



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 08:59 PM EDT

PDB ID : 3OMI  
Title : Catalytic core subunits (I and II) of cytochrome C oxidase from Rhodobacter sphaeroides with D132A mutation  
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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

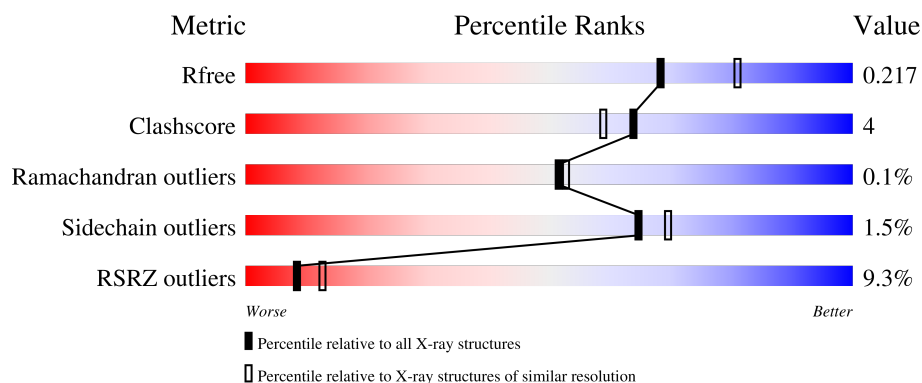
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	535	<div> <div>6%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	C	535	<div> <div>15%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>
2	B	256	<div> <div>4%</div> <div> <div></div> <div>97%</div> <div>.</div> </div> </div>
2	D	256	<div> <div>8%</div> <div> <div></div> <div>93%</div> <div>7%</div> </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
4	DMU	C	604	-	-	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 13416 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	0	0
			4167	2793	654	689	31			
1	C	530	Total	C	N	O	S	0	0	0
			4102	2749	641	681	31			

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

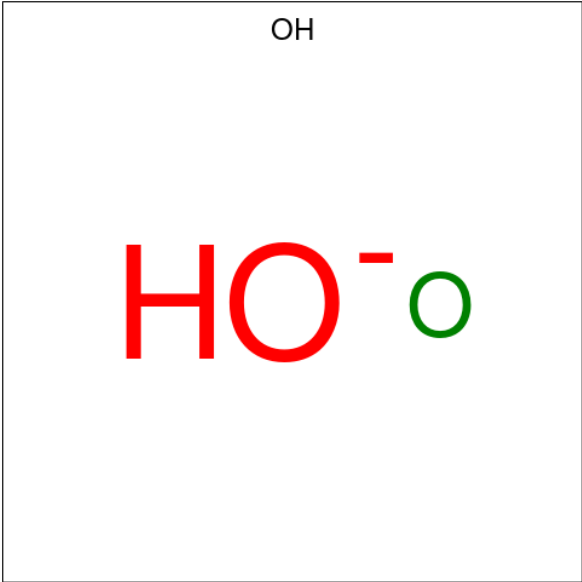
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			2008	1312	329	361	6			
2	D	256	Total	C	N	O	S	0	0	0
			2002	1307	326	363	6			

There are 8 discrepancies between the modelled and reference sequences:

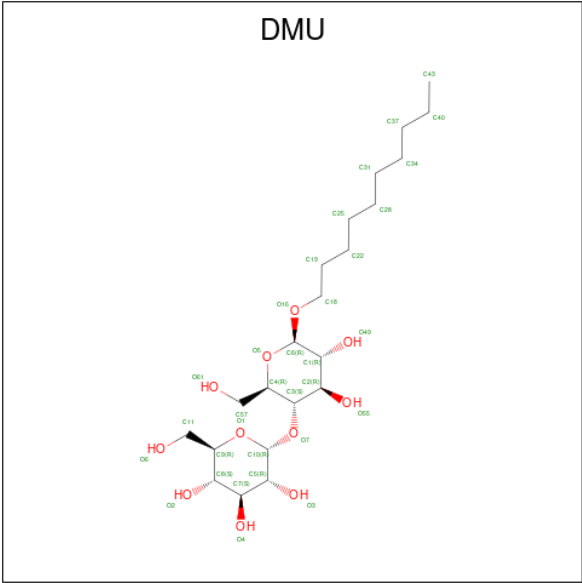
Chain	Residue	Modelled	Actual	Comment	Reference
B	282	HIS	-	EXPRESSION TAG	UNP Q3J5G0
B	283	HIS	-	EXPRESSION TAG	UNP Q3J5G0
B	284	HIS	-	EXPRESSION TAG	UNP Q3J5G0
B	285	HIS	-	EXPRESSION TAG	UNP Q3J5G0
D	282	HIS	-	EXPRESSION TAG	UNP Q3J5G0
D	283	HIS	-	EXPRESSION TAG	UNP Q3J5G0
D	284	HIS	-	EXPRESSION TAG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

- Molecule 3 is HYDROXIDE ION (three-letter code: 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 (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



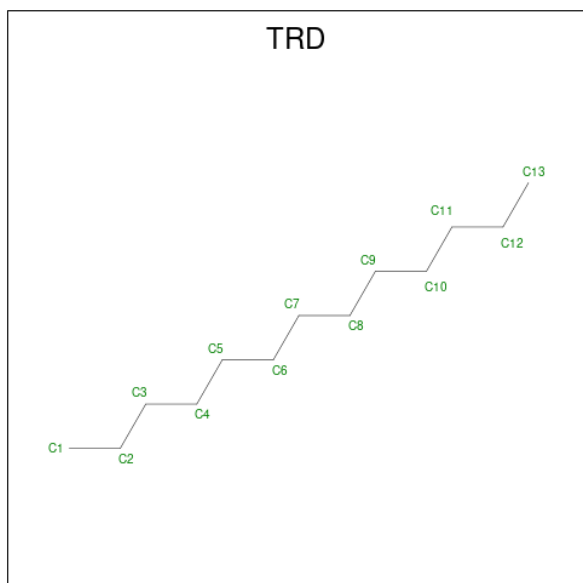
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 22 16 6	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			22	16	6		
4	B	1	Total	C	O	0	0
			33	22	11		
4	B	1	Total	C	O	0	0
			33	22	11		
4	B	1	Total	C	O	0	0
			33	22	11		
4	B	1	Total	C	O	0	0
			23	12	11		
4	C	1	Total	C	O	0	0
			33	22	11		
4	C	1	Total	C	O	0	0
			23	12	11		
4	C	1	Total	C	O	0	0
			23	12	11		
4	D	1	Total	C	O	0	0
			23	12	11		
4	D	1	Total	C	O	0	0
			23	12	11		

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



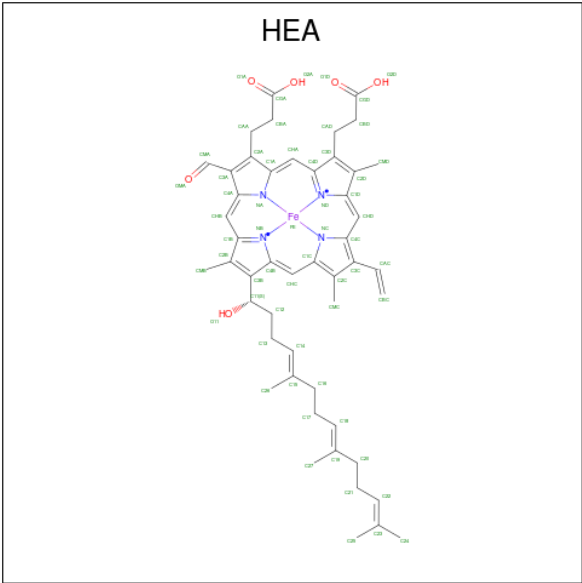
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 7 7	0	0
5	A	1	Total C 7 7	0	0
5	A	1	Total C 13 13	0	0
5	A	1	Total C 13 13	0	0
5	B	1	Total C 9 9	0	0
5	C	1	Total C 11 11	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 (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



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 60 49 1 4 6	0	0
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	
			60	49	1	4	6	
							0	0

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

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

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

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

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

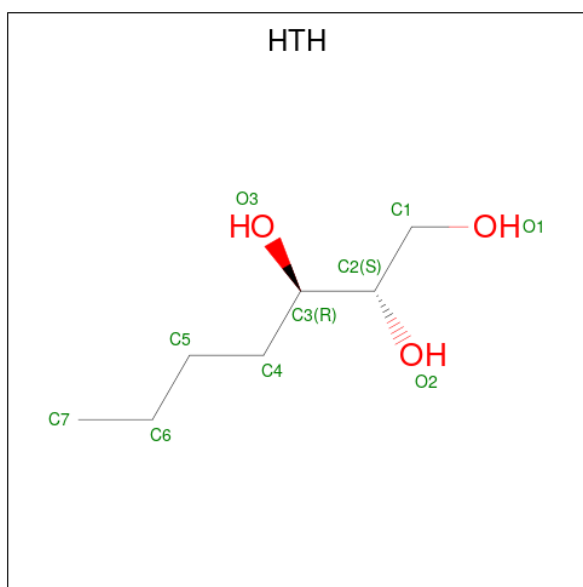
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Ca		
			1	1	0	0
9	C	1	Total	Ca		
			1	1	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 11 is (2S,3R)-heptane-1,2,3-triol (three-letter code: HTH) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).





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

- Molecule 12 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	1	Total	Cu	0	0
			1	1		
12	D	1	Total	Cu	0	0
			1	1		

- Molecule 13 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	142	Total	O	0	0
			142	142		
14	B	134	Total	O	0	0
			134	134		

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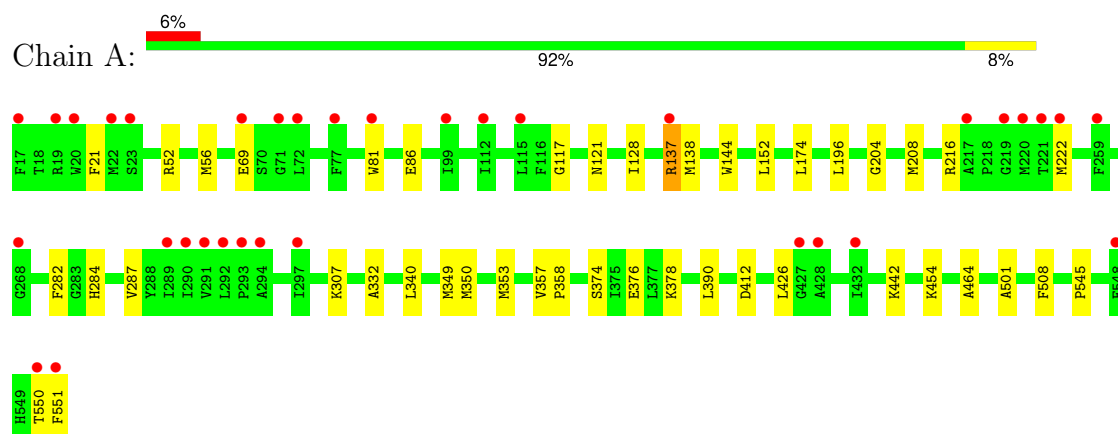
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	95	Total 95	O 95	0	0
14	D	120	Total 120	O 120	0	0

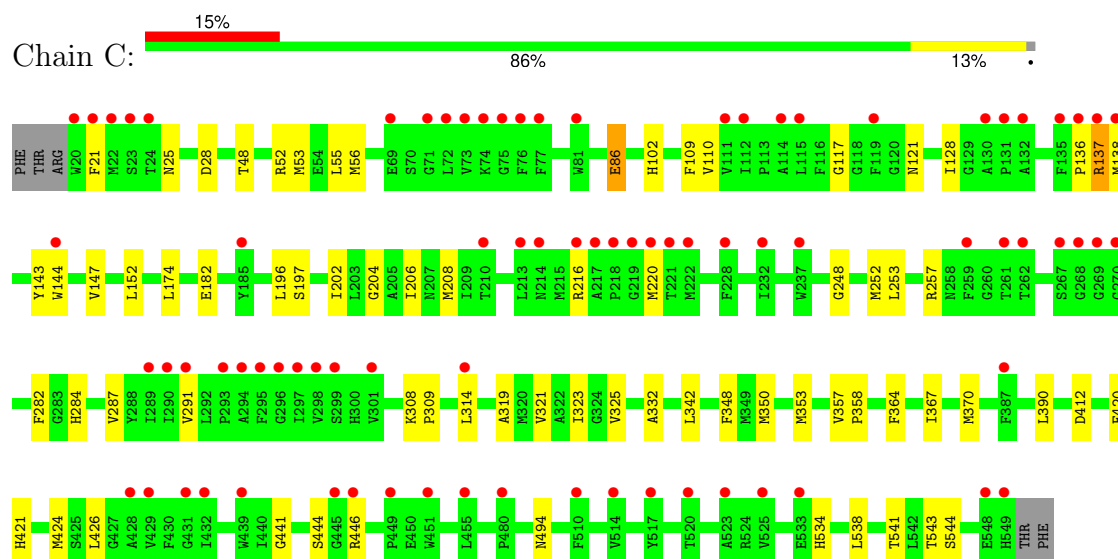
### 3 Residue-property plots [i](#)

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

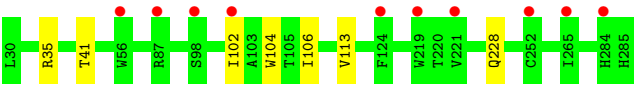


- Molecule 1: Cytochrome c oxidase, aa3 type, subunit I

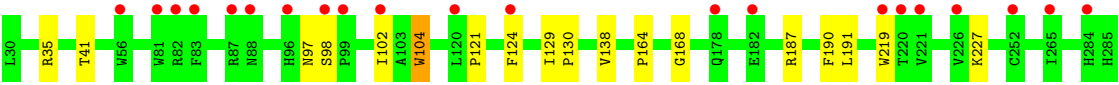
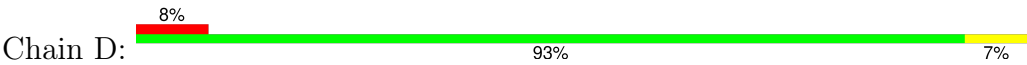


- Molecule 2: Cytochrome c oxidase subunit 2





● 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, $\alpha$ , $\beta$ , $\gamma$	125.06Å 131.52Å 175.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.84 – 2.15 35.84 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.5 (35.84-2.15) 96.5 (35.84-2.15)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.16Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.192 , 0.215 0.195 , 0.217	Depositor DCC
$R_{free}$ test set	4574 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.2	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 66.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13416	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CU, DMU, CA, HEA, CD, HTH, CL, OH, CU1, 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	0.57	1/4320 (0.0%)	0.55	0/5900
1	C	0.48	0/4251	0.53	0/5808
2	B	0.51	0/2069	0.56	0/2835
2	D	0.49	0/2063	0.54	0/2829
All	All	0.52	1/12703 (0.0%)	0.54	0/17372

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	GLU	CD-OE2	7.42	1.33	1.25

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	4167	0	4063	38	0
1	C	4102	0	4001	50	0
2	B	2008	0	1955	4	0
2	D	2002	0	1940	9	0
3	A	1	0	0	1	0
3	C	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	44	0	62	1	0
4	B	122	0	147	0	0
4	C	79	0	84	3	0
4	D	46	0	42	2	0
5	A	47	0	92	2	0
5	B	9	0	17	3	0
5	C	11	0	21	0	0
5	D	20	0	41	1	0
6	A	120	0	108	6	0
6	C	120	0	108	5	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	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	1	0	0	0	0
12	D	1	0	0	0	0
13	B	2	0	0	0	0
13	D	2	0	0	0	0
14	A	142	0	0	2	0
14	B	134	0	0	1	0
14	C	95	0	0	4	0
14	D	120	0	0	0	0
All	All	13416	0	12697	107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 107 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	1.07	1.16
1:C:534:HIS:HE1	14:C:794:HOH:O	1.44	1.00
1:C:534:HIS:HD2	14:C:791:HOH:O	1.47	0.98
1:A:426:LEU:HD21	1:A:464:ALA:CB	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:HH11	1:A:137:ARG:CG	1.87	0.88

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	533/535 (100%)	524 (98%)	9 (2%)	0	100	100
1	C	528/535 (99%)	517 (98%)	10 (2%)	1 (0%)	47	46
2	B	254/256 (99%)	248 (98%)	6 (2%)	0	100	100
2	D	254/256 (99%)	247 (97%)	6 (2%)	1 (0%)	34	29
All	All	1569/1582 (99%)	1536 (98%)	31 (2%)	2 (0%)	51	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	220	MET
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	423/434 (98%)	418 (99%)	5 (1%)	71	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	417/434 (96%)	409 (98%)	8 (2%)	57	61
2	B	210/215 (98%)	208 (99%)	2 (1%)	76	81
2	D	210/215 (98%)	206 (98%)	4 (2%)	57	61
All	All	1260/1298 (97%)	1241 (98%)	19 (2%)	65	69

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	412	ASP
2	D	187	ARG
2	D	227	LYS
2	D	104	TRP
1	C	86	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 2 are modelled with single atom and 16 are monoatomic - leaving 25 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	DMU	B	304	-	24,24,34	0.55	0	35,35,45	0.68	0
4	DMU	B	302	-	34,34,34	0.52	0	45,45,45	0.82	2 (4%)
5	TRD	B	305	-	8,8,12	0.23	0	7,7,11	0.50	0
5	TRD	D	303	-	12,12,12	0.21	0	11,11,11	0.63	0
5	TRD	A	604	-	6,6,12	0.29	0	5,5,11	0.38	0
4	DMU	C	603	-	24,24,34	0.54	0	35,35,45	0.74	0
11	HTH	B	306	-	9,9,9	0.42	0	10,10,10	0.67	0
6	HEA	A	607	1	58,67,67	1.34	6 (10%)	63,103,103	1.65	15 (23%)
4	DMU	B	303	-	34,34,34	0.48	0	45,45,45	0.61	0
5	TRD	A	609	-	12,12,12	0.26	0	11,11,11	0.56	0
4	DMU	C	602	-	34,34,34	0.57	0	45,45,45	0.80	0
5	TRD	A	606	-	6,6,12	0.31	0	5,5,11	0.40	0
6	HEA	A	608	1,14	58,67,67	1.37	6 (10%)	63,103,103	1.68	15 (23%)
4	DMU	A	603	-	22,22,34	0.55	0	27,27,45	0.84	1 (3%)
4	DMU	C	604	-	24,24,34	0.63	0	35,35,45	0.81	1 (2%)
5	TRD	A	610	-	12,12,12	0.36	0	11,11,11	0.43	0
4	DMU	D	301	-	24,24,34	0.54	0	35,35,45	0.61	0
5	TRD	C	607	-	10,10,12	0.33	0	9,9,11	0.44	0
6	HEA	C	605	1	58,67,67	1.31	5 (8%)	63,103,103	1.46	13 (20%)
4	DMU	B	301	-	34,34,34	0.44	0	45,45,45	0.90	2 (4%)
5	TRD	D	304	-	6,6,12	0.25	0	5,5,11	0.39	0
4	DMU	A	602	-	22,22,34	0.51	0	27,27,45	0.83	1 (3%)
5	TRD	A	605	-	6,6,12	0.27	0	5,5,11	0.46	0
6	HEA	C	606	1,14	58,67,67	1.41	5 (8%)	63,103,103	1.63	17 (26%)
4	DMU	D	302	-	24,24,34	0.56	0	35,35,45	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMU	B	304	-	-	3/8/48/59	0/2/2/2
4	DMU	B	302	-	-	9/19/59/59	0/2/2/2
5	TRD	B	305	-	-	1/6/6/10	-
5	TRD	D	303	-	-	5/10/10/10	-
5	TRD	A	604	-	-	2/4/4/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMU	C	603	-	-	2/8/48/59	0/2/2/2
11	HTH	B	306	-	-	4/10/10/10	-
6	HEA	A	607	1	-	4/32/76/76	-
4	DMU	B	303	-	-	5/19/59/59	0/2/2/2
5	TRD	A	609	-	-	7/10/10/10	-
4	DMU	C	602	-	-	9/19/59/59	0/2/2/2
5	TRD	A	606	-	-	0/4/4/10	-
6	HEA	A	608	1,14	-	7/32/76/76	-
4	DMU	A	603	-	-	3/13/33/59	0/1/1/2
4	DMU	C	604	-	-	4/8/48/59	0/2/2/2
5	TRD	A	610	-	-	3/10/10/10	-
4	DMU	D	301	-	-	4/8/48/59	0/2/2/2
5	TRD	C	607	-	-	2/8/8/10	-
6	HEA	C	605	1	-	6/32/76/76	-
4	DMU	B	301	-	-	5/19/59/59	0/2/2/2
5	TRD	D	304	-	-	1/4/4/10	-
4	DMU	A	602	-	-	6/13/33/59	0/1/1/2
5	TRD	A	605	-	-	0/4/4/10	-
6	HEA	C	606	1,14	-	4/32/76/76	-
4	DMU	D	302	-	-	2/8/48/59	0/2/2/2

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	607	HEA	C3A-C2A	-4.72	1.34	1.40
6	C	605	HEA	C3A-C2A	-4.51	1.34	1.40
6	A	608	HEA	C3A-C2A	-4.35	1.34	1.40
6	C	605	HEA	C3C-C2C	-4.30	1.34	1.40
6	C	606	HEA	C3A-C2A	-4.26	1.34	1.40

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	608	HEA	C4B-NB-C1B	3.73	109.62	105.21
6	A	608	HEA	C4A-CHB-C1B	3.65	127.38	122.56
6	A	607	HEA	C17-C18-C19	-3.59	119.40	127.62
6	A	607	HEA	C1D-ND-C4D	3.58	109.44	105.21
6	C	606	HEA	C4D-CHA-C1A	3.56	127.25	122.56

There are no chirality outliers.

5 of 98 torsion outliers are listed below:

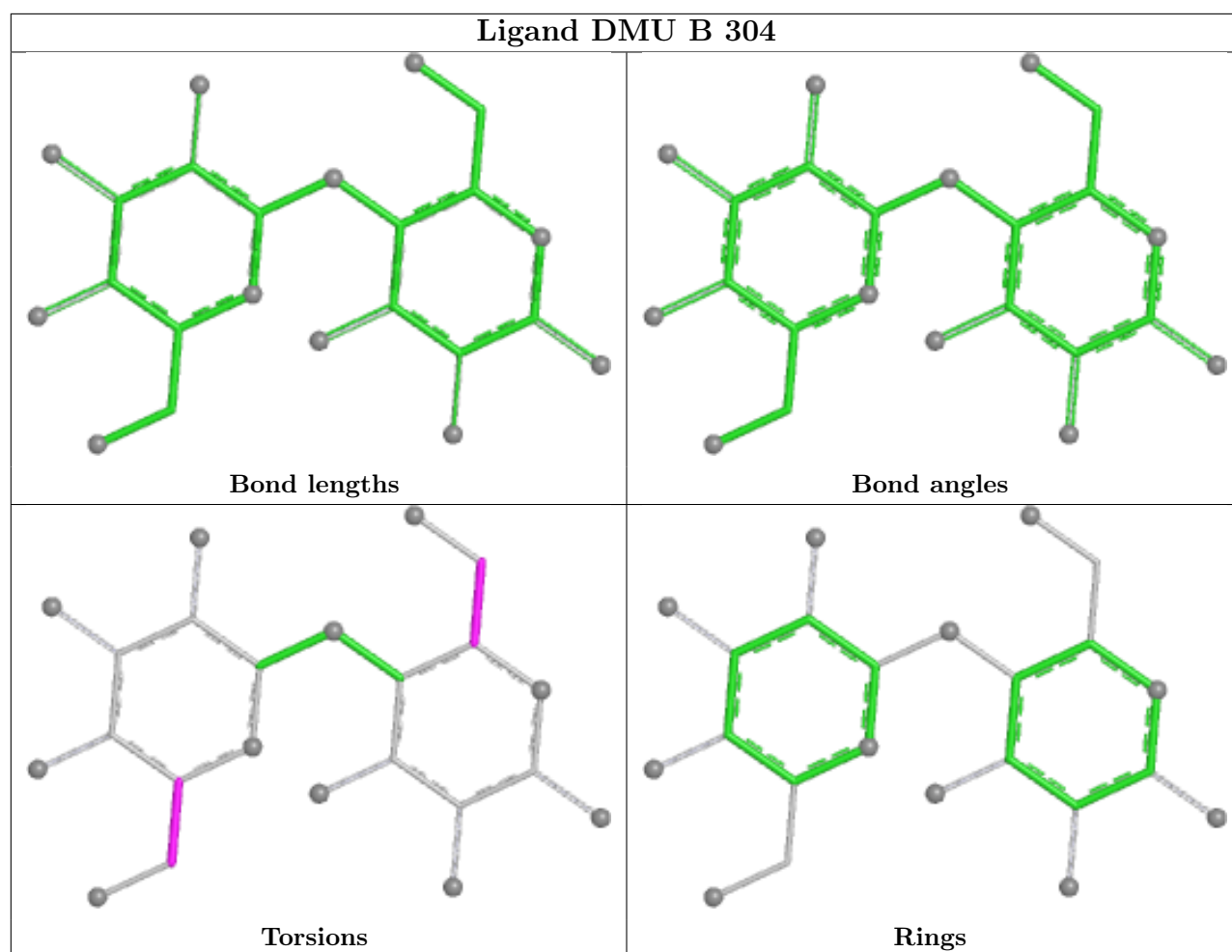
Mol	Chain	Res	Type	Atoms
4	B	302	DMU	C19-C18-O16-C6
11	B	306	HTH	O1-C1-C2-O2
4	C	604	DMU	O5-C4-C57-O61
4	C	604	DMU	O6-C11-C9-O1
4	D	301	DMU	O5-C4-C57-O61

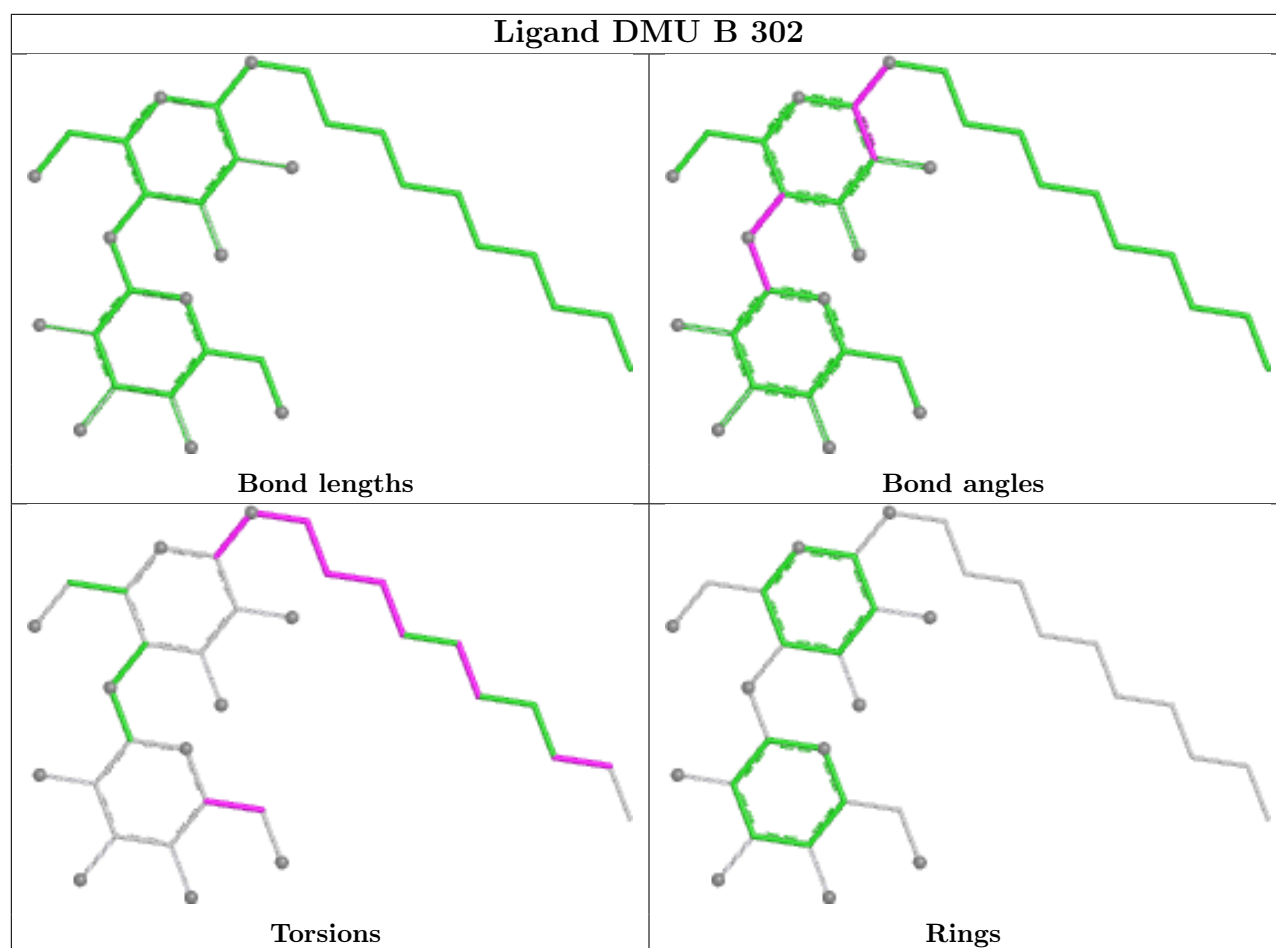
There are no ring outliers.

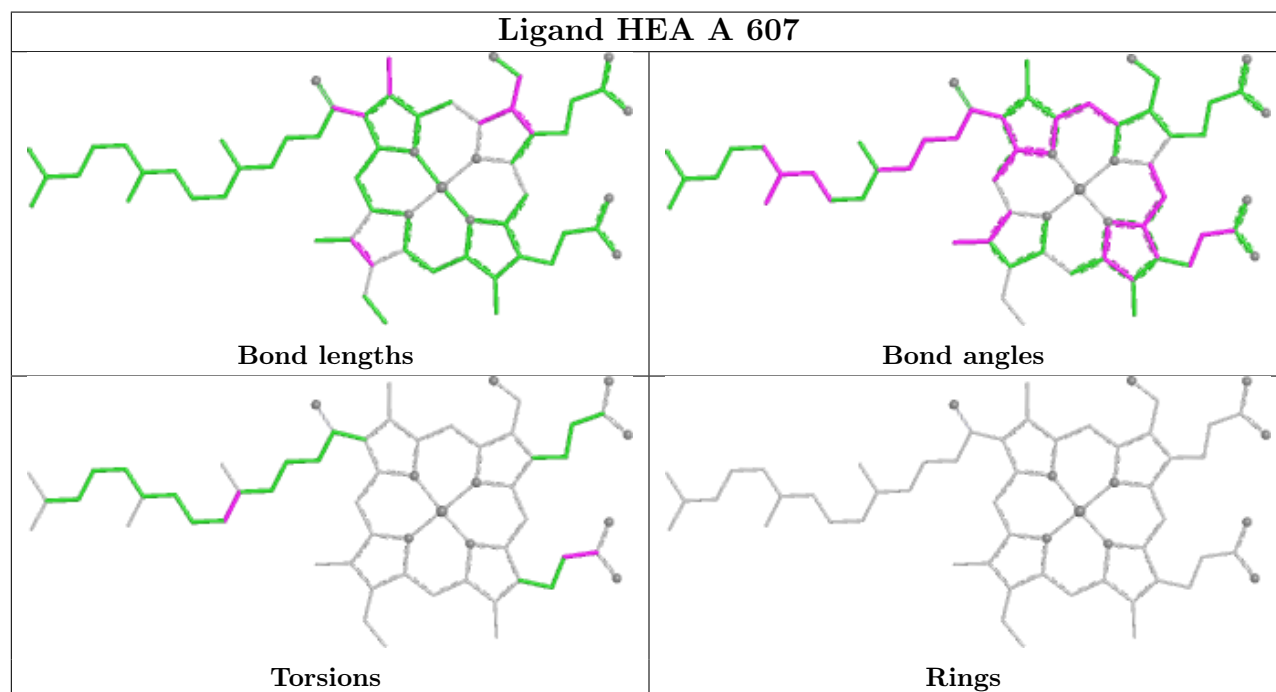
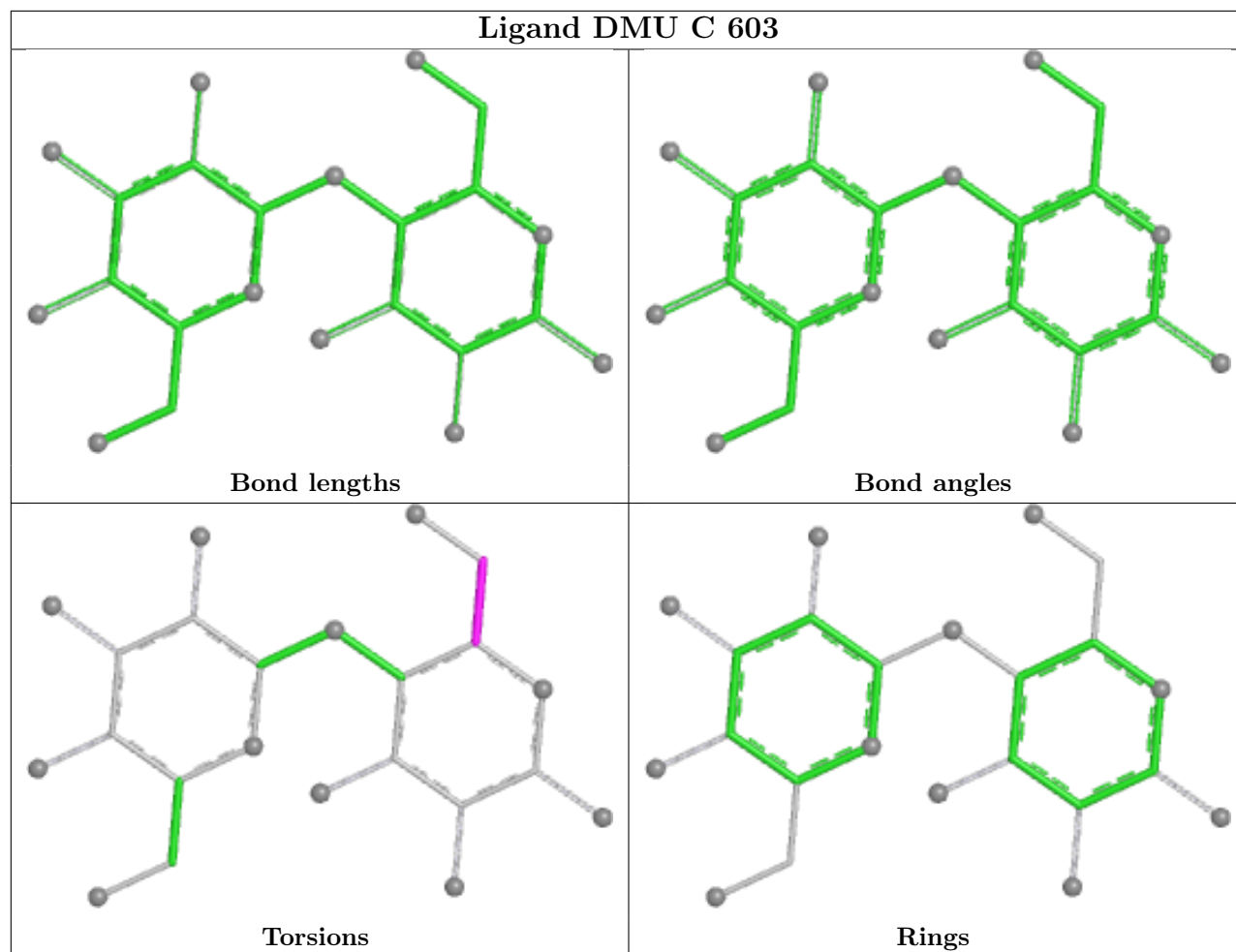
13 monomers are involved in 23 short contacts:

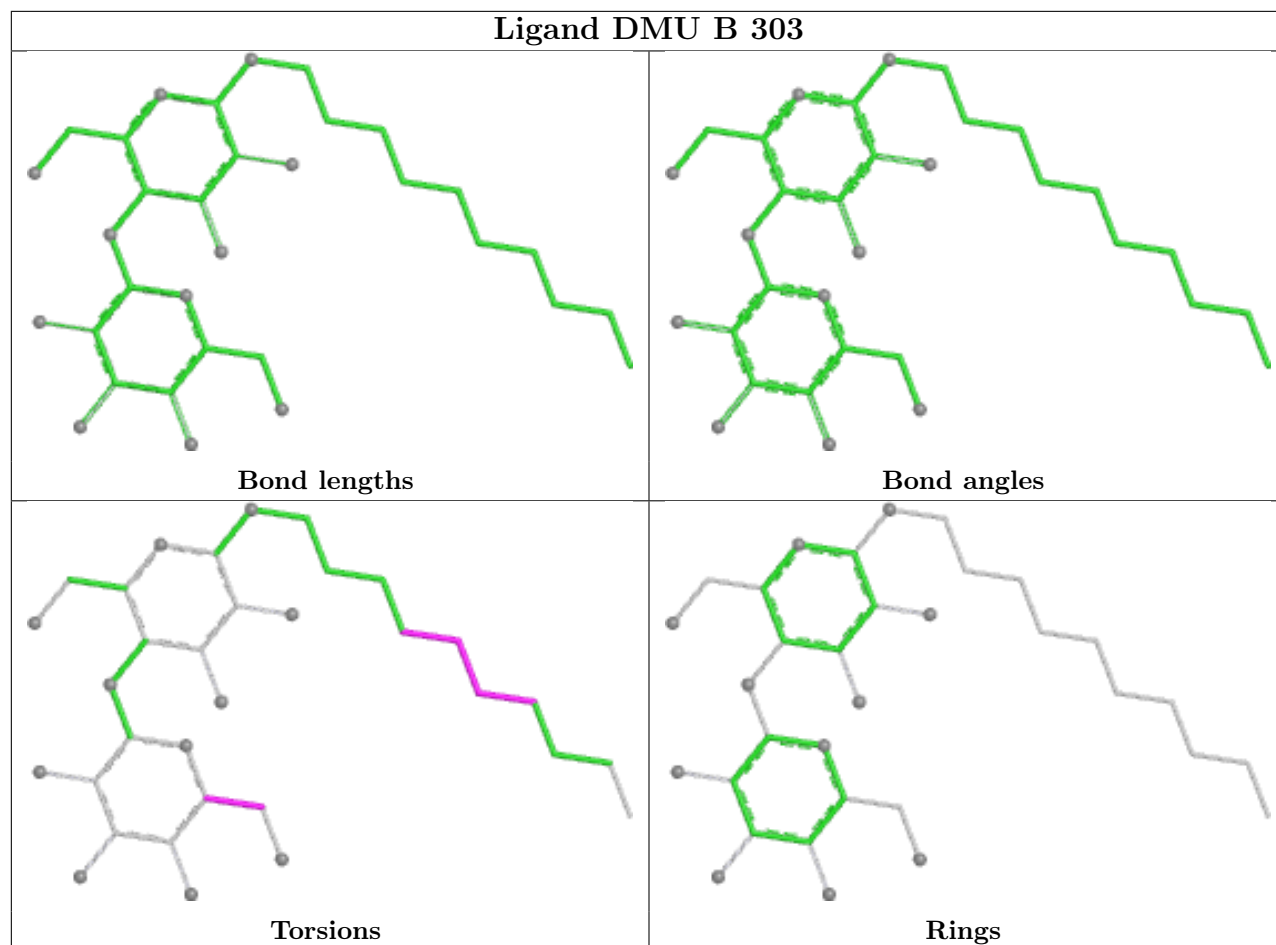
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	305	TRD	3	0
5	D	303	TRD	1	0
6	A	607	HEA	2	0
5	A	609	TRD	1	0
4	C	602	DMU	2	0
6	A	608	HEA	4	0
4	A	603	DMU	1	0
4	C	604	DMU	1	0
5	A	610	TRD	1	0
4	D	301	DMU	1	0
6	C	605	HEA	3	0
6	C	606	HEA	2	0
4	D	302	DMU	1	0

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

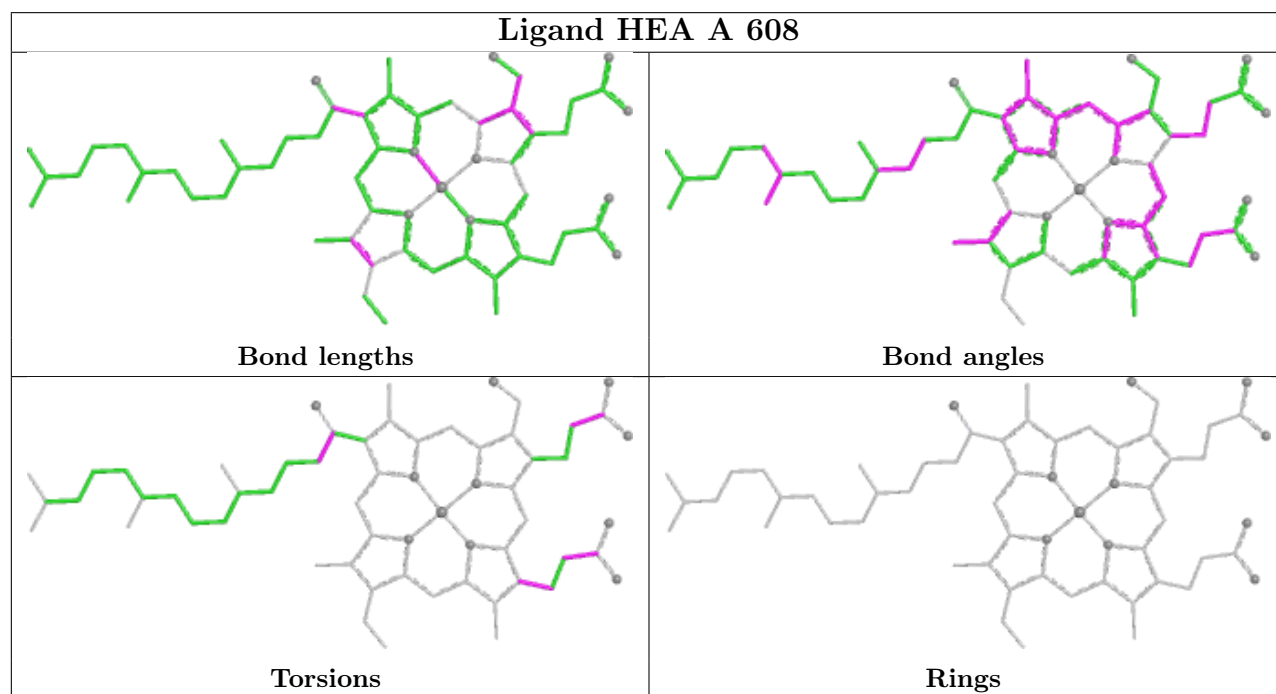
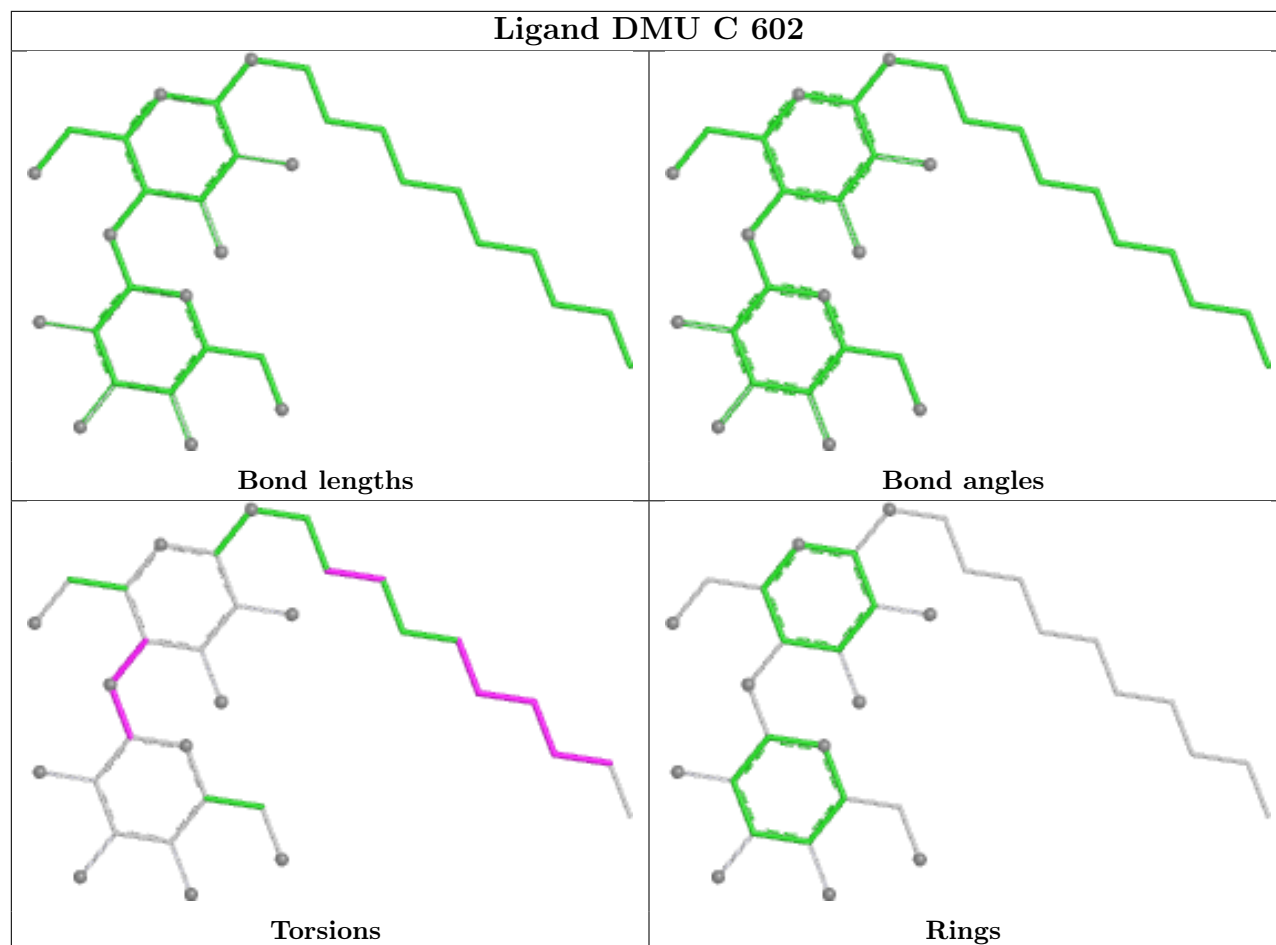


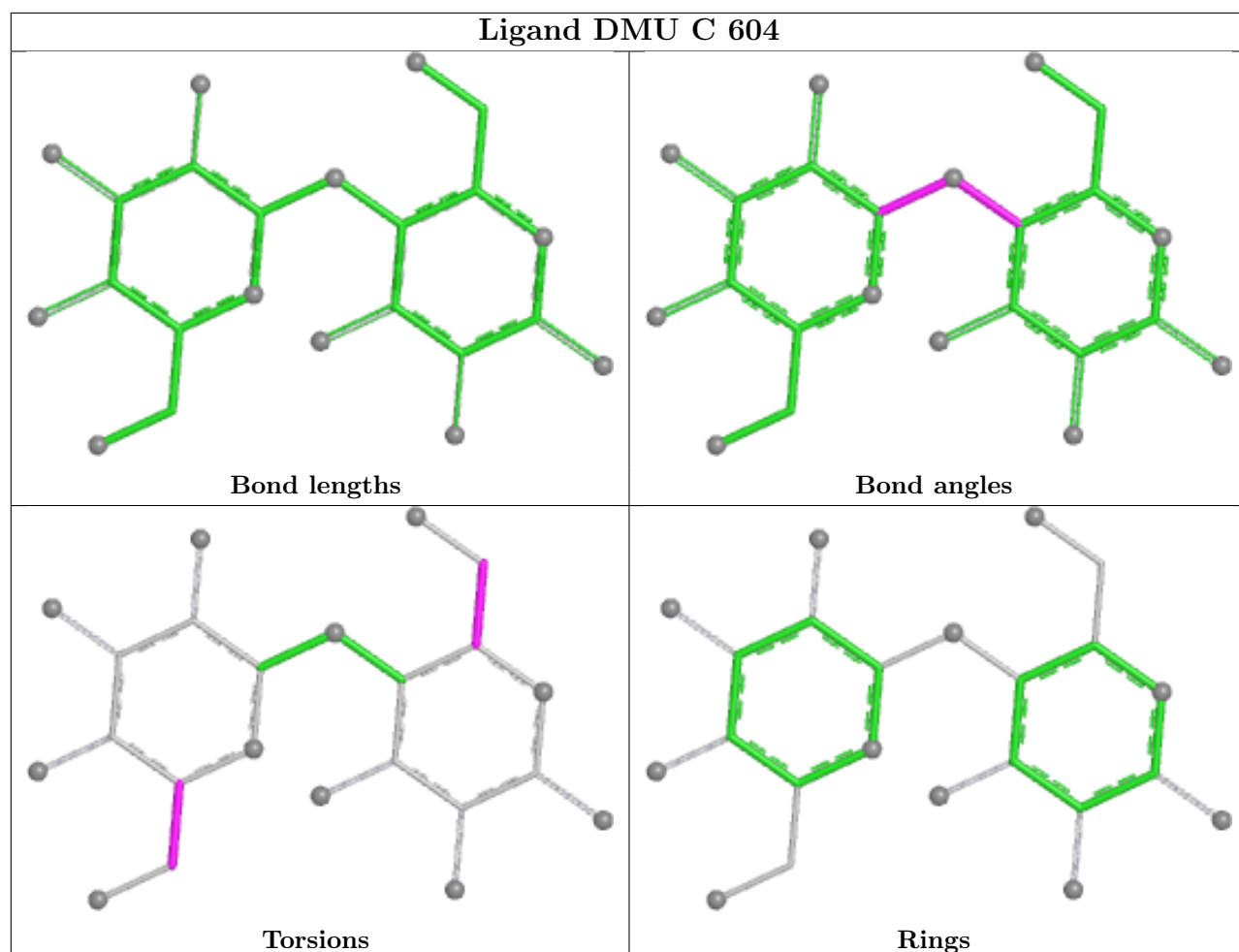
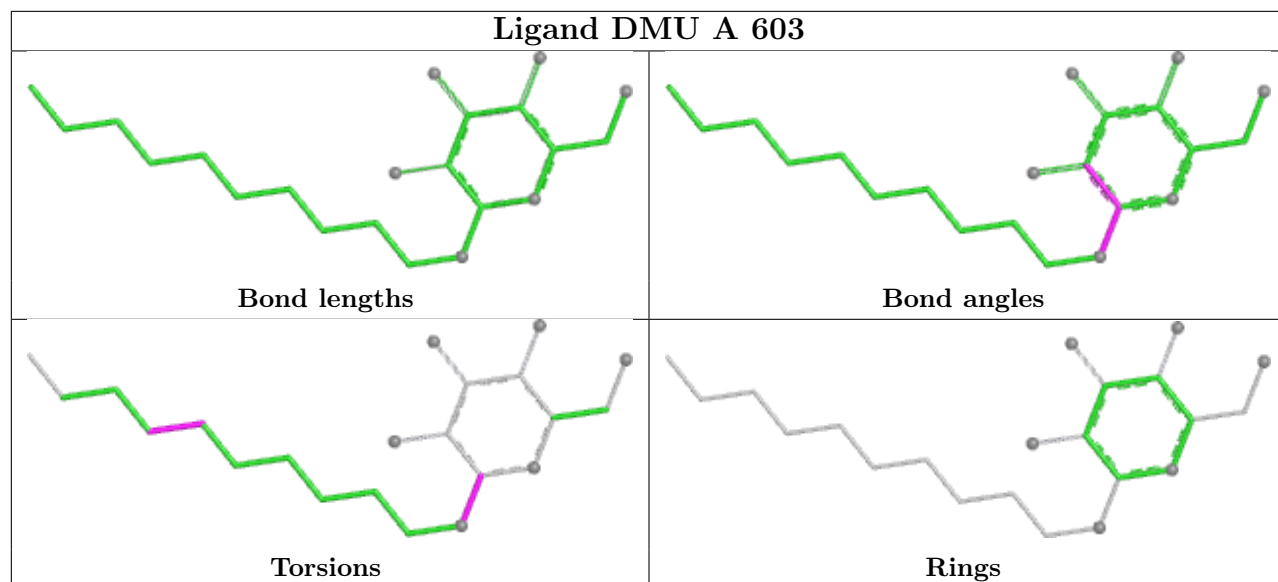


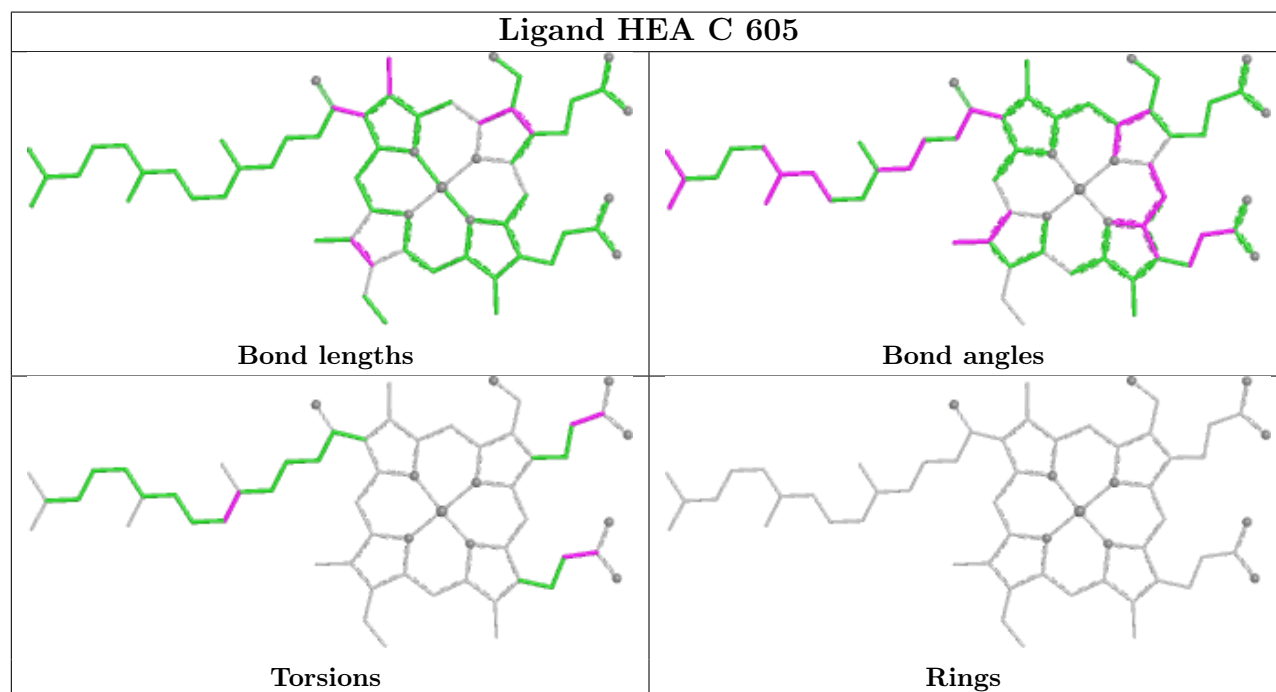
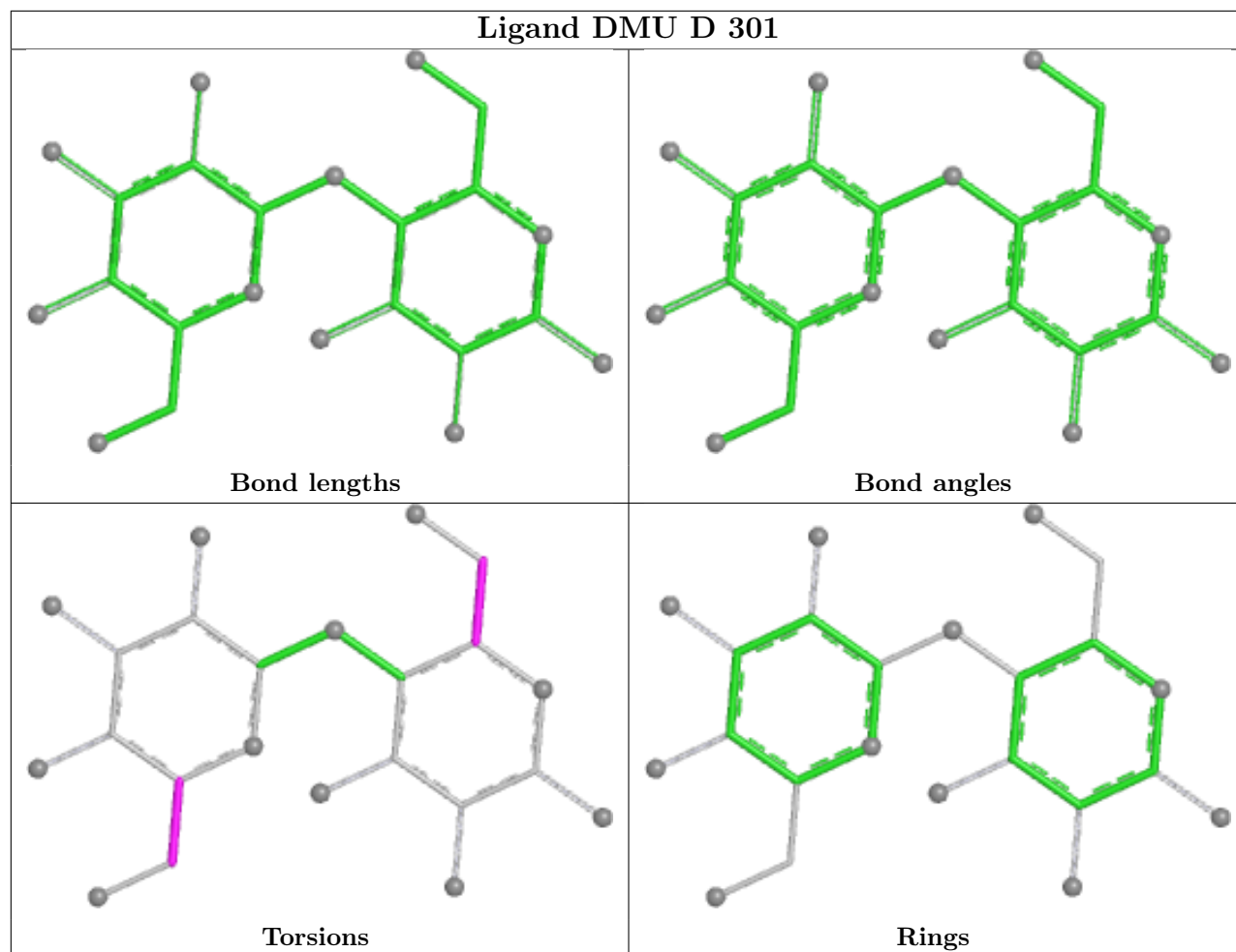


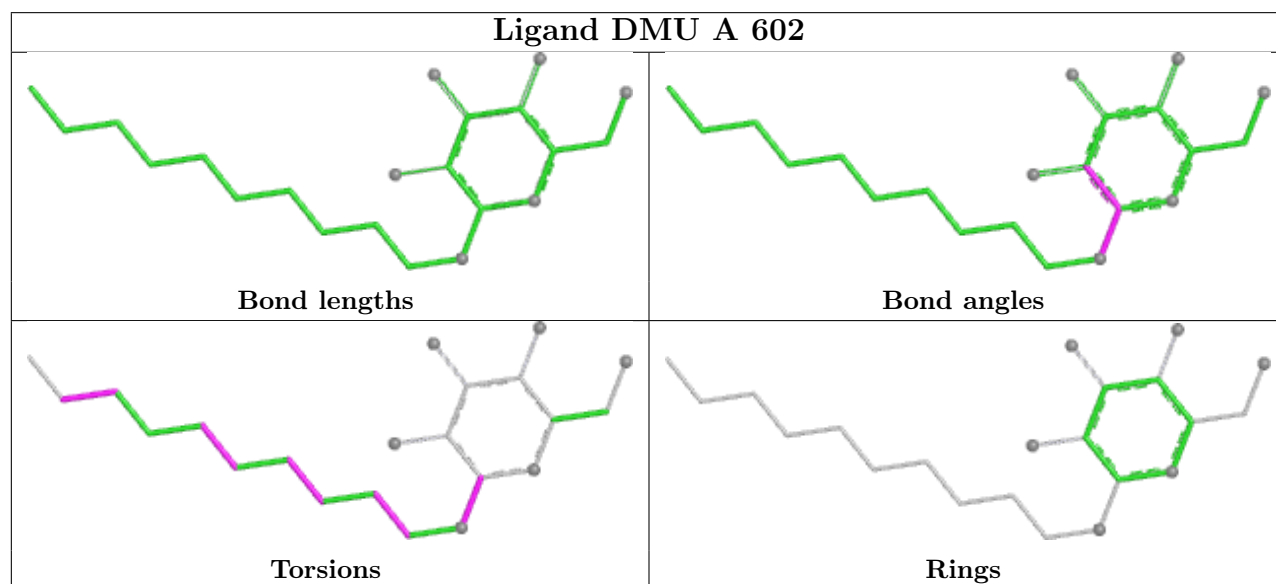
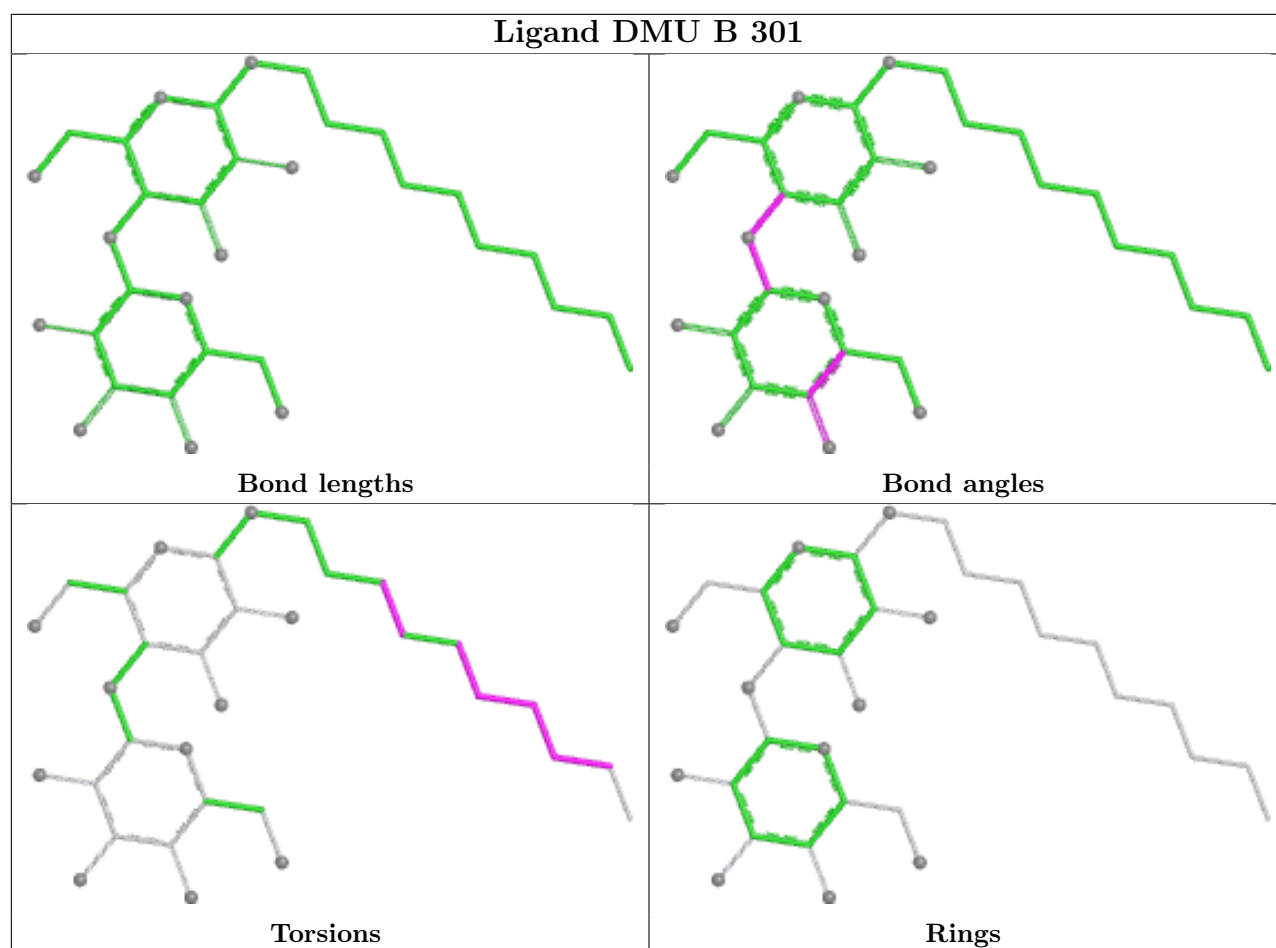


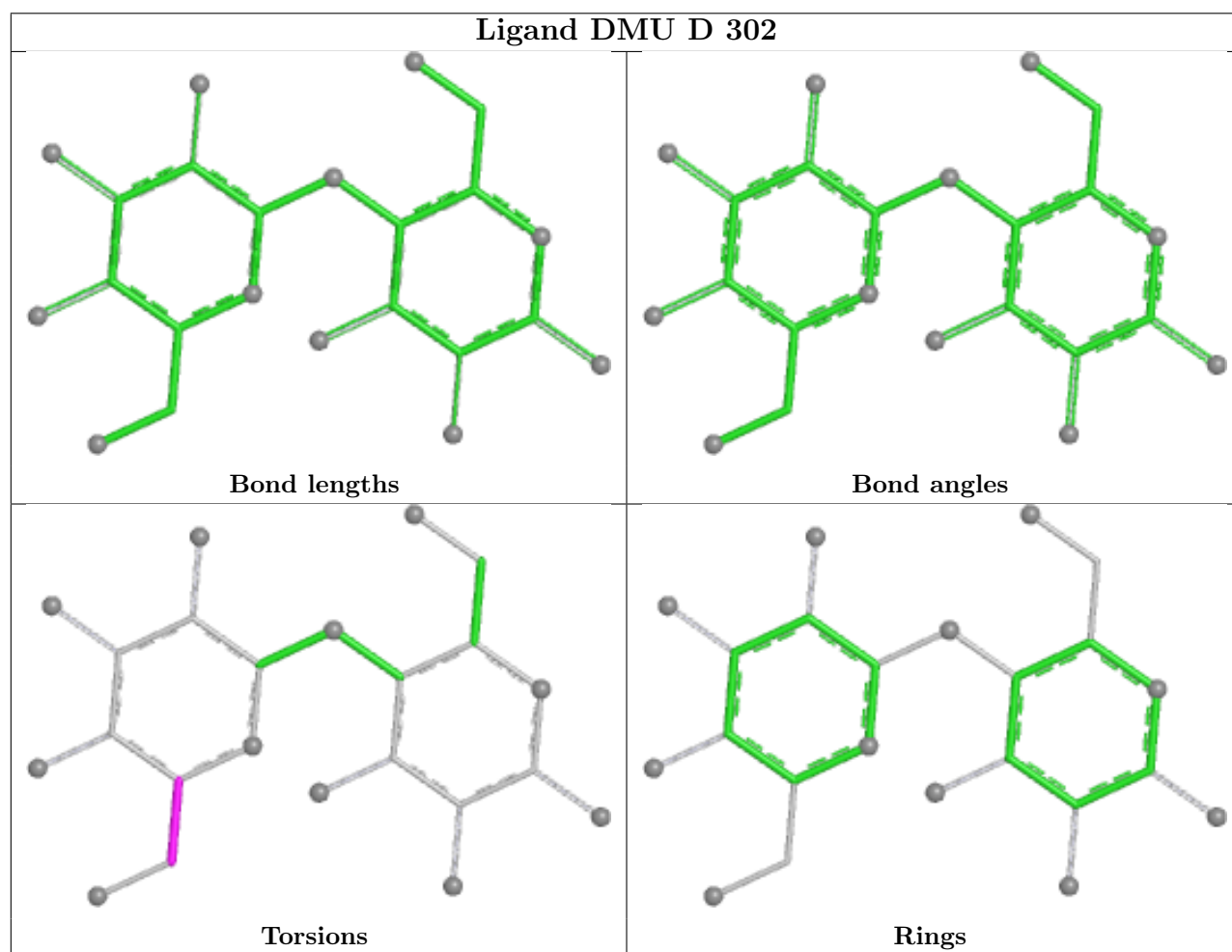
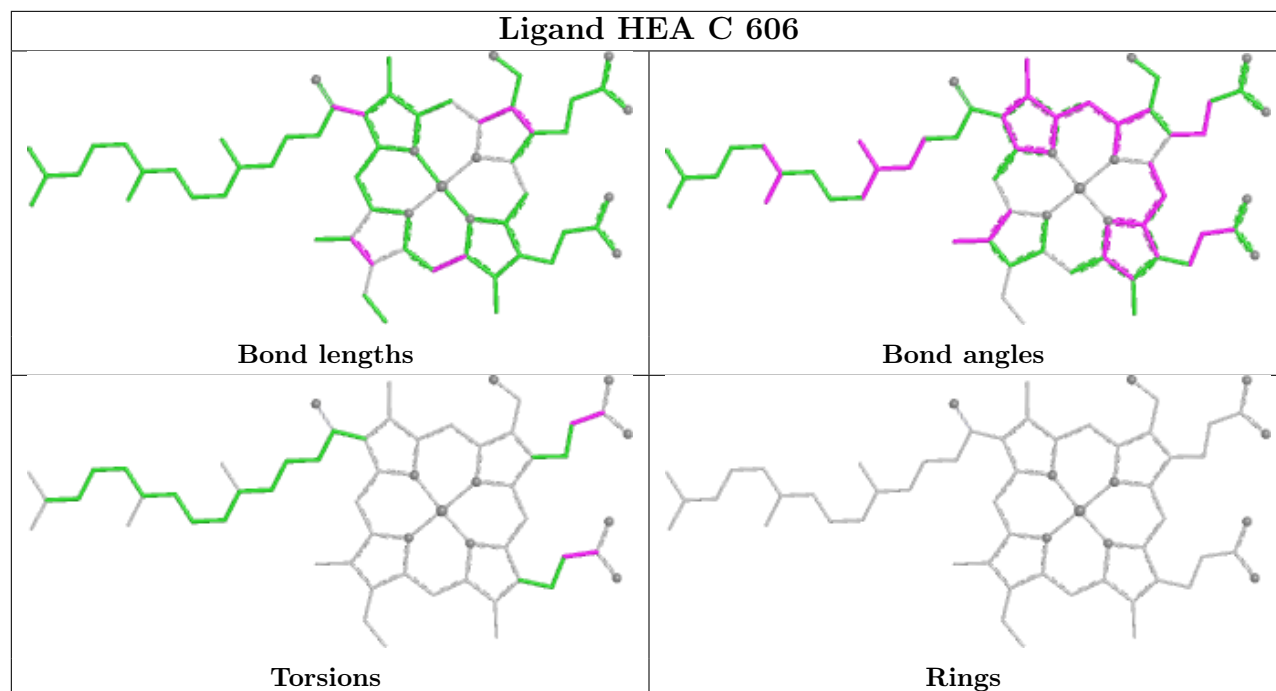












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	535/535 (100%)	0.09	34 (6%) 19 26	18, 30, 53, 75	0
1	C	530/535 (99%)	0.59	81 (15%) 2 2	25, 45, 68, 81	0
2	B	256/256 (100%)	-0.02	10 (3%) 39 48	18, 34, 47, 54	0
2	D	256/256 (100%)	0.20	21 (8%) 11 16	24, 38, 58, 67	0
All	All	1577/1582 (99%)	0.26	146 (9%) 8 13	18, 36, 61, 81	0

The worst 5 of 146 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	TRP	8.1
1	A	20	TRP	7.1
1	C	222	MET	5.6
1	C	73	VAL	5.4
1	A	22	MET	5.3

### 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 monosaccharides in this entry.

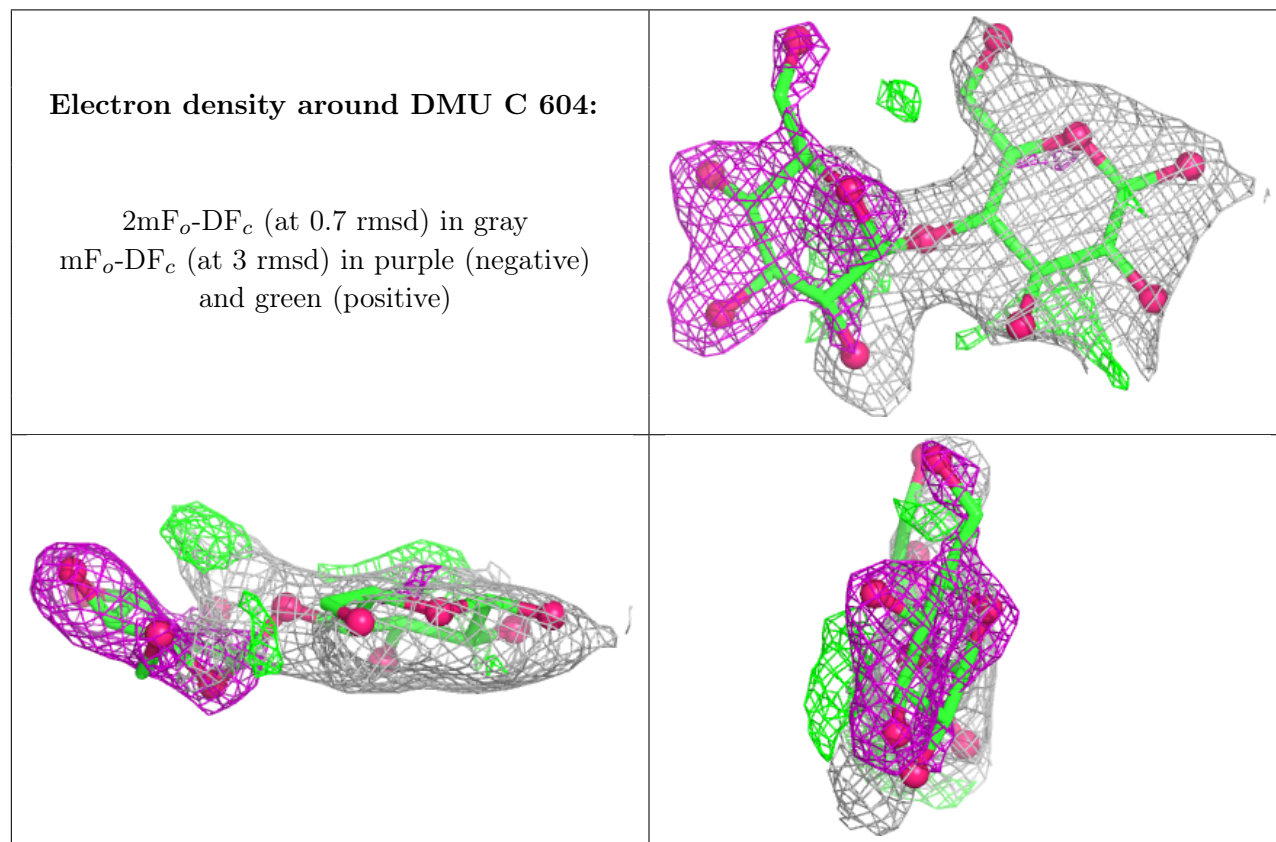
### 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	DMU	C	604	23/33	0.14	0.57	39,43,51,51	23
4	DMU	A	602	22/33	0.70	0.23	38,59,66,66	0
5	TRD	A	604	7/13	0.72	0.17	52,55,57,57	0
5	TRD	A	609	13/13	0.75	0.25	64,65,68,68	0
5	TRD	A	605	7/13	0.78	0.20	50,52,52,52	0
4	DMU	A	603	22/33	0.80	0.17	35,44,50,51	22
5	TRD	C	607	11/13	0.80	0.18	70,71,72,72	0
4	DMU	B	304	23/33	0.81	0.21	69,69,70,70	23
4	DMU	D	301	23/33	0.81	0.19	64,64,65,65	23
11	HTH	B	306	10/10	0.81	0.32	51,57,60,60	0
4	DMU	D	302	23/33	0.83	0.27	70,72,76,76	23
5	TRD	D	304	7/13	0.84	0.16	54,54,55,55	0
4	DMU	C	602	33/33	0.85	0.36	40,44,46,47	0
5	TRD	A	606	7/13	0.85	0.25	60,61,62,62	0
5	TRD	D	303	13/13	0.86	0.13	48,49,55,55	0
4	DMU	B	302	33/33	0.86	0.19	43,49,51,54	33
4	DMU	C	603	23/33	0.86	0.28	85,85,86,86	23
10	CL	C	611	1/1	0.88	0.08	66,66,66,66	0
5	TRD	A	610	13/13	0.88	0.12	37,41,46,46	0
5	TRD	B	305	9/13	0.90	0.13	39,40,41,43	9
4	DMU	B	303	33/33	0.90	0.18	46,51,57,59	33
4	DMU	B	301	33/33	0.96	0.10	20,31,51,53	0
6	HEA	A	608	60/60	0.97	0.14	19,24,36,39	0
6	HEA	C	606	60/60	0.97	0.11	25,31,41,42	0
6	HEA	C	605	60/60	0.98	0.16	25,29,42,43	0
9	CA	C	610	1/1	0.98	0.05	34,34,34,34	0
7	CU	A	611	1/1	0.99	0.11	28,28,28,28	0
7	CU	C	608	1/1	0.99	0.08	35,35,35,35	0
8	MG	A	612	1/1	0.99	0.21	16,16,16,16	0
3	OH	A	601	1/1	0.99	0.14	17,17,17,17	0
10	CL	A	614	1/1	0.99	0.07	39,39,39,39	0
3	OH	C	601	1/1	0.99	0.18	27,27,27,27	0
6	HEA	A	607	60/60	0.99	0.18	16,19,27,28	0
13	CD	B	309	1/1	0.99	0.06	37,37,37,37	0
13	CD	B	310	1/1	0.99	0.11	35,35,35,35	1
13	CD	D	307	1/1	0.99	0.05	36,36,36,36	0
13	CD	D	308	1/1	0.99	0.06	47,47,47,47	1
12	CU1	B	308	1/1	1.00	0.11	21,21,21,21	0
12	CU1	D	306	1/1	1.00	0.09	26,26,26,26	0
7	CU	D	305	1/1	1.00	0.10	27,27,27,27	0
7	CU	B	307	1/1	1.00	0.11	21,21,21,21	0
8	MG	C	609	1/1	1.00	0.19	20,20,20,20	0
9	CA	A	613	1/1	1.00	0.10	23,23,23,23	0

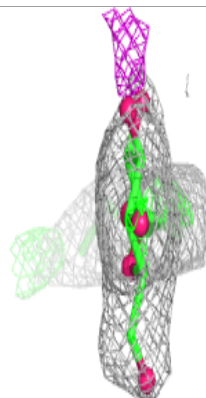
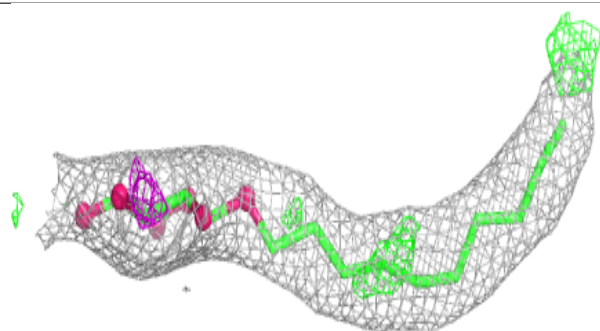
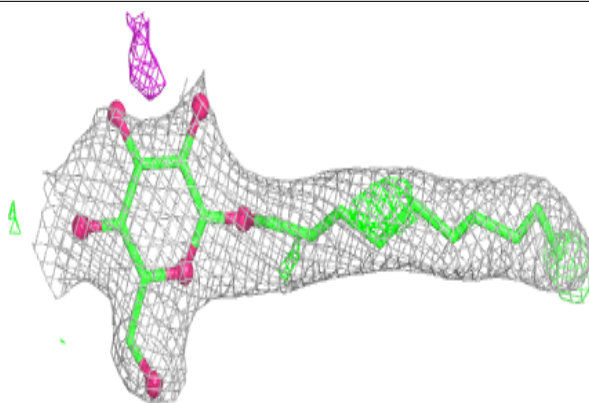


The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

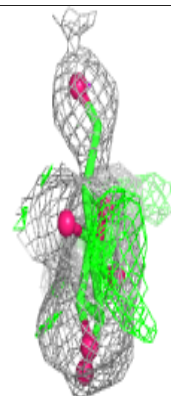
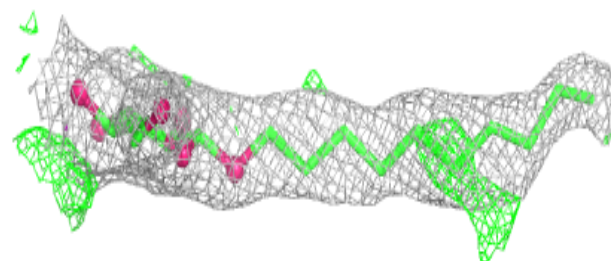
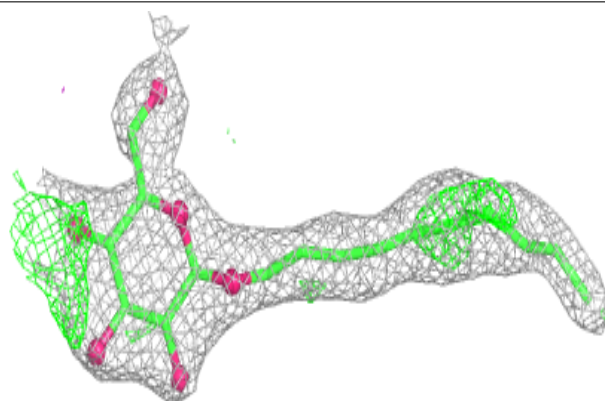


**Electron density around DMU A 602:**

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

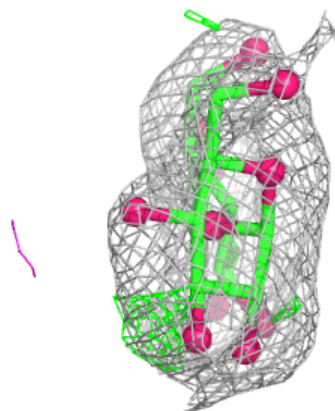
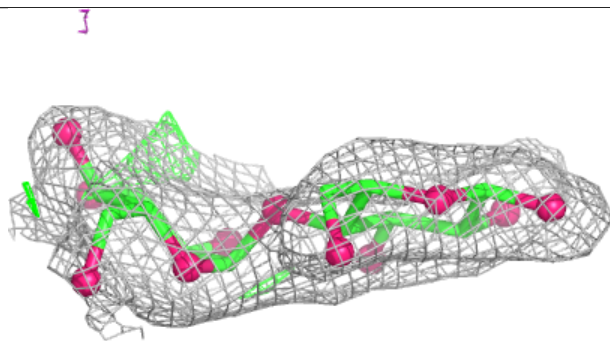
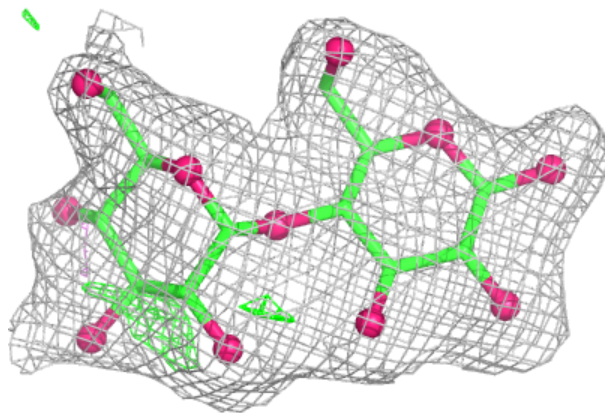
**Electron density around DMU A 603:**

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and green (positive)



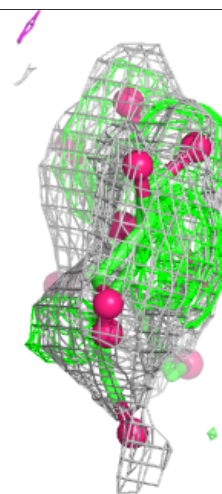
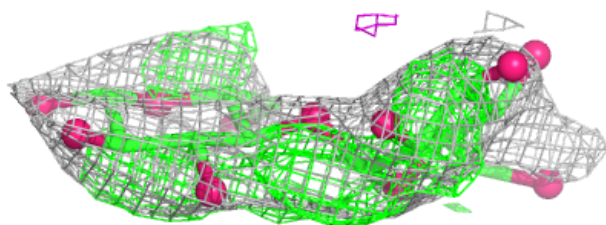
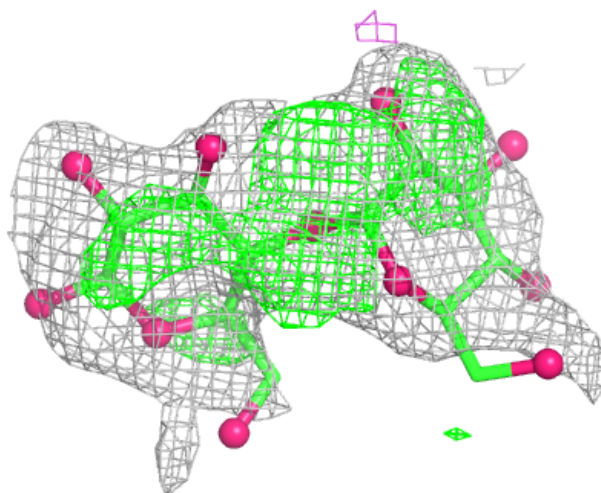
**Electron density around DMU B 304:**

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and green (positive)



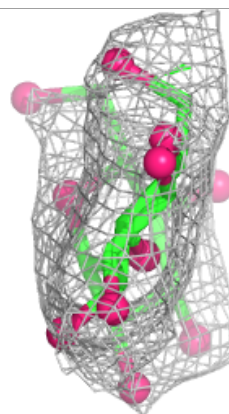
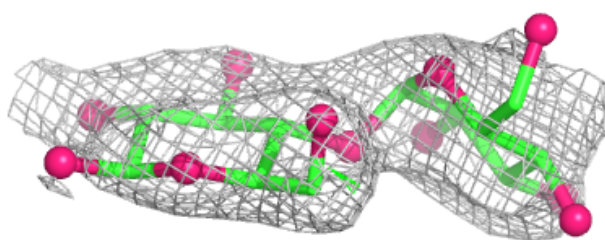
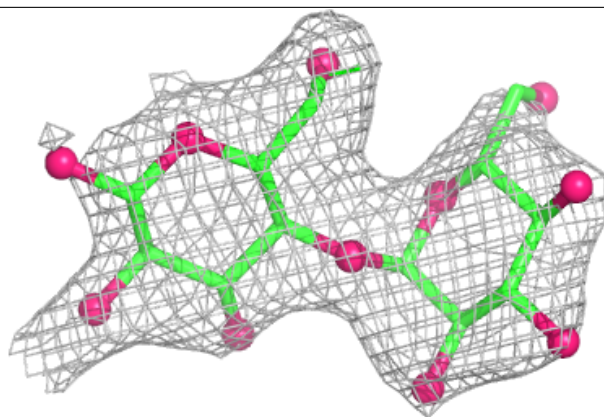
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and green (positive)

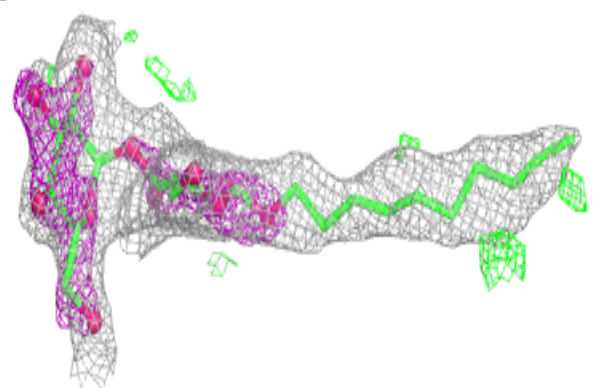
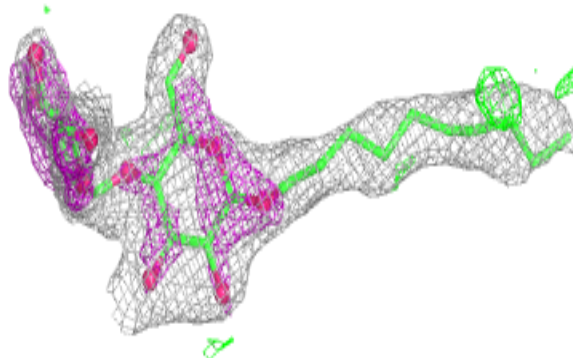


**Electron density around DMU D 302:**

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and green (positive)

**Electron density around DMU C 602:**

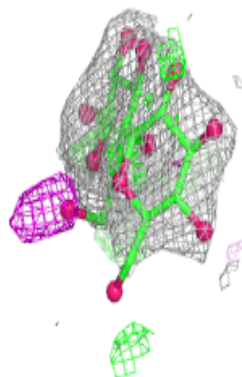
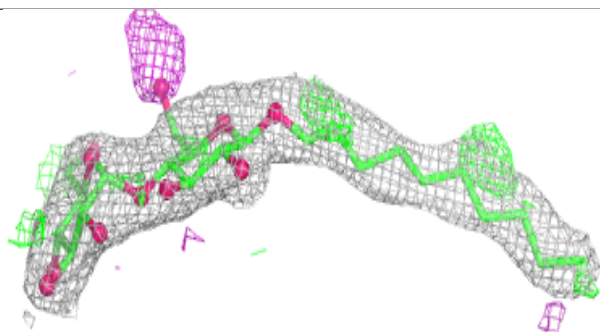
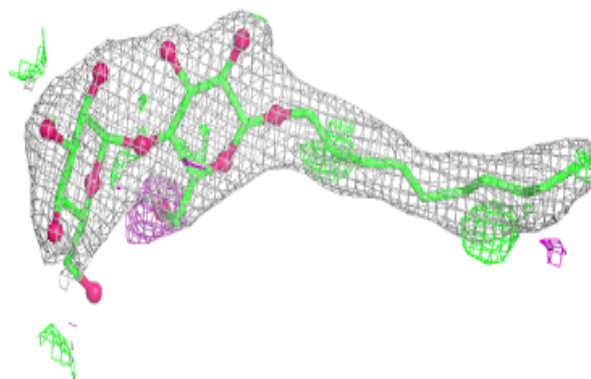
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and green (positive)



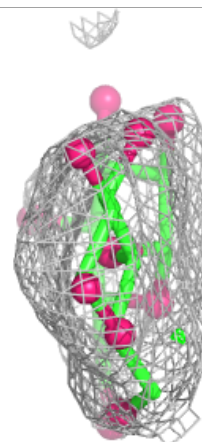
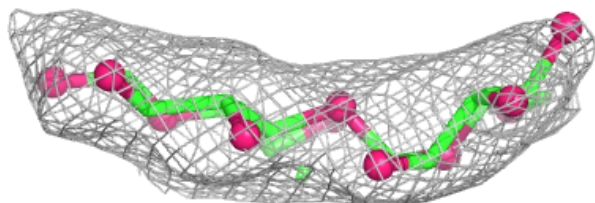
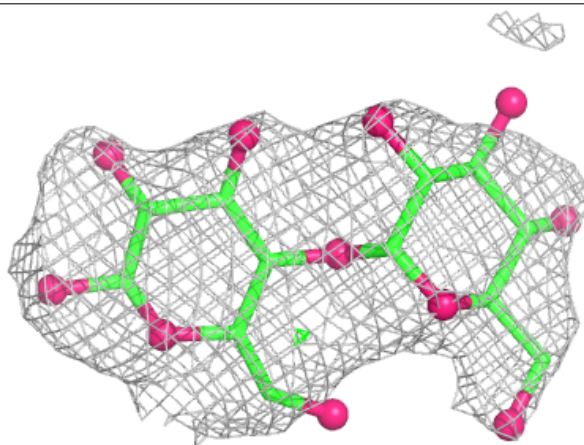


**Electron density around DMU B 302:**

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

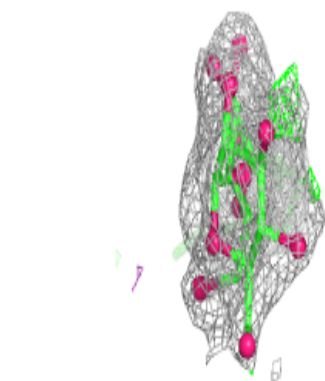
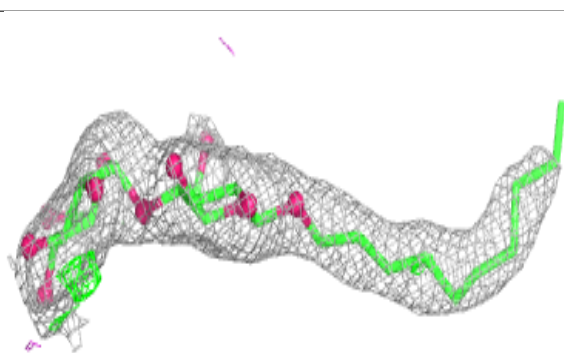
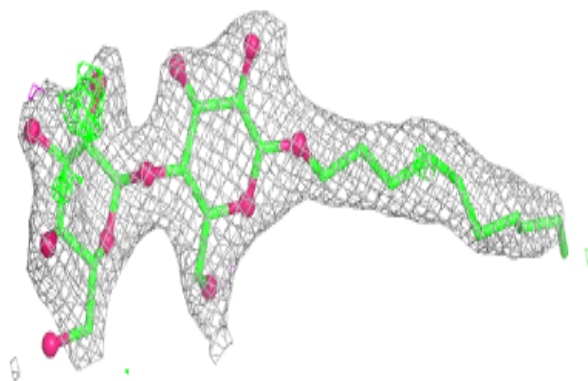
**Electron density around DMU C 603:**

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

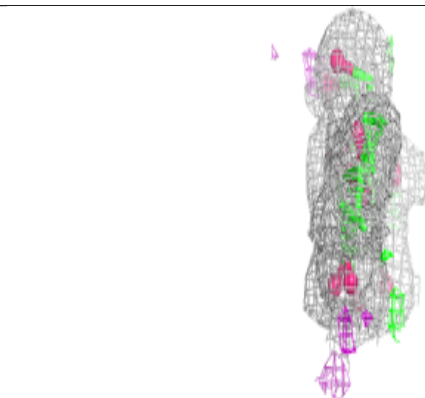
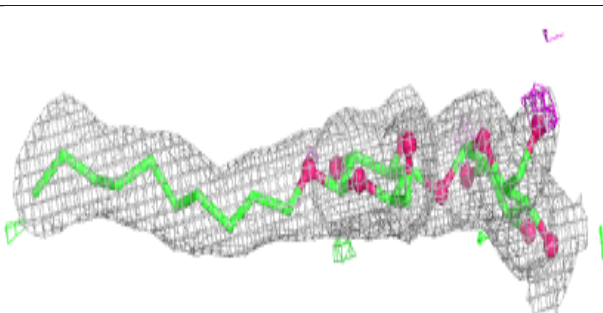
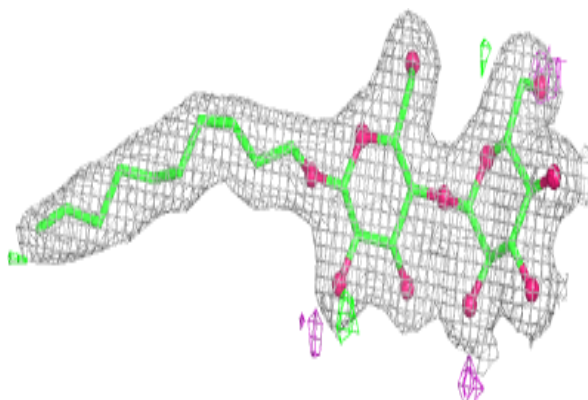


**Electron density around DMU B 303:**

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

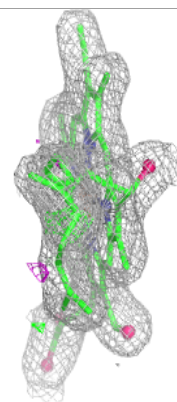
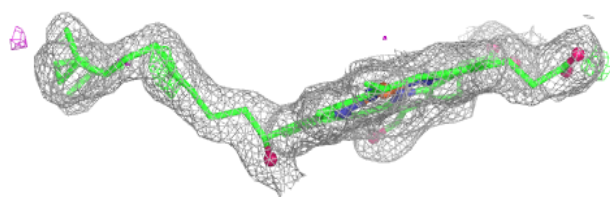
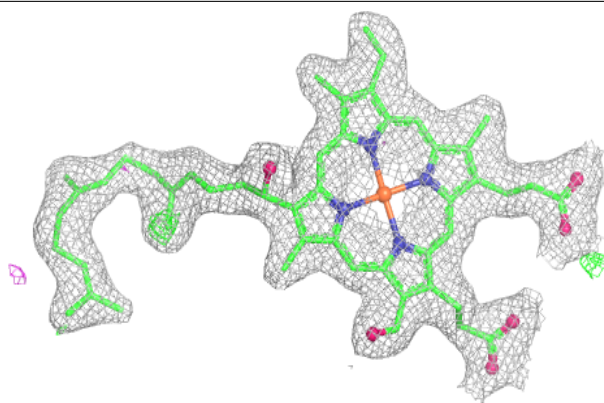
**Electron density around DMU B 301:**

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

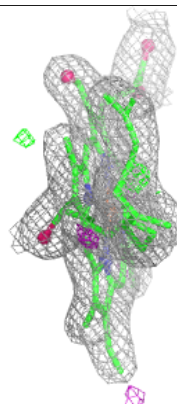
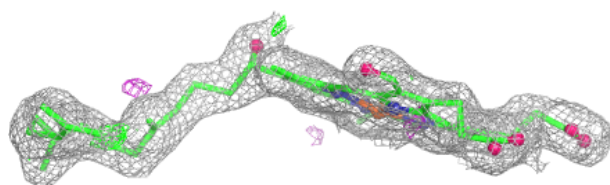
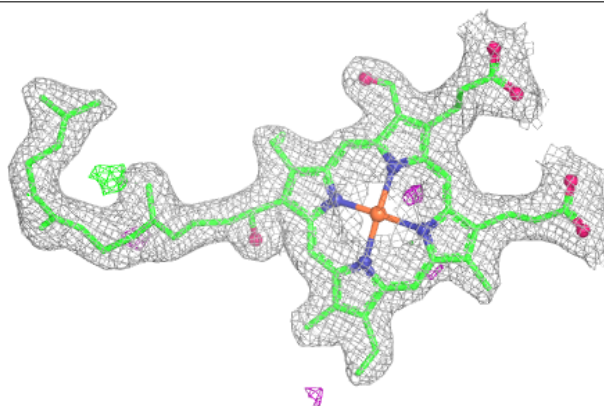


**Electron density around HEA A 608:**

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

**Electron density around HEA C 606:**

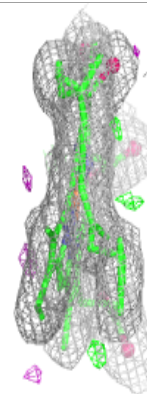
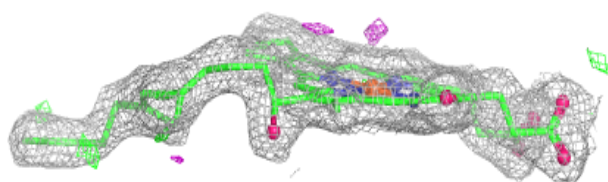
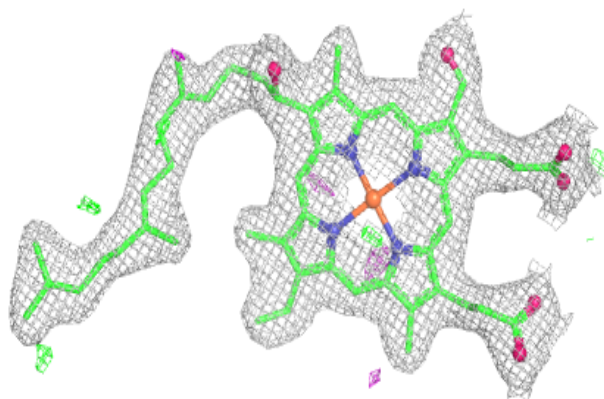
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



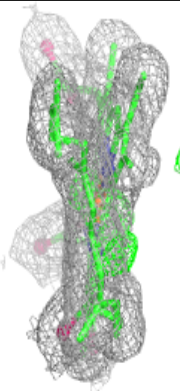
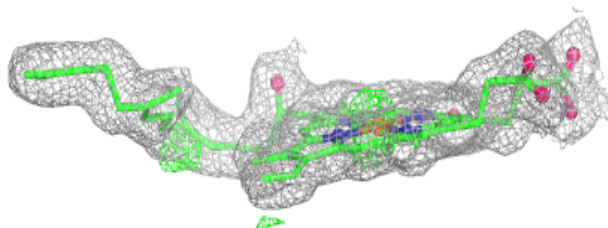
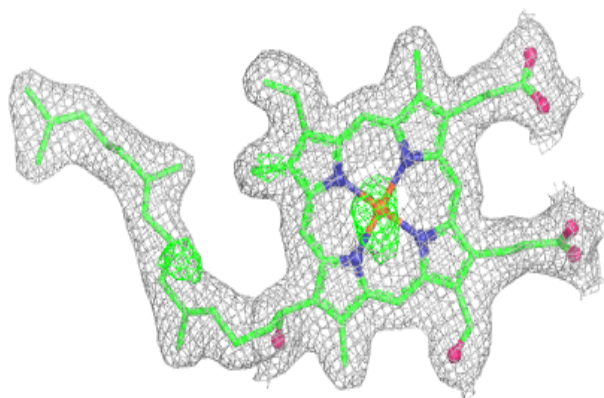


**Electron density around HEA C 605:**

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

**Electron density around HEA A 607:**

$2mF_o-DF_c$  (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.