



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 01:51 PM EDT

PDB ID : 2GSM  
Title : Catalytic Core (Subunits I and II) of Cytochrome c oxidase from Rhodobacter sphaeroides  
Authors : Qin, L.; Hiser, C.; Mulichak, A.; Garavito, R.M.; Ferguson-Miller, S.  
Deposited on : 2006-04-26  
Resolution : 2.00 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.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

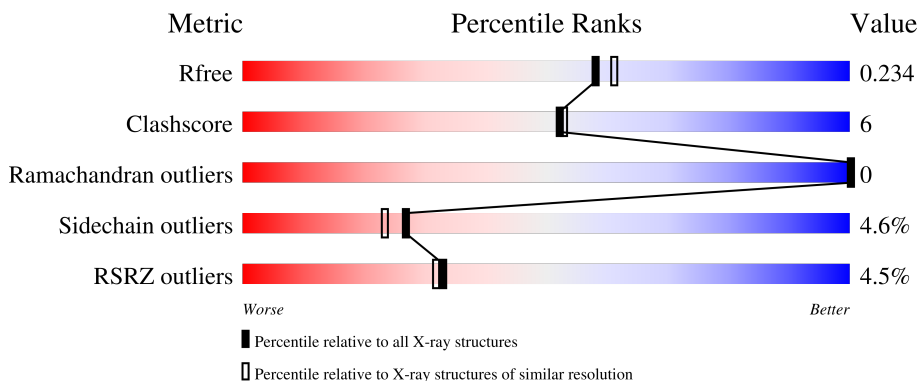
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	<div> <div>3%</div> <div>82%</div> <div>11%</div> <div>5%</div> </div>
1	C	566	<div> <div>7%</div> <div>81%</div> <div>12%</div> <div>6%</div> </div>
2	B	262	<div> <div>2%</div> <div>85%</div> <div>11%</div> <div>2%</div> </div>
2	D	262	<div> <div>3%</div> <div>85%</div> <div>11%</div> <div>2%</div> </div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13644 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	535	Total	C	N	O	S	26	0	0
			4212	2822	663	696	31			
1	C	534	Total	C	N	O	S	44	0	0
			4201	2813	662	695	31			

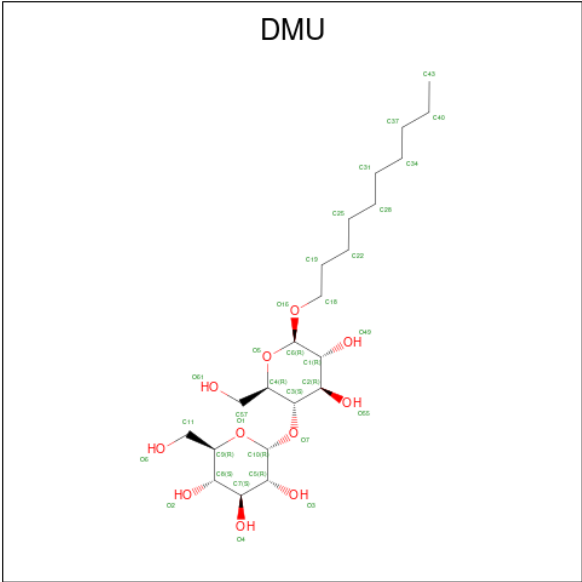
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	9	0	0
			2025	1321	333	365	6			
2	D	256	Total	C	N	O	S	13	0	0
			2025	1321	333	365	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
			33	22	11		
3	A	1	Total	C	O	11	0
			33	22	11		
3	B	1	Total	C	O	0	0
			33	22	11		
3	B	1	Total	C	O	0	0
			23	12	11		
3	C	1	Total	C	O	0	0
			23	12	11		
3	C	1	Total	C	O	11	0
			33	22	11		
3	C	1	Total	C	O	0	0
			33	22	11		
3	D	1	Total	C	O	0	0
			23	12	11		
3	D	1	Total	C	O	0	0
			23	12	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		

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

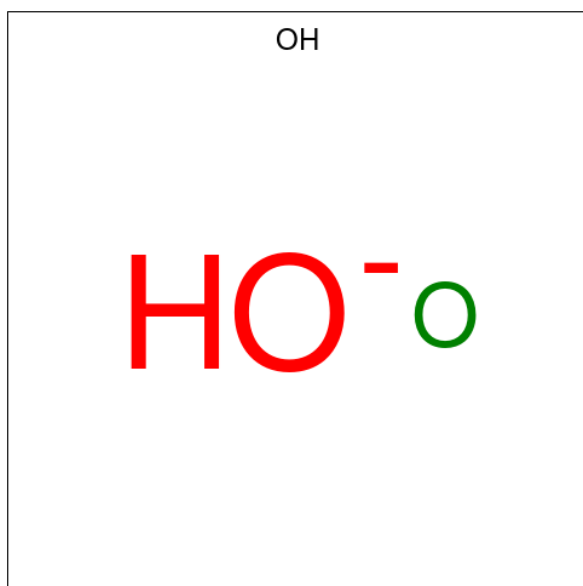
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

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



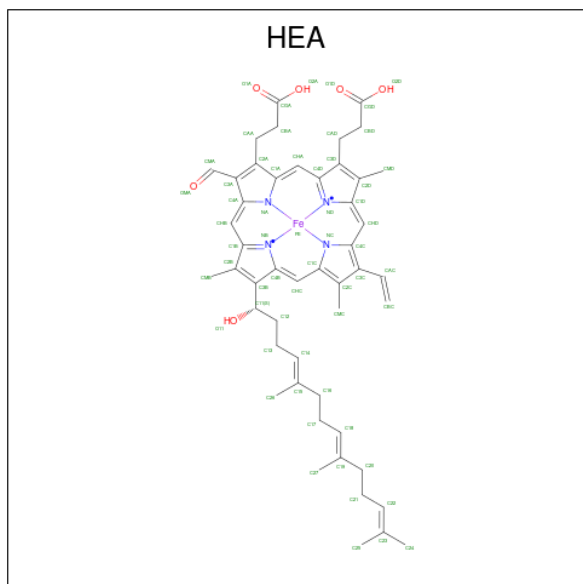
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	O 1	0	0

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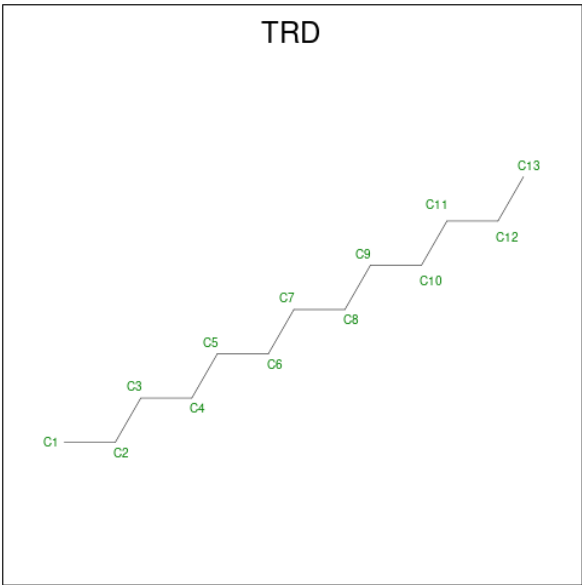
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total O 1 1	0	0

- Molecule 8 is HEME-A (three-letter code: HEA) (formula:  $\text{C}_{49}\text{H}_{56}\text{FeN}_4\text{O}_6$ ).



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

- Molecule 9 is TRIDECANE (three-letter code: TRD) (formula:  $\text{C}_{13}\text{H}_{28}$ ).



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

- Molecule 10 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 11 is water.

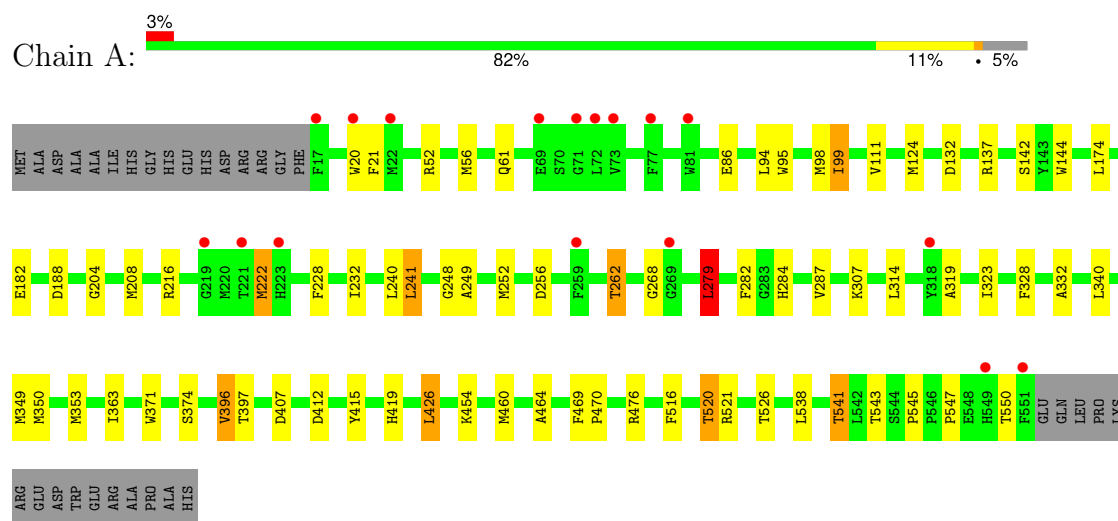
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	140	Total 140	O 140	0	0
11	B	142	Total 142	O 142	0	0
11	C	100	Total 100	O 100	0	0
11	D	121	Total 121	O 121	0	0



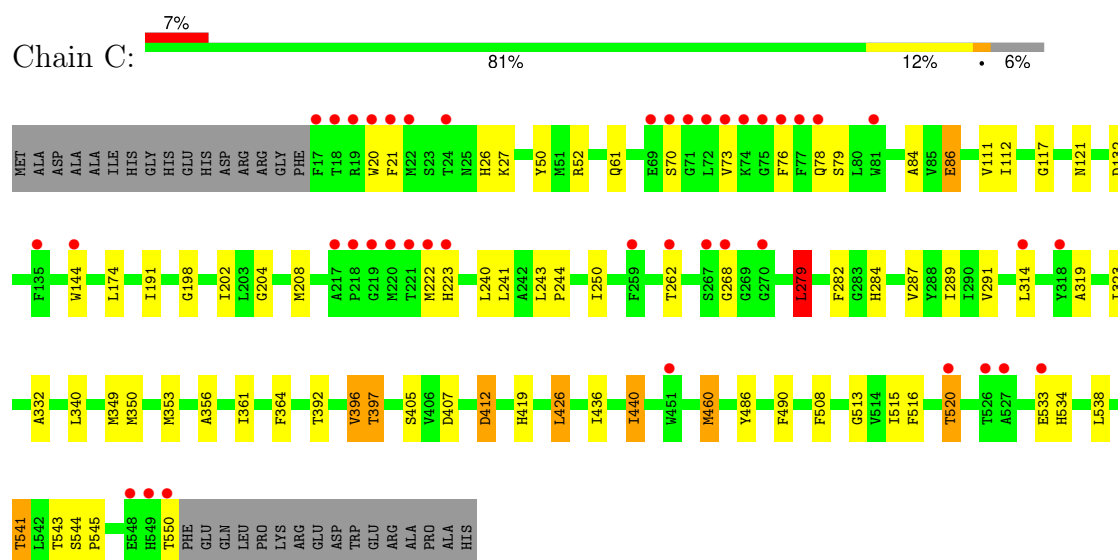
### 3 Residue-property plots [i](#)

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.

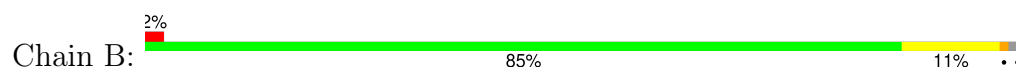
#### • Molecule 1: Cytochrome c oxidase subunit 1

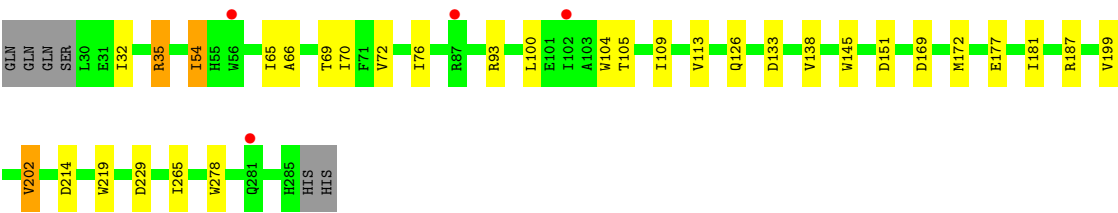


#### • Molecule 1: Cytochrome c oxidase subunit 1

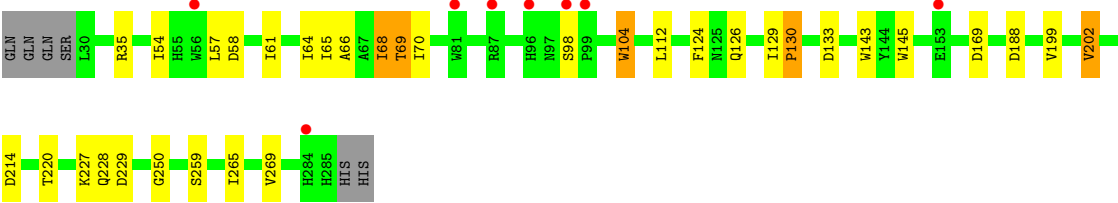
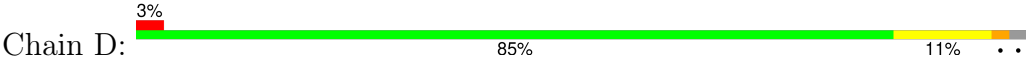


#### • Molecule 2: Cytochrome c oxidase subunit 2





● 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, $\alpha$ , $\beta$ , $\gamma$	125.02Å 131.64Å 176.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.91 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-2.00) 96.1 (19.91-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.24 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.214 , 0.232 0.215 , 0.234	Depositor DCC
$R_{free}$ test set	3780 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 66.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13644	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CA, HEA, CU, CD, OH, TRD, 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	0.60	0/4368	0.67	6/5961 (0.1%)
1	C	0.51	0/4356	0.63	5/5945 (0.1%)
2	B	0.53	0/2087	0.72	8/2857 (0.3%)
2	D	0.51	0/2087	0.69	5/2857 (0.2%)
All	All	0.54	0/12898	0.67	24/17620 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	229	ASP	CB-CG-OD2	8.12	125.61	118.30
1	A	407	ASP	CB-CG-OD2	6.63	124.27	118.30
2	D	169	ASP	CB-CG-OD2	6.37	124.03	118.30
2	B	214	ASP	CB-CG-OD2	6.26	123.93	118.30
2	B	133	ASP	CB-CG-OD2	6.15	123.83	118.30
2	D	229	ASP	CB-CG-OD2	6.09	123.78	118.30
2	D	58	ASP	CB-CG-OD2	5.99	123.69	118.30
1	C	132	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	426	LEU	CA-CB-CG	5.69	128.39	115.30
1	C	412	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	188	ASP	CB-CG-OD2	5.50	123.25	118.30
2	B	169	ASP	CB-CG-OD2	5.38	123.14	118.30
2	D	133	ASP	CB-CG-OD2	5.36	123.13	118.30
1	C	426	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	256	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	279	LEU	CA-CB-CG	-5.26	103.20	115.30
1	C	407	ASP	CB-CG-OD2	5.19	122.97	118.30
2	B	93	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	132	ASP	CB-CG-OD2	5.16	122.94	118.30
2	D	188	ASP	CB-CG-OD2	5.09	122.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	93	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	B	202	VAL	CB-CA-C	-5.05	101.80	111.40
2	B	151	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	279	LEU	CA-CB-CG	-5.01	103.78	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4212	0	4134	53	0
1	C	4201	0	4125	48	0
2	B	2025	0	1982	20	0
2	D	2025	0	1982	19	0
3	A	99	0	126	0	0
3	B	56	0	63	3	0
3	C	89	0	105	2	0
3	D	46	0	42	2	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	120	0	108	7	0
8	C	120	0	108	4	0
9	A	59	0	125	4	0
9	B	9	0	17	2	0
9	C	44	0	90	2	0
9	D	20	0	41	0	0
10	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	2	0	0	0	0
11	A	140	0	0	3	0
11	B	142	0	0	1	0
11	C	100	0	0	2	0
11	D	121	0	0	1	0
All	All	13644	0	13048	143	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 6.

All (143) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PHE:CE2	1:A:232:ILE:HD11	1.96	1.00
1:A:350:MET:HA	1:A:353:MET:HE3	1.51	0.91
1:C:397:THR:HG22	1:C:419:HIS:HB2	1.54	0.90
7:A:6501:OH:O	11:A:6506:HOH:O	1.95	0.83
1:A:460:MET:CE	1:A:464:ALA:HB2	2.08	0.83
7:C:7501:OH:O	11:C:1006:HOH:O	1.97	0.81
1:A:460:MET:HE2	1:A:464:ALA:HB2	1.62	0.81
2:B:54:ILE:HD11	2:B:126:GLN:HE21	1.46	0.81
8:A:2002:HEA:HMC1	8:A:2002:HEA:HBC1	1.63	0.80
1:A:21:PHE:HB3	1:A:144:TRP:HZ2	1.48	0.79
1:C:397:THR:CG2	1:C:419:HIS:HB2	2.13	0.79
1:C:350:MET:HA	1:C:353:MET:HE3	1.64	0.77
1:A:543:THR:HG23	1:A:545:PRO:O	1.85	0.77
1:A:550:THR:OG1	11:A:6611:HOH:O	2.05	0.75
1:C:543:THR:HG23	1:C:545:PRO:O	1.88	0.74
8:A:2001:HEA:HBC1	8:A:2001:HEA:HMC1	1.70	0.73
2:B:65:ILE:O	2:B:69:THR:HG23	1.88	0.73
2:B:32:ILE:HG22	2:B:35:ARG:HD3	1.70	0.73
1:A:319:ALA:O	1:A:323:ILE:HG12	1.90	0.72
1:C:84:ALA:HB1	1:C:86:GLU:OE1	1.90	0.72
1:C:460:MET:HE3	1:C:460:MET:HA	1.72	0.71
1:C:319:ALA:O	1:C:323:ILE:HG12	1.93	0.68
8:C:3001:HEA:HMC1	8:C:3001:HEA:HBC1	1.74	0.68
1:A:228:PHE:CZ	1:A:232:ILE:HD11	2.30	0.66
1:A:21:PHE:HB3	1:A:144:TRP:CZ2	2.31	0.66
1:C:515:ILE:HD13	3:C:6004:DMU:H20	1.78	0.66
1:A:396:VAL:HG13	2:B:65:ILE:HB	1.76	0.66
1:A:124:MET:HB2	1:A:232:ILE:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:ILE:O	2:D:69:THR:HG23	1.97	0.64
2:B:54:ILE:HD11	2:B:126:GLN:NE2	2.12	0.63
1:A:350:MET:HA	1:A:353:MET:CE	2.28	0.63
2:D:64:ILE:O	2:D:68:ILE:HD13	1.97	0.63
1:C:516:PHE:O	1:C:520:THR:HB	1.98	0.63
1:C:533:GLU:H	1:C:533:GLU:CD	2.02	0.61
1:A:332:ALA:HB1	1:A:340:LEU:HD11	1.83	0.60
1:C:86:GLU:H	1:C:86:GLU:CD	2.04	0.60
2:D:54:ILE:HD11	2:D:126:GLN:HE21	1.67	0.60
1:C:50:TYR:OH	1:C:79:SER:HB2	2.01	0.60
8:A:2002:HEA:HMC1	8:A:2002:HEA:CBC	2.32	0.60
2:D:202:VAL:HG13	2:D:269:VAL:HG12	1.83	0.59
1:A:86:GLU:H	1:A:86:GLU:CD	2.06	0.59
1:A:516:PHE:O	1:A:520:THR:HB	2.03	0.59
1:A:538:LEU:O	1:A:541:THR:HB	2.02	0.59
1:C:405:SER:O	2:D:54:ILE:HD12	2.03	0.58
1:C:287:VAL:HB	8:C:3002:HEA:CAC	2.33	0.58
1:A:543:THR:HG22	1:A:547:PRO:HD3	1.86	0.58
2:B:113:VAL:HA	9:B:5008:TRD:H41	1.85	0.58
2:D:57:LEU:O	2:D:61:ILE:HG12	2.04	0.57
1:A:204:GLY:O	1:A:208:MET:HG2	2.04	0.57
1:A:249:ALA:HA	1:A:252:MET:HE3	1.87	0.57
2:D:54:ILE:HD11	2:D:126:GLN:NE2	2.20	0.56
1:A:287:VAL:HB	8:A:2002:HEA:CAC	2.36	0.56
1:C:332:ALA:HB1	1:C:340:LEU:HD11	1.88	0.56
2:D:228:GLN:NE2	11:D:1207:HOH:O	2.38	0.55
2:B:145:TRP:NE1	2:B:265:ILE:HD11	2.21	0.55
1:A:396:VAL:CG1	2:B:65:ILE:HB	2.37	0.54
1:A:397:THR:HG22	1:A:419:HIS:HB2	1.89	0.54
1:A:520:THR:HG22	1:A:521:ARG:HG2	1.88	0.54
1:A:248:GLY:O	1:A:252:MET:HG3	2.06	0.54
2:B:100:LEU:HD22	3:B:5003:DMU:H9	1.89	0.53
1:C:117:GLY:O	1:C:121:ASN:HB2	2.07	0.53
3:D:6003:DMU:H35	3:D:6003:DMU:H29	1.89	0.53
2:B:100:LEU:HD21	3:B:5003:DMU:H12	1.91	0.53
1:C:396:VAL:HG13	2:D:65:ILE:HD12	1.89	0.52
1:C:350:MET:HA	1:C:353:MET:CE	2.36	0.51
1:C:513:GLY:HA3	9:C:6001:TRD:H111	1.92	0.51
1:C:534:HIS:ND1	11:C:1405:HOH:O	2.34	0.51
1:C:392:THR:O	1:C:396:VAL:HB	2.11	0.51
1:C:460:MET:HA	1:C:460:MET:CE	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PHE:CE2	1:A:232:ILE:CD1	2.84	0.50
2:B:199:VAL:HG13	2:B:278:TRP:CE2	2.47	0.50
1:C:349:MET:HG2	1:C:353:MET:CE	2.42	0.50
1:A:262:THR:HG21	1:A:268:GLY:HA3	1.94	0.49
2:B:145:TRP:CE2	2:B:265:ILE:HD11	2.47	0.49
2:B:35:ARG:HD2	11:B:5065:HOH:O	2.12	0.49
1:C:26:HIS:CE1	1:C:27:LYS:HG3	2.47	0.49
1:C:262:THR:OG1	1:C:268:GLY:HA3	2.12	0.49
1:A:454:LYS:HE3	11:A:6636:HOH:O	2.12	0.49
1:A:476:ARG:HH21	9:A:5007:TRD:H21	1.78	0.49
2:B:72:VAL:O	2:B:76:ILE:HG12	2.13	0.49
1:A:94:LEU:O	1:A:98:MET:HG2	2.13	0.48
3:C:6005:DMU:H14	9:C:6006:TRD:H101	1.96	0.48
1:C:396:VAL:HG13	2:D:65:ILE:HB	1.95	0.48
1:C:508:PHE:HB2	8:C:3001:HEA:H261	1.96	0.48
1:A:349:MET:O	1:A:353:MET:HE2	2.14	0.47
1:C:191:ILE:HG23	1:C:250:ILE:HB	1.96	0.47
1:A:287:VAL:HB	8:A:2002:HEA:C3C	2.44	0.47
1:A:95:TRP:CE2	1:A:99:ILE:HD13	2.49	0.47
8:A:2002:HEA:HBC1	8:A:2002:HEA:CMC	2.41	0.47
1:C:436:ILE:O	1:C:440:ILE:HB	2.14	0.47
1:A:262:THR:O	1:A:262:THR:CG2	2.63	0.47
1:C:538:LEU:O	1:C:541:THR:HB	2.14	0.47
2:D:145:TRP:CE2	2:D:265:ILE:HD11	2.50	0.46
1:A:397:THR:HG23	1:A:415:TYR:CE1	2.50	0.46
1:C:112:ILE:HD13	1:C:289:ILE:HG22	1.96	0.46
9:A:5005:TRD:H61	9:A:5006:TRD:H52	1.97	0.46
1:C:364:PHE:HB3	2:D:104:TRP:CE3	2.51	0.46
2:D:124:PHE:HB3	3:D:6011:DMU:H5	1.98	0.46
1:A:279:LEU:O	1:A:279:LEU:HG	2.11	0.45
1:C:287:VAL:HB	8:C:3002:HEA:HAC	1.99	0.45
9:A:5005:TRD:H81	9:A:5006:TRD:H72	1.98	0.45
1:A:314:LEU:HD12	1:A:314:LEU:HA	1.87	0.45
1:A:350:MET:HG2	9:B:5008:TRD:H51	1.98	0.45
1:C:349:MET:O	1:C:353:MET:HE2	2.16	0.45
1:A:262:THR:O	1:A:262:THR:HG23	2.17	0.45
1:C:279:LEU:O	1:C:279:LEU:HG	2.14	0.45
1:A:216:ARG:CZ	1:A:222:MET:HE3	2.47	0.45
2:D:66:ALA:O	2:D:70:ILE:HG12	2.17	0.45
1:A:476:ARG:NH2	9:A:5007:TRD:H21	2.32	0.44
1:C:544:SER:HA	1:C:545:PRO:HA	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ALA:HA	1:A:252:MET:CE	2.47	0.44
1:A:371:TRP:CG	3:B:5003:DMU:H10	2.52	0.44
1:C:284:HIS:CD2	1:C:284:HIS:C	2.90	0.44
1:A:241:LEU:HD13	1:A:328:PHE:CE1	2.53	0.44
1:C:21:PHE:HB3	1:C:144:TRP:HZ2	1.83	0.43
2:D:129:ILE:HA	2:D:130:PRO:HD3	1.82	0.43
1:C:204:GLY:O	1:C:208:MET:HG2	2.18	0.43
1:A:460:MET:HE1	1:A:464:ALA:HB2	1.96	0.43
1:C:349:MET:HG2	1:C:353:MET:HE1	2.01	0.43
1:A:284:HIS:CD2	1:A:284:HIS:C	2.92	0.42
1:A:363:ILE:HD13	8:A:2002:HEA:H172	2.01	0.42
2:B:105:THR:O	2:B:109:ILE:HG13	2.19	0.42
1:A:241:LEU:HB3	1:A:328:PHE:CZ	2.54	0.42
1:A:460:MET:HE2	1:A:464:ALA:CB	2.43	0.42
1:C:356:ALA:HB3	2:D:112:LEU:HD11	2.01	0.42
1:C:284:HIS:O	1:C:287:VAL:HG22	2.19	0.42
1:A:469:PHE:N	1:A:470:PRO:CD	2.83	0.42
1:A:349:MET:HG2	1:A:353:MET:HE2	2.02	0.41
2:B:54:ILE:HD13	2:B:54:ILE:N	2.34	0.41
2:B:66:ALA:O	2:B:70:ILE:HG12	2.20	0.41
1:C:396:VAL:CG1	2:D:65:ILE:HB	2.51	0.41
2:B:138:VAL:HG11	2:B:219:TRP:CD1	2.55	0.41
2:B:177:GLU:O	2:B:181:ILE:HG12	2.21	0.41
2:B:172:MET:HG2	2:B:187:ARG:HH21	1.85	0.41
1:C:223:HIS:CD2	1:C:314:LEU:HD11	2.56	0.41
1:C:486:TYR:CD2	1:C:490:PHE:HB2	2.55	0.41
2:D:143:TRP:CG	2:D:259:SER:HB2	2.55	0.41
2:D:220:THR:O	2:D:250:GLY:HA3	2.21	0.41
1:C:198:GLY:O	1:C:202:ILE:HG12	2.21	0.40
1:C:73:VAL:O	1:C:76:PHE:HB3	2.20	0.40
1:A:262:THR:CG2	1:A:268:GLY:HA3	2.51	0.40
1:A:307:LYS:HE2	1:A:374:SER:HB3	2.03	0.40
1:C:243:LEU:N	1:C:244:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	533/566 (94%)	520 (98%)	13 (2%)	0	100	100
1	C	532/566 (94%)	519 (98%)	13 (2%)	0	100	100
2	B	254/262 (97%)	248 (98%)	6 (2%)	0	100	100
2	D	254/262 (97%)	247 (97%)	7 (3%)	0	100	100
All	All	1573/1656 (95%)	1534 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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	435/459 (95%)	413 (95%)	22 (5%)	24	19
1	C	434/459 (95%)	410 (94%)	24 (6%)	21	17
2	B	215/221 (97%)	211 (98%)	4 (2%)	57	61
2	D	215/221 (97%)	205 (95%)	10 (5%)	26	22
All	All	1299/1360 (96%)	1239 (95%)	60 (5%)	27	23

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	TRP
1	A	52	ARG

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Mol	Chain	Res	Type
1	A	56	MET
1	A	61	GLN
1	A	99	ILE
1	A	111	VAL
1	A	137	ARG
1	A	142	SER
1	A	174	LEU
1	A	182	GLU
1	A	222	MET
1	A	240	LEU
1	A	241	LEU
1	A	262	THR
1	A	279	LEU
1	A	282	PHE
1	A	396	VAL
1	A	412	ASP
1	A	426	LEU
1	A	520	THR
1	A	526	THR
1	A	541	THR
2	B	35	ARG
2	B	54	ILE
2	B	104	TRP
2	B	202	VAL
1	C	20	TRP
1	C	52	ARG
1	C	61	GLN
1	C	70	SER
1	C	78	GLN
1	C	86	GLU
1	C	111	VAL
1	C	174	LEU
1	C	222	MET
1	C	240	LEU
1	C	241	LEU
1	C	279	LEU
1	C	282	PHE
1	C	291	VAL
1	C	361	ILE
1	C	396	VAL
1	C	397	THR
1	C	412	ASP

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Mol	Chain	Res	Type
1	C	426	LEU
1	C	440	ILE
1	C	460	MET
1	C	520	THR
1	C	541	THR
1	C	550	THR
2	D	35	ARG
2	D	68	ILE
2	D	69	THR
2	D	98	SER
2	D	104	TRP
2	D	130	PRO
2	D	199	VAL
2	D	202	VAL
2	D	214	ASP
2	D	227	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	534	HIS
2	B	209	GLN
2	B	228	GLN
2	B	251	GLN
1	C	26	HIS
1	C	127	HIS
1	C	223	HIS
2	D	88	ASN
2	D	237	GLN
2	D	251	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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 14 are monoatomic and 2 are modelled with single atom - leaving 26 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	5011	-	24,24,34	0.60	0	35,35,45	1.21	4 (11%)
3	DMU	D	6003	-	24,24,34	0.57	0	35,35,45	0.78	1 (2%)
9	TRD	A	5007	-	12,12,12	0.22	0	11,11,11	0.51	0
8	HEA	A	2001	1	58,67,67	1.45	6 (10%)	63,103,103	1.19	6 (9%)
3	DMU	B	5003	-	34,34,34	0.53	0	45,45,45	0.68	0
9	TRD	D	6008	-	6,6,12	0.25	0	5,5,11	0.41	0
3	DMU	C	6002	-	24,24,34	0.58	0	35,35,45	0.71	0
3	DMU	A	5001	-	34,34,34	0.50	0	45,45,45	1.02	1 (2%)
9	TRD	D	6007	-	12,12,12	0.24	0	11,11,11	0.62	0
8	HEA	A	2002	11,1	58,67,67	1.40	9 (15%)	63,103,103	1.70	13 (20%)
9	TRD	B	5008	-	8,8,12	0.27	0	7,7,11	0.48	0
3	DMU	A	5004	-	34,34,34	0.51	0	45,45,45	0.98	4 (8%)
3	DMU	C	6004	-	34,34,34	0.66	1 (2%)	45,45,45	0.87	1 (2%)
3	DMU	D	6011	-	24,24,34	0.56	0	35,35,45	1.30	6 (17%)
9	TRD	C	6001	-	12,12,12	0.31	0	11,11,11	0.51	0
8	HEA	C	3001	1	58,67,67	1.47	4 (6%)	63,103,103	1.19	6 (9%)
9	TRD	C	6009	-	8,8,12	0.30	0	7,7,11	0.48	0
9	TRD	A	5005	-	12,12,12	0.28	0	11,11,11	0.57	0
8	HEA	C	3002	11,1	58,67,67	1.48	6 (10%)	63,103,103	1.60	12 (19%)
9	TRD	A	5006	-	12,12,12	0.28	0	11,11,11	0.54	0
3	DMU	C	6005	-	34,34,34	0.69	1 (2%)	45,45,45	1.49	10 (22%)
3	DMU	A	5002	-	34,34,34	0.57	1 (2%)	45,45,45	0.96	3 (6%)
9	TRD	C	6010	-	8,8,12	0.31	0	7,7,11	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	TRD	A	5009	-	6,6,12	0.32	0	5,5,11	0.39	0
9	TRD	A	5010	-	12,12,12	0.27	0	11,11,11	0.56	0
9	TRD	C	6006	-	12,12,12	0.27	0	11,11,11	0.61	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	5011	-	-	4/8/48/59	0/2/2/2
3	DMU	D	6003	-	-	3/8/48/59	0/2/2/2
9	TRD	A	5007	-	-	5/10/10/10	-
8	HEA	A	2001	1	-	6/32/76/76	-
3	DMU	B	5003	-	-	7/19/59/59	0/2/2/2
9	TRD	D	6008	-	-	1/4/4/10	-
3	DMU	C	6002	-	-	4/8/48/59	0/2/2/2
3	DMU	A	5001	-	-	3/19/59/59	0/2/2/2
9	TRD	D	6007	-	-	6/10/10/10	-
8	HEA	A	2002	11,1	-	4/32/76/76	-
9	TRD	B	5008	-	-	4/6/6/10	-
3	DMU	A	5004	-	-	6/19/59/59	0/2/2/2
3	DMU	C	6004	-	-	9/19/59/59	0/2/2/2
3	DMU	D	6011	-	-	4/8/48/59	0/2/2/2
9	TRD	C	6001	-	-	3/10/10/10	-
8	HEA	C	3001	1	-	6/32/76/76	-
9	TRD	C	6009	-	-	2/6/6/10	-
9	TRD	A	5005	-	-	2/10/10/10	-
8	HEA	C	3002	11,1	-	4/32/76/76	-
9	TRD	A	5006	-	-	5/10/10/10	-
3	DMU	C	6005	-	-	9/19/59/59	0/2/2/2
3	DMU	A	5002	-	-	10/19/59/59	0/2/2/2
9	TRD	C	6010	-	-	4/6/6/10	-
9	TRD	A	5009	-	-	1/4/4/10	-
9	TRD	A	5010	-	-	6/10/10/10	-
9	TRD	C	6006	-	-	2/10/10/10	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2001	HEA	C3A-C2A	-6.20	1.32	1.40
8	C	3001	HEA	C3A-C2A	-5.90	1.32	1.40
8	C	3002	HEA	C3A-C2A	-4.35	1.34	1.40
8	C	3001	HEA	C3C-C2C	-4.21	1.34	1.40
8	A	2001	HEA	C3C-C2C	-4.01	1.34	1.40
8	C	3002	HEA	C3C-C2C	-3.92	1.35	1.40
8	C	3002	HEA	C11-C3B	3.79	1.56	1.51
8	A	2002	HEA	C3A-C2A	-3.73	1.35	1.40
8	A	2002	HEA	C3C-C2C	-3.50	1.35	1.40
8	C	3001	HEA	C11-C3B	3.39	1.55	1.51
8	C	3002	HEA	C3A-C4A	3.20	1.46	1.41
8	A	2002	HEA	C11-C3B	3.15	1.55	1.51
8	C	3001	HEA	C3A-C4A	2.92	1.45	1.41
8	A	2002	HEA	FE-NB	2.85	2.13	1.98
8	A	2002	HEA	C3A-C4A	2.76	1.45	1.41
8	A	2001	HEA	C11-C3B	2.72	1.54	1.51
8	C	3002	HEA	FE-NB	2.49	2.11	1.98
8	A	2002	HEA	C3A-CMA	2.40	1.52	1.46
8	A	2001	HEA	C3A-C4A	2.37	1.44	1.41
8	C	3002	HEA	CHD-C1D	2.29	1.40	1.34
8	A	2002	HEA	CHD-C1D	2.20	1.40	1.34
3	C	6005	DMU	O16-C6	2.15	1.43	1.40
8	A	2001	HEA	C3A-CMA	2.13	1.51	1.46
3	C	6004	DMU	O16-C6	2.13	1.43	1.40
3	A	5002	DMU	O16-C6	2.12	1.43	1.40
8	A	2002	HEA	CMD-C2D	2.04	1.54	1.50
8	A	2002	HEA	FE-ND	2.03	2.09	1.98
8	A	2001	HEA	CMD-C2D	2.01	1.54	1.50

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	6005	DMU	C10-O7-C3	-4.22	107.96	117.98
8	A	2002	HEA	C4A-CHB-C1B	4.19	128.09	122.56
8	A	2002	HEA	C4B-NB-C1B	4.08	110.04	105.21
8	C	3002	HEA	C4D-CHA-C1A	4.06	127.92	122.56
8	A	2002	HEA	CAD-CBD-CGD	-3.92	103.27	113.67
8	C	3002	HEA	C1D-ND-C4D	3.51	109.36	105.21
8	A	2002	HEA	C1D-ND-C4D	3.47	109.31	105.21
8	A	2001	HEA	C27-C19-C20	3.43	121.18	115.23
8	C	3002	HEA	C4B-NB-C1B	3.41	109.25	105.21
8	C	3002	HEA	C4A-CHB-C1B	3.27	126.87	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	6005	DMU	O1-C9-C8	3.05	115.20	109.70
8	A	2002	HEA	C3D-C4D-ND	-3.02	107.43	110.35
8	C	3001	HEA	C27-C19-C20	3.02	120.46	115.23
8	A	2001	HEA	C17-C18-C19	-2.98	120.80	127.62
8	C	3002	HEA	CAD-CBD-CGD	-2.91	105.94	113.67
8	A	2001	HEA	C12-C11-C3B	-2.90	107.59	112.12
3	C	6005	DMU	C2-C3-C4	-2.89	104.52	110.93
8	C	3002	HEA	CMC-C2C-C1C	-2.86	124.26	128.46
8	C	3001	HEA	C13-C14-C15	-2.85	121.09	127.62
8	A	2002	HEA	C2B-C1B-NB	-2.81	106.66	109.90
8	C	3002	HEA	C3D-C4D-ND	-2.81	107.64	110.35
8	C	3002	HEA	CBA-CAA-C2A	-2.73	108.06	112.55
3	C	6005	DMU	O1-C10-C5	2.72	115.96	110.37
8	C	3001	HEA	C12-C11-C3B	-2.67	107.94	112.12
8	A	2002	HEA	CMC-C2C-C1C	-2.67	124.54	128.46
8	A	2002	HEA	C3B-C4B-NB	-2.67	106.77	109.84
3	D	6011	DMU	C10-O1-C9	2.66	118.91	113.72
8	A	2002	HEA	C4D-CHA-C1A	2.65	126.06	122.56
8	A	2001	HEA	CMC-C2C-C1C	-2.63	124.61	128.46
8	C	3001	HEA	CMC-C2C-C1C	-2.57	124.69	128.46
3	D	6011	DMU	O5-C6-C1	-2.57	105.78	110.30
3	A	5004	DMU	C10-O7-C3	-2.55	111.93	117.98
8	C	3002	HEA	C27-C19-C20	2.54	119.64	115.23
3	D	6011	DMU	O7-C3-C4	-2.54	102.81	109.48
3	C	6005	DMU	C10-O1-C9	2.50	118.60	113.72
3	B	5011	DMU	O5-C6-C1	-2.49	105.92	110.30
3	B	5011	DMU	O5-C4-C3	2.48	114.85	109.72
8	A	2002	HEA	CMB-C2B-C3B	-2.48	125.48	130.28
3	C	6004	DMU	C10-O7-C3	-2.47	112.11	117.98
3	C	6005	DMU	O7-C10-C5	2.47	114.16	108.09
8	C	3002	HEA	C2D-C1D-ND	-2.45	107.02	109.84
3	A	5004	DMU	O16-C6-C1	2.45	111.99	108.27
3	D	6011	DMU	O5-C4-C3	2.44	114.77	109.72
8	A	2002	HEA	C2D-C1D-ND	-2.43	107.04	109.84
3	A	5002	DMU	C10-O1-C9	2.42	118.45	113.72
3	A	5002	DMU	C10-O7-C3	-2.37	112.36	117.98
3	D	6011	DMU	C2-C3-C4	2.36	116.17	110.93
3	A	5004	DMU	C18-O16-C6	-2.33	109.70	113.68
8	A	2002	HEA	C27-C19-C20	2.32	119.26	115.23
8	C	3001	HEA	C17-C18-C19	-2.30	122.36	127.62
3	A	5001	DMU	C10-O7-C3	-2.27	112.60	117.98
3	B	5011	DMU	C1-C2-C3	2.23	114.75	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2001	HEA	C27-C19-C18	-2.23	117.90	123.63
8	A	2002	HEA	C3A-C4A-NA	-2.22	106.76	110.94
3	B	5011	DMU	C2-C3-C4	2.21	115.83	110.93
3	C	6005	DMU	O7-C3-C4	2.19	115.22	109.48
3	D	6011	DMU	C1-C2-C3	2.19	114.64	109.68
3	A	5004	DMU	C2-C3-C4	-2.18	106.11	110.93
8	C	3002	HEA	C3B-C4B-NB	-2.16	107.35	109.84
8	C	3002	HEA	C2B-C1B-NB	-2.14	107.42	109.90
3	C	6005	DMU	C10-C5-C7	2.13	114.48	110.01
8	C	3001	HEA	C25-C23-C24	2.12	119.47	114.59
3	C	6005	DMU	O3-C5-C7	-2.11	105.41	110.38
8	A	2001	HEA	C13-C14-C15	-2.08	122.87	127.62
3	A	5002	DMU	O5-C4-C57	2.05	111.51	106.44
3	C	6005	DMU	O5-C4-C57	2.05	111.51	106.44
3	D	6003	DMU	O5-C4-C57	2.01	111.41	106.44

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5002	DMU	C19-C18-O16-C6
3	C	6005	DMU	O5-C6-O16-C18
3	B	5003	DMU	O6-C11-C9-C8
3	A	5002	DMU	O6-C11-C9-O1
3	B	5003	DMU	O6-C11-C9-O1
3	B	5011	DMU	O6-C11-C9-O1
3	D	6003	DMU	O6-C11-C9-O1
3	C	6002	DMU	O5-C4-C57-O61
3	A	5002	DMU	O6-C11-C9-C8
3	A	5002	DMU	O5-C6-O16-C18
3	C	6005	DMU	O5-C4-C57-O61
3	C	6004	DMU	O6-C11-C9-O1
3	C	6002	DMU	C3-C4-C57-O61
3	C	6004	DMU	O6-C11-C9-C8
3	A	5002	DMU	C1-C6-O16-C18
3	C	6005	DMU	C3-C4-C57-O61
3	B	5011	DMU	C3-C4-C57-O61
3	C	6002	DMU	O6-C11-C9-O1
3	B	5011	DMU	O6-C11-C9-C8
3	B	5003	DMU	O16-C18-C19-C22
3	C	6004	DMU	C1-C6-O16-C18
3	C	6005	DMU	C1-C6-O16-C18

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Mol	Chain	Res	Type	Atoms
3	C	6004	DMU	O5-C6-O16-C18
9	D	6008	TRD	C2-C3-C4-C5
3	B	5003	DMU	C25-C28-C31-C34
3	D	6011	DMU	O6-C11-C9-O1
3	A	5001	DMU	C19-C22-C25-C28
3	A	5002	DMU	C18-C19-C22-C25
9	D	6007	TRD	C2-C3-C4-C5
9	C	6001	TRD	C5-C6-C7-C8
9	C	6010	TRD	C4-C5-C6-C7
9	D	6007	TRD	C6-C7-C8-C9
3	D	6003	DMU	C3-C4-C57-O61
9	A	5010	TRD	C9-C10-C11-C12
3	C	6004	DMU	C19-C22-C25-C28
3	C	6004	DMU	C18-C19-C22-C25
9	A	5007	TRD	C11-C10-C9-C8
3	C	6005	DMU	O6-C11-C9-C8
3	A	5004	DMU	C1-C6-O16-C18
9	A	5006	TRD	C9-C10-C11-C12
3	B	5003	DMU	C18-C19-C22-C25
3	D	6003	DMU	O6-C11-C9-C8
9	A	5006	TRD	C11-C10-C9-C8
9	B	5008	TRD	C4-C5-C6-C7
3	A	5004	DMU	C25-C28-C31-C34
9	A	5007	TRD	C4-C5-C6-C7
9	A	5010	TRD	C2-C3-C4-C5
3	D	6011	DMU	O5-C4-C57-O61
3	C	6004	DMU	C25-C28-C31-C34
8	C	3001	HEA	C14-C15-C16-C17
9	A	5005	TRD	C2-C3-C4-C5
9	C	6009	TRD	C3-C4-C5-C6
8	C	3001	HEA	C26-C15-C16-C17
9	A	5006	TRD	C2-C3-C4-C5
3	D	6011	DMU	C2-C3-O7-C10
3	C	6004	DMU	C34-C37-C40-C43
9	A	5010	TRD	C4-C5-C6-C7
9	A	5009	TRD	C4-C5-C6-C7
3	A	5002	DMU	C31-C34-C37-C40
9	A	5007	TRD	C2-C3-C4-C5
3	C	6004	DMU	O16-C18-C19-C22
9	D	6007	TRD	C5-C6-C7-C8
3	C	6005	DMU	C31-C34-C37-C40
3	B	5003	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
9	C	6006	TRD	C2-C3-C4-C5
3	B	5011	DMU	O5-C4-C57-O61
9	A	5005	TRD	C4-C5-C6-C7
9	B	5008	TRD	C5-C6-C7-C8
9	C	6009	TRD	C4-C5-C6-C7
3	D	6011	DMU	C4-C3-O7-C10
9	D	6007	TRD	C4-C5-C6-C7
3	A	5004	DMU	O5-C6-O16-C18
9	C	6010	TRD	C6-C7-C8-C9
9	C	6001	TRD	C2-C3-C4-C5
9	C	6001	TRD	C4-C5-C6-C7
3	B	5003	DMU	C19-C22-C25-C28
9	B	5008	TRD	C3-C4-C5-C6
3	A	5002	DMU	O16-C18-C19-C22
9	D	6007	TRD	C11-C10-C9-C8
9	B	5008	TRD	C6-C7-C8-C9
9	D	6007	TRD	C9-C10-C11-C12
9	C	6010	TRD	C3-C4-C5-C6
9	A	5010	TRD	C1-C2-C3-C4
9	A	5007	TRD	C6-C7-C8-C9
3	A	5001	DMU	C28-C31-C34-C37
3	C	6005	DMU	C4-C3-O7-C10
9	A	5010	TRD	C11-C10-C9-C8
3	A	5004	DMU	O16-C18-C19-C22
3	A	5001	DMU	O5-C6-O16-C18
3	C	6005	DMU	C2-C3-O7-C10
3	C	6002	DMU	O6-C11-C9-C8
8	A	2001	HEA	C26-C15-C16-C17
9	A	5007	TRD	C10-C11-C12-C13
8	C	3002	HEA	CAA-CBA-CGA-O1A
8	A	2001	HEA	C14-C15-C16-C17
8	A	2002	HEA	CAA-CBA-CGA-O1A
3	A	5002	DMU	C22-C25-C28-C31
3	A	5002	DMU	C19-C22-C25-C28
8	A	2001	HEA	CAD-CBD-CGD-O2D
9	C	6006	TRD	C9-C10-C11-C12
8	A	2002	HEA	CAA-CBA-CGA-O2A
9	A	5006	TRD	C10-C11-C12-C13
8	A	2002	HEA	CAD-CBD-CGD-O1D
8	C	3002	HEA	CAD-CBD-CGD-O1D
8	A	2002	HEA	CAD-CBD-CGD-O2D
8	C	3002	HEA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
8	C	3002	HEA	CAD-CBD-CGD-O2D
8	C	3001	HEA	CAD-CBD-CGD-O2D
8	A	2001	HEA	CAD-CBD-CGD-O1D
8	C	3001	HEA	CAD-CBD-CGD-O1D
3	A	5004	DMU	C18-C19-C22-C25
3	C	6005	DMU	C25-C28-C31-C34
9	C	6010	TRD	C1-C2-C3-C4
8	A	2001	HEA	C16-C17-C18-C19
9	A	5006	TRD	C1-C2-C3-C4
3	A	5004	DMU	C19-C22-C25-C28
8	C	3001	HEA	CAA-CBA-CGA-O1A
9	A	5010	TRD	C5-C6-C7-C8
8	C	3001	HEA	CAA-CBA-CGA-O2A
8	A	2001	HEA	CAA-CBA-CGA-O1A

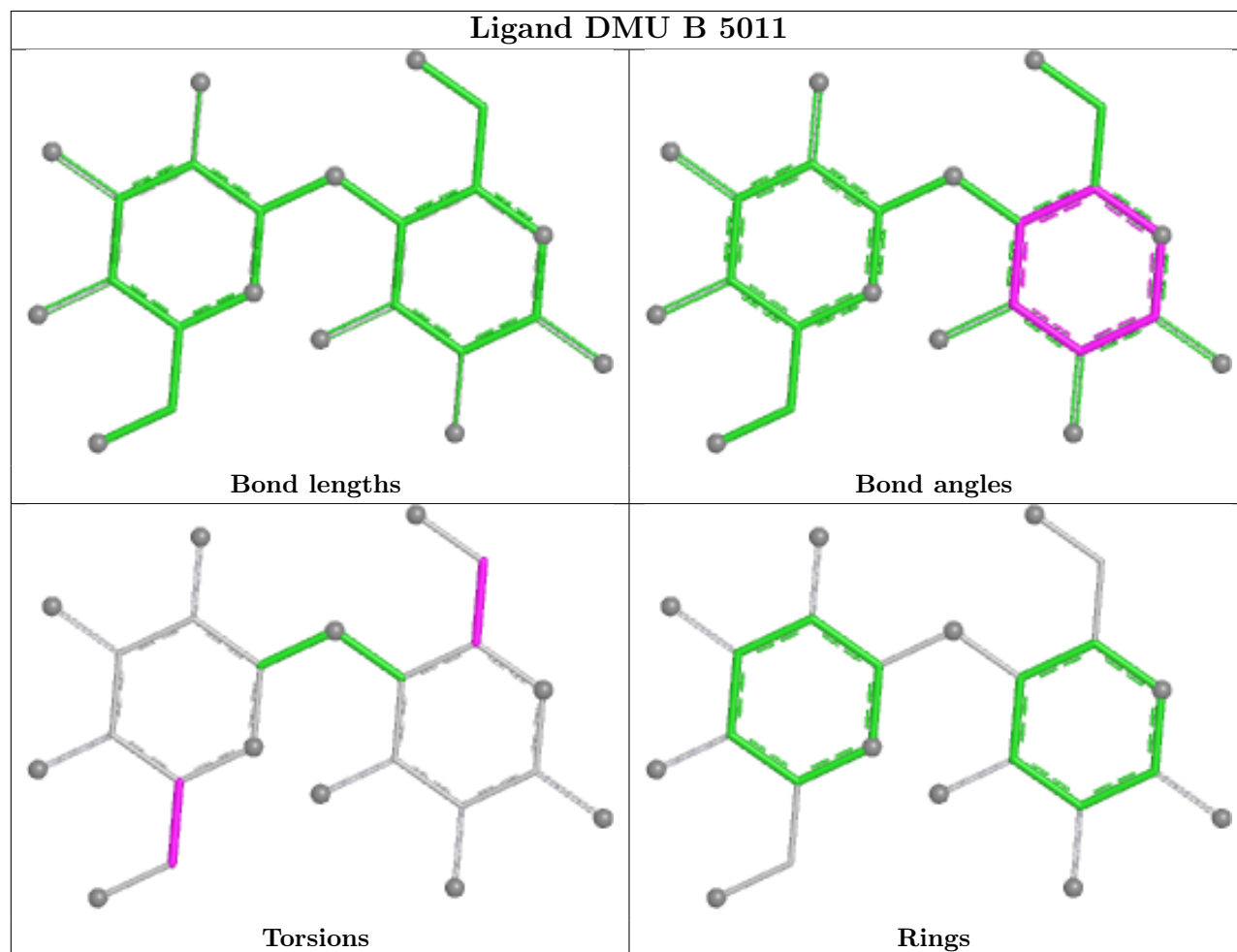
There are no ring outliers.

15 monomers are involved in 25 short contacts:

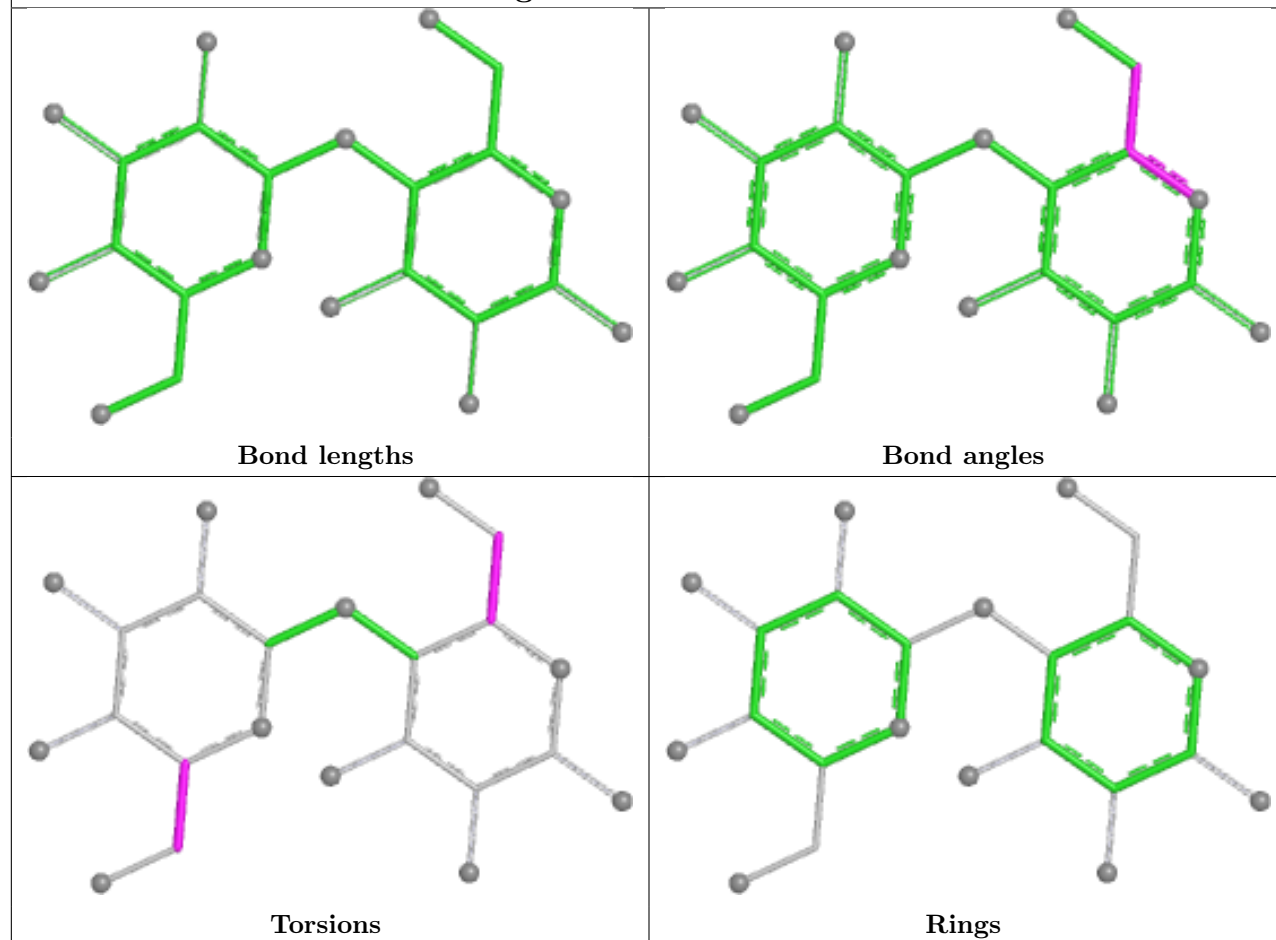
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	6003	DMU	1	0
9	A	5007	TRD	2	0
8	A	2001	HEA	1	0
3	B	5003	DMU	3	0
8	A	2002	HEA	6	0
9	B	5008	TRD	2	0
3	C	6004	DMU	1	0
3	D	6011	DMU	1	0
9	C	6001	TRD	1	0
8	C	3001	HEA	2	0
9	A	5005	TRD	2	0
8	C	3002	HEA	2	0
9	A	5006	TRD	2	0
3	C	6005	DMU	1	0
9	C	6006	TRD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

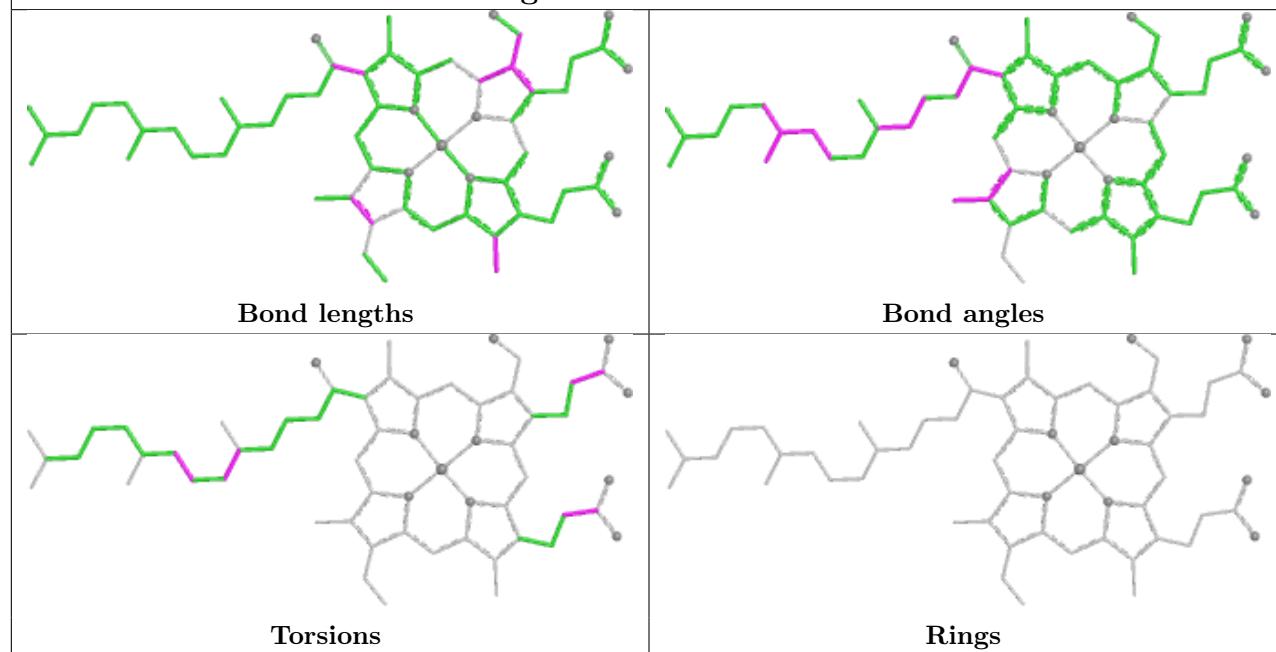
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

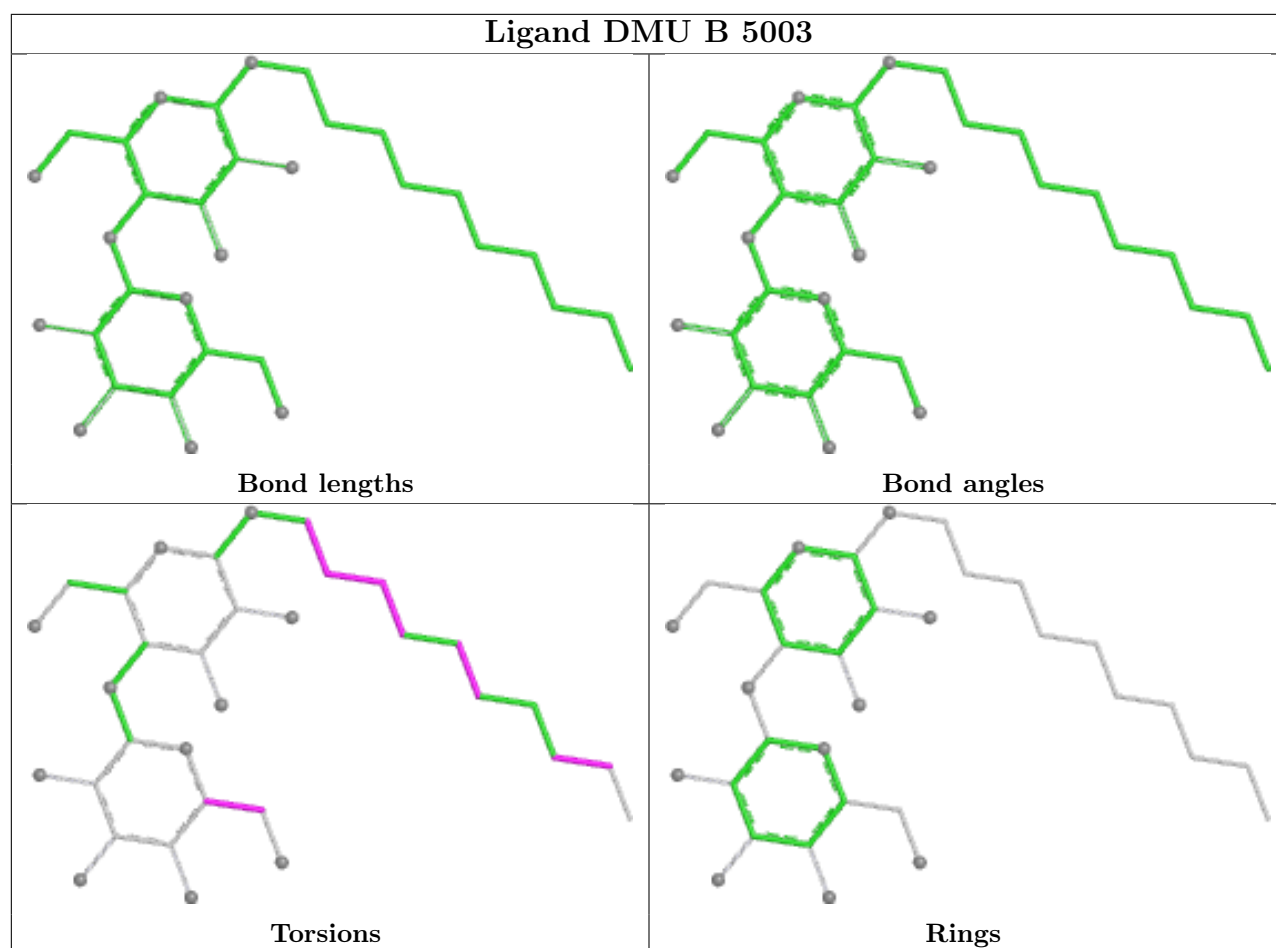


## Ligand DMU D 6003

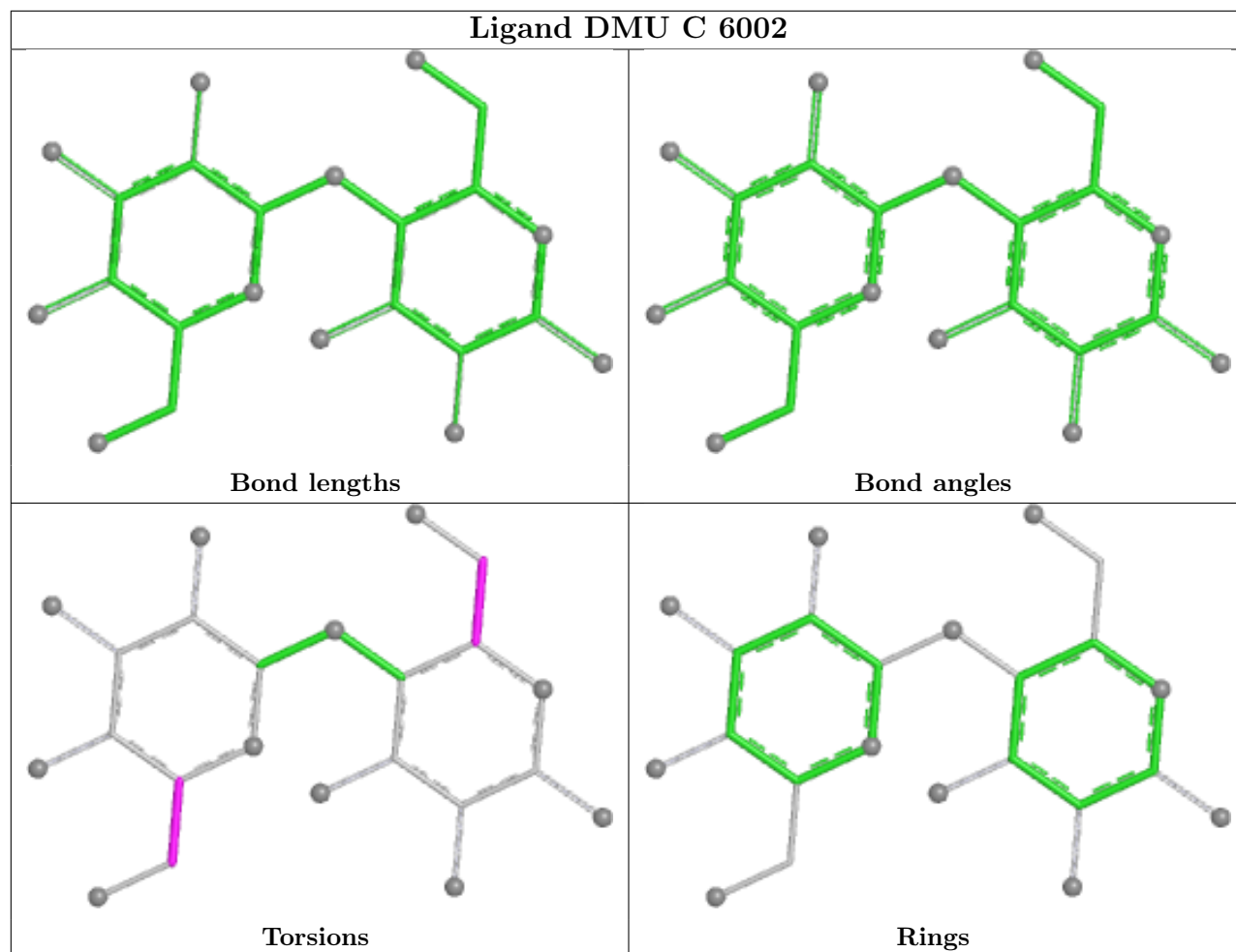


## Ligand HEA A 2001

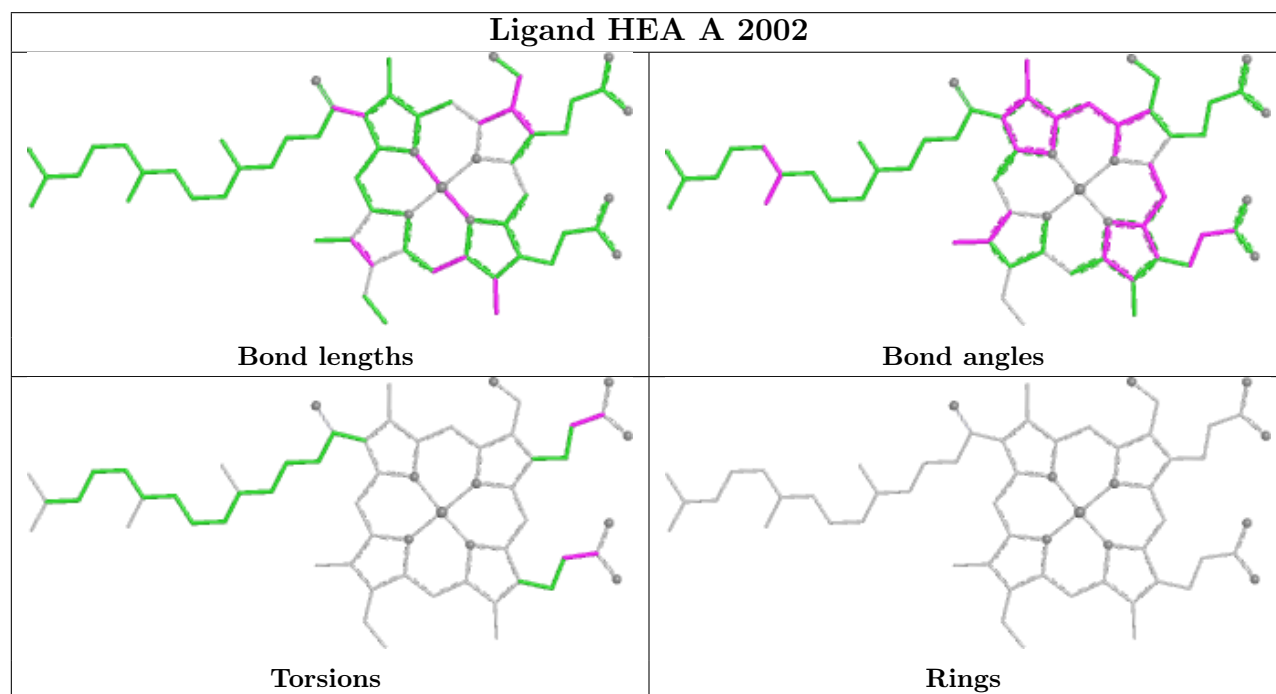
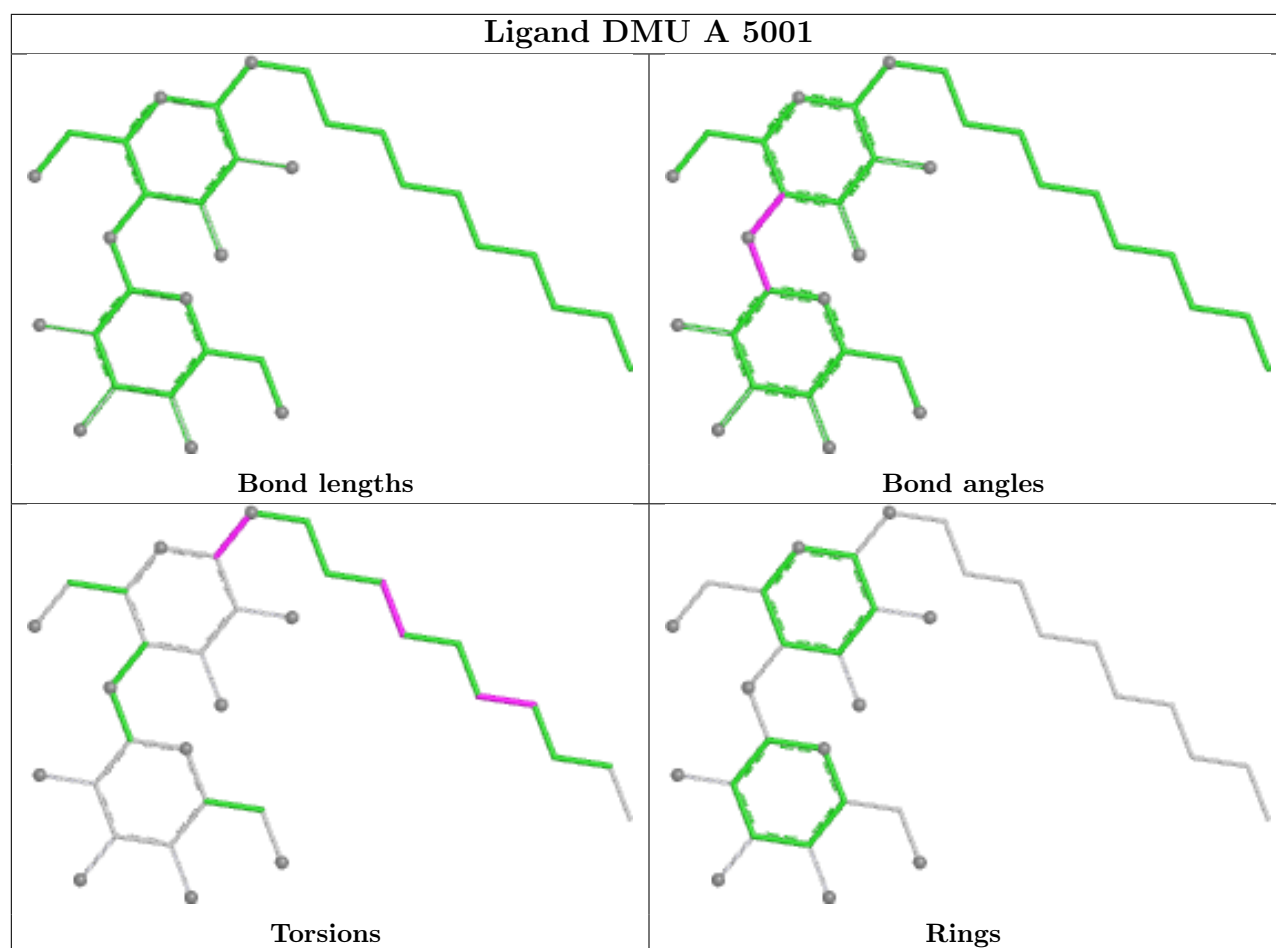


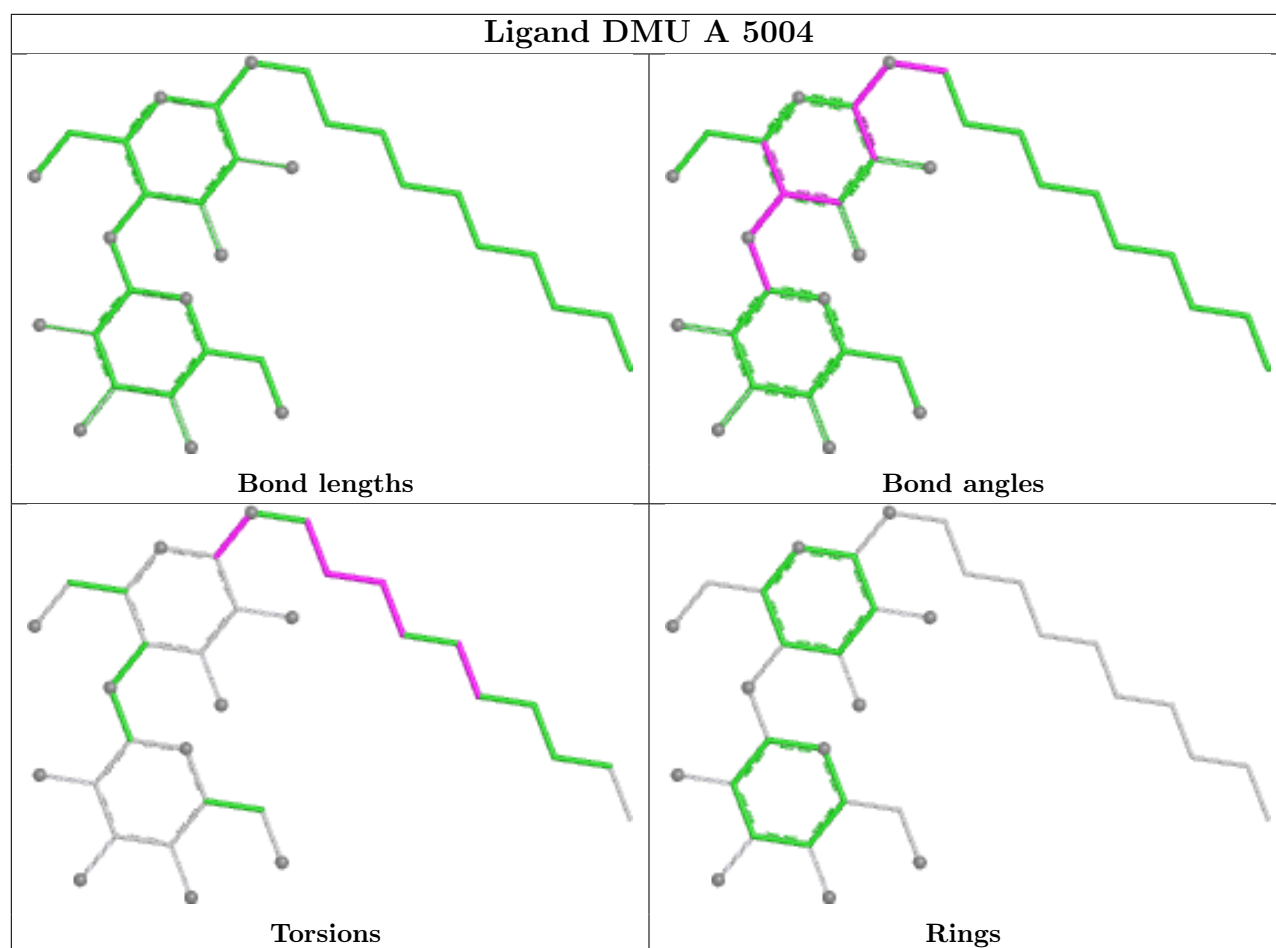


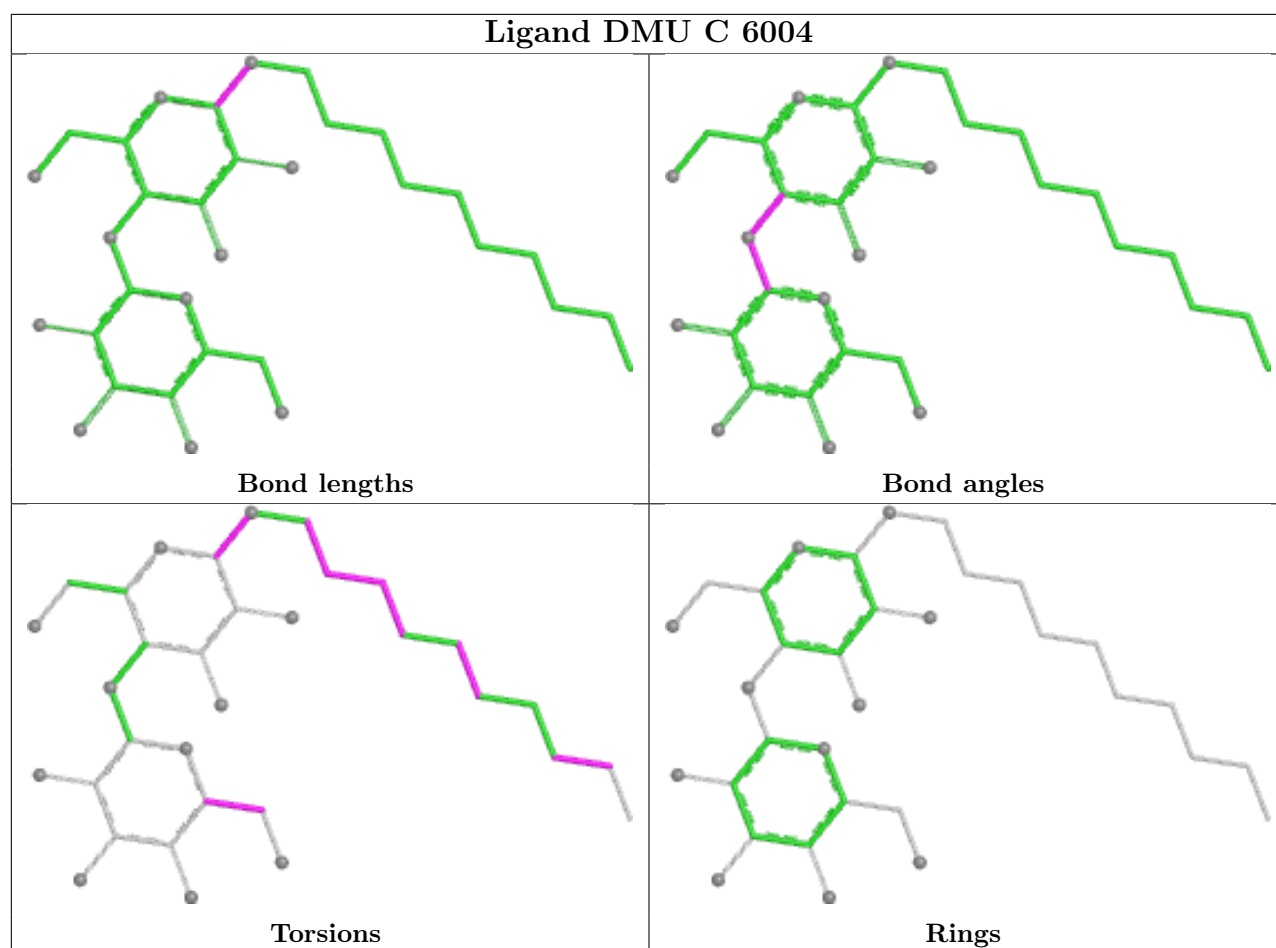
## Ligand DMU C 6002



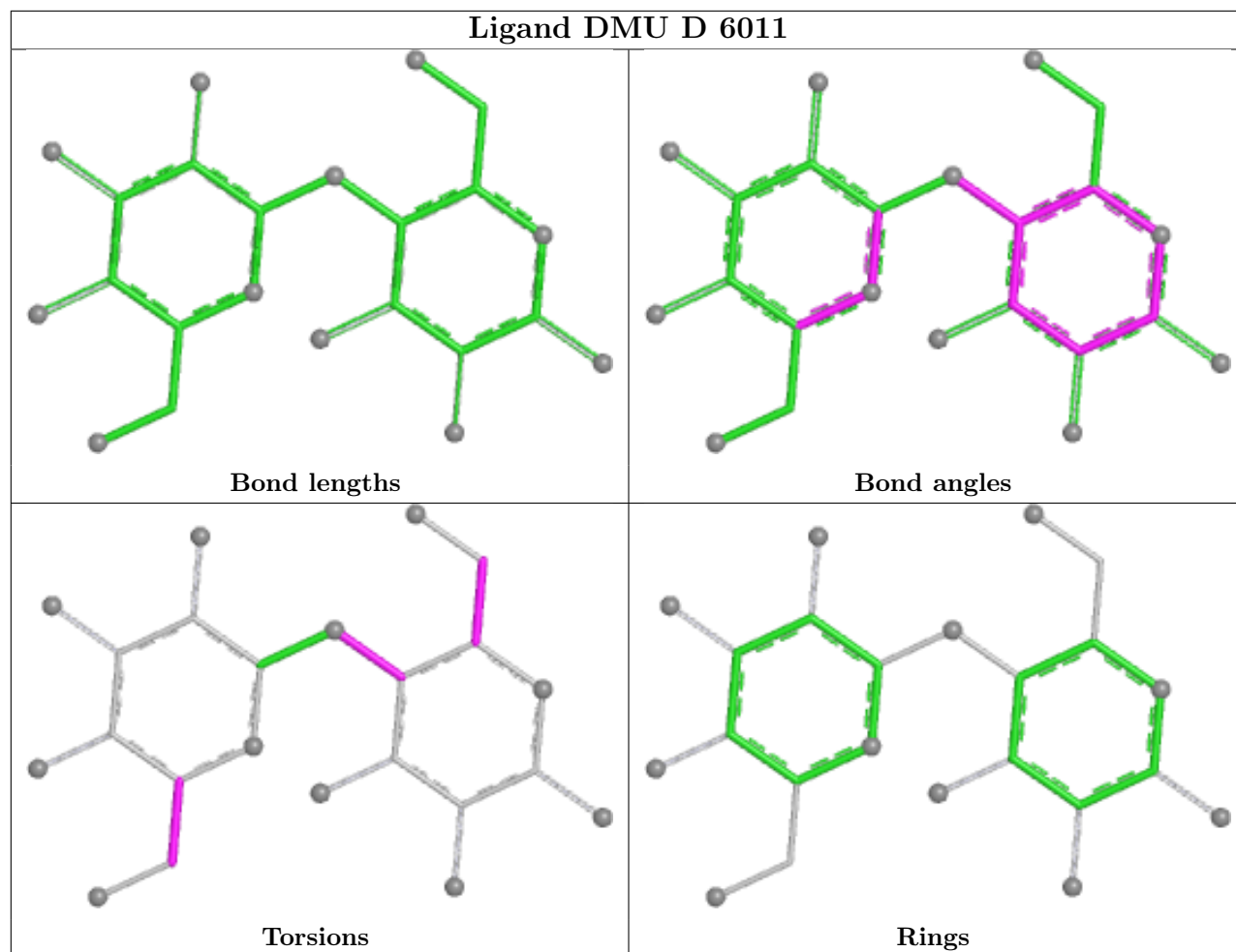




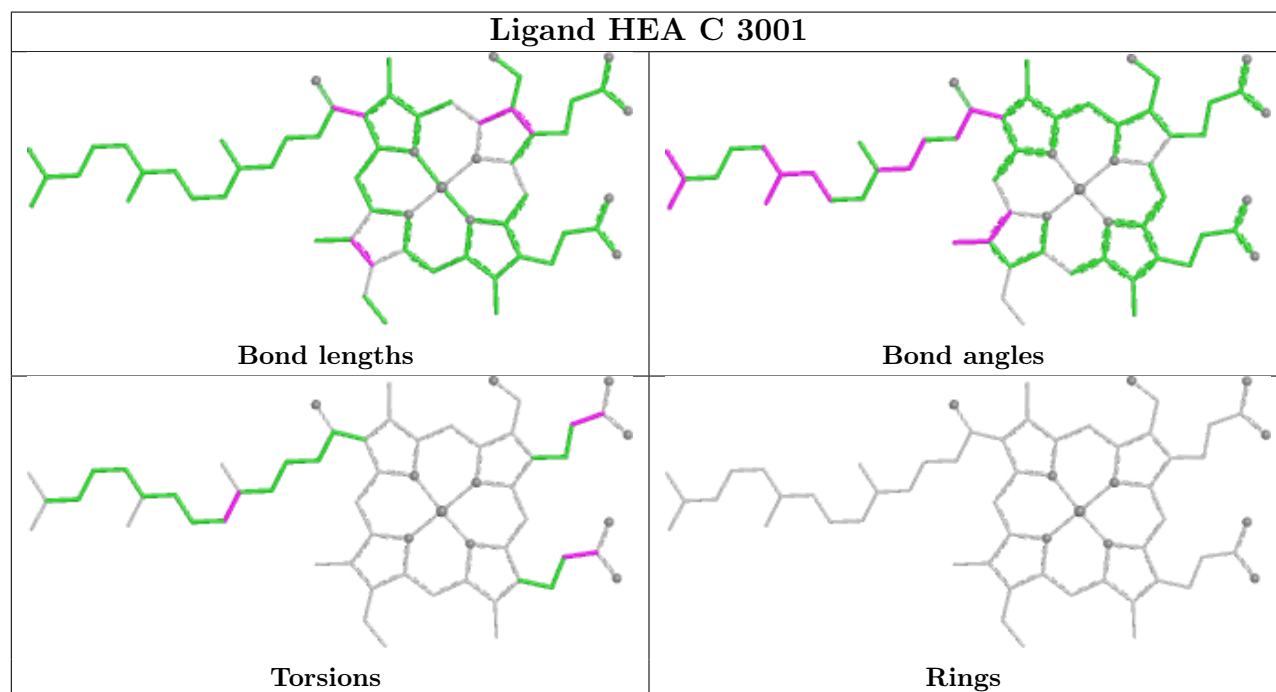




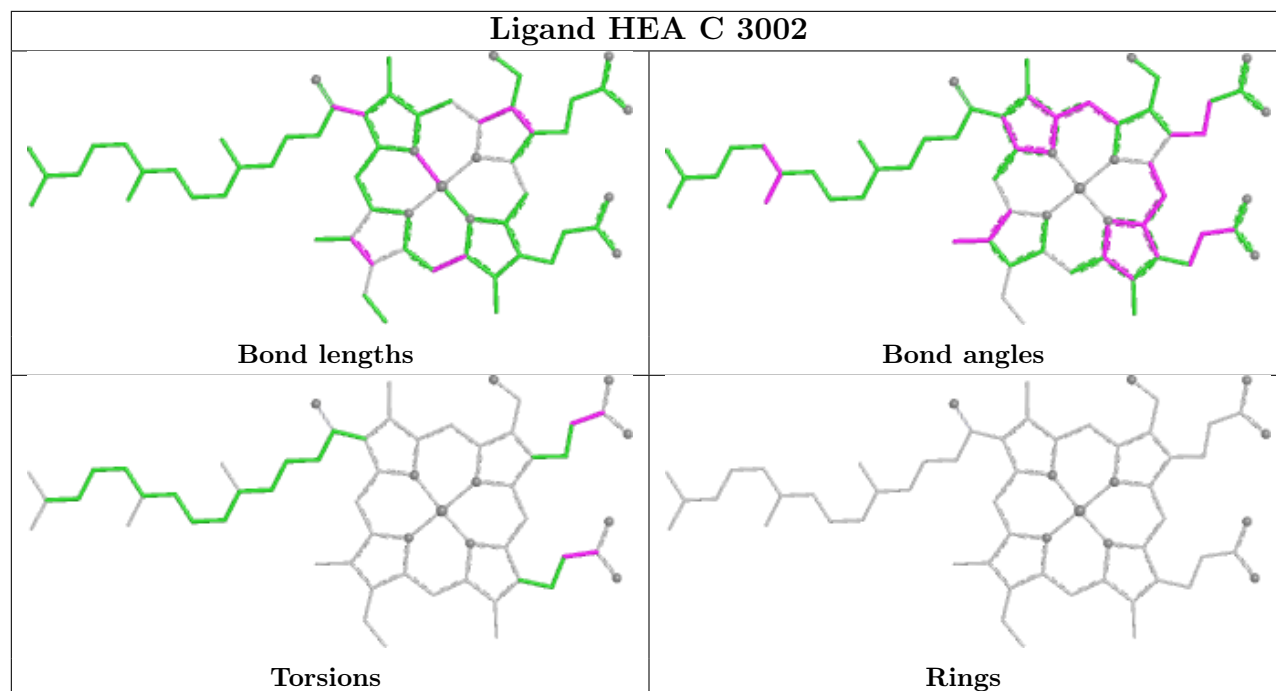
## Ligand DMU D 6011



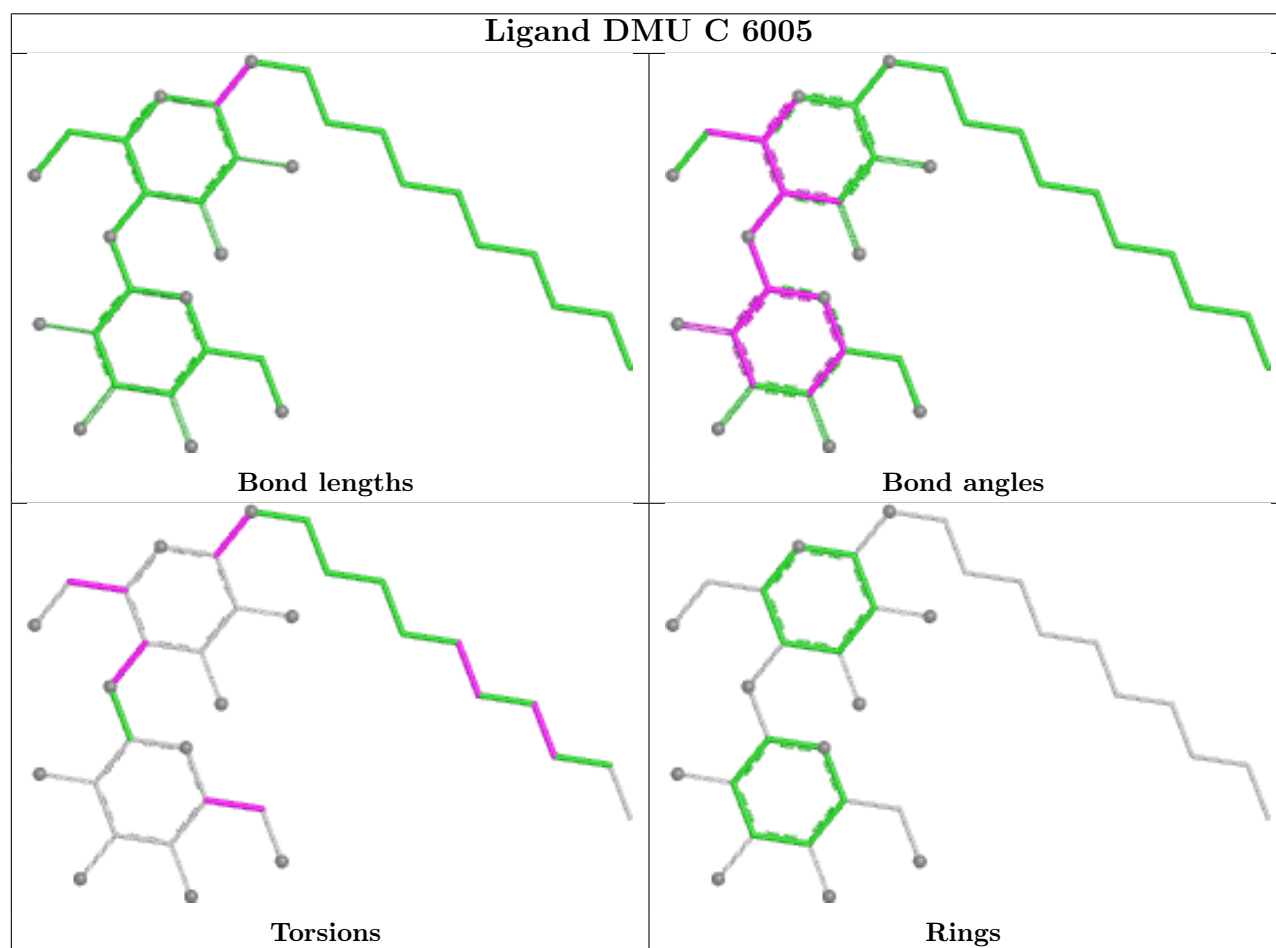
## Ligand HEA C 3001

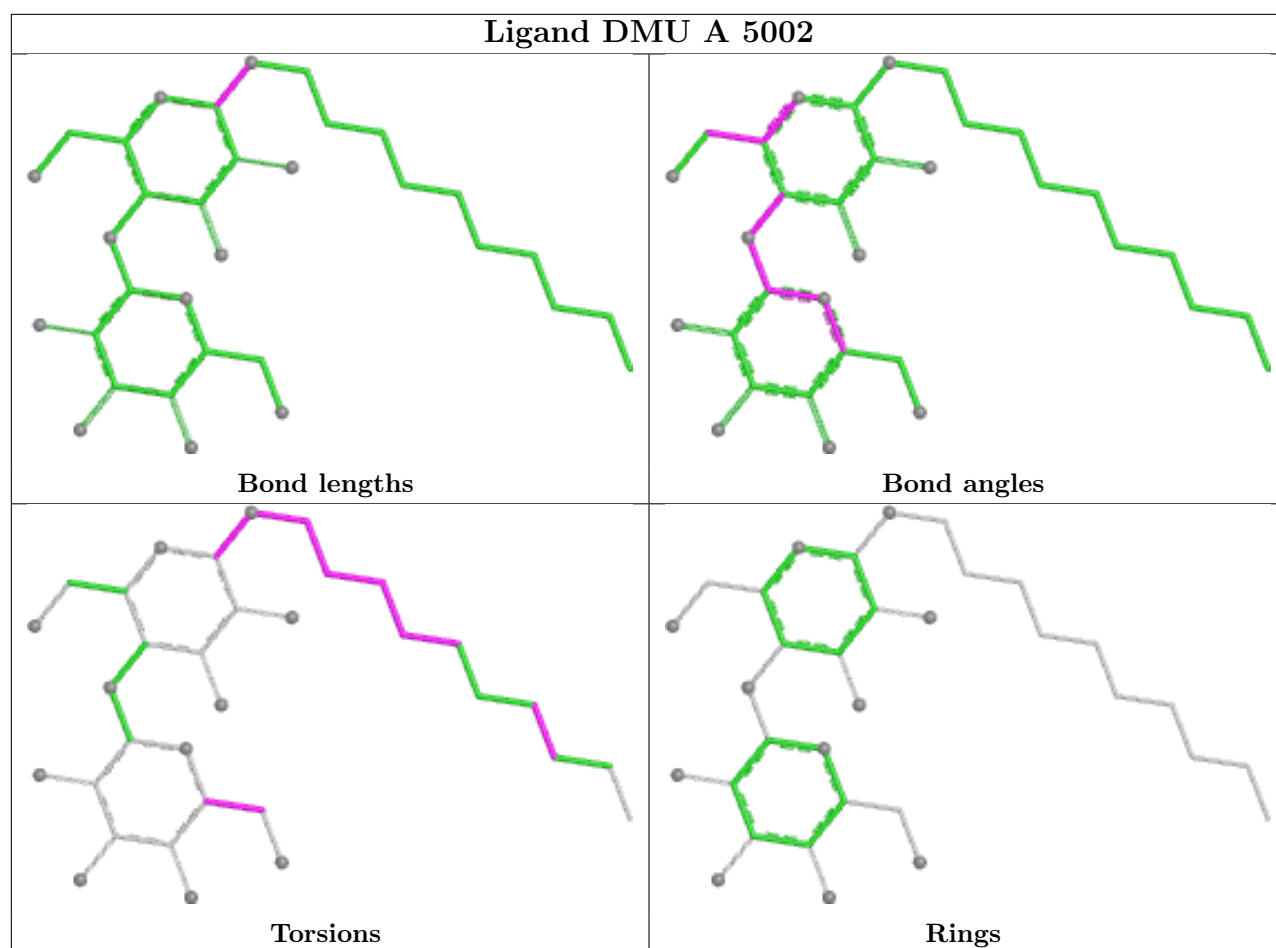


## Ligand HEA C 3002



## Ligand DMU C 6005





## 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	535/566 (94%)	-0.13	17 (3%)	47 46	19, 30, 47, 58	6 (1%)
1	C	534/566 (94%)	0.19	42 (7%)	12 11	25, 41, 54, 60	9 (1%)
2	B	256/262 (97%)	-0.19	4 (1%)	72 70	21, 33, 44, 50	2 (0%)
2	D	256/262 (97%)	-0.00	8 (3%)	49 48	26, 37, 50, 55	3 (1%)
All	All	1581/1656 (95%)	-0.01	71 (4%)	33 32	19, 35, 51, 60	20 (1%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	17	PHE	7.3
1	C	20	TRP	6.3
1	C	18	THR	6.1
1	C	81	TRP	5.9
1	C	222	MET	5.6
1	C	549	HIS	5.5
1	C	77	PHE	4.8
1	C	72	LEU	4.7
1	C	550	THR	4.6
1	A	20	TRP	4.6
1	A	72	LEU	4.5
2	B	56	TRP	4.4
1	C	73	VAL	4.4
1	C	71	GLY	4.2
1	C	218	PRO	4.2
1	C	259	PHE	4.1
1	C	223	HIS	4.1
2	D	56	TRP	4.1
1	A	17	PHE	4.0
1	A	81	TRP	3.9
1	A	69	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	22	MET	3.9
1	C	70	SER	3.6
1	C	69	GLU	3.6
1	C	268	GLY	3.6
1	A	219	GLY	3.4
2	D	99	PRO	3.4
1	A	259	PHE	3.3
1	A	549	HIS	3.2
1	C	21	PHE	3.2
1	C	267	SER	3.1
1	C	520	THR	3.0
1	C	533	GLU	3.0
1	A	73	VAL	2.9
1	A	77	PHE	2.9
1	C	262	THR	2.9
1	A	71	GLY	2.9
2	D	284	HIS	2.7
1	A	318	TYR	2.7
1	C	76	PHE	2.7
1	C	220	MET	2.7
1	A	551	PHE	2.6
1	C	318	TYR	2.6
1	C	75	GLY	2.6
1	C	135	PHE	2.6
2	B	87	ARG	2.5
1	C	24	THR	2.5
1	C	526	THR	2.5
1	C	219	GLY	2.5
1	C	217	ALA	2.4
2	B	102	ILE	2.4
1	A	22	MET	2.4
1	C	19	ARG	2.4
1	C	74	LYS	2.3
1	C	451	TRP	2.3
2	D	87	ARG	2.3
1	C	270	GLY	2.3
2	D	96	HIS	2.3
1	A	269	GLY	2.3
2	D	81	TRP	2.3
1	C	548	GLU	2.2
2	D	153	GLU	2.2
1	C	221	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	223	HIS	2.1
2	D	98	SER	2.1
1	C	78	GLN	2.1
1	C	314	LEU	2.0
1	C	144	TRP	2.0
1	A	221	THR	2.0
1	C	527	ALA	2.0
2	B	281	GLN	2.0

## 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(Å <sup>2</sup> )	Q<0.9
3	DMU	B	5011	23/33	0.63	0.24	51,54,57,59	23
3	DMU	C	6005	33/33	0.71	0.27	44,53,57,57	33
3	DMU	D	6011	23/33	0.71	0.28	53,55,57,57	23
9	TRD	A	5009	7/13	0.76	0.21	48,51,52,52	0
9	TRD	A	5010	13/13	0.78	0.28	46,49,56,56	0
3	DMU	C	6002	23/33	0.81	0.35	56,57,57,58	23
9	TRD	C	6009	9/13	0.81	0.32	48,49,53,53	0
3	DMU	C	6004	33/33	0.82	0.28	46,59,100,100	11
9	TRD	C	6001	13/13	0.82	0.20	49,50,53,53	0
3	DMU	A	5004	33/33	0.82	0.17	35,54,100,100	11
3	DMU	D	6003	23/33	0.83	0.23	50,52,55,56	23
3	DMU	A	5002	33/33	0.88	0.24	48,51,55,57	0
3	DMU	B	5003	33/33	0.88	0.24	48,52,58,58	0
9	TRD	D	6007	13/13	0.88	0.16	45,46,49,49	0
9	TRD	A	5006	13/13	0.90	0.30	49,51,53,53	0

*Continued on next page...*

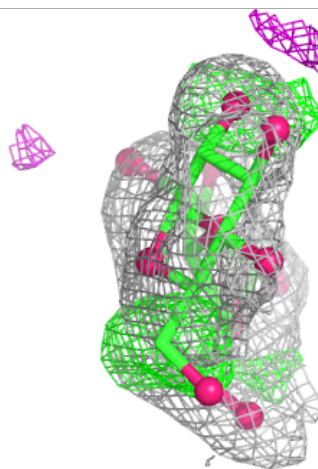
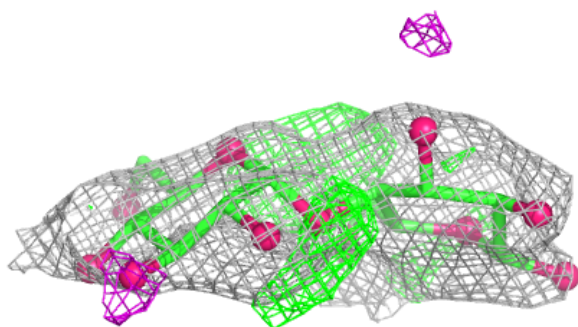
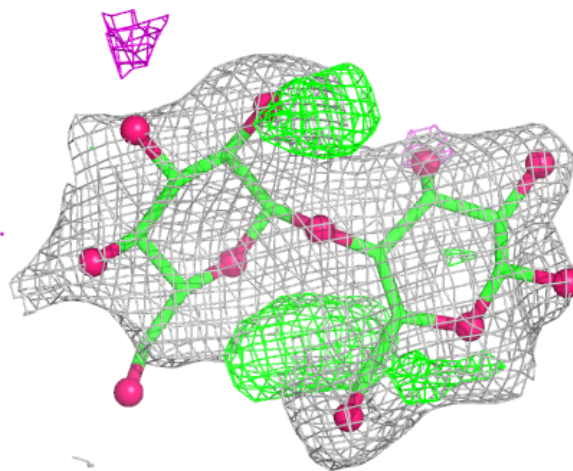
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	TRD	C	6010	9/13	0.90	0.21	50,51,52,52	0
9	TRD	C	6006	13/13	0.90	0.34	51,52,53,54	0
9	TRD	B	5008	9/13	0.92	0.20	44,45,46,46	0
9	TRD	A	5005	13/13	0.92	0.12	39,41,48,48	0
9	TRD	D	6008	7/13	0.92	0.18	44,44,45,45	0
9	TRD	A	5007	13/13	0.93	0.12	35,38,40,42	0
3	DMU	A	5001	33/33	0.94	0.11	24,33,44,44	0
7	OH	A	6501	1/1	0.97	0.12	26,26,26,26	0
7	OH	C	7501	1/1	0.97	0.09	35,35,35,35	0
8	HEA	A	2002	60/60	0.98	0.09	21,25,32,35	0
8	HEA	C	3001	60/60	0.98	0.10	26,29,40,41	0
8	HEA	C	3002	60/60	0.98	0.08	26,30,38,39	0
6	CA	C	4007	1/1	0.98	0.05	34,34,34,34	0
8	HEA	A	2001	60/60	0.98	0.11	17,21,26,27	0
6	CA	A	3007	1/1	0.99	0.09	24,24,24,24	0
4	CU	A	3005	1/1	0.99	0.06	27,27,27,27	0
4	CU	C	4005	1/1	0.99	0.04	33,33,33,33	0
5	MG	A	3006	1/1	0.99	0.18	10,10,10,10	0
5	MG	C	4006	1/1	0.99	0.14	12,12,12,12	0
10	CD	B	3008	1/1	0.99	0.05	35,35,35,35	0
10	CD	B	3009	1/1	0.99	0.04	40,40,40,40	1
10	CD	D	4008	1/1	0.99	0.05	35,35,35,35	0
10	CD	D	4009	1/1	0.99	0.02	42,42,42,42	1
4	CU	D	4003	1/1	1.00	0.08	27,27,27,27	0
4	CU	D	4004	1/1	1.00	0.09	29,29,29,29	0
4	CU	B	3004	1/1	1.00	0.10	24,24,24,24	0
4	CU	B	3003	1/1	1.00	0.07	24,24,24,24	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.

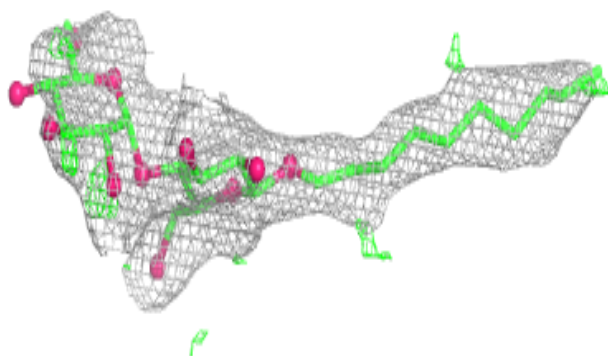
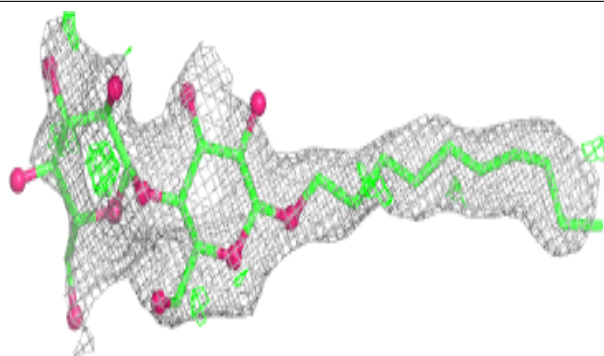
**Electron density around DMU B 5011:**

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

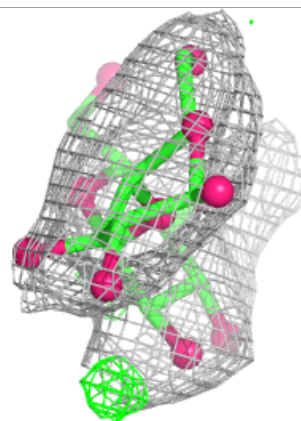
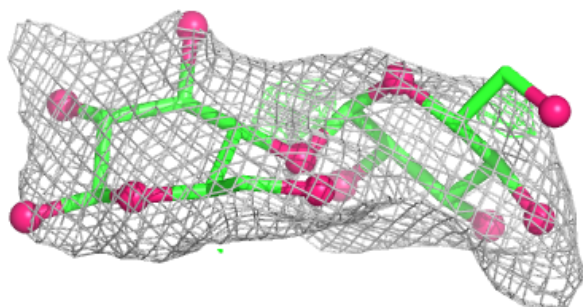
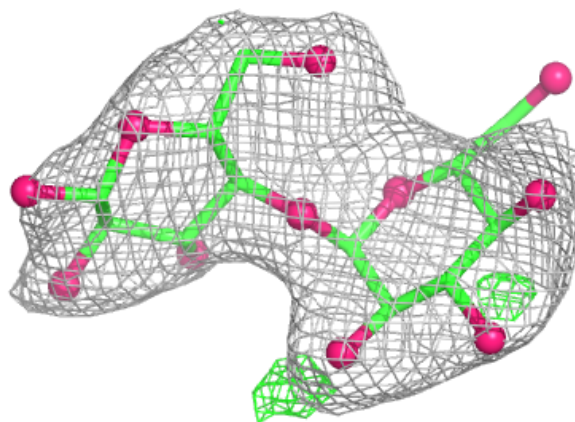


**Electron density around DMU C 6005:**

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

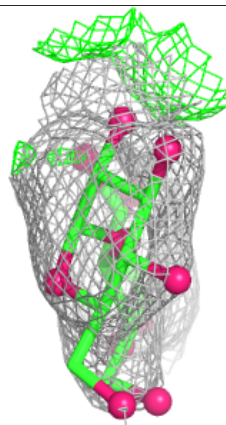
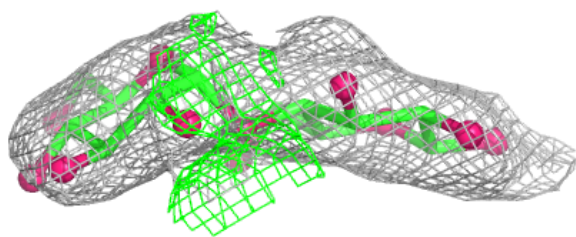
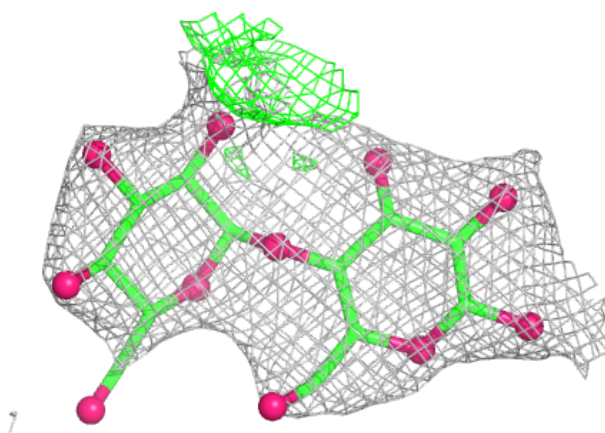
**Electron density around DMU D 6011:**

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

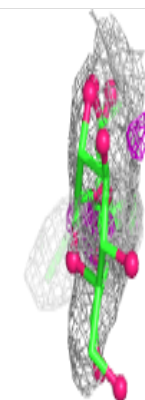
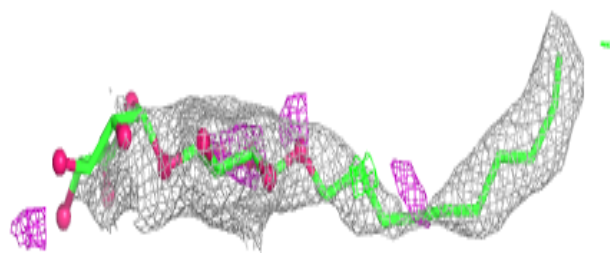
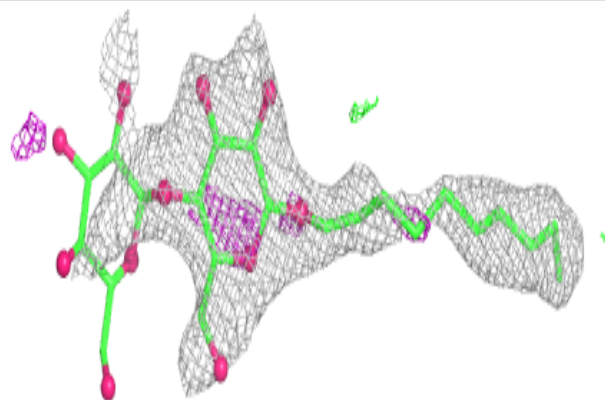


**Electron density around DMU C 6002:**

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

**Electron density around DMU C 6004:**

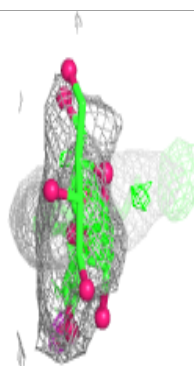
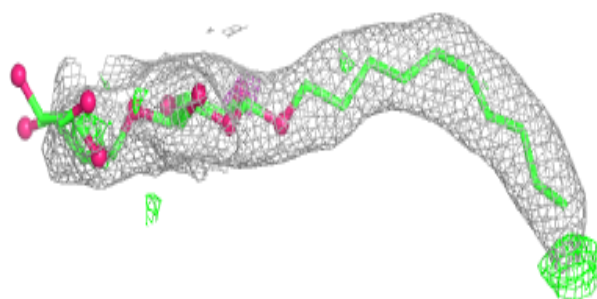
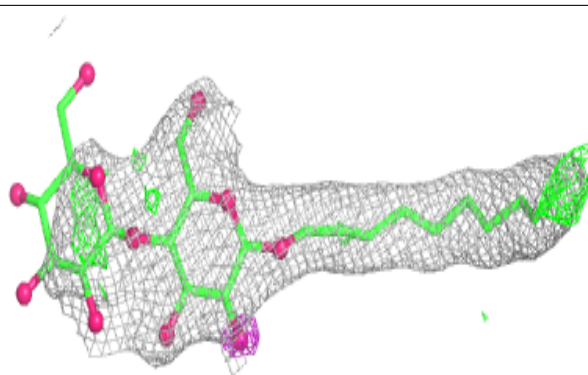
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





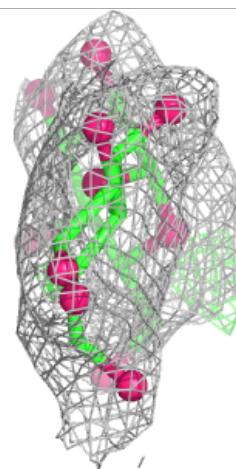
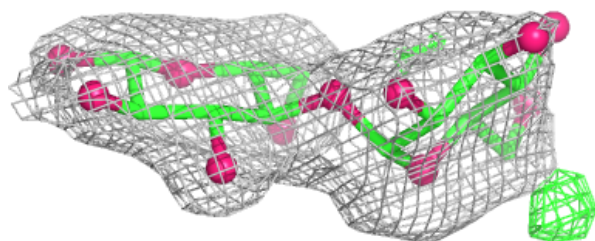
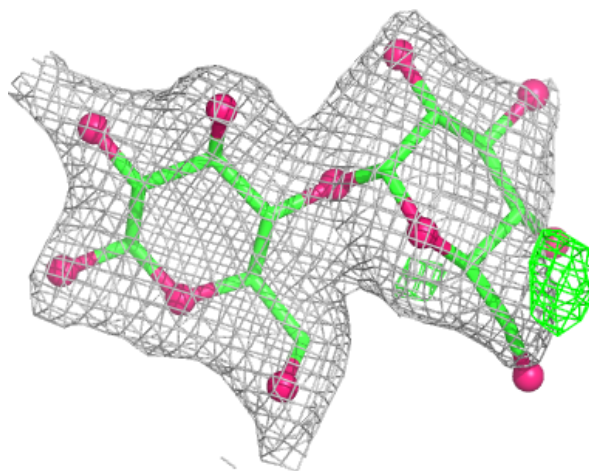
**Electron density around DMU A 5004:**

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



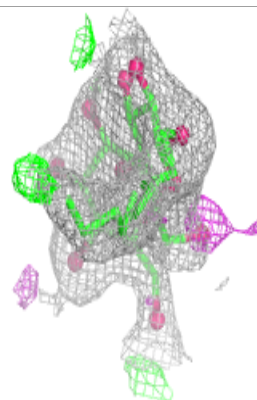
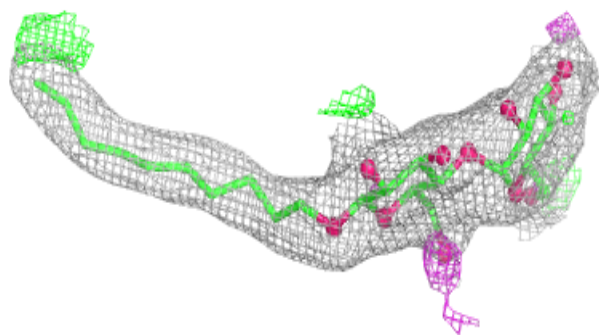
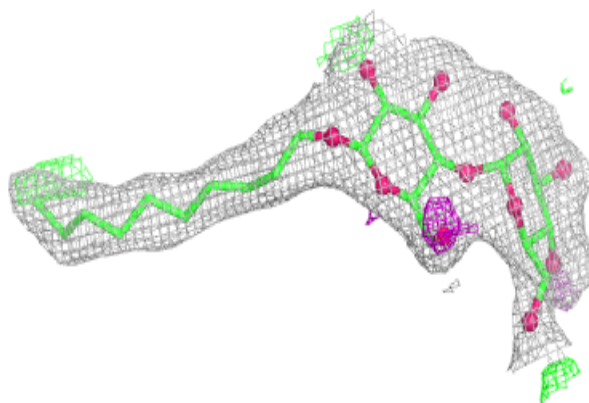
**Electron density around DMU D 6003:**

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

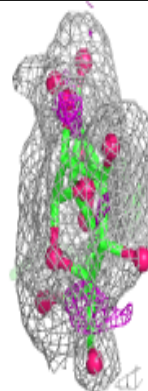
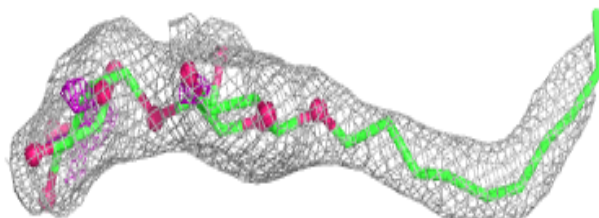
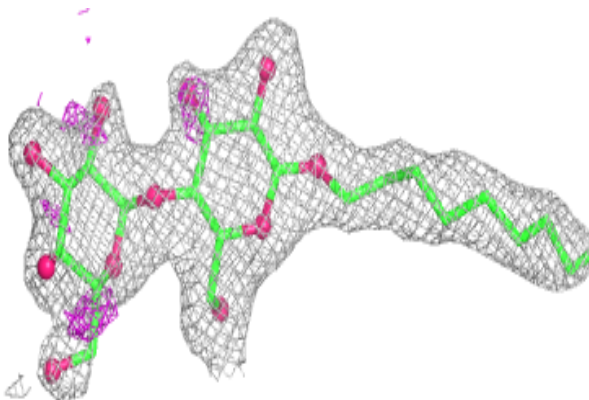


**Electron density around DMU A 5002:**

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

**Electron density around DMU B 5003:**

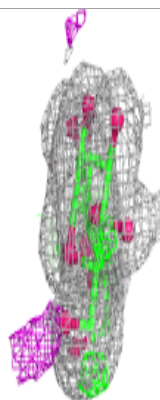
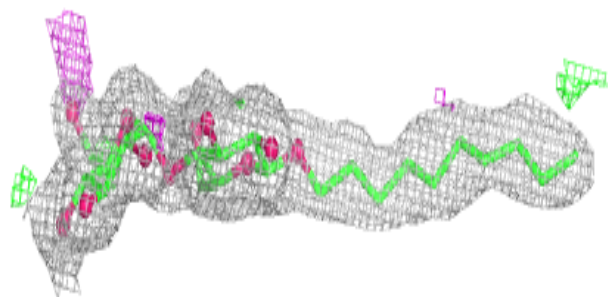
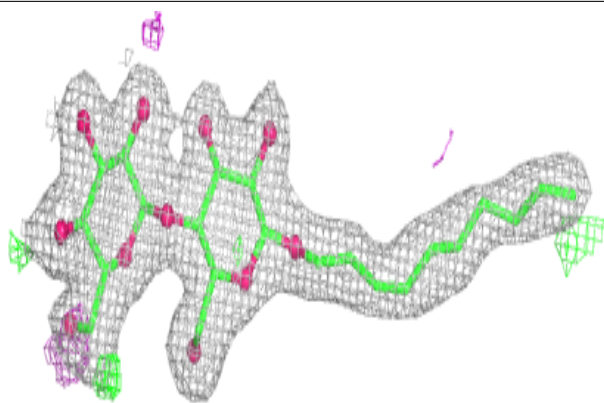
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



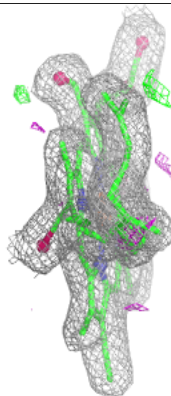
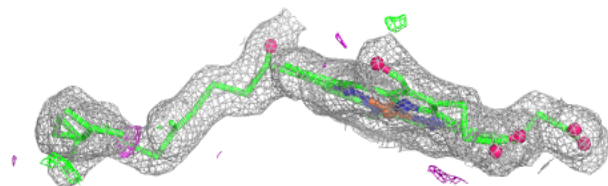
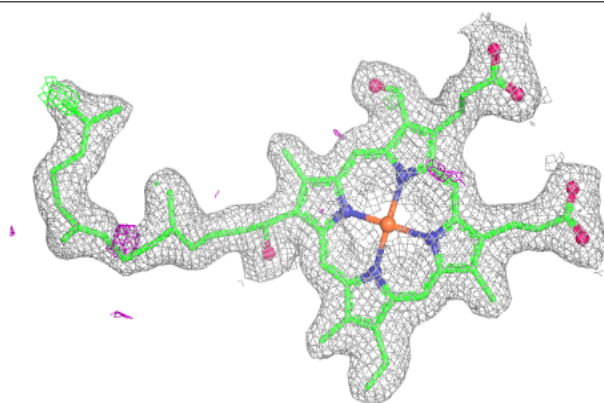


**Electron density around DMU A 5001:**

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

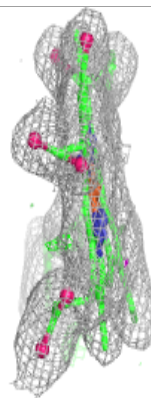
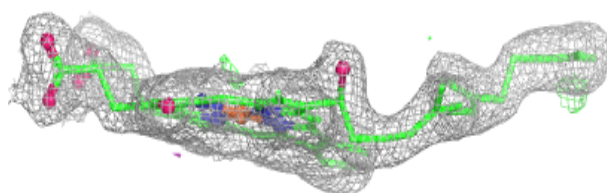
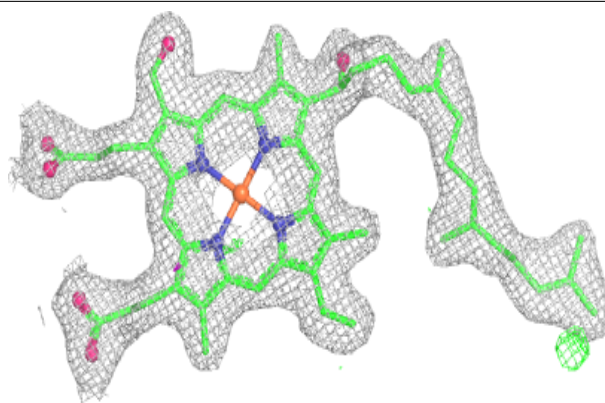
**Electron density around HEA A 2002:**

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

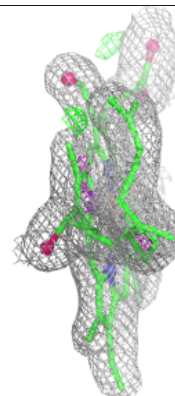
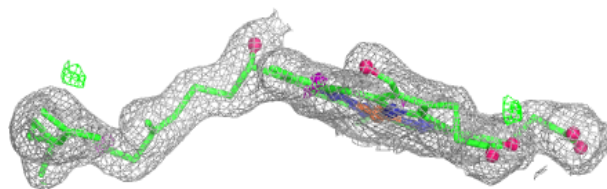
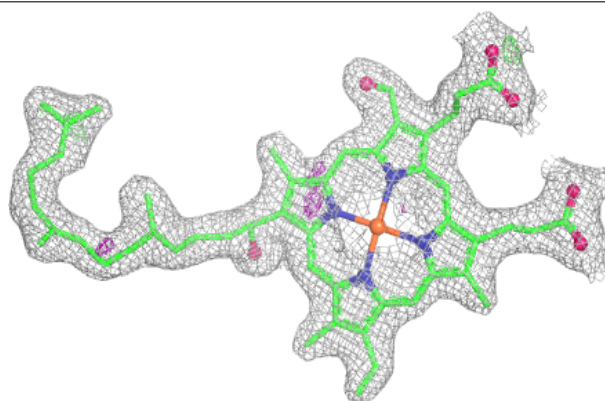


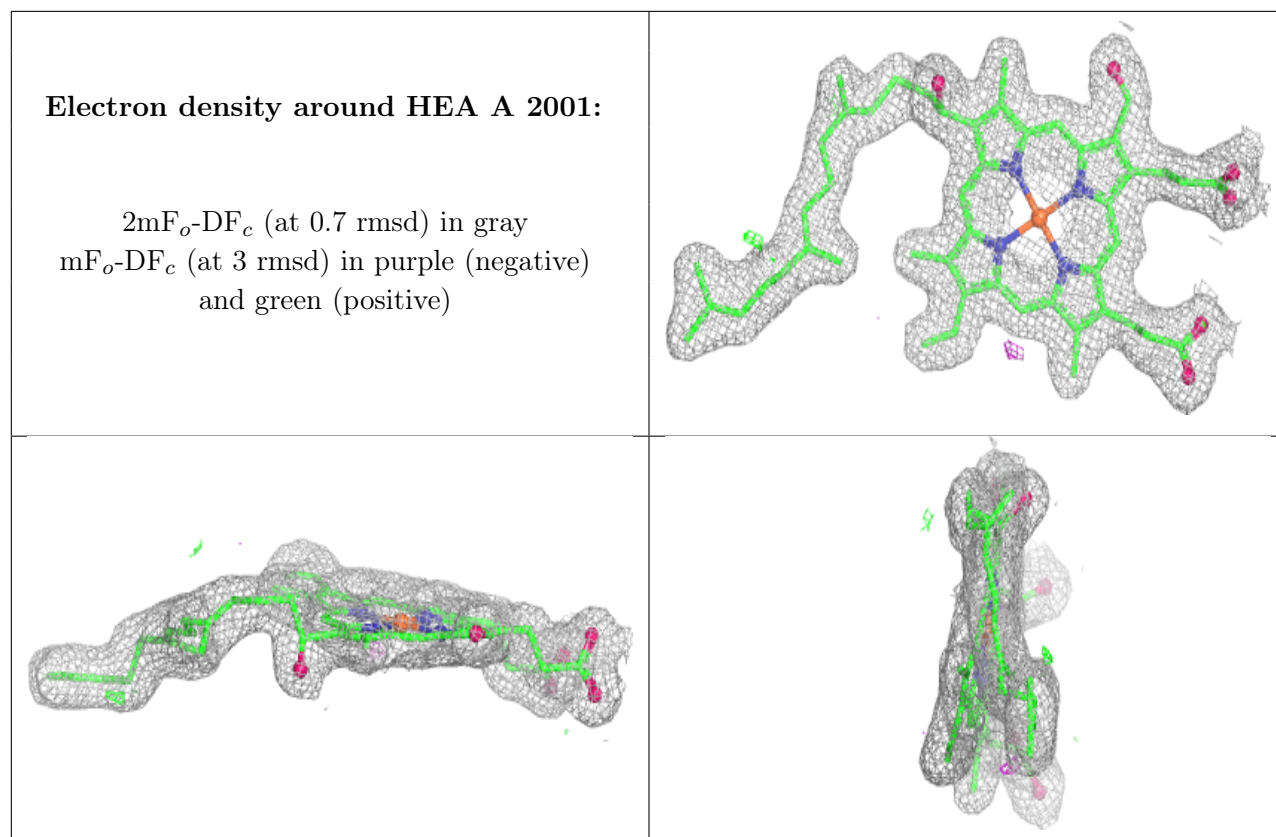
**Electron density around HEA C 3001:**

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

**Electron density around HEA C 3002:**

$2mF_o-DF_c$  (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.