



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 29, 2024 – 10:26 AM EDT

PDB ID : 3DTU  
Title : Catalytic core subunits (I and II) of cytochrome c oxidase from *Rhodobacter sphaeroides* complexed with deoxycholic acid  
Authors : Qin, L.; Mills, D.A.; Buhrow, L.; Hiser, C.; Ferguson-Miller, S.  
Deposited on : 2008-07-15  
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	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

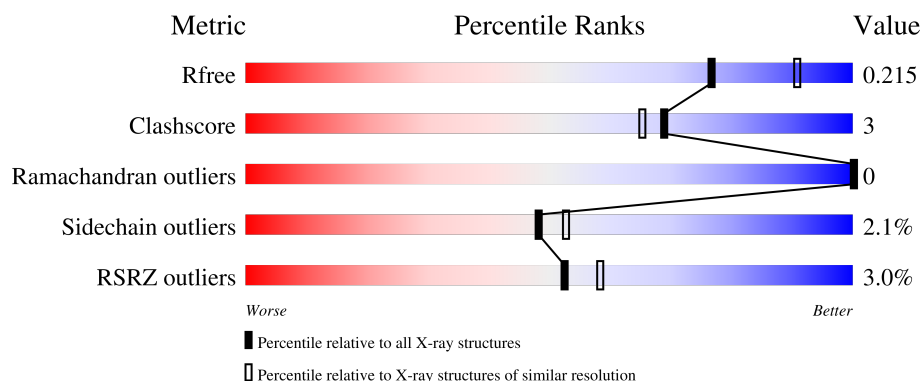
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

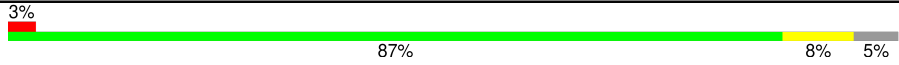

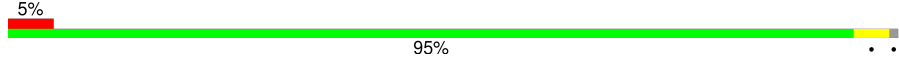
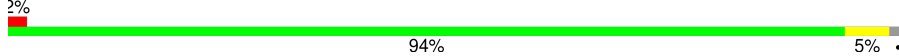
The reported resolution of this entry is 2.15 Å.

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))
$R_{free}$	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (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	566	
1	C	566	
2	B	262	
2	D	262	

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
10	TRD	C	581	-	-	-	X
10	TRD	C	584	-	-	X	-
12	HTO	B	1	X	-	-	-
3	DMU	A	1002	-	-	-	X
3	DMU	B	1003	-	-	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 13976 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	539	Total	C	N	O	S	33	0	0
			4249	2845	673	700	31			
1	C	536	Total	C	N	O	S	32	0	0
			4221	2827	664	699	31			

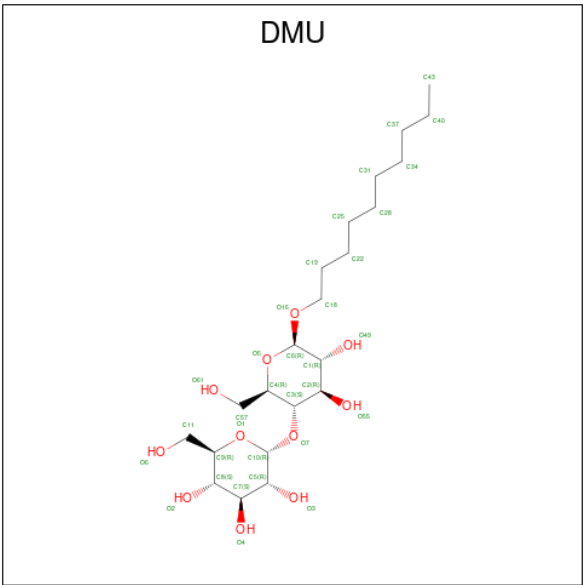
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	259	Total	C	N	O	S	21	0	0
			2051	1336	340	369	6			
2	D	258	Total	C	N	O	S	15	0	0
			2040	1329	336	369	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	282	HIS	-	expression tag	UNP Q03736
B	283	HIS	-	expression tag	UNP Q03736
B	284	HIS	-	expression tag	UNP Q03736
B	285	HIS	-	expression tag	UNP Q03736
B	286	HIS	-	expression tag	UNP Q03736
B	287	HIS	-	expression tag	UNP Q03736
D	282	HIS	-	expression tag	UNP Q03736
D	283	HIS	-	expression tag	UNP Q03736
D	284	HIS	-	expression tag	UNP Q03736
D	285	HIS	-	expression tag	UNP Q03736
D	286	HIS	-	expression tag	UNP Q03736
D	287	HIS	-	expression tag	UNP Q03736

- Molecule 3 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula:  $C_{22}H_{42}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			33	22	11		
3	A	1	Total	C	O	0	0
			22	11	11		
3	A	1	Total	C	O	0	0
			22	16	6		
3	A	1	Total	C	O	0	0
			33	22	11		
3	B	1	Total	C	O	0	0
			23	17	6		
3	B	1	Total	C	O	0	0
			23	12	11		
3	C	1	Total	C	O	0	0
			33	22	11		
3	C	1	Total	C	O	0	0
			33	22	11		
3	D	1	Total	C	O	0	0
			33	22	11		

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	2	Total Cu 2 2	0	0

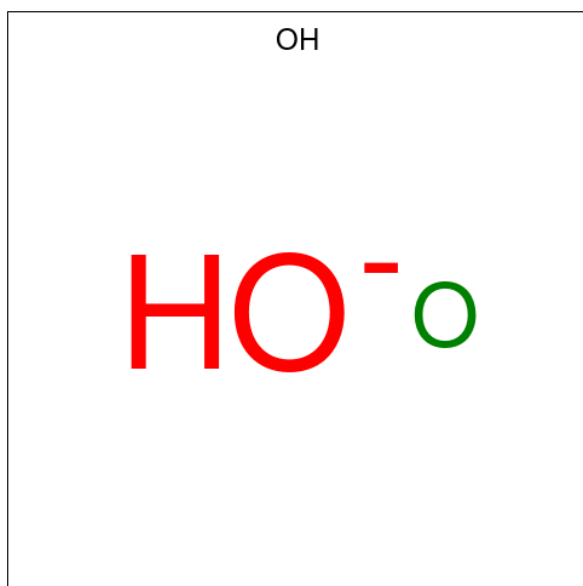
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

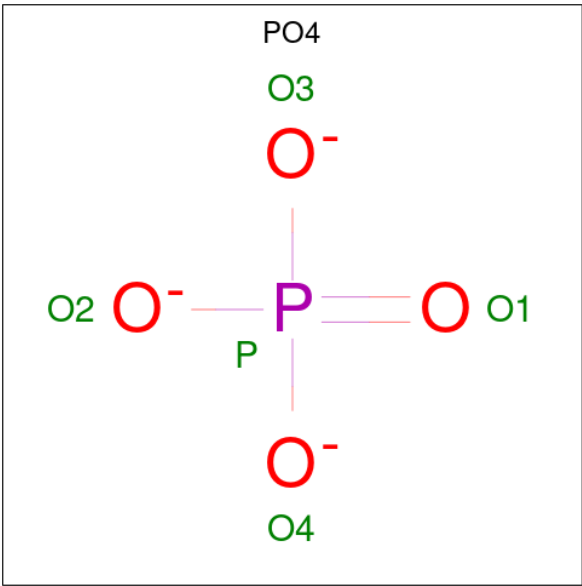
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0
6	C	1	Total Ca 1 1	0	0

- Molecule 7 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



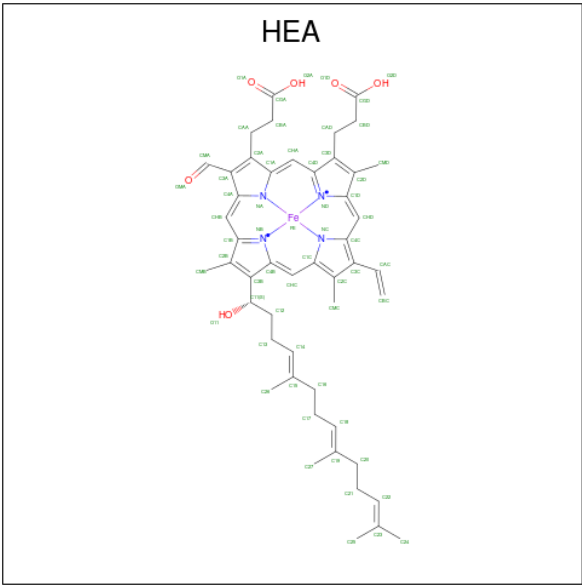
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0
7	C	1	Total O 1 1	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	O	P		0	0
			5	4	1			
8	C	1	Total	O	P		0	0
			5	4	1			

- Molecule 9 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



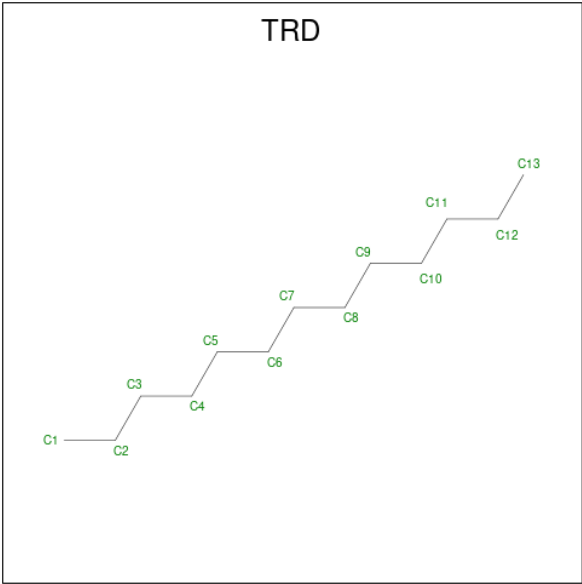
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	Fe	N O	0	0
			60	49	1 4	6		

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

- Molecule 10 is TRIDECANE (three-letter code: TRD) (formula: C<sub>13</sub>H<sub>28</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	C		
			13	13	0	0
10	A	1	Total	C		
			11	11	0	0
10	A	1	Total	C		
			13	13	0	0
10	A	1	Total	C		
			7	7	0	0
10	A	1	Total	C		
			11	11	0	0
10	A	1	Total	C		
			7	7	0	0
10	A	1	Total	C		
			7	7	0	0
10	A	1	Total	C		
			11	11	0	0

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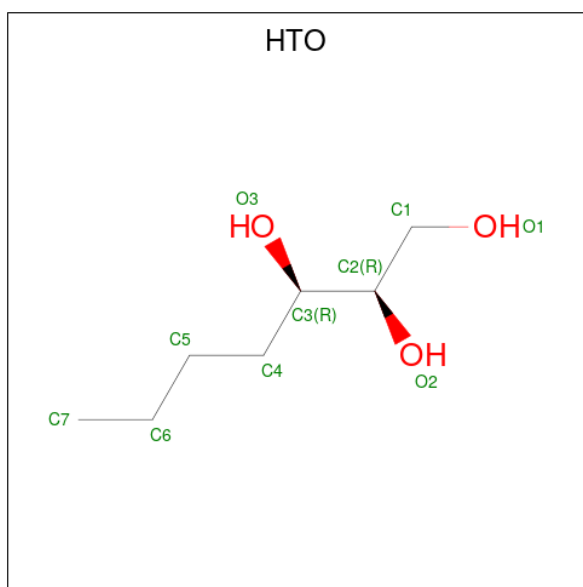
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C 9 9	0	0
10	B	1	Total C 9 9	0	0
10	B	1	Total C 9 9	0	0
10	C	1	Total C 13 13	0	0
10	C	1	Total C 11 11	0	0
10	C	1	Total C 7 7	0	0
10	C	1	Total C 9 9	0	0
10	C	1	Total C 11 11	0	0
10	C	1	Total C 7 7	0	0
10	C	1	Total C 7 7	0	0
10	C	1	Total C 7 7	0	0
10	D	1	Total C 13 13	0	0
10	D	1	Total C 9 9	0	0
10	D	1	Total C 11 11	0	0
10	D	1	Total C 7 7	0	0

- Molecule 11 is CADMIUM ION (three-letter code: CD) (formula: Cd).

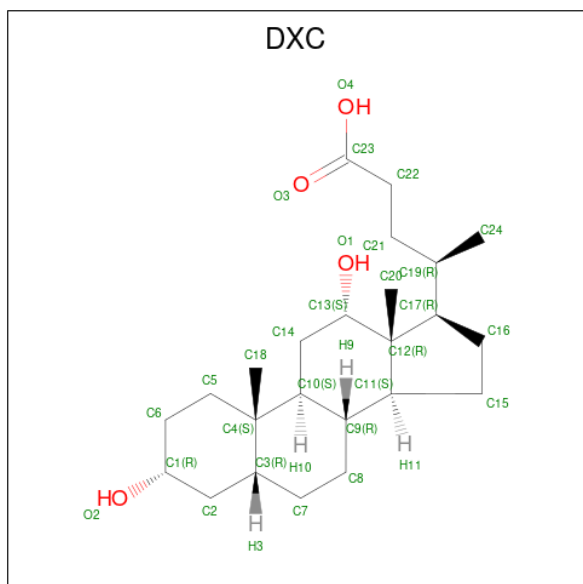
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	3	Total Cd 3 3	0	0
11	D	2	Total Cd 2 2	0	0

- Molecule 12 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).



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

- Molecule 13 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (three-letter code: DXC) (formula:  $C_{24}H_{40}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			28	24	4		

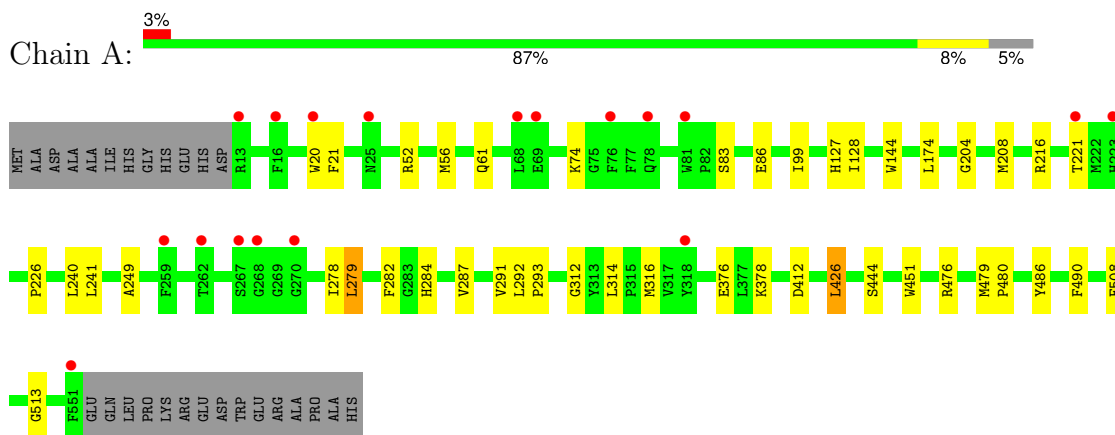
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	144	Total 144	O 144	0	0
14	B	160	Total 160	O 160	0	0
14	C	169	Total 169	O 169	0	0
14	D	163	Total 163	O 163	0	0

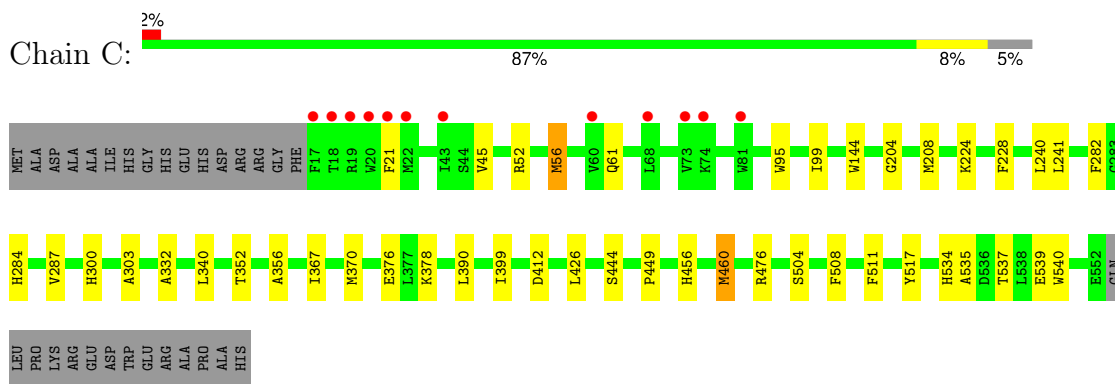
### 3 Residue-property plots [i](#)

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

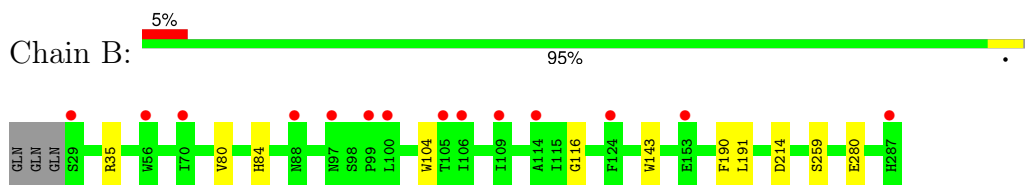
#### • Molecule 1: Cytochrome c oxidase subunit 1



#### • Molecule 1: Cytochrome c oxidase subunit 1

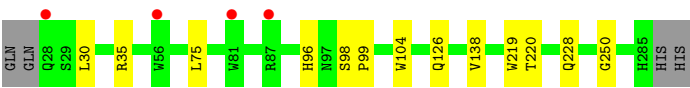


#### • Molecule 2: Cytochrome c oxidase subunit 2



#### • 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, $\alpha$ , $\beta$ , $\gamma$	123.24Å 132.05Å 167.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.15 40.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.9 (40.00-2.15) 96.9 (40.00-2.15)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.184 , 0.212 0.184 , 0.215	Depositor DCC
$R_{free}$ test set	3612 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.5	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13976	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 3.21% 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: CA, PO4, HEA, HTO, DXC, OH, MG, DMU, TRD, CU, CD

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	0.50	0/4406	0.55	2/6010 (0.0%)
1	C	0.53	0/4377	0.56	0/5973
2	B	0.48	0/2115	0.54	0/2895
2	D	0.53	0/2102	0.57	0/2877
All	All	0.51	0/13000	0.56	2/17755 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	LEU	CA-CB-CG	6.12	129.38	115.30
1	A	279	LEU	CA-CB-CG	-5.14	103.48	115.30

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	4249	0	4172	30	0
1	C	4221	0	4140	39	0
2	B	2051	0	2001	5	0
2	D	2040	0	1995	6	0
3	A	110	0	131	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	46	0	52	0	0
3	C	66	0	84	1	0
3	D	33	0	42	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	1	0
7	C	1	0	0	1	0
8	A	5	0	0	0	0
8	C	5	0	0	0	0
9	A	120	0	108	5	0
9	C	120	0	108	8	0
10	A	80	0	158	7	0
10	B	27	0	51	1	0
10	C	72	0	139	13	0
10	D	40	0	79	2	0
11	B	3	0	0	0	0
11	D	2	0	0	0	0
12	B	10	0	16	1	0
13	C	28	0	39	0	0
14	A	144	0	0	1	0
14	B	160	0	0	0	0
14	C	169	0	0	3	0
14	D	163	0	0	1	0
All	All	13976	0	13315	91	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 91 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:303:ALA:HB3	10:C:584:TRD:H21	1.38	1.05
3:A:1002:DMU:C2	3:A:1002:DMU:C6	2.49	0.90
7:C:572:OH:O	14:C:589:HOH:O	1.89	0.90
9:C:574:HEA:HMC1	9:C:574:HEA:HBC1	1.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1501:OH:O	14:A:1511:HOH:O	2.00	0.79

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	537/566 (95%)	525 (98%)	12 (2%)	0	100	100
1	C	534/566 (94%)	526 (98%)	8 (2%)	0	100	100
2	B	257/262 (98%)	250 (97%)	7 (3%)	0	100	100
2	D	256/262 (98%)	251 (98%)	5 (2%)	0	100	100
All	All	1584/1656 (96%)	1552 (98%)	32 (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	438/459 (95%)	426 (97%)	12 (3%)	40	42
1	C	436/459 (95%)	427 (98%)	9 (2%)	48	53
2	B	218/221 (99%)	215 (99%)	3 (1%)	62	68
2	D	217/221 (98%)	213 (98%)	4 (2%)	54	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1309/1360 (96%)	1281 (98%)	28 (2%)	48 53

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	214	ASP
2	D	126	GLN
1	C	61	GLN
2	D	30	LEU
1	C	56	MET

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

Mol	Chain	Res	Type
2	D	228	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 57 ligands modelled in this entry, 15 are monoatomic and 2 are modelled with single atom - leaving 40 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	DMU	C	567	-	34,34,34	0.65	1 (2%)	45,45,45	0.74	1 (2%)
3	DMU	A	1005	-	34,34,34	0.60	0	45,45,45	0.67	0
10	TRD	D	12	-	10,10,12	0.27	0	9,9,11	0.41	0
10	TRD	A	1506	-	12,12,12	0.24	0	11,11,11	0.52	0
10	TRD	A	1010	-	10,10,12	0.25	0	9,9,11	0.51	0
10	TRD	C	583	-	6,6,12	0.22	0	5,5,11	0.45	0
10	TRD	C	582	-	6,6,12	0.25	0	5,5,11	0.39	0
13	DXC	C	576	11	31,31,31	0.60	0	49,49,49	1.31	7 (14%)
10	TRD	C	577	-	12,12,12	0.29	0	11,11,11	0.42	0
10	TRD	D	288	-	8,8,12	0.24	0	7,7,11	0.44	0
10	TRD	C	584	-	6,6,12	0.10	0	5,5,11	0.58	0
9	HEA	A	1503	1,14	58,67,67	1.41	5 (8%)	63,103,103	1.62	13 (20%)
3	DMU	A	1002	-	21,21,34	0.56	0	26,28,45	0.82	0
10	TRD	A	1504	-	12,12,12	0.28	0	11,11,11	0.45	0
10	TRD	C	581	-	10,10,12	0.27	0	9,9,11	0.50	0
10	TRD	C	580	-	8,8,12	0.25	0	7,7,11	0.45	0
3	DMU	A	567	-	34,34,34	0.55	0	45,45,45	0.76	1 (2%)
3	DMU	D	11	-	34,34,34	0.57	0	45,45,45	0.79	1 (2%)
10	TRD	D	23	-	6,6,12	0.22	0	5,5,11	0.44	0
10	TRD	A	1505	-	10,10,12	0.26	0	9,9,11	0.47	0
9	HEA	C	575	1,14	58,67,67	1.41	7 (12%)	63,103,103	1.60	13 (20%)
10	TRD	A	1013	-	6,6,12	0.28	0	5,5,11	0.31	0
10	TRD	D	7	-	12,12,12	0.24	0	11,11,11	0.58	0
10	TRD	A	1014	-	6,6,12	0.22	0	5,5,11	0.43	0
8	PO4	C	573	-	4,4,4	0.92	0	6,6,6	0.37	0
10	TRD	C	579	-	6,6,12	0.26	0	5,5,11	0.31	0
10	TRD	B	1023	-	8,8,12	0.25	0	7,7,11	0.45	0
3	DMU	A	1004	-	22,22,34	0.62	1 (4%)	27,27,45	0.89	1 (3%)
3	DMU	B	1003	-	23,23,34	0.56	0	28,28,45	0.64	0
8	PO4	A	1001	-	4,4,4	0.94	0	6,6,6	0.46	0
10	TRD	C	578	-	10,10,12	0.30	0	9,9,11	0.39	0
3	DMU	B	1011	-	24,24,34	0.50	0	35,35,45	0.75	0
10	TRD	A	1015	-	10,10,12	0.27	0	9,9,11	0.50	0
9	HEA	C	574	1	58,67,67	1.43	6 (10%)	63,103,103	1.02	4 (6%)
10	TRD	B	1031	-	8,8,12	0.28	0	7,7,11	0.37	0
10	TRD	A	1009	-	6,6,12	0.23	0	5,5,11	0.41	0
12	HTO	B	1	-	9,9,9	0.21	0	10,10,10	0.82	0
9	HEA	A	1502	1	58,67,67	1.49	7 (12%)	63,103,103	1.13	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DMU	C	568	-	34,34,34	0.58	1 (2%)	45,45,45	0.80	1 (2%)
10	TRD	B	1012	-	8,8,12	0.26	0	7,7,11	0.43	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
3	DMU	C	567	-	-	7/19/59/59	0/2/2/2
3	DMU	A	1005	-	-	11/19/59/59	0/2/2/2
10	TRD	D	12	-	-	4/8/8/10	-
10	TRD	A	1506	-	-	7/10/10/10	-
10	TRD	A	1010	-	-	4/8/8/10	-
10	TRD	C	583	-	-	3/4/4/10	-
10	TRD	C	582	-	-	4/4/4/10	-
13	DXC	C	576	11	-	5/9/71/71	0/4/4/4
10	TRD	C	577	-	-	4/10/10/10	-
10	TRD	D	288	-	-	3/6/6/10	-
10	TRD	C	584	-	-	2/4/4/10	-
9	HEA	A	1503	1,14	-	7/32/76/76	-
3	DMU	A	1002	-	-	2/16/37/59	0/1/1/2
10	TRD	A	1504	-	-	4/10/10/10	-
10	TRD	C	581	-	-	3/8/8/10	-
10	TRD	C	580	-	-	3/6/6/10	-
3	DMU	A	567	-	-	9/19/59/59	0/2/2/2
3	DMU	D	11	-	-	4/19/59/59	0/2/2/2
10	TRD	D	23	-	-	2/4/4/10	-
10	TRD	A	1505	-	-	6/8/8/10	-
9	HEA	C	575	1,14	-	5/32/76/76	-
10	TRD	A	1013	-	-	2/4/4/10	-
10	TRD	D	7	-	-	6/10/10/10	-
10	TRD	A	1014	-	-	3/4/4/10	-
10	TRD	C	579	-	-	1/4/4/10	-
10	TRD	B	1023	-	-	1/6/6/10	-
3	DMU	A	1004	-	-	8/13/33/59	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMU	B	1003	-	-	9/15/35/59	0/1/1/2
10	TRD	C	578	-	-	4/8/8/10	-
3	DMU	B	1011	-	-	4/8/48/59	0/2/2/2
10	TRD	A	1015	-	-	4/8/8/10	-
9	HEA	C	574	1	-	5/32/76/76	-
10	TRD	B	1031	-	-	3/6/6/10	-
10	TRD	A	1009	-	-	3/4/4/10	-
12	HTO	B	1	-	1/1/2/2	5/10/10/10	-
9	HEA	A	1502	1	-	6/32/76/76	-
3	DMU	C	568	-	-	9/19/59/59	0/2/2/2
10	TRD	B	1012	-	-	4/6/6/10	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1502	HEA	C3A-C2A	-5.51	1.32	1.40
9	C	574	HEA	C3A-C2A	-5.02	1.33	1.40
9	C	575	HEA	C3A-C2A	-4.73	1.34	1.40
9	C	574	HEA	C3C-C2C	-4.69	1.34	1.40
9	A	1502	HEA	C3C-C2C	-4.55	1.34	1.40

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	575	HEA	CAD-CBD-CGD	-4.76	101.03	113.67
9	A	1503	HEA	CBA-CAA-C2A	-3.90	106.12	112.55
9	A	1503	HEA	CMC-C2C-C1C	-3.75	122.96	128.46
9	C	575	HEA	CMC-C2C-C1C	-3.73	122.99	128.46
9	A	1503	HEA	C4A-CHB-C1B	3.57	127.27	122.56

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	B	1	HTO	C2

5 of 176 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	567	DMU	C19-C18-O16-C6

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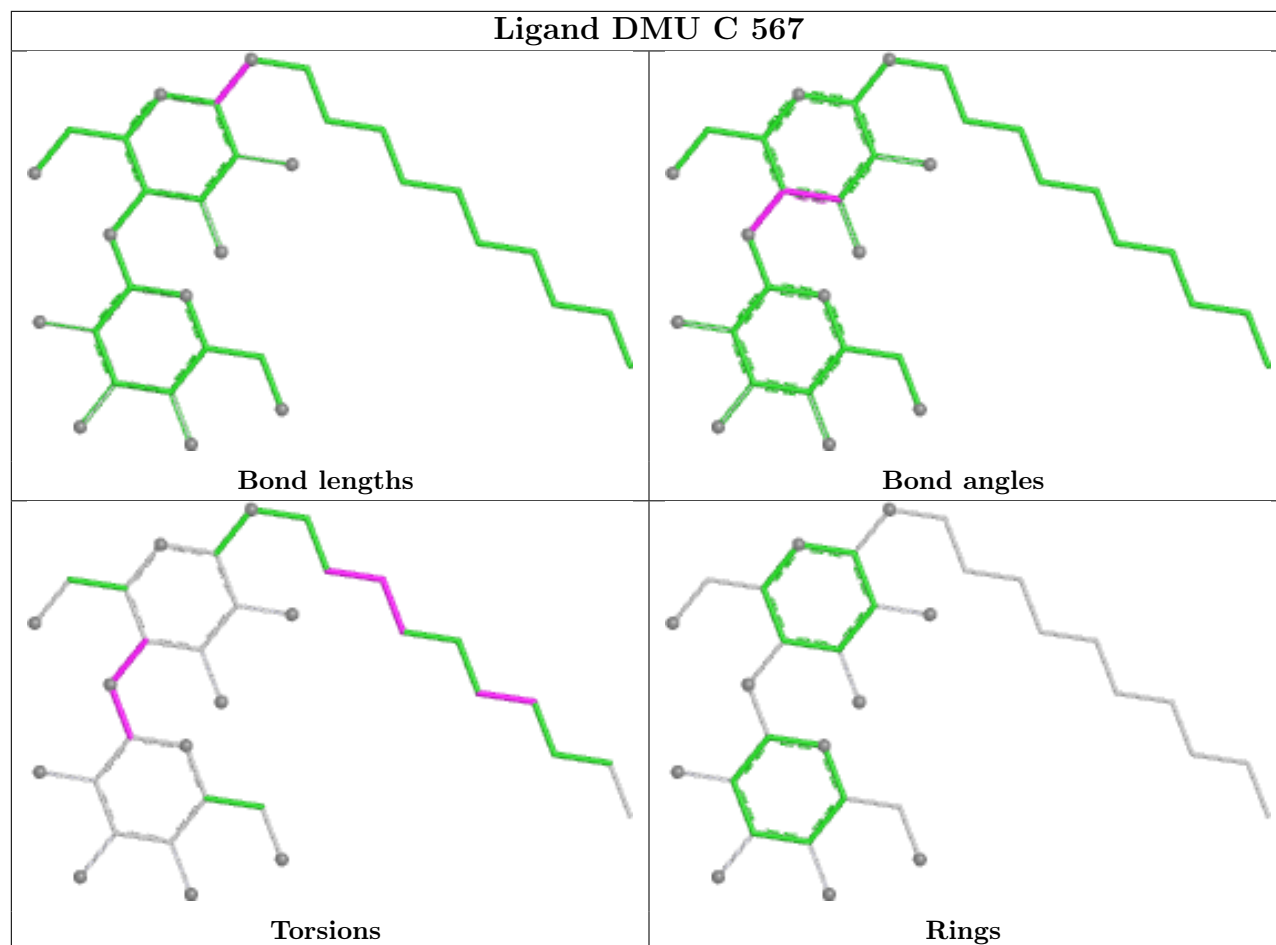
Mol	Chain	Res	Type	Atoms
3	A	1002	DMU	C3-C4-O5-C6
3	A	1002	DMU	C57-C4-O5-C6
3	A	1004	DMU	C1-C6-O16-C18
3	A	1004	DMU	O5-C6-O16-C18

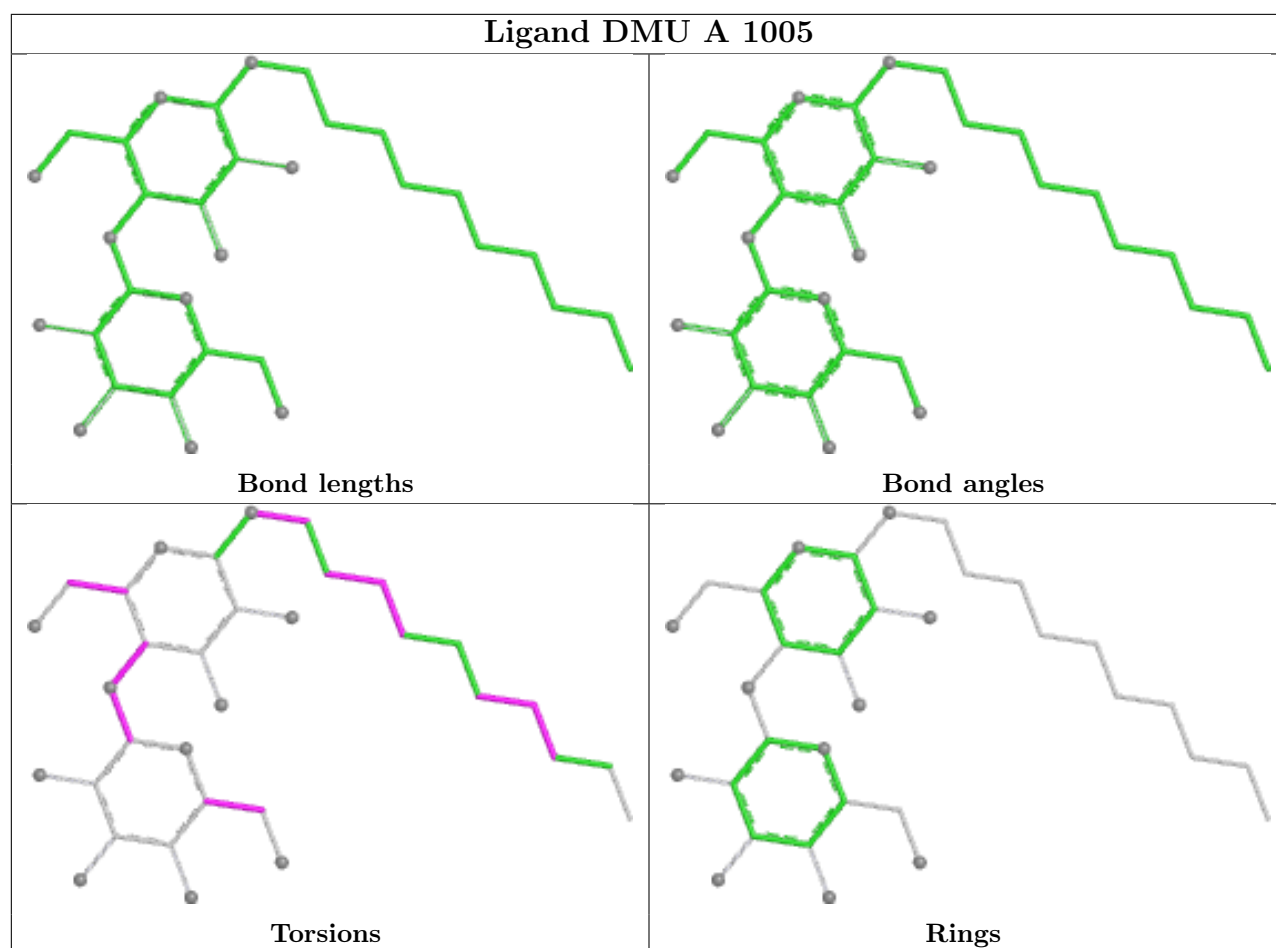
There are no ring outliers.

16 monomers are involved in 48 short contacts:

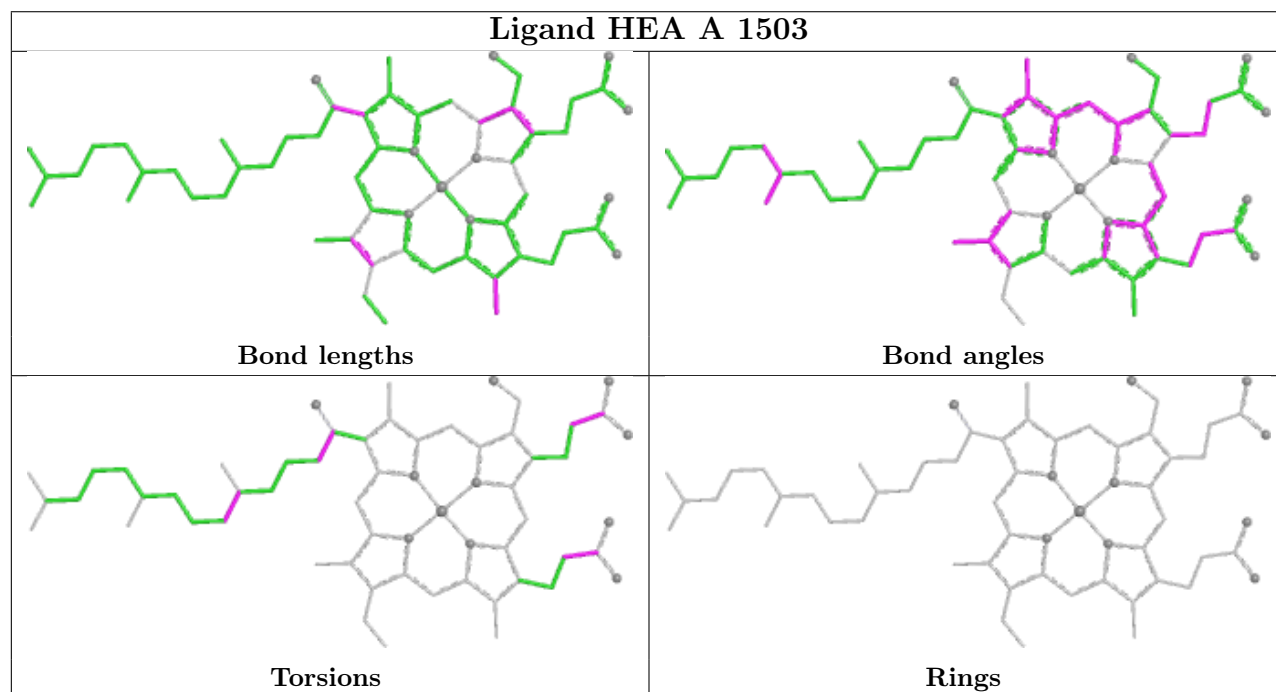
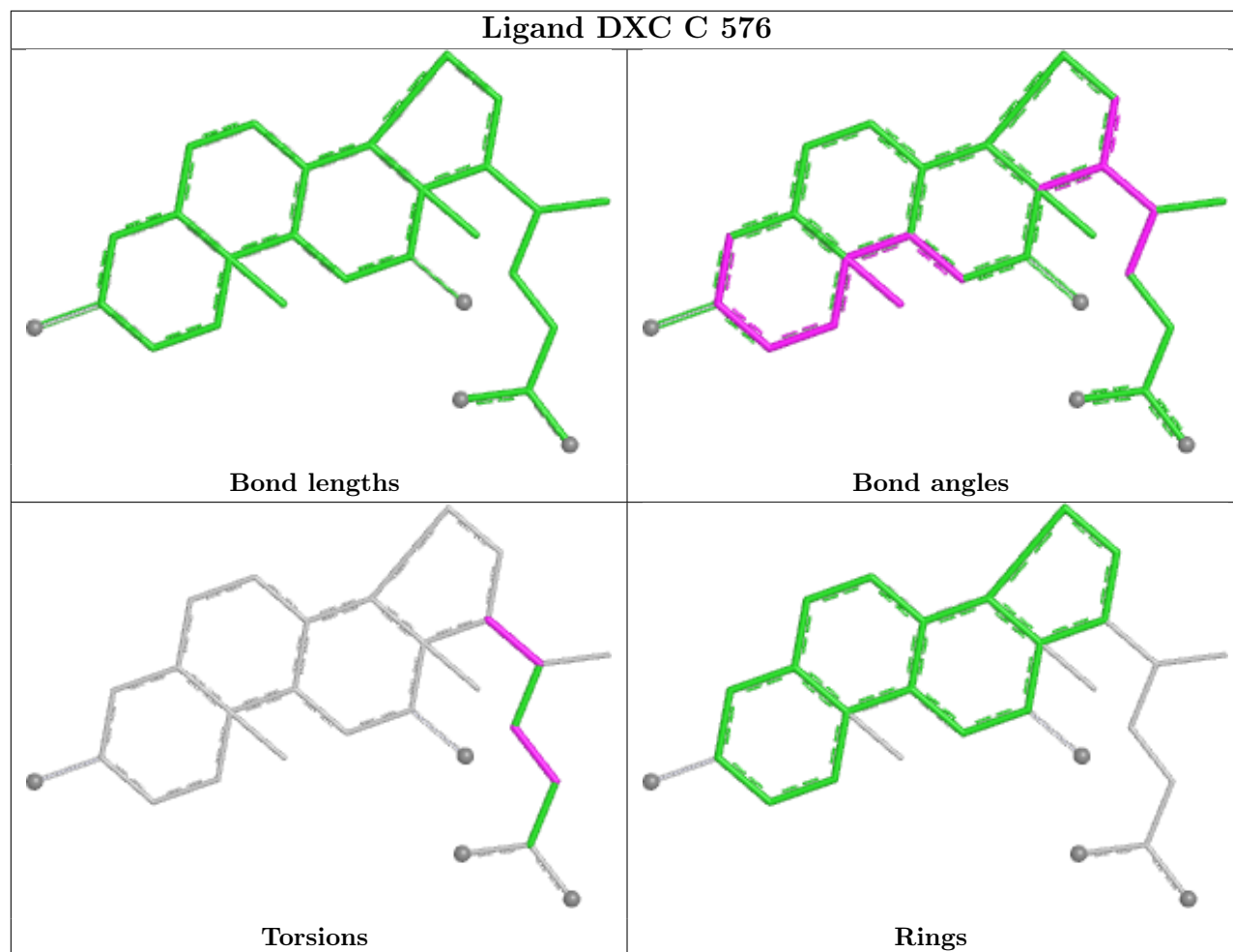
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	567	DMU	1	0
3	A	1005	DMU	1	0
10	A	1506	TRD	3	0
10	C	577	TRD	1	0
10	C	584	TRD	12	0
9	A	1503	HEA	1	0
3	A	1002	DMU	3	0
10	A	1504	TRD	4	0
3	A	567	DMU	3	0
9	C	575	HEA	4	0
10	D	7	TRD	2	0
10	B	1023	TRD	1	0
3	A	1004	DMU	3	0
9	C	574	HEA	4	0
12	B	1	HTO	1	0
9	A	1502	HEA	4	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.

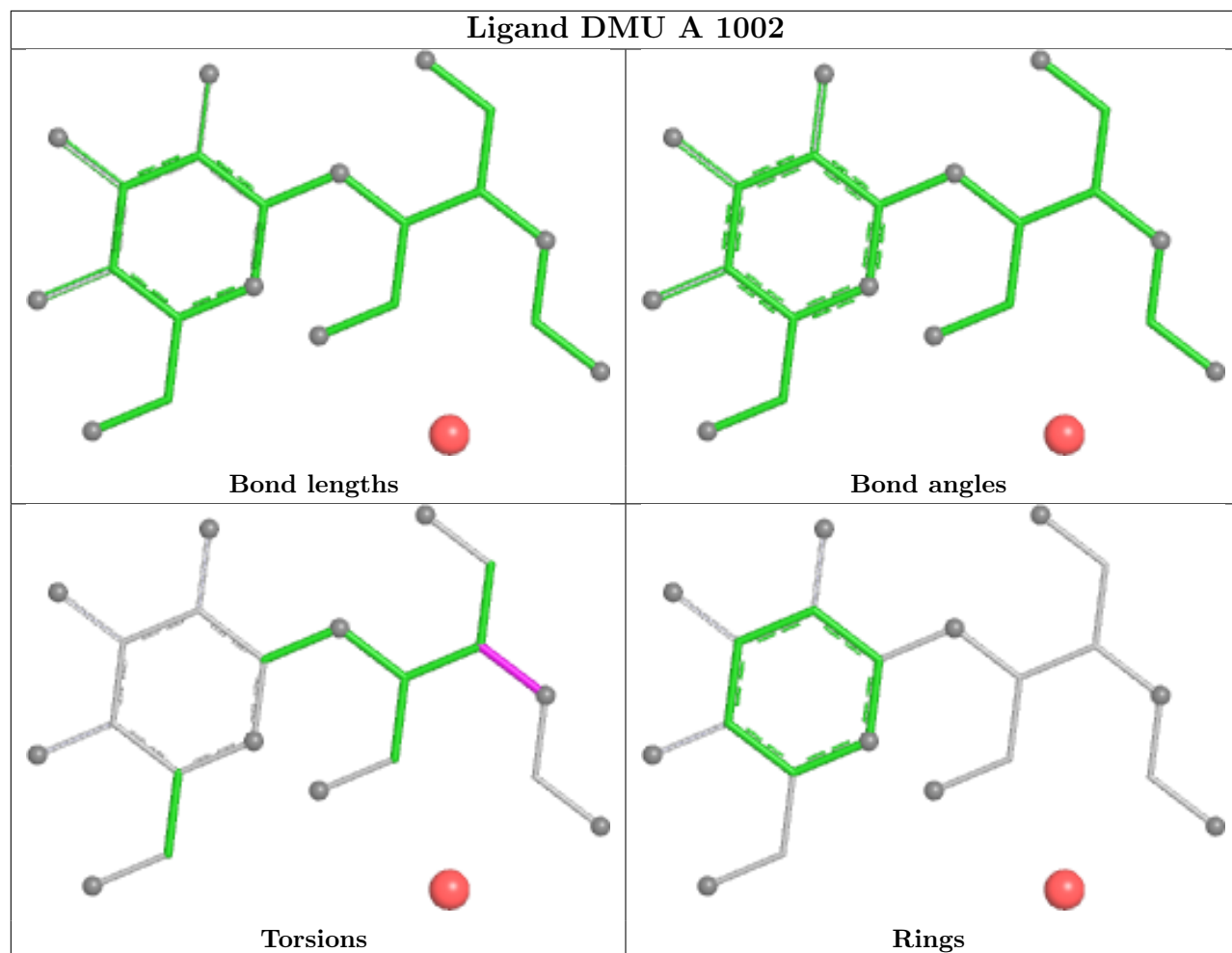


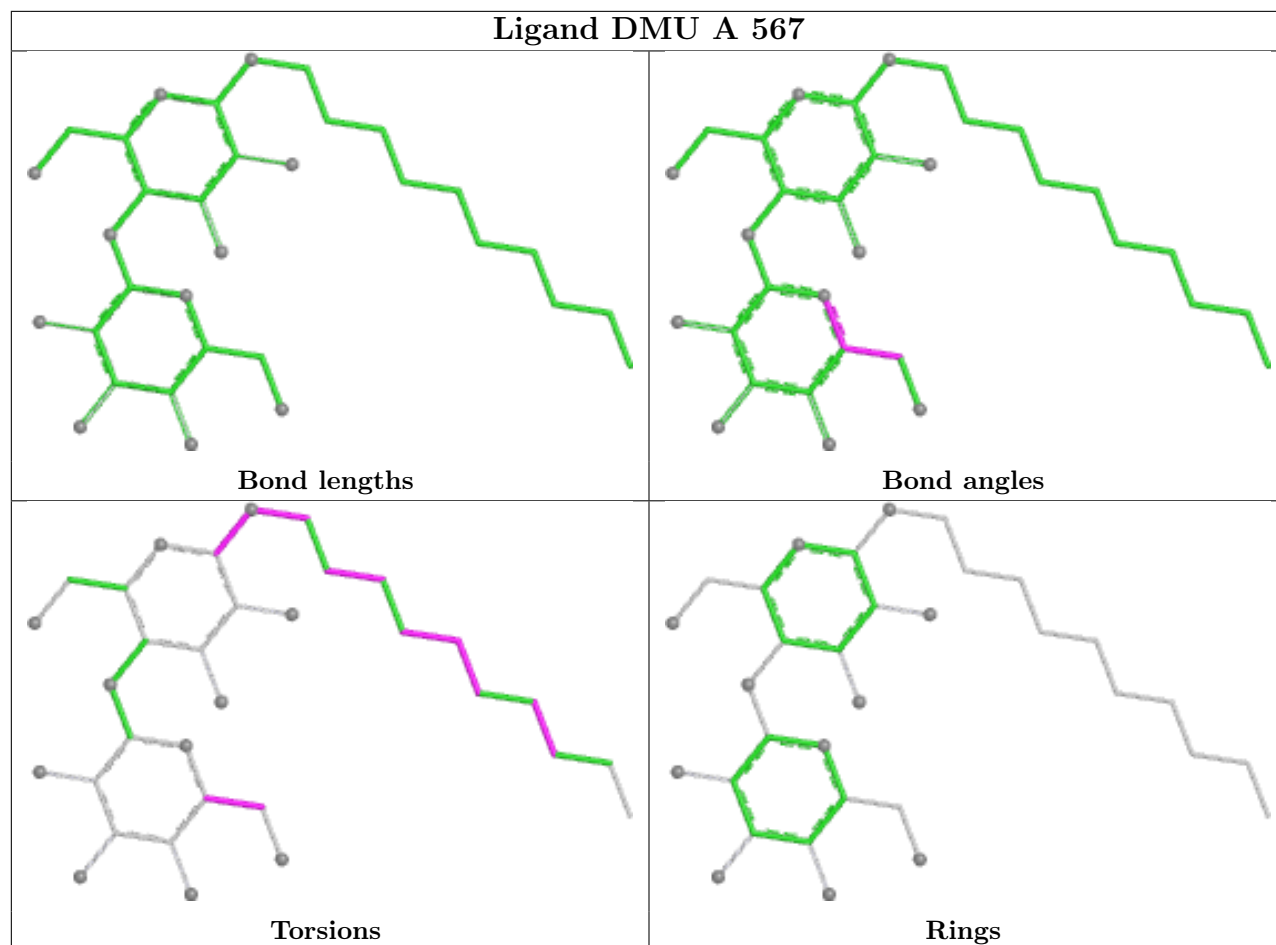


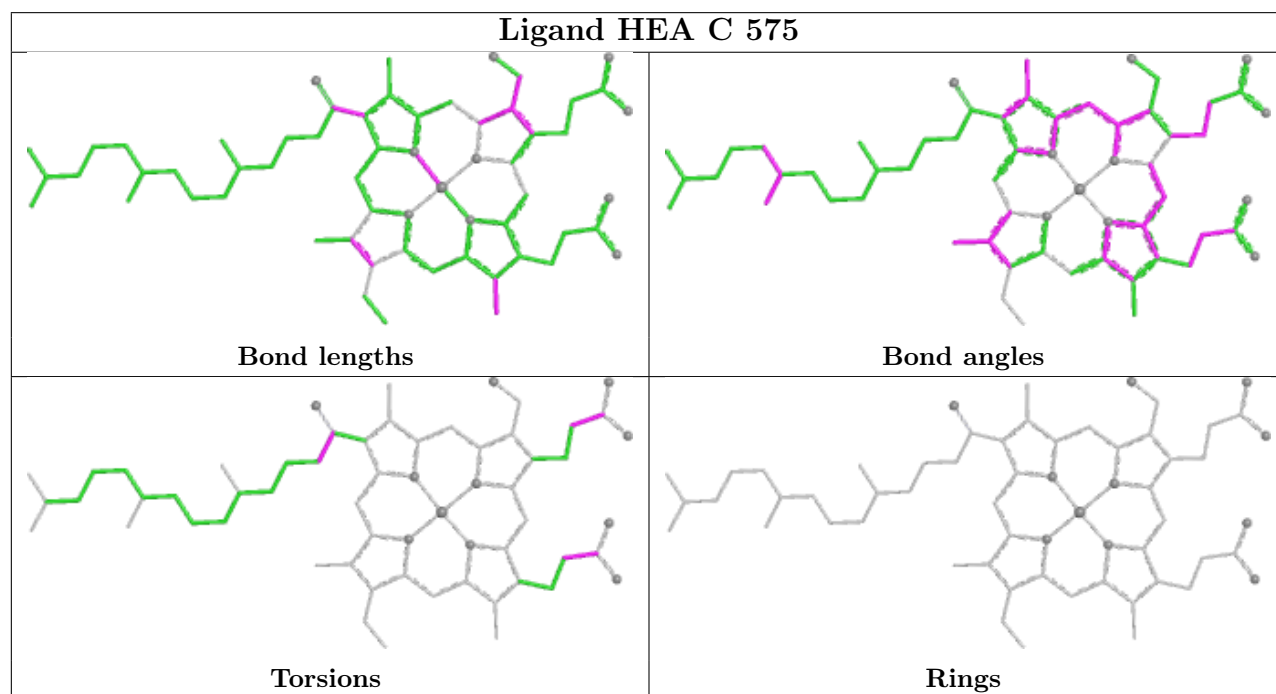
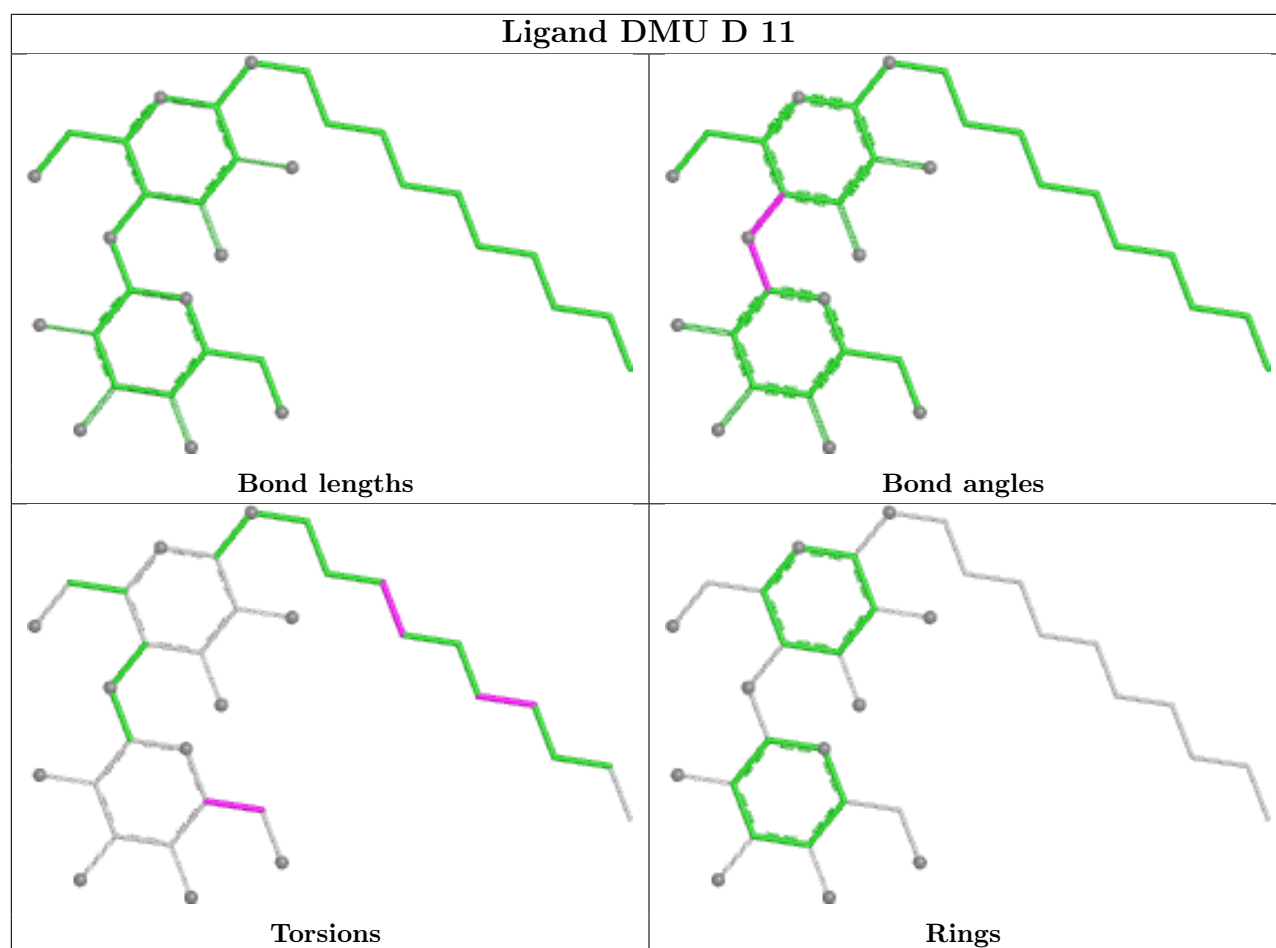


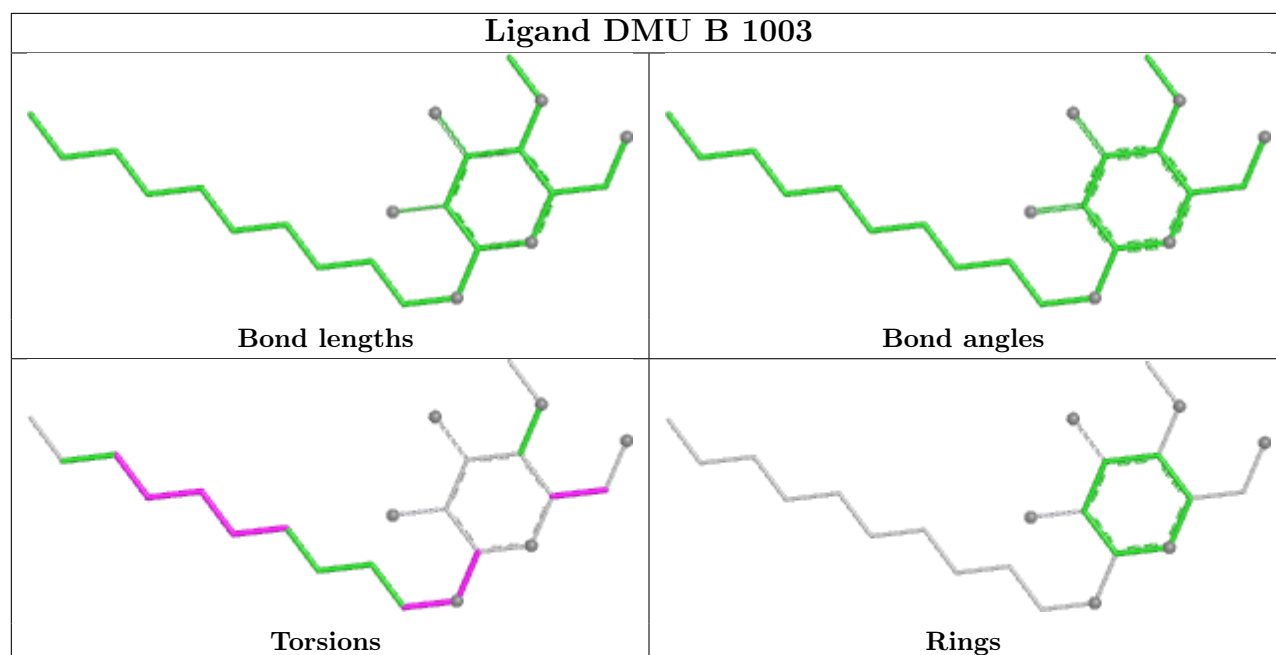
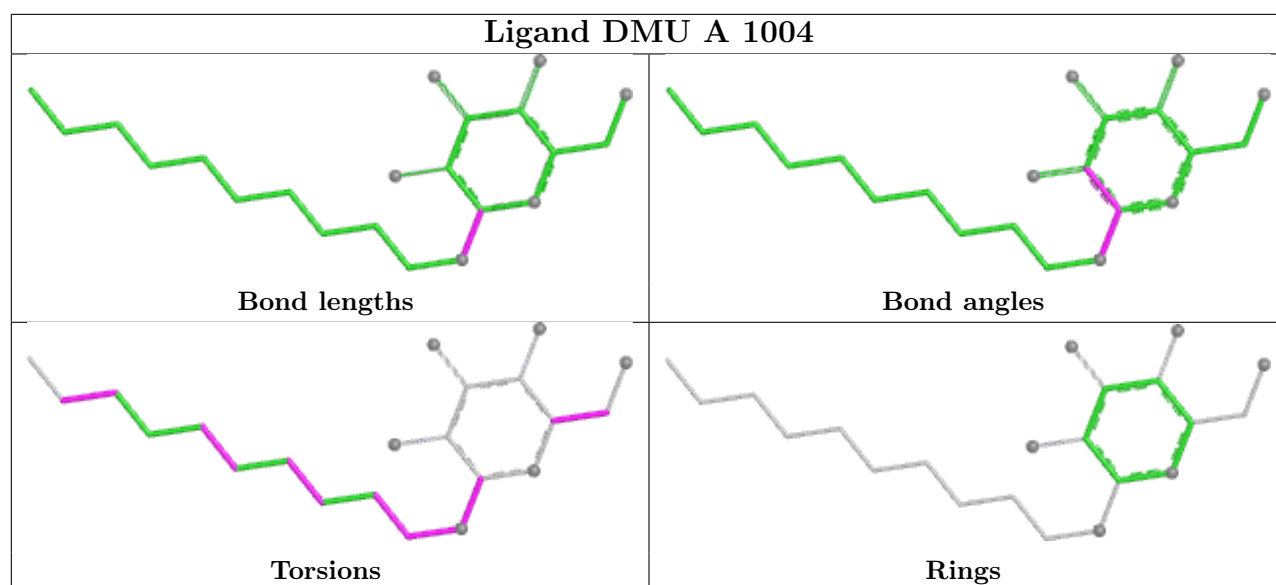


## Ligand DMU A 1002

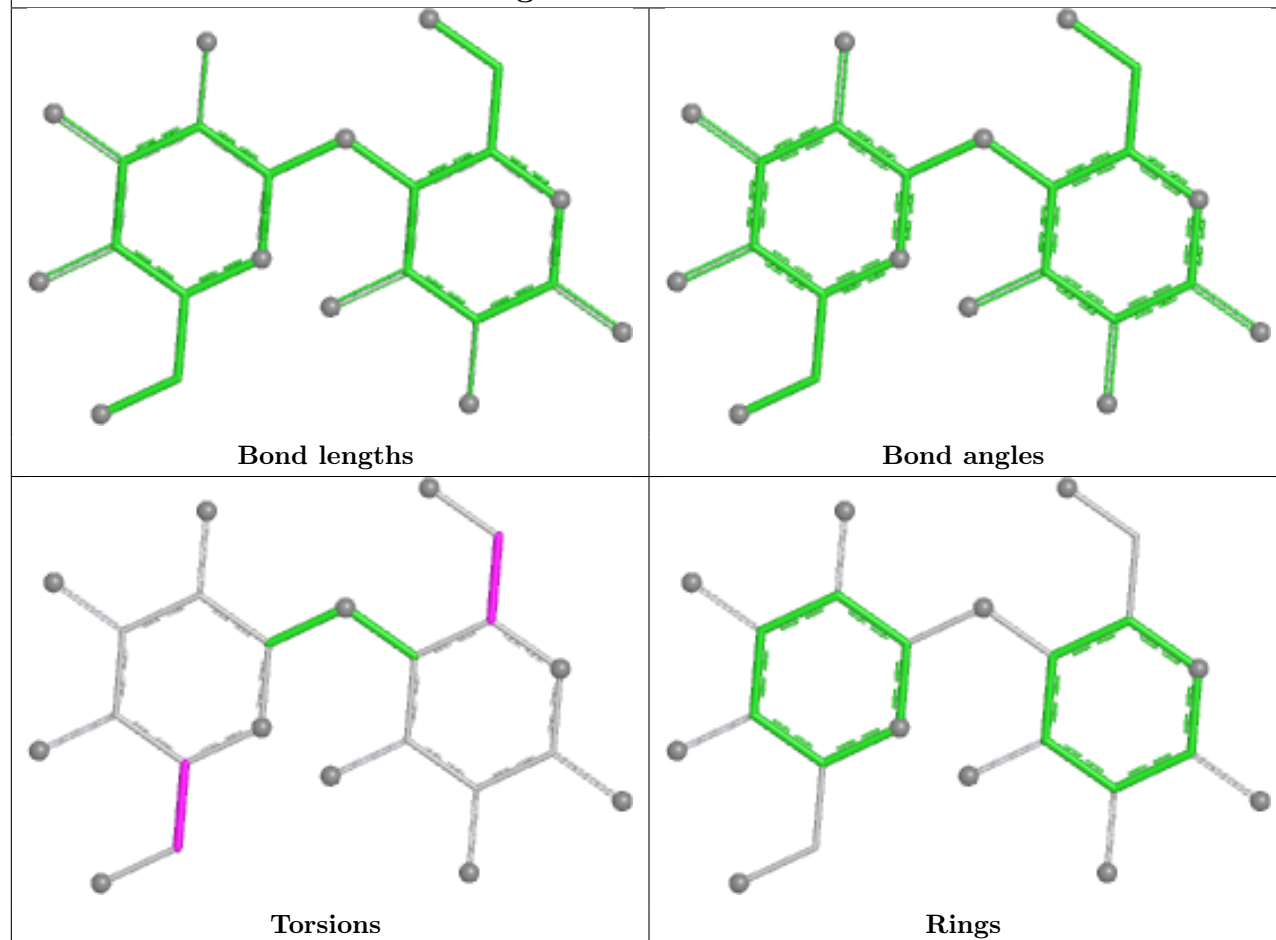




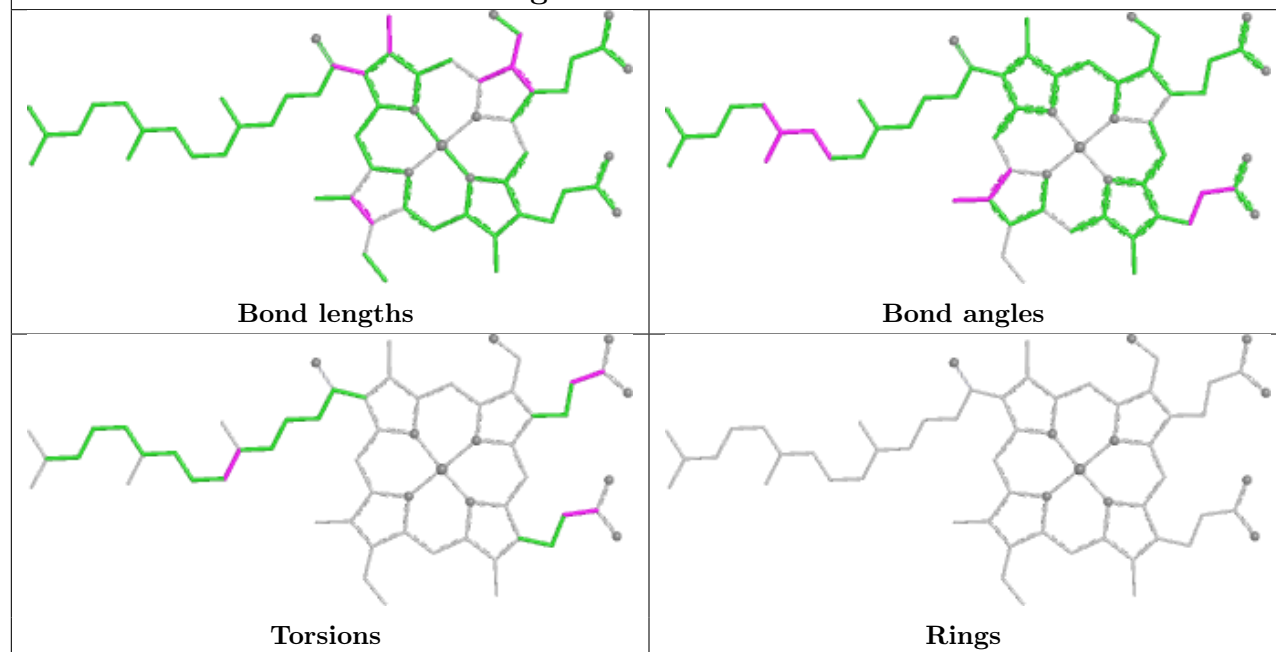


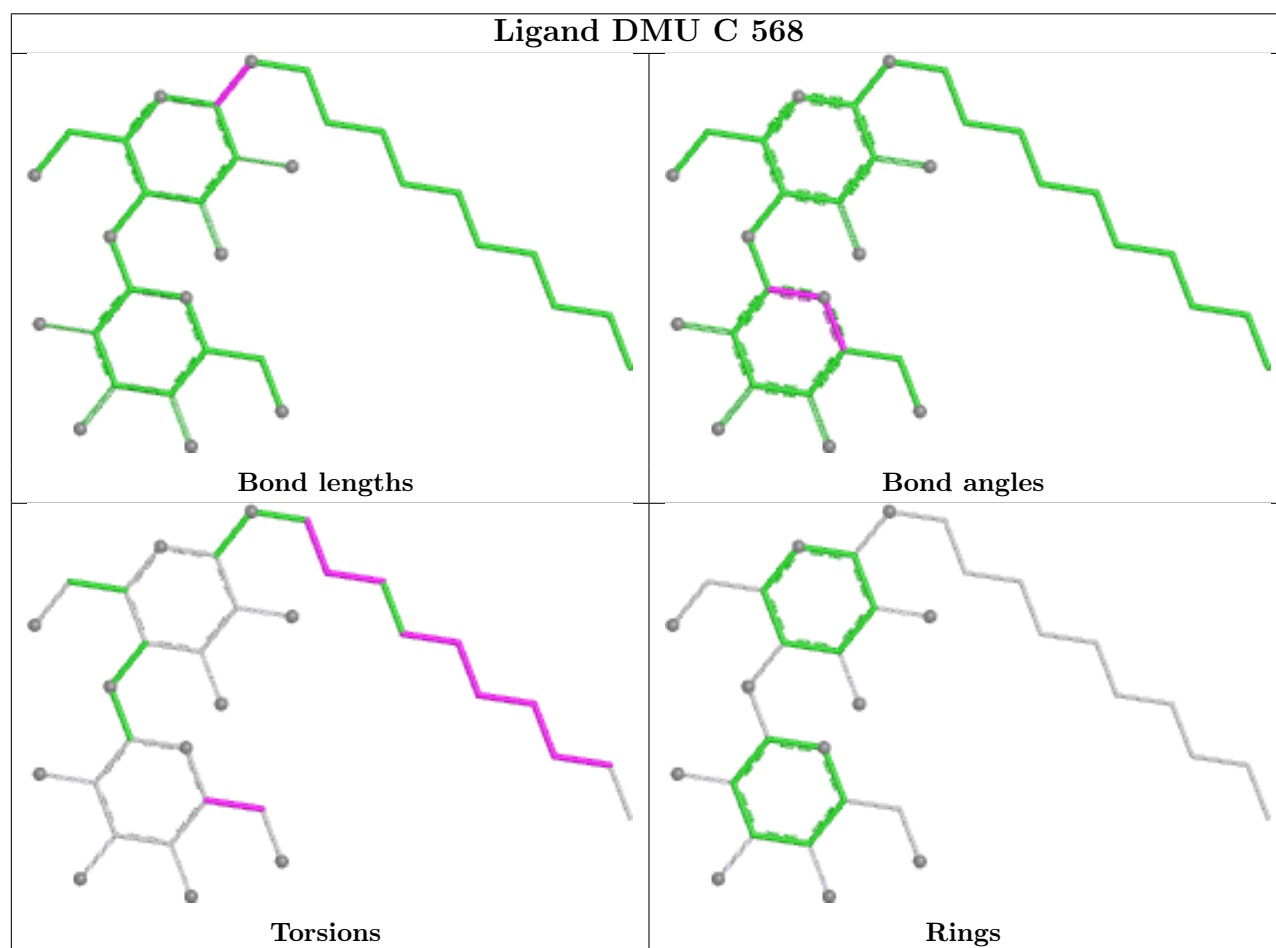
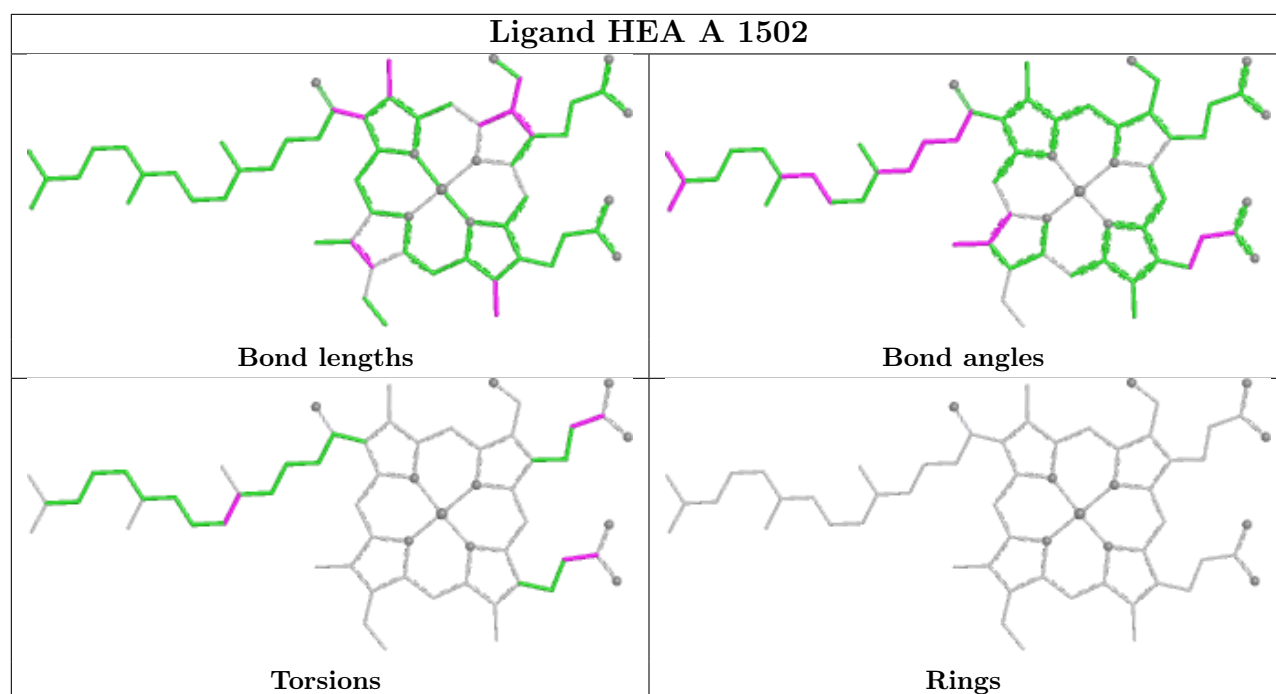


## Ligand DMU B 1011



## Ligand HEA C 574





## 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(Å²)	Q<0.9
1	A	539/566 (95%)	0.20	18 (3%)	49	55	22, 37, 58, 76	7 (1%)
1	C	536/566 (94%)	0.09	12 (2%)	62	67	20, 33, 48, 67	7 (1%)
2	B	259/262 (98%)	0.24	14 (5%)	32	38	23, 37, 52, 65	5 (1%)
2	D	258/262 (98%)	0.10	4 (1%)	70	73	20, 35, 45, 57	4 (1%)
All	All	1592/1656 (96%)	0.15	48 (3%)	52	58	20, 35, 51, 76	23 (1%)

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	TRP	4.7
1	A	81	TRP	4.6
2	D	56	TRP	4.1
2	B	99	PRO	3.8
1	A	268	GLY	3.8

### 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
10	TRD	A	1015	11/13	0.70	0.39	63,65,70,70	11
10	TRD	A	1013	7/13	0.71	0.30	53,54,55,55	0
3	DMU	B	1003	23/33	0.71	0.42	49,54,56,56	23
3	DMU	B	1011	23/33	0.72	0.36	57,58,58,58	23
3	DMU	C	567	33/33	0.73	0.22	77,81,82,83	0
10	TRD	A	1505	11/13	0.73	0.39	64,65,66,66	11
10	TRD	C	581	11/13	0.73	0.42	74,75,77,77	11
3	DMU	A	1002	22/33	0.74	0.45	66,66,67,67	22
10	TRD	C	582	7/13	0.74	0.35	67,67,67,67	7
8	PO4	C	573	5/5	0.77	0.23	53,53,54,55	5
10	TRD	C	579	7/13	0.78	0.31	68,68,69,69	0
10	TRD	C	580	9/13	0.80	0.36	62,64,64,64	9
10	TRD	C	578	11/13	0.80	0.22	61,62,63,63	0
3	DMU	D	11	33/33	0.80	0.23	70,73,74,75	33
10	TRD	C	577	13/13	0.81	0.18	45,50,53,54	0
8	PO4	A	1001	5/5	0.81	0.23	69,69,70,70	5
10	TRD	D	23	7/13	0.82	0.29	61,61,62,62	7
10	TRD	B	1031	9/13	0.83	0.23	53,55,58,58	0
10	TRD	A	1009	7/13	0.83	0.23	60,60,62,62	0
10	TRD	B	1012	9/13	0.84	0.26	74,75,77,77	0
3	DMU	A	1004	22/33	0.84	0.20	44,61,65,66	22
10	TRD	C	583	7/13	0.84	0.26	57,57,59,59	0
3	DMU	A	1005	33/33	0.84	0.17	50,57,61,61	33
3	DMU	C	568	33/33	0.85	0.15	65,68,69,70	0
10	TRD	C	584	7/13	0.85	0.21	46,50,54,55	0
10	TRD	B	1023	9/13	0.85	0.18	58,59,60,61	0
10	TRD	A	1504	13/13	0.86	0.23	56,58,61,62	0
10	TRD	D	12	11/13	0.86	0.29	58,58,58,59	11
10	TRD	A	1010	11/13	0.86	0.31	58,59,59,60	11
3	DMU	A	567	33/33	0.87	0.15	48,63,67,68	0
10	TRD	A	1014	7/13	0.89	0.39	73,73,74,74	7
10	TRD	D	7	13/13	0.89	0.15	41,43,50,50	0
10	TRD	D	288	9/13	0.89	0.19	52,53,56,56	0
10	TRD	A	1506	13/13	0.89	0.18	45,46,51,53	0
7	OH	A	1501	1/1	0.89	0.16	35,35,35,35	0
13	DXC	C	576	28/28	0.91	0.12	46,50,52,52	0
12	HTO	B	1	10/10	0.93	0.15	51,54,55,56	0
7	OH	C	572	1/1	0.95	0.08	28,28,28,28	0
9	HEA	A	1503	60/60	0.97	0.08	26,29,41,42	0
11	CD	B	1009	1/1	0.97	0.04	45,45,45,45	1
9	HEA	C	574	60/60	0.98	0.07	23,26,32,33	0
9	HEA	A	1502	60/60	0.98	0.06	23,26,33,34	0
6	CA	C	571	1/1	0.98	0.03	32,32,32,32	0

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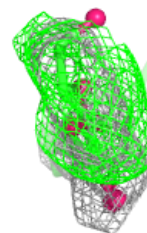
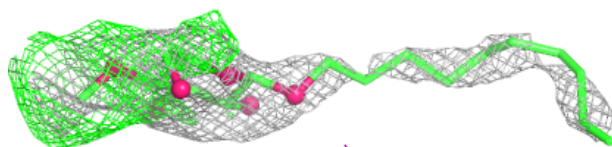
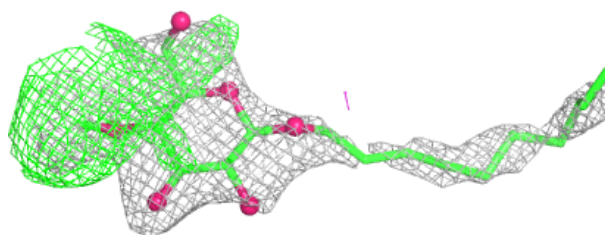
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	HEA	C	575	60/60	0.99	0.05	21,24,32,33	0
11	CD	B	1010	1/1	0.99	0.09	53,53,53,53	1
11	CD	D	8	1/1	0.99	0.02	36,36,36,36	0
11	CD	D	9	1/1	0.99	0.02	46,46,46,46	0
4	CU	A	1023	1/1	0.99	0.02	32,32,32,32	0
11	CD	B	1008	1/1	0.99	0.02	35,35,35,35	0
6	CA	A	1007	1/1	1.00	0.02	27,27,27,27	0
4	CU	B	1022	1/1	1.00	0.01	28,28,28,28	0
4	CU	B	1004	1/1	1.00	0.01	29,29,29,29	0
4	CU	C	569	1/1	1.00	0.02	26,26,26,26	0
4	CU	D	3	1/1	1.00	0.02	28,28,28,28	0
4	CU	D	4	1/1	1.00	0.01	28,28,28,28	0
5	MG	A	1006	1/1	1.00	0.05	16,16,16,16	0
5	MG	C	570	1/1	1.00	0.05	15,15,15,15	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.

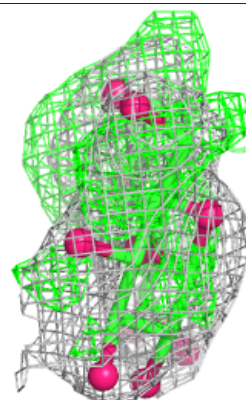
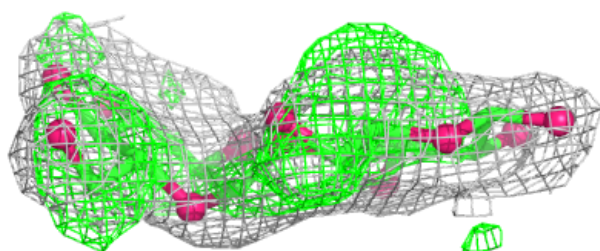
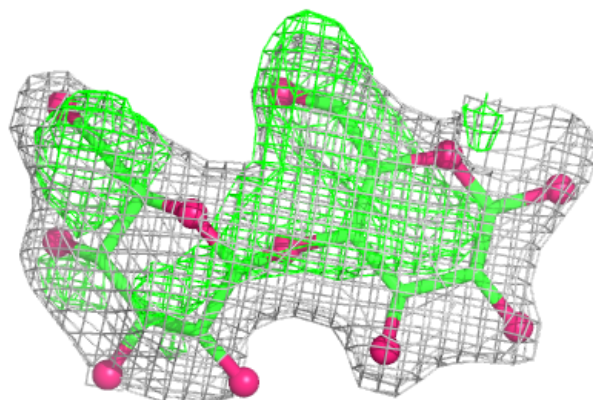
**Electron density around DMU B 1003:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

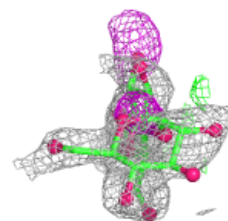
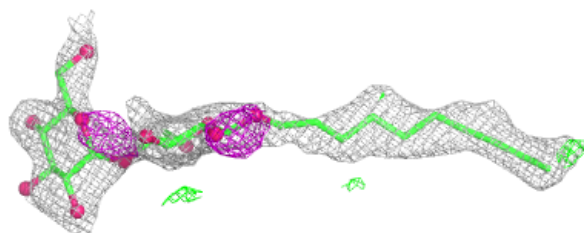
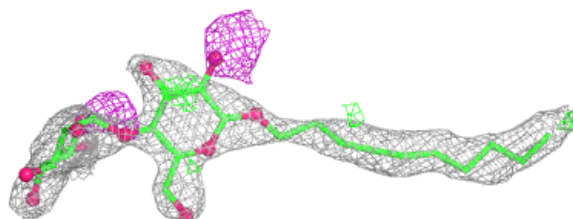


**Electron density around DMU B 1011:**

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

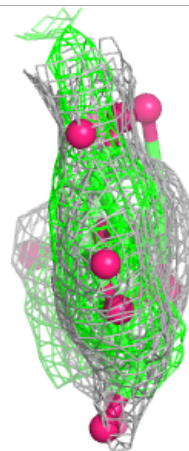
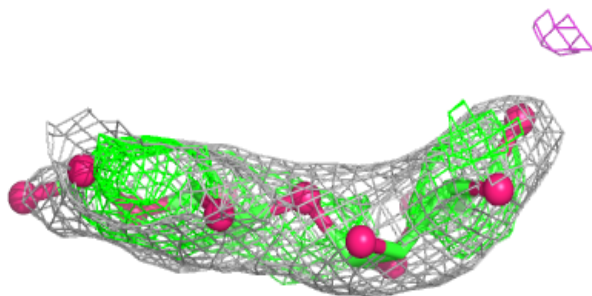
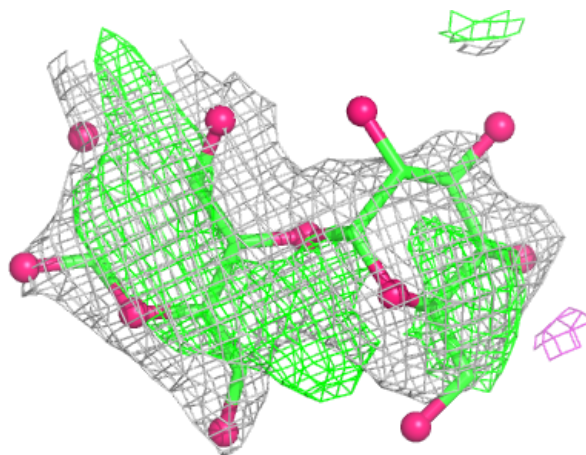
**Electron density around DMU C 567:**

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



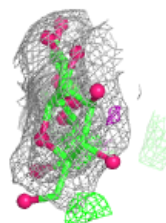
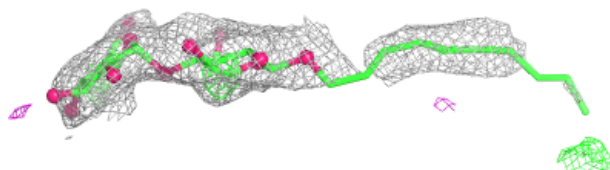
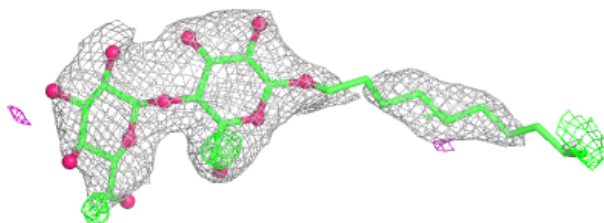
**Electron density around DMU A 1002:**

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

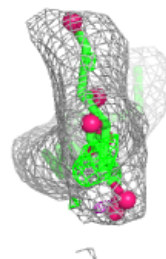
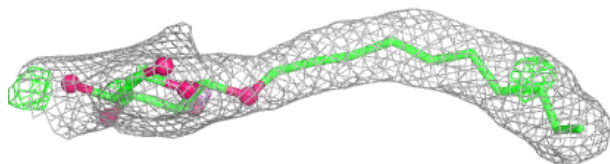
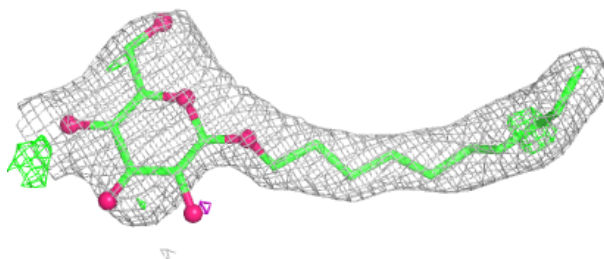


**Electron density around DMU D 11:**

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

**Electron density around DMU A 1004:**

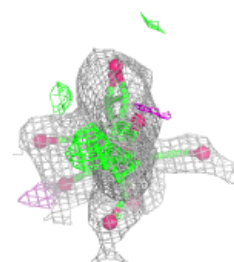
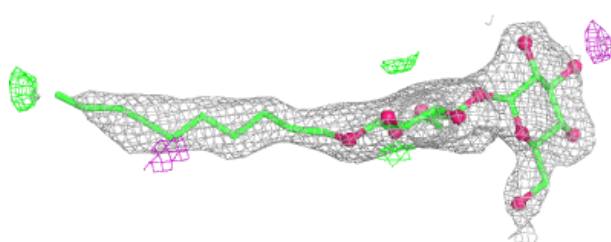
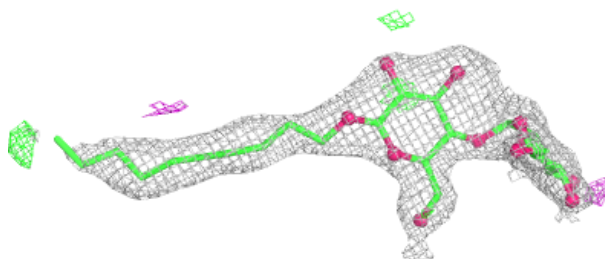
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



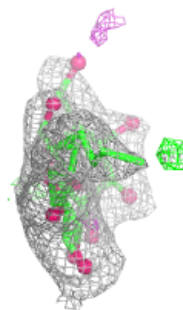
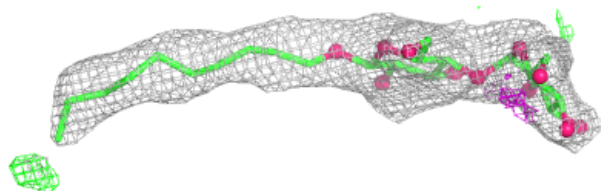
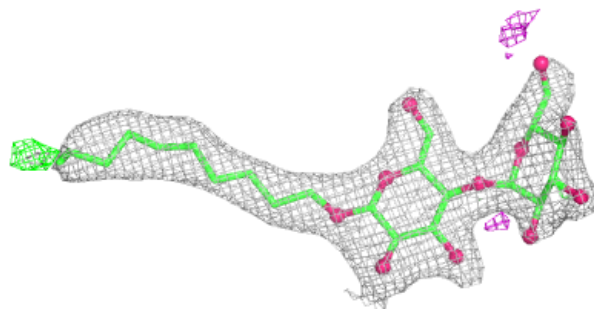


**Electron density around DMU A 1005:**

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

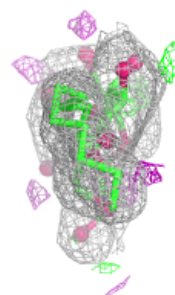
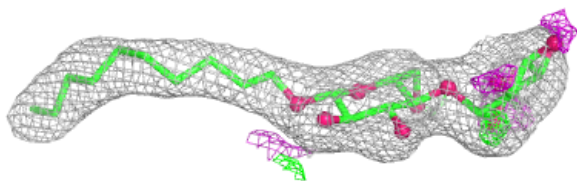
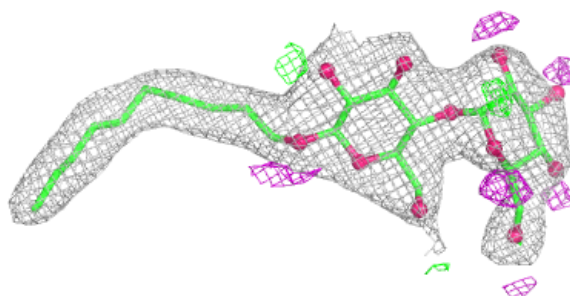
**Electron density around DMU C 568:**

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

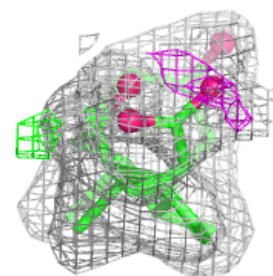
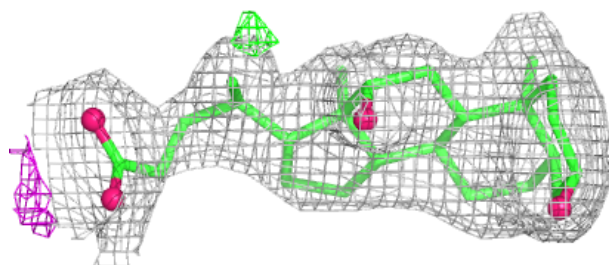
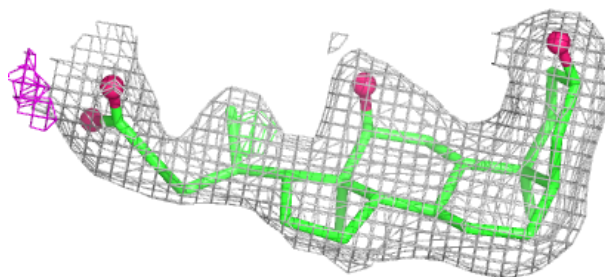


**Electron density around DMU A 567:**

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

**Electron density around DXC C 576:**

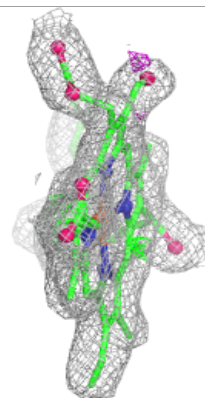
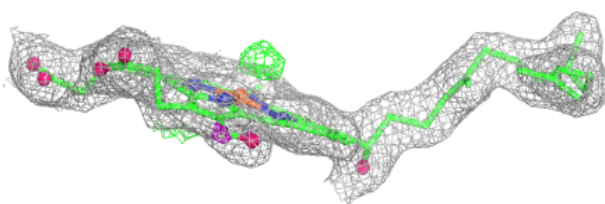
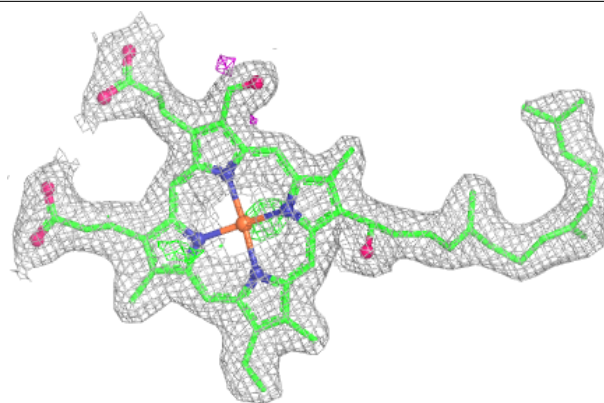
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



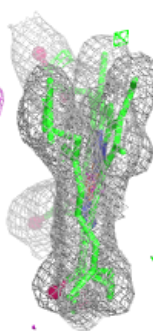
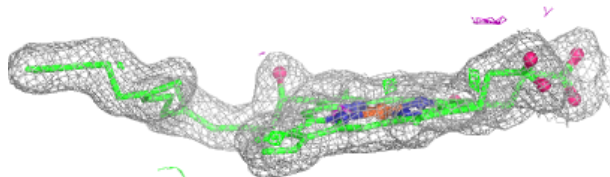
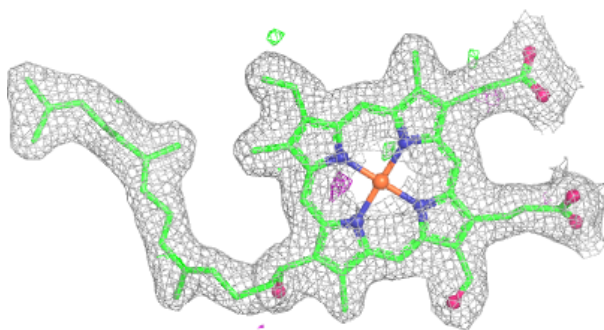


**Electron density around HEA A 1503:**

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

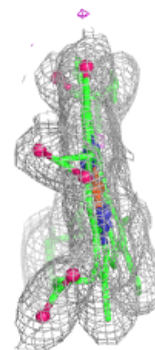
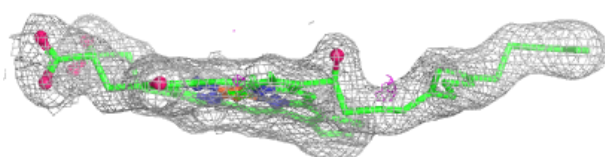
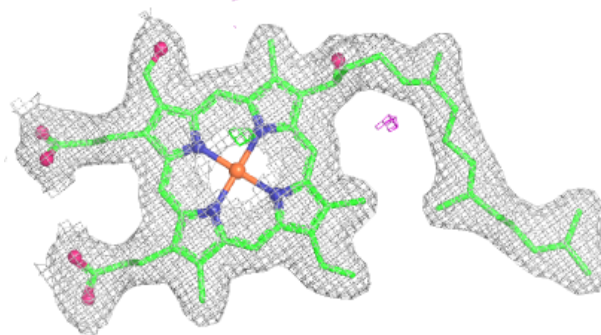
**Electron density around HEA C 574:**

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

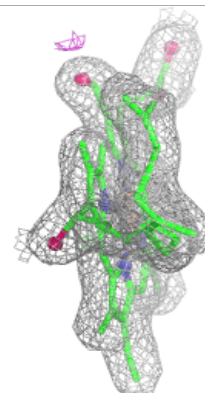
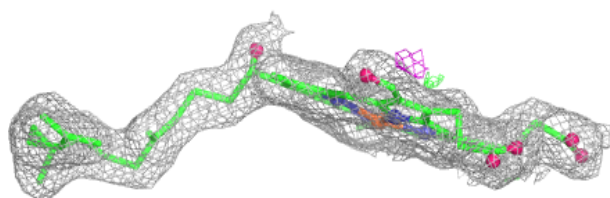
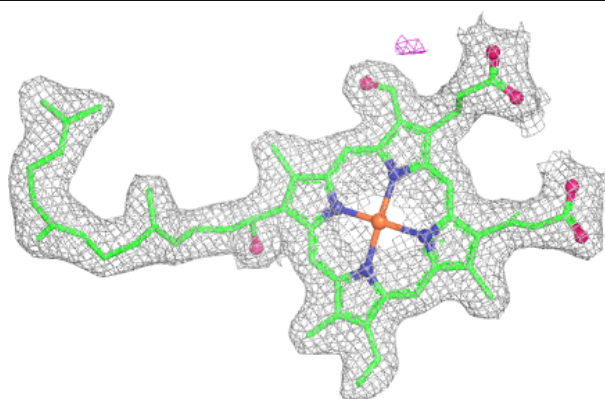


**Electron density around HEA A 1502:**

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

**Electron density around HEA C 575:**

$2mF_o-DF_c$  (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.