



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 05:06 PM UTC

PDB ID : 2GSM / pdb_00002gsm
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

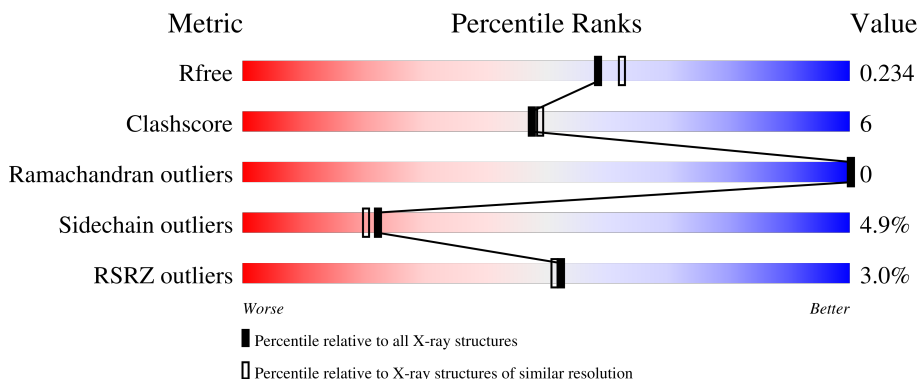
1 Overall quality at a glance ⓘ

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 ≥ 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	2% 82% 10% 5%
1	C	566	5% 79% 13% 6%
2	B	262	% 87% 9% ..
2	D	262	2% 86% 9% ..

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			

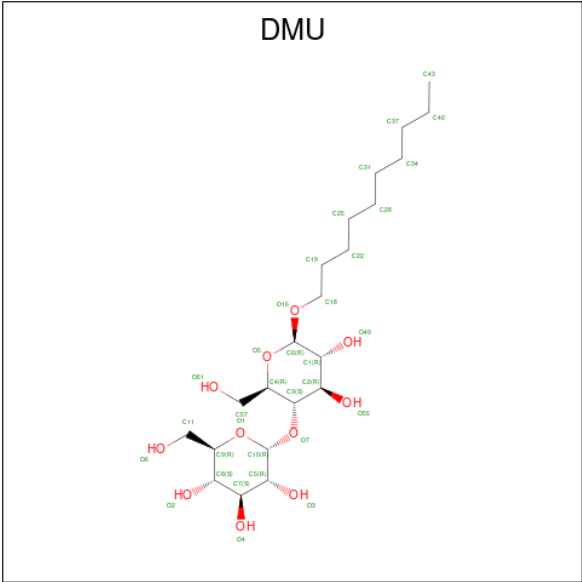
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

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 (CCD ID: 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 (CCD ID: 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

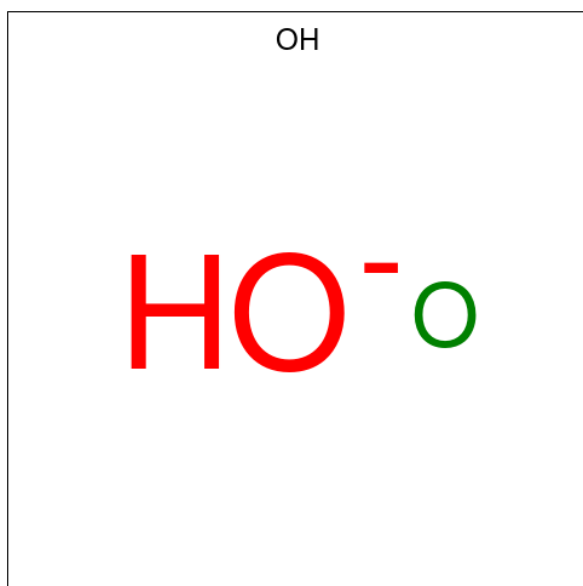
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 (CCD ID: 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 (CCD ID: OH) (formula: HO).



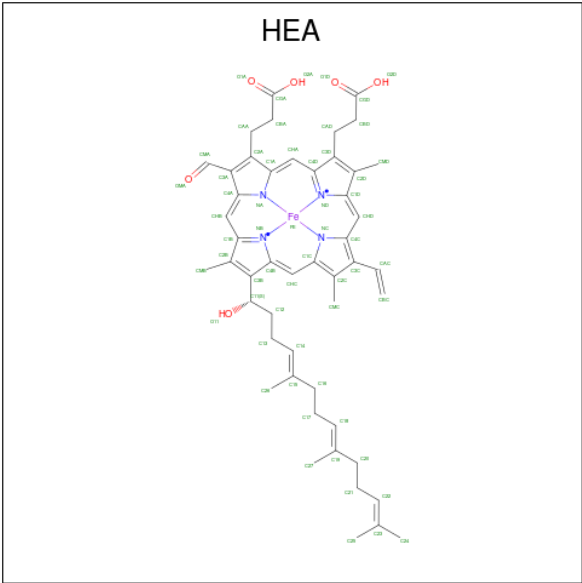
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	O 1	0	0

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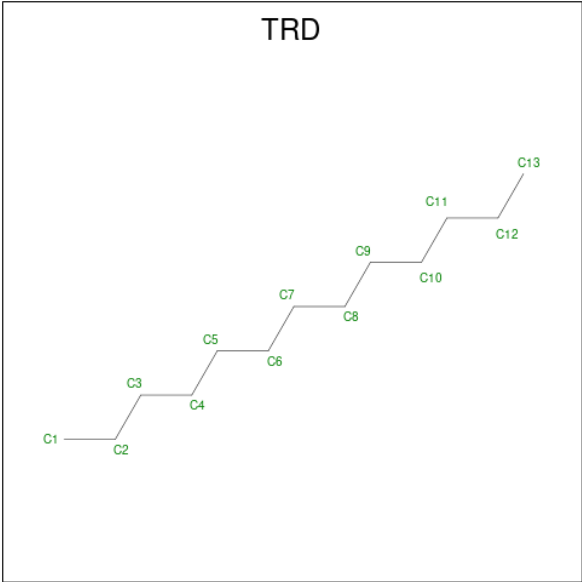
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	O	0	0
			1	1		

- Molecule 8 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- Molecule 9 is TRIDECANE (CCD ID: TRD) (formula: C₁₃H₂₈).



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

- Molecule 10 is CADMIUM ION (CCD ID: 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

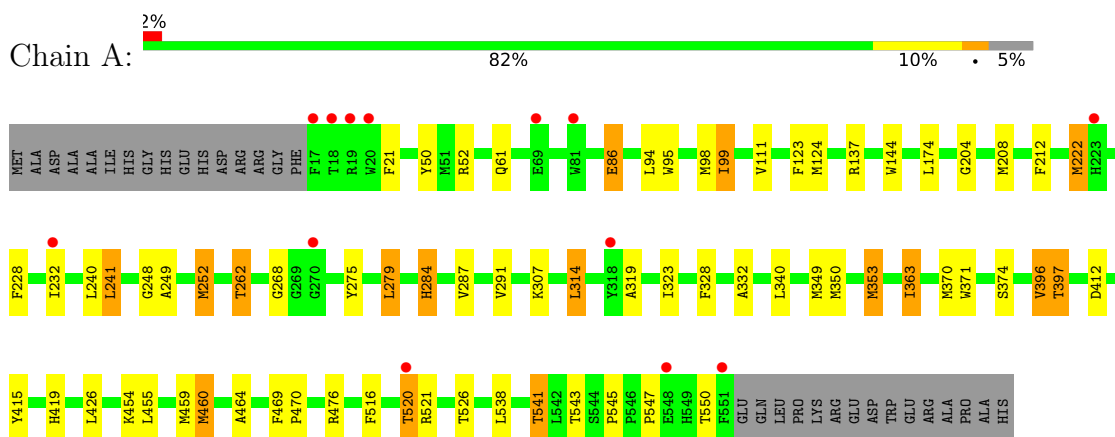
- Molecule 11 is water.

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

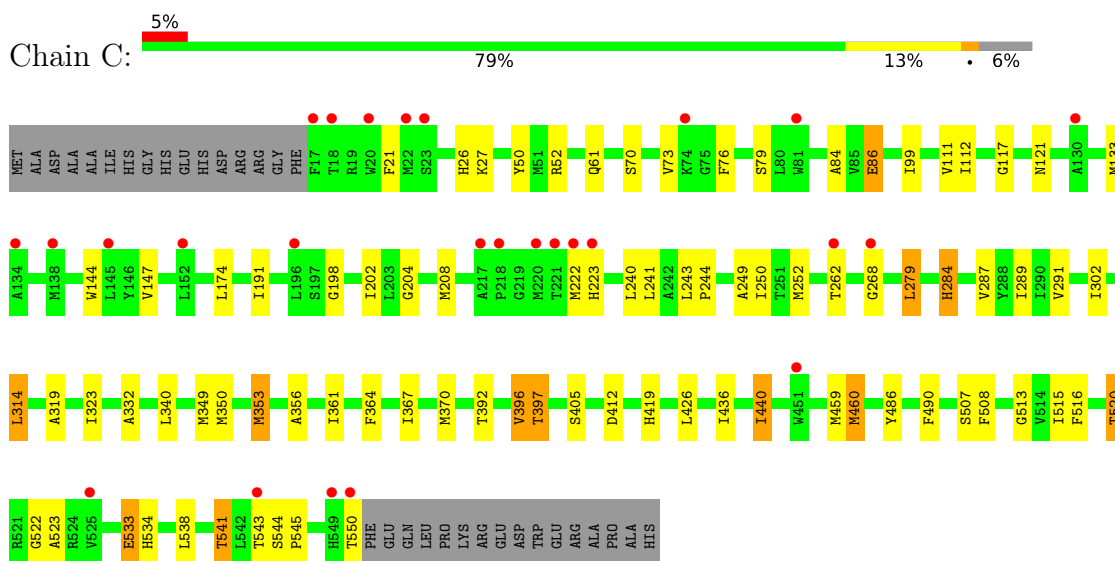
3 Residue-property plots

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.

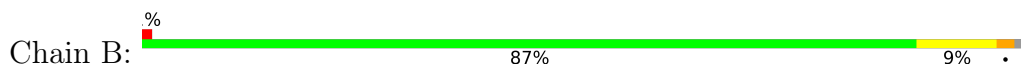
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2





Amino Acid	Number of Mutations
S269	1
I265	1
V269	1
H284	2
H285	2
HIS	1
GLN	1
SER	1
L30	1
T54	1
H55	2
Y56	2
Y57	2
L61	3
T64	1
T65	1
A66	1
A67	1
T68	1
T69	1
T70	1
L74	2
L86	2
H97	1
S98	1
P99	1
V104	3
V107	1
P108	2
I109	2
L112	1
F124	1
M125	1
Q126	1
I129	1
P130	1
W143	1
Y144	1
V145	1
V199	2
V202	3
D214	1
T220	1
Q228	1
G250	1
T258	1

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.02Å 131.64Å 176.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-2.00) 96.0 (20.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (1.93%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.73	4/4368 (0.1%)	0.91	2/5961 (0.0%)
1	C	0.60	1/4356 (0.0%)	0.93	1/5945 (0.0%)
2	B	0.66	0/2087	0.88	1/2857 (0.0%)
2	D	0.63	1/2087 (0.0%)	0.90	1/2857 (0.0%)
All	All	0.66	6/12898 (0.0%)	0.91	5/17620 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	MET	SD-CE	-11.26	1.51	1.79
1	A	460	MET	SD-CE	-7.28	1.61	1.79
2	D	107	VAL	CA-CB	6.54	1.57	1.54
1	C	353	MET	SD-CE	-6.41	1.63	1.79
1	A	252	MET	SD-CE	-6.01	1.64	1.79

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	HIS	N-CA-CB	8.34	118.31	110.39
1	C	284	HIS	N-CA-CB	7.23	117.26	110.39
2	B	202	VAL	CB-CA-C	-6.31	101.80	111.08
1	A	123	PHE	N-CA-C	5.27	119.80	112.90
2	D	258	ILE	N-CA-C	5.17	117.52	111.05

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	52	0
2	B	2025	0	1982	20	0
2	D	2025	0	1982	20	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	6	0
8	C	120	0	108	3	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
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	146	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.

The worst 5 of 146 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:460:MET:HE2	1:A:464:ALA:HB2	1.48	0.95
1:A:350:MET:HA	1:A:353:MET:HE3	1.50	0.94
1:C:350:MET:HA	1:C:353:MET:HE3	1.51	0.91
1:C:397:THR:HG22	1:C:419:HIS:HB2	1.54	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	533/566 (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 [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	435/459 (95%)	413 (95%)	22 (5%)	21	19
1	C	434/459 (95%)	408 (94%)	26 (6%)	17	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	215/221 (97%)	209 (97%)	6 (3%)	38	41
2	D	215/221 (97%)	205 (95%)	10 (5%)	23	22
All	All	1299/1360 (96%)	1235 (95%)	64 (5%)	22	20

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	70	ILE
2	D	104	TRP
2	B	68	ILE
2	B	54	ILE
2	D	109	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	170	ASN
2	D	96	HIS
1	C	67	HIS
2	D	88	ASN
1	C	26	HIS

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 oligosaccharides 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	5003	-	34,34,34	0.53	0	45,45,45	0.68	0
9	TRD	A	5006	-	12,12,12	0.28	0	11,11,11	0.54	0
9	TRD	D	6007	-	12,12,12	0.24	0	11,11,11	0.62	0
9	TRD	A	5010	-	12,12,12	0.27	0	11,11,11	0.56	0
3	DMU	D	6011	-	24,24,34	0.56	0	35,35,45	1.30	6 (17%)
9	TRD	A	5009	-	6,6,12	0.32	0	5,5,11	0.39	0
9	TRD	A	5005	-	12,12,12	0.28	0	11,11,11	0.57	0
9	TRD	C	6010	-	8,8,12	0.31	0	7,7,11	0.47	0
3	DMU	C	6005	-	34,34,34	0.69	1 (2%)	45,45,45	1.49	10 (22%)
3	DMU	A	5004	-	34,34,34	0.51	0	45,45,45	0.98	4 (8%)
9	TRD	C	6001	-	12,12,12	0.31	0	11,11,11	0.51	0
3	DMU	A	5002	-	34,34,34	0.57	1 (2%)	45,45,45	0.96	3 (6%)
8	HEA	C	3001	1	67,67,67	1.06	3 (4%)	81,103,103	1.06	5 (6%)
8	HEA	C	3002	1,11	67,67,67	1.59	7 (10%)	81,103,103	1.40	10 (12%)
3	DMU	A	5001	-	34,34,34	0.50	0	45,45,45	1.02	1 (2%)
9	TRD	B	5008	-	8,8,12	0.27	0	7,7,11	0.48	0
9	TRD	C	6009	-	8,8,12	0.30	0	7,7,11	0.48	0
8	HEA	A	2002	1,11	67,67,67	1.56	8 (11%)	81,103,103	1.54	13 (16%)
9	TRD	C	6006	-	12,12,12	0.27	0	11,11,11	0.61	0
9	TRD	A	5007	-	12,12,12	0.22	0	11,11,11	0.51	0
3	DMU	B	5011	-	24,24,34	0.60	0	35,35,45	1.21	4 (11%)
3	DMU	C	6002	-	24,24,34	0.58	0	35,35,45	0.71	0
9	TRD	D	6008	-	6,6,12	0.25	0	5,5,11	0.41	0
8	HEA	A	2001	1	67,67,67	1.03	5 (7%)	81,103,103	1.06	5 (6%)
3	DMU	C	6004	-	34,34,34	0.66	1 (2%)	45,45,45	0.87	1 (2%)
3	DMU	D	6003	-	24,24,34	0.57	0	35,35,45	0.78	1 (2%)

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	5003	-	-	7/19/59/59	0/2/2/2
9	TRD	A	5006	-	-	5/10/10/10	-
9	TRD	D	6007	-	-	6/10/10/10	-
9	TRD	A	5010	-	-	6/10/10/10	-
3	DMU	D	6011	-	-	4/8/48/59	0/2/2/2
9	TRD	A	5009	-	-	1/4/4/10	-
9	TRD	A	5005	-	-	2/10/10/10	-
9	TRD	C	6010	-	-	4/6/6/10	-
3	DMU	C	6005	-	-	9/19/59/59	0/2/2/2
3	DMU	A	5004	-	-	6/19/59/59	0/2/2/2
9	TRD	C	6001	-	-	3/10/10/10	-
3	DMU	A	5002	-	-	10/19/59/59	0/2/2/2
8	HEA	C	3001	1	-	6/36/76/76	-
8	HEA	C	3002	1,11	-	4/36/76/76	-
3	DMU	A	5001	-	-	3/19/59/59	0/2/2/2
9	TRD	B	5008	-	-	4/6/6/10	-
9	TRD	C	6009	-	-	2/6/6/10	-
8	HEA	A	2002	1,11	-	4/36/76/76	-
9	TRD	C	6006	-	-	2/10/10/10	-
9	TRD	A	5007	-	-	5/10/10/10	-
3	DMU	B	5011	-	-	4/8/48/59	0/2/2/2
3	DMU	C	6002	-	-	4/8/48/59	0/2/2/2
9	TRD	D	6008	-	-	1/4/4/10	-
8	HEA	A	2001	1	-	6/36/76/76	-
3	DMU	C	6004	-	-	9/19/59/59	0/2/2/2
3	DMU	D	6003	-	-	3/8/48/59	0/2/2/2

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2002	HEA	FE-NB	6.18	2.13	1.94
8	C	3002	HEA	FE-NB	5.53	2.11	1.94
8	A	2002	HEA	FE-ND	4.69	2.09	1.94
8	C	3002	HEA	FE-NA	4.68	2.10	1.95
8	A	2002	HEA	FE-NA	4.49	2.10	1.95

The worst 5 of 63 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	C4B-NB-C1B	4.08	110.04	105.21
8	A	2002	HEA	CAD-CBD-CGD	-3.92	103.27	113.67
8	A	2002	HEA	C2A-C1A-NA	-3.57	106.88	110.32
8	C	3002	HEA	C1D-ND-C4D	3.51	109.36	105.21

There are no chirality outliers.

5 of 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

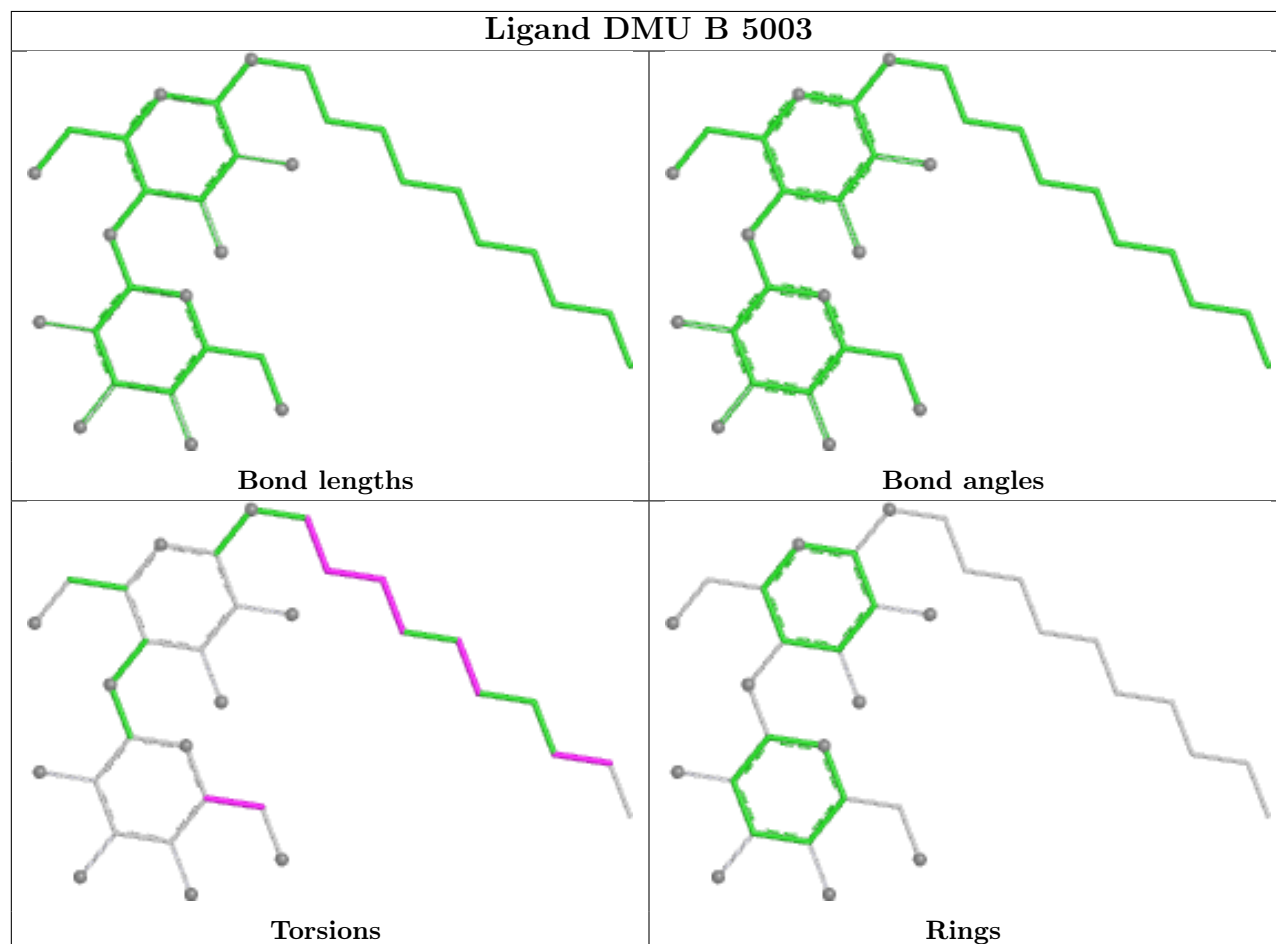
There are no ring outliers.

15 monomers are involved in 23 short contacts:

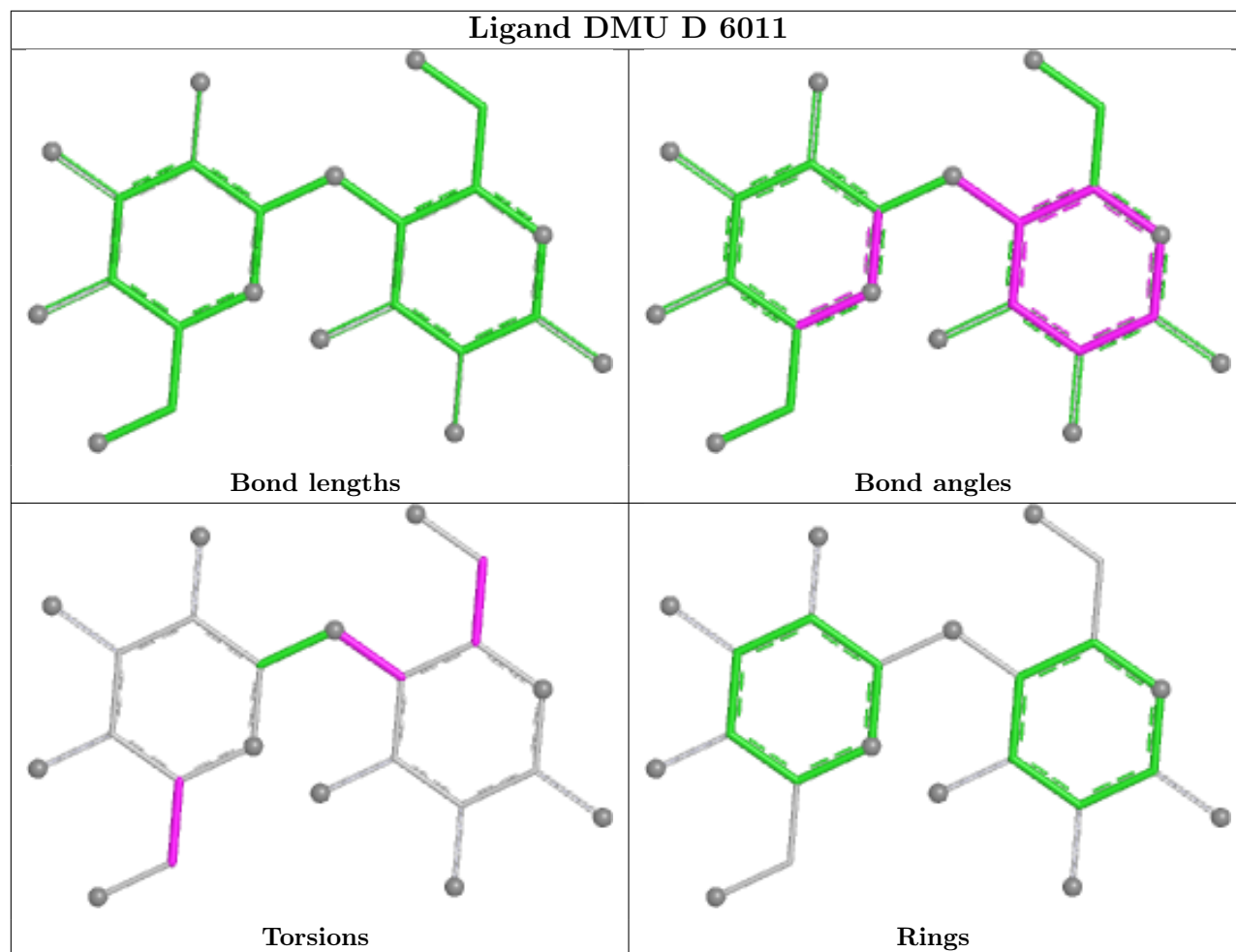
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5003	DMU	3	0
9	A	5006	TRD	2	0
3	D	6011	DMU	1	0
9	A	5005	TRD	2	0
3	C	6005	DMU	1	0
9	C	6001	TRD	1	0
8	C	3001	HEA	1	0
8	C	3002	HEA	2	0
9	B	5008	TRD	2	0
8	A	2002	HEA	5	0
9	C	6006	TRD	1	0
9	A	5007	TRD	2	0
8	A	2001	HEA	1	0
3	C	6004	DMU	1	0
3	D	6003	DMU	1	0

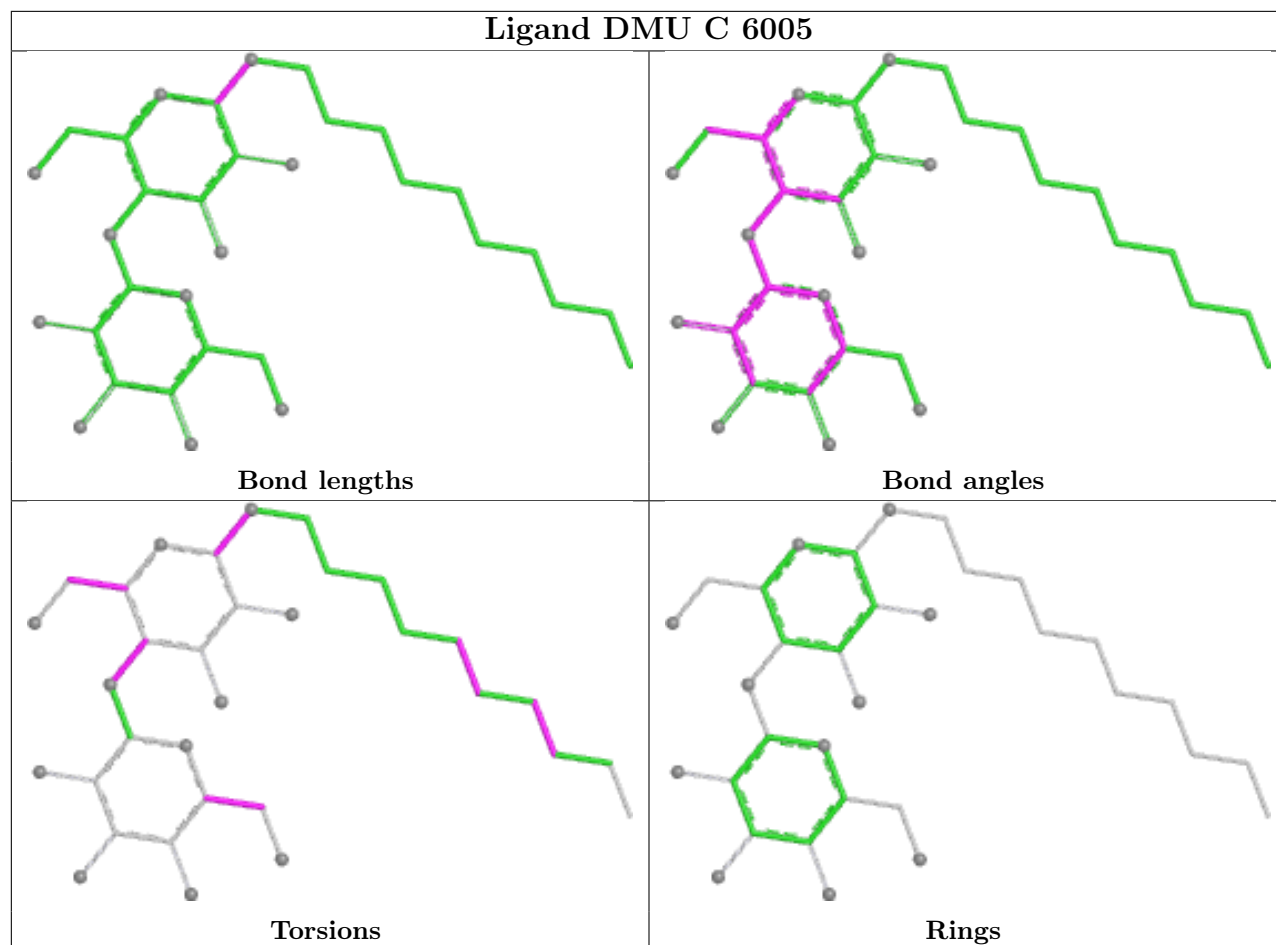
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

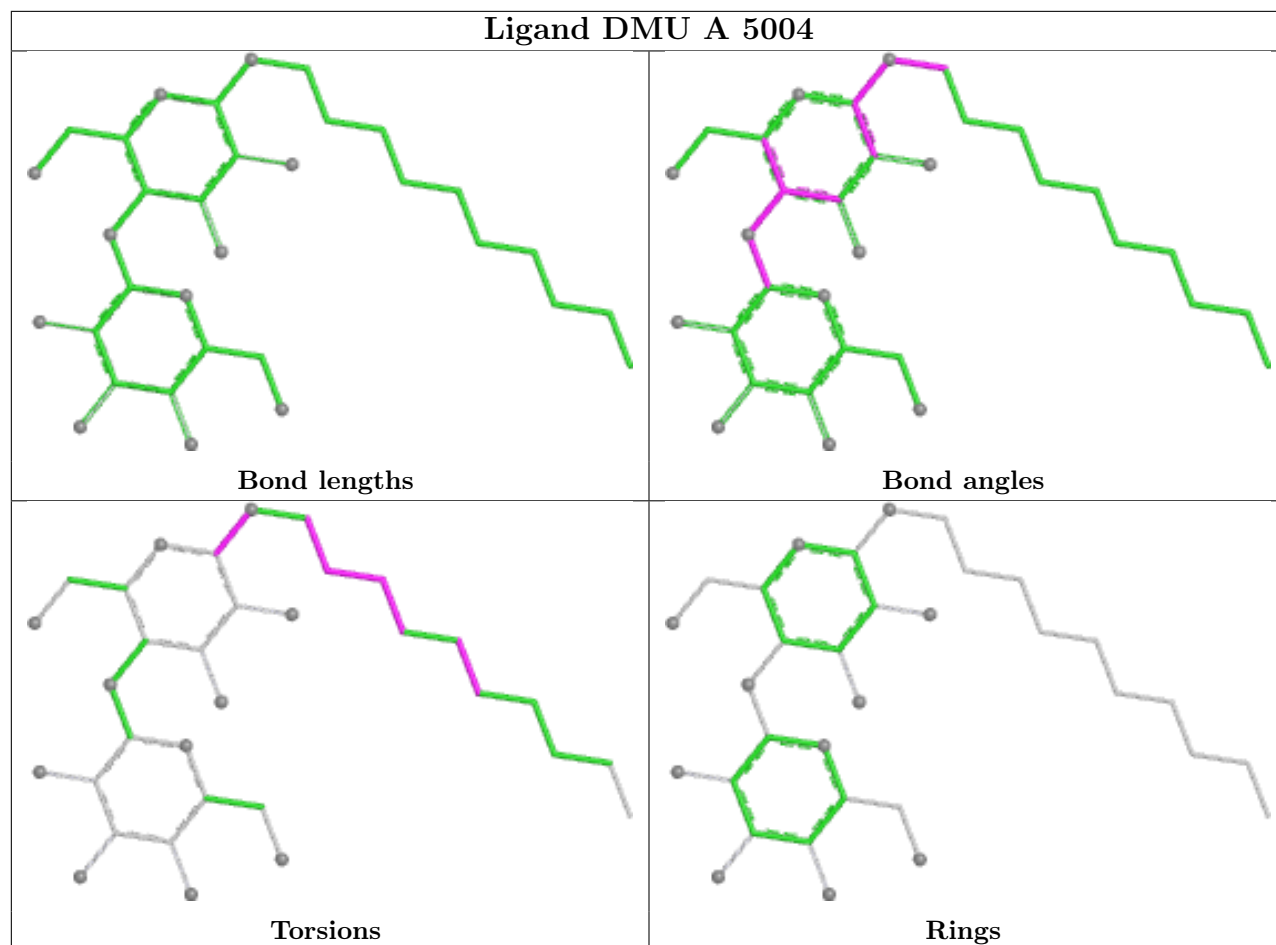
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

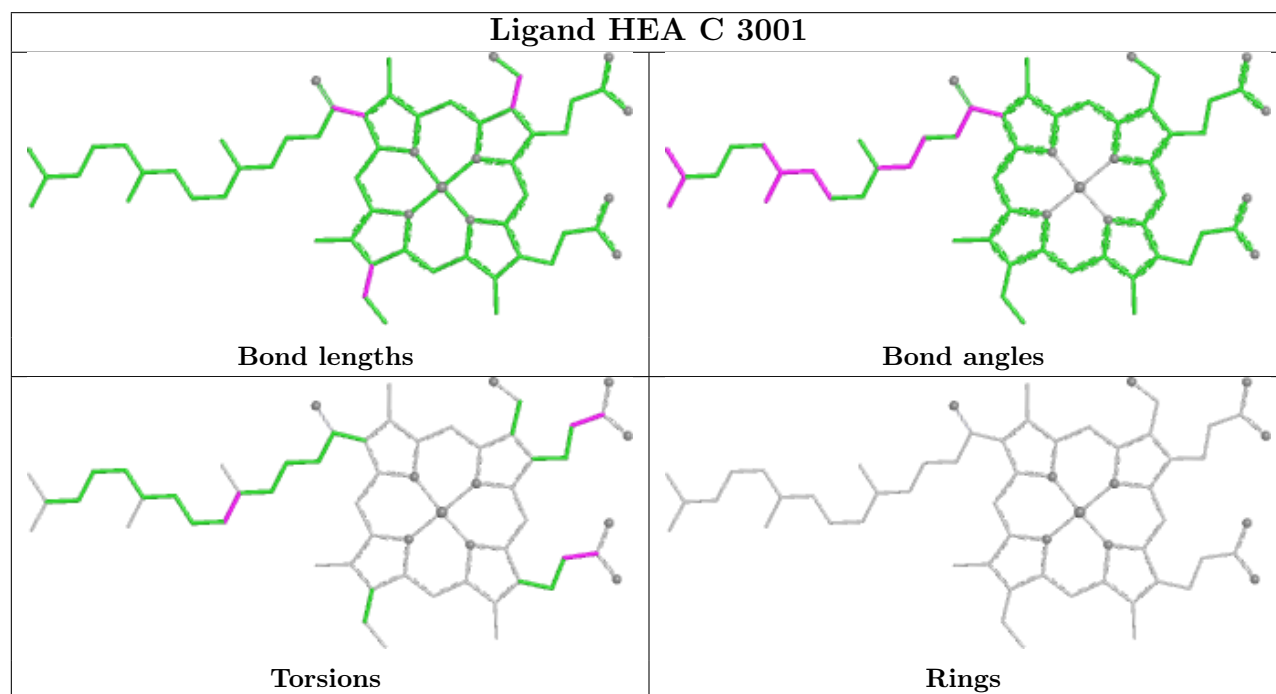
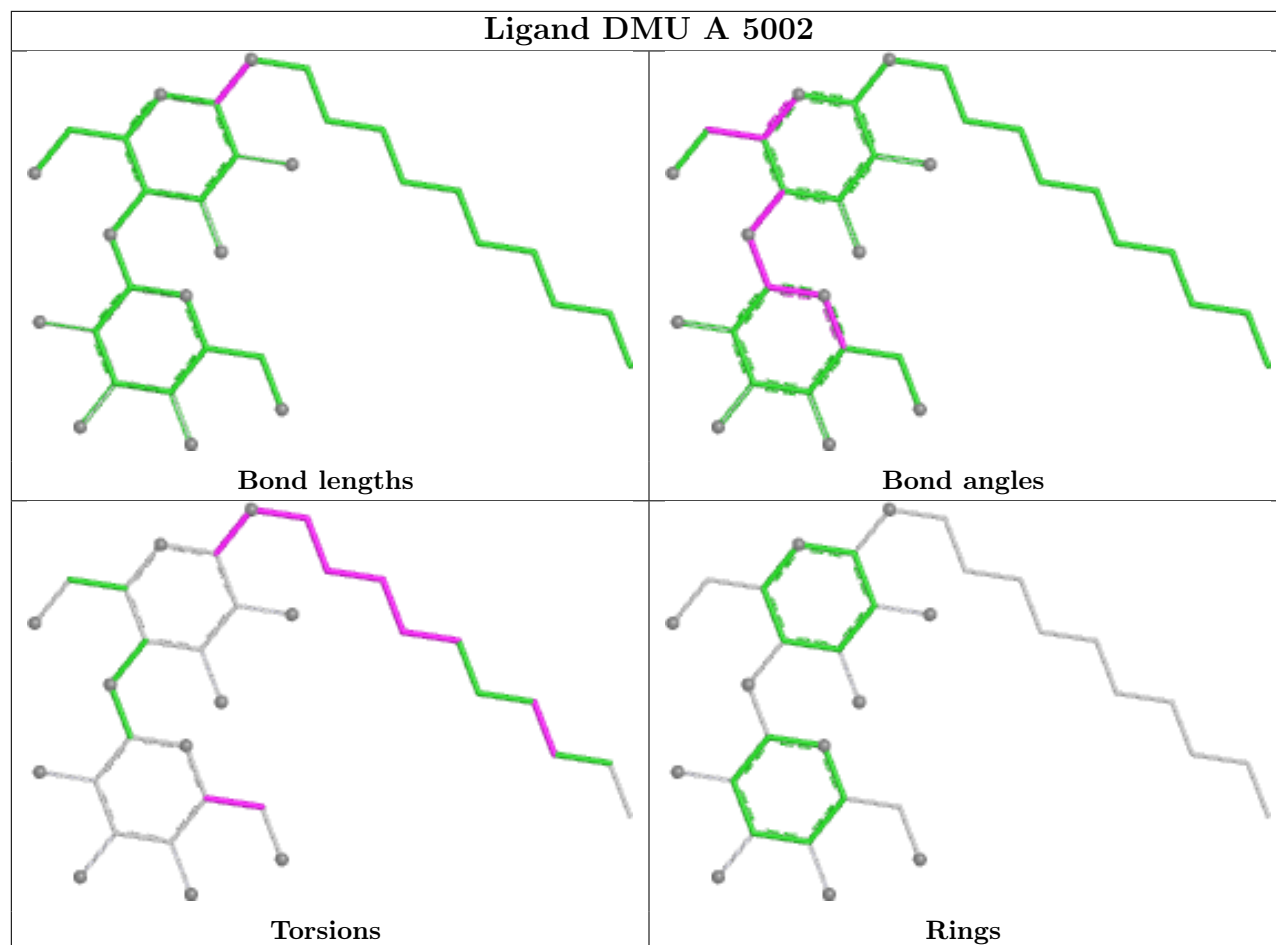


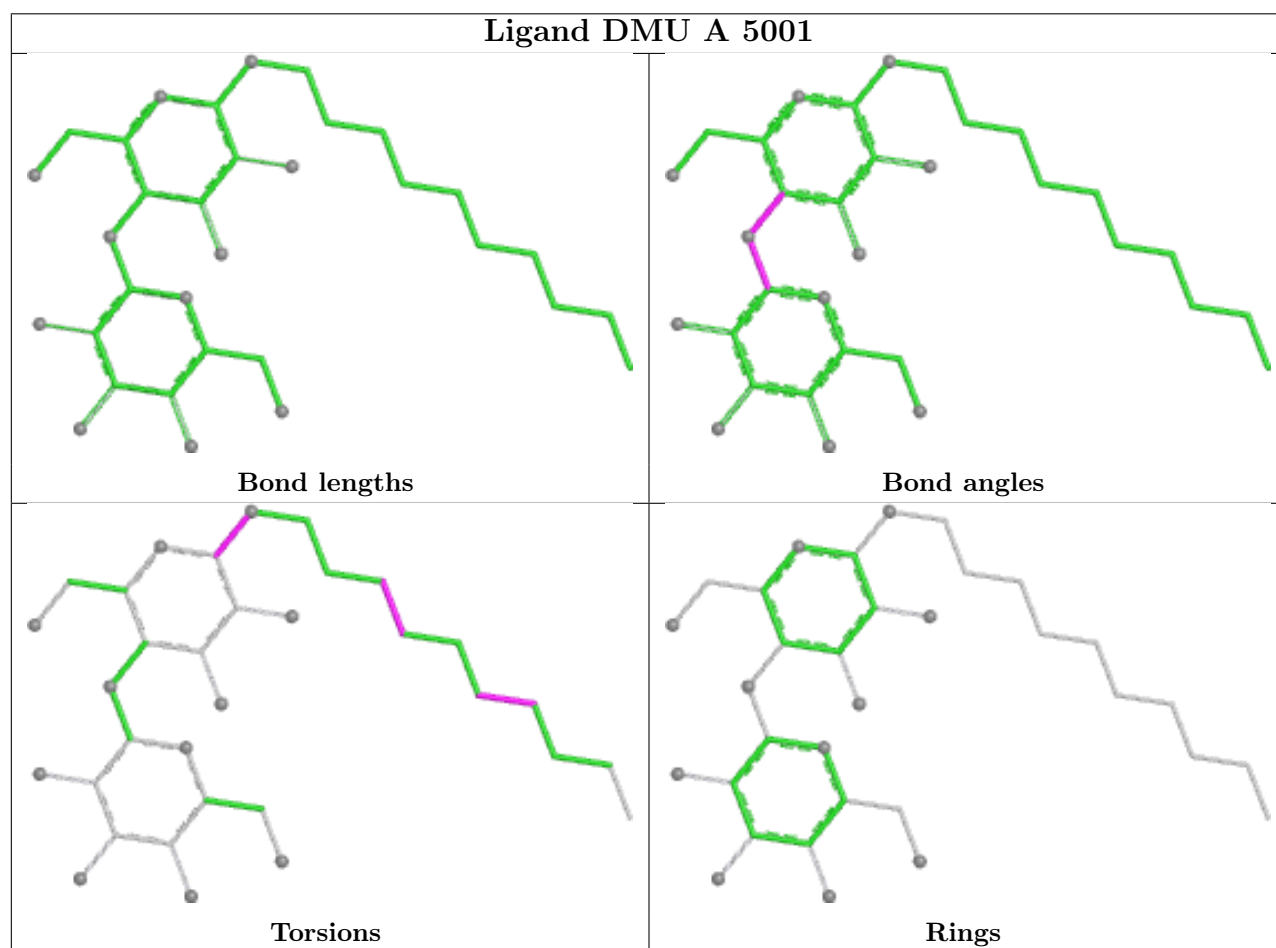
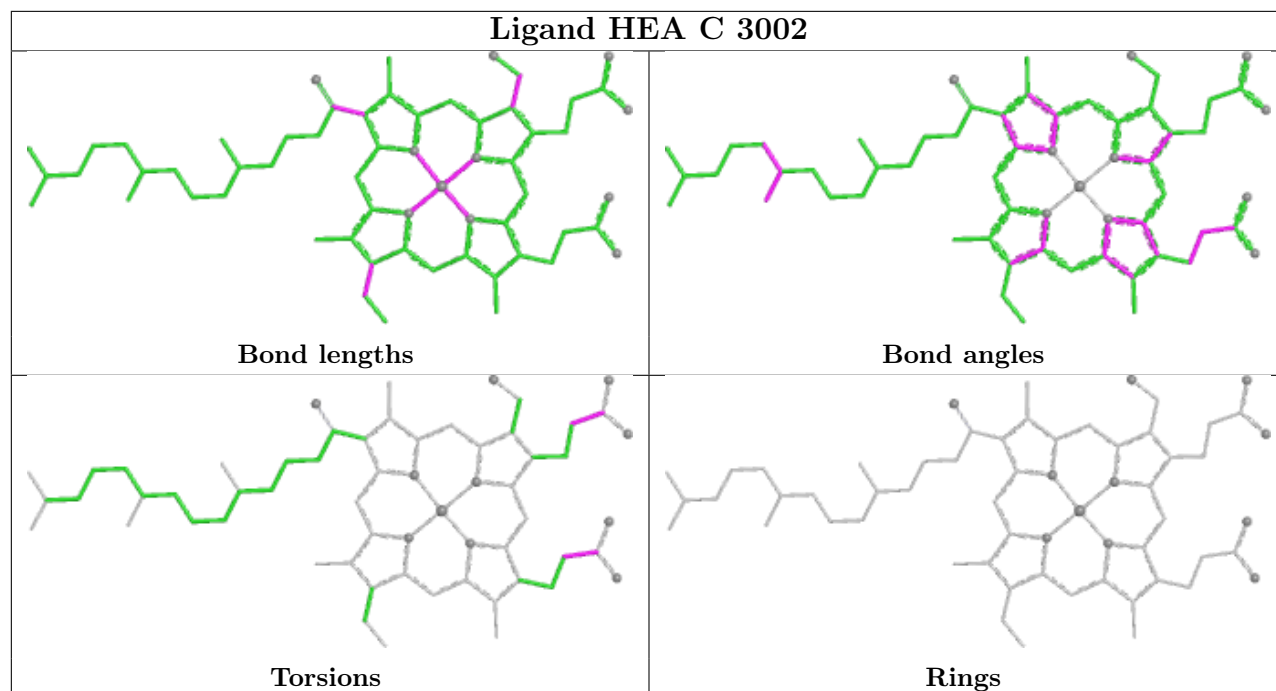
Ligand DMU D 6011

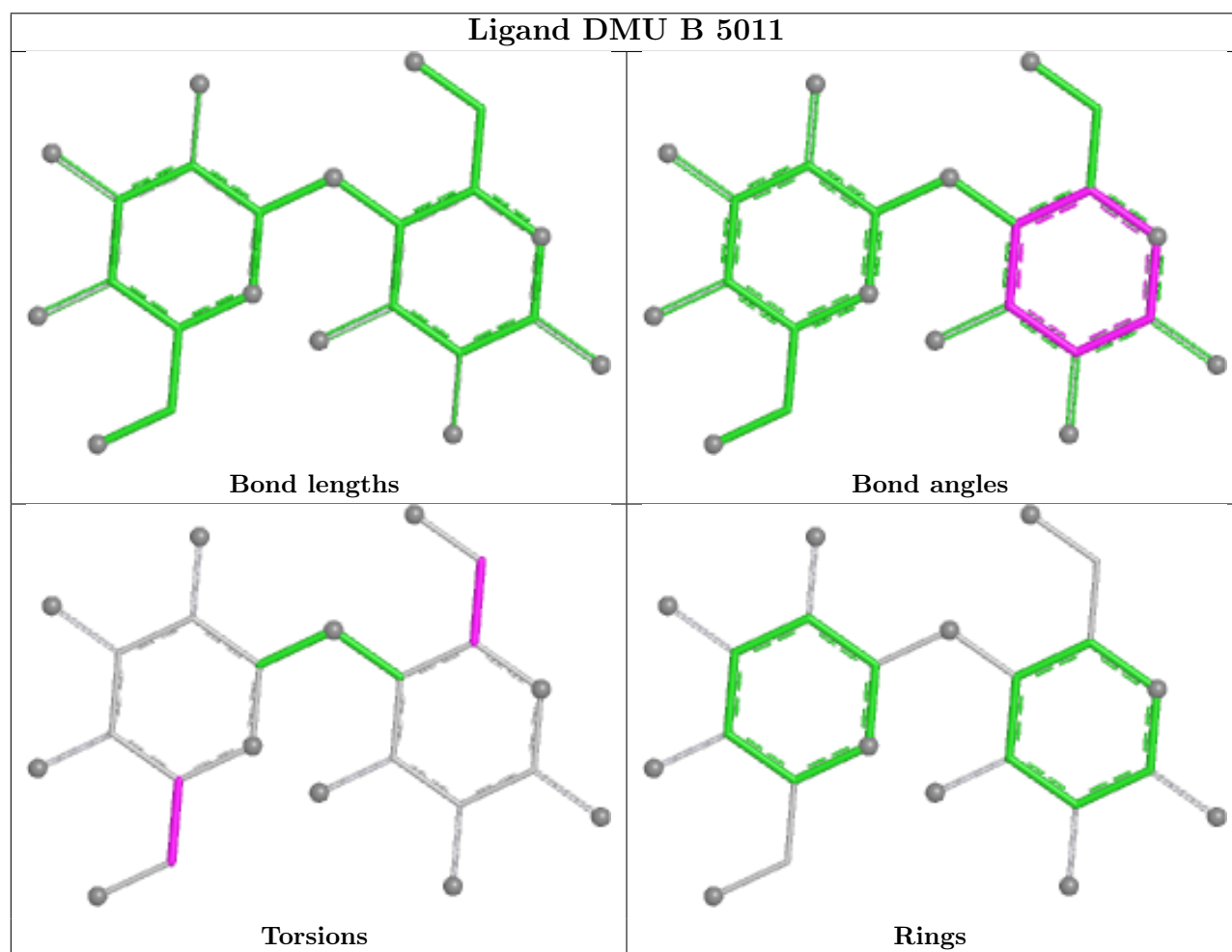
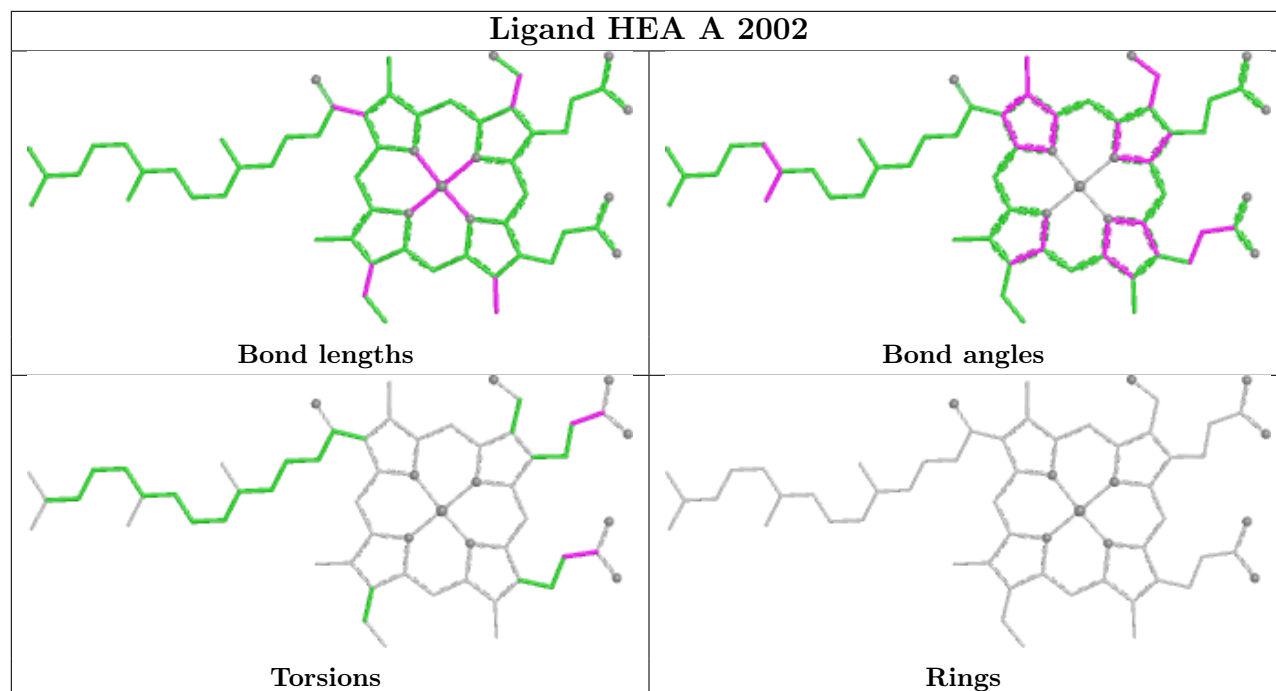


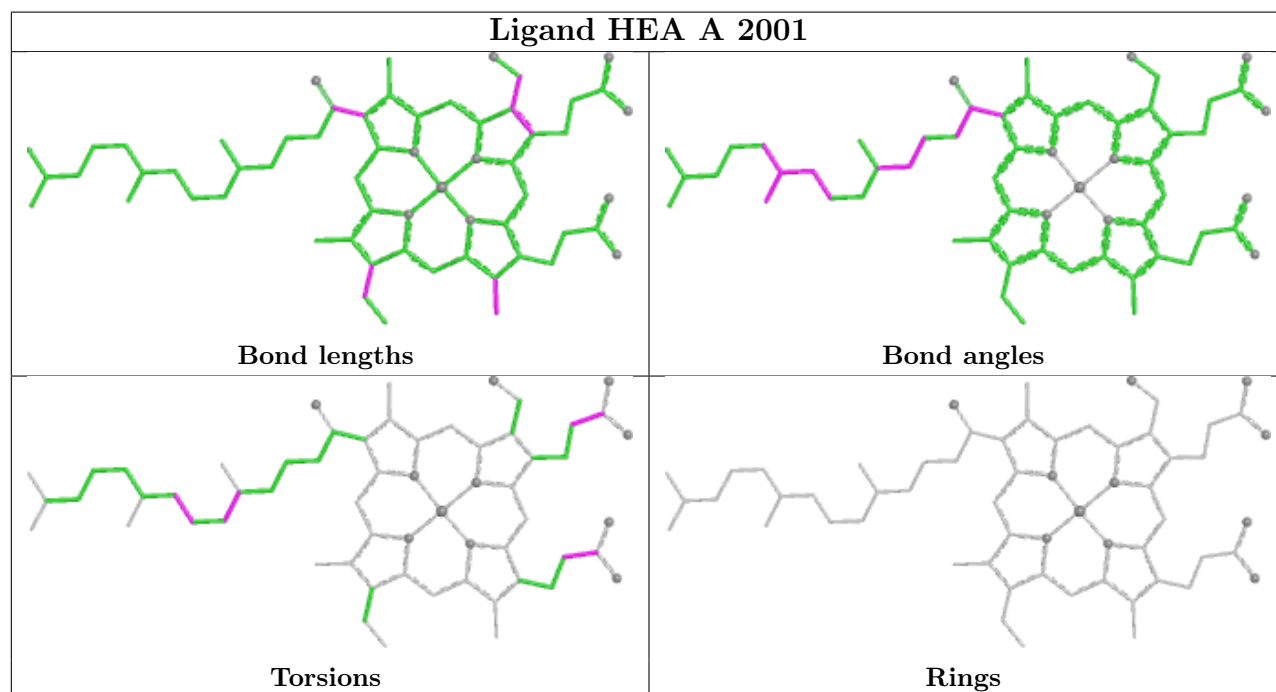
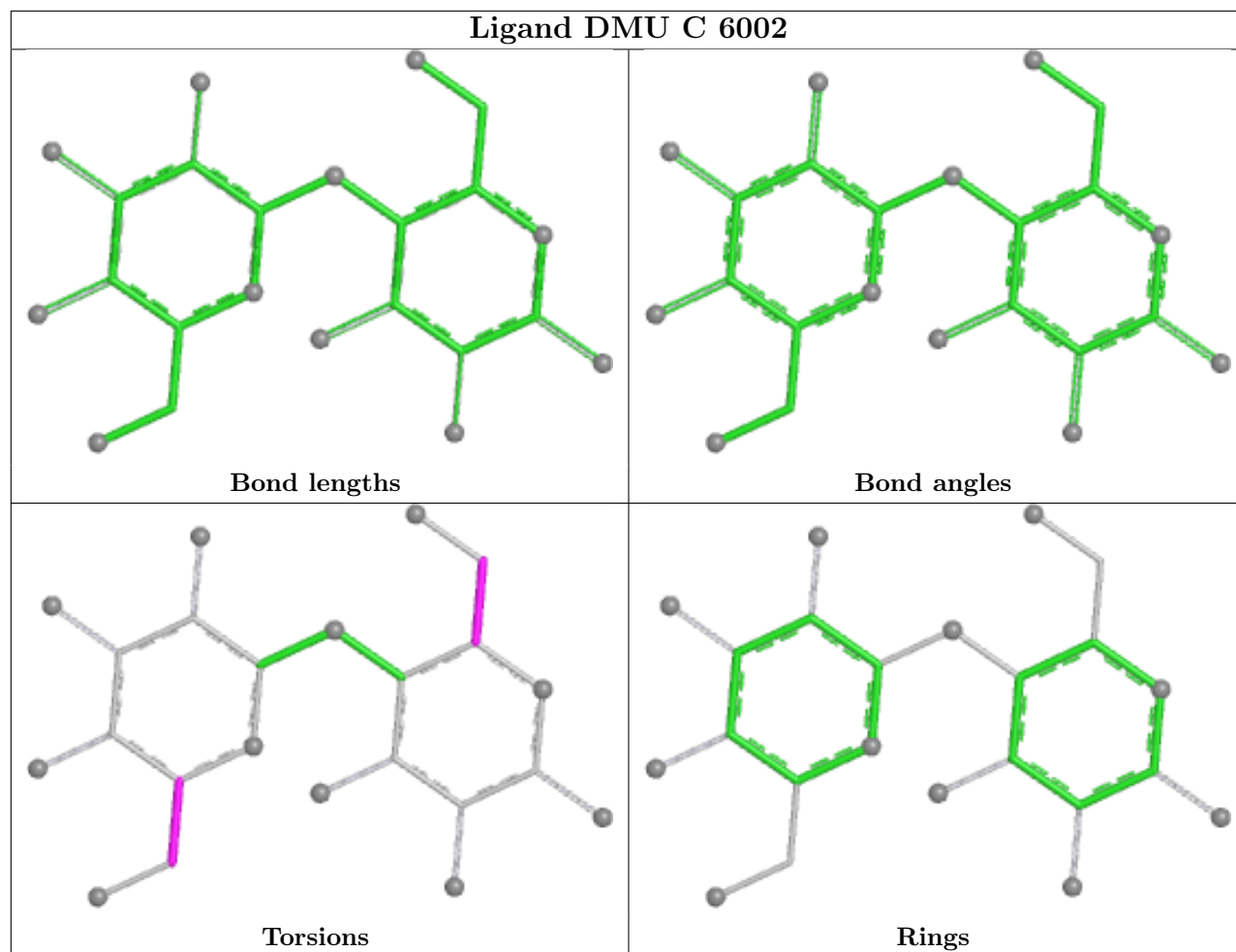


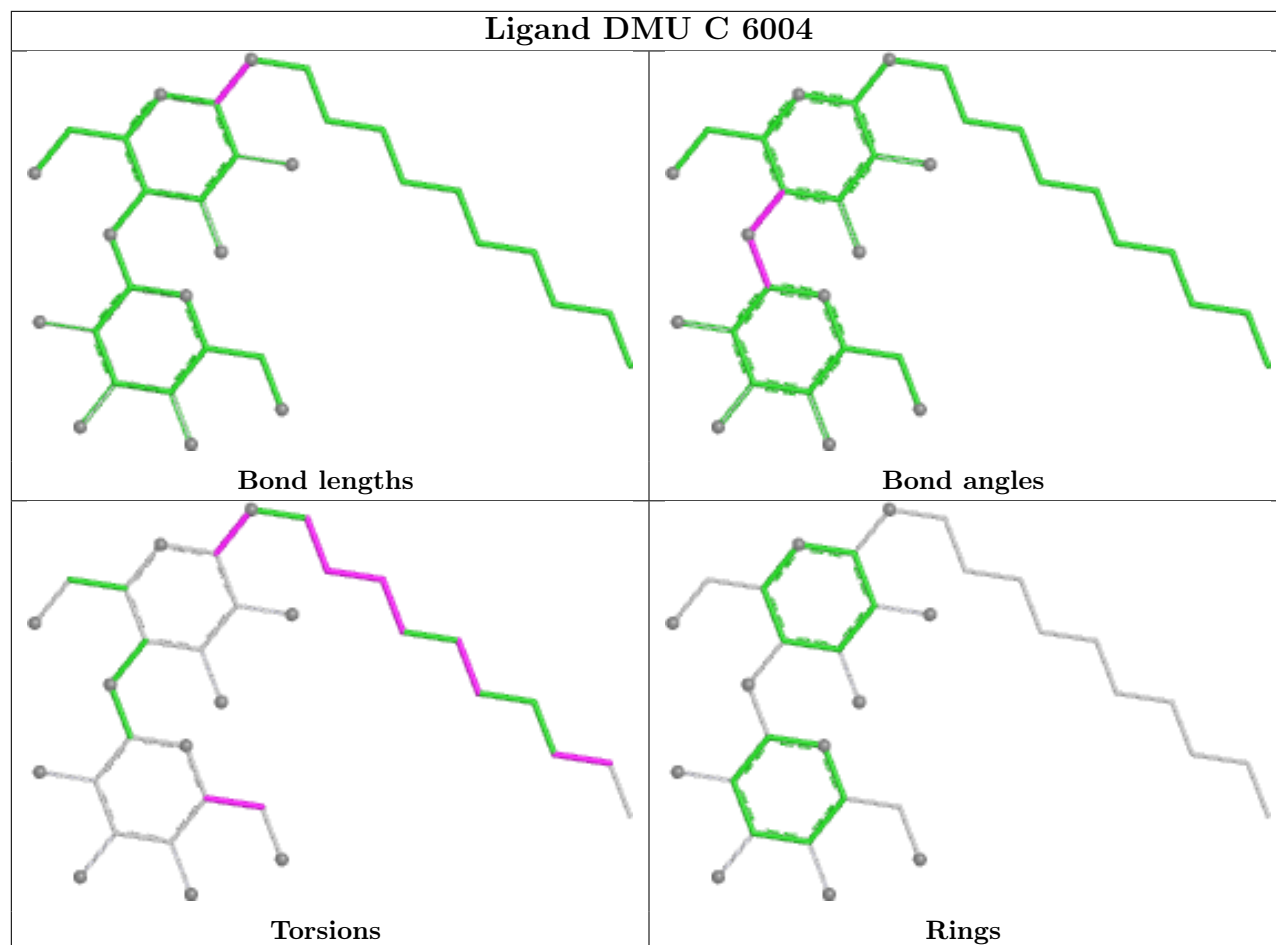


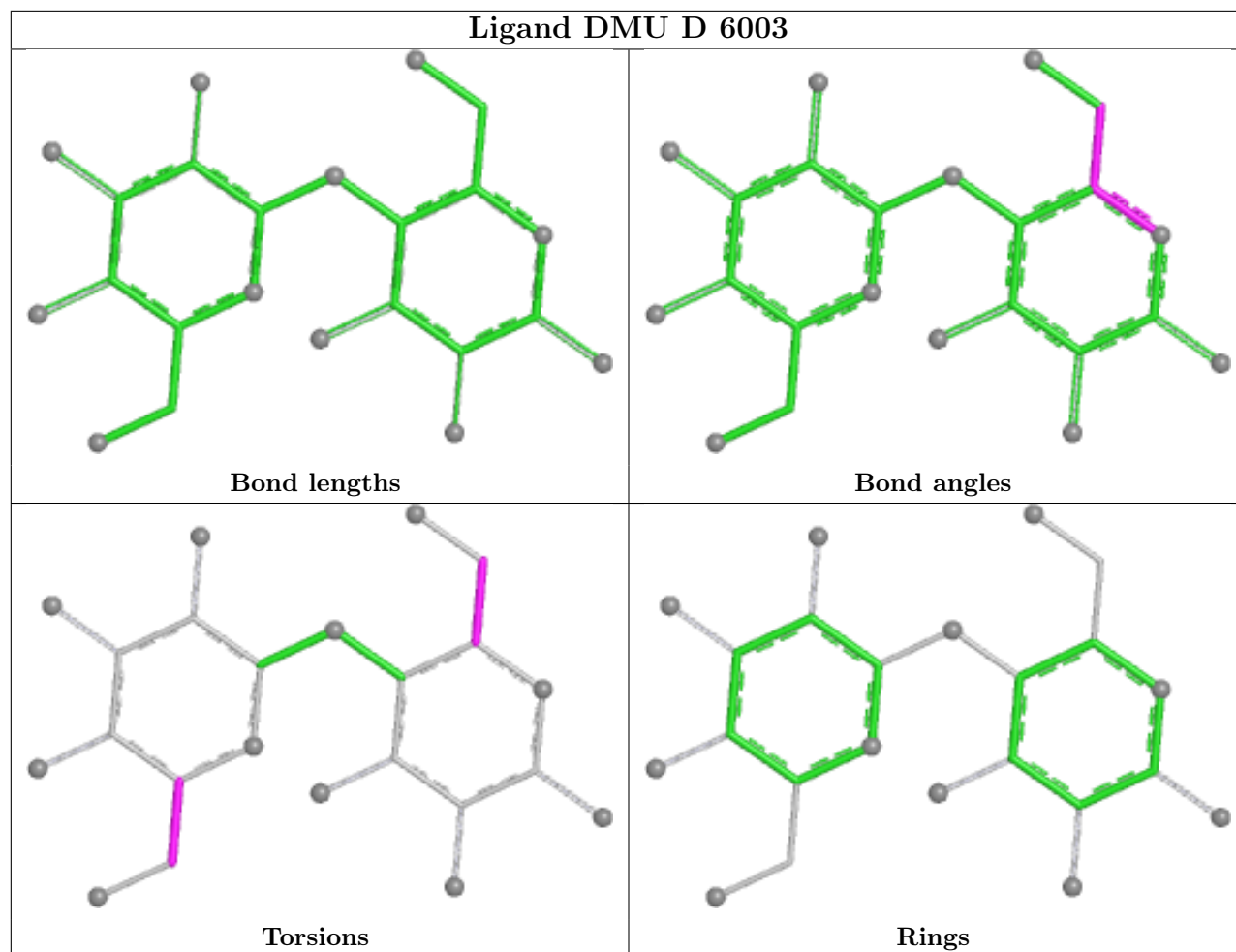












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	535/566 (94%)	-0.09	13 (2%) 59 59	19, 30, 44, 57	6 (1%)
1	C	534/566 (94%)	0.39	26 (4%) 35 34	22, 41, 53, 60	9 (1%)
2	B	256/262 (97%)	-0.07	2 (0%) 82 82	21, 33, 44, 50	2 (0%)
2	D	256/262 (97%)	0.13	6 (2%) 61 60	23, 37, 50, 55	3 (1%)
All	All	1581/1656 (95%)	0.11	47 (2%) 52 51	19, 35, 50, 60	20 (1%)

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	222	MET	5.0
1	A	17	PHE	4.2
1	A	20	TRP	4.0
1	C	81	TRP	3.7
2	D	56	TRP	3.5

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

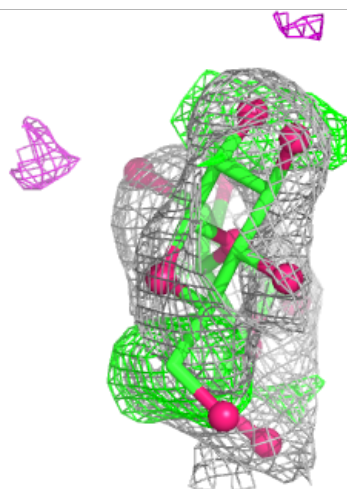
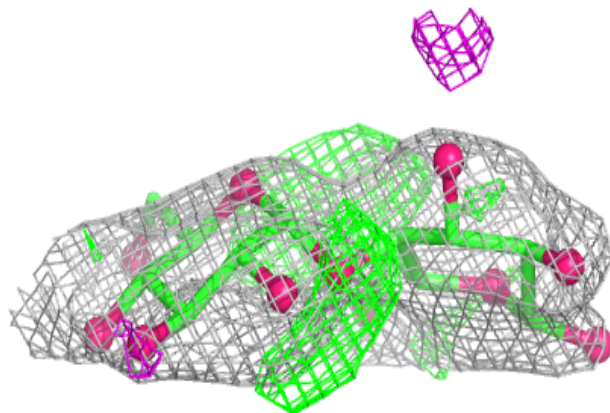
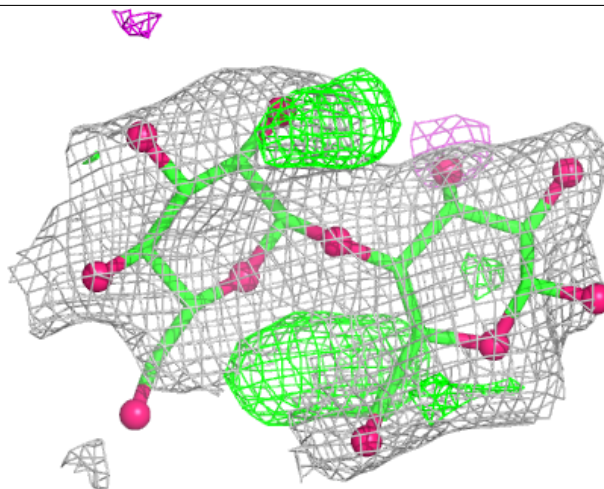
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMU	B	5011	23/33	0.59	0.19	51,54,57,59	23
9	TRD	C	6001	13/13	0.64	0.23	49,50,53,53	0
3	DMU	D	6011	23/33	0.65	0.18	53,55,57,57	23
9	TRD	C	6009	9/13	0.66	0.18	48,49,53,53	0
9	TRD	C	6006	13/13	0.68	0.17	51,52,53,54	0
3	DMU	C	6002	23/33	0.69	0.13	56,57,57,58	23
3	DMU	D	6003	23/33	0.72	0.15	50,52,55,56	23
9	TRD	A	5010	13/13	0.73	0.21	46,49,56,56	0
3	DMU	C	6005	33/33	0.73	0.18	44,53,57,57	33
3	DMU	C	6004	33/33	0.77	0.14	46,59,100,100	11
9	TRD	A	5009	7/13	0.77	0.19	48,51,52,52	0
9	TRD	A	5005	13/13	0.80	0.15	39,41,48,48	0
9	TRD	D	6007	13/13	0.80	0.19	45,46,49,49	0
3	DMU	A	5004	33/33	0.81	0.13	35,54,100,100	11
9	TRD	B	5008	9/13	0.84	0.13	44,45,46,46	0
9	TRD	A	5006	13/13	0.85	0.14	49,51,53,53	0
3	DMU	B	5003	33/33	0.86	0.12	48,52,58,58	0
9	TRD	A	5007	13/13	0.86	0.15	35,38,40,42	0
3	DMU	A	5002	33/33	0.86	0.11	48,51,55,57	0
9	TRD	C	6010	9/13	0.88	0.13	50,51,52,52	0
9	TRD	D	6008	7/13	0.89	0.14	44,44,45,45	0
3	DMU	A	5001	33/33	0.94	0.09	24,33,44,44	0
7	OH	C	7501	1/1	0.94	0.09	35,35,35,35	0
7	OH	A	6501	1/1	0.97	0.07	26,26,26,26	0
6	CA	C	4007	1/1	0.98	0.03	34,34,34,34	0
8	HEA	A	2002	60/60	0.98	0.06	21,25,32,35	0
8	HEA	C	3001	60/60	0.98	0.06	26,29,40,41	0
8	HEA	C	3002	60/60	0.98	0.06	26,30,38,39	0
4	CU	C	4005	1/1	0.99	0.02	33,33,33,33	0
5	MG	A	3006	1/1	0.99	0.11	10,10,10,10	0
8	HEA	A	2001	60/60	0.99	0.04	17,21,26,27	0
5	MG	C	4006	1/1	0.99	0.07	12,12,12,12	0
6	CA	A	3007	1/1	0.99	0.03	24,24,24,24	0
4	CU	A	3005	1/1	0.99	0.03	27,27,27,27	0
10	CD	B	3008	1/1	0.99	0.02	35,35,35,35	0
10	CD	B	3009	1/1	0.99	0.03	40,40,40,40	1
10	CD	D	4008	1/1	0.99	0.02	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	0.01	27,27,27,27	0
4	CU	D	4004	1/1	1.00	0.02	29,29,29,29	0
4	CU	B	3004	1/1	1.00	0.04	24,24,24,24	0
4	CU	B	3003	1/1	1.00	0.02	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.

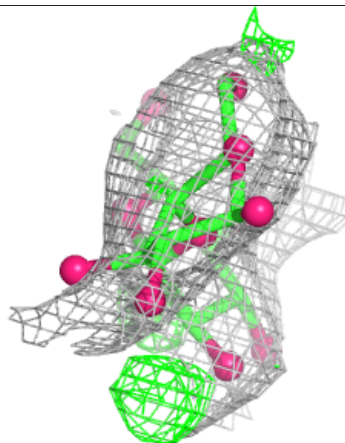
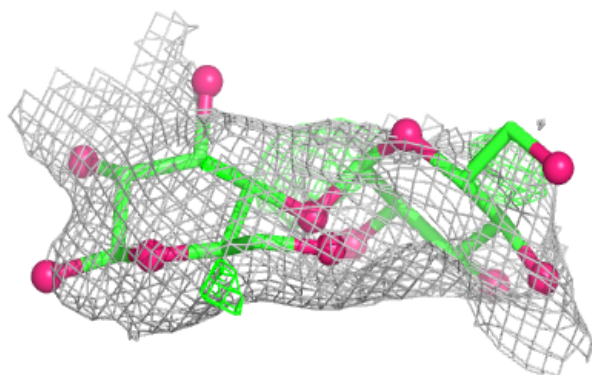
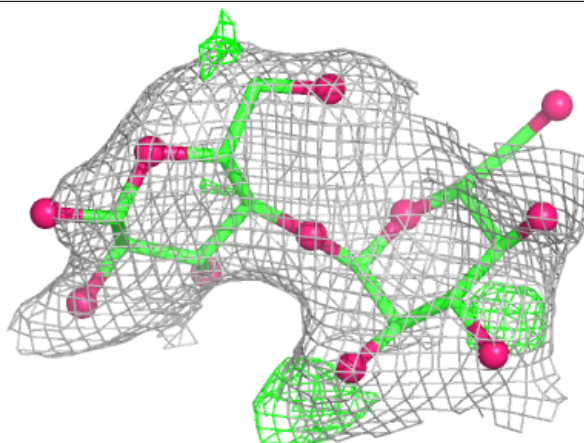
Electron density around DMU B 5011:

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



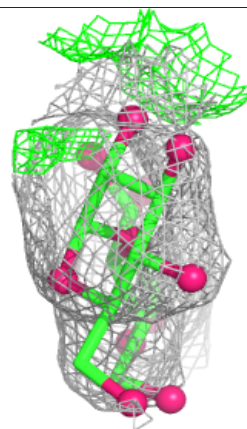
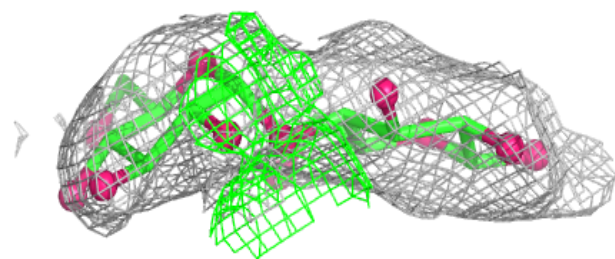
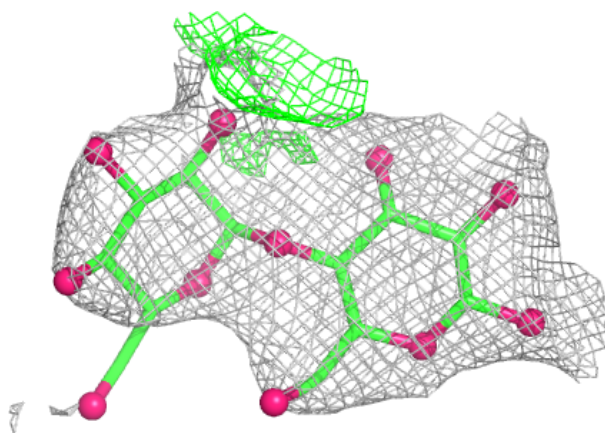
Electron density around DMU D 6011:

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



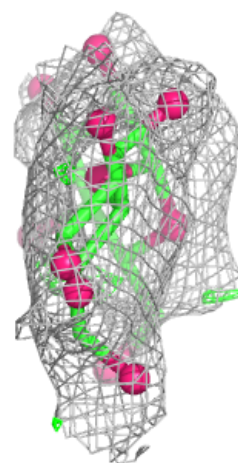
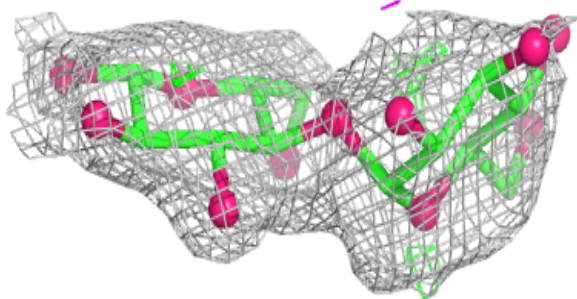
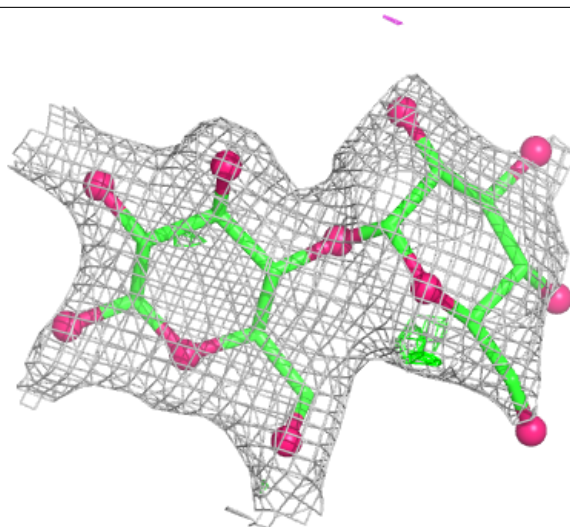
Electron density around DMU C 6002:

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



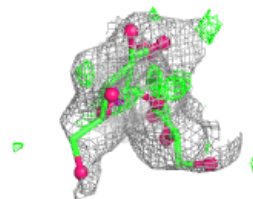
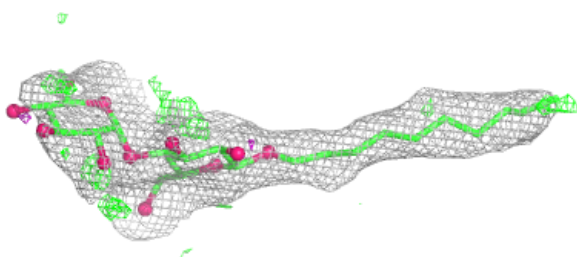
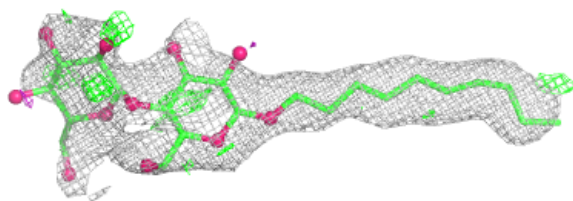
Electron density around DMU D 6003:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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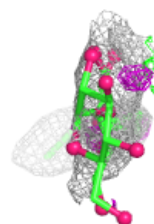
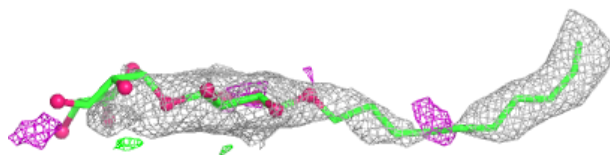
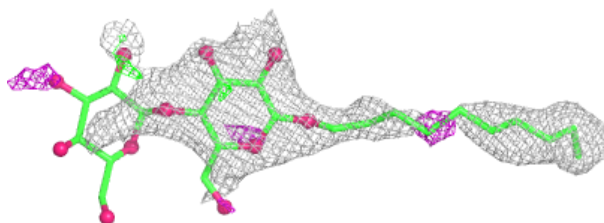


Electron density around DMU C 6005:

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and green (positive)

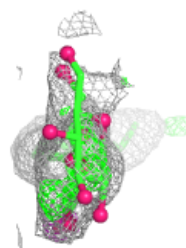
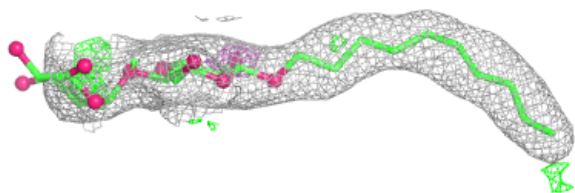
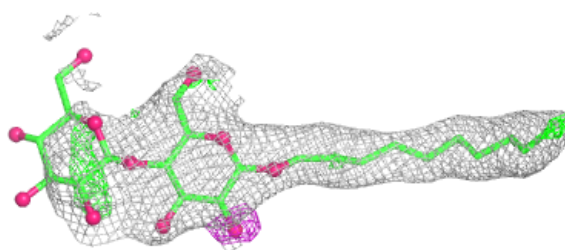
**Electron density around DMU C 6004:**

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

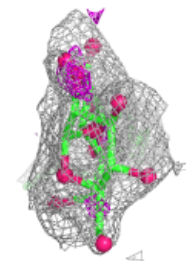
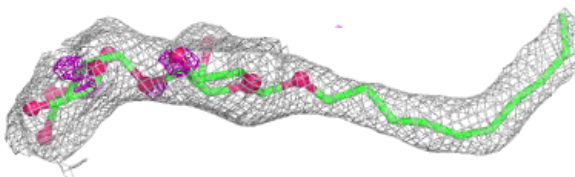
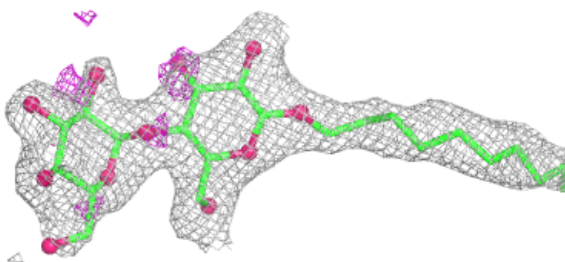


Electron density around DMU A 5004:

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and green (positive)

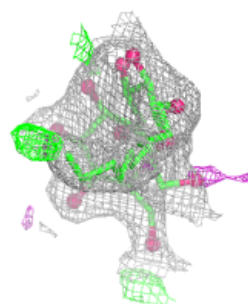
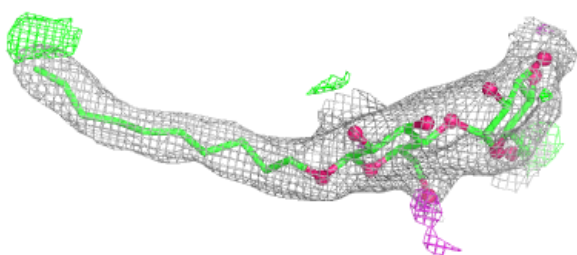
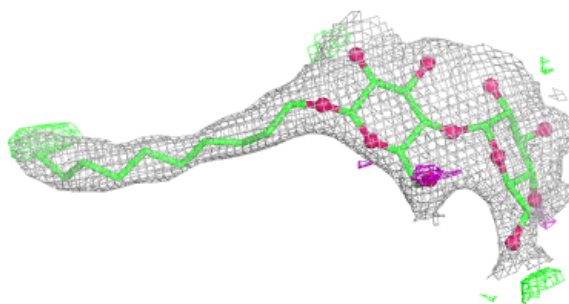
**Electron density around DMU B 5003:**

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

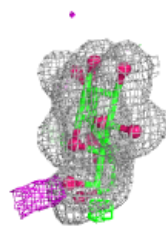
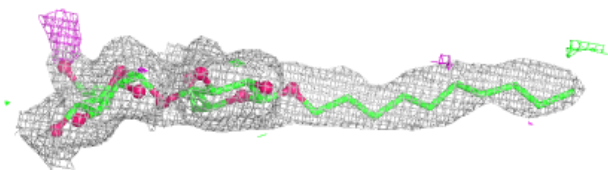
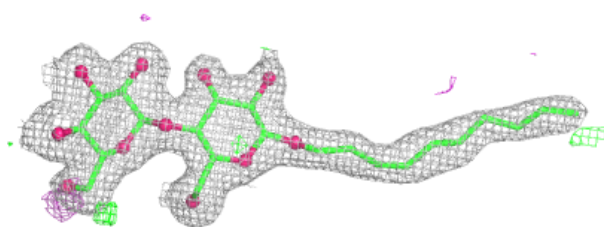


Electron density around DMU A 5002:

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

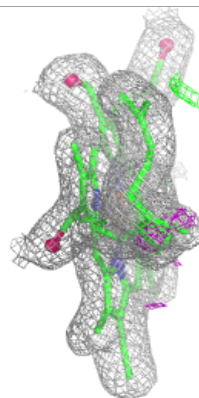
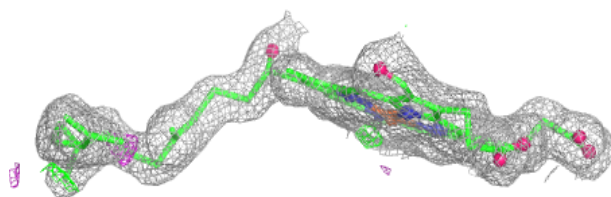
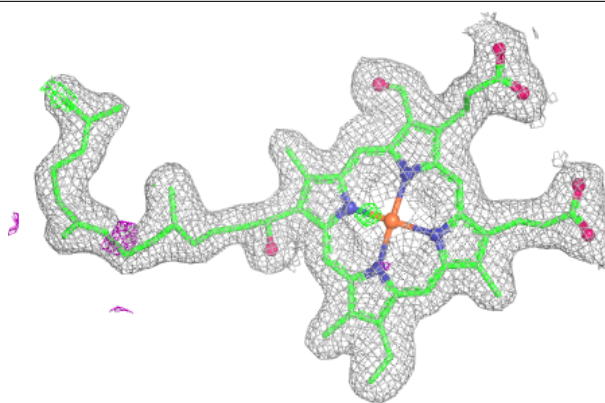
**Electron density around DMU A 5001:**

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

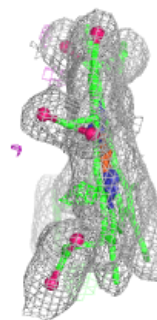
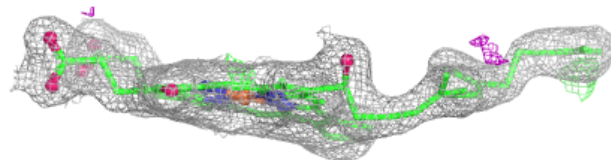
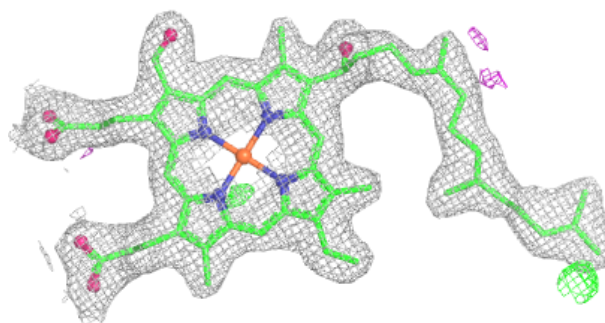


Electron density around HEA A 2002:

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

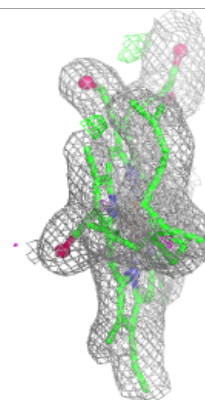
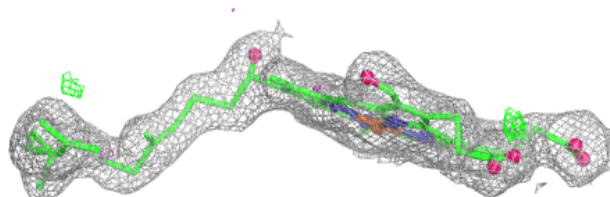
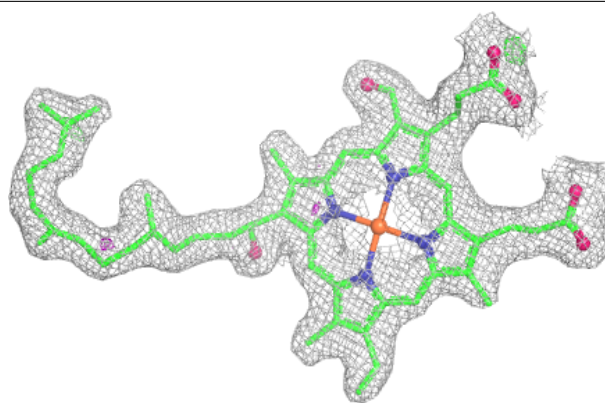
**Electron density around HEA C 3001:**

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

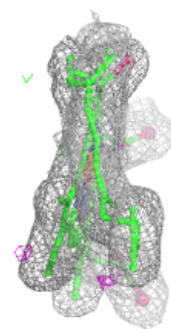
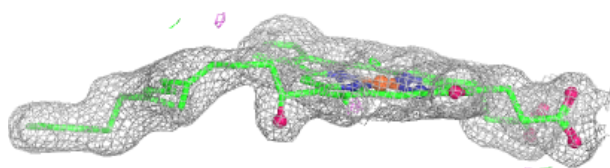
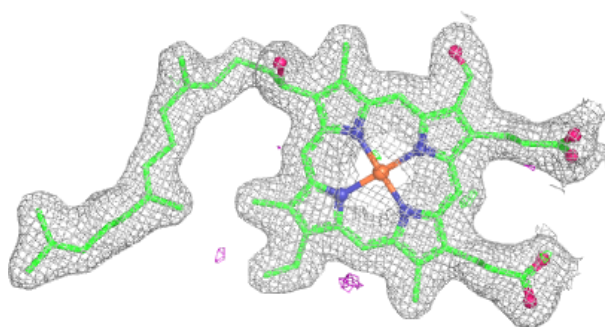


Electron density around HEA C 3002:

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

**Electron density around HEA A 2001:**

$2mF_o-DF_c$ (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.