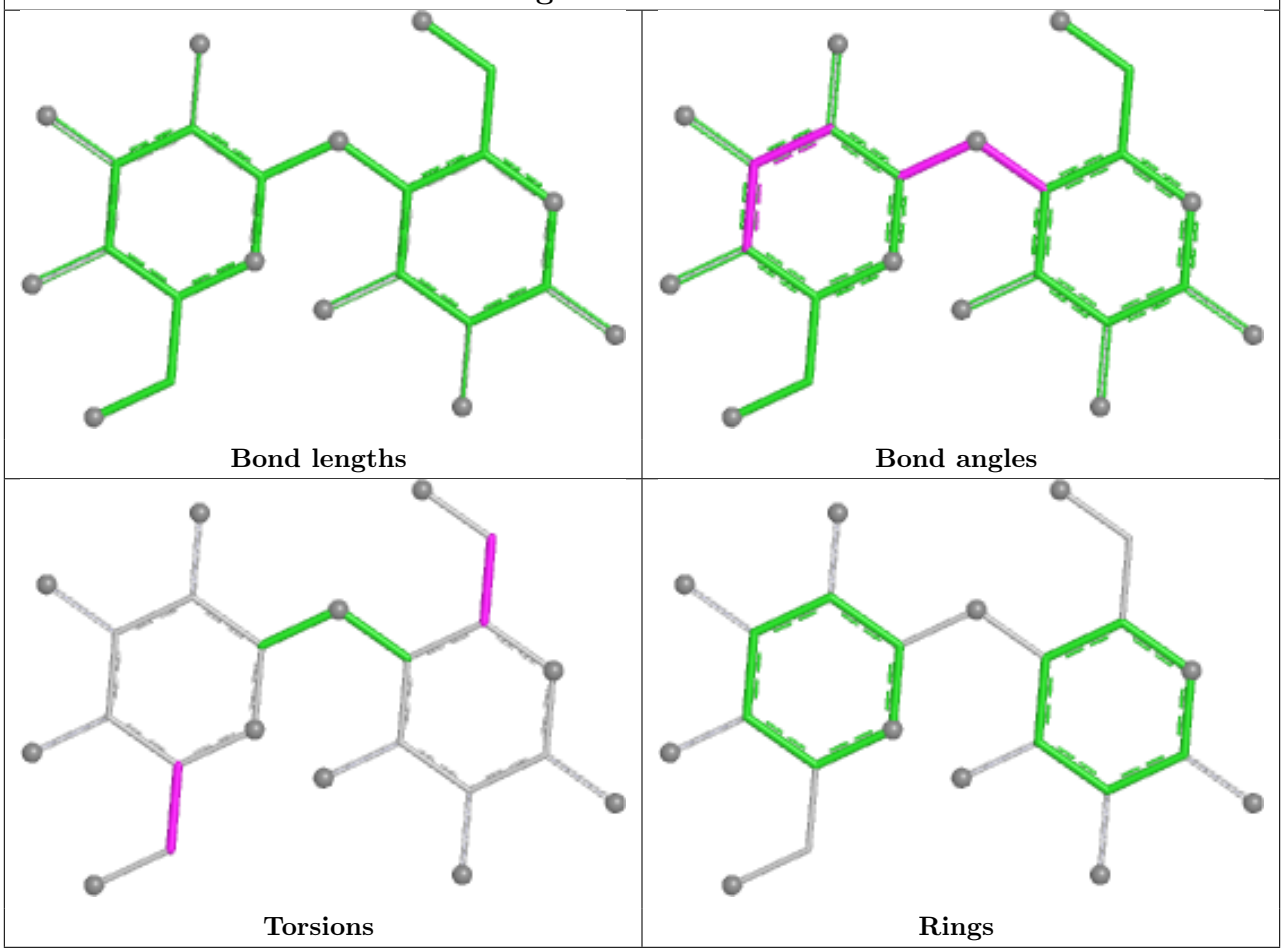
13 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3	TRD	1	0
4	C	9	DMU	1	0
6	C	2[B]	HEA	7	0
6	C	1	HEA	7	0
6	C	2[A]	HEA	7	0
4	D	8	DMU	1	0
4	C	10	DMU	1	0
6	A	2[B]	HEA	9	0
5	A	553	TRD	1	0
6	A	2[A]	HEA	7	0
5	C	552	TRD	1	0
6	A	1	HEA	4	0
4	A	1005	DMU	2	0

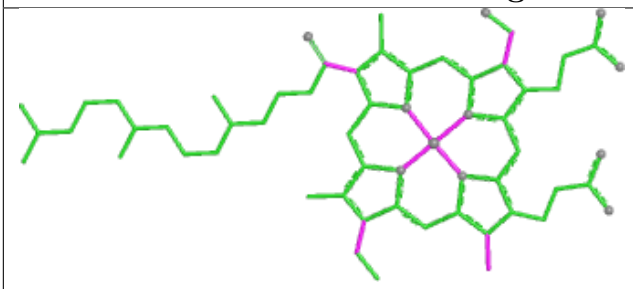
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

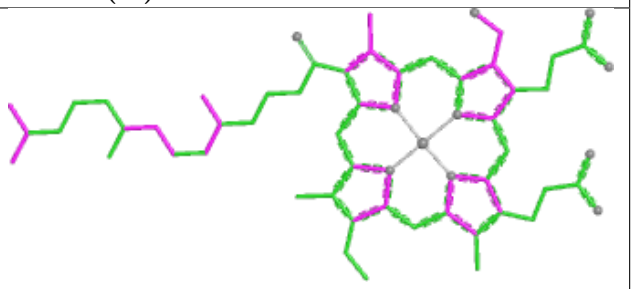
Ligand DMU C 9



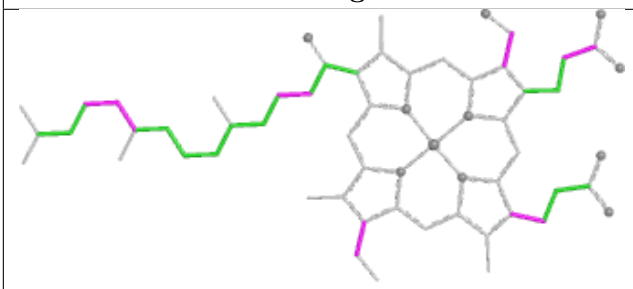
Ligand HEA C 2 (B)



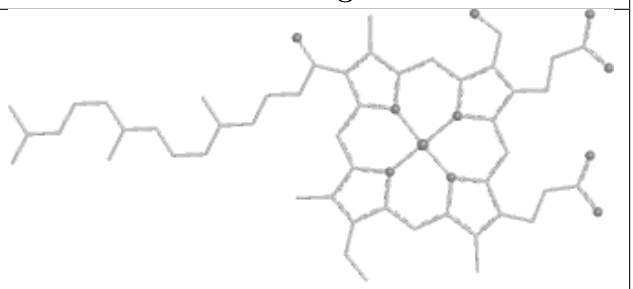
Bond lengths



Bond angles

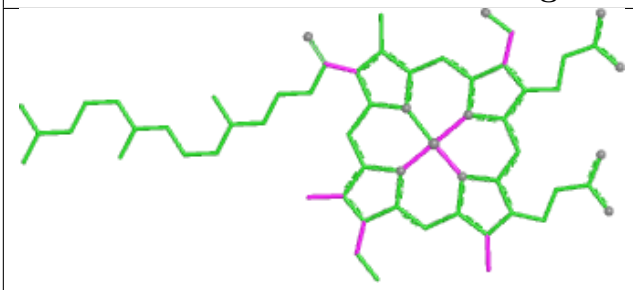


Torsions

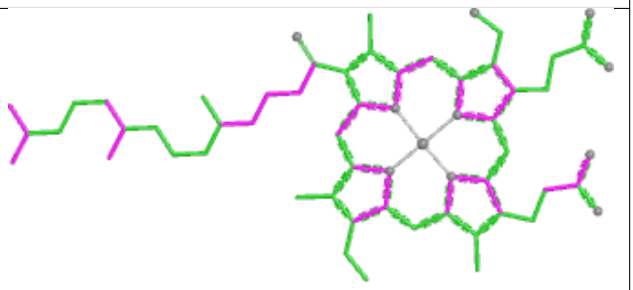


Rings

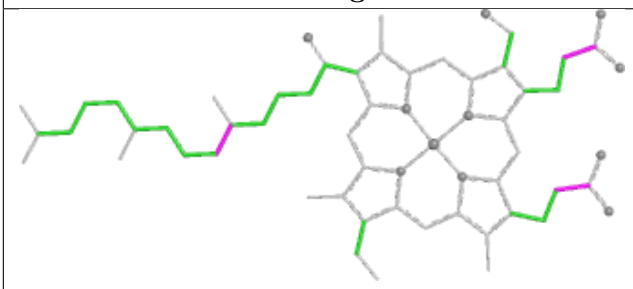
Ligand HEA C 1



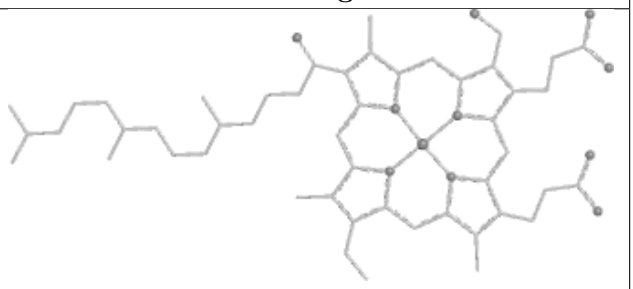
Bond lengths



Bond angles

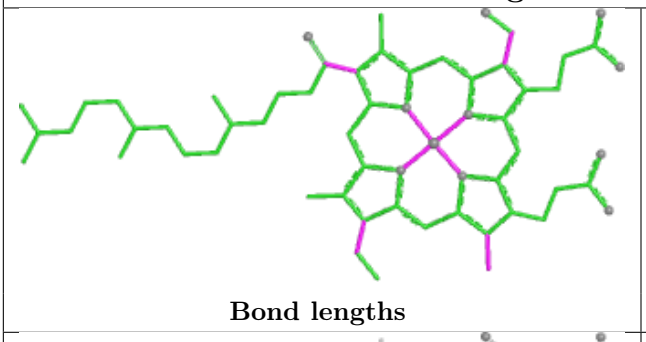


Torsions

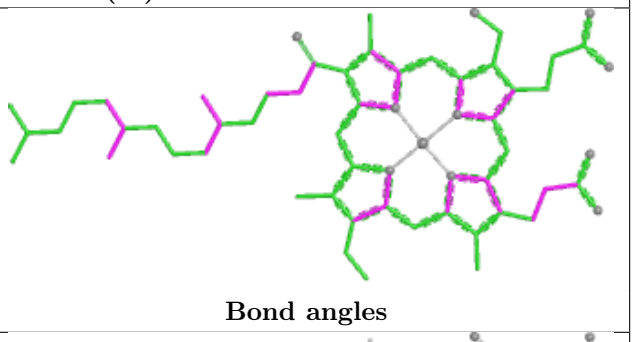


Rings

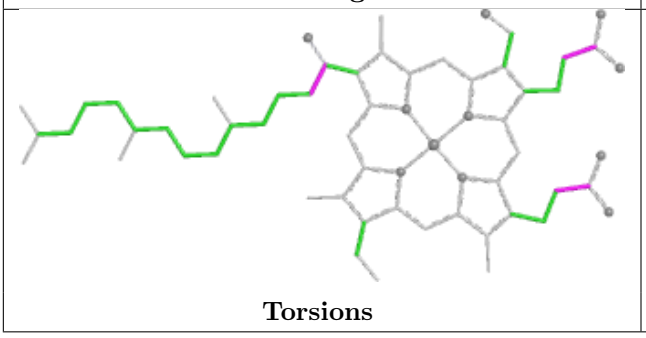
Ligand HEA C 2 (A)



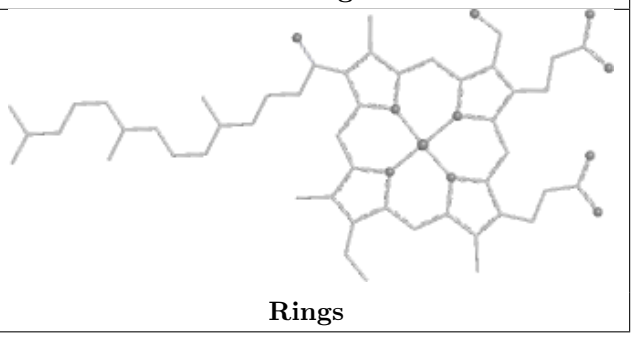
Bond lengths



Bond angles

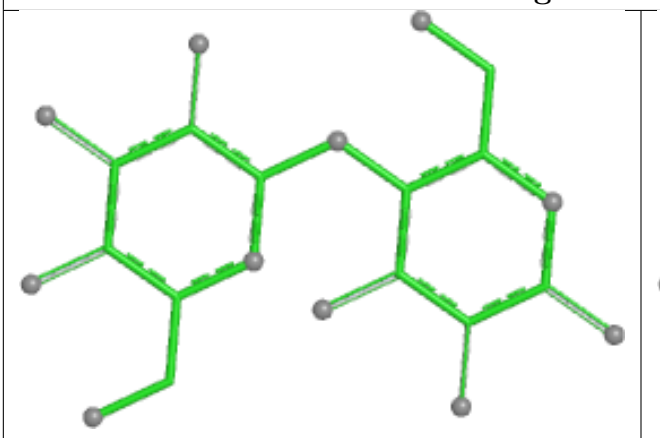


Torsions

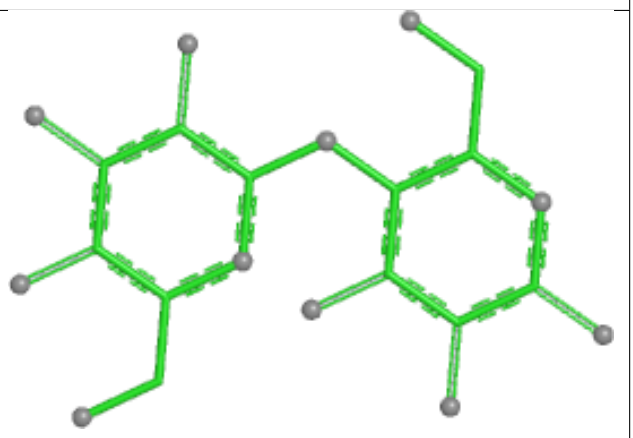


Rings

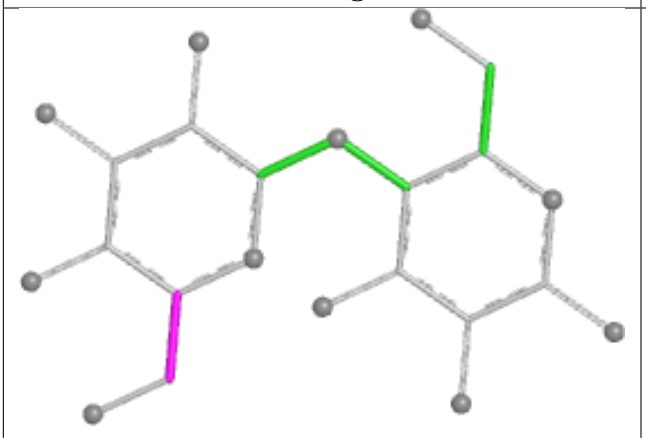
Ligand DMU D 8



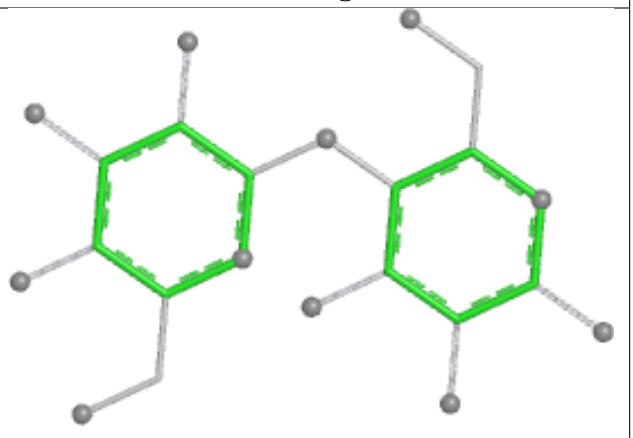
Bond lengths



Bond angles

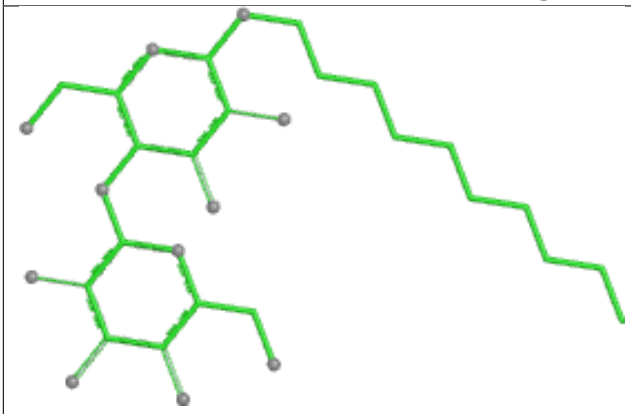


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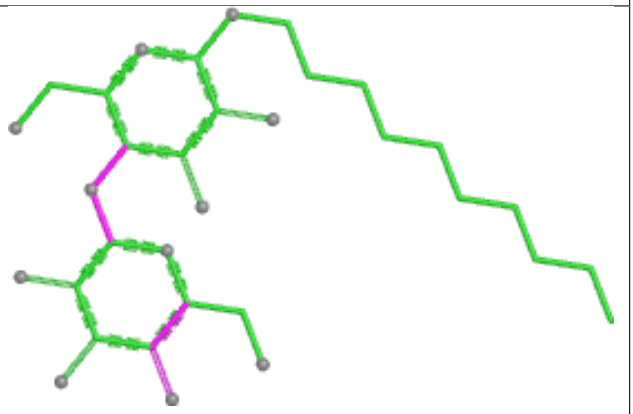


Rings

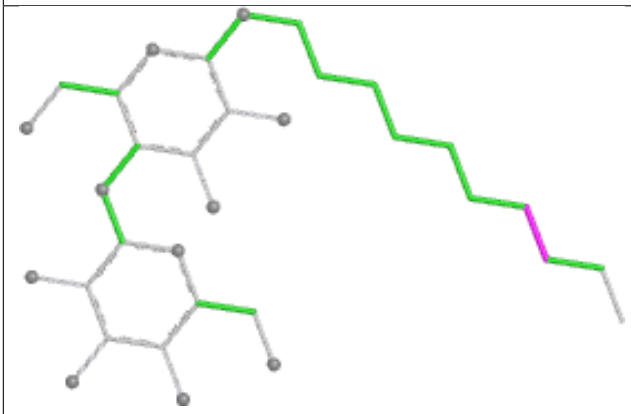
Ligand DMU B 1



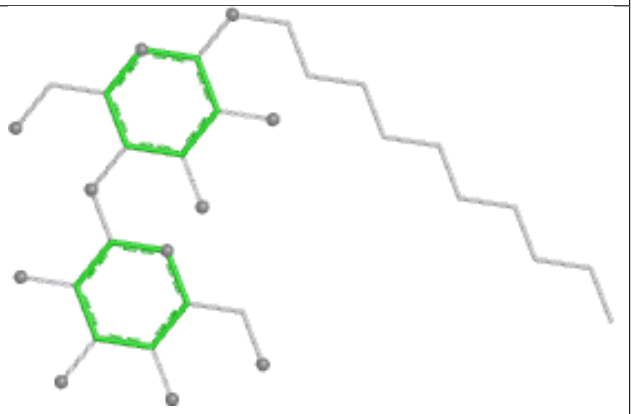
Bond lengths



Bond angles

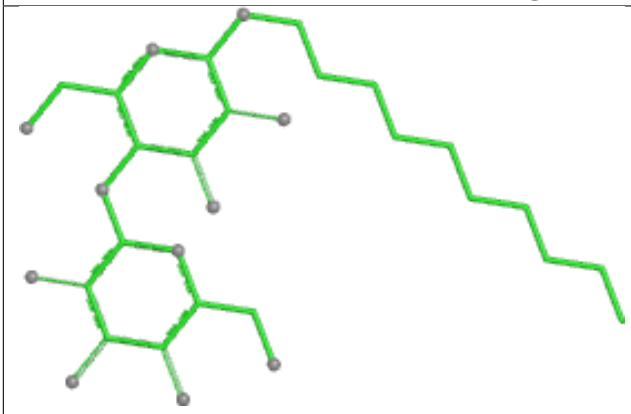


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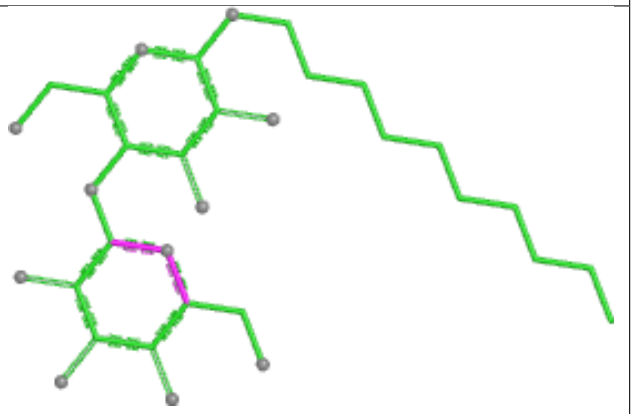


Rings

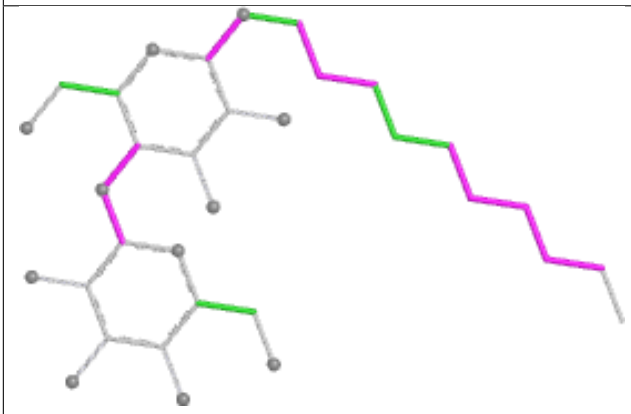
Ligand DMU C 10



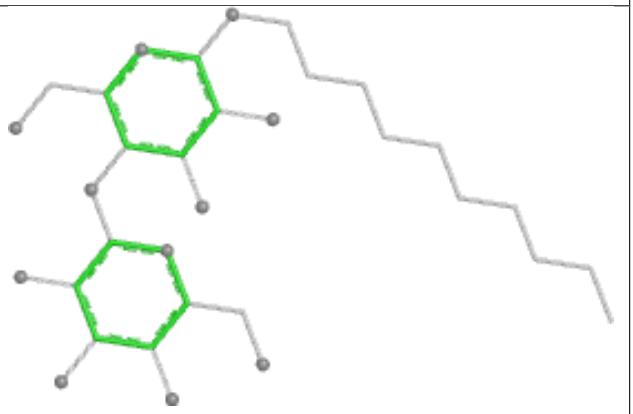
Bond lengths



Bond angles

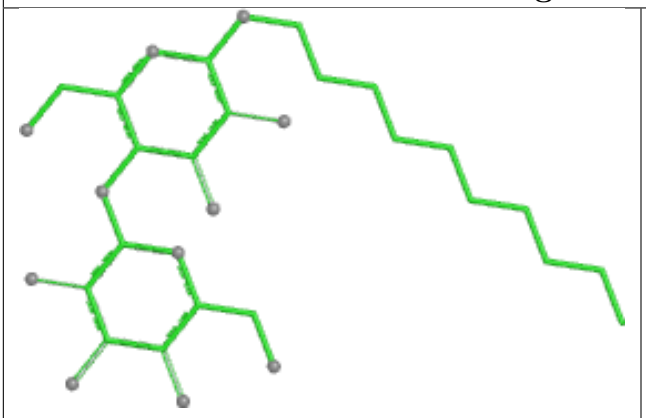


Torsions

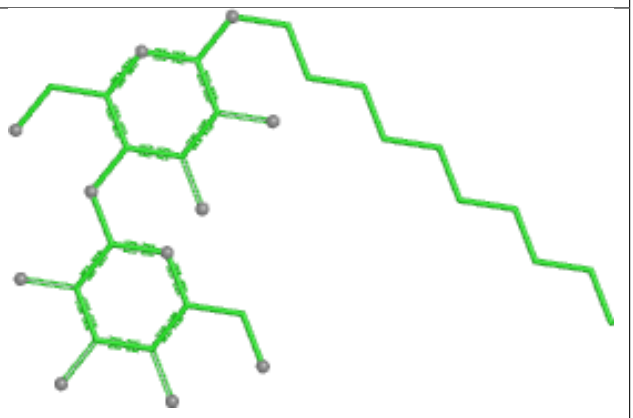


Rings

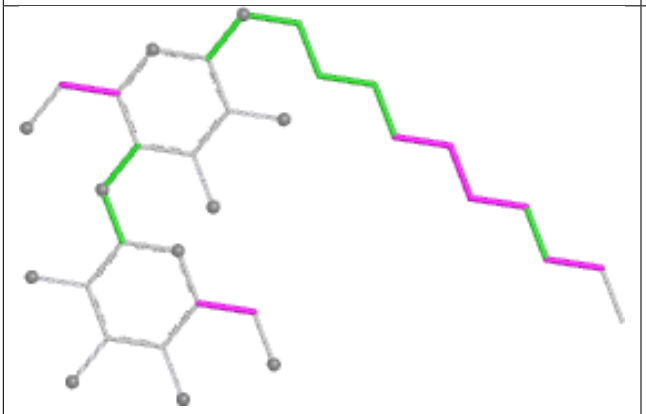
Ligand DMU B 3



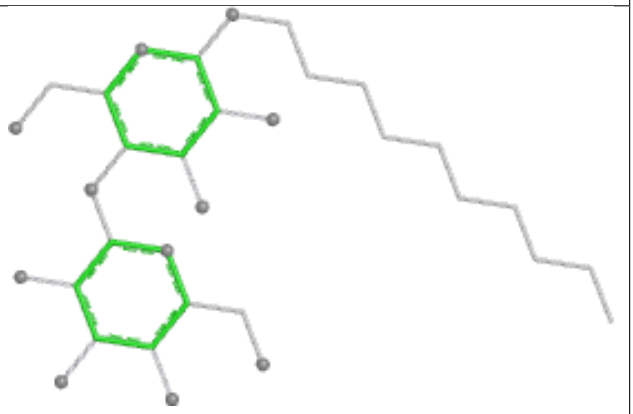
Bond lengths



Bond angles

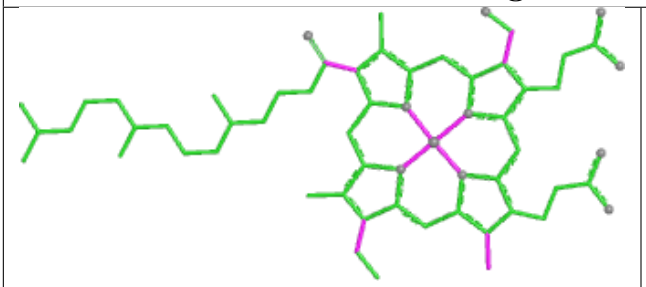


Torsions

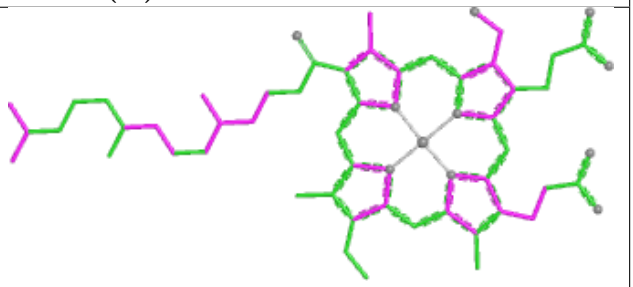


Rings

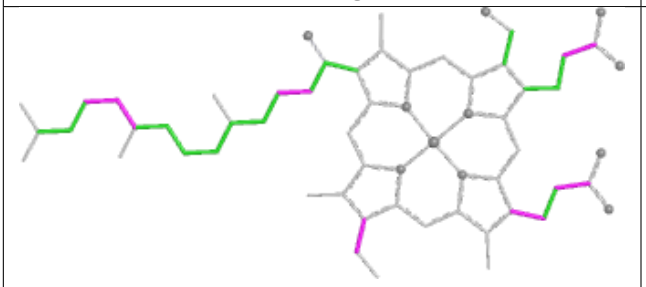
Ligand HEA A 2 (B)



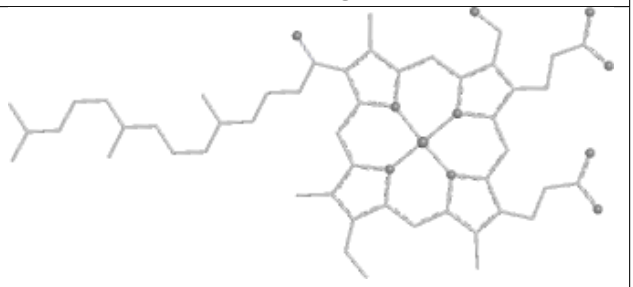
Bond lengths



Bond angles

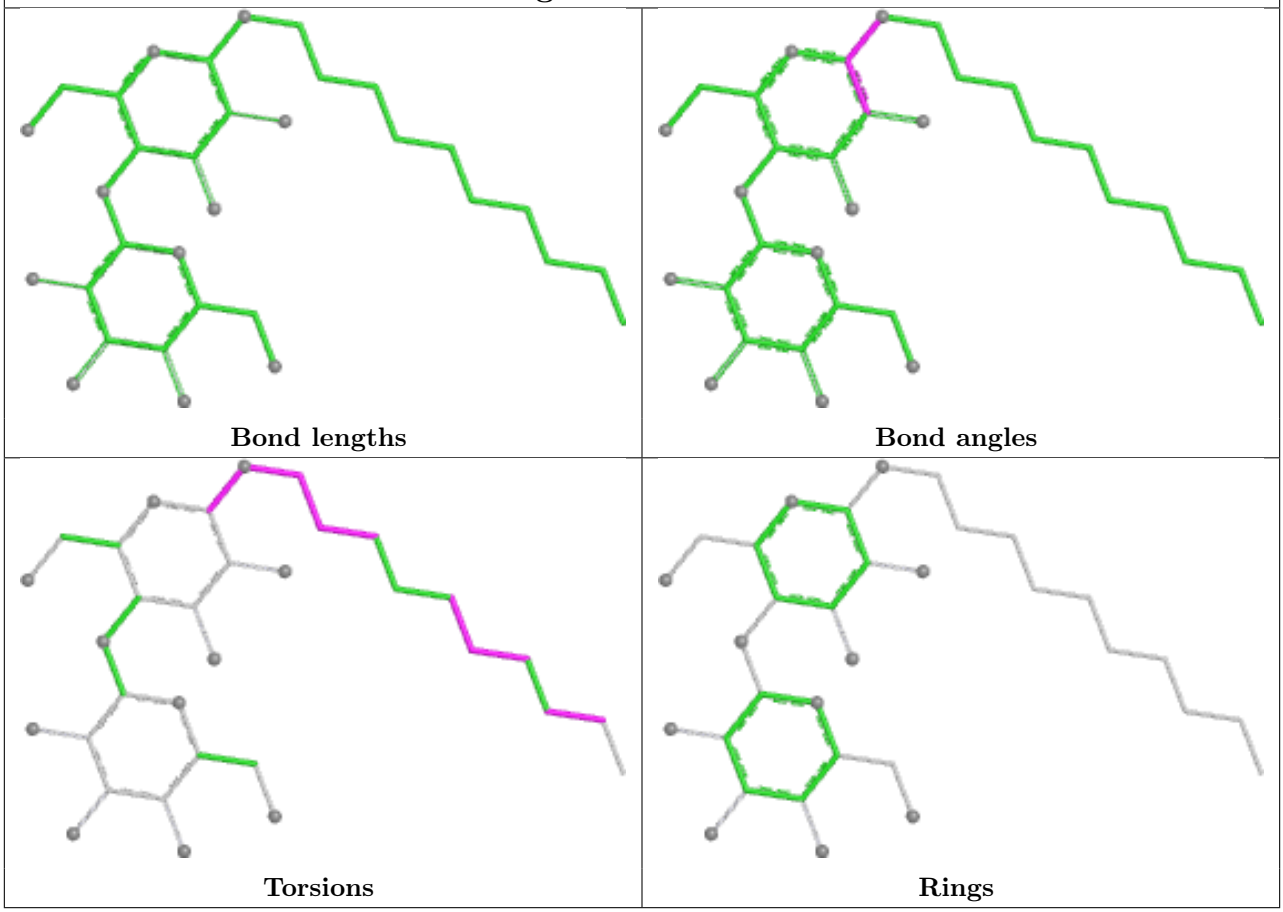


Torsions

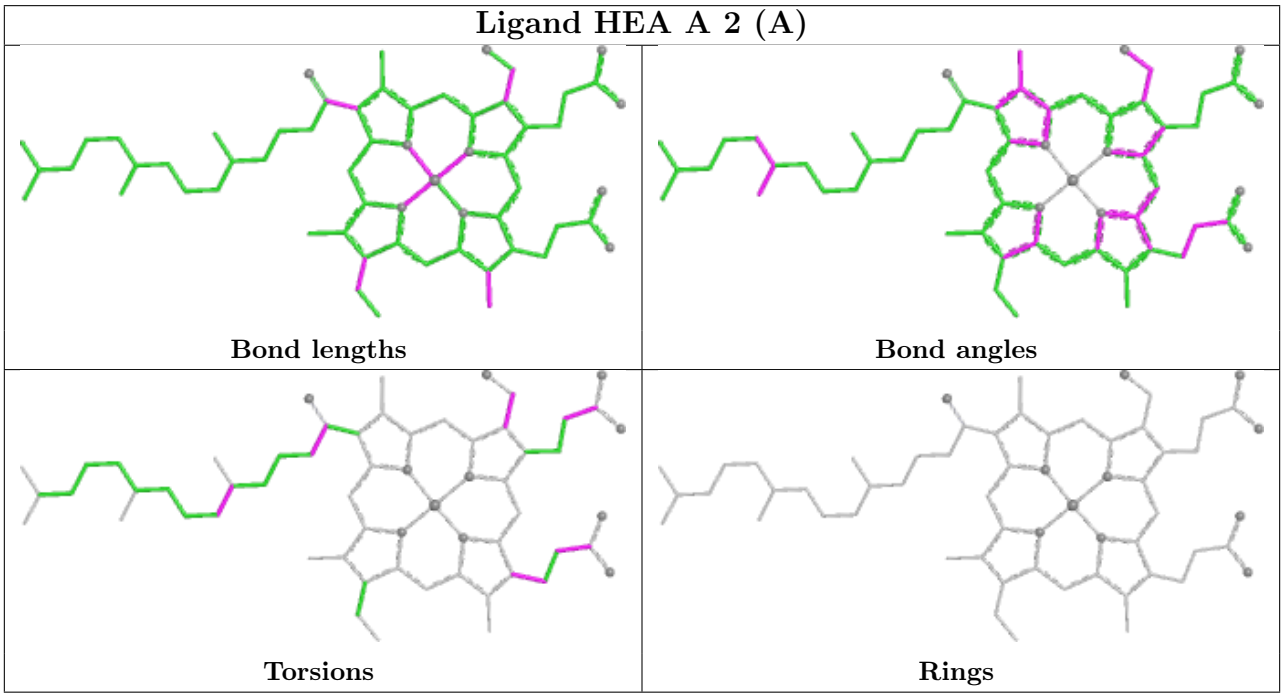


Rings

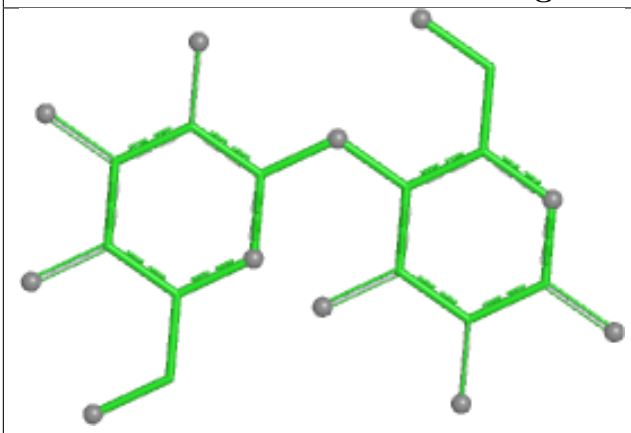
Ligand DMU B 2



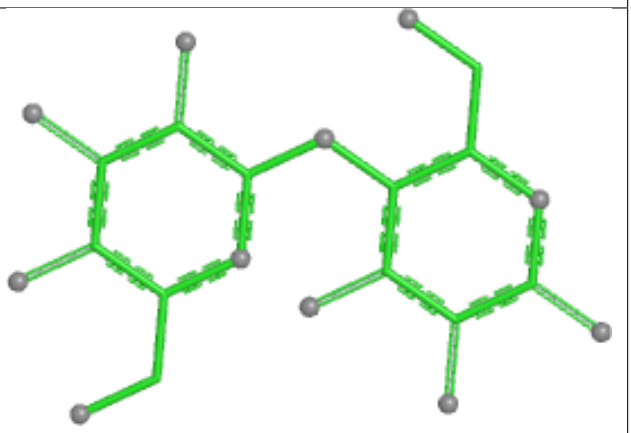
Ligand HEA A 2 (A)



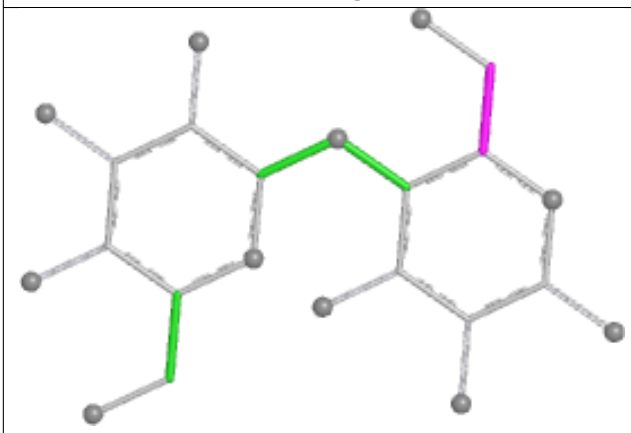
Ligand DMU C 5



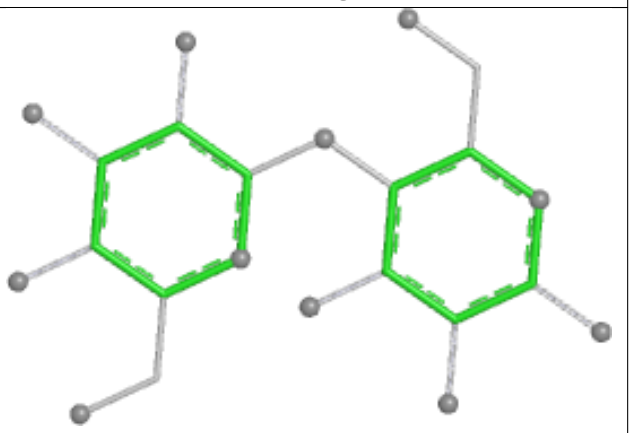
Bond lengths



Bond angles

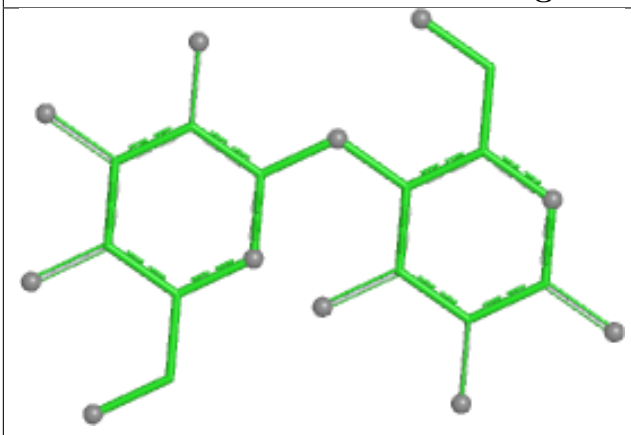


Torsions

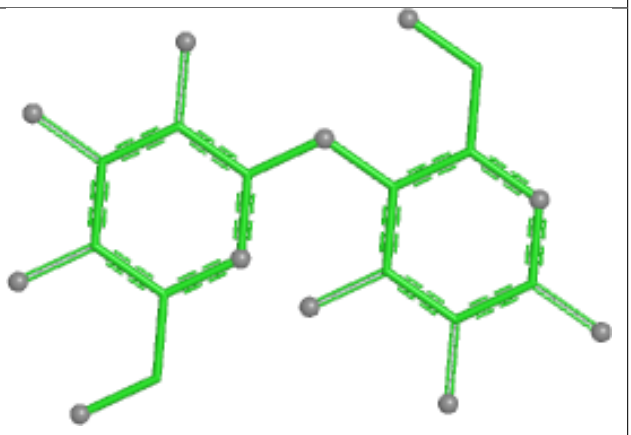


Rings

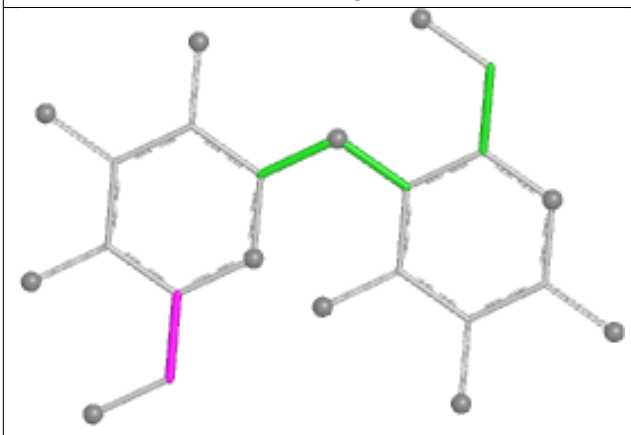
Ligand DMU B 6



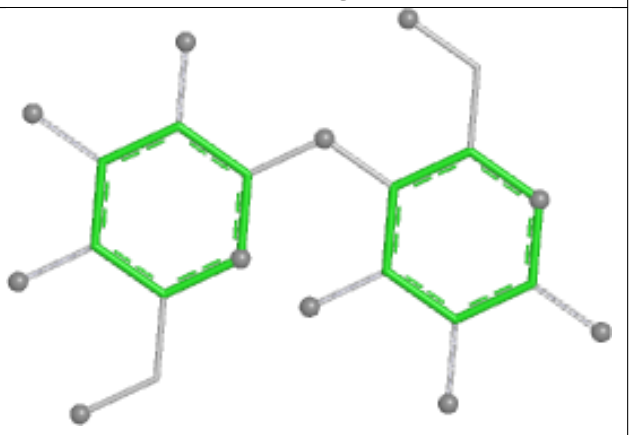
Bond lengths



Bond angles

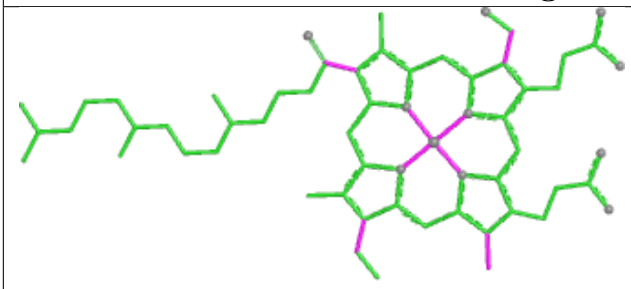


Torsions

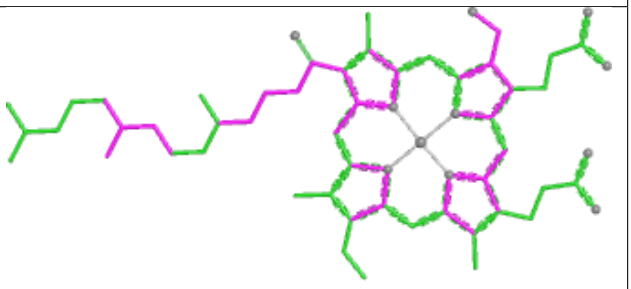


Rings

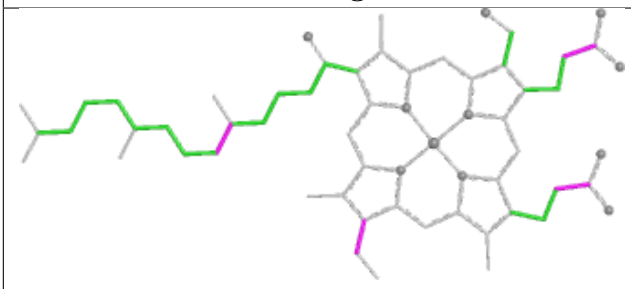
Ligand HEA A 1



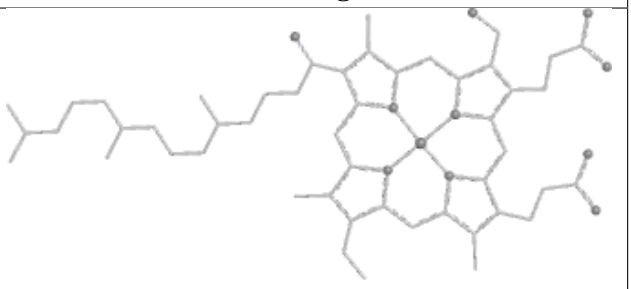
Bond lengths



Bond angles

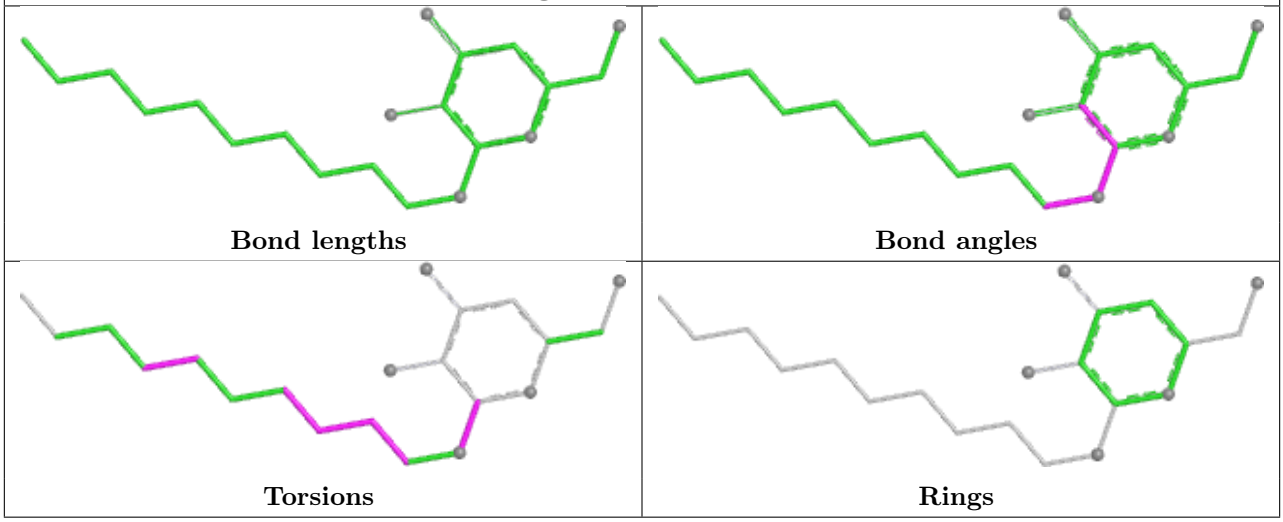


Torsions

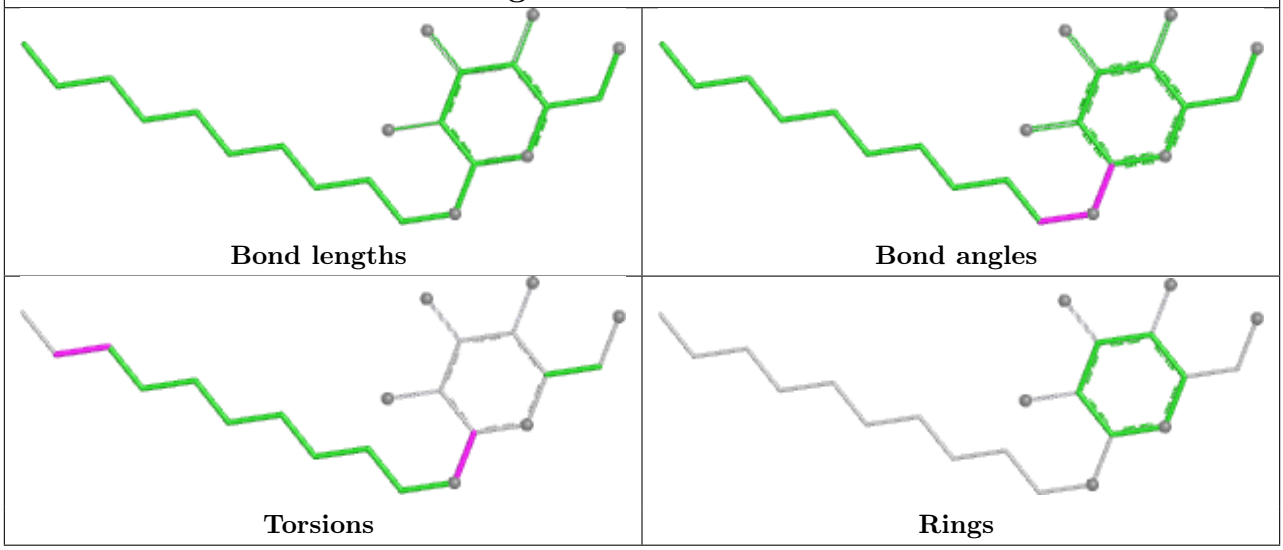


Rings

Ligand DMU A 7



Ligand DMU A 1005



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	535/535 (100%)	0.36	40 (7%) 20 23	13, 35, 57, 81	13 (2%)
1	C	531/535 (99%)	1.29	107 (20%) 3 3	16, 52, 76, 88	13 (2%)
2	B	256/256 (100%)	0.34	11 (4%) 40 45	23, 39, 55, 59	0
2	D	256/256 (100%)	0.68	26 (10%) 12 13	30, 44, 64, 72	0
All	All	1578/1582 (99%)	0.72	184 (11%) 9 10	13, 42, 67, 88	26 (1%)

The worst 5 of 184 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	361[A]	ILE	15.3
1	A	361[A]	ILE	13.2
1	C	20	TRP	7.8
2	B	56	TRP	7.2
2	D	284	HIS	5.6

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

There are no oligosaccharides in this entry.

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
4	DMU	C	9	23/33	0.63	0.22	85,86,89,89	23
4	DMU	C	5	23/33	0.67	0.23	97,98,98,99	23
4	DMU	D	8	23/33	0.72	0.23	89,90,93,93	23
5	TRD	A	1013	7/13	0.72	0.31	54,56,57,57	0
5	TRD	A	552	6/13	0.77	0.28	62,63,63,63	0
4	DMU	D	4	23/33	0.78	0.29	91,91,91,91	23
5	TRD	A	553	13/13	0.81	0.26	71,71,73,73	0
4	DMU	B	2	33/33	0.82	0.23	49,54,56,57	33
5	TRD	C	552	13/13	0.82	0.31	80,82,83,84	0
5	TRD	B	4	8/13	0.83	0.20	35,36,37,37	0
4	DMU	A	7	21/33	0.83	0.18	43,59,70,72	0
4	DMU	B	6	23/33	0.84	0.20	76,77,78,78	23
5	TRD	A	3	13/13	0.84	0.22	46,49,53,54	0
5	TRD	D	3	13/13	0.85	0.25	55,58,61,61	0
10	CL	C	554	1/1	0.85	0.21	68,68,68,68	0
4	DMU	A	1005	22/33	0.87	0.17	44,49,53,54	22
4	DMU	C	10	33/33	0.87	0.15	73,74,76,76	0
5	TRD	D	14	7/13	0.87	0.22	65,65,65,65	0
4	DMU	B	3	33/33	0.87	0.15	73,78,82,83	0
5	TRD	A	1009	7/13	0.89	0.19	57,58,58,58	0
11	HTH	B	286	10/10	0.90	0.19	56,60,61,61	0
4	DMU	B	1	33/33	0.94	0.09	26,35,46,48	0
6	HEA	C	2[B]	60/60	0.95	0.10	35,40,48,48	60
3	OH	C	802	1/1	0.95	0.34	21,21,21,21	1
6	HEA	C	2[A]	60/60	0.95	0.10	25,28,33,34	60
6	HEA	A	2[A]	60/60	0.96	0.09	21,22,30,32	60
6	HEA	A	2[B]	60/60	0.96	0.09	30,33,41,41	60
10	CL	A	10	1/1	0.97	0.06	41,41,41,41	0
3	OH	A	802	1/1	0.97	0.08	8,8,8,8	1
6	HEA	C	1	60/60	0.97	0.08	31,34,47,47	0
12	CD	D	9	1/1	0.97	0.07	63,63,63,63	1
12	CD	B	9	1/1	0.98	0.11	39,39,39,39	1
6	HEA	A	1	60/60	0.99	0.06	21,25,30,32	0
7	CU1	A	5	1/1	0.99	0.05	37,37,37,37	0
7	CU1	C	553	1/1	0.99	0.04	45,45,45,45	0
12	CD	B	8	1/1	0.99	0.02	41,41,41,41	0
8	MG	C	6	1/1	0.99	0.08	18,18,18,18	0
12	CD	D	288	1/1	0.99	0.02	40,40,40,40	0
9	CA	C	7	1/1	0.99	0.05	38,38,38,38	0
7	CU1	D	287	1/1	1.00	0.02	32,32,32,32	0
8	MG	A	6	1/1	1.00	0.08	13,13,13,13	0
7	CU1	B	288	1/1	1.00	0.02	26,26,26,26	0
9	CA	A	554	1/1	1.00	0.01	27,27,27,27	0

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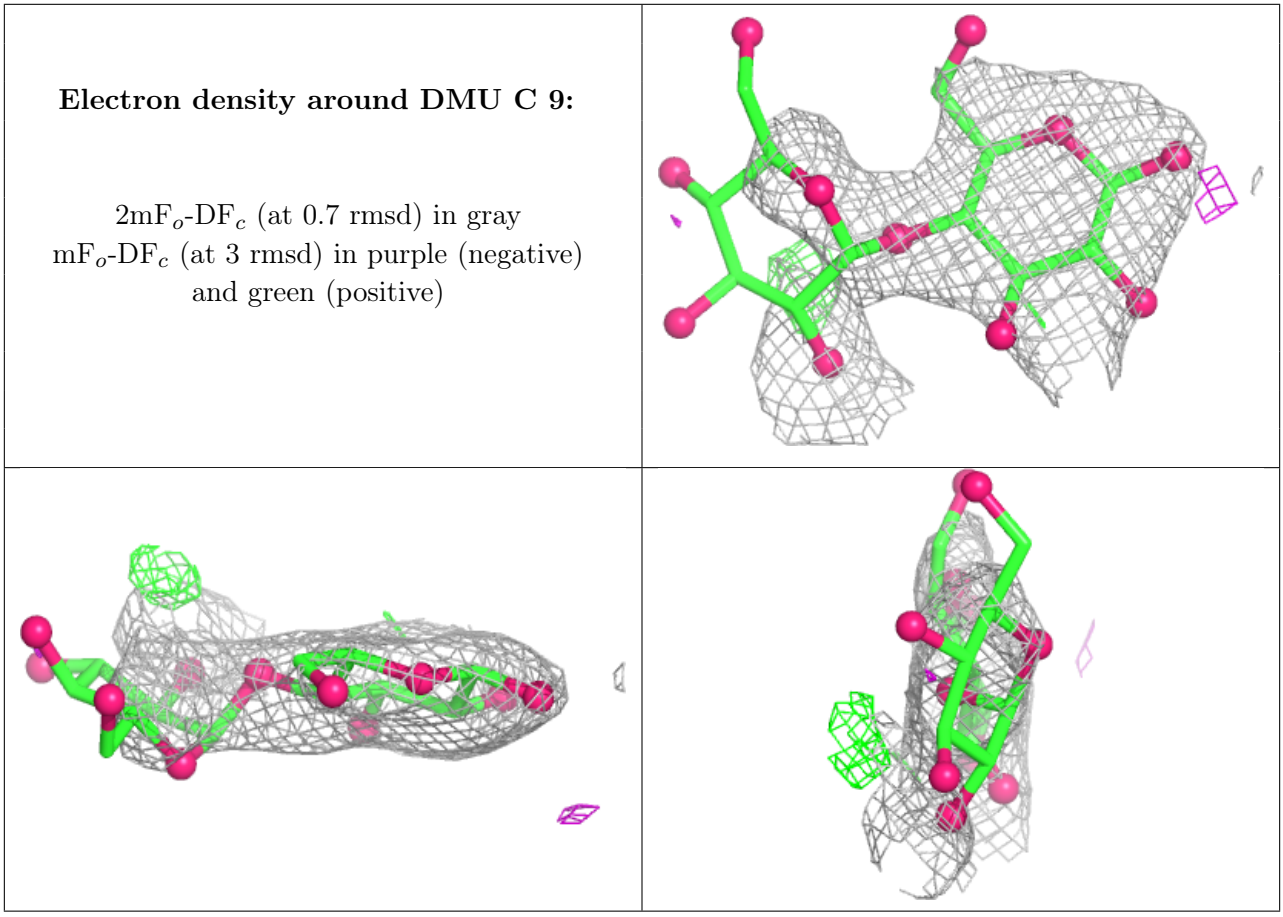
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CU1	B	287	1/1	1.00	0.01	25,25,25,25	0
7	CU1	D	286	1/1	1.00	0.02	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.

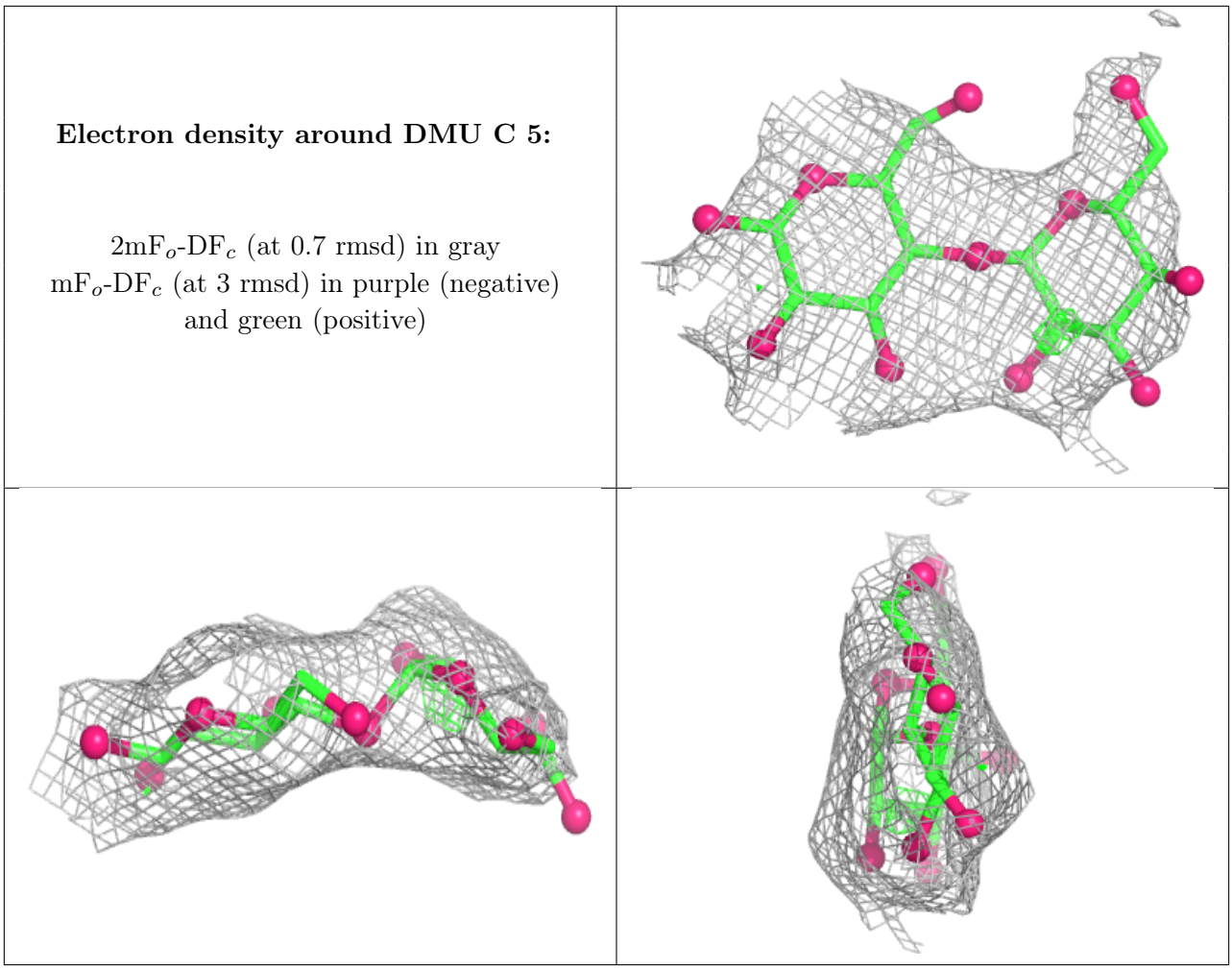
Electron density around DMU C 9:

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



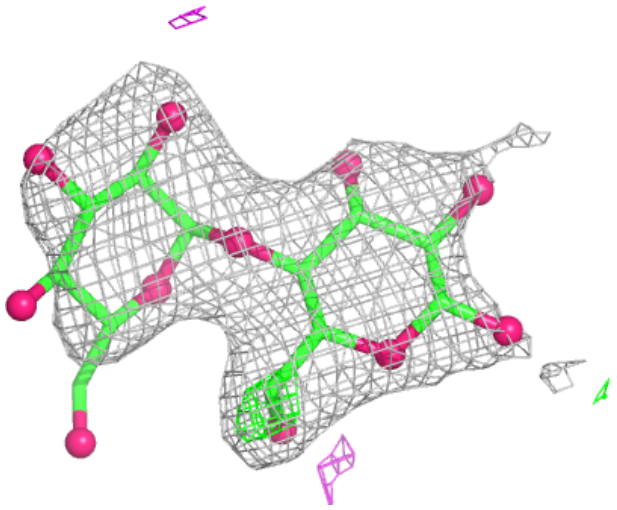
Electron density around DMU C 5:

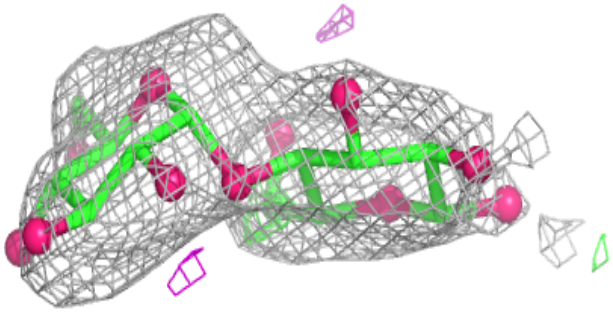
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

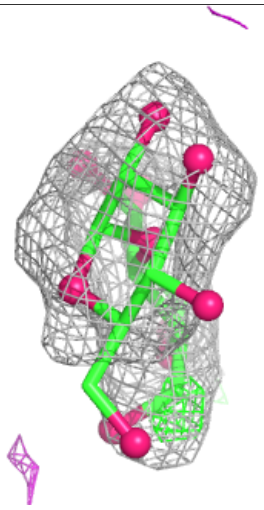


Electron density around DMU D 8:

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

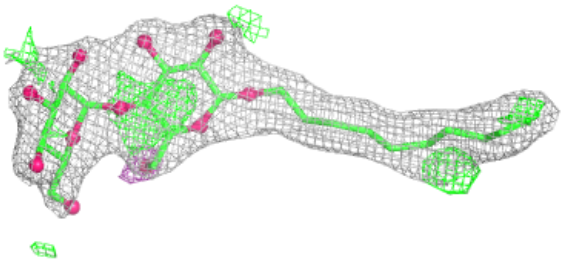


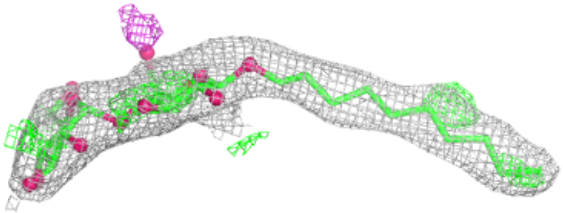


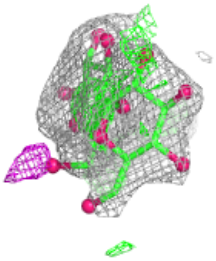


Electron density around DMU B 2:

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

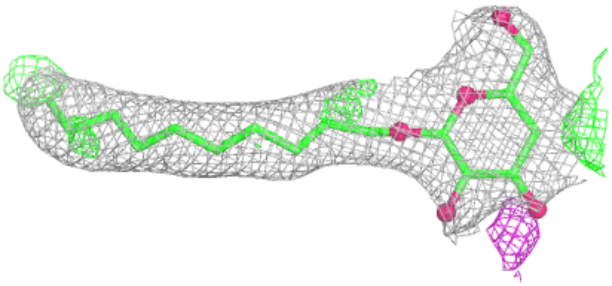


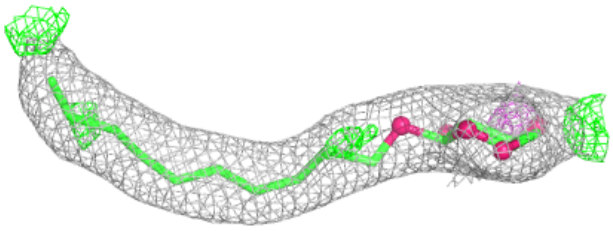


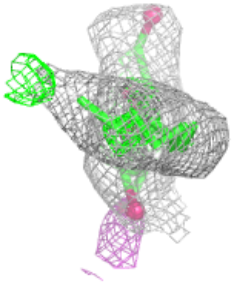


Electron density around DMU A 7:

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

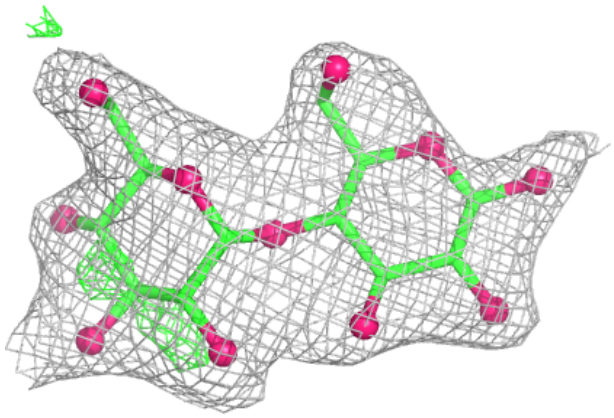


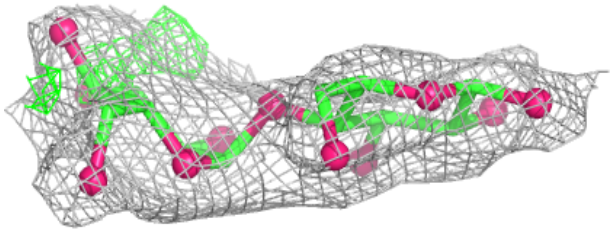


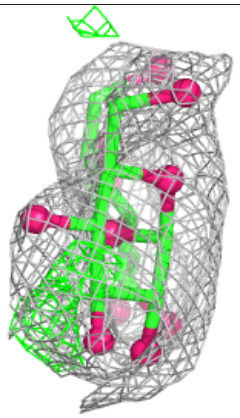


Electron density around DMU B 6:

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

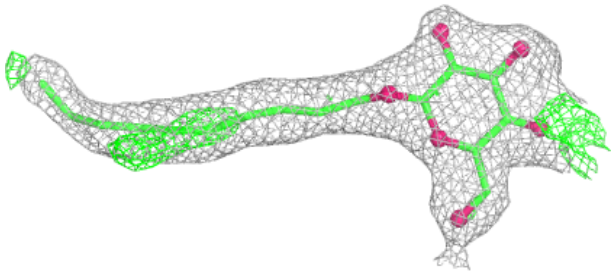


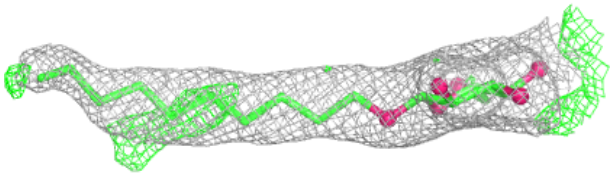


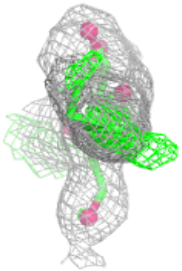


Electron density around DMU A 1005:

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

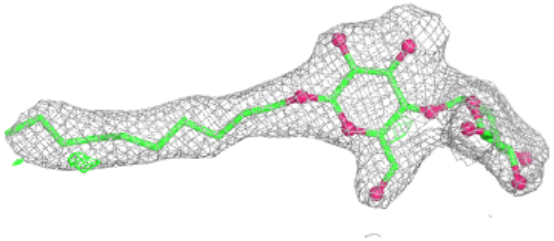


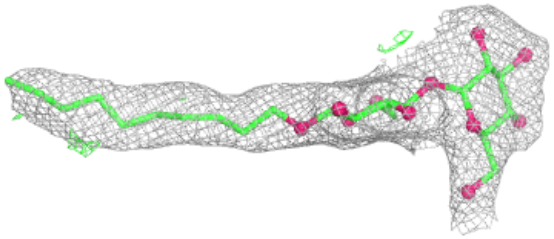


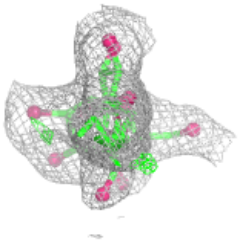


Electron density around DMU C 10:

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

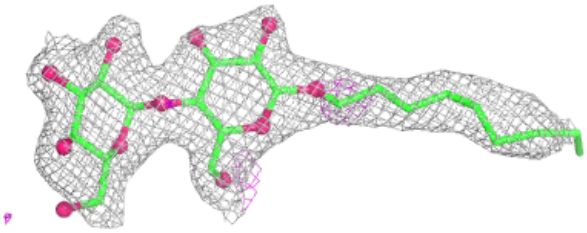


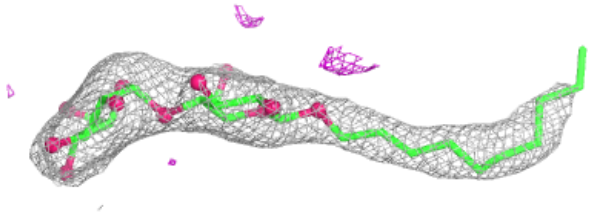


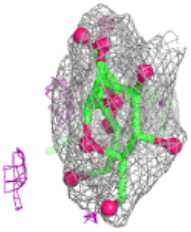


Electron density around DMU B 3:

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

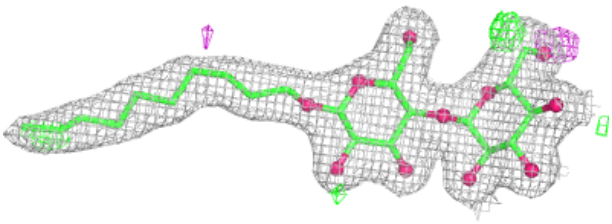


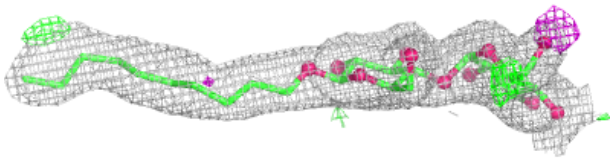




Electron density around DMU B 1:

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

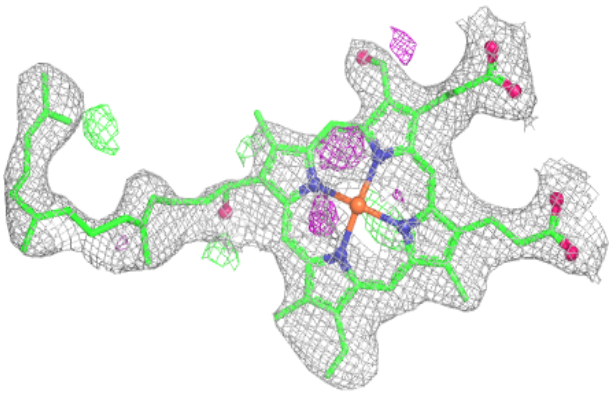


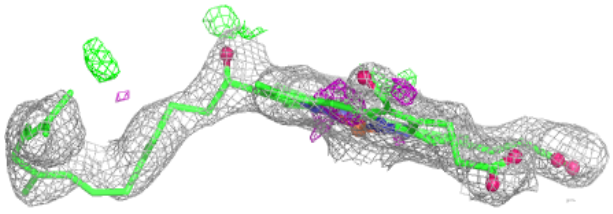


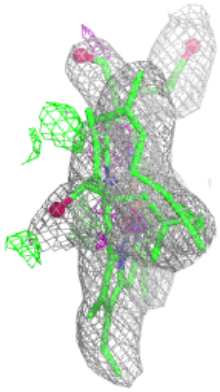


Electron density around HEA C 2 (B):

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

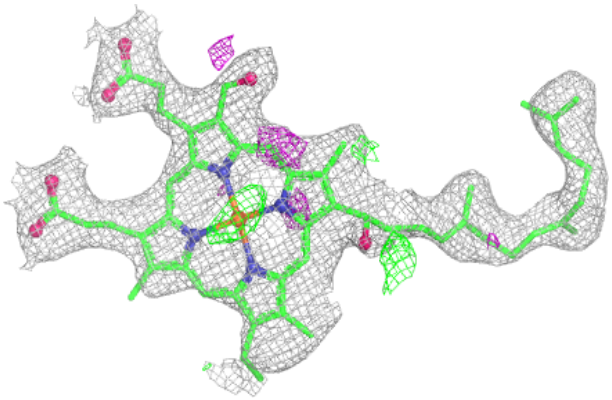


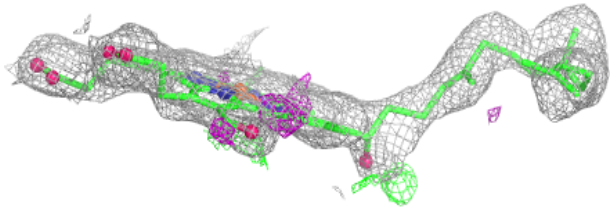


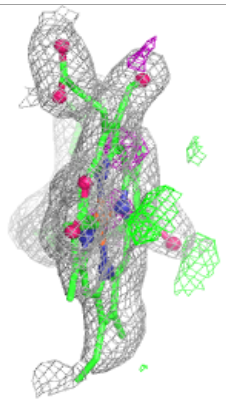


Electron density around HEA C 2 (A):

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

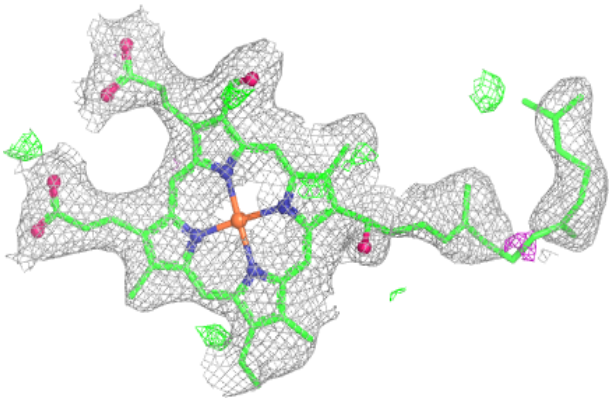


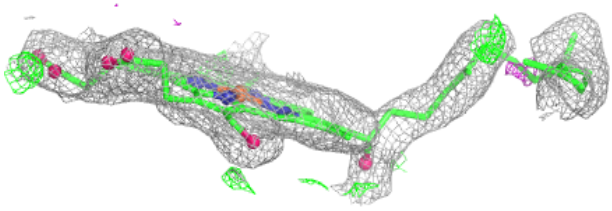


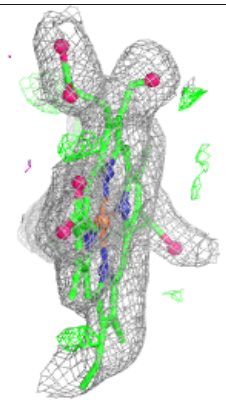


Electron density around HEA A 2 (A):

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

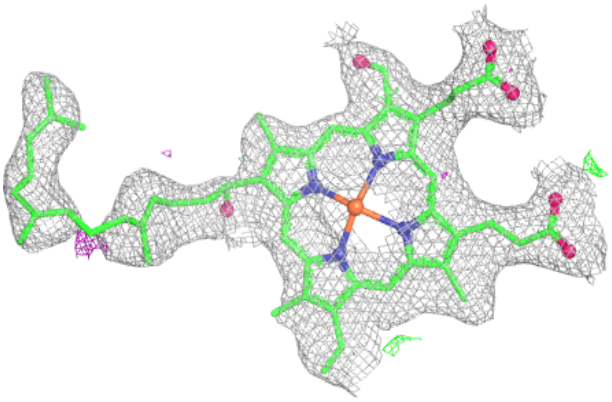


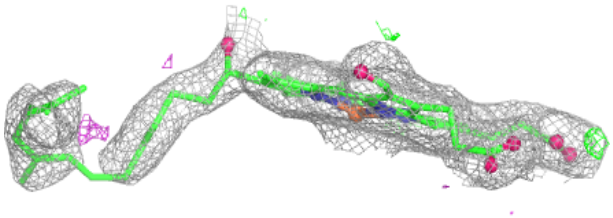


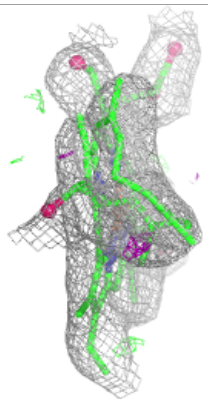


Electron density around HEA A 2 (B):

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

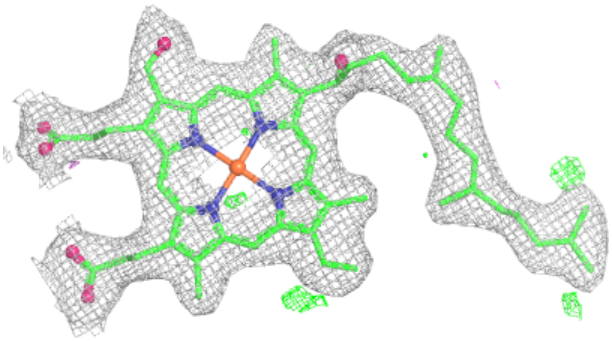


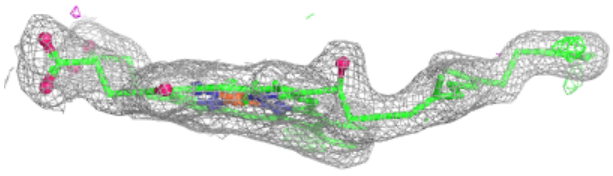


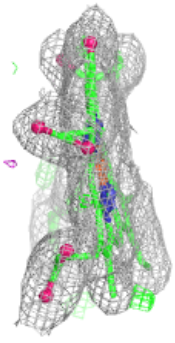


Electron density around HEA C 1:

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

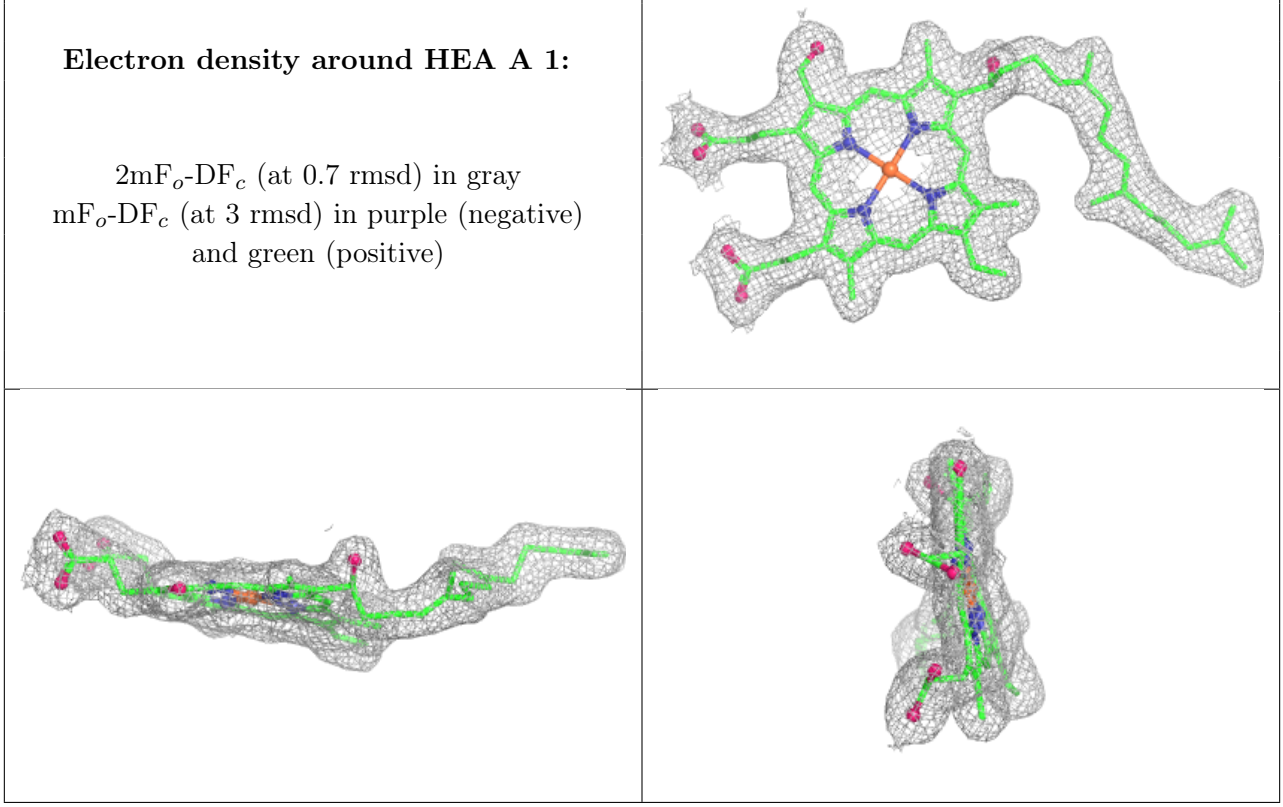






Electron density around HEA A 1:

$2mF_o$-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.