



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 19, 2019 – 10:51 AM EST

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 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

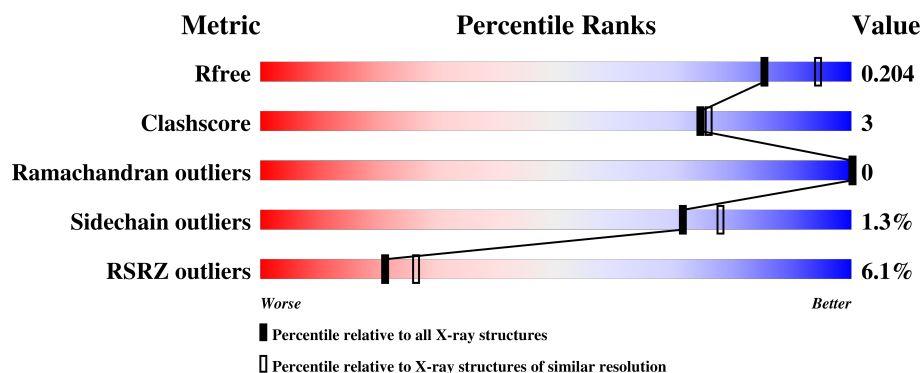
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	534	<div> <div>5%</div> <div>92%</div> <div>8%</div> </div>
1	C	534	<div> <div>10%</div> <div>90%</div> <div>10%</div> </div>
2	B	257	<div> <div>2%</div> <div>94%</div> <div>5%</div> </div>
2	D	257	<div> <div>4%</div> <div>95%</div> <div>5%</div> </div>

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
3	TRD	A	605	-	-	-	X
3	TRD	A	607	-	-	-	X
5	HEA	A	615	X	-	-	-
5	HEA	A	616	X	-	-	-
5	HEA	C	604	X	-	-	-
5	HEA	C	605	X	-	-	-

2 Entry composition

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			

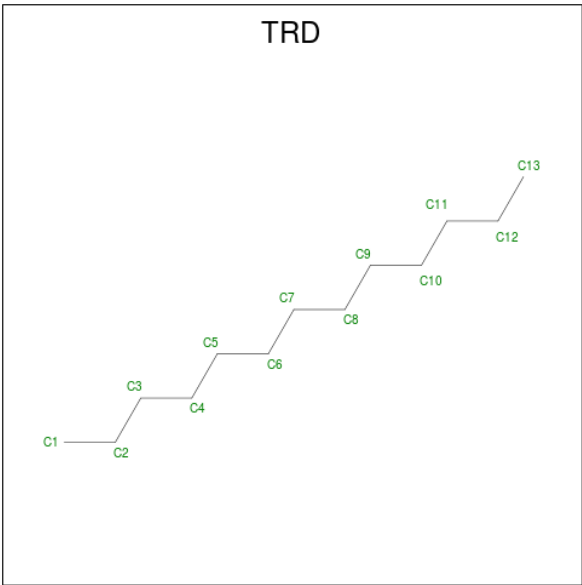
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

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:

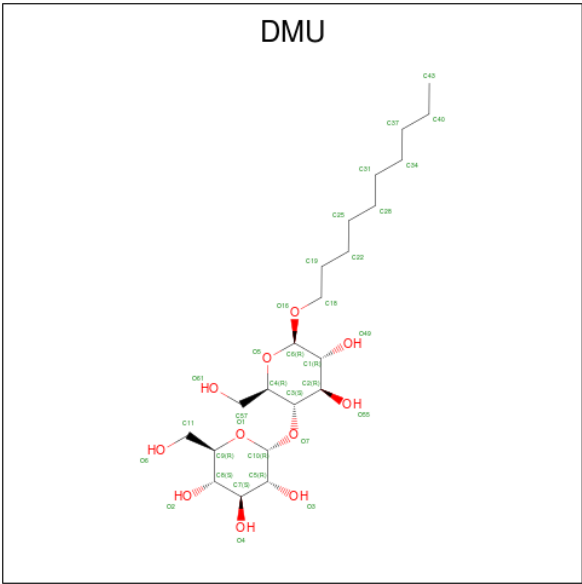
Chain	Residue	Modelled	Actual	Comment	Reference
B	29	ALA	-	expression tag	UNP Q3J5G0
B	282	HIS	-	expression tag	UNP Q3J5G0
B	283	HIS	-	expression tag	UNP Q3J5G0
B	284	HIS	-	expression tag	UNP Q3J5G0
B	285	HIS	-	expression tag	UNP Q3J5G0
D	29	ALA	-	expression tag	UNP Q3J5G0
D	282	HIS	-	expression tag	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 TRIDECANE (three-letter code: TRD) (formula: C₁₃H₂₈).



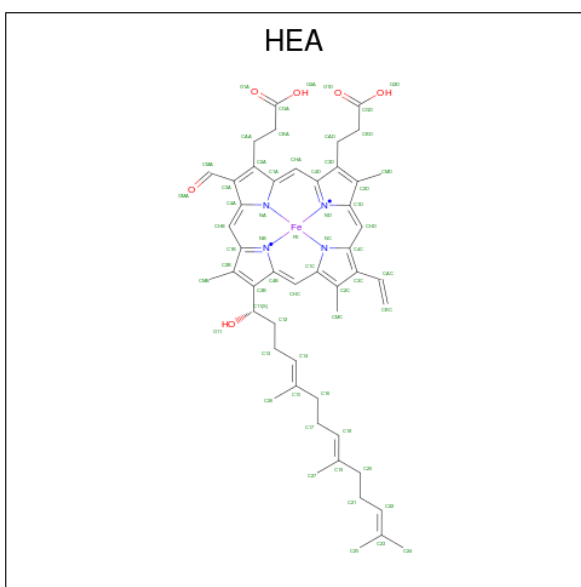
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 13 13	0	0
3	A	1	Total C 13 13	0	0
3	A	1	Total C 13 13	0	0
3	A	1	Total C 13 13	0	0
3	A	1	Total C 7 7	0	0
3	A	1	Total C 13 13	0	0
3	A	1	Total C 13 13	0	0
3	A	1	Total C 13 13	0	0
3	A	1	Total C 13 13	0	0
3	A	1	Total C 13 13	0	0
3	B	1	Total C 13 13	0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

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



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

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



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

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

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

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

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

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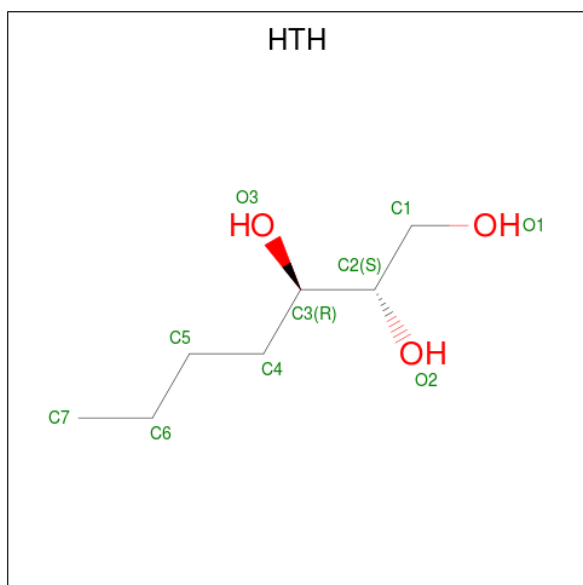
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg	0	0
			1	1		

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

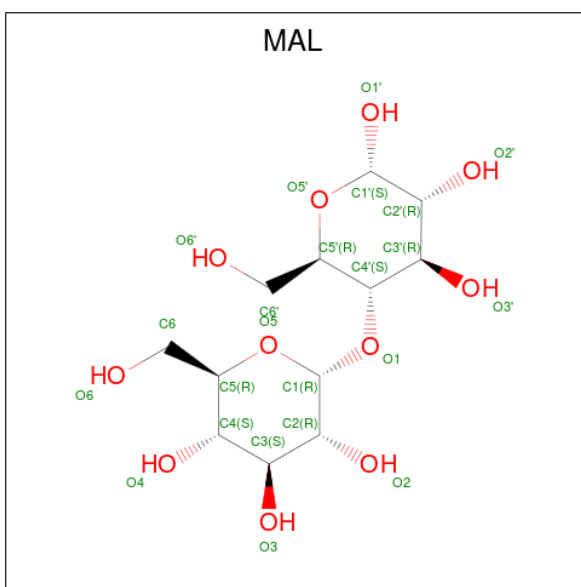
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		
8	C	1	Total	Ca	0	0
			1	1		

- Molecule 9 is (2S,3R)-heptane-1,2,3-triol (three-letter code: HTH) (formula: C₇H₁₆O₃).



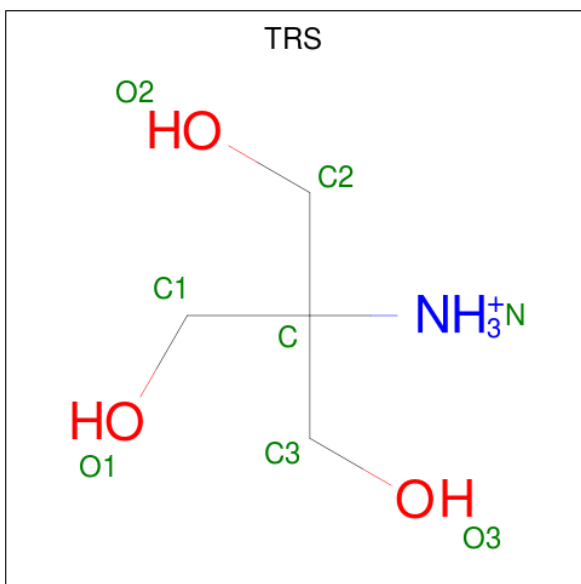
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			10	7	3		
9	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is MALTOSE (three-letter code: MAL) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			23	12	11		
10	D	1	Total	C	O	0	0
			23	12	11		

- 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	0	0
			8	4	1	3		

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

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

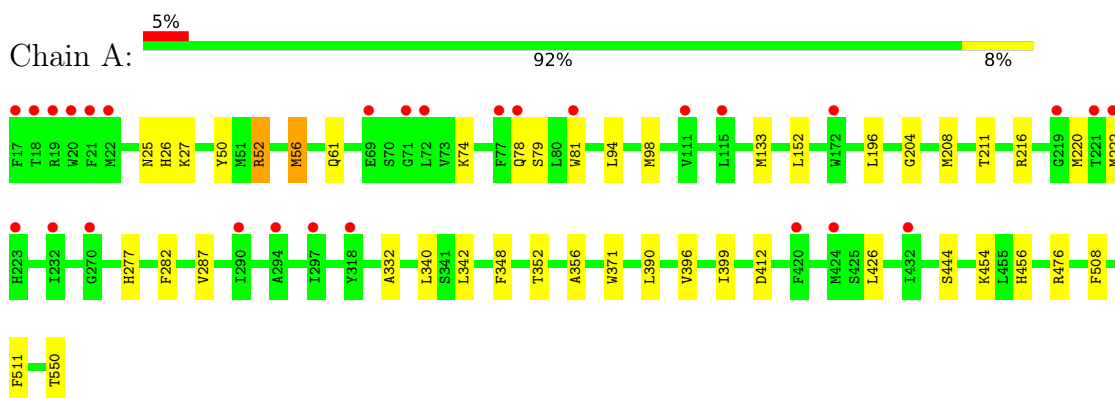
- Molecule 13 is water.

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

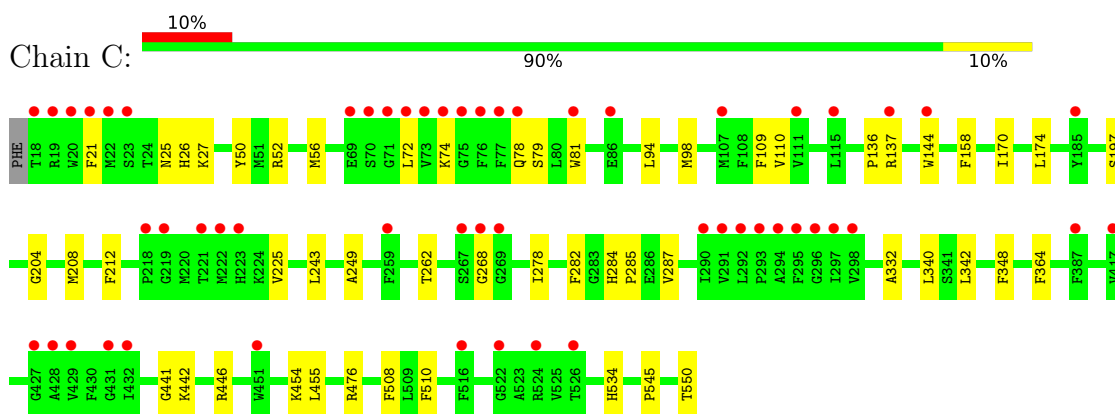
3 Residue-property plots [i](#)

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

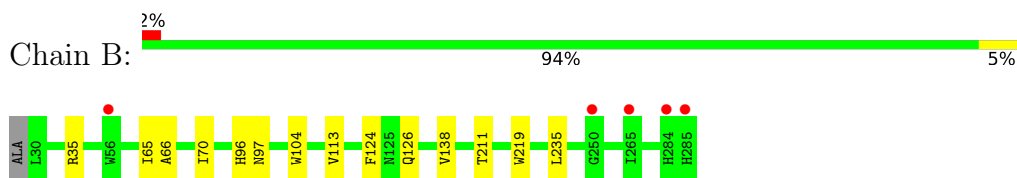
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 1: Cytochrome c oxidase subunit 1

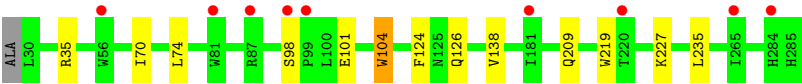


• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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	A	124	0	265	6	0
3	B	13	0	28	0	0
3	C	26	0	56	1	0
3	D	9	0	17	0	0
4	A	132	0	168	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	30	0	33	3	0
4	C	23	0	31	0	0
5	A	120	0	108	8	0
5	C	120	0	108	6	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	A	10	0	16	1	0
9	B	10	0	16	0	0
10	B	23	0	22	0	0
10	D	23	0	22	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	12932	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.

The worst 5 of 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
5:A:615:HEA:HMC1	5:A:615:HEA:HBC1	1.68	0.75
5:C:604:HEA:HMC1	5:C:604:HEA:HBC1	1.72	0.72

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%)	81	85
1	C	426/434 (98%)	422 (99%)	4 (1%)	81	85
2	B	214/215 (100%)	211 (99%)	3 (1%)	69	76
2	D	210/215 (98%)	205 (98%)	5 (2%)	52	56
All	All	1275/1298 (98%)	1259 (99%)	16 (1%)	71	78

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	52	ARG
1	C	56	MET
2	D	98	SER

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Mol	Chain	Res	Type
2	B	126	GLN
2	D	104	TRP

Some 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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 14 are monoatomic - leaving 29 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	$\# Z > 2$
3	TRD	A	601	-	12,12,12	0.16	0	11,11,11	0.64	0
3	TRD	A	602	-	12,12,12	0.18	0	11,11,11	0.80	0
3	TRD	A	603	-	12,12,12	0.17	0	11,11,11	0.71	0
3	TRD	A	604	-	12,12,12	0.18	0	11,11,11	0.62	0
3	TRD	A	605	-	6,6,12	0.18	0	5,5,11	0.52	0
3	TRD	A	606	-	12,12,12	0.14	0	11,11,11	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TRD	A	607	-	12,12,12	0.11	0	11,11,11	0.85	0
3	TRD	A	608	-	12,12,12	0.16	0	11,11,11	0.70	0
3	TRD	A	609	-	12,12,12	0.14	0	11,11,11	0.80	0
3	TRD	A	610	-	12,12,12	0.17	0	11,11,11	0.72	0
4	DMU	A	611	-	34,34,34	1.94	13 (38%)	45,45,45	1.25	4 (8%)
4	DMU	A	612	-	34,34,34	1.76	8 (23%)	45,45,45	1.23	5 (11%)
4	DMU	A	613	-	34,34,34	1.93	10 (29%)	45,45,45	1.38	6 (13%)
4	DMU	A	614	-	34,34,34	1.91	13 (38%)	45,45,45	1.87	11 (24%)
5	HEA	A	615	1	44,67,67	1.90	11 (25%)	37,103,103	2.52	13 (35%)
5	HEA	A	616	1,13	44,67,67	1.80	11 (25%)	37,103,103	2.27	8 (21%)
9	HTH	A	620	-	9,9,9	0.57	0	10,10,10	1.31	1 (10%)
3	TRD	B	301	-	12,12,12	0.16	0	11,11,11	0.74	0
4	DMU	B	302	-	31,31,34	1.96	13 (41%)	42,42,45	1.24	4 (9%)
10	MAL	B	303	-	24,24,24	0.49	0	35,35,35	0.73	0
11	TRS	B	304	-	7,7,7	0.36	0	9,9,9	1.45	1 (11%)
9	HTH	B	309	-	9,9,9	0.56	0	10,10,10	1.15	2 (20%)
3	TRD	C	601	-	12,12,12	0.15	0	11,11,11	0.91	0
3	TRD	C	602	-	12,12,12	0.16	0	11,11,11	0.68	0
4	DMU	C	603	-	23,23,34	1.80	6 (26%)	28,28,45	1.01	2 (7%)
5	HEA	C	604	1	44,67,67	1.94	11 (25%)	37,103,103	2.43	13 (35%)
5	HEA	C	605	1,13	44,67,67	1.87	11 (25%)	37,103,103	2.33	10 (27%)
3	TRD	D	301	-	8,8,12	0.14	0	7,7,11	0.79	0
10	MAL	D	302	-	24,24,24	0.58	0	35,35,35	1.41	7 (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	TRD	A	601	-	-	0/10/10/10	-
3	TRD	A	602	-	-	2/10/10/10	-
3	TRD	A	603	-	-	4/10/10/10	-
3	TRD	A	604	-	-	5/10/10/10	-
3	TRD	A	605	-	-	1/4/4/10	-
3	TRD	A	606	-	-	3/10/10/10	-
3	TRD	A	607	-	-	4/10/10/10	-
3	TRD	A	608	-	-	7/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRD	A	609	-	-	3/10/10/10	-
3	TRD	A	610	-	-	3/10/10/10	-
4	DMU	A	611	-	-	13/19/59/59	0/2/2/2
4	DMU	A	612	-	-	3/19/59/59	0/2/2/2
4	DMU	A	613	-	-	6/19/59/59	0/2/2/2
4	DMU	A	614	-	-	8/19/59/59	0/2/2/2
5	HEA	A	615	1	2/2/7/16	2/24/76/76	-
5	HEA	A	616	1,13	2/2/7/16	0/24/76/76	-
9	HTH	A	620	-	-	7/10/10/10	-
3	TRD	B	301	-	-	3/10/10/10	-
4	DMU	B	302	-	-	8/16/56/59	0/2/2/2
10	MAL	B	303	-	-	2/8/48/48	0/2/2/2
11	TRS	B	304	-	-	8/9/9/9	-
9	HTH	B	309	-	-	5/10/10/10	-
3	TRD	C	601	-	-	3/10/10/10	-
3	TRD	C	602	-	-	2/10/10/10	-
4	DMU	C	603	-	-	5/15/35/59	0/1/1/2
5	HEA	C	604	1	2/2/7/16	2/24/76/76	-
5	HEA	C	605	1,13	2/2/7/16	0/24/76/76	-
3	TRD	D	301	-	-	1/6/6/10	-
10	MAL	D	302	-	-	2/8/48/48	0/2/2/2

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	604	HEA	C3B-C11	-7.45	1.47	1.52
5	A	615	HEA	C3B-C11	-7.16	1.47	1.52
5	C	605	HEA	C3B-C11	-5.80	1.48	1.52
5	A	616	HEA	C3B-C11	-5.20	1.48	1.52
5	C	604	HEA	C3C-C2C	5.18	1.47	1.40

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	604	HEA	C1B-C2B-C3B	-7.90	101.50	107.00
5	A	615	HEA	C1B-C2B-C3B	-7.33	101.89	107.00
5	A	616	HEA	C4B-C3B-C2B	-6.45	102.36	106.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	605	HEA	C1B-C2B-C3B	-6.43	102.52	107.00
5	A	616	HEA	CAD-CBD-CGD	-6.29	101.92	112.66

5 of 8 chirality outliers are listed below:

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

5 of 112 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	620	HTH	C1-C2-C3-O3
9	A	620	HTH	C1-C2-C3-C4
9	A	620	HTH	O2-C2-C3-O3
9	A	620	HTH	O2-C2-C3-C4
4	B	302	DMU	O5-C6-O16-C18

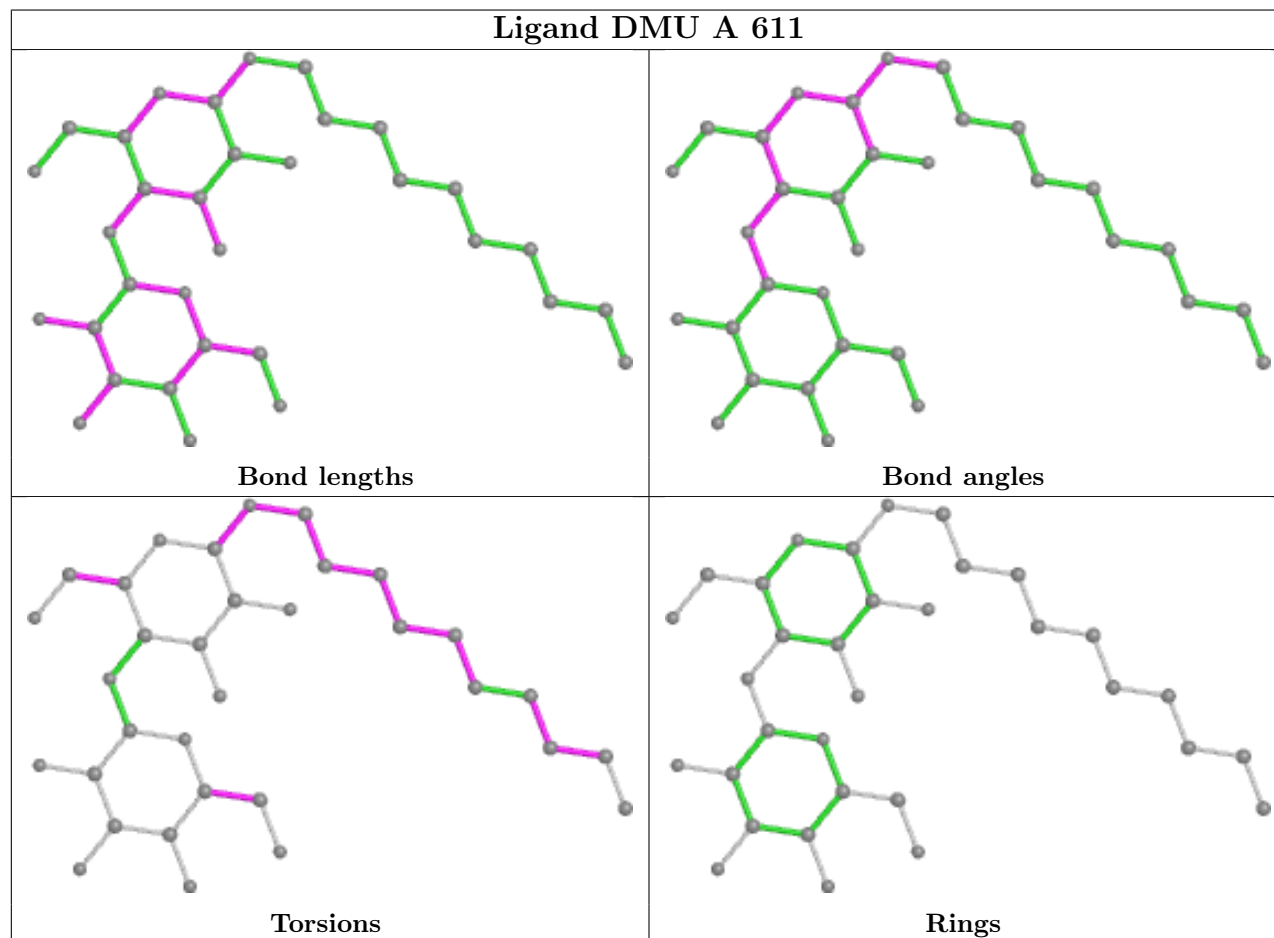
There are no ring outliers.

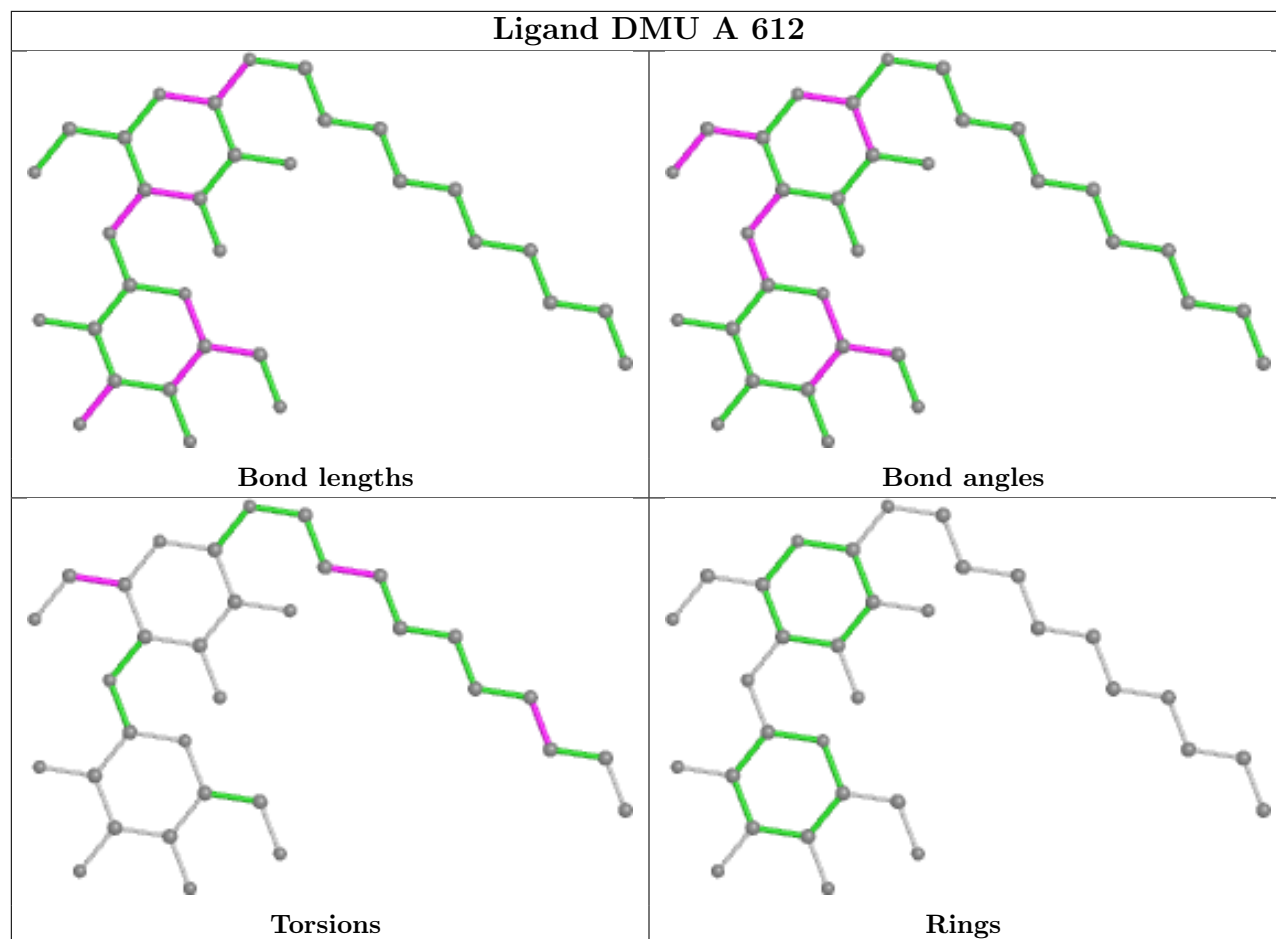
14 monomers are involved in 30 short contacts:

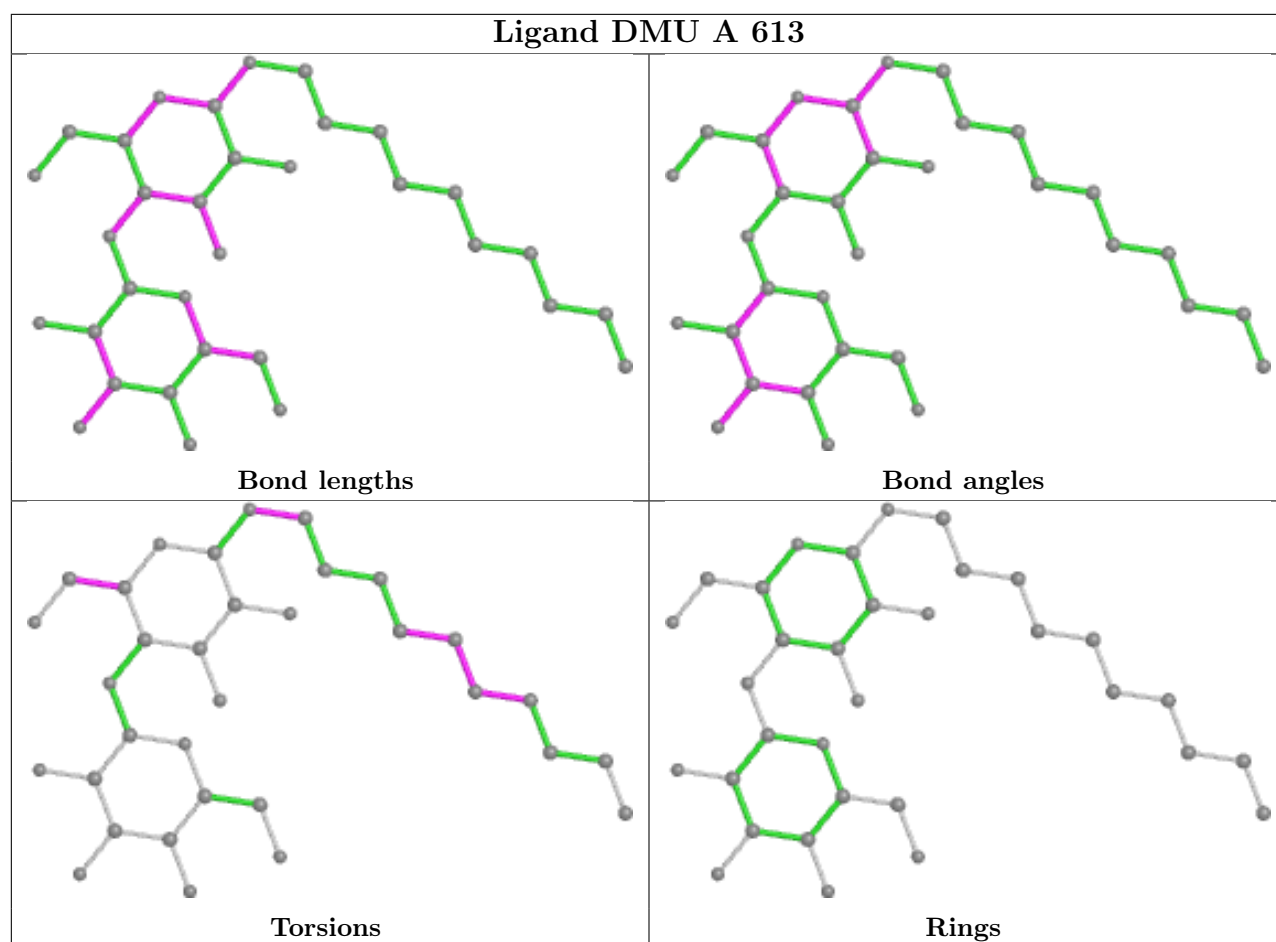
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	TRD	1	0
3	A	604	TRD	2	0
3	A	606	TRD	1	0
3	A	607	TRD	1	0
3	A	609	TRD	1	0
4	A	611	DMU	1	0
4	A	614	DMU	4	0
5	A	615	HEA	3	0
5	A	616	HEA	5	0
9	A	620	HTH	1	0
4	B	302	DMU	3	0
3	C	601	TRD	1	0
5	C	604	HEA	3	0
5	C	605	HEA	3	0

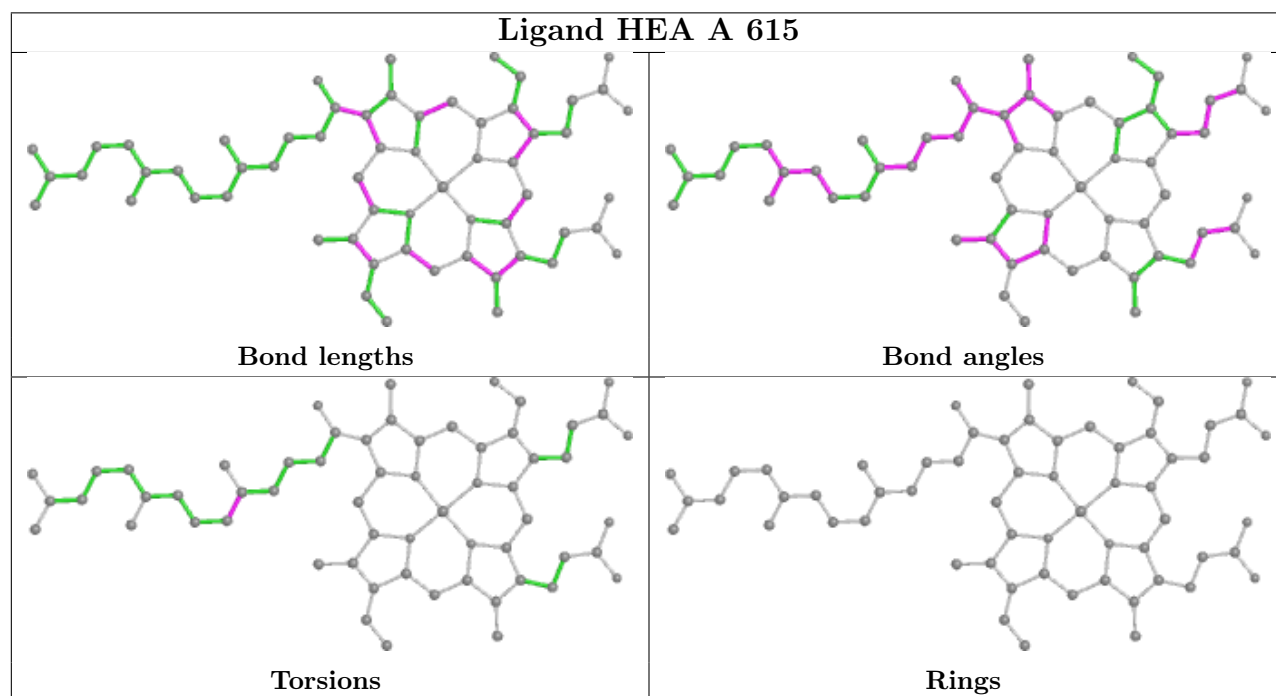
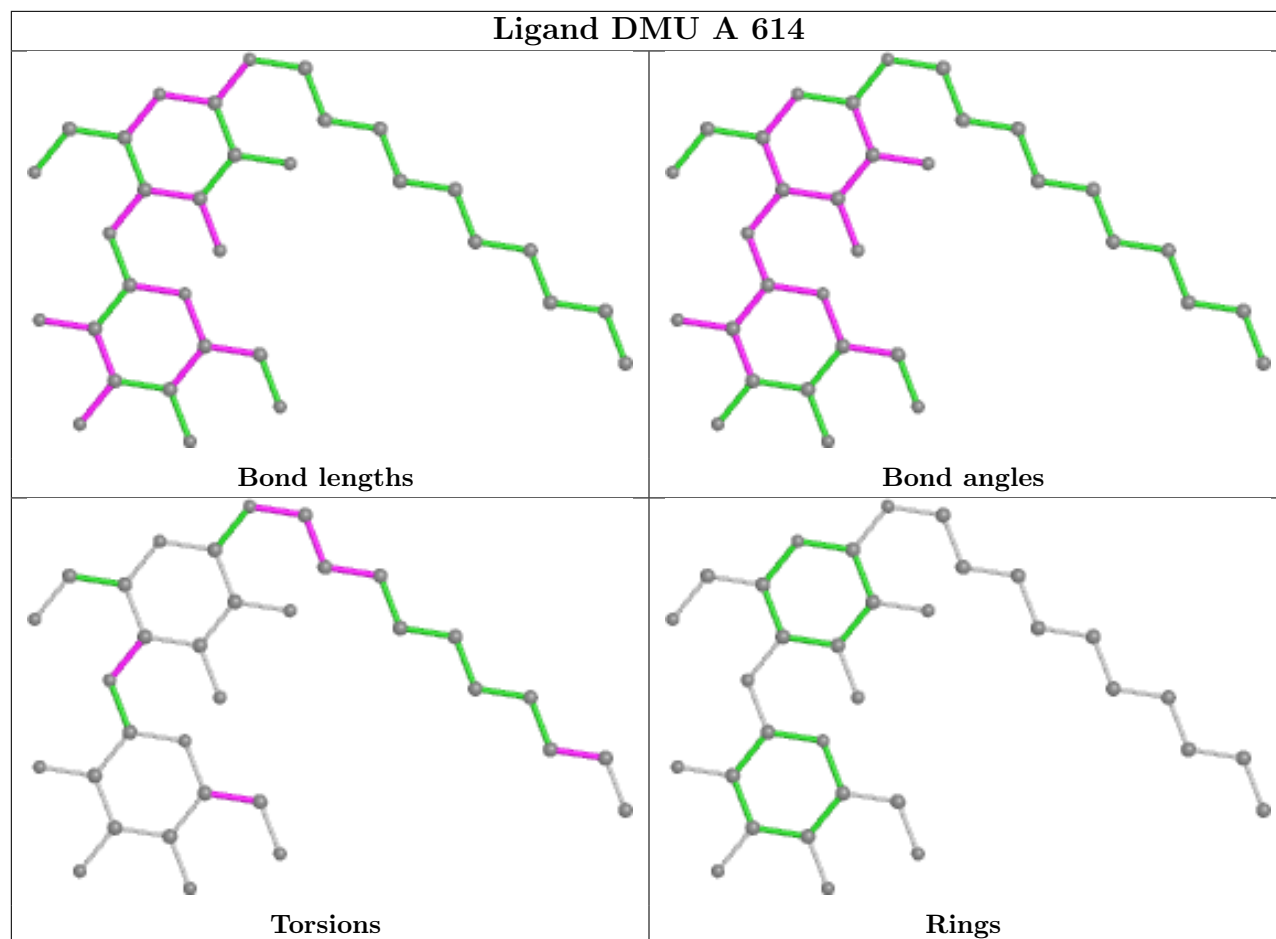
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

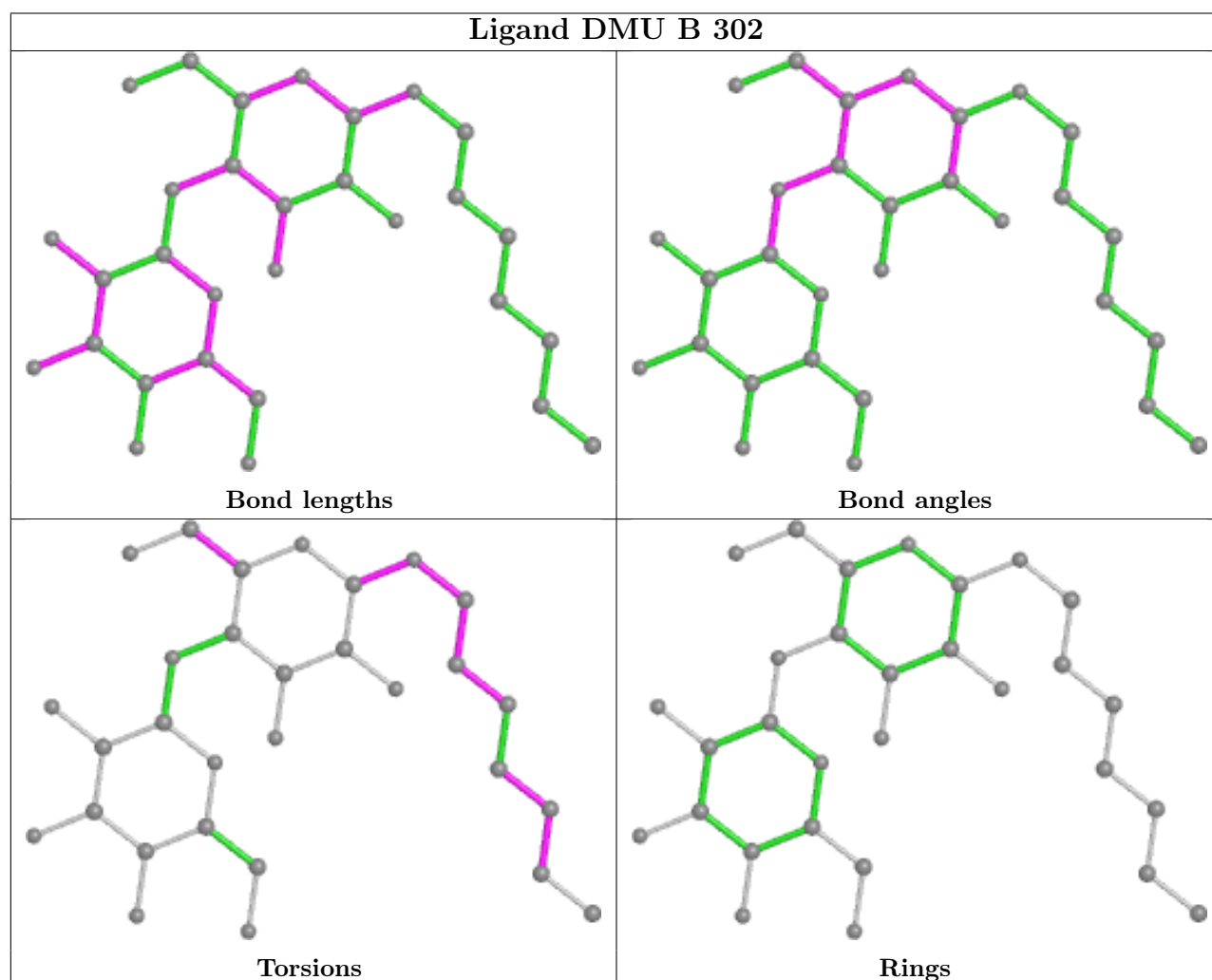
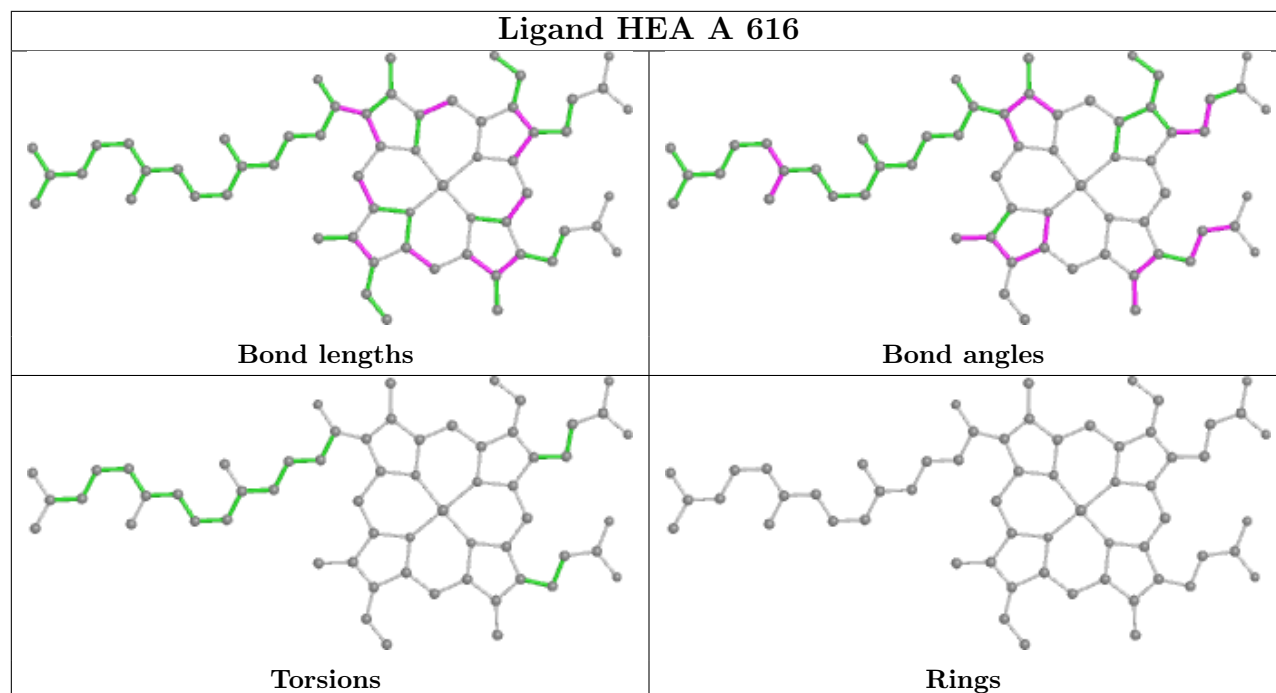
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

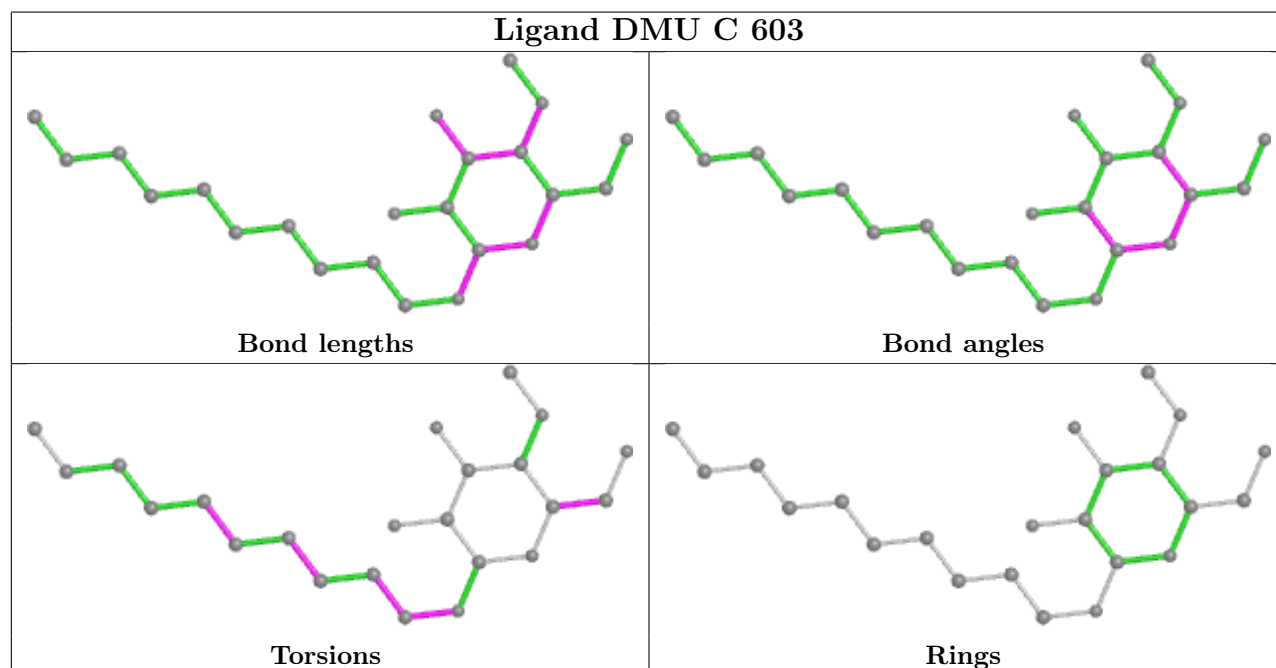
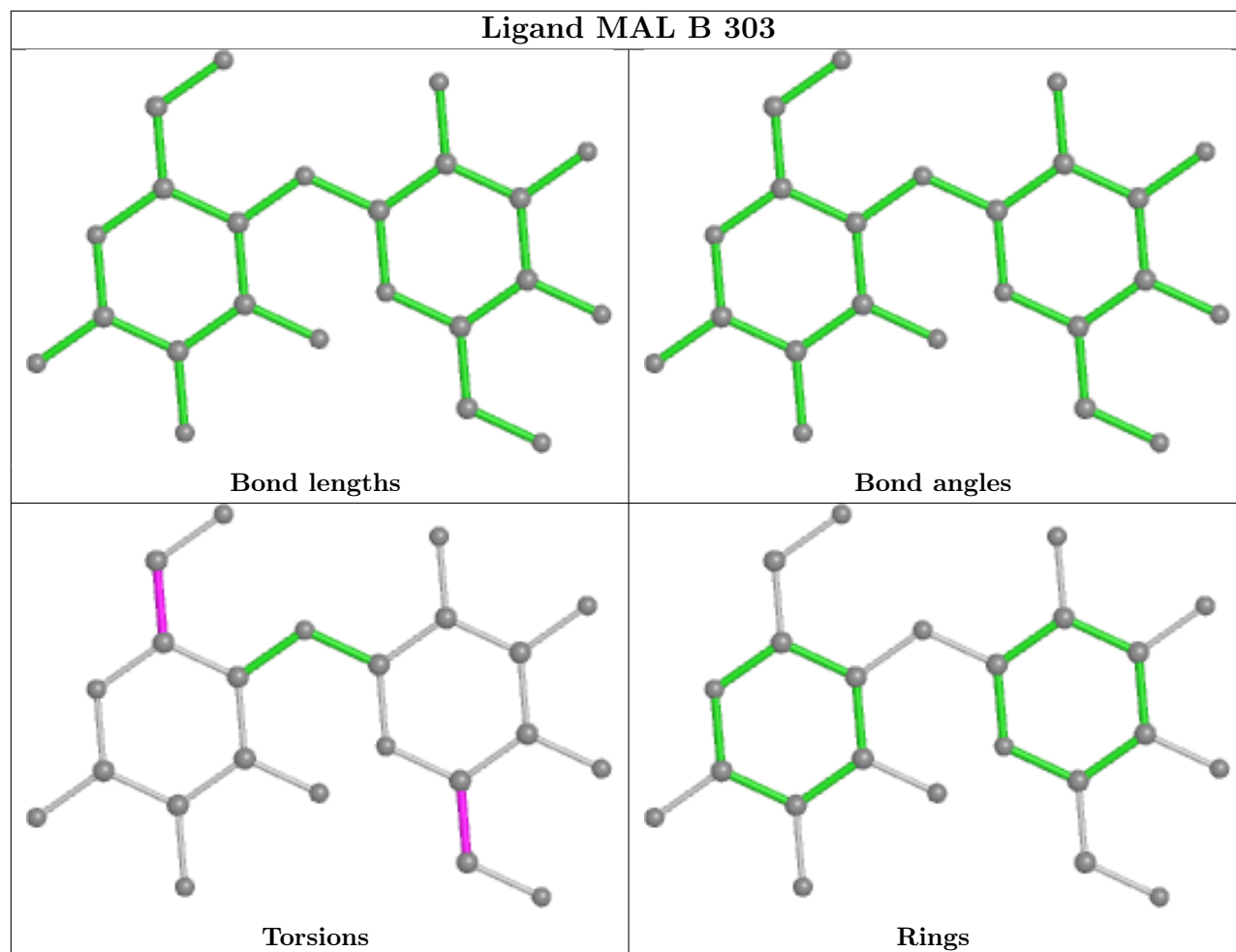


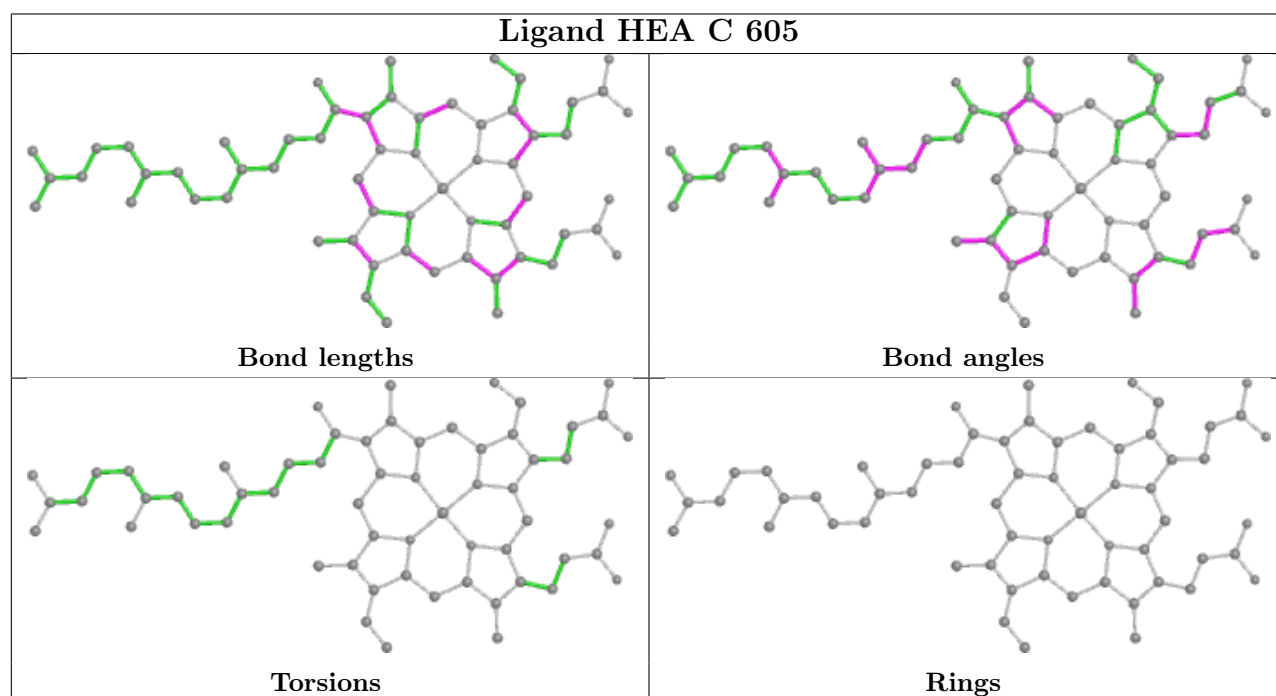
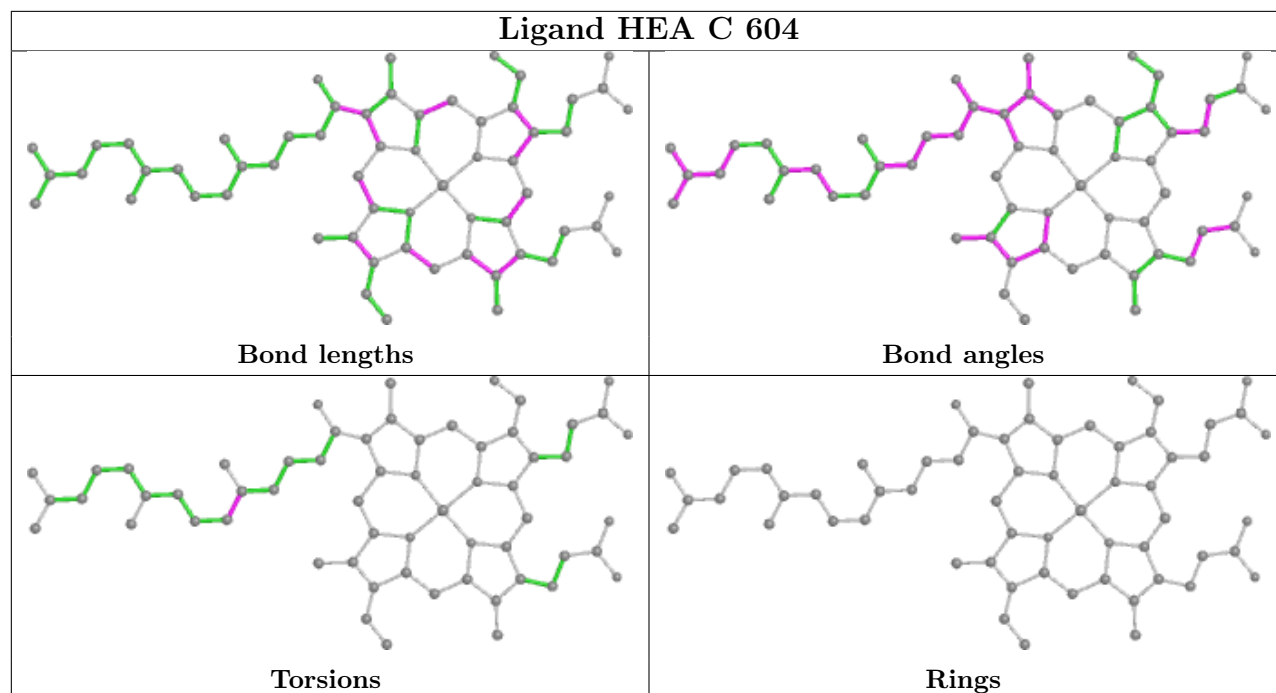


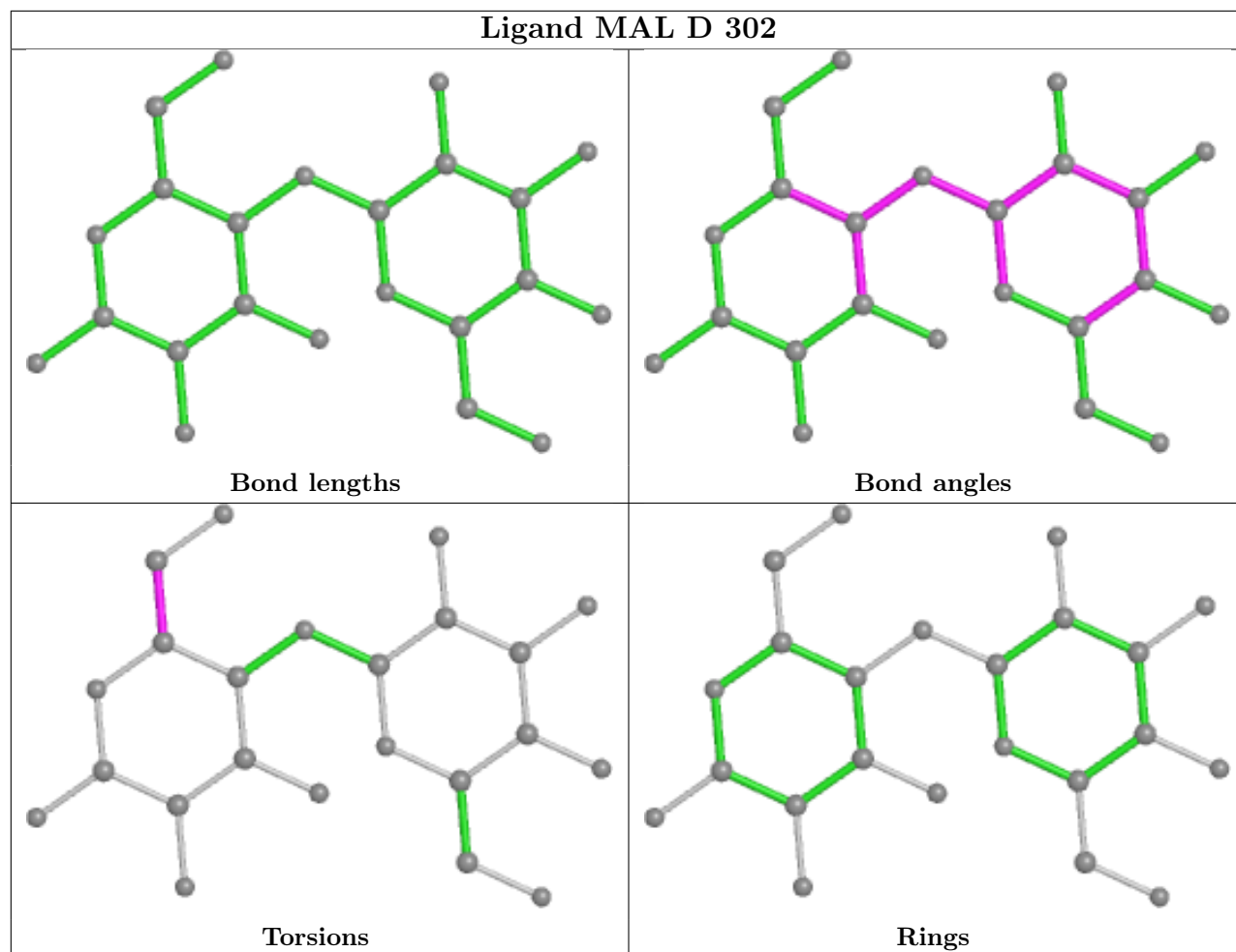












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 33	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 51	28, 40, 57, 67	0
All	All	1579/1582 (99%)	-0.10	96 (6%) 21 26	24, 38, 58, 92	1 (0%)

The worst 5 of 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

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](#)

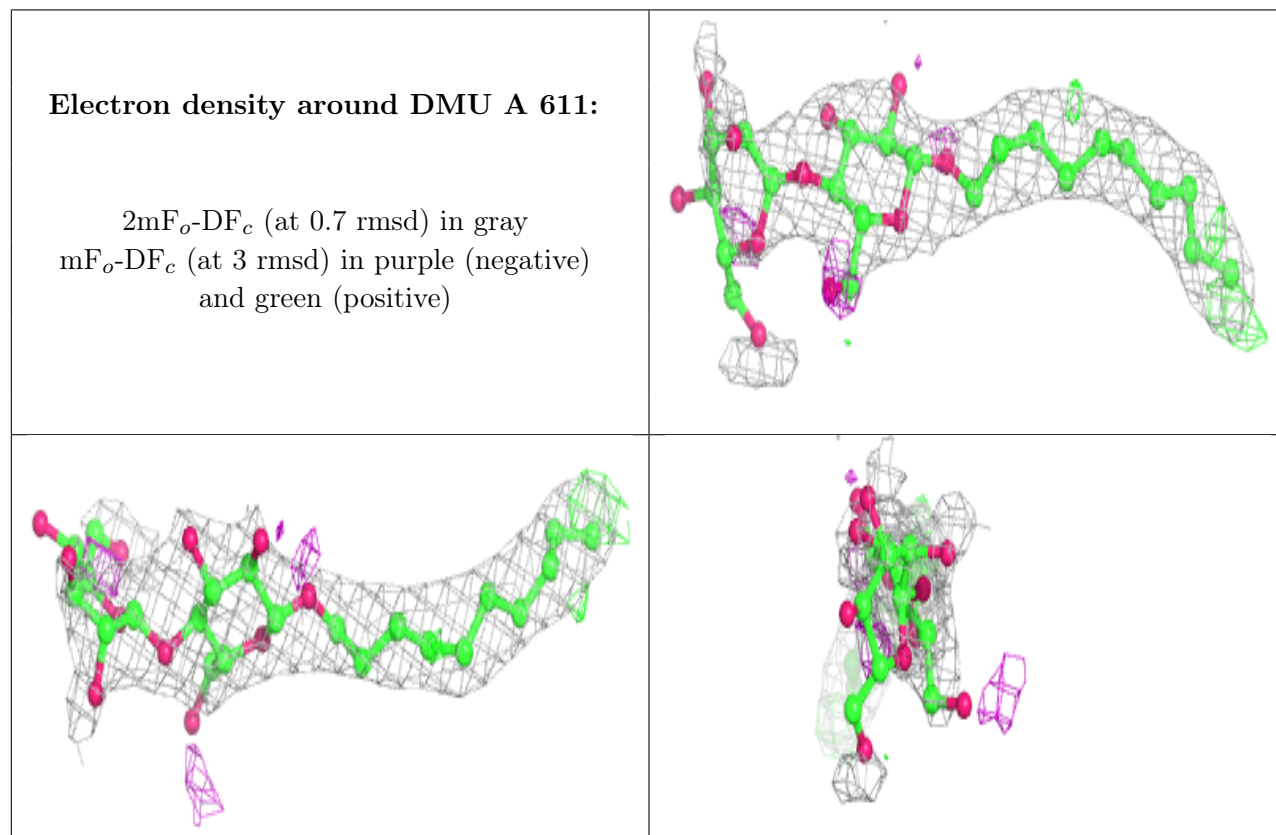
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

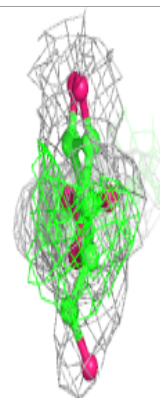
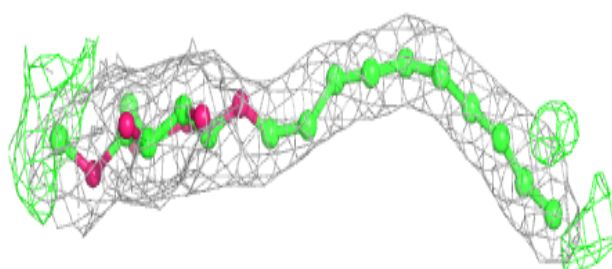
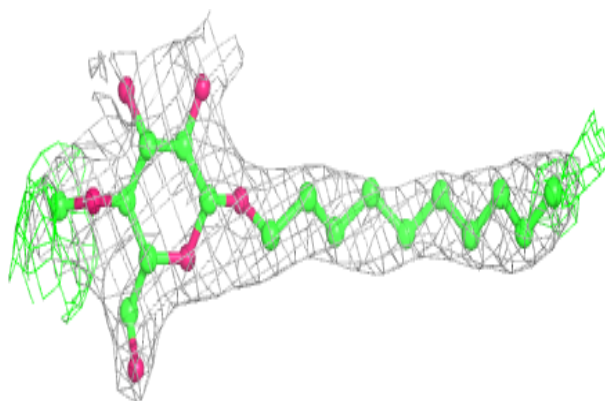
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DMU	A	611	33/33	0.52	0.33	43,73,102,108	0
3	TRD	A	604	13/13	0.54	0.24	45,52,57,58	0
3	TRD	B	301	13/13	0.58	0.31	52,57,61,66	0
3	TRD	A	610	13/13	0.64	0.28	47,53,58,59	0
11	TRS	B	304	8/8	0.64	0.16	52,59,64,71	0
3	TRD	A	605	7/13	0.65	0.50	51,55,59,59	0
9	HTH	A	620	10/10	0.68	0.30	42,51,59,71	0
3	TRD	A	602	13/13	0.69	0.35	50,56,64,65	0
3	TRD	A	608	13/13	0.69	0.34	50,55,70,72	0
4	DMU	C	603	23/33	0.70	0.24	49,73,86,91	0
10	MAL	D	302	23/23	0.73	0.28	69,74,79,81	0
3	TRD	A	607	13/13	0.74	0.64	52,61,66,66	0
3	TRD	A	603	13/13	0.78	0.18	44,50,63,66	0
3	TRD	C	602	13/13	0.78	0.23	59,64,72,72	0
4	DMU	A	614	33/33	0.79	0.29	44,59,75,81	0
3	TRD	A	601	13/13	0.83	0.15	51,55,68,68	0
4	DMU	A	613	33/33	0.85	0.25	47,61,67,70	0
3	TRD	A	606	13/13	0.86	0.21	46,52,63,64	0
10	MAL	B	303	23/23	0.86	0.27	66,71,79,82	0
4	DMU	B	302	30/33	0.87	0.19	46,57,62,67	0
3	TRD	A	609	13/13	0.88	0.17	37,43,49,54	0
9	HTH	B	309	10/10	0.89	0.18	39,48,51,60	10
3	TRD	C	601	13/13	0.92	0.10	41,45,46,52	0
3	TRD	D	301	9/13	0.94	0.09	48,50,53,55	0
4	DMU	A	612	33/33	0.95	0.09	26,35,48,52	0
5	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
12	CD	D	306	1/1	0.98	0.04	62,62,62,62	1
7	MG	C	607	1/1	0.98	0.21	19,19,19,19	0
5	HEA	C	605	60/60	0.98	0.14	26,31,40,43	0
5	HEA	A	615	60/60	0.98	0.19	20,25,30,33	0
8	CA	C	608	1/1	0.98	0.06	33,33,33,33	0
5	HEA	A	616	60/60	0.98	0.14	23,27,36,39	0
6	CU	C	606	1/1	0.99	0.10	34,34,34,34	0
7	MG	A	618	1/1	0.99	0.16	15,15,15,15	0
6	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	CA	A	619	1/1	0.99	0.08	28,28,28,28	0
12	CD	B	307	1/1	1.00	0.08	40,40,40,40	0
6	CU	B	306	1/1	1.00	0.08	25,25,25,25	0
6	CU	D	304	1/1	1.00	0.08	31,31,31,31	0
6	CU	A	617	1/1	1.00	0.09	30,30,30,30	0
6	CU	B	305	1/1	1.00	0.07	25,25,25,25	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.

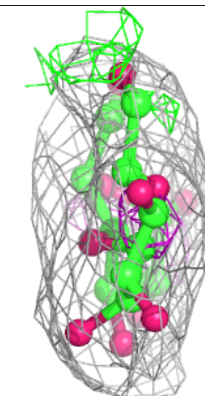
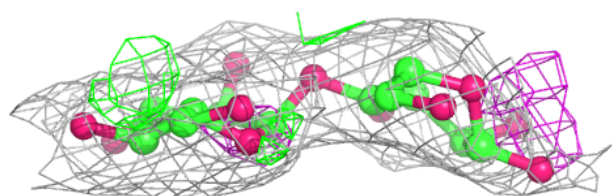
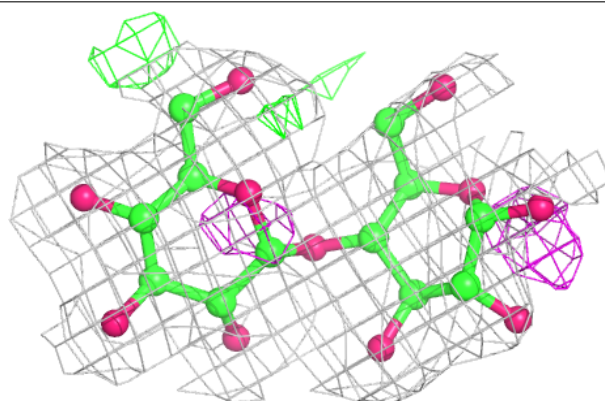


Electron density around DMU C 603:

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

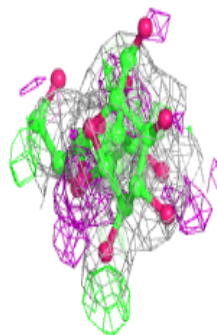
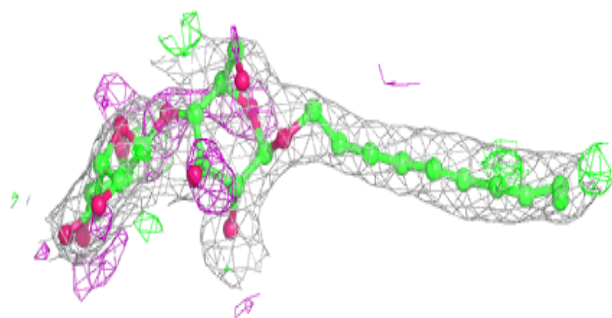
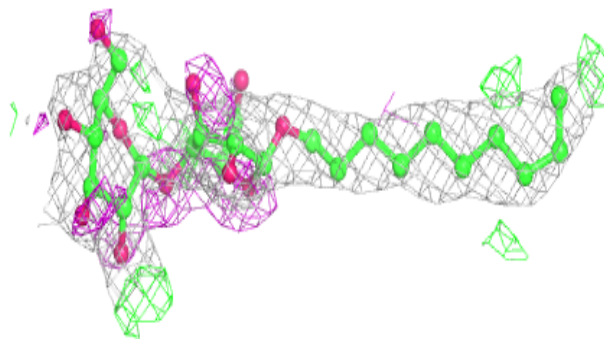
**Electron density around MAL D 302:**

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

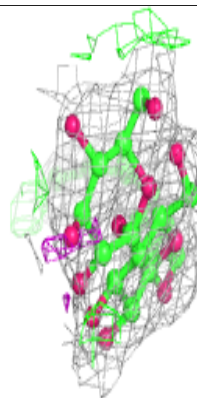
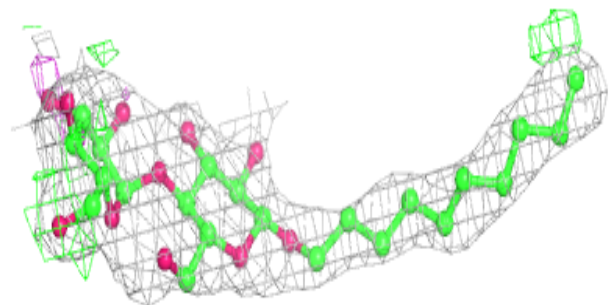
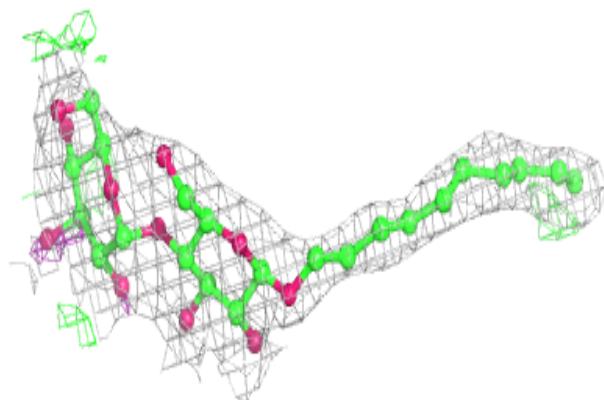


Electron density around DMU A 614:

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

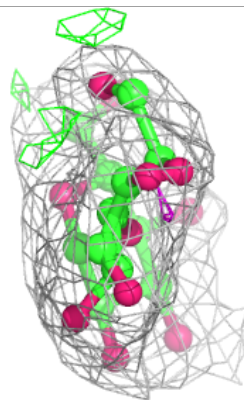
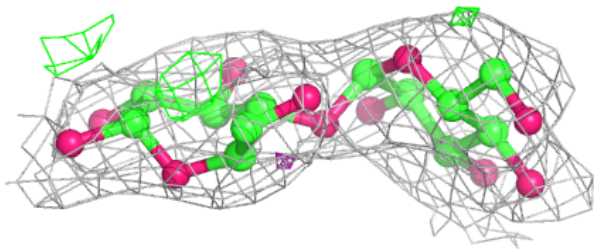
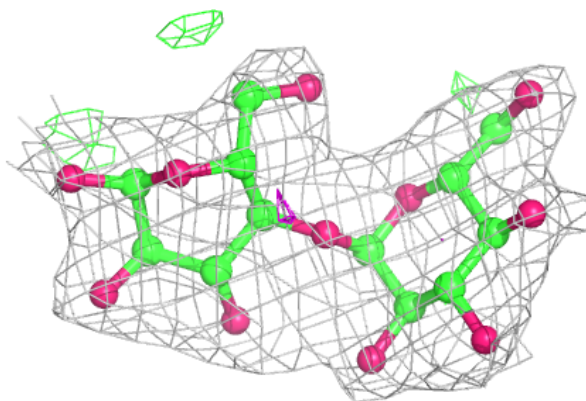
**Electron density around DMU A 613:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

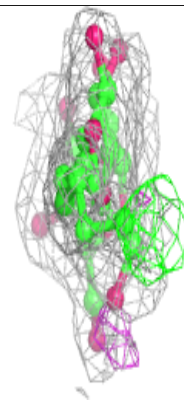
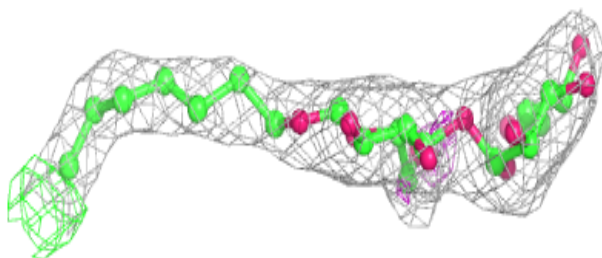
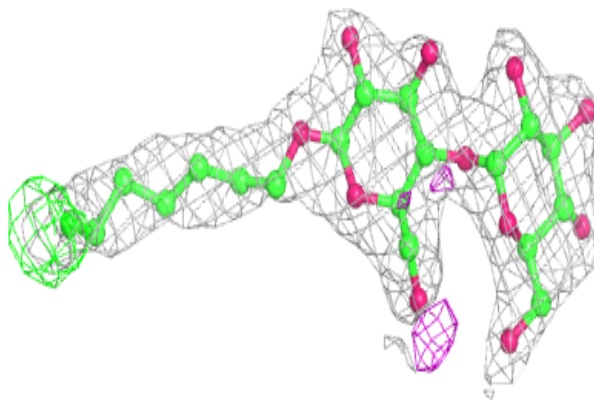


Electron density around MAL B 303:

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

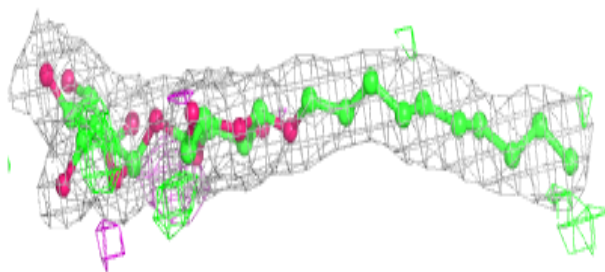
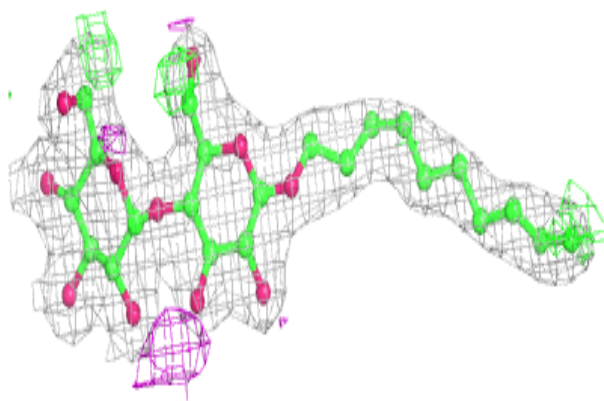
**Electron density around DMU B 302:**

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

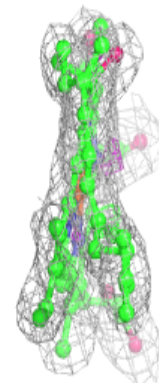
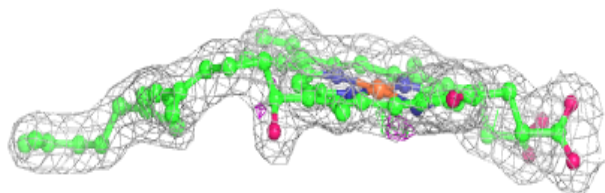
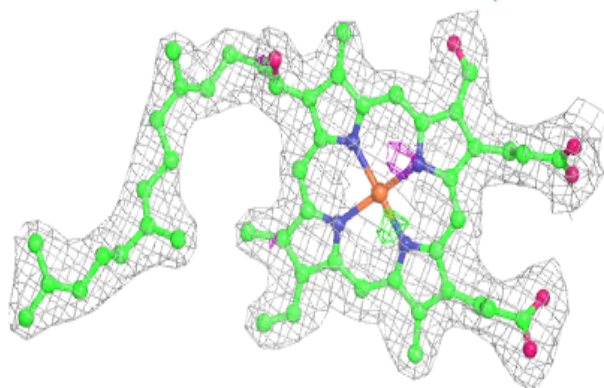


Electron density around DMU A 612:

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

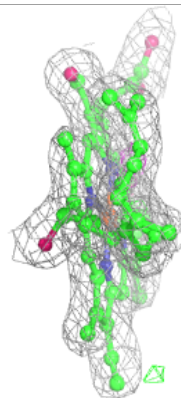
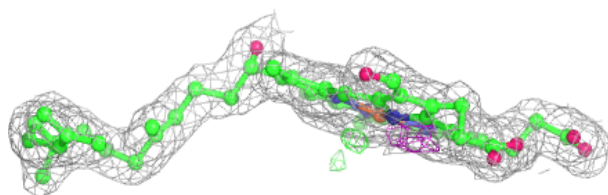
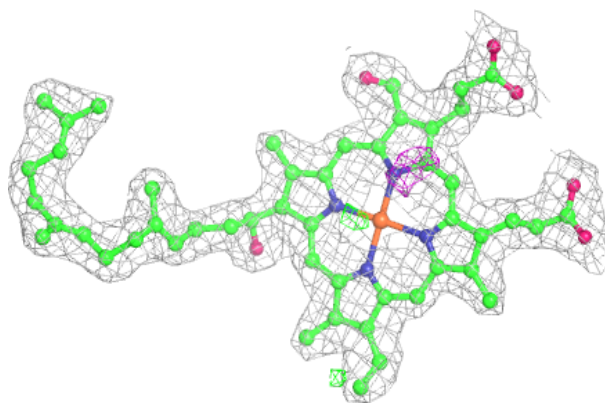
**Electron density around HEA C 604:**

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

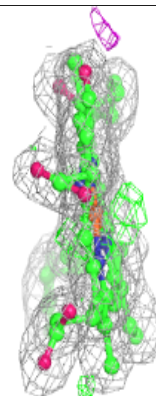
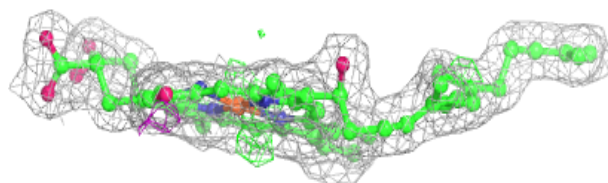
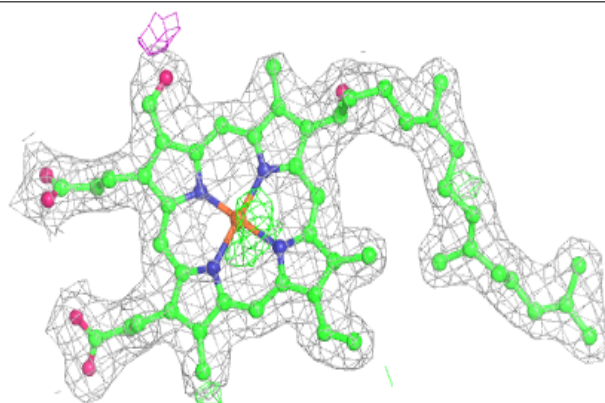


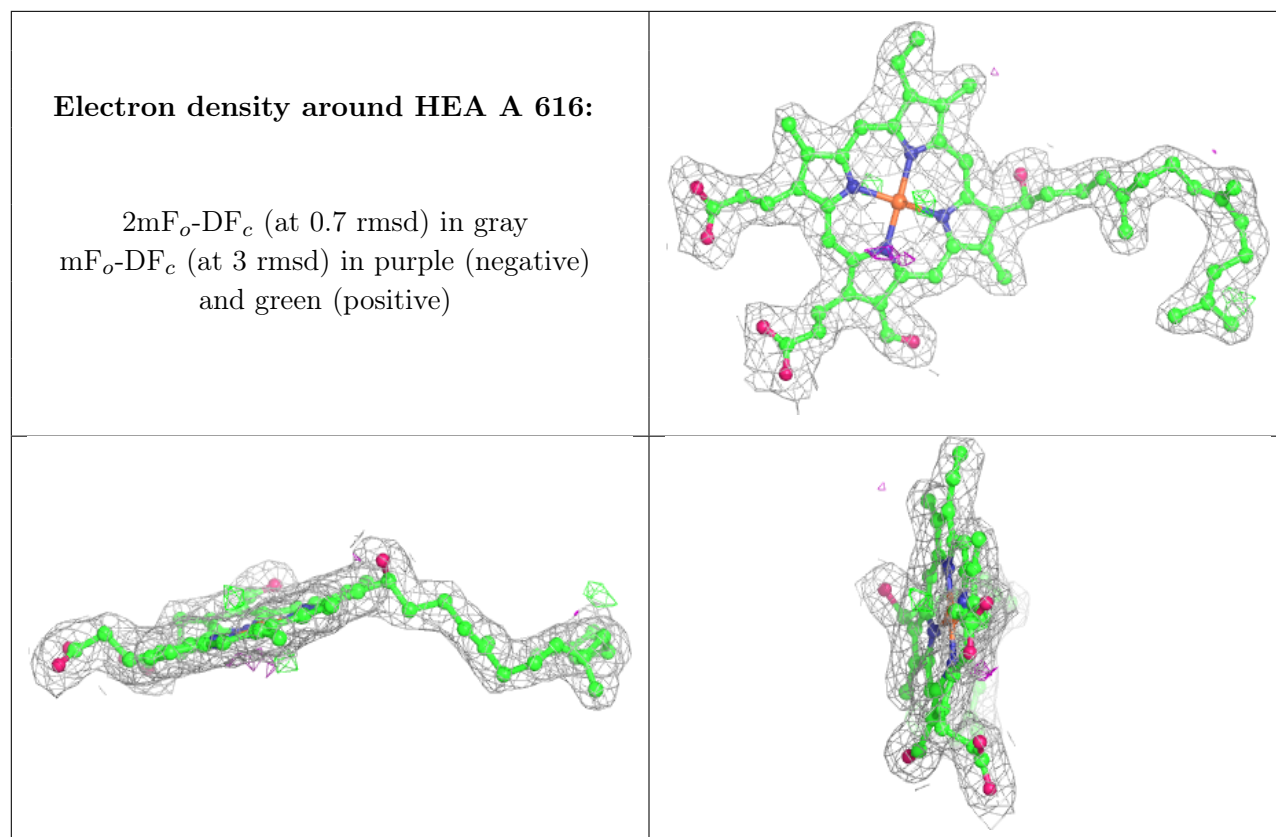
Electron density around HEA C 605:

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

**Electron density around HEA A 615:**

$2mF_o-DF_c$ (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.