



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 08:17 PM EDT

PDB ID : 3OMA
Title : Catalytic core subunits (I and II) of cytochrome C oxidase from Rhodobacter sphaeroides with K362M mutation
Authors : Liu, J.; Qin, L.; Ferguson-Miller, S.
Deposited on : 2010-08-26
Resolution : 2.30 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

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	:	4.02b-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

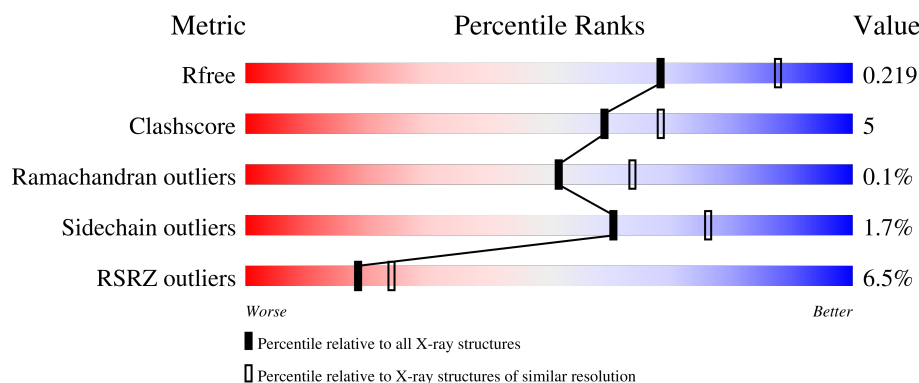
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	535	<div> <div>5%</div> <div>90%</div> <div>9%</div> </div>
1	C	535	<div> <div>10%</div> <div>86%</div> <div>13%</div> </div>
2	B	256	<div> <div>2%</div> <div>95%</div> <div></div> </div>
2	D	256	<div> <div>7%</div> <div>92%</div> <div>7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	HTH	B	286	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 13395 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c oxidase, aa3 type, subunit I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4159	2784	654	689	32			
1	C	531	Total	C	N	O	S	0	0	0
			4121	2761	646	683	31			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	MET	LYS	ENGINEERED MUTATION	UNP Q3J5A7
C	362	MET	LYS	ENGINEERED MUTATION	UNP Q3J5A7

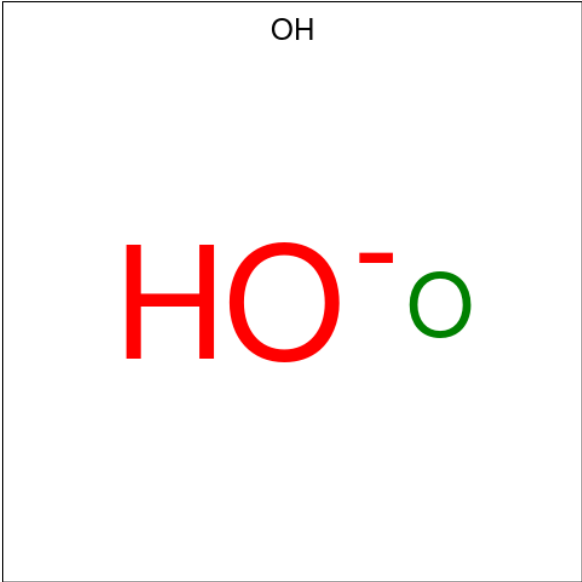
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			2018	1316	333	363	6			
2	D	256	Total	C	N	O	S	0	0	0
			1999	1305	326	362	6			

There are 8 discrepancies between the modelled and reference sequences:

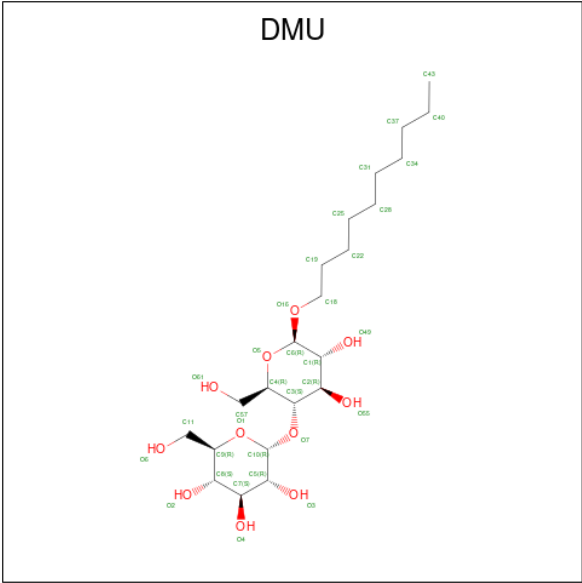
Chain	Residue	Modelled	Actual	Comment	Reference
B	282	HIS	-	EXPRESSION TAG	UNP Q3J5G0
B	283	HIS	-	EXPRESSION TAG	UNP Q3J5G0
B	284	HIS	-	EXPRESSION TAG	UNP Q3J5G0
B	285	HIS	-	EXPRESSION TAG	UNP Q3J5G0
D	282	HIS	-	EXPRESSION TAG	UNP Q3J5G0
D	283	HIS	-	EXPRESSION TAG	UNP Q3J5G0
D	284	HIS	-	EXPRESSION TAG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

- Molecule 3 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



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

- Molecule 4 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



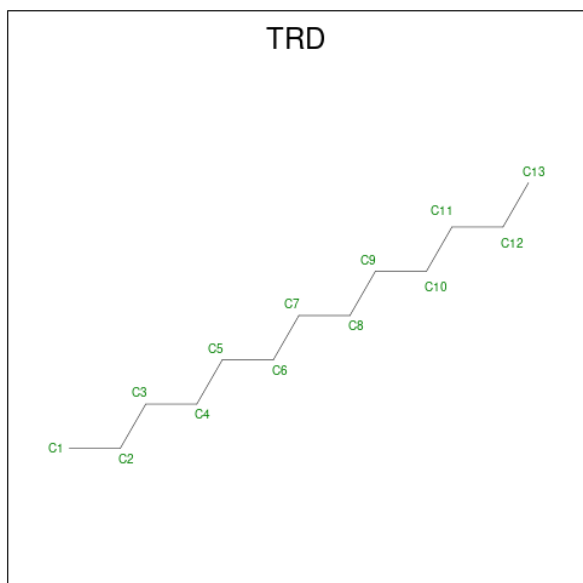
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 22 16 6	0	0

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

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



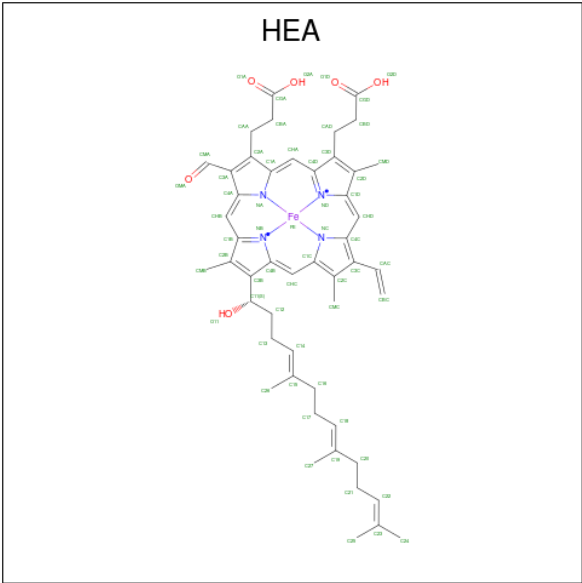
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 7 7	0	0

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

- Molecule 6 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

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

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

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

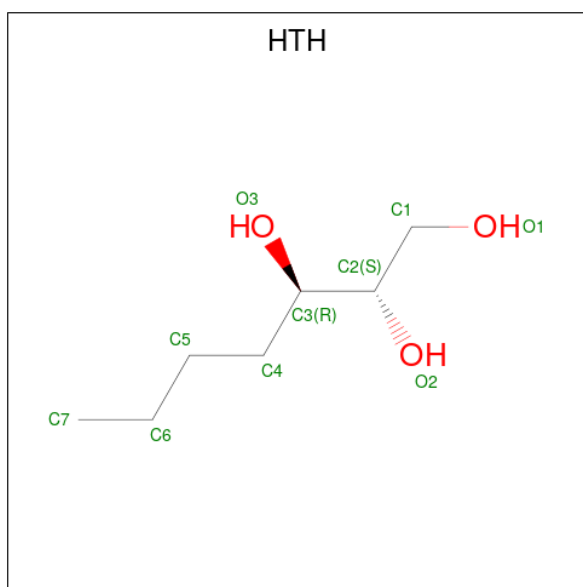
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 10 is (2S,3R)-heptane-1,2,3-triol (three-letter code: HTH) (formula: C₇H₁₆O₃).



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

- Molecule 11 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

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

- Molecule 12 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	132	Total	O	0	0
			132	132		
13	B	134	Total	O	0	0
			134	134		

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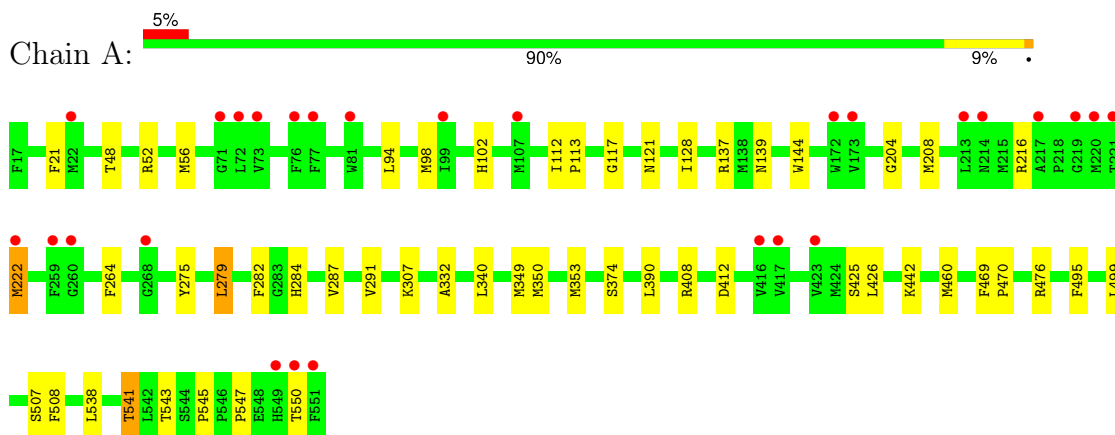
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	82	Total 82	O 82	0	0
13	D	104	Total 104	O 104	0	0

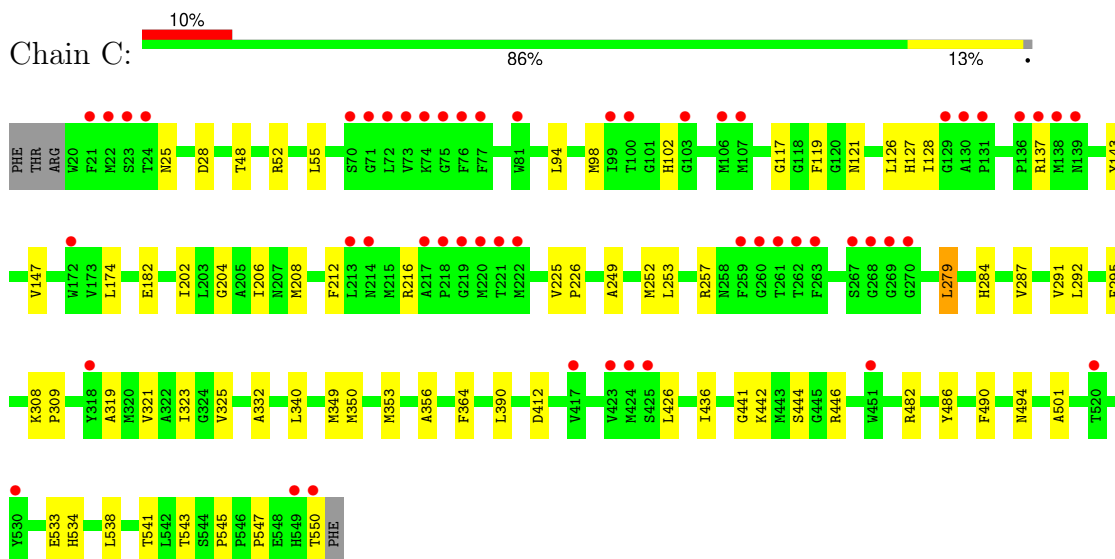
3 Residue-property plots [i](#)

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

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

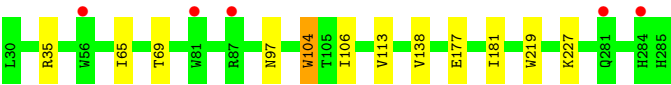


- Molecule 1: Cytochrome c oxidase, aa3 type, subunit I

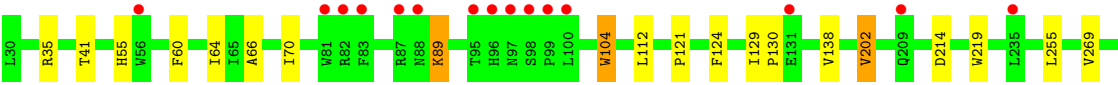
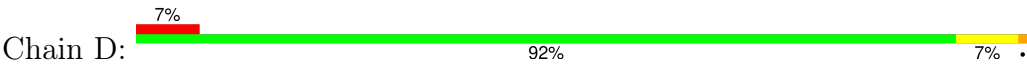


- Molecule 2: Cytochrome c oxidase subunit 2





● Molecule 2: Cytochrome c oxidase subunit 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.02Å 131.58Å 176.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.37 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-2.30) 97.6 (49.37-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.29Å)	Xtriage
Refinement program	REFMAC, CNS	Depositor
R, R_{free}	0.191 , 0.219 0.192 , 0.219	Depositor DCC
R_{free} test set	3771 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13395	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: TRD, HTH, CA, HEA, CU1, DMU, CU, MG, CD, OH

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	0/4311	0.56	0/5888
1	C	0.53	0/4272	0.54	0/5837
2	B	0.62	0/2080	0.57	0/2848
2	D	0.52	0/2060	0.54	0/2824
All	All	0.57	0/12723	0.55	0/17397

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4159	0	4051	43	0
1	C	4121	0	4015	48	0
2	B	2018	0	1969	7	0
2	D	1999	0	1936	17	0
3	A	1	0	0	1	0
3	C	1	0	0	1	0
4	A	44	0	62	1	0
4	B	122	0	147	0	0
4	C	79	0	84	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	46	0	42	3	0
5	A	47	0	92	1	0
5	B	9	0	17	1	0
5	C	13	0	28	0	0
5	D	20	0	41	1	0
6	A	120	0	108	6	0
6	C	120	0	108	5	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	B	10	0	16	1	0
11	B	1	0	0	0	0
11	D	1	0	0	0	0
12	B	2	0	0	0	0
12	D	2	0	0	0	0
13	A	132	0	0	4	0
13	B	134	0	0	1	0
13	C	82	0	0	4	0
13	D	104	0	0	1	0
All	All	13395	0	12716	120	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 5.

All (120) 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)
2:D:89:LYS:NZ	2:D:89:LYS:HB3	1.43	1.06
2:D:89:LYS:HB3	2:D:89:LYS:HZ2	0.85	0.99
1:C:534:HIS:HD2	13:C:623:HOH:O	1.44	0.98
2:D:89:LYS:NZ	2:D:89:LYS:CB	2.30	0.89
2:D:89:LYS:HZ2	2:D:89:LYS:CB	1.81	0.86
10:B:286:HTH:O2	13:B:496:HOH:O	1.98	0.82
6:A:1:HEA:HMC1	6:A:1:HEA:HBC1	1.65	0.76
3:A:706:OH:O	13:A:727:HOH:O	2.05	0.75
1:A:350:MET:HA	1:A:353:MET:HE3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:706:OH:O	13:C:556:HOH:O	2.09	0.70
1:A:350:MET:HA	1:A:353:MET:CE	2.21	0.70
1:A:543:THR:HG22	1:A:547:PRO:HD3	1.75	0.69
1:A:287:VAL:HB	6:A:2:HEA:CAC	2.22	0.68
6:C:1:HEA:HBC1	6:C:1:HEA:HMC1	1.75	0.68
1:C:128:ILE:HB	1:C:216:ARG:HG2	1.74	0.68
1:A:216:ARG:CZ	1:A:222:MET:HE3	2.24	0.68
1:A:21:PHE:HB3	1:A:144:TRP:HZ2	1.60	0.66
2:D:66:ALA:O	2:D:70:ILE:HG12	1.96	0.65
1:C:534:HIS:HE1	13:C:720:HOH:O	1.79	0.64
1:A:307:LYS:HE2	1:A:374:SER:HB3	1.81	0.62
1:C:182:GLU:O	1:C:257:ARG:NH1	2.34	0.61
1:A:204:GLY:O	1:A:208:MET:HG2	2.00	0.61
1:A:216:ARG:CZ	1:A:222:MET:CE	2.80	0.60
1:A:550:THR:OG1	13:A:814:HOH:O	2.15	0.60
2:D:202:VAL:HG13	2:D:269:VAL:HG12	1.84	0.59
4:D:4:DMU:H35	4:D:4:DMU:H29	1.84	0.59
1:A:550:THR:OG1	13:A:803:HOH:O	2.17	0.58
1:A:460:MET:HE3	1:A:507:SER:OG	2.03	0.58
1:A:543:THR:CG2	1:A:547:PRO:HD3	2.33	0.58
1:C:204:GLY:O	1:C:208:MET:HG2	2.03	0.58
1:C:319:ALA:O	1:C:323:ILE:HG12	2.03	0.58
1:C:350:MET:HA	1:C:353:MET:CE	2.34	0.57
2:B:65:ILE:O	2:B:69:THR:HG23	2.03	0.57
1:C:287:VAL:HB	6:C:2:HEA:CAC	2.35	0.57
1:A:287:VAL:HB	6:A:2:HEA:HAC	1.87	0.56
1:C:332:ALA:HB1	1:C:340:LEU:HD11	1.88	0.56
1:A:408:ARG:O	2:B:227:LYS:HE2	2.07	0.55
1:C:543:THR:HG23	1:C:545:PRO:O	2.07	0.55
1:C:533:GLU:H	1:C:533:GLU:CD	2.11	0.54
1:C:350:MET:HA	1:C:353:MET:HE2	1.90	0.54
1:C:321:VAL:O	1:C:325:VAL:HG23	2.08	0.53
6:C:2:HEA:HMC1	6:C:2:HEA:HBC1	1.89	0.53
2:D:121:PRO:HB3	4:D:4:DMU:H40	1.91	0.52
1:A:543:THR:HG23	1:A:545:PRO:O	2.10	0.52
2:B:177:GLU:O	2:B:181:ILE:HG12	2.08	0.52
1:C:202:ILE:O	1:C:206:ILE:HG12	2.09	0.52
1:C:534:HIS:CE1	13:C:720:HOH:O	2.60	0.52
1:C:349:MET:O	1:C:353:MET:HG3	2.10	0.52
1:C:279:LEU:O	1:C:279:LEU:HG	2.09	0.51
1:A:216:ARG:NH2	1:A:222:MET:CE	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:LEU:O	1:C:257:ARG:HG3	2.11	0.50
1:A:332:ALA:HB1	1:A:340:LEU:HD11	1.93	0.50
1:C:538:LEU:O	1:C:541:THR:HB	2.12	0.50
2:D:60:PHE:O	2:D:64:ILE:HG12	2.12	0.49
1:A:287:VAL:HB	6:A:2:HEA:C3C	2.43	0.49
1:C:308:LYS:HG3	1:C:309:PRO:HD2	1.94	0.48
1:A:538:LEU:O	1:A:541:THR:HB	2.12	0.48
1:A:56:MET:HE1	4:A:1005:DMU:H6	1.95	0.48
2:B:113:VAL:HA	5:B:4:TRD:H61	1.95	0.48
1:C:444:SER:HA	4:C:9:DMU:H5	1.95	0.48
2:D:55:HIS:HE1	13:D:330:HOH:O	1.96	0.48
1:A:390:LEU:HD13	1:A:426:LEU:HB3	1.96	0.47
2:B:104:TRP:C	2:B:104:TRP:CD1	2.86	0.47
2:D:124:PHE:HB3	4:D:4:DMU:H33	1.97	0.47
1:C:48:THR:CG2	1:C:102:HIS:CE1	2.99	0.46
1:C:547:PRO:HD2	1:C:550:THR:HG22	1.97	0.46
6:C:2:HEA:HMC1	6:C:2:HEA:CBC	2.46	0.46
1:A:425:SER:C	1:A:426:LEU:HD12	2.36	0.45
1:A:442:LYS:O	1:A:545:PRO:HA	2.16	0.45
1:C:543:THR:HG22	1:C:547:PRO:HD3	1.98	0.45
1:A:279:LEU:O	1:A:279:LEU:HG	2.17	0.45
1:C:356:ALA:HB3	2:D:112:LEU:HD11	1.98	0.45
1:A:216:ARG:NH2	1:A:222:MET:HE1	2.31	0.45
2:D:138:VAL:HG11	2:D:219:TRP:CD1	2.52	0.45
1:A:495:PHE:CE2	1:A:499:LEU:HD11	2.52	0.44
1:C:212:PHE:CE2	1:C:225:VAL:HG11	2.52	0.44
1:C:284:HIS:O	1:C:287:VAL:HG22	2.15	0.44
1:A:128:ILE:HB	1:A:216:ARG:HG2	1.99	0.44
1:A:94:LEU:O	1:A:98:MET:HG2	2.17	0.44
1:A:460:MET:HE1	6:A:1:HEA:H262	1.98	0.44
1:C:126:LEU:O	1:C:538:LEU:HB2	2.18	0.44
1:A:508:PHE:HB2	6:A:1:HEA:H261	1.99	0.44
1:C:119:PHE:HZ	1:C:436:ILE:HG13	1.83	0.43
2:D:104:TRP:CD1	2:D:104:TRP:C	2.91	0.43
1:A:117:GLY:O	1:A:121:ASN:HB2	2.18	0.43
1:C:127:HIS:HB3	1:C:226:PRO:HG2	2.00	0.43
1:A:426:LEU:HD12	1:A:426:LEU:N	2.34	0.43
1:A:469:PHE:N	1:A:470:PRO:CD	2.82	0.43
1:C:441:GLY:HA2	1:C:446:ARG:O	2.18	0.43
1:C:284:HIS:CD2	1:C:284:HIS:C	2.91	0.43
1:A:216:ARG:NH2	1:A:222:MET:HE3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ALA:HA	1:C:252:MET:HE3	2.01	0.42
1:C:486:TYR:CD2	1:C:490:PHE:HB2	2.54	0.42
2:B:138:VAL:HG11	2:B:219:TRP:CD1	2.54	0.42
1:C:143:TYR:O	1:C:147:VAL:HG23	2.19	0.42
1:A:476:ARG:HH21	5:A:3:TRD:H31	1.85	0.42
1:C:364:PHE:HB3	2:D:104:TRP:CE3	2.55	0.42
1:A:112:ILE:HB	1:A:113:PRO:HD3	2.00	0.42
1:A:284:HIS:CD2	1:A:284:HIS:C	2.93	0.42
1:A:139:ASN:HA	13:A:824:HOH:O	2.20	0.42
1:C:52:ARG:HG3	1:C:501:ALA:CB	2.50	0.42
1:C:55:LEU:O	1:C:494:ASN:HB3	2.19	0.41
1:A:48:THR:CG2	1:A:102:HIS:CE1	3.04	0.41
1:C:390:LEU:HD13	1:C:426:LEU:HB3	2.02	0.41
1:A:349:MET:O	1:A:353:MET:HE2	2.20	0.41
1:C:94:LEU:O	1:C:98:MET:HG2	2.20	0.41
1:C:442:LYS:O	1:C:545:PRO:HA	2.21	0.41
1:A:350:MET:HA	1:A:353:MET:HE2	2.00	0.41
1:A:264:PHE:CE1	1:A:275:TYR:HB2	2.56	0.41
2:D:129:ILE:HA	2:D:130:PRO:HD3	1.91	0.41
6:C:1:HEA:HMC1	6:C:1:HEA:CB	2.49	0.41
2:B:104:TRP:C	2:B:104:TRP:HD1	2.25	0.40
1:C:117:GLY:O	1:C:121:ASN:HB2	2.21	0.40
1:C:292:LEU:HD23	1:C:292:LEU:HA	1.80	0.40
1:C:350:MET:HA	1:C:353:MET:HE3	2.00	0.40
2:D:41:THR:OG1	5:D:3:TRD:H12	2.21	0.40
1:C:48:THR:HG21	1:C:102:HIS:CE1	2.56	0.40
1:C:482:ARG:HD3	2:D:255:LEU:HB2	2.03	0.40
1:C:25:ASN:HB3	1:C:28:ASP:OD2	2.22	0.40
1:C:292:LEU:O	1:C:295:PHE:HB2	2.21	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	533/535 (100%)	520 (98%)	13 (2%)	0	100	100
1	C	529/535 (99%)	516 (98%)	13 (2%)	0	100	100
2	B	254/256 (99%)	248 (98%)	5 (2%)	1 (0%)	34	42
2	D	254/256 (99%)	245 (96%)	9 (4%)	0	100	100
All	All	1570/1582 (99%)	1529 (97%)	40 (2%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	97	ASN

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	424/435 (98%)	416 (98%)	8 (2%)	57	73
1	C	420/435 (97%)	415 (99%)	5 (1%)	71	84
2	B	213/215 (99%)	210 (99%)	3 (1%)	67	81
2	D	209/215 (97%)	204 (98%)	5 (2%)	49	66
All	All	1266/1300 (97%)	1245 (98%)	21 (2%)	60	76

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	137	ARG
1	A	222	MET
1	A	279	LEU
1	A	282	PHE
1	A	291	VAL
1	A	412	ASP
1	A	541	THR
2	B	35	ARG
2	B	104	TRP

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Mol	Chain	Res	Type
2	B	106	ILE
1	C	137	ARG
1	C	174	LEU
1	C	279	LEU
1	C	291	VAL
1	C	412	ASP
2	D	35	ARG
2	D	89	LYS
2	D	104	TRP
2	D	202	VAL
2	D	214	ASP

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 2 are modelled with single atom and 14 are monoatomic - leaving 25 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMU	D	4	-	24,24,34	0.53	0	35,35,45	0.63	0
5	TRD	A	1009	-	6,6,12	0.31	0	5,5,11	0.37	0
4	DMU	D	8	-	24,24,34	0.54	0	35,35,45	0.68	0
10	HTH	B	286	-	9,9,9	0.35	0	10,10,10	0.73	0
4	DMU	A	1005	-	22,22,34	0.58	1 (4%)	27,27,45	0.82	1 (3%)
5	TRD	A	1013	-	6,6,12	0.32	0	5,5,11	0.38	0
4	DMU	B	2	-	34,34,34	0.55	1 (2%)	45,45,45	0.93	3 (6%)
6	HEA	A	2	1,13	58,67,67	1.32	6 (10%)	63,103,103	1.64	15 (23%)
4	DMU	B	3	-	34,34,34	0.57	0	45,45,45	0.60	0
5	TRD	A	3	-	12,12,12	0.37	0	11,11,11	0.34	0
4	DMU	C	9	-	24,24,34	0.58	0	35,35,45	0.94	2 (5%)
6	HEA	A	1	1	58,67,67	1.30	6 (10%)	63,103,103	1.57	11 (17%)
4	DMU	C	10	-	34,34,34	0.64	1 (2%)	45,45,45	0.83	0
6	HEA	C	2	1,13	58,67,67	1.39	5 (8%)	63,103,103	1.53	14 (22%)
5	TRD	A	552	-	12,12,12	0.27	0	11,11,11	0.47	0
4	DMU	C	5	-	24,24,34	0.52	0	35,35,45	0.65	0
5	TRD	B	4	-	8,8,12	0.26	0	7,7,11	0.45	0
4	DMU	A	7	-	22,22,34	0.56	0	27,27,45	0.77	1 (3%)
5	TRD	C	552	-	12,12,12	0.26	0	11,11,11	0.52	0
4	DMU	B	6	-	24,24,34	0.53	0	35,35,45	0.74	0
4	DMU	B	1	-	34,34,34	0.58	0	45,45,45	1.17	3 (6%)
5	TRD	A	1015	-	6,6,12	0.32	0	5,5,11	0.37	0
5	TRD	D	14	-	6,6,12	0.26	0	5,5,11	0.39	0
5	TRD	D	3	-	12,12,12	0.20	0	11,11,11	0.59	0
6	HEA	C	1	1	58,67,67	1.33	5 (8%)	63,103,103	1.56	12 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMU	D	4	-	-	3/8/48/59	0/2/2/2
5	TRD	A	1009	-	-	2/4/4/10	-
4	DMU	D	8	-	-	0/8/48/59	0/2/2/2
10	HTH	B	286	-	-	3/10/10/10	-
4	DMU	A	1005	-	-	5/13/33/59	0/1/1/2
5	TRD	A	1013	-	-	0/4/4/10	-
4	DMU	B	2	-	-	10/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEA	A	2	1,13	-	6/32/76/76	-
4	DMU	B	3	-	-	6/19/59/59	0/2/2/2
5	TRD	A	3	-	-	4/10/10/10	-
4	DMU	C	9	-	-	4/8/48/59	0/2/2/2
6	HEA	A	1	1	-	6/32/76/76	-
4	DMU	C	10	-	-	11/19/59/59	0/2/2/2
6	HEA	C	2	1,13	-	8/32/76/76	-
5	TRD	A	552	-	-	4/10/10/10	-
4	DMU	C	5	-	-	3/8/48/59	0/2/2/2
5	TRD	B	4	-	-	1/6/6/10	-
4	DMU	A	7	-	-	4/13/33/59	0/1/1/2
5	TRD	C	552	-	-	2/10/10/10	-
4	DMU	B	6	-	-	4/8/48/59	0/2/2/2
4	DMU	B	1	-	-	6/19/59/59	0/2/2/2
5	TRD	A	1015	-	-	2/4/4/10	-
5	TRD	D	14	-	-	1/4/4/10	-
5	TRD	D	3	-	-	5/10/10/10	-
6	HEA	C	1	1	-	5/32/76/76	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1	HEA	C3A-C2A	-4.74	1.33	1.40
6	C	1	HEA	C3A-C2A	-4.53	1.34	1.40
6	C	2	HEA	C3A-C2A	-4.17	1.34	1.40
6	C	2	HEA	C3C-C2C	-4.07	1.34	1.40
6	C	2	HEA	C11-C3B	4.02	1.56	1.51
6	A	2	HEA	C11-C3B	4.00	1.56	1.51
6	A	2	HEA	C3A-C2A	-3.75	1.35	1.40
6	C	1	HEA	C11-C3B	3.72	1.55	1.51
6	C	1	HEA	C3C-C2C	-3.55	1.35	1.40
6	A	2	HEA	C3C-C2C	-3.27	1.35	1.40
6	A	1	HEA	C3C-C2C	-3.06	1.36	1.40
6	A	1	HEA	C11-C3B	2.96	1.55	1.51
6	C	2	HEA	C3A-C4A	2.78	1.45	1.41
6	A	2	HEA	C3A-C4A	2.67	1.45	1.41
6	C	1	HEA	C3A-C4A	2.66	1.45	1.41
6	A	1	HEA	C3A-C4A	2.54	1.45	1.41
6	A	1	HEA	CMD-C2D	2.33	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2	HEA	CHD-C1D	2.28	1.40	1.34
6	A	2	HEA	CHD-C1D	2.17	1.39	1.34
6	C	1	HEA	CMD-C2D	2.17	1.55	1.50
6	A	2	HEA	C3A-CMA	2.16	1.51	1.46
4	C	10	DMU	O16-C6	2.12	1.43	1.40
4	B	2	DMU	O16-C6	2.10	1.43	1.40
6	A	1	HEA	CMB-C2B	2.08	1.55	1.50
4	A	1005	DMU	O16-C6	2.04	1.43	1.40

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2	HEA	C4D-CHA-C1A	4.26	128.18	122.56
6	C	1	HEA	C4D-CHA-C1A	4.21	128.11	122.56
6	A	2	HEA	C4D-CHA-C1A	3.91	127.72	122.56
6	A	1	HEA	CMC-C2C-C1C	-3.83	122.85	128.46
6	A	2	HEA	CMC-C2C-C1C	-3.69	123.05	128.46
6	C	1	HEA	CMC-C2C-C1C	-3.62	123.16	128.46
6	A	1	HEA	C4A-CHB-C1B	3.36	126.99	122.56
6	A	2	HEA	C27-C19-C20	3.28	120.92	115.23
6	A	1	HEA	C1D-ND-C4D	3.14	108.92	105.21
4	B	2	DMU	O16-C6-C1	3.00	112.83	108.27
4	B	2	DMU	C10-O7-C3	-2.94	111.00	117.98
6	A	1	HEA	C13-C14-C15	-2.91	120.96	127.62
6	C	1	HEA	C27-C19-C20	2.91	120.28	115.23
6	C	2	HEA	CAD-CBD-CGD	-2.87	106.05	113.67
4	C	9	DMU	C10-O7-C3	-2.86	111.20	117.98
6	C	1	HEA	C13-C14-C15	-2.85	121.09	127.62
6	A	2	HEA	C4B-NB-C1B	2.81	108.53	105.21
6	C	1	HEA	C17-C18-C19	-2.79	121.23	127.62
6	C	1	HEA	C3D-C4D-ND	-2.79	107.66	110.35
6	C	2	HEA	C27-C19-C20	2.77	120.04	115.23
6	A	1	HEA	C3D-C4D-ND	-2.76	107.68	110.35
6	A	2	HEA	C1D-ND-C4D	2.73	108.44	105.21
6	A	2	HEA	CAD-CBD-CGD	-2.72	106.45	113.67
6	C	2	HEA	C1D-ND-C4D	2.71	108.42	105.21
6	C	2	HEA	C4B-NB-C1B	2.68	108.38	105.21
6	A	2	HEA	C4A-CHB-C1B	2.66	126.06	122.56
6	A	1	HEA	C27-C19-C20	2.61	119.76	115.23
6	A	2	HEA	CMB-C2B-C3B	-2.57	125.30	130.28
6	C	2	HEA	C3D-C4D-ND	-2.56	107.87	110.35
6	A	2	HEA	C3D-C4D-ND	-2.56	107.88	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	7	DMU	O16-C6-C1	2.55	112.15	108.27
6	C	2	HEA	CMC-C2C-C1C	-2.51	124.77	128.46
6	C	1	HEA	CHA-C4D-ND	2.45	127.07	124.44
4	A	1005	DMU	O16-C6-C1	2.44	111.98	108.27
6	A	1	HEA	C17-C18-C19	-2.40	122.14	127.62
4	B	1	DMU	O2-C8-C9	2.38	115.19	109.32
6	A	1	HEA	C4B-NB-C1B	2.34	107.98	105.21
6	C	2	HEA	CHA-C4D-ND	2.32	126.93	124.44
6	A	1	HEA	C2D-C1D-ND	-2.28	107.22	109.84
6	C	2	HEA	C26-C15-C16	2.28	119.18	115.23
6	C	1	HEA	C4B-NB-C1B	2.26	107.89	105.21
6	C	2	HEA	C2D-C1D-ND	-2.24	107.27	109.84
6	A	2	HEA	CHA-C4D-ND	2.21	126.81	124.44
6	C	1	HEA	C1D-ND-C4D	2.20	107.81	105.21
6	A	2	HEA	C2D-C1D-ND	-2.20	107.31	109.84
6	C	1	HEA	CAD-CBD-CGD	-2.19	107.85	113.67
6	C	1	HEA	C3A-C4A-NA	-2.18	106.82	110.94
6	A	2	HEA	C3B-C4B-NB	-2.17	107.34	109.84
4	B	1	DMU	O16-C6-C1	2.15	111.53	108.27
6	A	2	HEA	C13-C14-C15	-2.14	122.73	127.62
6	C	1	HEA	CHB-C1B-NB	2.13	126.72	124.44
6	A	1	HEA	C4D-CHA-C1A	2.12	125.35	122.56
6	C	2	HEA	C13-C12-C11	-2.10	111.04	114.39
6	C	2	HEA	C4A-CHB-C1B	2.10	125.33	122.56
6	A	2	HEA	C2B-C1B-NB	-2.08	107.50	109.90
6	A	2	HEA	CMC-C2C-C3C	2.07	128.83	124.68
4	B	2	DMU	C10-O1-C9	2.07	117.77	113.72
4	C	9	DMU	C8-C7-C5	2.04	114.41	110.83
6	A	1	HEA	C13-C12-C11	-2.03	111.15	114.39
4	B	1	DMU	C8-C7-C5	-2.02	107.29	110.83
6	C	2	HEA	C3B-C4B-NB	-2.02	107.52	109.84
6	C	2	HEA	C3A-C4A-NA	-2.00	107.16	110.94

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2	DMU	C19-C18-O16-C6
10	B	286	HTH	C2-C3-C4-C5
10	B	286	HTH	O3-C3-C4-C5
4	C	9	DMU	O5-C4-C57-O61
4	B	6	DMU	O6-C11-C9-O1

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Mol	Chain	Res	Type	Atoms
4	D	4	DMU	O6-C11-C9-C8
4	C	10	DMU	O1-C10-O7-C3
4	B	3	DMU	O6-C11-C9-C8
4	C	9	DMU	C3-C4-C57-O61
4	B	2	DMU	O6-C11-C9-O1
4	A	7	DMU	O5-C6-O16-C18
4	B	1	DMU	O5-C6-O16-C18
4	B	2	DMU	O5-C6-O16-C18
4	C	5	DMU	O5-C4-C57-O61
4	C	9	DMU	O6-C11-C9-O1
4	D	4	DMU	O6-C11-C9-O1
4	C	9	DMU	O6-C11-C9-C8
4	B	6	DMU	O6-C11-C9-C8
4	A	7	DMU	C1-C6-O16-C18
4	B	1	DMU	C1-C6-O16-C18
4	B	2	DMU	C1-C6-O16-C18
4	B	2	DMU	O6-C11-C9-C8
4	C	5	DMU	C3-C4-C57-O61
4	B	3	DMU	O6-C11-C9-O1
4	C	10	DMU	C3-C4-C57-O61
4	B	2	DMU	C18-C19-C22-C25
5	D	3	TRD	C4-C5-C6-C7
4	B	1	DMU	C28-C31-C34-C37
4	C	10	DMU	C18-C19-C22-C25
5	A	3	TRD	C11-C10-C9-C8
4	B	3	DMU	C25-C28-C31-C34
5	D	3	TRD	C11-C10-C9-C8
5	A	3	TRD	C2-C3-C4-C5
4	B	1	DMU	C18-C19-C22-C25
4	B	3	DMU	C28-C31-C34-C37
4	B	6	DMU	C3-C4-C57-O61
6	C	1	HEA	C26-C15-C16-C17
4	A	1005	DMU	O5-C6-O16-C18
4	B	1	DMU	C25-C28-C31-C34
4	A	1005	DMU	C1-C6-O16-C18
5	D	3	TRD	C6-C7-C8-C9
4	B	2	DMU	C19-C22-C25-C28
5	A	3	TRD	C4-C5-C6-C7
4	B	1	DMU	C22-C25-C28-C31
4	B	2	DMU	O16-C18-C19-C22
4	A	7	DMU	C25-C28-C31-C34
5	D	3	TRD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	A	1005	DMU	C28-C31-C34-C37
6	C	1	HEA	C14-C15-C16-C17
5	A	552	TRD	C2-C3-C4-C5
4	B	3	DMU	C22-C25-C28-C31
5	C	552	TRD	C2-C3-C4-C5
6	C	2	HEA	C3B-C11-C12-C13
5	A	552	TRD	C1-C2-C3-C4
4	B	2	DMU	C34-C37-C40-C43
5	D	3	TRD	C5-C6-C7-C8
5	C	552	TRD	C3-C4-C5-C6
4	C	10	DMU	C31-C34-C37-C40
6	A	2	HEA	C4D-C3D-CAD-CBD
4	C	5	DMU	O6-C11-C9-O1
4	A	7	DMU	C34-C37-C40-C43
4	B	6	DMU	O5-C4-C57-O61
5	A	1009	TRD	C1-C2-C3-C4
5	B	4	TRD	C6-C7-C8-C9
10	B	286	HTH	O1-C1-C2-O2
5	D	14	TRD	C3-C4-C5-C6
4	C	10	DMU	O5-C4-C57-O61
4	A	1005	DMU	C19-C22-C25-C28
5	A	552	TRD	C10-C11-C12-C13
4	C	10	DMU	O6-C11-C9-C8
5	A	1009	TRD	C4-C5-C6-C7
6	A	2	HEA	C2D-C3D-CAD-CBD
4	D	4	DMU	C3-C4-C57-O61
6	C	2	HEA	CAD-CBD-CGD-O1D
6	A	2	HEA	CAD-CBD-CGD-O2D
6	C	1	HEA	CAD-CBD-CGD-O2D
6	A	2	HEA	CAD-CBD-CGD-O1D
4	B	3	DMU	C3-C4-C57-O61
5	A	1015	TRD	C6-C7-C8-C9
5	A	3	TRD	C5-C6-C7-C8
4	C	10	DMU	C2-C3-O7-C10
6	A	2	HEA	CAA-CBA-CGA-O1A
6	C	2	HEA	CAD-CBD-CGD-O2D
5	A	552	TRD	C6-C7-C8-C9
4	C	10	DMU	C34-C37-C40-C43
6	C	2	HEA	CAA-CBA-CGA-O1A
6	A	1	HEA	C26-C15-C16-C17
6	A	2	HEA	CAA-CBA-CGA-O2A
6	C	1	HEA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
5	A	1015	TRD	C5-C6-C7-C8
6	C	2	HEA	CAA-CBA-CGA-O2A
6	A	1	HEA	CAD-CBD-CGD-O2D
6	A	1	HEA	C14-C15-C16-C17
4	C	10	DMU	C4-C3-O7-C10
6	C	2	HEA	C4D-C3D-CAD-CBD
6	C	2	HEA	O11-C11-C12-C13
6	A	1	HEA	CAD-CBD-CGD-O1D
4	A	1005	DMU	C31-C34-C37-C40
4	C	10	DMU	O16-C18-C19-C22
4	C	10	DMU	O5-C6-O16-C18
6	A	1	HEA	CAA-CBA-CGA-O1A
4	B	2	DMU	C25-C28-C31-C34
6	C	1	HEA	CAA-CBA-CGA-O1A
6	C	2	HEA	C2D-C3D-CAD-CBD
6	A	1	HEA	CAA-CBA-CGA-O2A

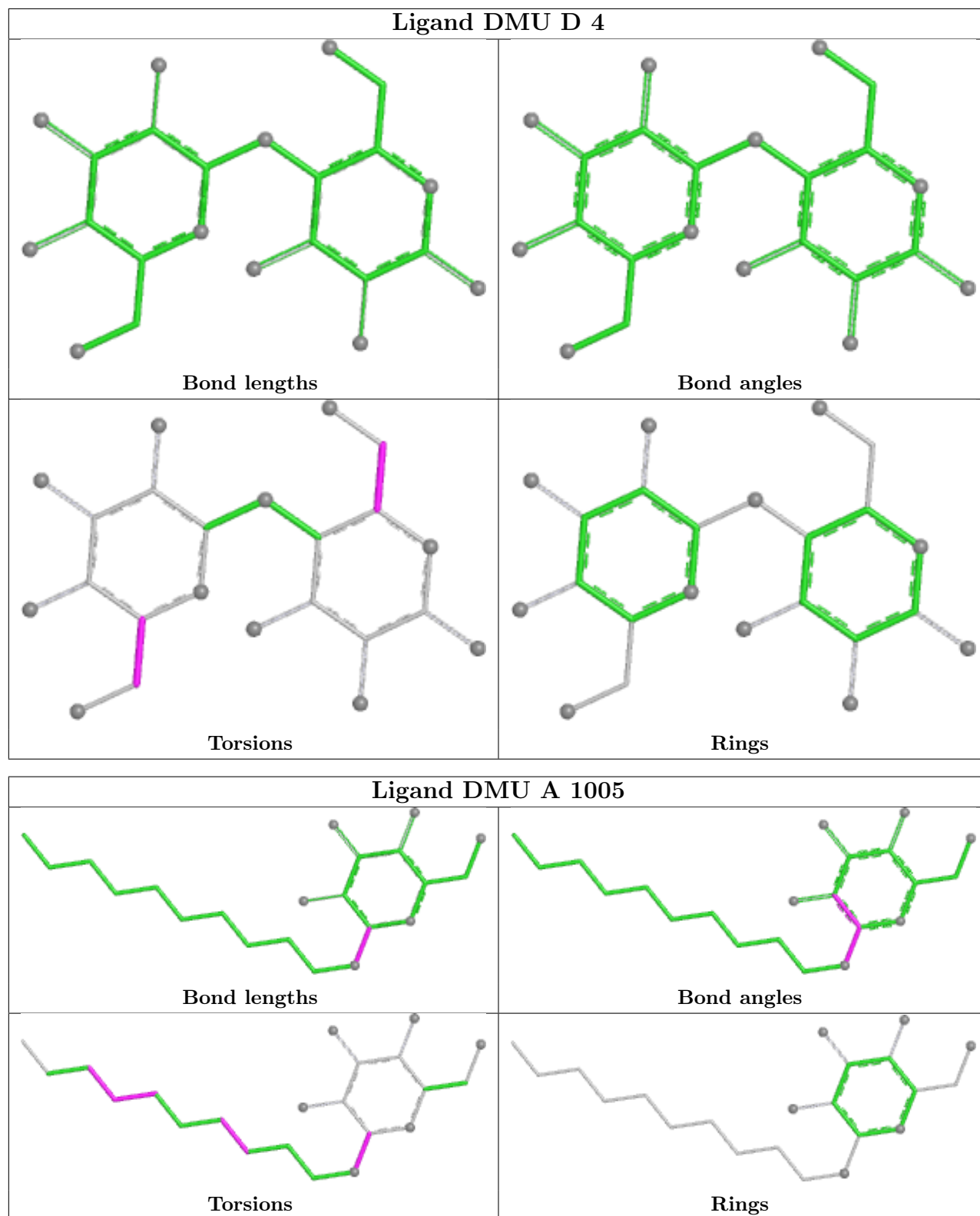
There are no ring outliers.

11 monomers are involved in 20 short contacts:

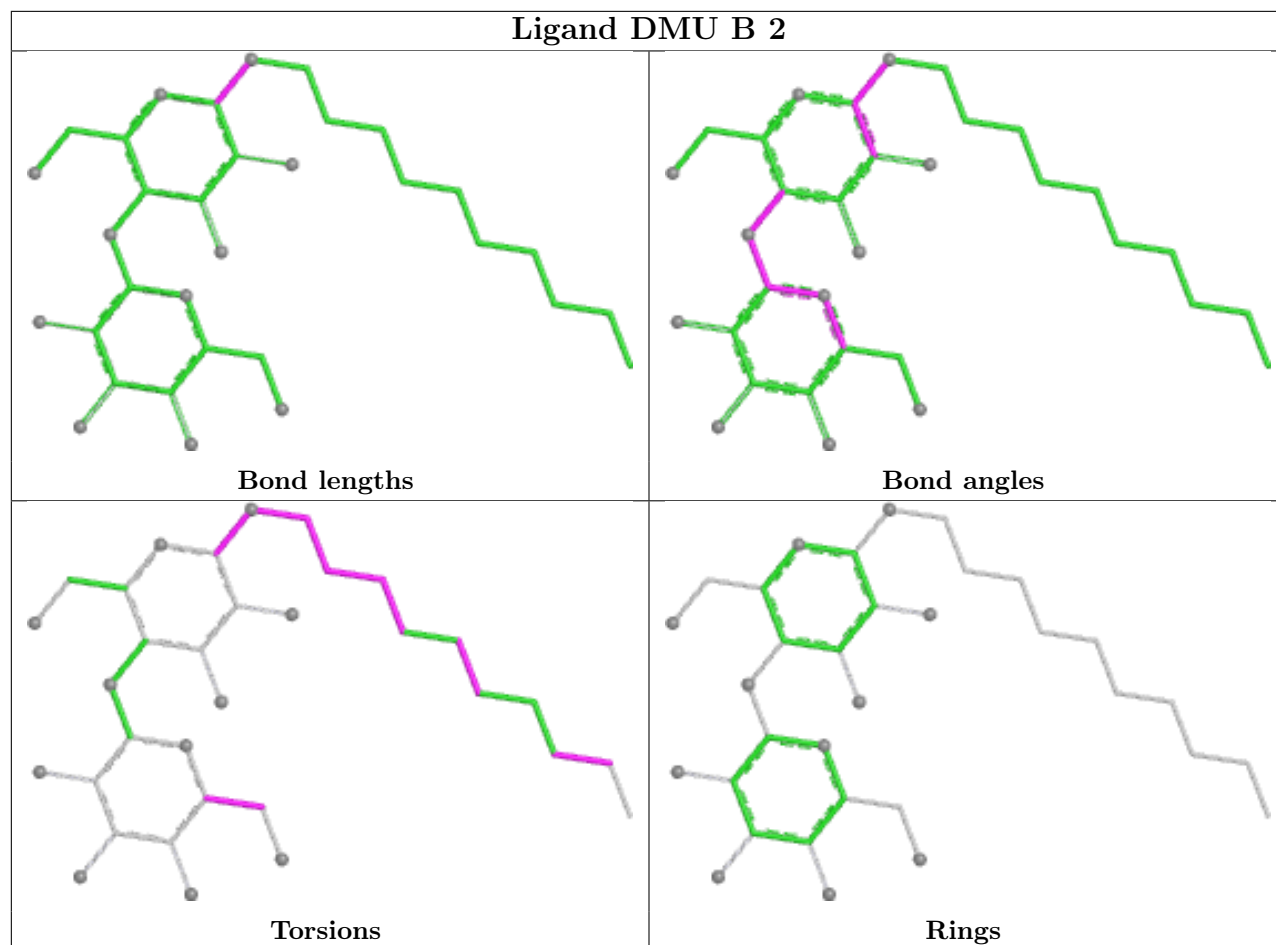
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	4	DMU	3	0
10	B	286	HTH	1	0
4	A	1005	DMU	1	0
6	A	2	HEA	3	0
5	A	3	TRD	1	0
4	C	9	DMU	1	0
6	A	1	HEA	3	0
6	C	2	HEA	3	0
5	B	4	TRD	1	0
5	D	3	TRD	1	0
6	C	1	HEA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

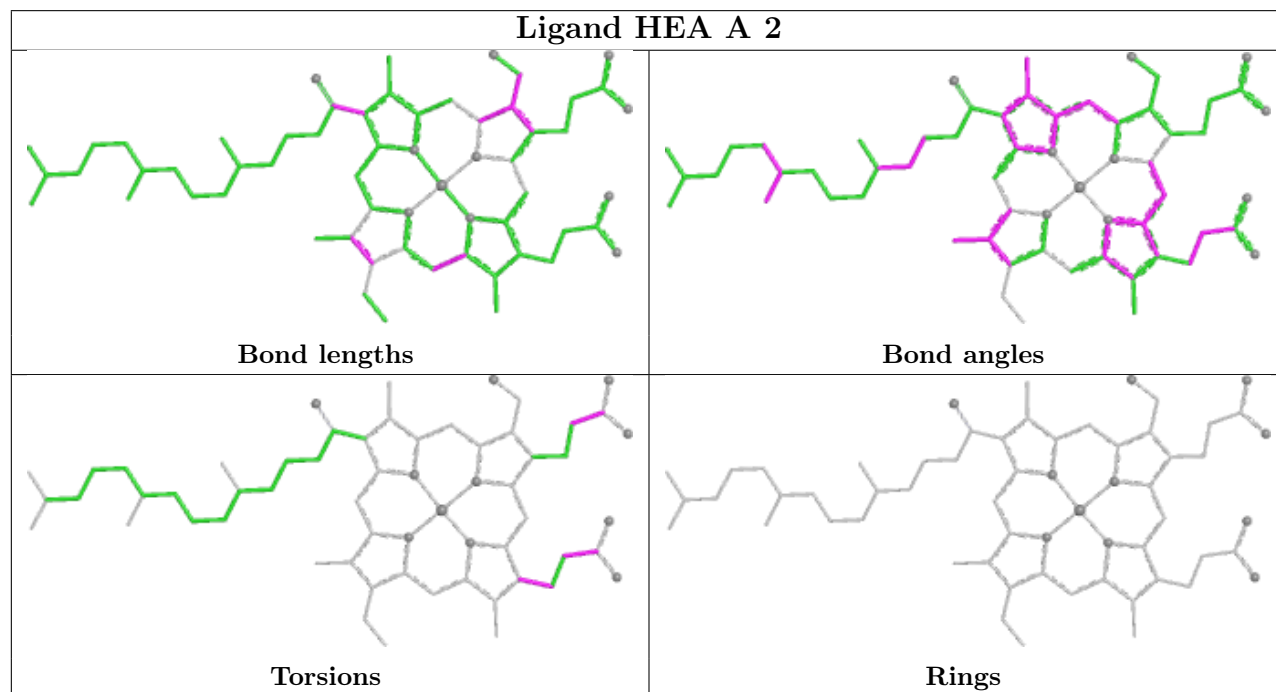
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

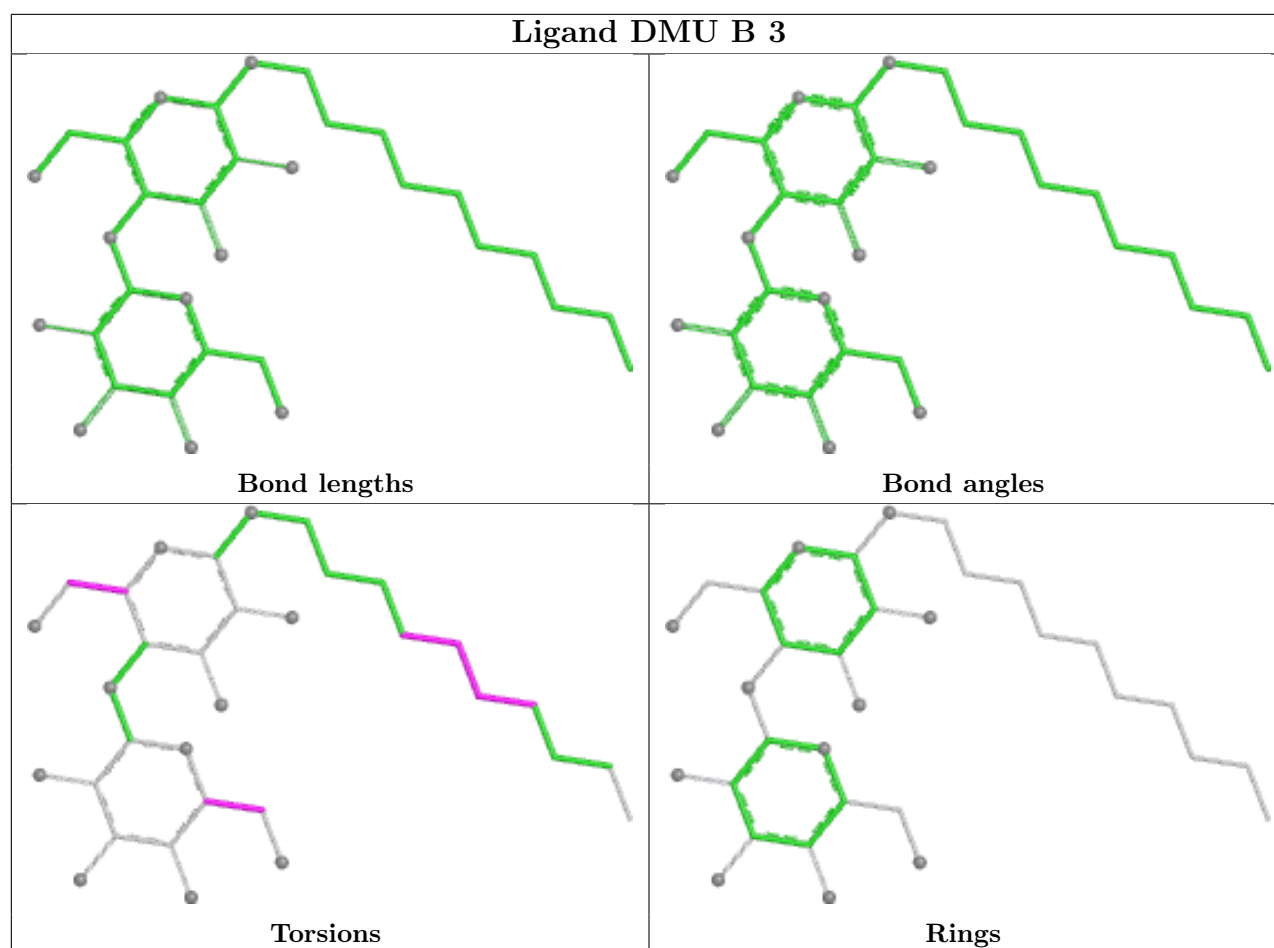


Ligand DMU B 2

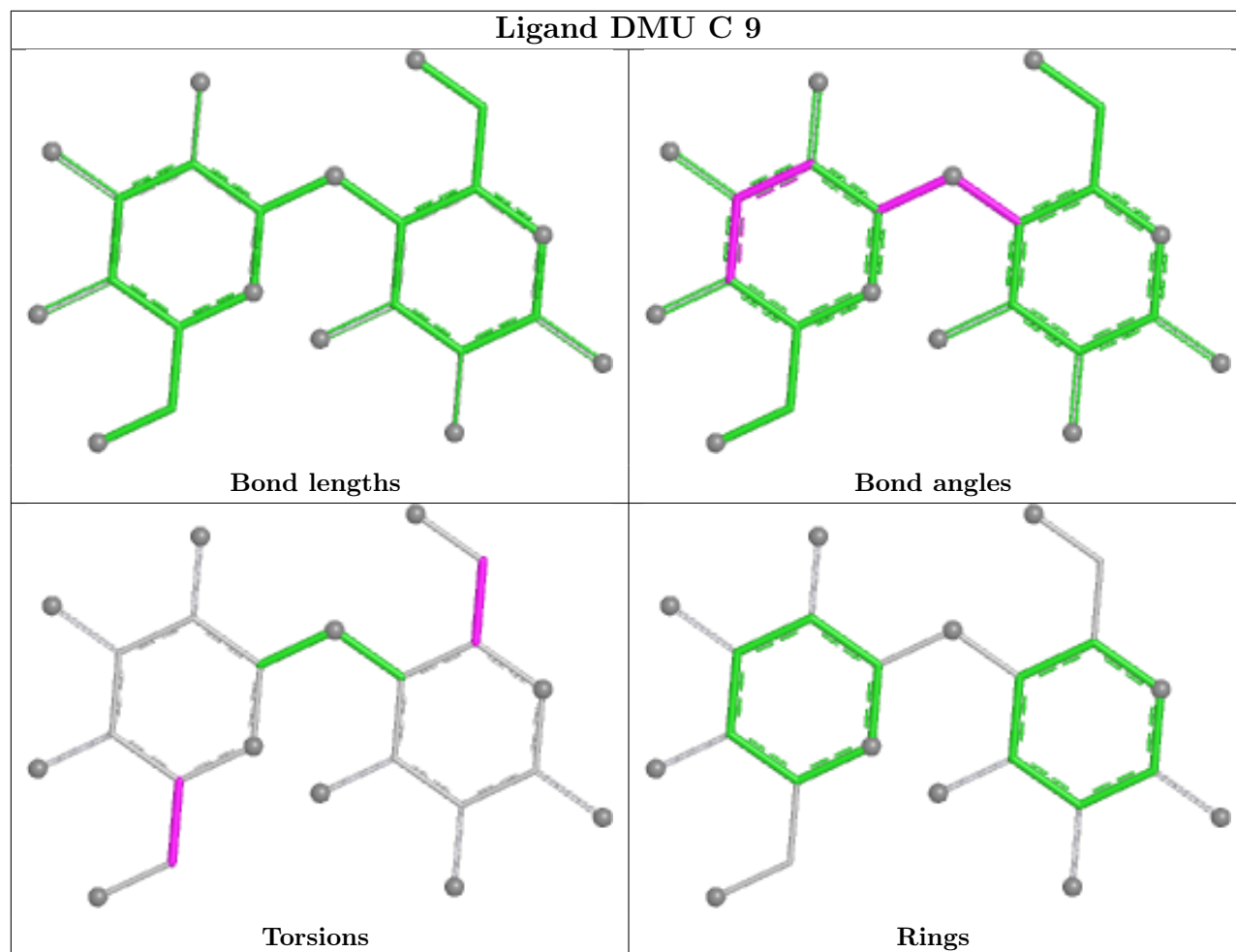


Ligand HEA A 2

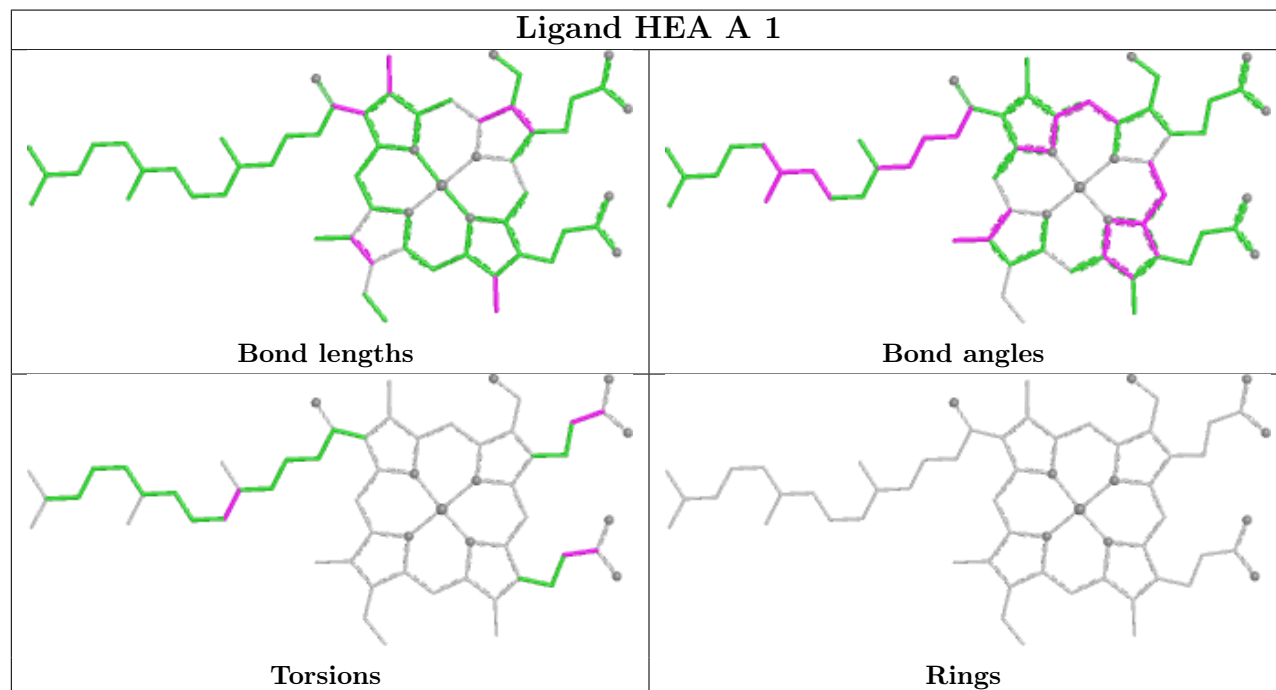




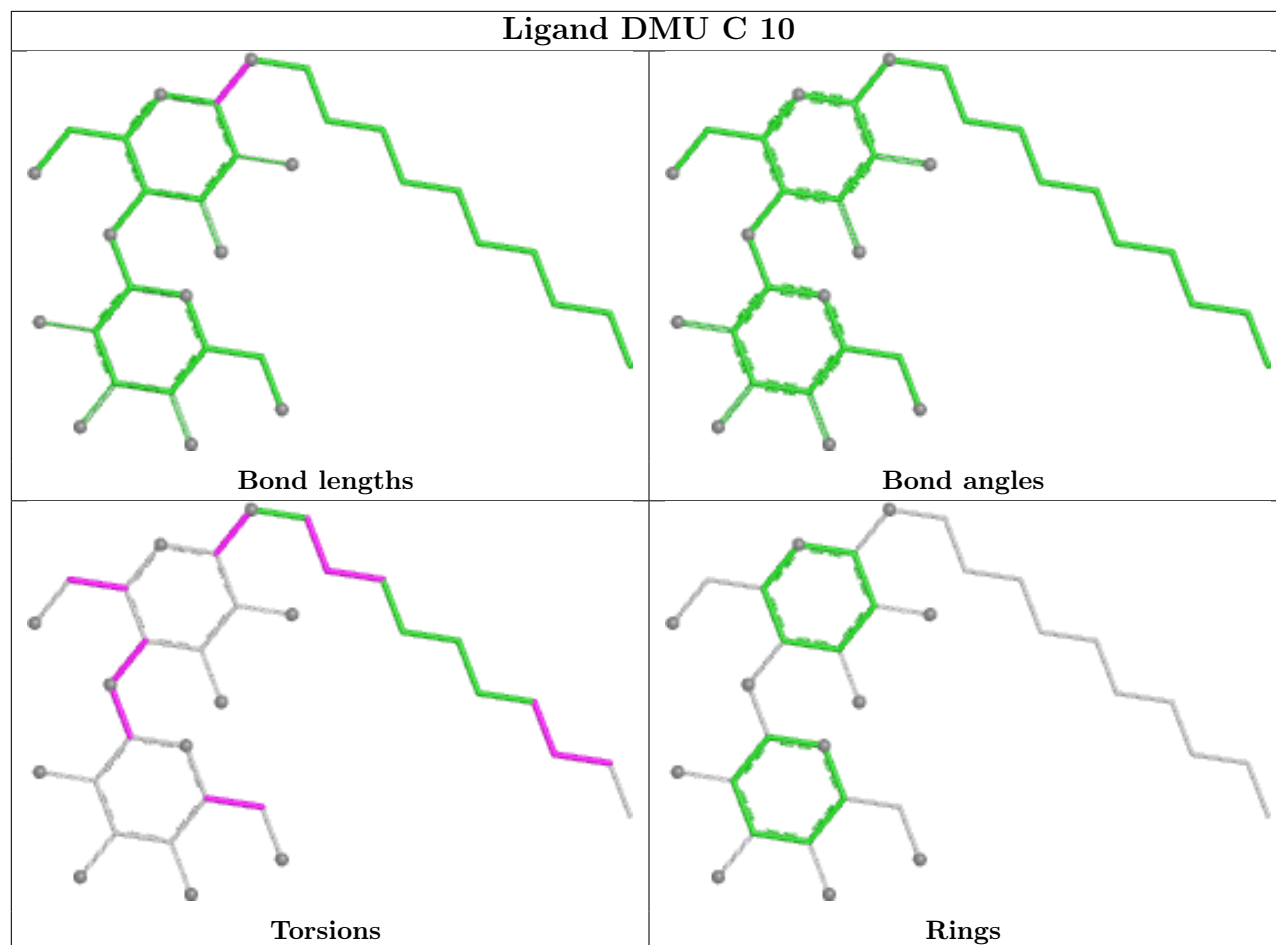
Ligand DMU C 9



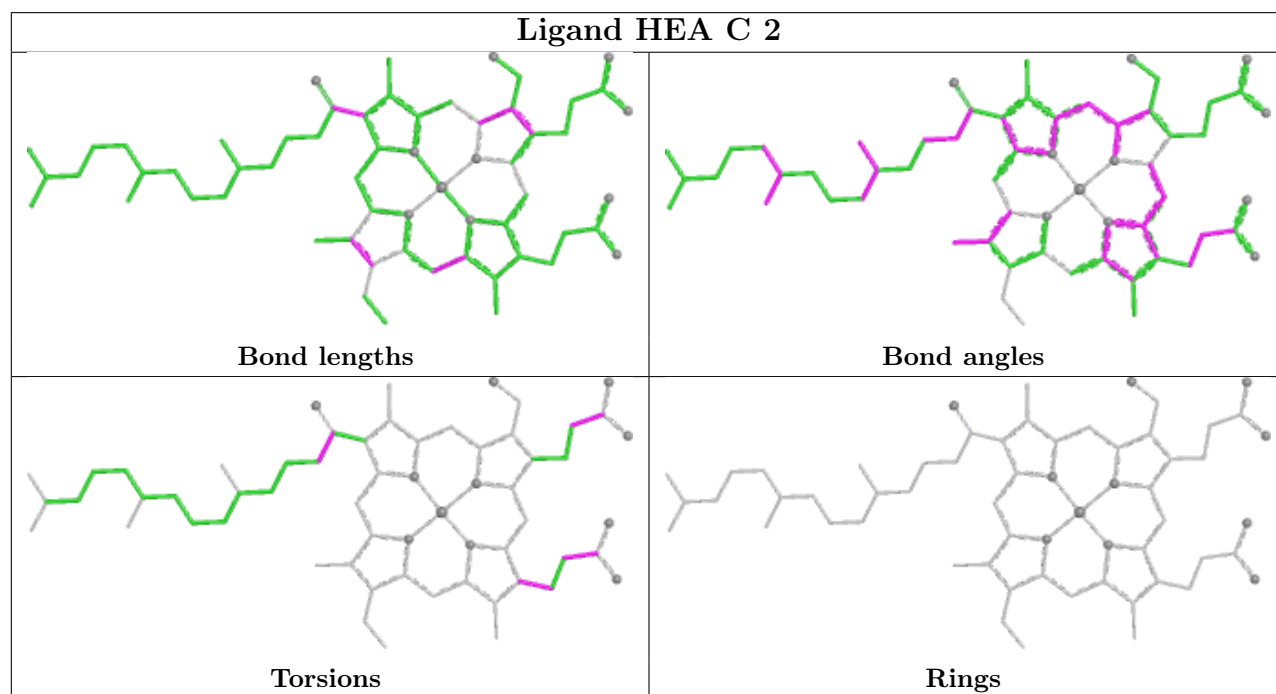
Ligand HEA A 1



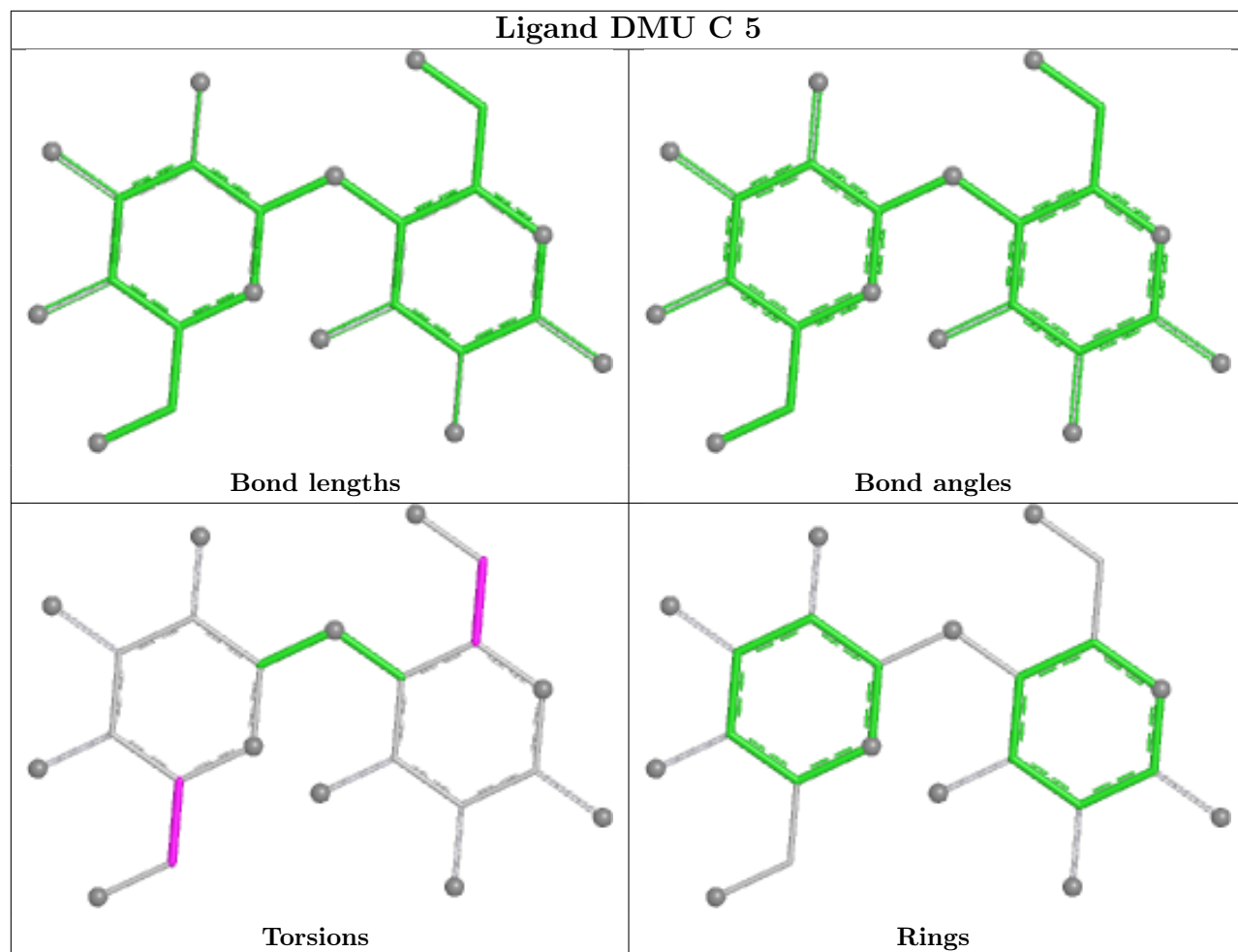
Ligand DMU C 10



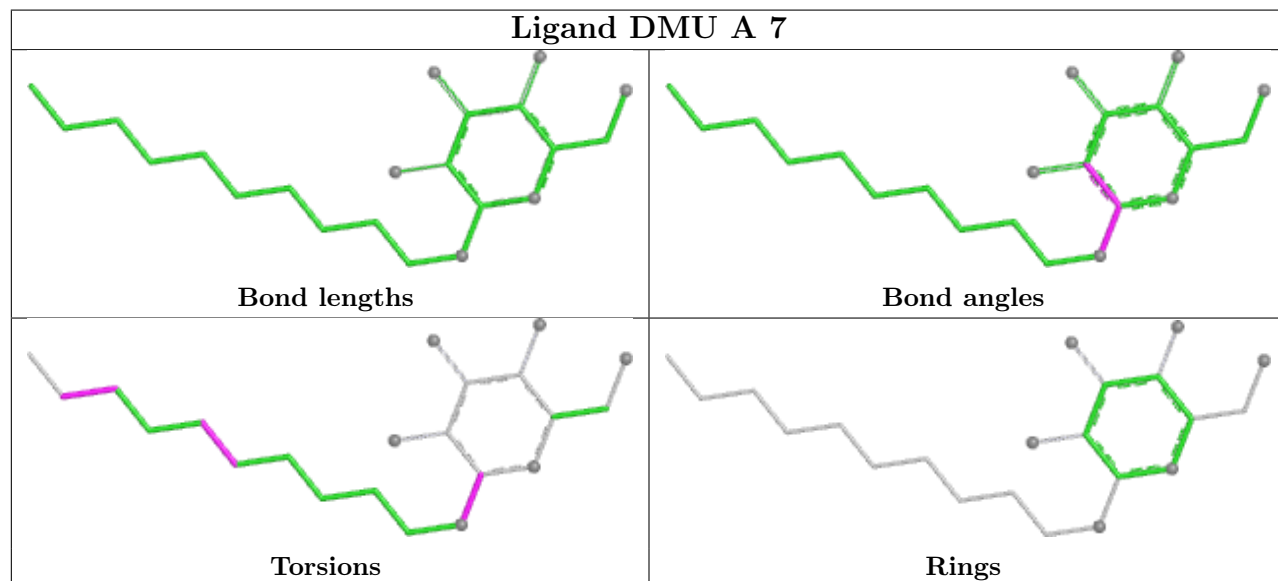
Ligand HEA C 2



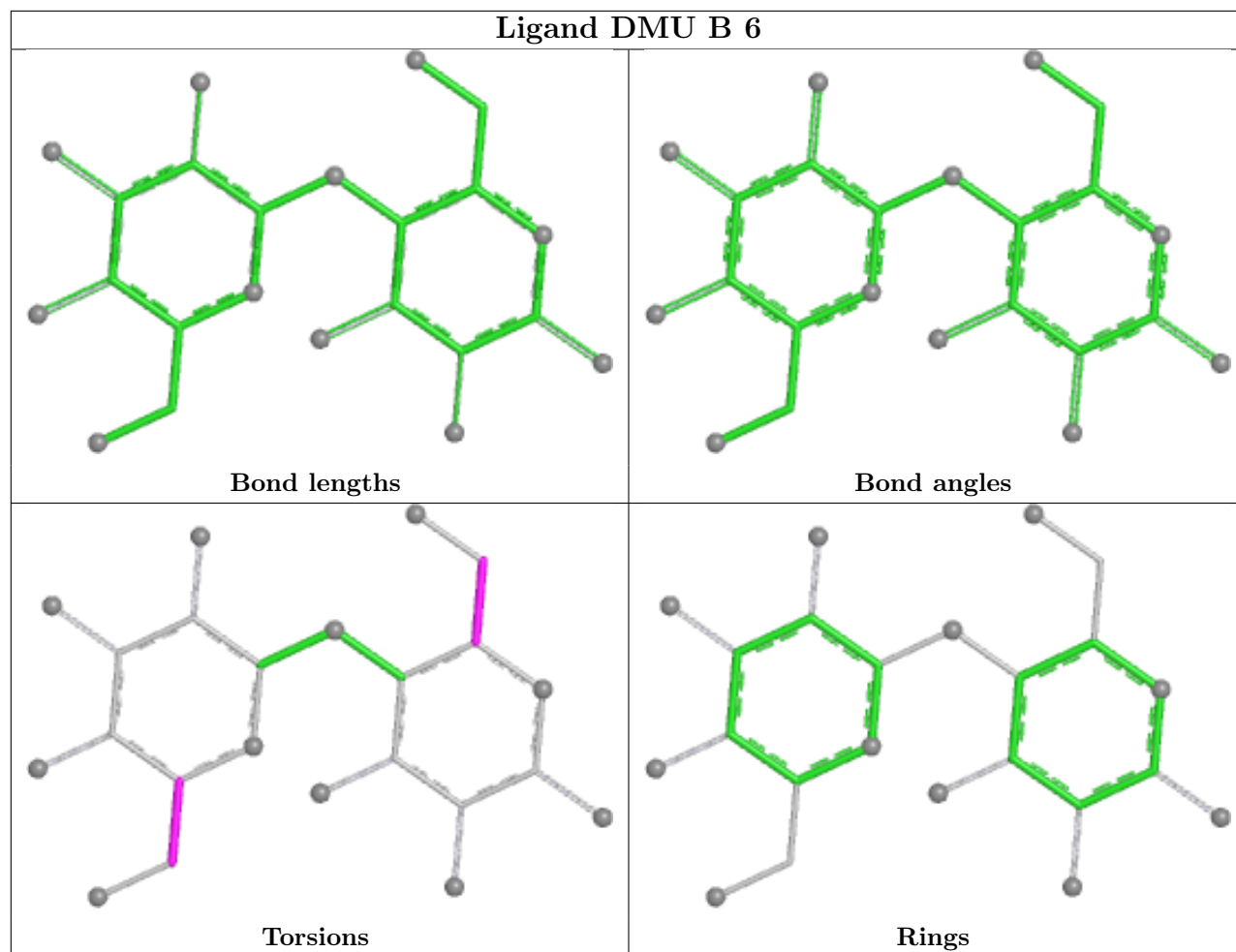
Ligand DMU C 5

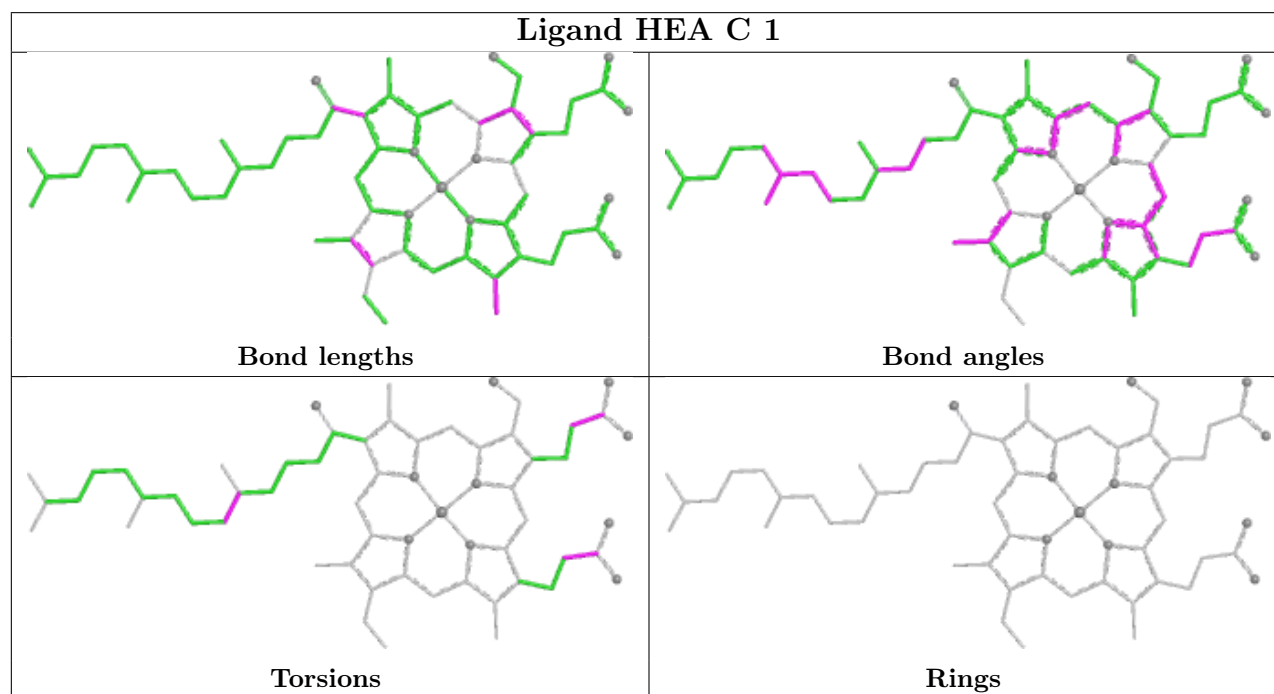
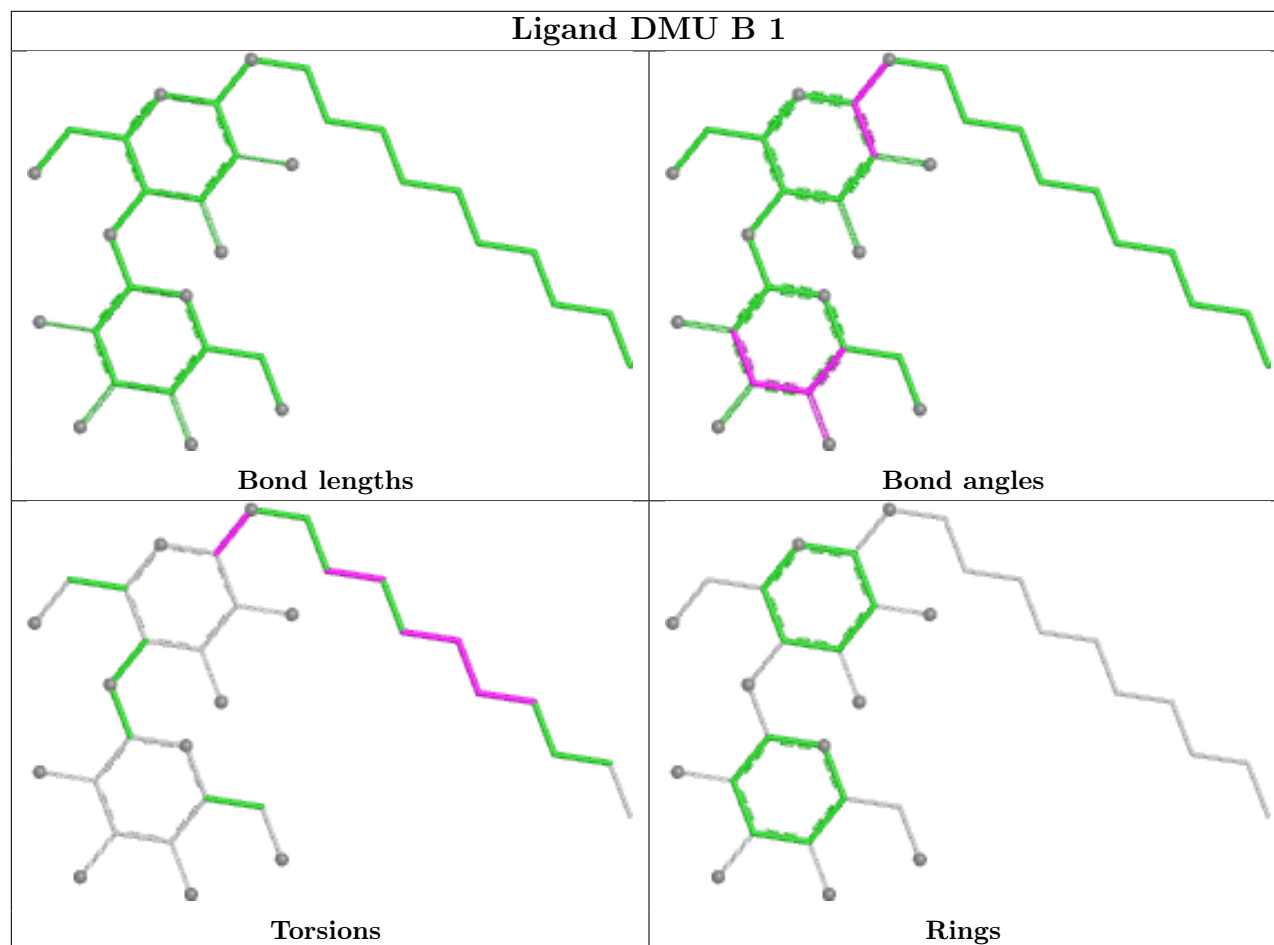


Ligand DMU A 7



Ligand DMU B 6





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, 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	535/535 (100%)	0.10	27 (5%) 28 35	25, 38, 60, 78	0
1	C	531/535 (99%)	0.49	53 (9%) 7 10	32, 54, 78, 92	0
2	B	256/256 (100%)	-0.11	5 (1%) 65 71	25, 42, 60, 66	0
2	D	256/256 (100%)	0.02	17 (6%) 18 23	32, 47, 68, 77	0
All	All	1578/1582 (99%)	0.18	102 (6%) 18 24	25, 45, 70, 92	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	222	MET	6.1
1	C	218	PRO	6.0
1	C	217	ALA	5.6
1	C	549	HIS	5.5
1	C	77	PHE	5.0
1	C	137	ARG	4.8
1	C	259	PHE	4.8
1	C	73	VAL	4.8
1	C	550	THR	4.7
1	C	81	TRP	4.6
1	C	76	PHE	4.5
1	C	262	THR	4.4
2	D	99	PRO	4.2
1	C	74	LYS	4.2
1	C	21	PHE	4.1
1	A	73	VAL	4.0
2	D	235	LEU	4.0
2	D	87	ARG	3.9
1	A	220	MET	3.9
2	D	96	HIS	3.9
2	D	98	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	219	GLY	3.8
1	C	138	MET	3.7
1	C	130	ALA	3.7
1	C	220	MET	3.7
1	A	81	TRP	3.6
2	B	56	TRP	3.6
1	C	213	LEU	3.6
1	A	222	MET	3.5
1	A	217	ALA	3.5
1	C	268	GLY	3.5
2	D	284	HIS	3.5
1	C	318	TYR	3.3
1	C	75	GLY	3.3
1	A	259	PHE	3.3
1	C	520	THR	3.3
2	B	284	HIS	3.2
1	A	71	GLY	3.2
2	D	82	ARG	3.2
1	C	269	GLY	3.2
1	A	22	MET	3.2
1	A	221	THR	3.2
1	A	551	PHE	3.2
1	C	261	THR	3.2
1	C	72	LEU	3.1
1	A	550	THR	3.1
2	B	87	ARG	3.0
1	C	100	THR	3.0
1	C	99	ILE	3.0
1	C	71	GLY	2.9
1	C	136	PRO	2.9
2	D	100	LEU	2.9
1	C	23	SER	2.8
2	B	81	TRP	2.8
2	D	88	ASN	2.8
1	C	103	GLY	2.7
2	D	131	GLU	2.7
1	A	172	TRP	2.7
1	C	172	TRP	2.7
1	C	70	SER	2.7
1	C	424	MET	2.6
1	C	214	ASN	2.6
1	A	549	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	106	MET	2.6
2	D	56	TRP	2.6
1	C	139	ASN	2.6
1	C	22	MET	2.6
2	D	285	HIS	2.6
1	C	131	PRO	2.6
1	C	221	THR	2.5
1	A	213	LEU	2.5
1	A	72	LEU	2.5
2	D	95	THR	2.5
1	C	270	GLY	2.4
1	A	423	VAL	2.4
1	C	451	TRP	2.4
1	C	417	VAL	2.4
1	A	260	GLY	2.4
1	C	107	MET	2.4
1	C	263	PHE	2.4
1	A	173	VAL	2.3
1	C	129	GLY	2.3
2	D	83	PHE	2.3
1	A	214	ASN	2.2
1	C	425	SER	2.2
1	A	99	ILE	2.2
2	D	97	ASN	2.2
1	C	267	SER	2.2
2	B	281	GLN	2.2
2	D	81	TRP	2.2
2	D	209	GLN	2.1
1	A	417	VAL	2.1
1	C	24	THR	2.1
1	C	423	VAL	2.1
1	C	530	TYR	2.1
1	A	219	GLY	2.1
1	C	260	GLY	2.1
1	A	416	VAL	2.1
1	A	107	MET	2.0
1	A	76	PHE	2.0
1	A	77	PHE	2.0
1	A	268	GLY	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, 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(\AA^2)	Q<0.9
4	DMU	C	9	23/33	0.52	0.29	96,98,102,102	23
5	TRD	A	1015	7/13	0.71	0.35	70,70,70,70	0
5	TRD	B	4	9/13	0.73	0.30	70,71,75,75	0
5	TRD	A	1009	7/13	0.74	0.30	64,66,67,67	0
10	HTH	B	286	10/10	0.76	0.41	71,76,77,77	0
4	DMU	A	7	22/33	0.78	0.20	46,66,74,76	0
4	DMU	D	8	23/33	0.78	0.33	92,93,97,97	23
4	DMU	B	2	33/33	0.78	0.29	67,69,78,79	25
5	TRD	A	1013	7/13	0.79	0.23	56,56,57,57	0
5	TRD	C	552	13/13	0.82	0.33	83,84,85,85	0
4	DMU	B	6	23/33	0.82	0.19	76,77,77,77	23
4	DMU	C	10	33/33	0.83	0.23	81,83,85,85	0
4	DMU	C	5	23/33	0.85	0.22	95,95,96,96	23
5	TRD	A	552	13/13	0.86	0.24	72,72,75,75	0
4	DMU	A	1005	22/33	0.87	0.20	45,50,56,57	22
4	DMU	D	4	23/33	0.88	0.21	81,82,83,83	23
4	DMU	B	3	33/33	0.89	0.26	83,88,92,93	0
5	TRD	D	14	7/13	0.90	0.11	56,56,59,59	0
5	TRD	D	3	13/13	0.90	0.27	54,55,59,59	0
12	CD	D	9	1/1	0.91	0.04	64,64,64,64	1
5	TRD	A	3	13/13	0.92	0.20	42,44,53,54	0
4	DMU	B	1	33/33	0.96	0.11	30,41,58,60	0
6	HEA	A	2	60/60	0.96	0.21	28,33,46,48	0
6	HEA	C	1	60/60	0.97	0.23	31,35,51,53	0
6	HEA	C	2	60/60	0.97	0.16	31,38,48,50	0
9	CA	C	7	1/1	0.98	0.05	45,45,45,45	0
3	OH	C	706	1/1	0.98	0.22	48,48,48,48	0

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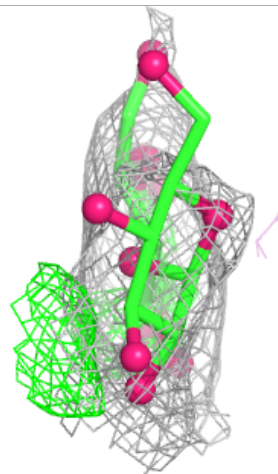
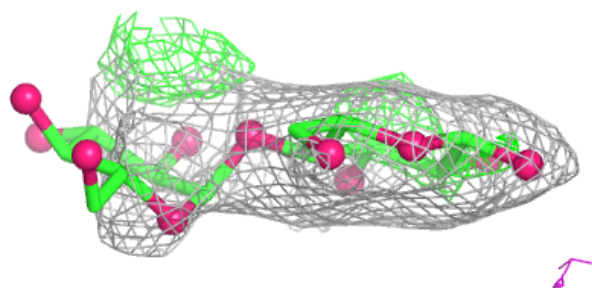
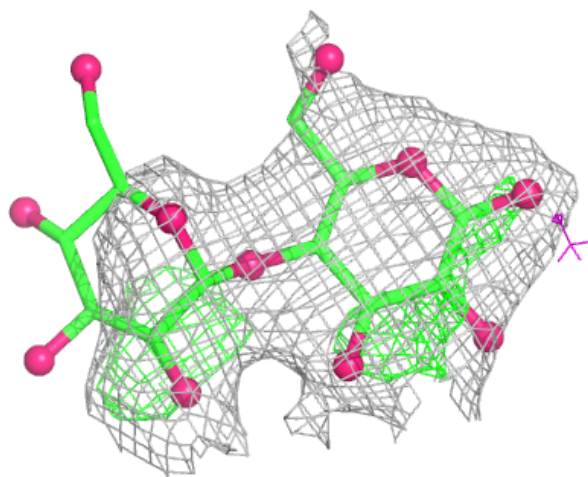
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	MG	A	6	1/1	0.98	0.24	20,20,20,20	0
8	MG	C	6	1/1	0.99	0.19	20,20,20,20	0
9	CA	A	553	1/1	0.99	0.11	30,30,30,30	0
3	OH	A	706	1/1	0.99	0.14	36,36,36,36	0
7	CU	A	5	1/1	0.99	0.15	35,35,35,35	0
12	CD	B	8	1/1	0.99	0.07	44,44,44,44	0
12	CD	B	9	1/1	0.99	0.05	53,53,53,53	1
12	CD	D	288	1/1	0.99	0.06	43,43,43,43	0
6	HEA	A	1	60/60	0.99	0.19	23,26,34,35	0
11	CU1	D	287	1/1	1.00	0.11	35,35,35,35	0
7	CU	D	286	1/1	1.00	0.11	35,35,35,35	0
7	CU	B	287	1/1	1.00	0.11	28,28,28,28	0
7	CU	C	553	1/1	1.00	0.13	42,42,42,42	0
11	CU1	B	288	1/1	1.00	0.14	27,27,27,27	0

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

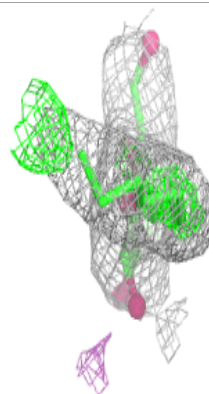
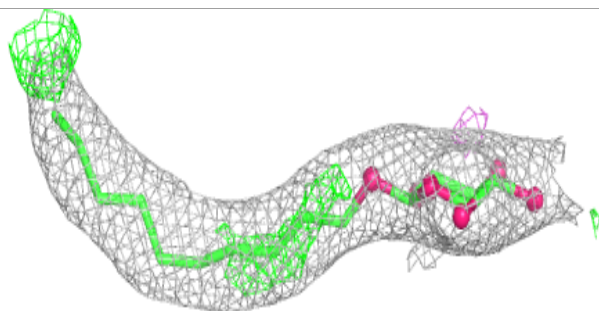
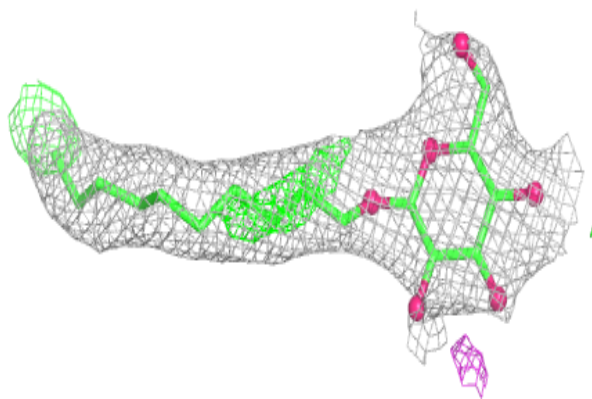
Electron density around DMU C 9:

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

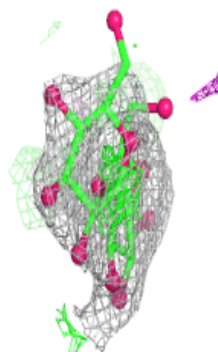
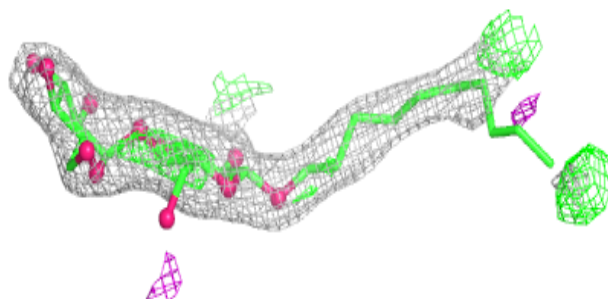
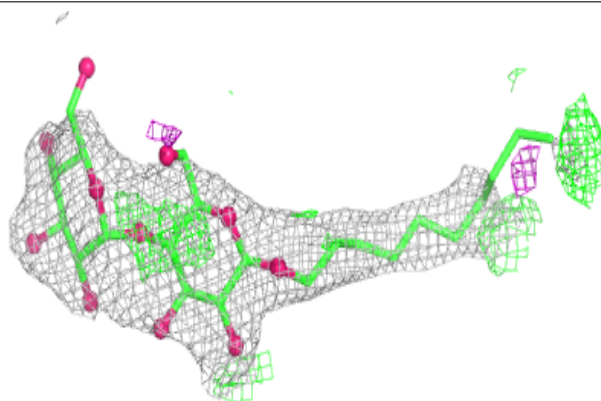


Electron density around DMU A 7:

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

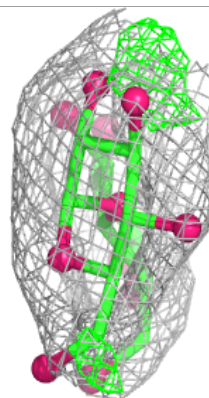
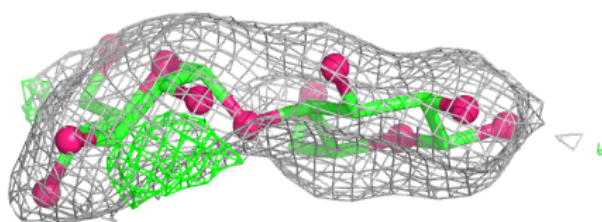
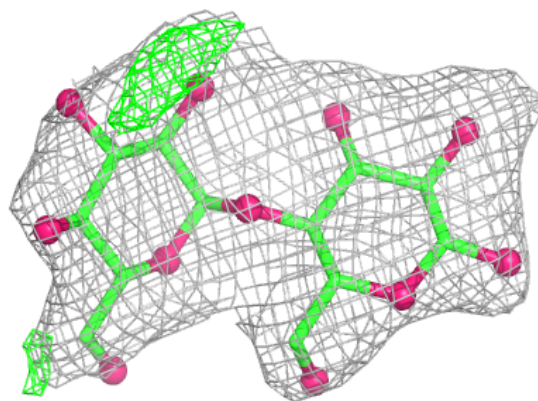
**Electron density around DMU B 2:**

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

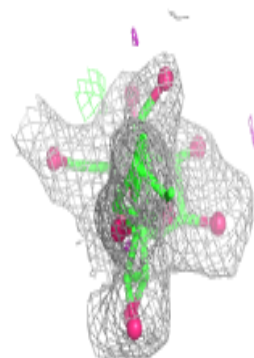
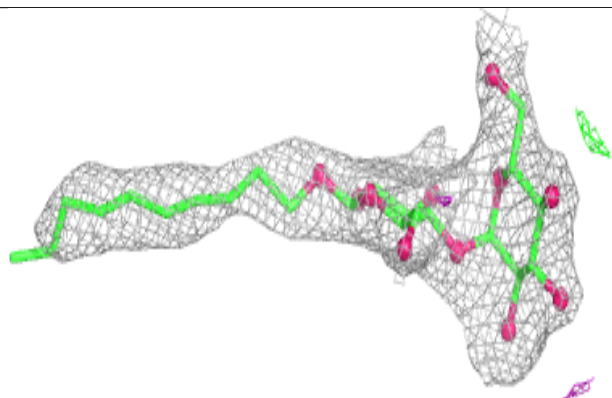
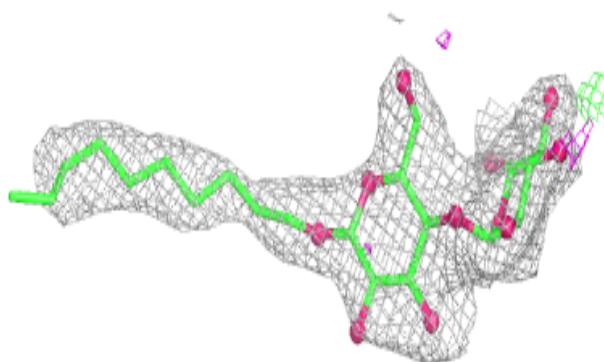


Electron density around DMU B 6:

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

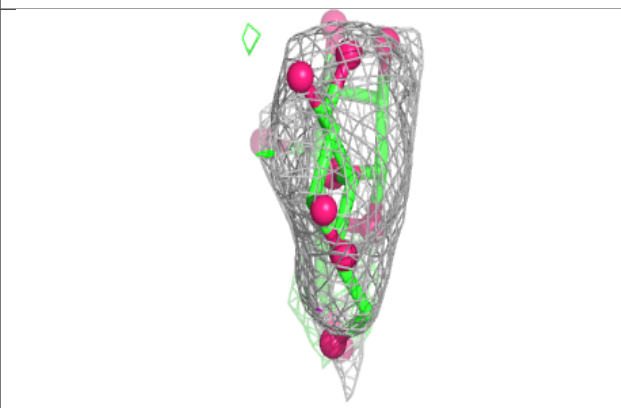
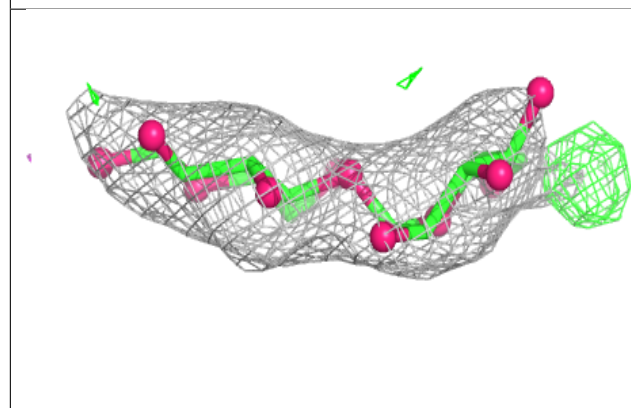
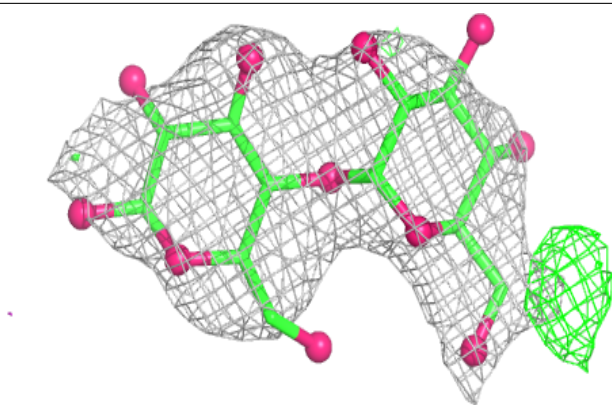
**Electron density around DMU C 10:**

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

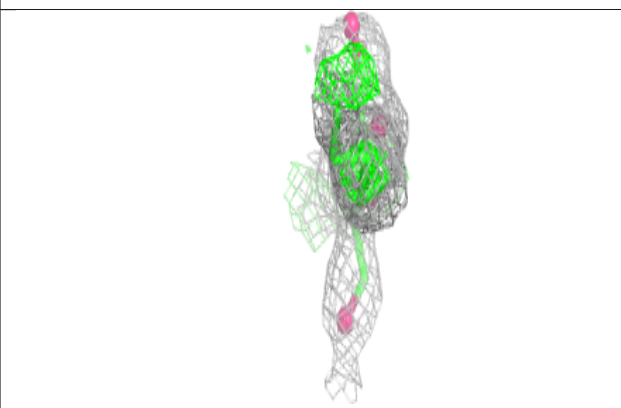
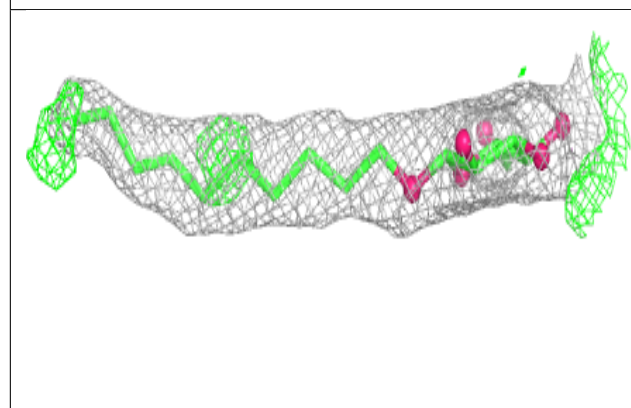
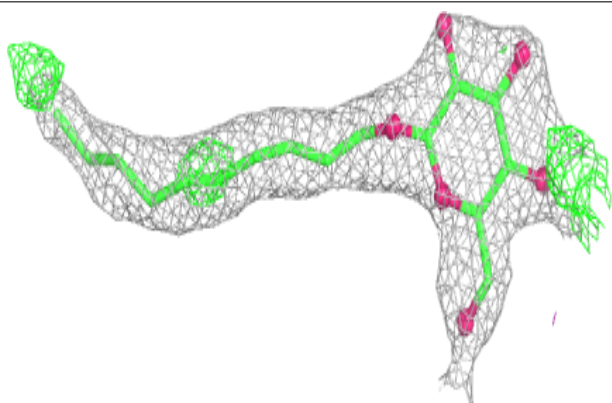


Electron density around DMU C 5:

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

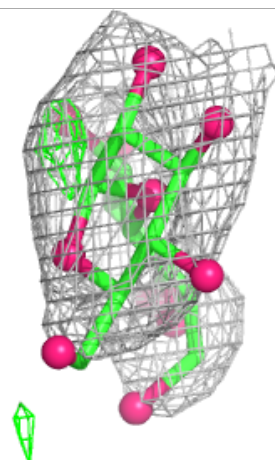
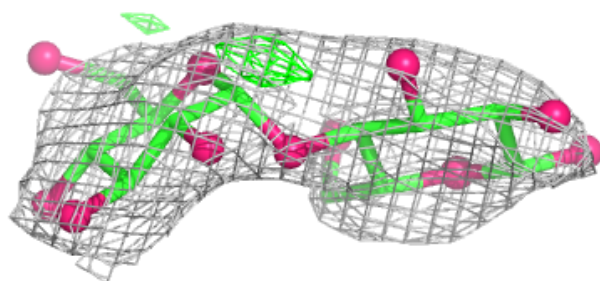
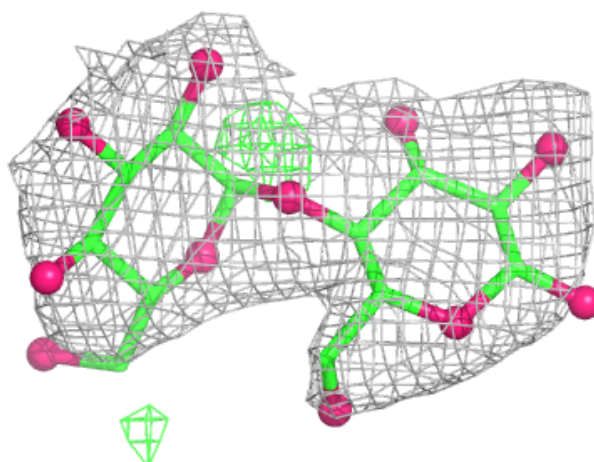
**Electron density around DMU A 1005:**

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



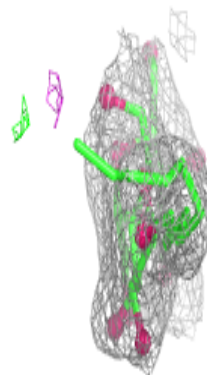
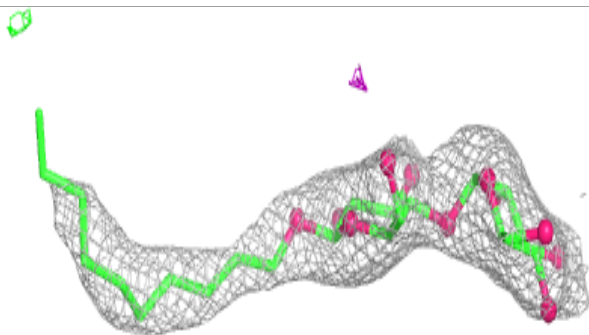
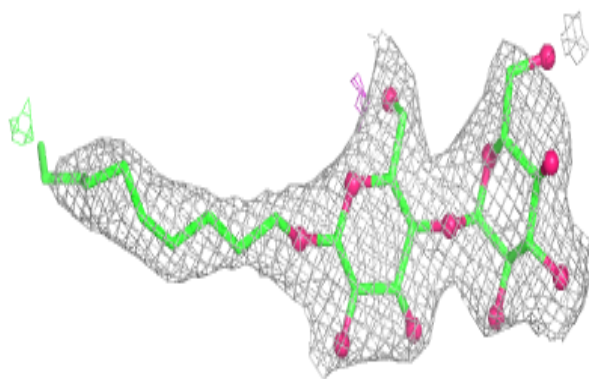
Electron density around DMU D 4:

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

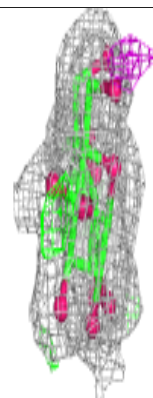
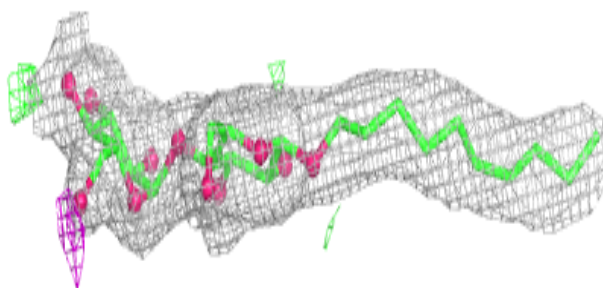
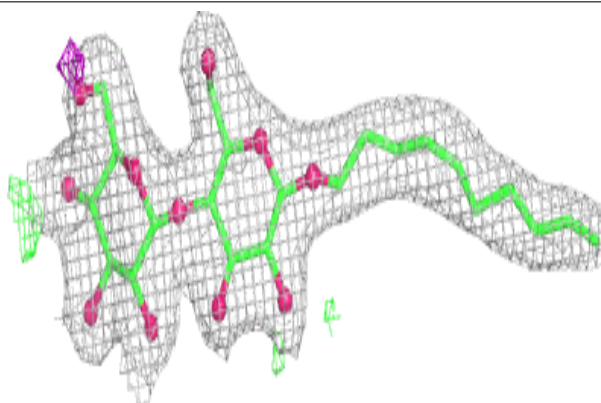


Electron density around DMU B 3:

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

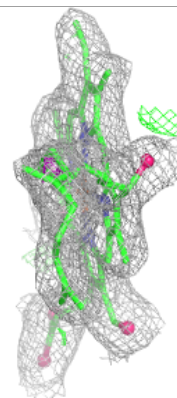
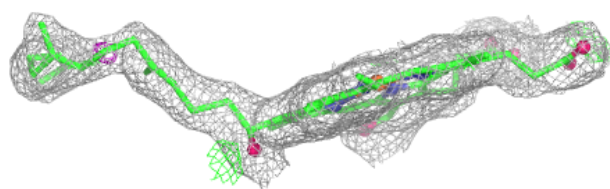
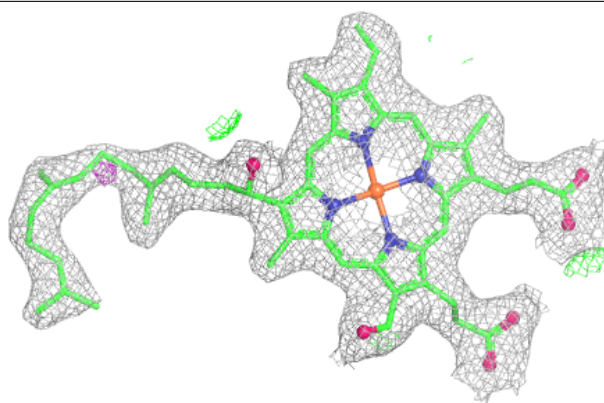
**Electron density around DMU B 1:**

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

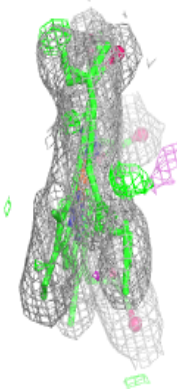
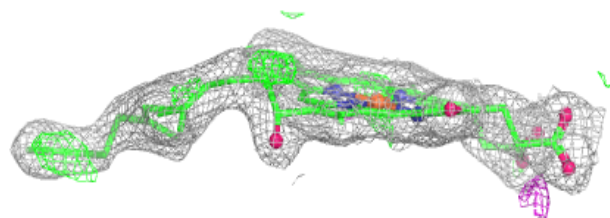
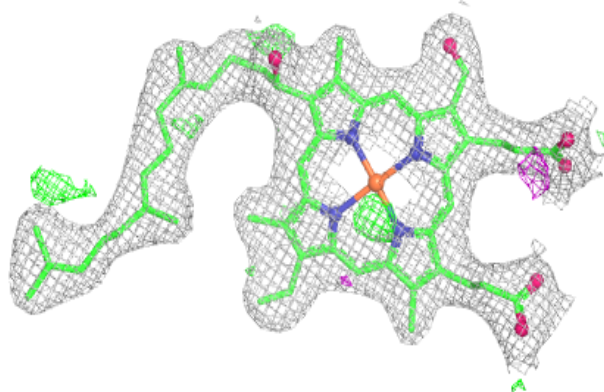


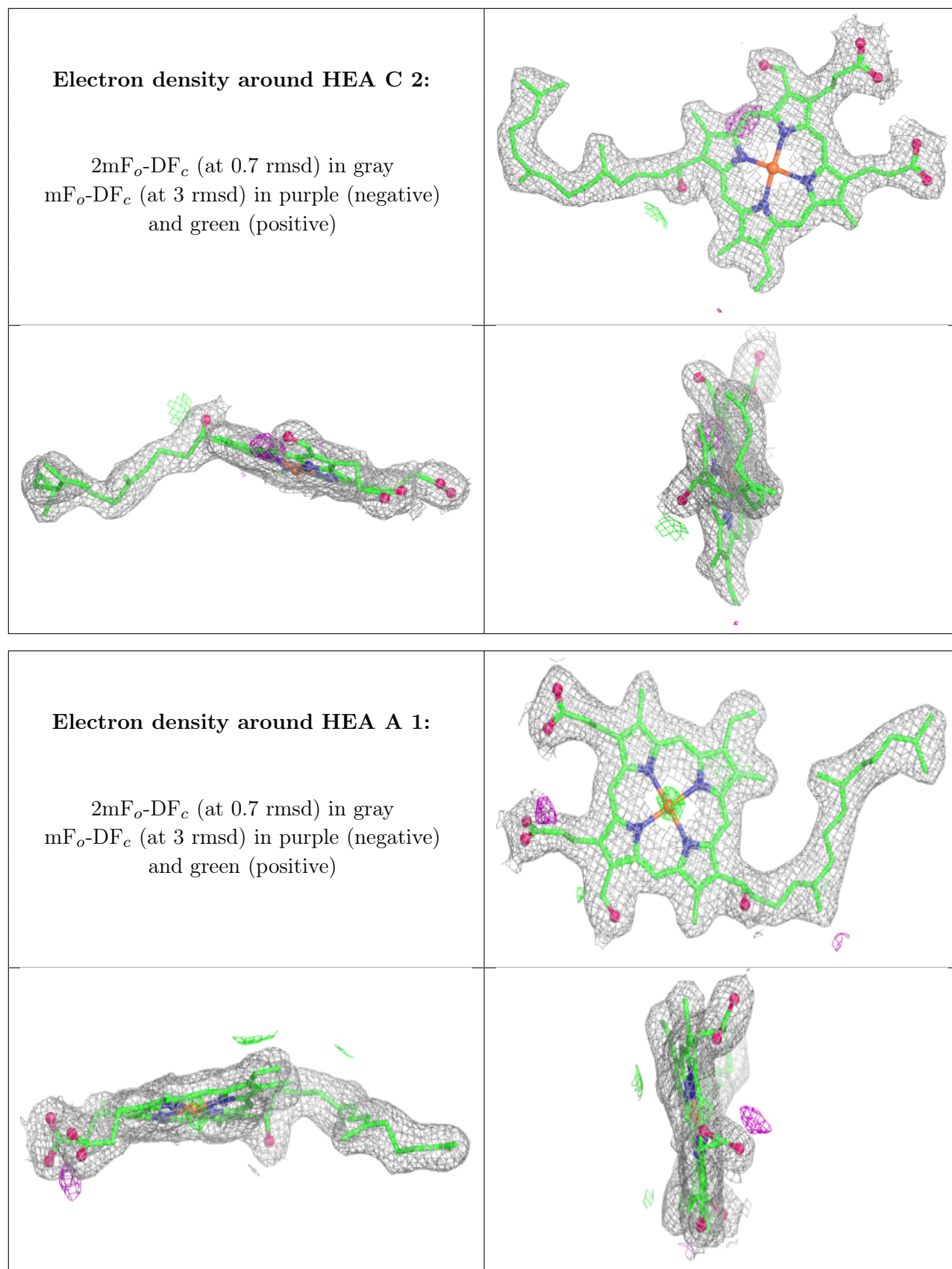
Electron density around HEA A 2:

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

**Electron density around HEA C 1:**

$2mF_o-DF_c$ (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.