



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:46 pm BST

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 Full wwPDB X-ray Structure Validation 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

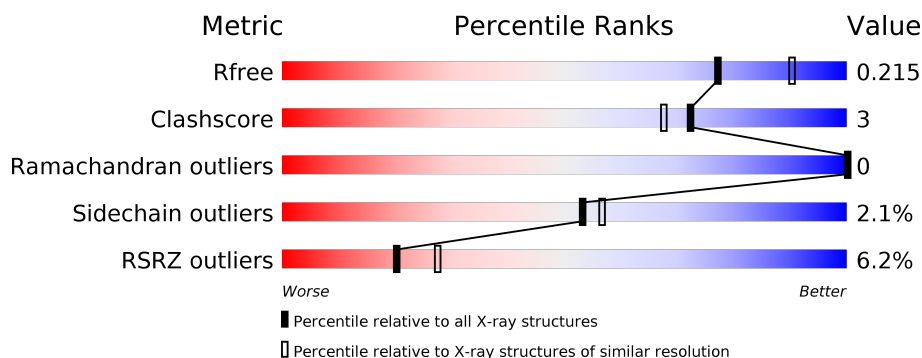
# 1 Overall quality at a glance

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 on 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	<div> <div>7%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
1	C	566	<div> <div>8%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
2	B	262	<div> <div>3%</div> <div>95%</div> <div>•</div> </div>
2	D	262	<div> <div>2%</div> <div>94%</div> <div>5%</div> <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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	TRD	C	584	-	-	X	-
12	HTO	B	1	X	-	-	-
9	HEA	A	1502	X	-	-	-
9	HEA	A	1503	X	-	-	-
9	HEA	C	574	X	-	-	-
9	HEA	C	575	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			

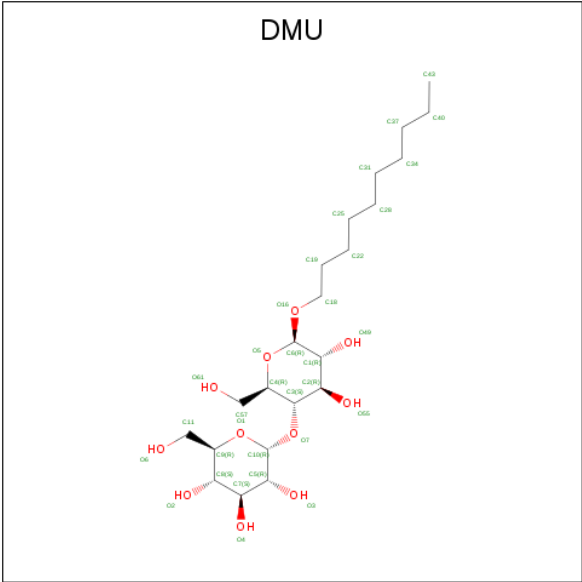
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

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	B	2	Total	Cu	0	0
			2	2		
4	A	1	Total	Cu	0	0
			1	1		
4	D	2	Total	Cu	0	0
			2	2		

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

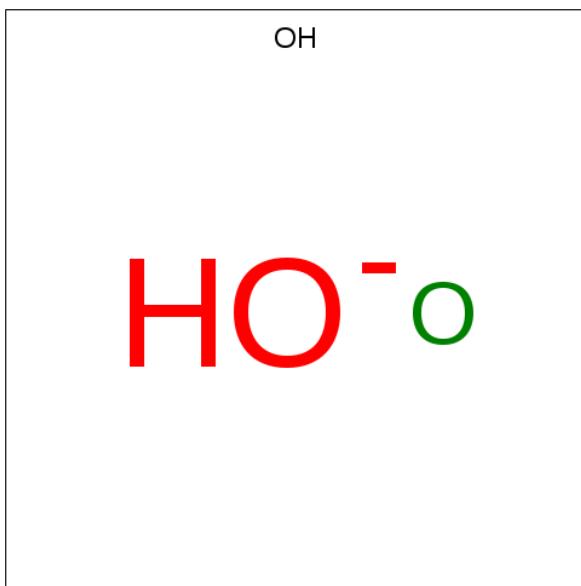
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

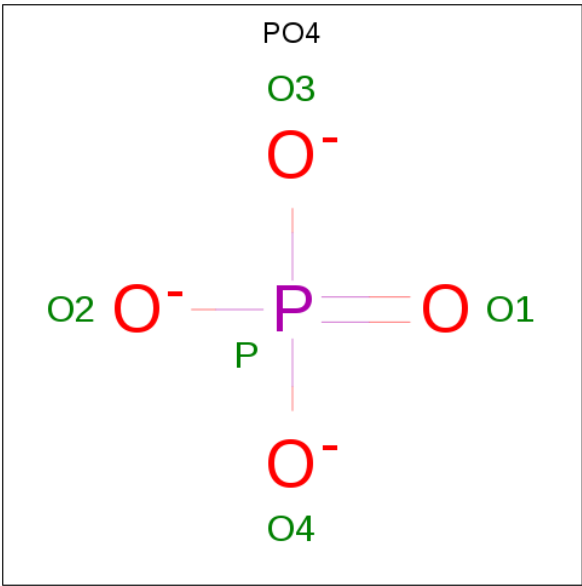
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0
6	C	1	Total Ca 1 1	0	0

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



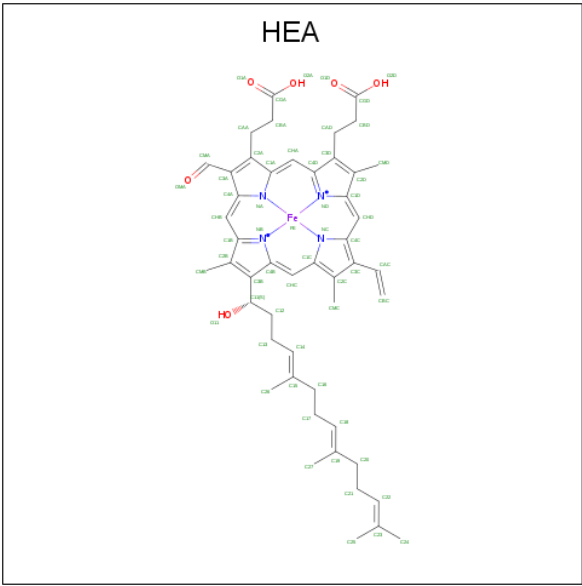
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0
7	C	1	Total O 1 1	0	0

- 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>).



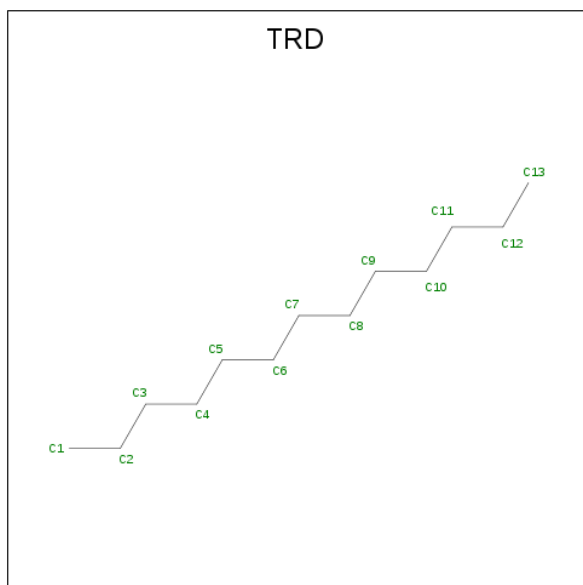
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

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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:  $C_{13}H_{28}$ ).



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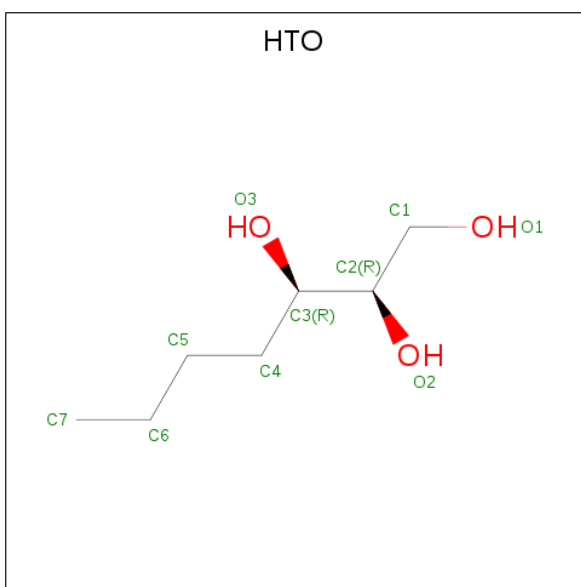
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C 9 9	0	0
10	B	1	Total C 9 9	0	0
10	B	1	Total C 9 9	0	0
10	C	1	Total C 13 13	0	0
10	C	1	Total C 11 11	0	0
10	C	1	Total C 7 7	0	0
10	C	1	Total C 9 9	0	0
10	C	1	Total C 11 11	0	0
10	C	1	Total C 7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

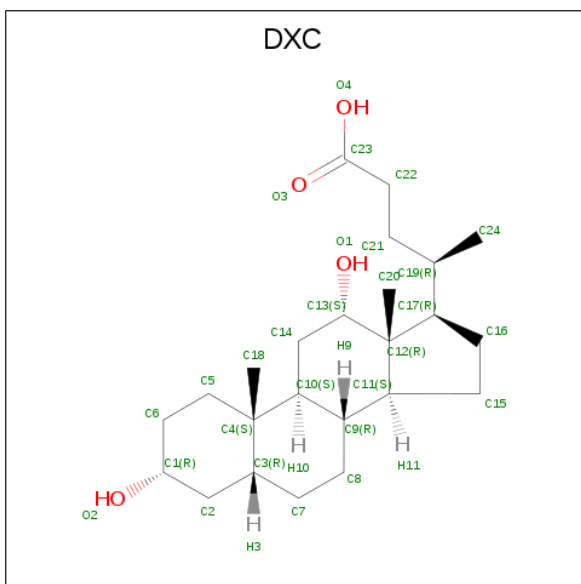
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	3	Total Cd 3 3	0	0
11	D	2	Total Cd 2 2	0	0

- 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		

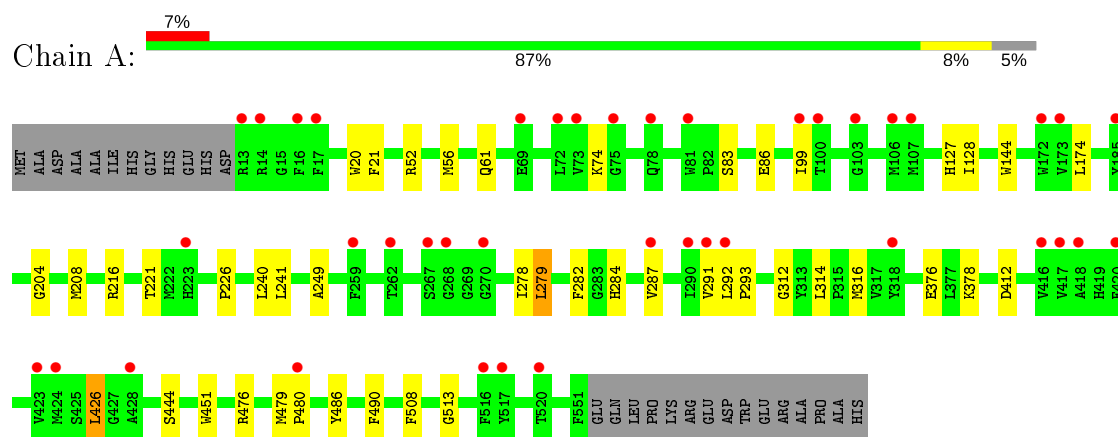
- Molecule 14 is water.

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

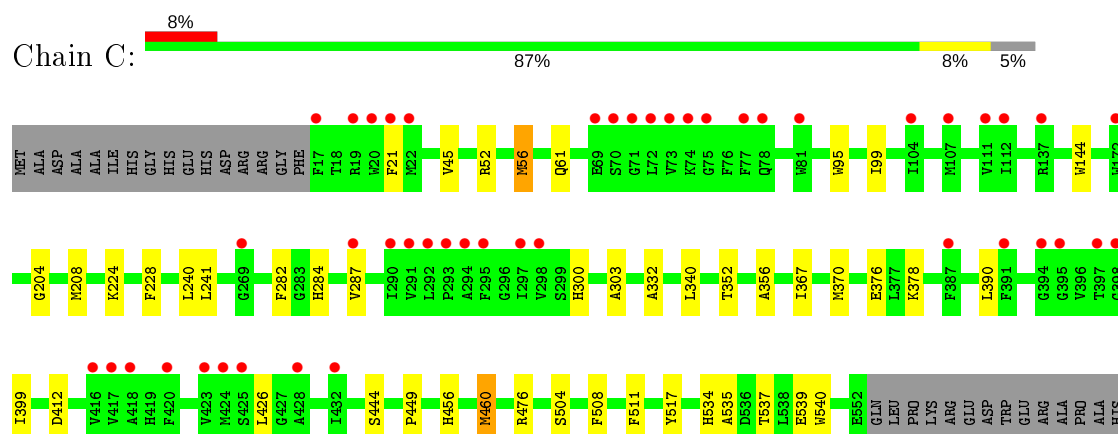
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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.

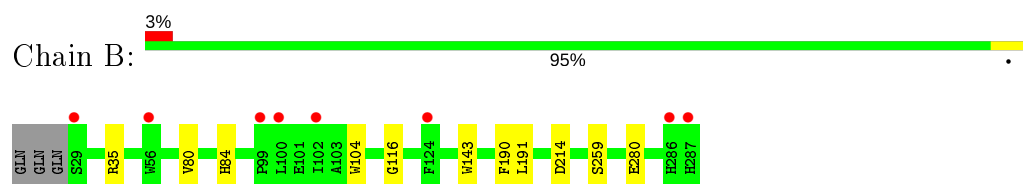
#### • Molecule 1: Cytochrome c oxidase subunit 1



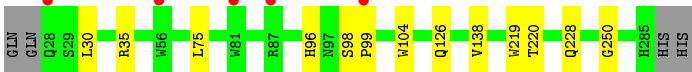
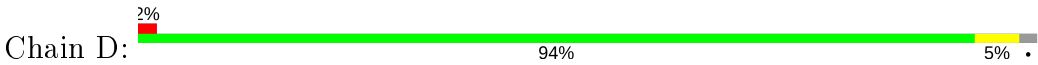
#### • Molecule 1: Cytochrome c oxidase subunit 1



#### • 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, $\alpha$ , $\beta$ , $\gamma$	123.24Å 132.05Å 167.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.15 39.90 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.9 (40.00-2.15) 96.9 (39.90-2.15)	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> )	0.35 , 69.5	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	0.95	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: MG, OH, HTO, PO4, TRD, CD, HEA, DXC, CA, CU, DMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.50	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.

All (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:HBC1	9:C:574:HEA:HMC1	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
1:A:56:MET:HE1	3:A:1005:DMU:H7	1.65	0.79
1:C:390:LEU:HD13	1:C:426:LEU:HD12	1.65	0.78
1:C:540:TRP:HE1	10:C:584:TRD:H61	1.49	0.76
1:A:20:TRP:HH2	3:A:1004:DMU:H1	1.52	0.74
1:C:460:MET:HA	1:C:460:MET:CE	2.20	0.72
1:C:228:PHE:H	1:C:300:HIS:HE2	1.38	0.70
9:A:1502:HEA:HMC1	9:A:1502:HEA:HBC1	1.72	0.69
3:A:567:DMU:H35	3:A:567:DMU:H29	1.75	0.69
3:A:1002:DMU:C2	3:A:1002:DMU:O49	2.41	0.69
1:C:303:ALA:CB	10:C:584:TRD:H21	2.18	0.68
1:C:537:THR:OG1	10:C:584:TRD:H51	1.94	0.68
1:C:534:HIS:ND1	14:C:747:HOH:O	2.27	0.67
1:C:476:ARG:HH21	10:D:7:TRD:H12	1.61	0.66
1:A:451:TRP:HZ2	10:A:1504:TRD:H52	1.60	0.66
3:A:1002:DMU:O49	3:A:1002:DMU:C6	2.43	0.66
1:A:513:GLY:HA3	10:A:1504:TRD:H101	1.80	0.63
1:C:303:ALA:HB3	10:C:584:TRD:C2	2.22	0.63
1:C:300:HIS:ND1	10:C:584:TRD:C7	2.62	0.62
1:A:451:TRP:HE1	10:A:1504:TRD:H32	1.66	0.60
1:A:20:TRP:CH2	3:A:1004:DMU:H1	2.36	0.58
1:C:460:MET:HA	1:C:460:MET:HE3	1.84	0.58
10:C:584:TRD:H11	14:C:686:HOH:O	2.02	0.58
1:C:460:MET:HE1	1:C:504:SER:HB3	1.86	0.57
1:A:204:GLY:O	1:A:208:MET:HG2	2.04	0.57
1:C:456:HIS:CE1	1:C:511:PHE:HB2	2.40	0.56
1:A:21:PHE:HB3	1:A:144:TRP:HZ2	1.70	0.56
1:C:21:PHE:HB3	1:C:144:TRP:HZ2	1.70	0.56
1:C:204:GLY:O	1:C:208:MET:HG2	2.06	0.56
1:C:332:ALA:HB1	1:C:340:LEU:HD11	1.88	0.55
1:C:287:VAL:HB	9:C:575:HEA:CAC	2.36	0.55
1:A:476:ARG:HH21	10:A:1506:TRD:C2	2.20	0.54
1:C:540:TRP:HE1	10:C:584:TRD:C6	2.18	0.53
1:A:287:VAL:HB	9:A:1503:HEA:CAC	2.38	0.53
1:C:460:MET:HA	1:C:460:MET:HE2	1.90	0.52
9:C:574:HEA:CBC	9:C:574:HEA:HMC1	2.35	0.52
1:C:535:ALA:HA	10:C:584:TRD:H31	1.91	0.52
1:C:367:ILE:HA	1:C:370:MET:HE2	1.92	0.51
1:A:127:HIS:HB3	1:A:226:PRO:HG2	1.92	0.50
1:C:376:GLU:OE2	1:C:378:LYS:HE2	2.11	0.50
1:C:56:MET:HE1	3:C:567:DMU:H7	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ILE:HG13	9:A:1502:HEA:HBA1	1.94	0.50
1:C:539:GLU:OE2	10:C:584:TRD:C7	2.60	0.50
1:C:444:SER:HA	10:C:577:TRD:H42	1.94	0.49
9:C:575:HEA:HMC1	9:C:575:HEA:HBC1	1.93	0.49
1:C:287:VAL:HB	9:C:575:HEA:C3C	2.44	0.48
1:A:249:ALA:HB2	1:A:278:ILE:HG22	1.95	0.47
1:C:300:HIS:HB3	10:C:584:TRD:H62	1.96	0.47
1:A:86:GLU:HG3	2:D:96:HIS:CG	2.49	0.47
1:A:476:ARG:HH21	10:A:1506:TRD:H21	1.79	0.46
1:A:284:HIS:CD2	1:A:284:HIS:C	2.87	0.46
1:C:95:TRP:CE2	1:C:99:ILE:HD13	2.50	0.46
1:C:284:HIS:CD2	1:C:284:HIS:C	2.89	0.46
1:C:508:PHE:HB2	9:C:574:HEA:H261	1.97	0.46
1:A:486:TYR:CD2	1:A:490:PHE:HB2	2.50	0.46
1:A:83:SER:HA	3:A:567:DMU:H41	1.98	0.45
1:C:45:VAL:HG21	9:C:574:HEA:H171	1.96	0.45
9:A:1502:HEA:HMC1	9:A:1502:HEA:CBC	2.43	0.45
2:B:280:GLU:HB2	12:B:1:HTO:H73	1.98	0.45
1:A:451:TRP:CZ2	10:A:1504:TRD:H52	2.46	0.45
3:A:567:DMU:H18	2:D:75:LEU:HD13	1.97	0.45
2:D:228:GLN:NE2	14:D:387:HOH:O	2.47	0.45
1:A:279:LEU:O	1:A:279:LEU:HG	2.14	0.44
2:B:190:PHE:O	2:B:191:LEU:HB2	2.17	0.44
2:B:80:VAL:O	2:B:84:HIS:HB2	2.17	0.44
1:A:476:ARG:HH21	10:A:1506:TRD:H22	1.81	0.44
1:C:370:MET:HB2	1:C:370:MET:HE2	1.83	0.44
1:A:21:PHE:HB3	1:A:144:TRP:CZ2	2.50	0.44
1:A:376:GLU:HG2	1:A:378:LYS:HG2	2.00	0.44
1:A:444:SER:HA	3:A:1004:DMU:H5	1.99	0.44
1:A:284:HIS:O	1:A:284:HIS:CD2	2.71	0.43
1:A:128:ILE:HB	1:A:216:ARG:HG2	2.00	0.43
1:A:508:PHE:HB2	9:A:1502:HEA:H261	2.01	0.42
2:D:98:SER:HB3	2:D:99:PRO:HD3	2.01	0.42
1:C:537:THR:HG23	10:C:584:TRD:H42	2.01	0.42
2:B:116:GLY:HA3	10:B:1023:TRD:H42	2.02	0.42
2:B:143:TRP:CG	2:B:259:SER:HB2	2.55	0.41
2:D:220:THR:O	2:D:250:GLY:HA3	2.20	0.41
1:A:479:MET:HA	1:A:480:PRO:HD3	1.89	0.41
1:C:352:THR:HG22	9:C:575:HEA:HMB2	2.02	0.41
1:C:449:PRO:HG3	1:C:517:TYR:CE2	2.56	0.41
1:C:460:MET:CA	1:C:460:MET:CE	2.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:HB2	1:A:293:PRO:HD3	2.03	0.41
1:C:356:ALA:HB2	1:C:399:ILE:HD11	2.03	0.41
1:C:476:ARG:NH2	10:D:7:TRD:H12	2.33	0.41
1:A:312:GLY:O	1:A:316:MET:HG2	2.21	0.40
2:D:138:VAL:HG11	2:D:219:TRP:CD1	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	44	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	436/459 (95%)	427 (98%)	9 (2%)	53	57
2	B	218/221 (99%)	215 (99%)	3 (1%)	67	72
2	D	217/221 (98%)	213 (98%)	4 (2%)	59	63
All	All	1309/1360 (96%)	1281 (98%)	28 (2%)	53	57

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	61	GLN
1	A	74	LYS
1	A	174	LEU
1	A	221	THR
1	A	240	LEU
1	A	241	LEU
1	A	282	PHE
1	A	291	VAL
1	A	314	LEU
1	A	412	ASP
1	A	426	LEU
2	B	35	ARG
2	B	104	TRP
2	B	214	ASP
1	C	52	ARG
1	C	56	MET
1	C	61	GLN
1	C	224	LYS
1	C	240	LEU
1	C	241	LEU
1	C	282	PHE
1	C	412	ASP
1	C	460	MET
2	D	30	LEU
2	D	35	ARG
2	D	104	TRP
2	D	126	GLN

Some 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 [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 57 ligands modelled in this entry, 2 are modelled with single atom and 15 are monoatomic - 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	B	1003	-	23,23,34	0.56	0	28,28,45	0.64	0
10	TRD	C	577	-	12,12,12	0.29	0	11,11,11	0.42	0
10	TRD	C	580	-	8,8,12	0.26	0	7,7,11	0.45	0
10	TRD	A	1505	-	10,10,12	0.26	0	9,9,11	0.47	0
10	TRD	A	1504	-	12,12,12	0.28	0	11,11,11	0.45	0
9	HEA	A	1502	1	44,67,67	1.66	6 (13%)	37,103,103	1.42	7 (18%)
3	DMU	B	1011	-	24,24,34	0.50	0	35,35,45	0.74	0
8	PO4	C	573	-	4,4,4	0.88	0	6,6,6	0.34	0
13	DXC	C	576	11	28,31,31	0.49	0	46,49,49	1.34	7 (15%)
3	DMU	A	1005	-	34,34,34	0.60	0	45,45,45	0.65	0
10	TRD	A	1013	-	6,6,12	0.27	0	5,5,11	0.30	0
10	TRD	C	579	-	6,6,12	0.26	0	5,5,11	0.29	0

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	0.72	1 (2%)
3	DMU	A	567	-	34,34,34	0.55	0	45,45,45	0.76	1 (2%)
10	TRD	B	1023	-	8,8,12	0.25	0	7,7,11	0.45	0
10	TRD	C	583	-	6,6,12	0.22	0	5,5,11	0.43	0
10	TRD	A	1015	-	10,10,12	0.27	0	9,9,11	0.50	0
10	TRD	B	1031	-	8,8,12	0.27	0	7,7,11	0.37	0
10	TRD	D	23	-	6,6,12	0.22	0	5,5,11	0.42	0
12	HTO	B	1	-	9,9,9	0.21	0	10,10,10	0.79	0
10	TRD	C	578	-	10,10,12	0.29	0	9,9,11	0.38	0
3	DMU	A	1004	-	22,22,34	0.62	1 (4%)	27,27,45	0.88	1 (3%)
10	TRD	A	1506	-	12,12,12	0.24	0	11,11,11	0.52	0
10	TRD	C	582	-	6,6,12	0.25	0	5,5,11	0.38	0
10	TRD	D	7	-	12,12,12	0.24	0	11,11,11	0.57	0
10	TRD	B	1012	-	8,8,12	0.26	0	7,7,11	0.42	0
10	TRD	A	1009	-	6,6,12	0.24	0	5,5,11	0.39	0
9	HEA	C	575	1,14	44,67,67	1.49	6 (13%)	37,103,103	1.84	8 (21%)
3	DMU	D	11	-	34,34,34	0.57	0	45,45,45	0.78	0
10	TRD	D	288	-	8,8,12	0.24	0	7,7,11	0.44	0
10	TRD	C	584	-	6,6,12	0.12	0	5,5,11	0.56	0
9	HEA	A	1503	1,14	44,67,67	1.53	6 (13%)	37,103,103	1.70	8 (21%)
9	HEA	C	574	1	44,67,67	1.62	7 (15%)	37,103,103	1.32	5 (13%)
3	DMU	A	1002	-	21,21,34	0.56	0	26,28,45	0.83	0
8	PO4	A	1001	-	4,4,4	0.90	0	6,6,6	0.43	0
10	TRD	D	12	-	10,10,12	0.27	0	9,9,11	0.40	0
10	TRD	C	581	-	10,10,12	0.27	0	9,9,11	0.50	0
3	DMU	C	568	-	34,34,34	0.58	0	45,45,45	0.80	1 (2%)
10	TRD	A	1010	-	10,10,12	0.25	0	9,9,11	0.51	0
10	TRD	A	1014	-	6,6,12	0.22	0	5,5,11	0.41	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	B	1003	-	-	9/15/35/59	0/1/1/2
10	TRD	C	577	-	-	4/10/10/10	-
10	TRD	C	580	-	-	3/6/6/10	-
10	TRD	A	1505	-	-	6/8/8/10	-
10	TRD	A	1504	-	-	4/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HEA	A	1502	1	2/2/7/16	2/24/76/76	-
3	DMU	B	1011	-	-	4/8/48/59	0/2/2/2
13	DXC	C	576	11	-	5/7/71/71	0/4/4/4
3	DMU	A	1005	-	-	11/19/59/59	0/2/2/2
10	TRD	A	1013	-	-	2/4/4/10	-
10	TRD	C	579	-	-	1/4/4/10	-
9	HEA	C	574	1	2/2/7/16	1/24/76/76	-
3	DMU	A	567	-	-	9/19/59/59	0/2/2/2
10	TRD	B	1023	-	-	1/6/6/10	-
10	TRD	C	583	-	-	3/4/4/10	-
10	TRD	A	1015	-	-	4/8/8/10	-
10	TRD	B	1031	-	-	3/6/6/10	-
10	TRD	D	23	-	-	2/4/4/10	-
12	HTO	B	1	-	1/1/2/2	5/10/10/10	-
10	TRD	C	578	-	-	4/8/8/10	-
3	DMU	A	1004	-	-	8/13/33/59	0/1/1/2
10	TRD	A	1506	-	-	7/10/10/10	-
10	TRD	C	582	-	-	4/4/4/10	-
10	TRD	D	7	-	-	6/10/10/10	-
10	TRD	B	1012	-	-	4/6/6/10	-
10	TRD	A	1009	-	-	3/4/4/10	-
9	HEA	C	575	1,14	3/3/7/16	2/24/76/76	-
3	DMU	D	11	-	-	4/19/59/59	0/2/2/2
10	TRD	D	288	-	-	3/6/6/10	-
10	TRD	C	584	-	-	2/4/4/10	-
9	HEA	A	1503	1,14	2/2/7/16	3/24/76/76	-
3	DMU	C	567	-	-	7/19/59/59	0/2/2/2
3	DMU	A	1002	-	-	2/16/37/59	0/1/1/2
10	TRD	D	12	-	-	4/8/8/10	-
10	TRD	C	581	-	-	3/8/8/10	-
3	DMU	C	568	-	-	9/19/59/59	0/2/2/2
10	TRD	A	1010	-	-	4/8/8/10	-
10	TRD	A	1014	-	-	3/4/4/10	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1502	HEA	C3A-C2A	-5.38	1.32	1.40
9	C	574	HEA	C3A-C2A	-4.90	1.33	1.40
9	A	1503	HEA	C3B-C11	4.77	1.56	1.52
9	C	575	HEA	C3A-C2A	-4.62	1.34	1.40
9	C	574	HEA	C3C-C2C	-4.58	1.34	1.40
9	A	1502	HEA	C3C-C2C	-4.44	1.34	1.40
9	A	1503	HEA	C3A-C2A	-4.20	1.34	1.40
9	C	575	HEA	C3B-C11	3.83	1.55	1.52
9	A	1503	HEA	C3C-C2C	-3.60	1.35	1.40
9	C	575	HEA	C3C-C2C	-3.59	1.35	1.40
9	C	574	HEA	C3B-C11	3.43	1.55	1.52
9	A	1502	HEA	C3C-CAC	3.25	1.54	1.47
9	A	1503	HEA	C3C-CAC	3.14	1.54	1.47
9	C	575	HEA	C3C-CAC	3.02	1.54	1.47
9	A	1502	HEA	C3B-C11	2.86	1.55	1.52
9	C	574	HEA	C3C-CAC	2.85	1.53	1.47
9	A	1502	HEA	C3B-C2B	-2.47	1.33	1.41
9	A	1502	HEA	C3A-CMA	2.45	1.52	1.46
9	C	574	HEA	C3B-C2B	-2.35	1.33	1.41
9	A	1503	HEA	C3B-C2B	-2.17	1.34	1.41
3	A	1004	DMU	O16-C6	2.11	1.43	1.40
9	C	574	HEA	C3A-CMA	2.07	1.51	1.46
9	C	575	HEA	C3A-CMA	2.07	1.51	1.46
9	C	574	HEA	CAD-C3D	2.03	1.55	1.52
3	C	567	DMU	O16-C6	2.03	1.43	1.40
9	C	575	HEA	C3B-C2B	-2.01	1.34	1.41
9	A	1503	HEA	C3A-CMA	2.01	1.51	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	575	HEA	CAD-CBD-CGD	-6.94	101.03	112.67
9	A	1503	HEA	CAD-CBD-CGD	-3.96	106.02	112.67
9	A	1502	HEA	CAD-CBD-CGD	-3.71	106.45	112.67
9	A	1503	HEA	CMC-C2C-C1C	-3.58	122.96	128.46
9	C	575	HEA	CMC-C2C-C1C	-3.56	122.99	128.46
13	C	576	DXC	C21-C19-C17	3.53	117.57	110.28
9	A	1503	HEA	CBA-CAA-C2A	-3.45	106.12	112.48
9	C	574	HEA	CAD-CBD-CGD	-3.25	107.21	112.67
13	C	576	DXC	C16-C17-C19	3.04	116.85	112.15
9	A	1503	HEA	C1B-C2B-C3B	2.98	109.07	107.00
9	A	1503	HEA	C27-C19-C20	2.86	120.08	115.27
3	A	1004	DMU	O16-C6-C1	2.79	112.65	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	574	HEA	C27-C19-C20	2.74	119.88	115.27
9	C	575	HEA	CBA-CAA-C2A	-2.70	107.50	112.48
9	A	1503	HEA	C3A-C4A-NA	-2.68	105.88	110.94
13	C	576	DXC	C2-C1-C6	2.60	113.65	110.55
13	C	576	DXC	C12-C17-C19	-2.49	116.52	119.50
13	C	576	DXC	C5-C6-C1	2.49	113.66	110.47
9	A	1502	HEA	C17-C18-C19	-2.46	121.73	127.66
9	C	575	HEA	CMC-C2C-C3C	2.39	129.15	124.68
9	C	574	HEA	C4B-C3B-C2B	2.39	108.53	106.87
13	C	576	DXC	C18-C4-C5	-2.37	104.44	108.26
9	A	1502	HEA	CMC-C2C-C1C	-2.29	124.94	128.46
9	A	1502	HEA	C13-C12-C11	-2.28	110.93	114.35
9	A	1503	HEA	CMC-C2C-C3C	2.23	128.86	124.68
9	A	1502	HEA	CMB-C2B-C1B	-2.19	125.09	128.46
9	A	1502	HEA	C25-C23-C24	2.19	119.45	114.60
9	C	575	HEA	CBD-CAD-C3D	2.18	116.50	112.49
9	C	575	HEA	C27-C19-C20	2.17	118.91	115.27
3	C	568	DMU	C10-O1-C9	2.16	117.94	113.69
9	C	574	HEA	C17-C18-C19	-2.13	122.52	127.66
9	C	575	HEA	C3A-C4A-NA	-2.10	106.99	110.94
13	C	576	DXC	C14-C10-C4	2.09	115.88	113.73
9	A	1503	HEA	CBD-CAD-C3D	2.07	116.30	112.49
9	C	574	HEA	C13-C12-C11	-2.06	111.25	114.35
9	A	1502	HEA	C4B-C3B-C2B	2.06	108.30	106.87
3	A	567	DMU	O1-C9-C11	2.05	111.53	106.44
3	C	567	DMU	O7-C3-C2	2.01	112.63	107.28
9	C	575	HEA	OMA-CMA-C3A	-2.01	120.53	124.91

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	1502	HEA	ND
9	A	1502	HEA	NB
12	B	1	HTO	C2
9	C	575	HEA	ND
9	C	575	HEA	NA
9	C	575	HEA	NB
9	A	1503	HEA	ND
9	A	1503	HEA	NB
9	C	574	HEA	ND
9	C	574	HEA	NB

All (161) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	567	DMU	C19-C18-O16-C6
12	B	1	HTO	O1-C1-C2-C3
12	B	1	HTO	C2-C3-C4-C5
3	A	1004	DMU	C1-C6-O16-C18
3	A	1004	DMU	O5-C6-O16-C18
9	C	575	HEA	O11-C11-C12-C13
9	A	1503	HEA	C3B-C11-C12-C13
9	A	1503	HEA	O11-C11-C12-C13
3	A	1002	DMU	C3-C4-O5-C6
3	A	1002	DMU	C57-C4-O5-C6
12	B	1	HTO	O1-C1-C2-O2
3	A	567	DMU	O6-C11-C9-O1
3	D	11	DMU	O6-C11-C9-O1
3	C	568	DMU	O6-C11-C9-O1
3	B	1011	DMU	O5-C4-C57-O61
3	D	11	DMU	O6-C11-C9-C8
3	B	1011	DMU	O6-C11-C9-O1
3	B	1011	DMU	C3-C4-C57-O61
13	C	576	DXC	C12-C17-C19-C21
3	C	568	DMU	O6-C11-C9-C8
3	B	1003	DMU	O5-C4-C57-O61
13	C	576	DXC	C16-C17-C19-C21
3	A	567	DMU	O5-C6-O16-C18
3	B	1003	DMU	C3-C4-C57-O61
3	A	1005	DMU	O1-C10-O7-C3
3	C	567	DMU	O1-C10-O7-C3
10	D	12	TRD	C3-C4-C5-C6
13	C	576	DXC	C19-C21-C22-C23
3	A	567	DMU	O6-C11-C9-C8
10	C	578	TRD	C6-C7-C8-C9
10	A	1010	TRD	C5-C6-C7-C8
10	C	580	TRD	C2-C3-C4-C5
3	C	567	DMU	C28-C31-C34-C37
10	A	1015	TRD	C5-C6-C7-C8
10	B	1031	TRD	C2-C3-C4-C5
10	C	581	TRD	C4-C5-C6-C7
10	C	580	TRD	C3-C4-C5-C6
10	A	1504	TRD	C5-C6-C7-C8
3	B	1003	DMU	C1-C6-O16-C18
3	A	567	DMU	C1-C6-O16-C18
10	D	23	TRD	C2-C3-C4-C5
10	C	577	TRD	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	C	568	DMU	C22-C25-C28-C31
10	C	577	TRD	C4-C5-C6-C7
10	A	1506	TRD	C4-C5-C6-C7
10	D	12	TRD	C6-C7-C8-C9
3	C	568	DMU	C28-C31-C34-C37
10	C	578	TRD	C7-C8-C9-C10
3	B	1003	DMU	O5-C6-O16-C18
10	A	1505	TRD	C6-C7-C8-C9
3	D	11	DMU	C19-C22-C25-C28
10	C	582	TRD	C2-C3-C4-C5
10	C	582	TRD	C3-C4-C5-C6
3	B	1003	DMU	C25-C28-C31-C34
10	C	577	TRD	C3-C4-C5-C6
3	B	1003	DMU	C19-C18-O16-C6
3	A	1005	DMU	C19-C18-O16-C6
12	B	1	HTO	O3-C3-C4-C5
3	A	1004	DMU	C19-C18-O16-C6
3	A	1005	DMU	C18-C19-C22-C25
3	B	1003	DMU	C31-C34-C37-C40
10	A	1010	TRD	C4-C5-C6-C7
10	A	1014	TRD	C2-C3-C4-C5
10	A	1504	TRD	C3-C4-C5-C6
3	C	568	DMU	C18-C19-C22-C25
10	A	1505	TRD	C5-C6-C7-C8
10	A	1015	TRD	C7-C8-C9-C10
10	C	581	TRD	C3-C4-C5-C6
10	A	1506	TRD	C2-C3-C4-C5
3	D	11	DMU	C28-C31-C34-C37
10	A	1505	TRD	C4-C5-C6-C7
10	D	7	TRD	C6-C7-C8-C9
10	C	584	TRD	C3-C4-C5-C6
3	C	567	DMU	C18-C19-C22-C25
10	B	1012	TRD	C3-C4-C5-C6
3	A	1005	DMU	C28-C31-C34-C37
10	A	1010	TRD	C6-C7-C8-C9
3	A	567	DMU	C22-C25-C28-C31
10	A	1505	TRD	C7-C8-C9-C10
3	C	568	DMU	C25-C28-C31-C34
10	A	1506	TRD	C9-C10-C11-C12
10	A	1506	TRD	C11-C10-C9-C8
10	D	12	TRD	C4-C5-C6-C7
10	B	1012	TRD	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
10	C	583	TRD	C1-C2-C3-C4
10	A	1014	TRD	C1-C2-C3-C4
10	A	1506	TRD	C5-C6-C7-C8
10	C	580	TRD	C1-C2-C3-C4
10	A	1015	TRD	C1-C2-C3-C4
10	D	7	TRD	C1-C2-C3-C4
10	A	1013	TRD	C1-C2-C3-C4
10	A	1010	TRD	C11-C10-C9-C8
10	B	1023	TRD	C5-C6-C7-C8
10	C	578	TRD	C11-C10-C9-C8
10	A	1506	TRD	C6-C7-C8-C9
13	C	576	DXC	C16-C17-C19-C24
10	A	1009	TRD	C4-C5-C6-C7
3	B	1003	DMU	C28-C31-C34-C37
3	C	568	DMU	C34-C37-C40-C43
10	A	1505	TRD	C11-C10-C9-C8
10	A	1505	TRD	C2-C3-C4-C5
10	B	1031	TRD	C5-C6-C7-C8
10	C	582	TRD	C1-C2-C3-C4
10	B	1031	TRD	C6-C7-C8-C9
3	A	1004	DMU	C25-C28-C31-C34
3	A	1005	DMU	C2-C3-O7-C10
10	C	579	TRD	C2-C3-C4-C5
10	D	7	TRD	C4-C5-C6-C7
10	C	584	TRD	C4-C5-C6-C7
3	A	1005	DMU	C4-C3-O7-C10
13	C	576	DXC	C12-C17-C19-C24
3	A	1004	DMU	C19-C22-C25-C28
10	D	23	TRD	C4-C5-C6-C7
10	C	582	TRD	C4-C5-C6-C7
3	B	1003	DMU	C22-C25-C28-C31
10	A	1014	TRD	C3-C4-C5-C6
10	D	288	TRD	C6-C7-C8-C9
3	C	567	DMU	C2-C3-O7-C10
10	D	7	TRD	C11-C10-C9-C8
3	A	567	DMU	C18-C19-C22-C25
3	A	1004	DMU	O16-C18-C19-C22
10	C	583	TRD	C4-C5-C6-C7
10	B	1012	TRD	C4-C5-C6-C7
3	C	567	DMU	C4-C3-O7-C10
3	A	1005	DMU	C19-C22-C25-C28
3	C	568	DMU	O16-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
10	C	583	TRD	C2-C3-C4-C5
10	A	1504	TRD	C1-C2-C3-C4
10	D	7	TRD	C5-C6-C7-C8
3	A	1005	DMU	C31-C34-C37-C40
10	A	1506	TRD	C1-C2-C3-C4
10	D	7	TRD	C9-C10-C11-C12
10	B	1012	TRD	C1-C2-C3-C4
10	C	581	TRD	C1-C2-C3-C4
10	A	1013	TRD	C3-C4-C5-C6
3	A	1005	DMU	C3-C4-C57-O61
10	C	577	TRD	C7-C8-C9-C10
3	A	1004	DMU	O5-C4-C57-O61
10	A	1504	TRD	C6-C7-C8-C9
10	D	12	TRD	C11-C10-C9-C8
10	A	1009	TRD	C2-C3-C4-C5
10	D	288	TRD	C3-C4-C5-C6
12	B	1	HTO	C4-C5-C6-C7
3	B	1011	DMU	O6-C11-C9-C8
10	A	1009	TRD	C1-C2-C3-C4
3	C	567	DMU	C19-C22-C25-C28
9	A	1502	HEA	C26-C15-C16-C17
9	C	574	HEA	C26-C15-C16-C17
3	A	567	DMU	C25-C28-C31-C34
3	A	1004	DMU	C34-C37-C40-C43
10	D	288	TRD	C1-C2-C3-C4
10	A	1015	TRD	C11-C10-C9-C8
9	A	1502	HEA	C14-C15-C16-C17
3	A	1005	DMU	O6-C11-C9-C8
3	C	567	DMU	C5-C10-O7-C3
3	C	568	DMU	C31-C34-C37-C40
3	A	1005	DMU	C5-C10-O7-C3
3	A	567	DMU	C31-C34-C37-C40
9	C	575	HEA	C3B-C11-C12-C13
9	A	1503	HEA	C26-C15-C16-C17
10	C	578	TRD	C5-C6-C7-C8

There are no ring outliers.

16 monomers are involved in 48 short contacts:

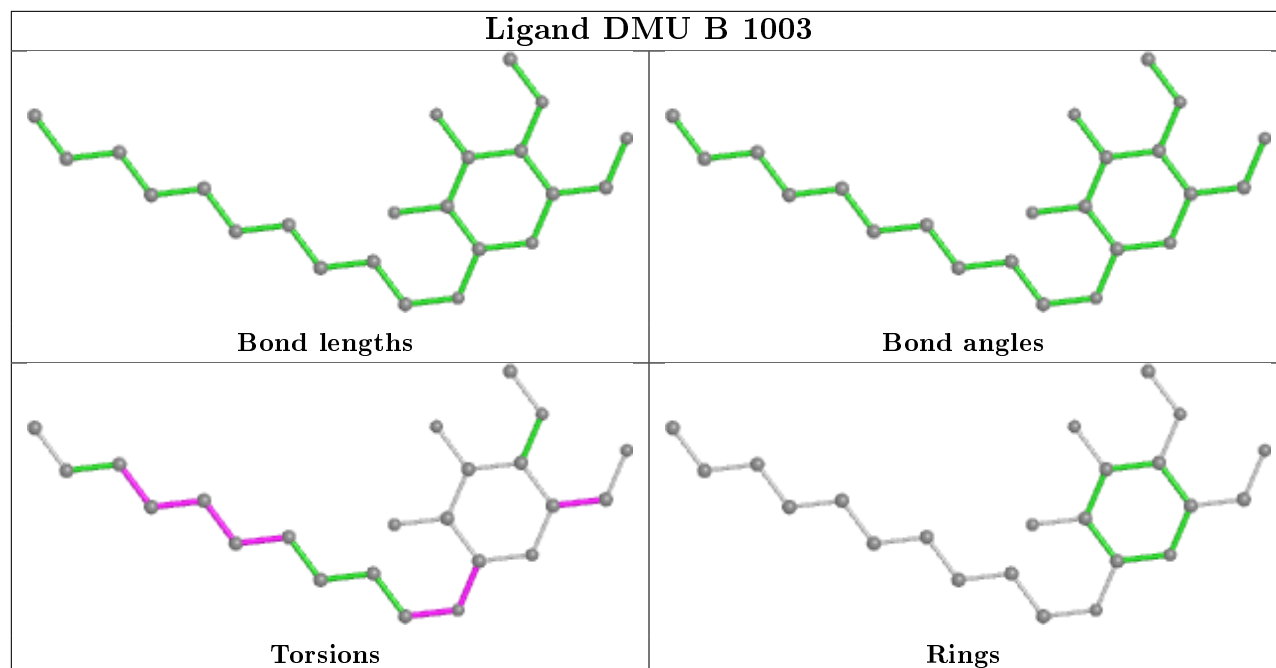
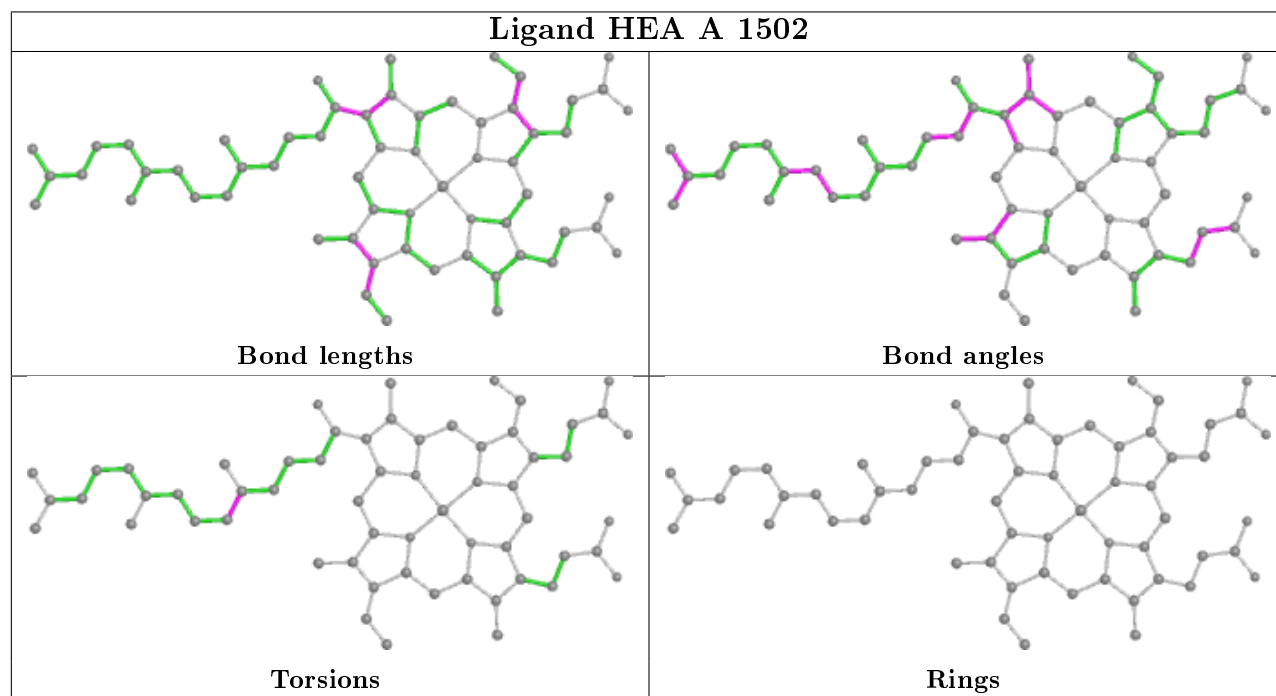
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	577	TRD	1	0
10	A	1504	TRD	4	0

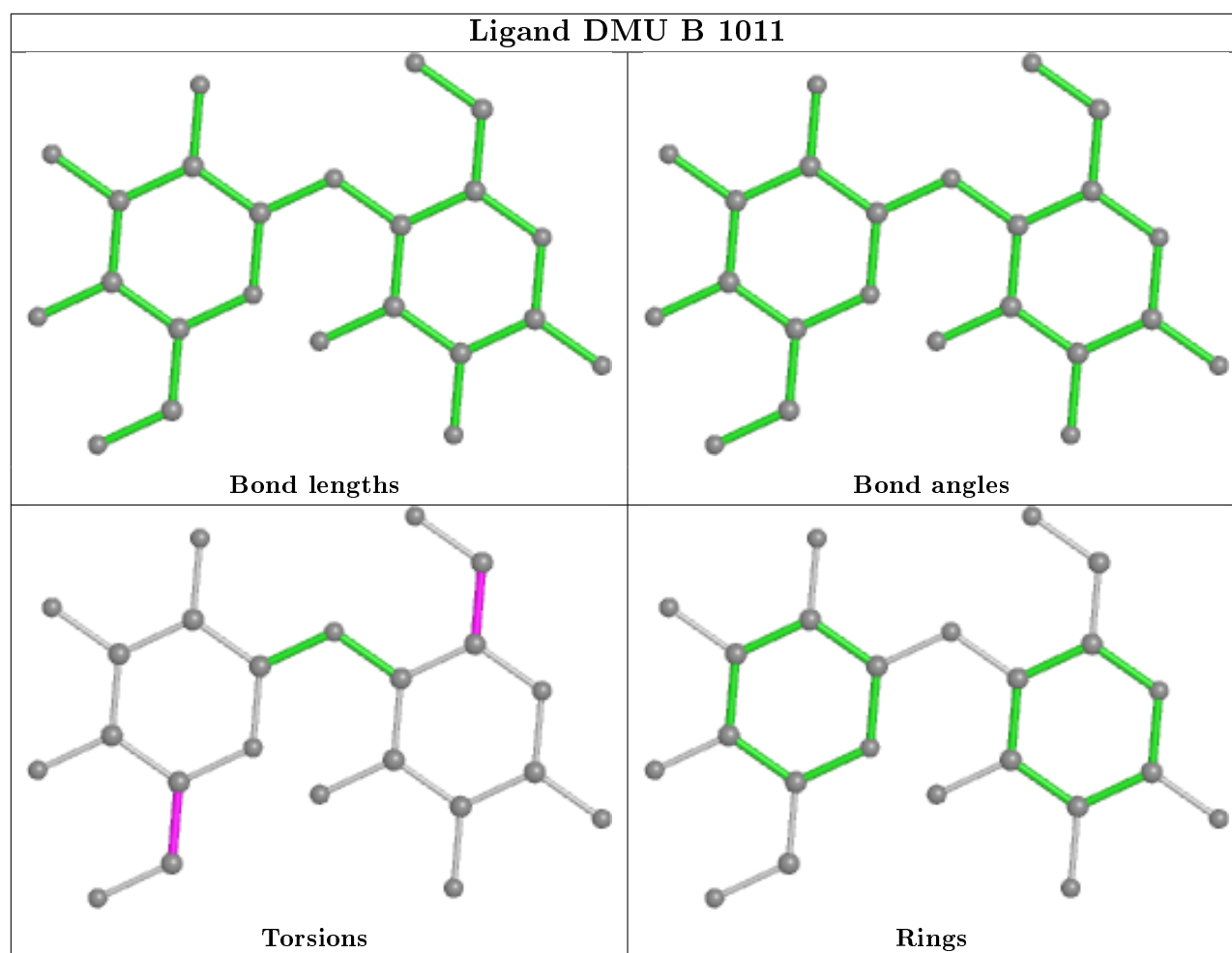
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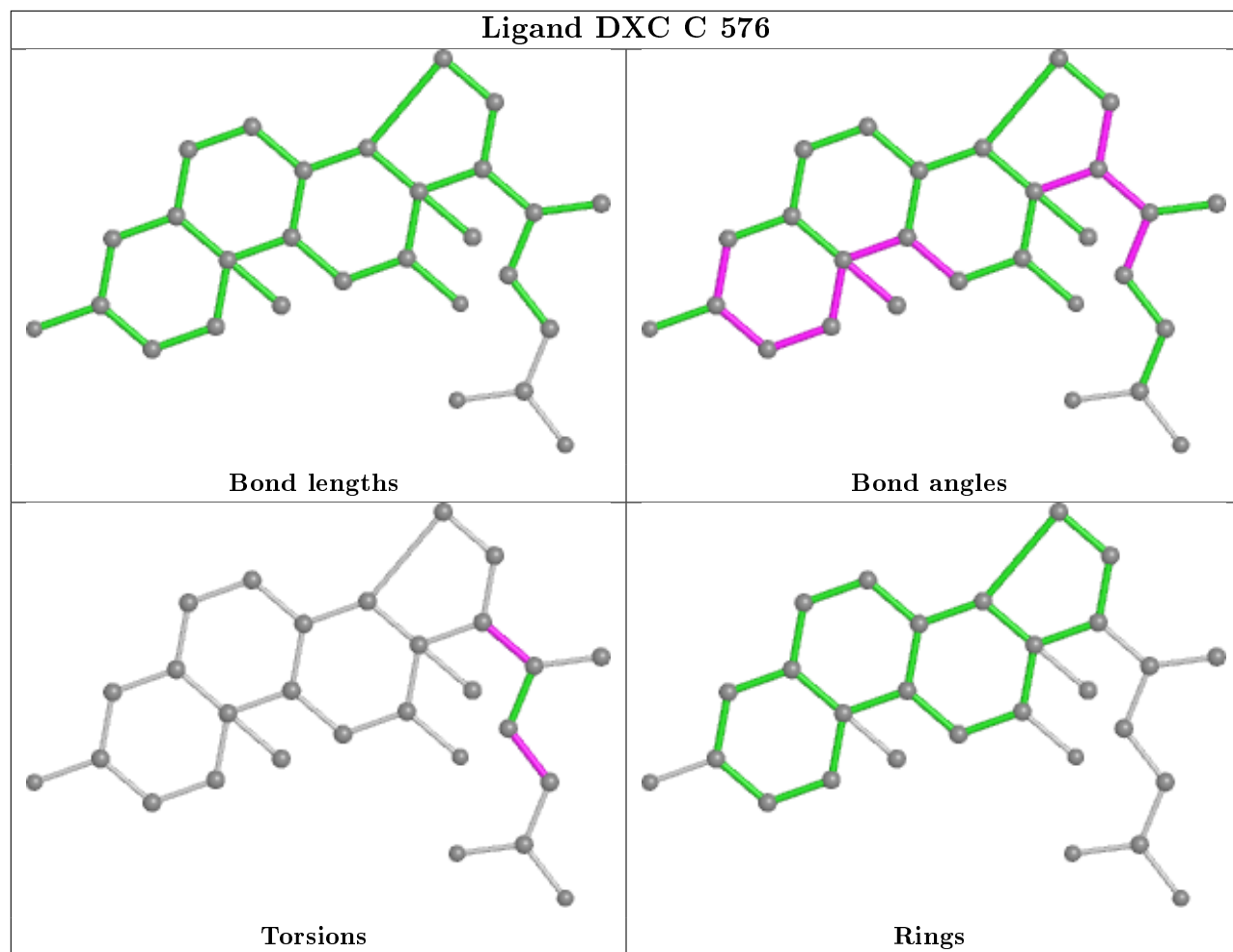
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1502	HEA	4	0
3	A	1005	DMU	1	0
3	C	567	DMU	1	0
3	A	567	DMU	3	0
10	B	1023	TRD	1	0
12	B	1	HTO	1	0
3	A	1004	DMU	3	0
10	A	1506	TRD	3	0
10	D	7	TRD	2	0
9	C	575	HEA	4	0
10	C	584	TRD	12	0
9	A	1503	HEA	1	0
9	C	574	HEA	4	0
3	A	1002	DMU	3	0

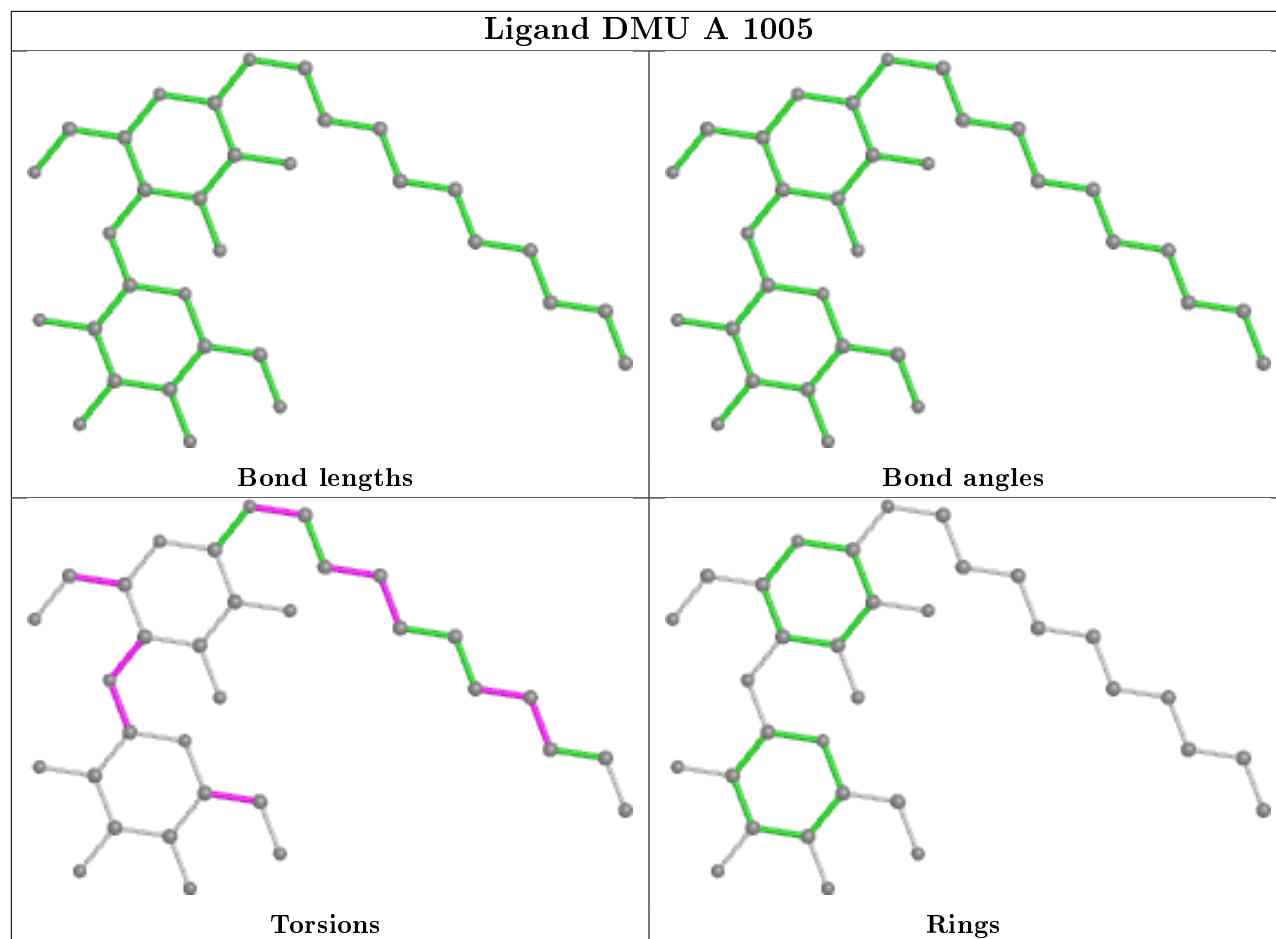
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

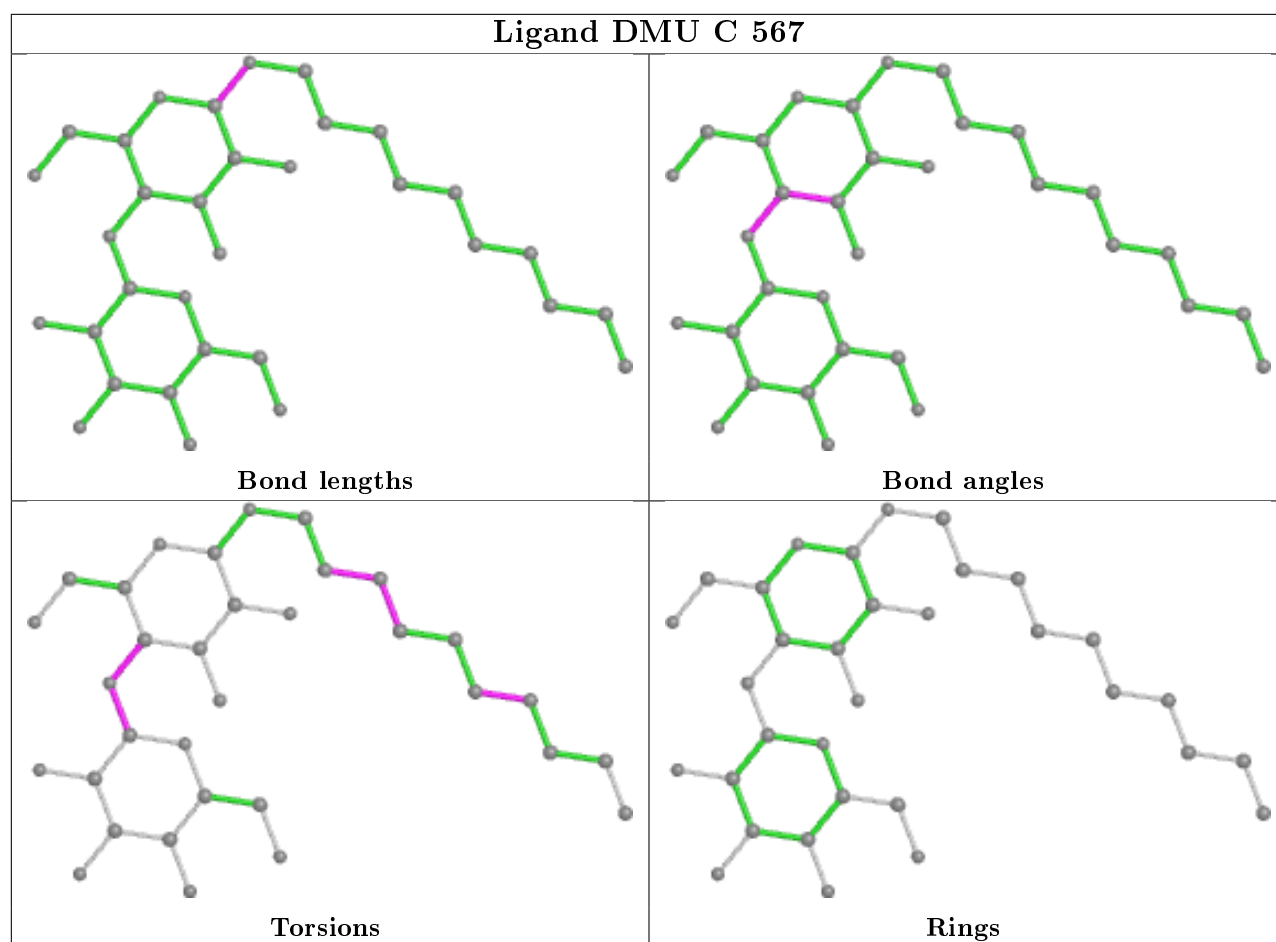
**Ligand DMU B 1003****Ligand HEA A 1502**

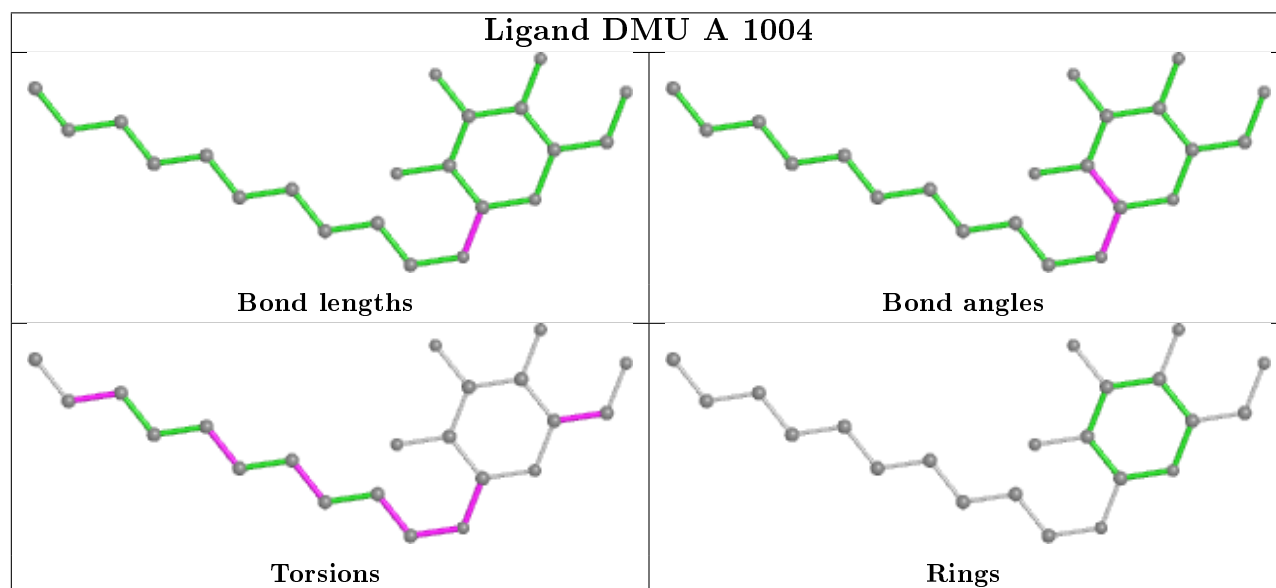
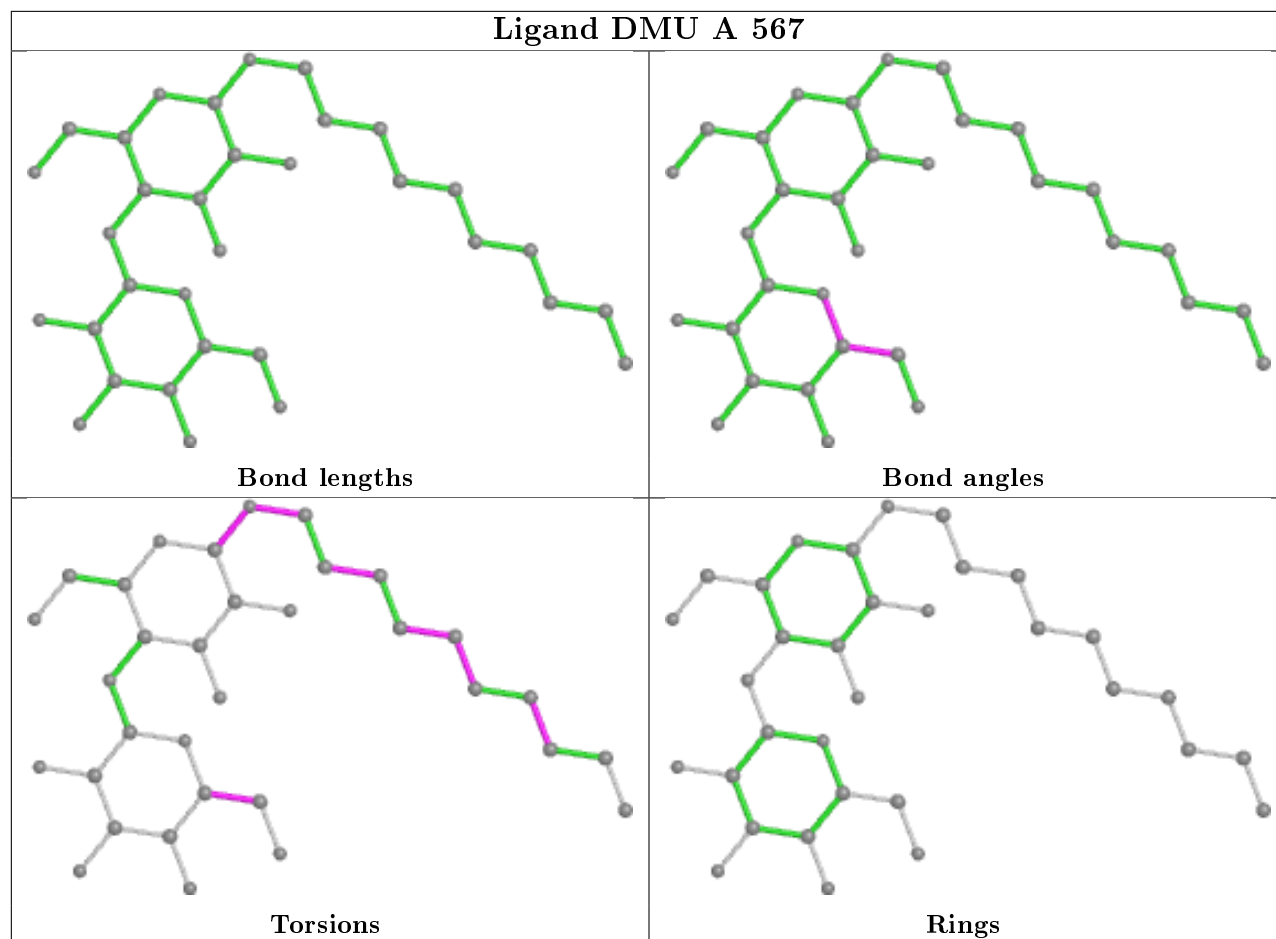


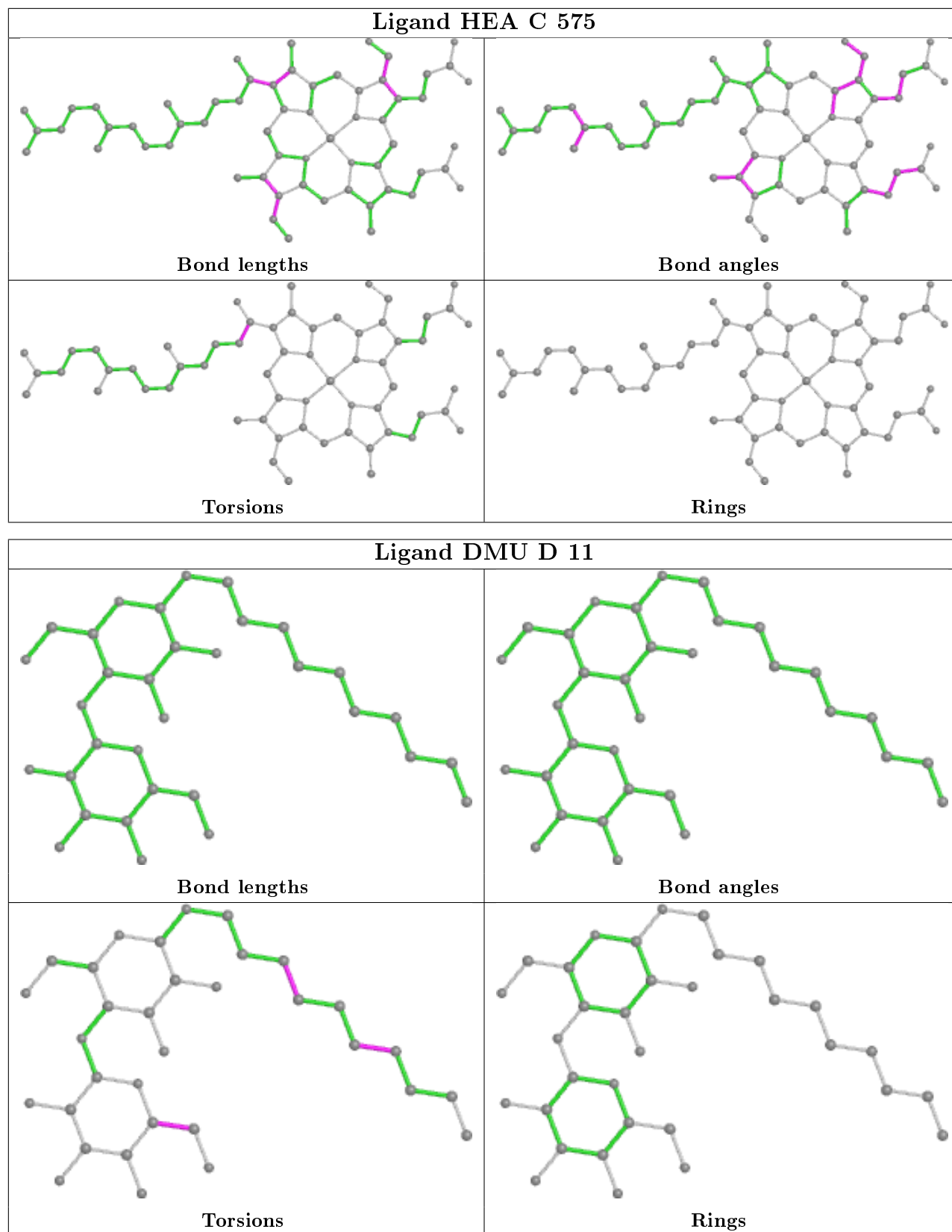


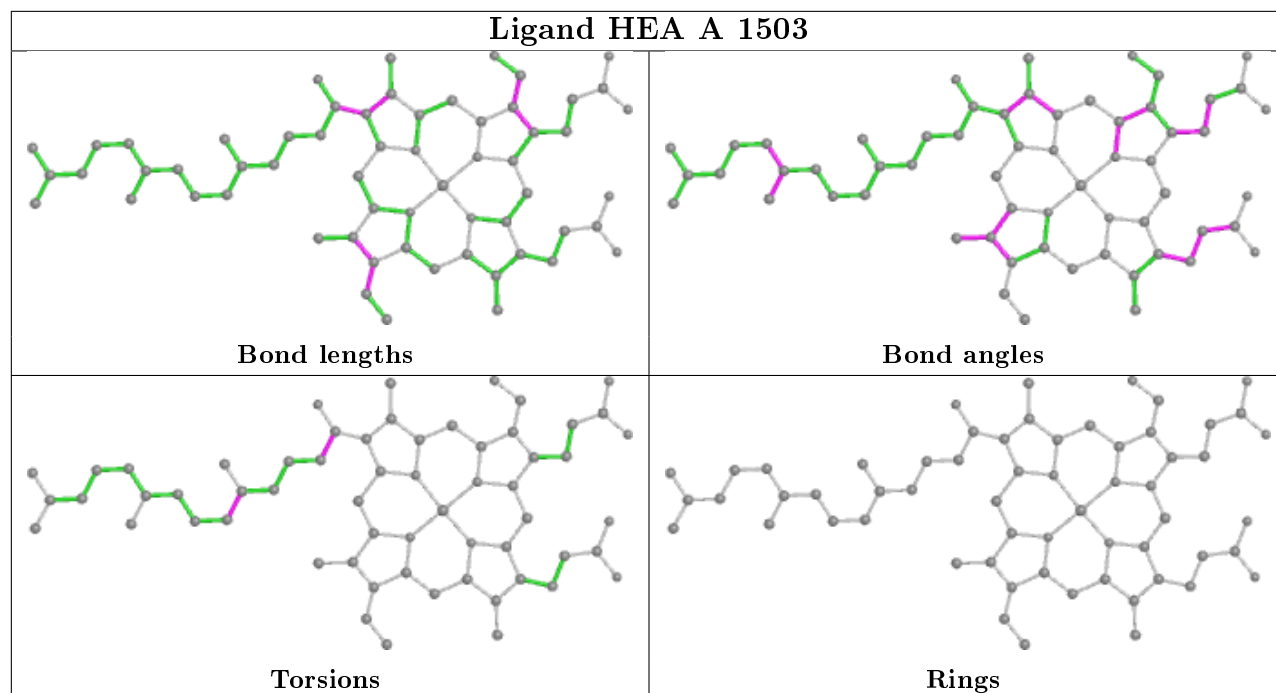
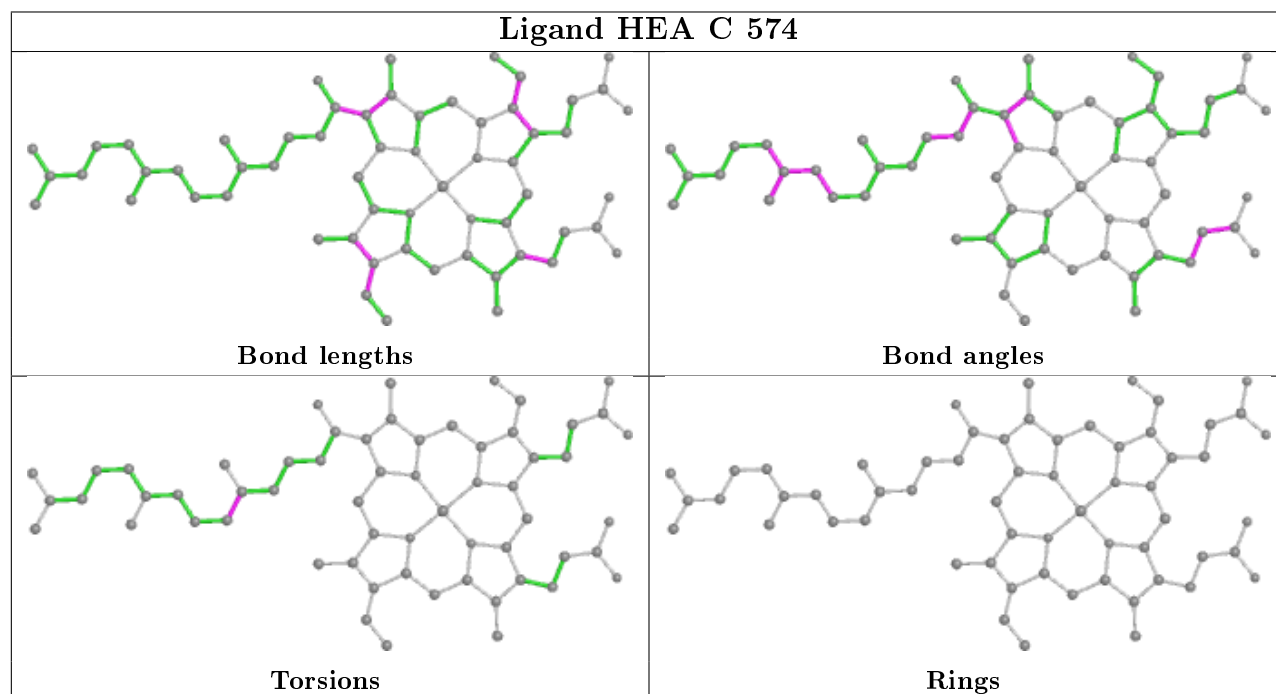




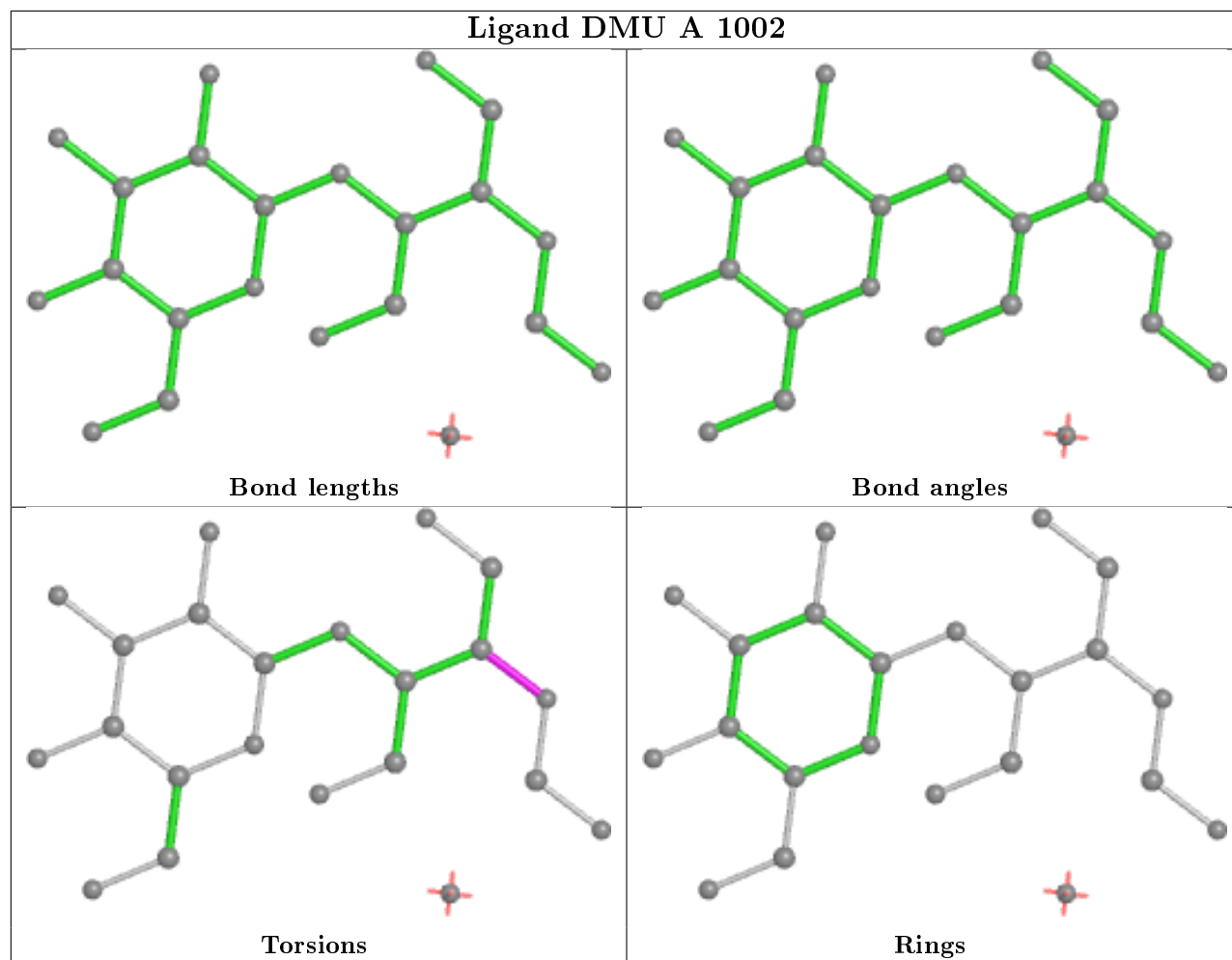


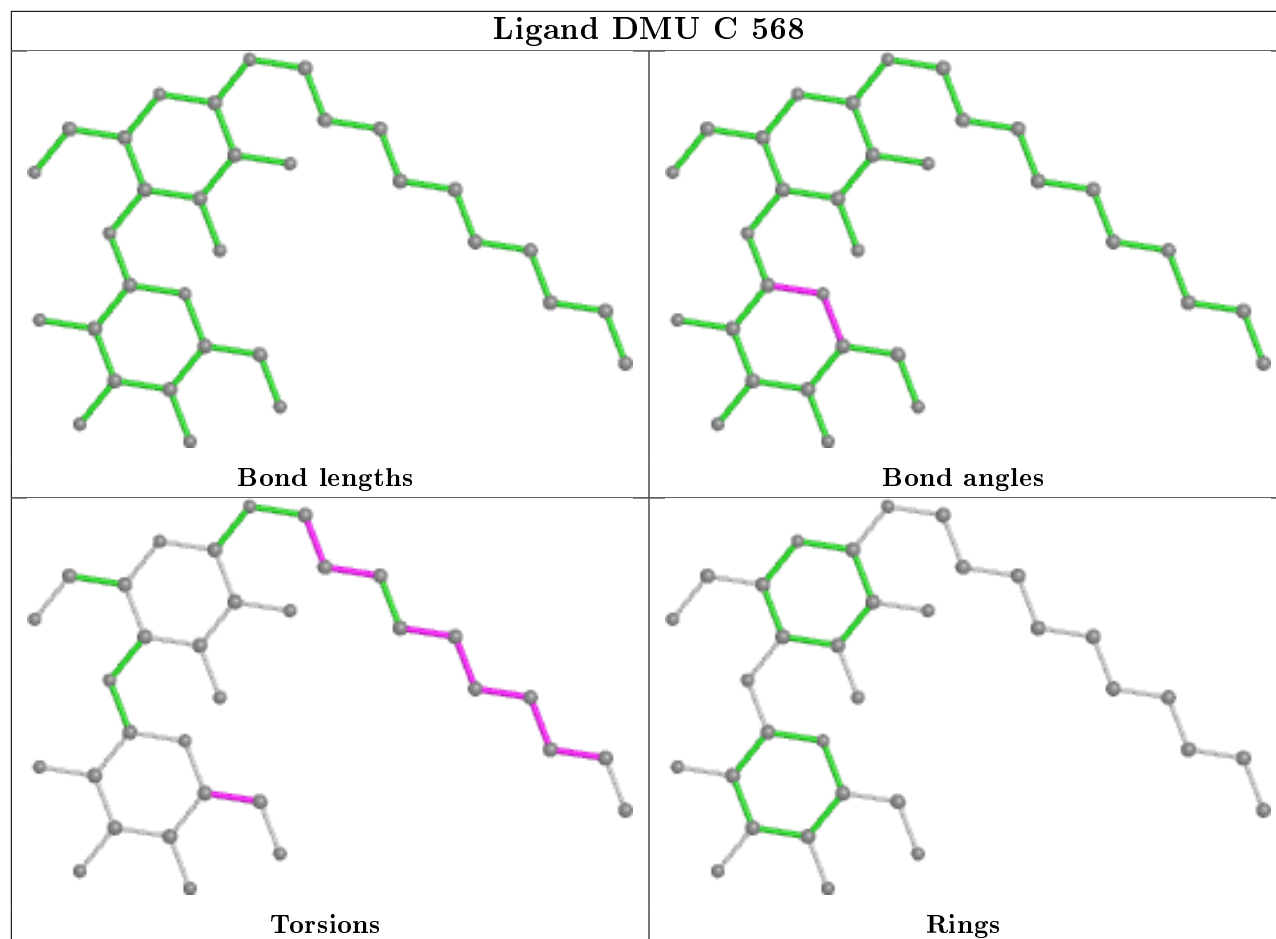




**Ligand HEA A 1503****Ligand HEA C 574**

## Ligand DMU A 1002





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	539/566 (95%)	0.21	40 (7%)	14 20	26, 37, 60, 76	7 (1%)
1	C	536/566 (94%)	0.24	46 (8%)	10 15	22, 33, 49, 67	7 (1%)
2	B	259/262 (98%)	-0.17	8 (3%)	49 58	26, 38, 52, 65	5 (1%)
2	D	258/262 (98%)	-0.23	5 (1%)	66 74	24, 35, 46, 57	4 (1%)
All	All	1592/1656 (96%)	0.09	99 (6%)	20 27	22, 35, 52, 76	23 (1%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	TRP	7.4
1	C	17	PHE	6.9
1	A	81	TRP	6.3
1	C	73	VAL	5.3
1	C	81	TRP	5.1
1	A	259	PHE	5.1
2	D	81	TRP	4.8
1	C	21	PHE	4.7
1	C	420	PHE	4.4
1	A	72	LEU	4.1
1	A	16	PHE	4.1
1	C	417	VAL	4.0
1	A	172	TRP	4.0
1	C	72	LEU	4.0
1	C	290	ILE	3.9
1	C	19	ARG	3.9
1	C	291	VAL	3.9
2	B	99	PRO	3.9
1	C	416	VAL	3.8
1	A	69	GLU	3.8
2	B	287	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	70	SER	3.7
1	A	262	THR	3.7
2	B	29	SER	3.6
2	D	56	TRP	3.5
1	C	287	VAL	3.4
1	C	424	MET	3.4
1	C	428	ALA	3.4
1	A	287	VAL	3.4
1	A	290	ILE	3.4
1	C	137	ARG	3.4
1	C	423	VAL	3.3
1	C	172	TRP	3.3
2	D	87	ARG	3.3
1	A	268	GLY	3.2
1	A	420	PHE	3.2
1	C	77	PHE	3.2
1	A	99	ILE	3.1
1	A	267	SER	3.1
1	C	75	GLY	3.0
1	A	73	VAL	3.0
1	A	291	VAL	3.0
1	A	520	THR	2.9
1	C	432	ILE	2.9
1	C	74	LYS	2.9
1	C	111	VAL	2.9
1	A	516	PHE	2.9
1	C	294	ALA	2.9
1	C	395	GLY	2.8
2	B	56	TRP	2.8
1	C	107	MET	2.8
1	A	423	VAL	2.7
1	A	424	MET	2.7
1	C	387	PHE	2.7
1	C	71	GLY	2.7
1	A	418	ALA	2.7
1	C	69	GLU	2.6
1	A	185	TYR	2.6
1	C	394	GLY	2.6
1	C	292	LEU	2.6
1	A	103	GLY	2.6
1	A	417	VAL	2.5
1	C	397	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	28	GLN	2.5
1	C	293	PRO	2.4
1	C	391	PHE	2.4
1	A	173	VAL	2.4
1	C	418	ALA	2.4
1	A	107	MET	2.4
2	B	100	LEU	2.4
1	A	270	GLY	2.4
1	A	78	GLN	2.4
1	A	318	TYR	2.4
1	A	106	MET	2.4
1	C	398	GLY	2.3
1	A	428	ALA	2.3
1	C	22	MET	2.3
1	A	480	PRO	2.3
1	C	104	ILE	2.3
1	C	298	VAL	2.3
1	A	75	GLY	2.3
1	C	269	GLY	2.3
1	C	297	ILE	2.3
1	C	78	GLN	2.2
1	C	425	SER	2.2
1	A	100	THR	2.2
1	C	112	ILE	2.2
1	A	292	LEU	2.2
1	A	223	HIS	2.1
2	B	124	PHE	2.1
2	B	286	HIS	2.1
1	A	416	VAL	2.1
2	B	102	ILE	2.1
1	A	14	ARG	2.1
1	A	17	PHE	2.1
1	C	295	PHE	2.1
1	A	517	TYR	2.0
1	A	13	ARG	2.0
2	D	99	PRO	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	C	581	11/13	0.47	0.26	74,75,77,77	11
10	TRD	A	1505	11/13	0.64	0.21	64,65,66,66	11
10	TRD	A	1015	11/13	0.66	0.17	63,65,70,70	11
3	DMU	C	567	33/33	0.66	0.40	77,81,82,83	0
10	TRD	A	1014	7/13	0.66	0.36	73,73,74,74	7
10	TRD	C	582	7/13	0.69	0.20	67,67,67,67	7
3	DMU	B	1003	23/33	0.70	0.33	49,54,56,56	23
10	TRD	C	580	9/13	0.70	0.19	62,64,64,64	9
10	TRD	C	578	11/13	0.72	0.20	61,62,63,63	0
10	TRD	A	1013	7/13	0.72	0.25	53,54,55,55	0
3	DMU	A	1004	22/33	0.73	0.23	44,61,65,66	22
3	DMU	B	1011	23/33	0.75	0.16	57,58,58,58	23
10	TRD	A	1009	7/13	0.75	0.25	60,60,62,62	0
10	TRD	D	12	11/13	0.78	0.22	58,58,58,59	11
3	DMU	A	1002	22/33	0.80	0.18	66,66,67,67	22
3	DMU	A	1005	33/33	0.80	0.23	50,57,61,61	33
10	TRD	B	1012	9/13	0.80	0.21	74,75,77,77	0
10	TRD	A	1010	11/13	0.80	0.21	58,59,59,60	11
10	TRD	B	1031	9/13	0.80	0.22	53,55,58,58	0
10	TRD	C	583	7/13	0.82	0.27	57,57,59,59	0
10	TRD	C	579	7/13	0.82	0.20	68,68,69,69	0
3	DMU	D	11	33/33	0.82	0.27	70,73,74,75	33
10	TRD	D	288	9/13	0.82	0.19	52,53,56,56	0
10	TRD	D	23	7/13	0.82	0.12	61,61,62,62	7
10	TRD	A	1504	13/13	0.84	0.19	56,58,61,62	0
8	PO4	C	573	5/5	0.85	0.27	53,53,54,55	5
3	DMU	C	568	33/33	0.85	0.19	65,68,69,70	0
10	TRD	B	1023	9/13	0.86	0.13	58,59,60,61	0
8	PO4	A	1001	5/5	0.86	0.25	69,69,70,70	5
10	TRD	C	584	7/13	0.87	0.34	46,50,54,55	0
10	TRD	C	577	13/13	0.87	0.14	45,50,53,54	0
10	TRD	D	7	13/13	0.87	0.20	41,43,50,50	0

*Continued on next page...*

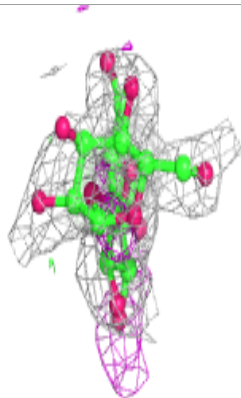
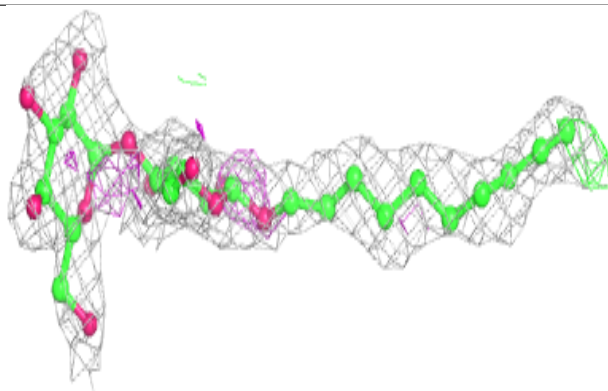
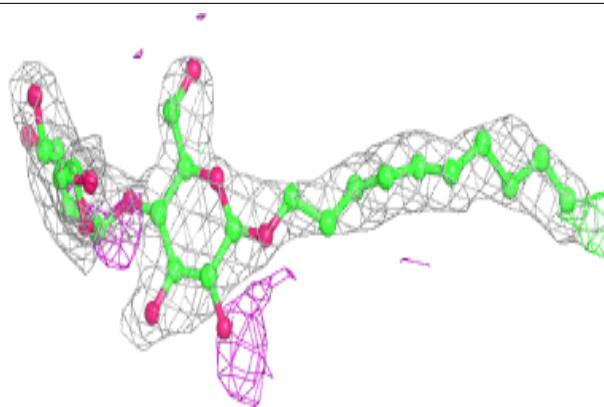
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DMU	A	567	33/33	0.88	0.15	48,63,67,68	0
10	TRD	A	1506	13/13	0.91	0.15	45,46,51,53	0
13	DXC	C	576	28/28	0.92	0.17	46,50,52,52	0
12	HTO	B	1	10/10	0.92	0.26	51,54,55,56	0
7	OH	A	1501	1/1	0.93	0.23	35,35,35,35	0
11	CD	B	1010	1/1	0.96	0.08	53,53,53,53	1
9	HEA	A	1503	60/60	0.96	0.19	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	0.97	0.20	23,26,32,33	0
9	HEA	A	1502	60/60	0.98	0.19	23,26,33,34	0
9	HEA	C	575	60/60	0.98	0.22	21,24,32,33	0
6	CA	C	571	1/1	0.98	0.05	32,32,32,32	0
4	CU	B	1022	1/1	0.99	0.10	28,28,28,28	0
7	OH	C	572	1/1	0.99	0.22	28,28,28,28	0
11	CD	D	9	1/1	0.99	0.05	46,46,46,46	0
11	CD	B	1008	1/1	0.99	0.06	35,35,35,35	0
6	CA	A	1007	1/1	0.99	0.07	27,27,27,27	0
4	CU	D	3	1/1	1.00	0.07	28,28,28,28	0
4	CU	A	1023	1/1	1.00	0.12	32,32,32,32	0
11	CD	D	8	1/1	1.00	0.05	36,36,36,36	0
5	MG	A	1006	1/1	1.00	0.21	16,16,16,16	0
4	CU	C	569	1/1	1.00	0.13	26,26,26,26	0
5	MG	C	570	1/1	1.00	0.20	15,15,15,15	0
4	CU	B	1004	1/1	1.00	0.08	29,29,29,29	0
4	CU	D	4	1/1	1.00	0.09	28,28,28,28	0

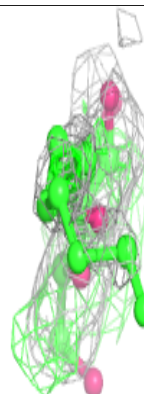
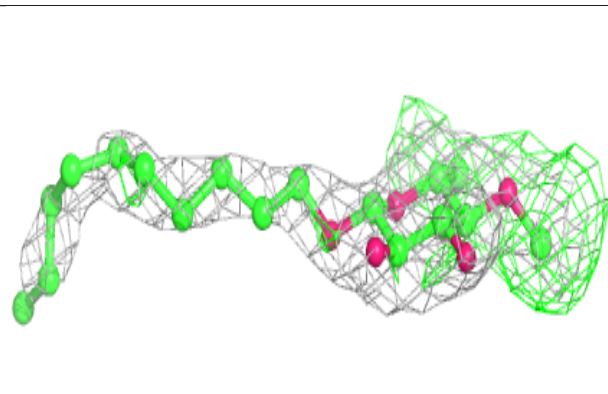
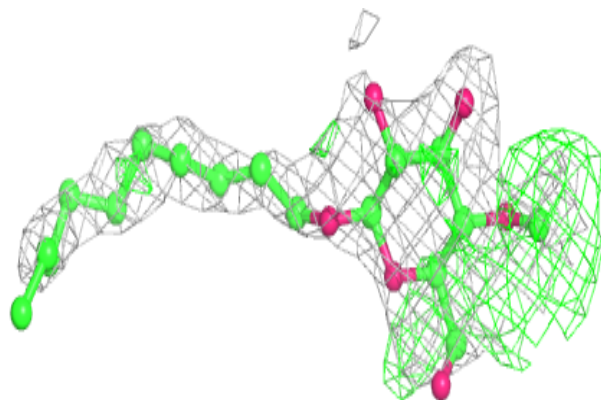
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around DMU C 567:**

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

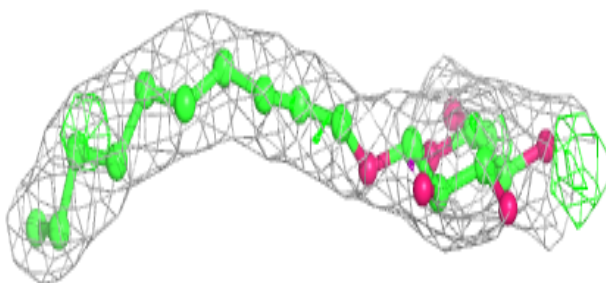
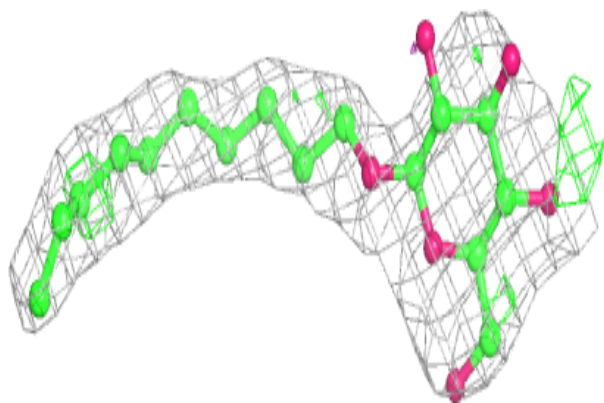
**Electron density around DMU B 1003:**

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

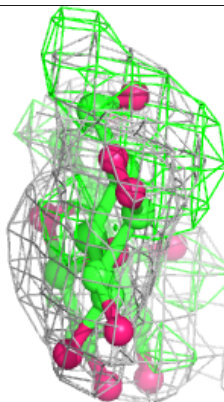
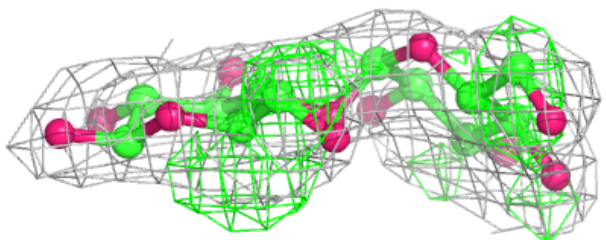
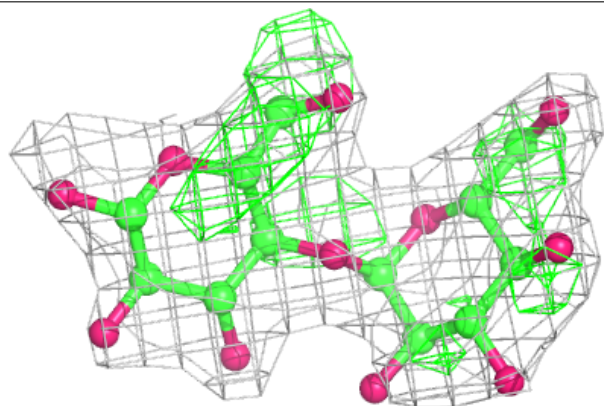


**Electron density around DMU A 1004:**

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

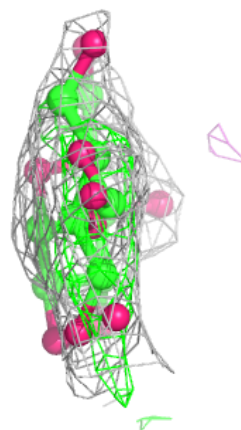
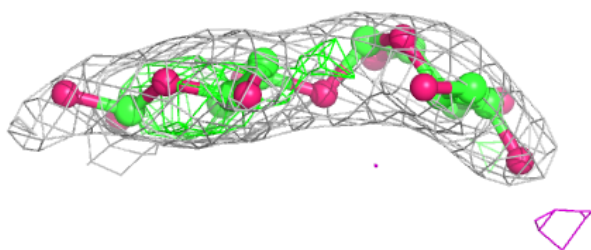
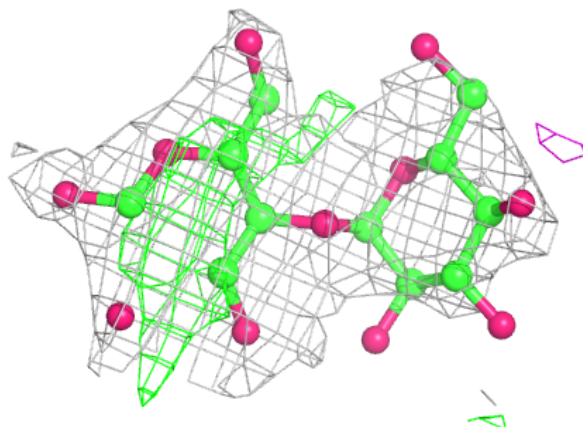
**Electron density around DMU B 1011:**

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

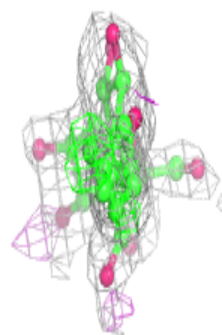
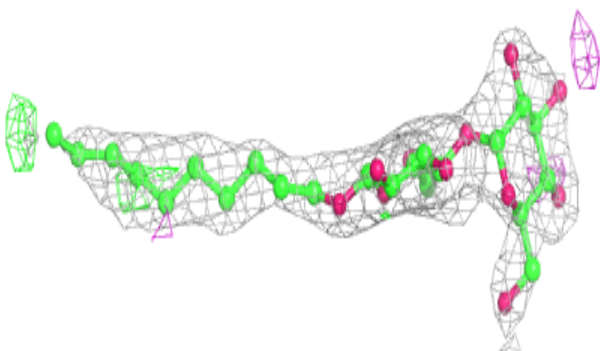
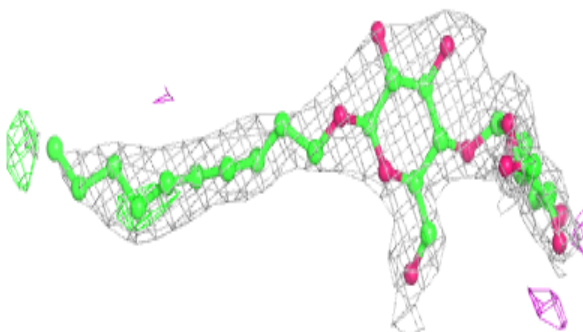


**Electron density around DMU A 1002:**

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

**Electron density around DMU A 1005:**

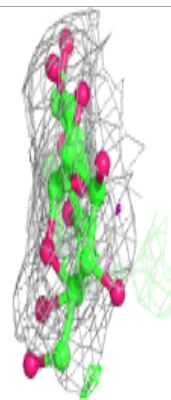
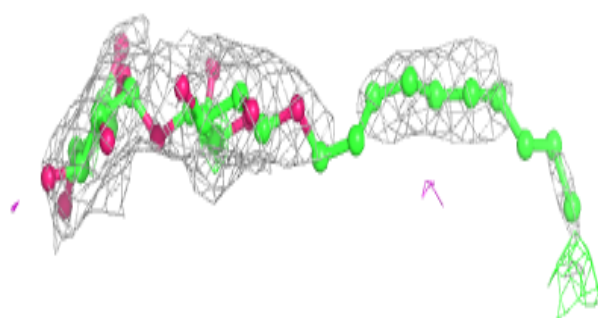
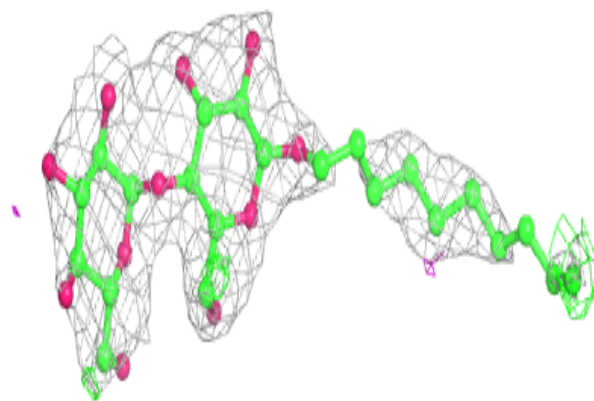
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



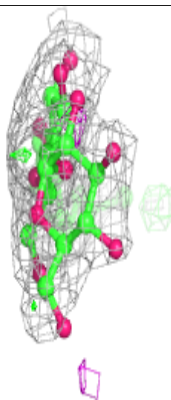
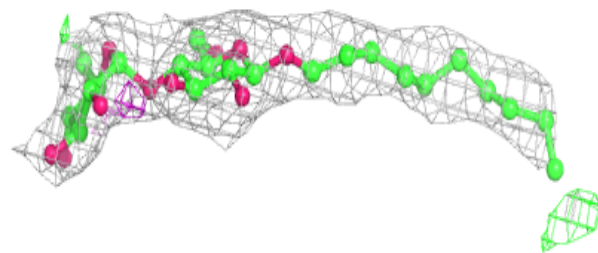
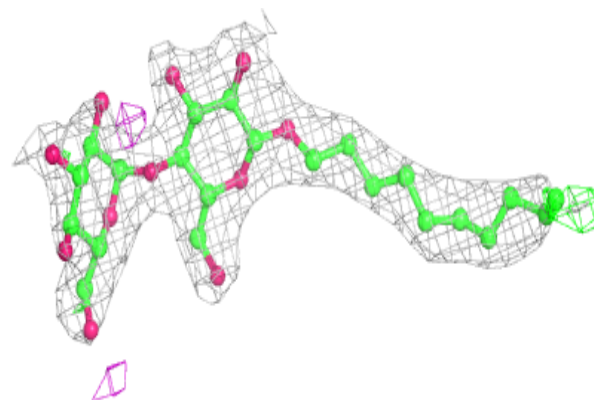


**Electron density around DMU D 11:**

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

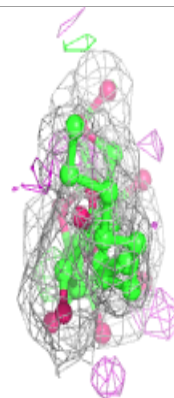
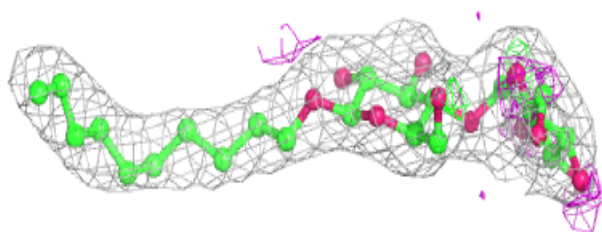
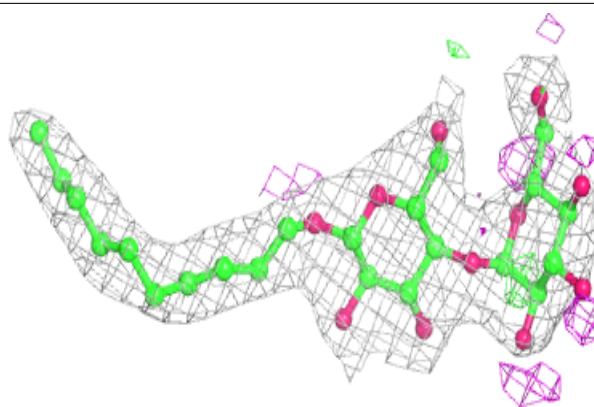
**Electron density around DMU C 568:**

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

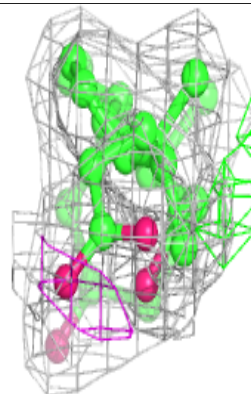
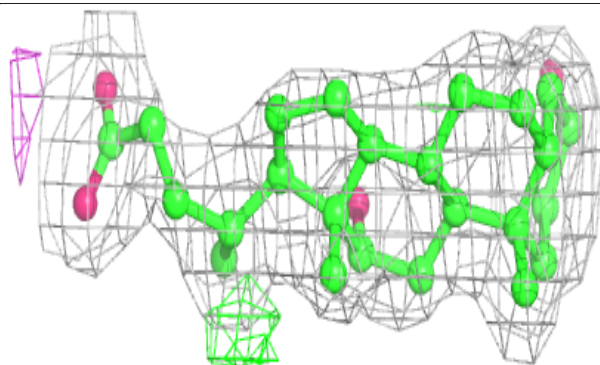
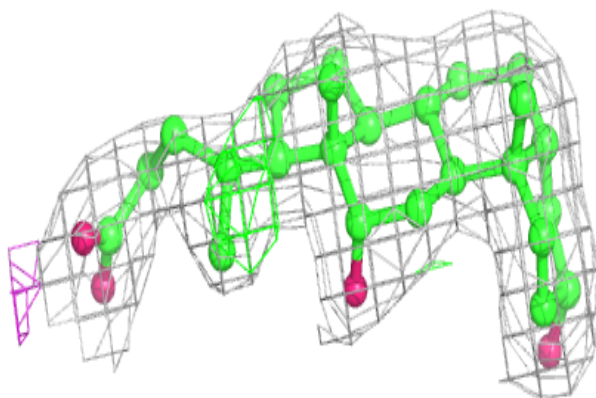


**Electron density around DMU A 567:**

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

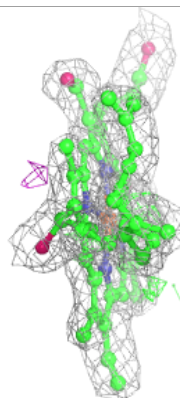
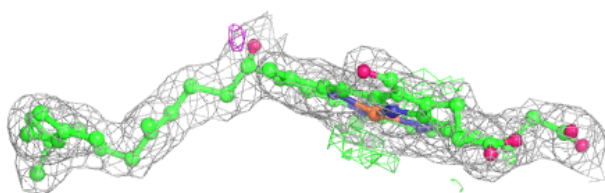
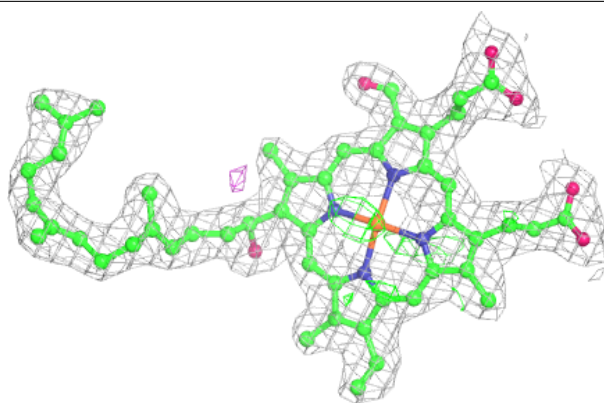
**Electron density around DXC C 576:**

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

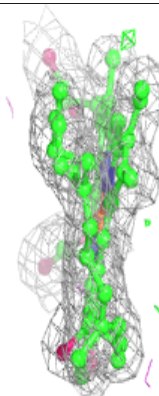
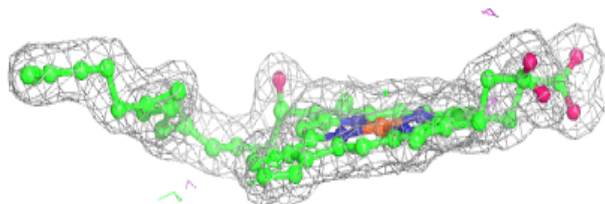
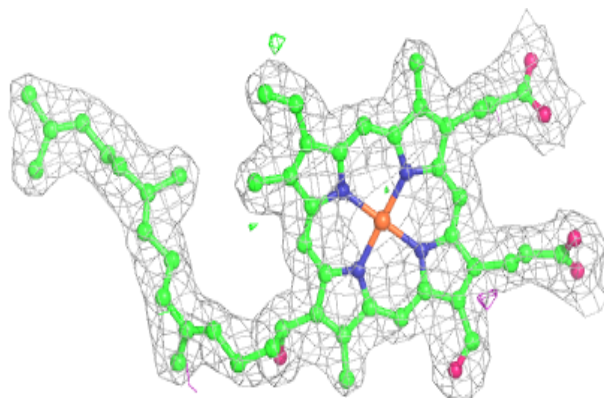


**Electron density around HEA A 1503:**

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

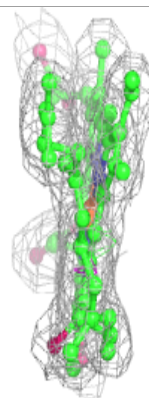
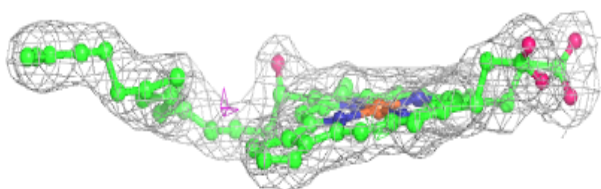
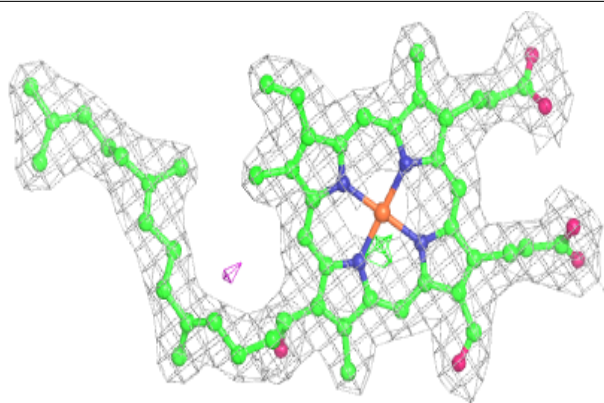
**Electron density around HEA C 574:**

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

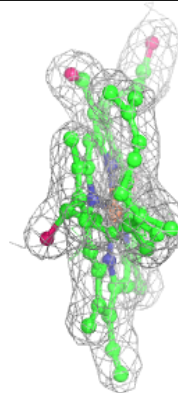
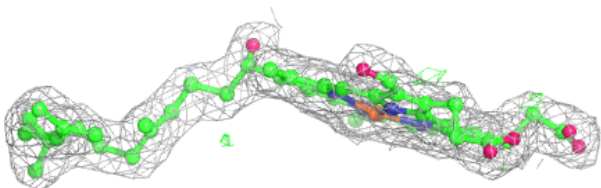
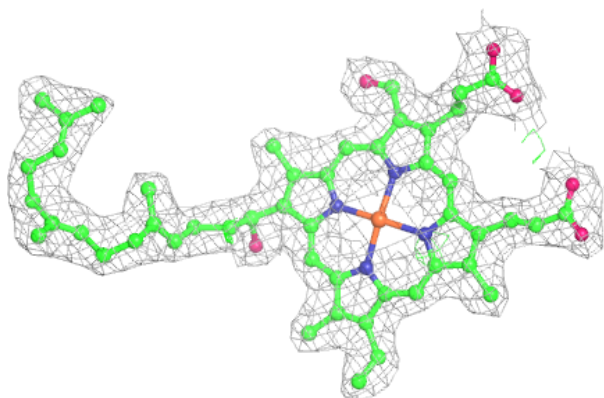


**Electron density around HEA A 1502:**

$2mF_o-DF_c$  (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

There are no such residues in this entry.