



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:31 PM UTC

PDB ID : 3OMI / pdb_00003omi
Title : Catalytic core subunits (I and II) of cytochrome C oxidase from Rhodobacter sphaeroides with D132A mutation
Authors : Liu, J.; Qin, L.; Ferguson-Miller, S.
Deposited on : 2010-08-27
Resolution : 2.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

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

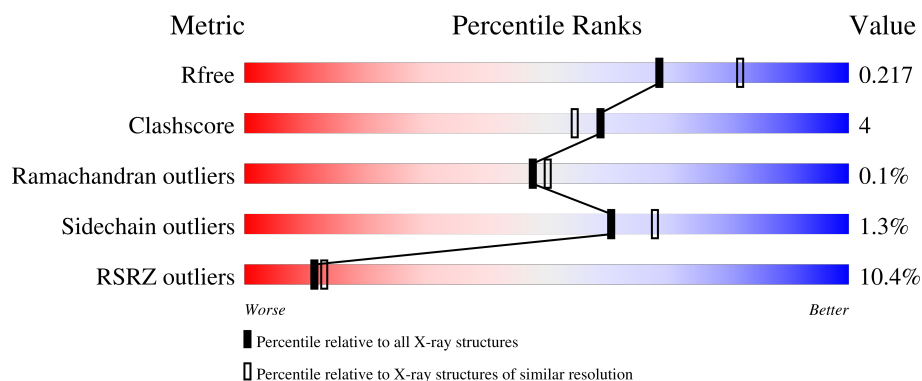
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	7% 91% 9% .
1	C	535	17% 85% 13% ..
2	B	256	4% 98% .
2	D	256	11% 93% 6%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 13416 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
			4167	2793	654	689	31			
1	C	530	Total	C	N	O	S	0	0	0
			4102	2749	641	681	31			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	ALA	ASP	engineered mutation	UNP Q3J5A7
C	132	ALA	ASP	engineered mutation	UNP Q3J5A7

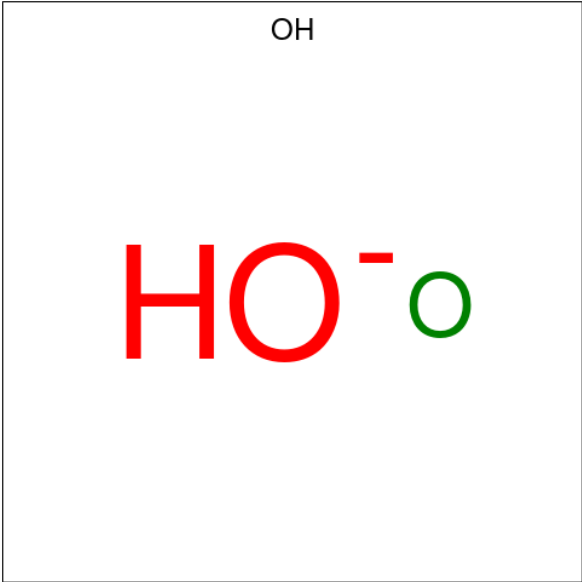
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			2008	1312	329	361	6			
2	D	256	Total	C	N	O	S	0	0	0
			2002	1307	326	363	6			

There are 8 discrepancies between the modelled and reference sequences:

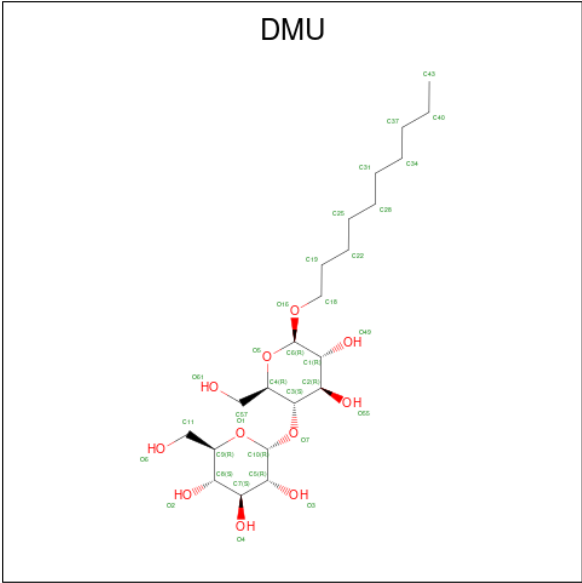
Chain	Residue	Modelled	Actual	Comment	Reference
B	282	HIS	-	expression tag	UNP Q3J5G0
B	283	HIS	-	expression tag	UNP Q3J5G0
B	284	HIS	-	expression tag	UNP Q3J5G0
B	285	HIS	-	expression tag	UNP Q3J5G0
D	282	HIS	-	expression tag	UNP Q3J5G0
D	283	HIS	-	expression tag	UNP Q3J5G0
D	284	HIS	-	expression tag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

- Molecule 3 is HYDROXIDE ION (CCD ID: 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 (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



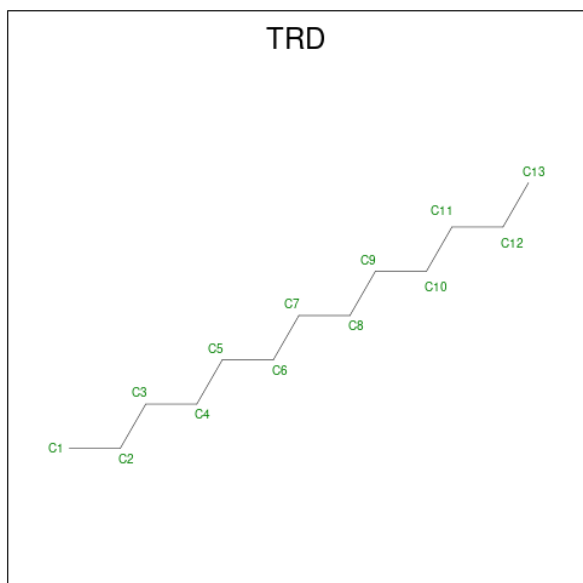
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 22 16 6	0	0

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

- Molecule 5 is TRIDECANE (CCD ID: TRD) (formula: $C_{13}H_{28}$).



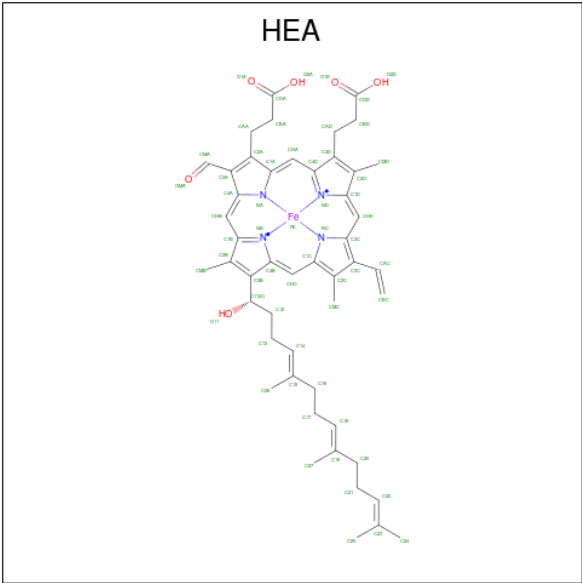
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C	0	0
			7	7		

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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 11 11	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 (CCD ID: 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 (CCD ID: 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 (CCD ID: 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

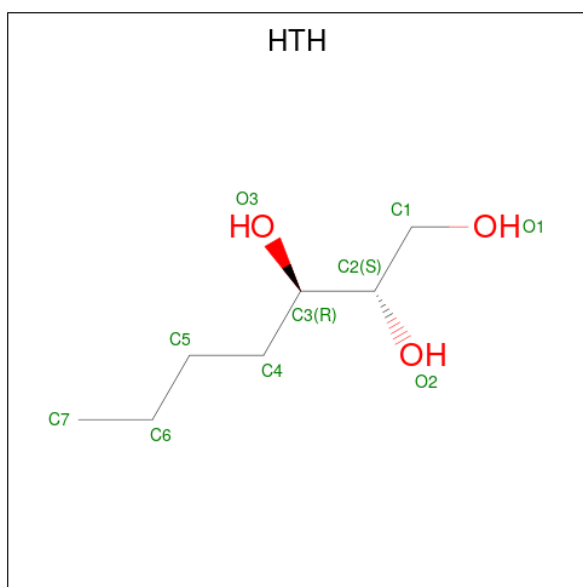
- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Cl		
			1	1	0	0
10	C	1	Total	Cl		
			1	1	0	0

- Molecule 11 is (2S,3R)-heptane-1,2,3-triol (CCD ID: HTH) (formula: C₇H₁₆O₃).



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

- Molecule 12 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

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

- Molecule 13 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	142	Total	O	0	0
			142	142		
14	B	134	Total	O	0	0
			134	134		

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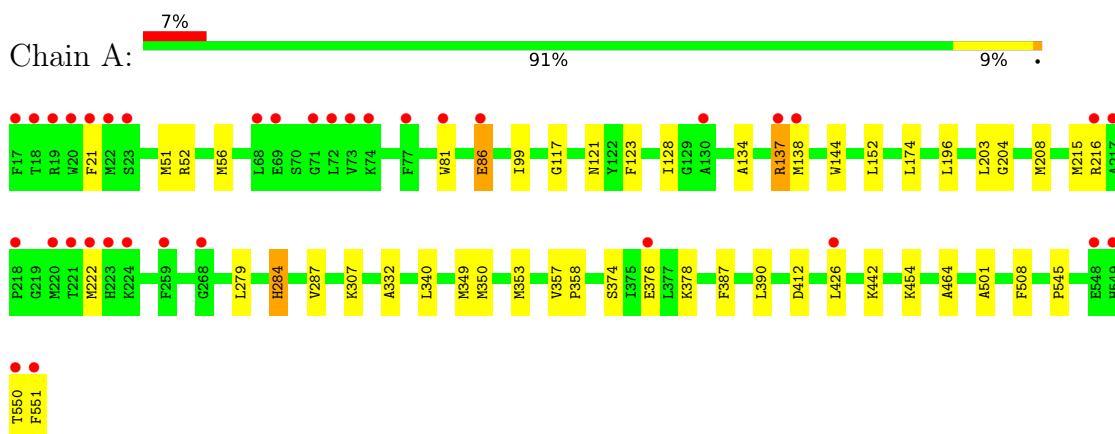
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	95	Total 95	O 95	0	0
14	D	120	Total 120	O 120	0	0

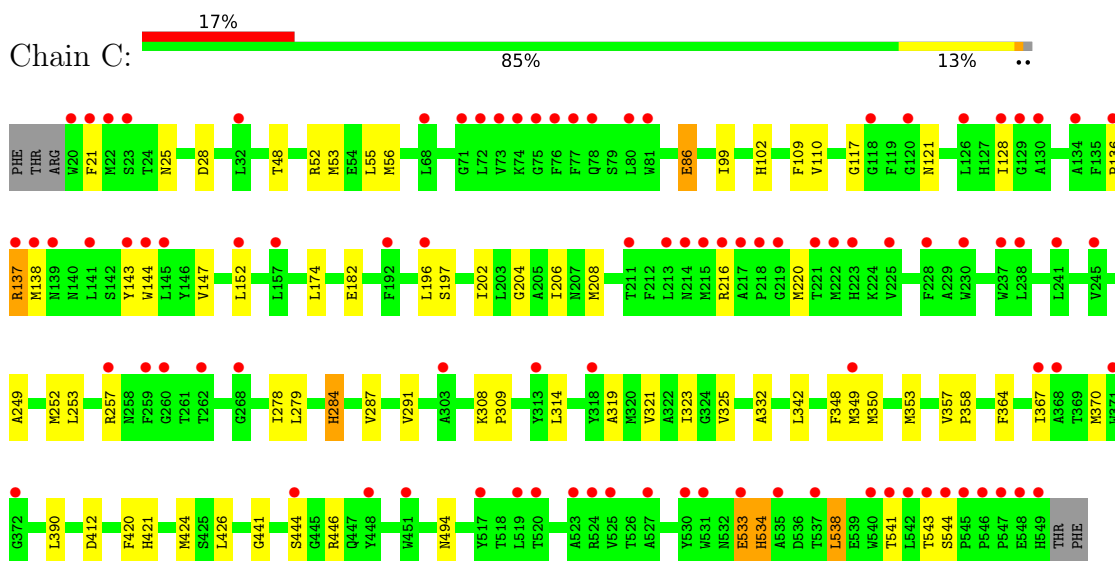
3 Residue-property plots [i](#)

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

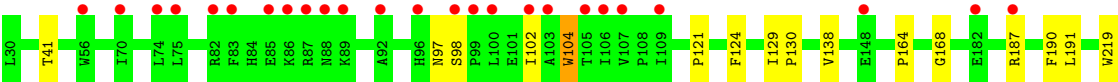
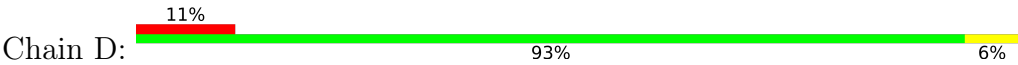


- Molecule 2: Cytochrome c oxidase subunit 2





● 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	125.06Å 131.52Å 175.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.84 – 2.15 35.84 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.5 (35.84-2.15) 96.5 (35.84-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.16Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.215 0.195 , 0.217	Depositor DCC
R_{free} test set	4574 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13416	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: CL, HTH, MG, CU, OH, TRD, DMU, HEA, CD, CU1, CA

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	0.67	1/4320 (0.0%)	0.87	2/5900 (0.0%)
1	C	0.59	2/4251 (0.0%)	0.91	4/5808 (0.1%)
2	B	0.62	0/2069	0.79	0/2835
2	D	0.58	0/2063	0.80	0/2829
All	All	0.62	3/12703 (0.0%)	0.86	6/17372 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	534	HIS	ND1-CE1	5.26	1.37	1.32
1	A	284	HIS	CE1-NE2	5.12	1.37	1.32
1	C	284	HIS	CE1-NE2	5.05	1.37	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	HIS	N-CA-CB	7.92	117.91	110.39
1	C	284	HIS	N-CA-CB	7.64	117.65	110.39
1	C	534	HIS	CB-CG-CD2	-6.70	122.49	131.20
1	C	534	HIS	CB-CG-ND1	5.69	131.24	122.70
1	A	123	PHE	N-CA-C	5.12	119.65	113.41

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	4167	0	4063	41	0
1	C	4102	0	4001	54	0
2	B	2008	0	1955	4	0
2	D	2002	0	1940	11	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	3	0
4	D	46	0	42	2	0
5	A	47	0	92	2	0
5	B	9	0	17	2	0
5	C	11	0	21	0	0
5	D	20	0	41	1	0
6	A	120	0	108	4	0
6	C	120	0	108	3	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	A	1	0	0	0	0
10	C	1	0	0	0	0
11	B	10	0	16	0	0
12	B	1	0	0	0	0
12	D	1	0	0	0	0
13	B	2	0	0	0	0
13	D	2	0	0	0	0
14	A	142	0	0	2	0
14	B	134	0	0	1	0
14	C	95	0	0	4	0
14	D	120	0	0	0	0
All	All	13416	0	12697	112	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 4.

The worst 5 of 112 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:137:ARG:HG3	1:A:137:ARG:HH11	1.07	1.16
1:C:534:HIS:HE1	14:C:794:HOH:O	1.44	1.00
1:C:534:HIS:HD2	14:C:791:HOH:O	1.47	0.98
1:A:426:LEU:HD21	1:A:464:ALA:CB	1.95	0.96
1:A:350:MET:HA	1:A:353:MET:HE3	1.47	0.95

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	533/535 (100%)	524 (98%)	9 (2%)	0	100	100
1	C	528/535 (99%)	517 (98%)	10 (2%)	1 (0%)	43	44
2	B	254/256 (99%)	248 (98%)	6 (2%)	0	100	100
2	D	254/256 (99%)	247 (97%)	6 (2%)	1 (0%)	30	26
All	All	1569/1582 (99%)	1536 (98%)	31 (2%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	220	MET
2	D	97	ASN

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	423/434 (98%)	418 (99%)	5 (1%)	63	70
1	C	417/434 (96%)	408 (98%)	9 (2%)	45	51
2	B	210/215 (98%)	209 (100%)	1 (0%)	81	87
2	D	210/215 (98%)	208 (99%)	2 (1%)	68	75
All	All	1260/1298 (97%)	1243 (99%)	17 (1%)	61	68

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	533	GLU
2	D	187	ARG
1	C	86	GLU
1	C	99	ILE
1	C	137	ARG

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	178	GLN
2	D	125	ASN
2	B	203	ASN
1	C	165	GLN
2	B	170	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 43 ligands modelled in this entry, 2 are modelled with single atom and 16 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
6	HEA	C	606	14,1	67,67,67	1.57	7 (10%)	81,103,103	1.46	17 (20%)
5	TRD	A	606	-	6,6,12	0.31	0	5,5,11	0.40	0
4	DMU	D	301	-	24,24,34	0.54	0	35,35,45	0.61	0
6	HEA	A	607	1	67,67,67	1.39	8 (11%)	81,103,103	1.50	15 (18%)
4	DMU	B	303	-	34,34,34	0.48	0	45,45,45	0.61	0
5	TRD	D	303	-	12,12,12	0.21	0	11,11,11	0.63	0
4	DMU	C	603	-	24,24,34	0.54	0	35,35,45	0.74	0
4	DMU	C	604	-	24,24,34	0.63	0	35,35,45	0.81	1 (2%)
11	HTH	B	306	-	9,9,9	0.42	0	10,10,10	0.67	0
5	TRD	B	305	-	8,8,12	0.23	0	7,7,11	0.50	0
5	TRD	A	605	-	6,6,12	0.27	0	5,5,11	0.46	0
5	TRD	C	607	-	10,10,12	0.33	0	9,9,11	0.44	0
4	DMU	B	304	-	24,24,34	0.55	0	35,35,45	0.68	0
4	DMU	D	302	-	24,24,34	0.56	0	35,35,45	0.60	0
6	HEA	A	608	14,1	67,67,67	1.51	7 (10%)	81,103,103	1.53	13 (16%)
4	DMU	B	301	-	34,34,34	0.44	0	45,45,45	0.90	2 (4%)
4	DMU	B	302	-	34,34,34	0.52	0	45,45,45	0.82	2 (4%)
6	HEA	C	605	1	67,67,67	1.35	7 (10%)	81,103,103	1.38	13 (16%)
4	DMU	C	602	-	34,34,34	0.57	0	45,45,45	0.80	0
5	TRD	A	610	-	12,12,12	0.36	0	11,11,11	0.43	0
4	DMU	A	603	-	22,22,34	0.55	0	27,27,45	0.84	1 (3%)
5	TRD	A	609	-	12,12,12	0.26	0	11,11,11	0.56	0
5	TRD	A	604	-	6,6,12	0.29	0	5,5,11	0.38	0
4	DMU	A	602	-	22,22,34	0.51	0	27,27,45	0.83	1 (3%)
5	TRD	D	304	-	6,6,12	0.25	0	5,5,11	0.39	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
6	HEA	C	606	14,1	-	4/36/76/76	-
5	TRD	A	606	-	-	0/4/4/10	-
4	DMU	D	301	-	-	4/8/48/59	0/2/2/2
6	HEA	A	607	1	-	4/36/76/76	-
4	DMU	B	303	-	-	5/19/59/59	0/2/2/2
5	TRD	D	303	-	-	5/10/10/10	-
4	DMU	C	603	-	-	2/8/48/59	0/2/2/2
4	DMU	C	604	-	-	4/8/48/59	0/2/2/2
11	HTH	B	306	-	-	4/10/10/10	-
5	TRD	B	305	-	-	1/6/6/10	-
5	TRD	A	605	-	-	0/4/4/10	-
5	TRD	C	607	-	-	2/8/8/10	-
4	DMU	B	304	-	-	3/8/48/59	0/2/2/2
4	DMU	D	302	-	-	2/8/48/59	0/2/2/2
6	HEA	A	608	14,1	-	7/36/76/76	-
4	DMU	B	301	-	-	5/19/59/59	0/2/2/2
4	DMU	B	302	-	-	9/19/59/59	0/2/2/2
6	HEA	C	605	1	-	6/36/76/76	-
4	DMU	C	602	-	-	9/19/59/59	0/2/2/2
5	TRD	A	610	-	-	3/10/10/10	-
4	DMU	A	603	-	-	3/13/33/59	0/1/1/2
5	TRD	A	609	-	-	7/10/10/10	-
5	TRD	A	604	-	-	2/4/4/10	-
4	DMU	A	602	-	-	6/13/33/59	0/1/1/2
5	TRD	D	304	-	-	1/4/4/10	-

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	606	HEA	FE-NC	6.16	2.15	1.95
6	C	605	HEA	FE-NA	5.67	2.13	1.95
6	A	608	HEA	FE-NA	5.56	2.13	1.95
6	A	608	HEA	FE-NB	4.72	2.09	1.94
6	C	606	HEA	FE-NA	4.65	2.10	1.95

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	608	HEA	C2A-C1A-NA	-4.03	106.44	110.32
6	C	605	HEA	C2A-C1A-NA	-3.98	106.48	110.32
6	A	608	HEA	C4B-NB-C1B	3.73	109.62	105.21
6	A	607	HEA	C17-C18-C19	-3.59	119.40	127.62
6	A	607	HEA	C1D-ND-C4D	3.58	109.44	105.21

There are no chirality outliers.

5 of 98 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	302	DMU	C19-C18-O16-C6
11	B	306	HTH	O1-C1-C2-O2
4	C	604	DMU	O5-C4-C57-O61
4	C	604	DMU	O6-C11-C9-O1
4	D	301	DMU	O5-C4-C57-O61

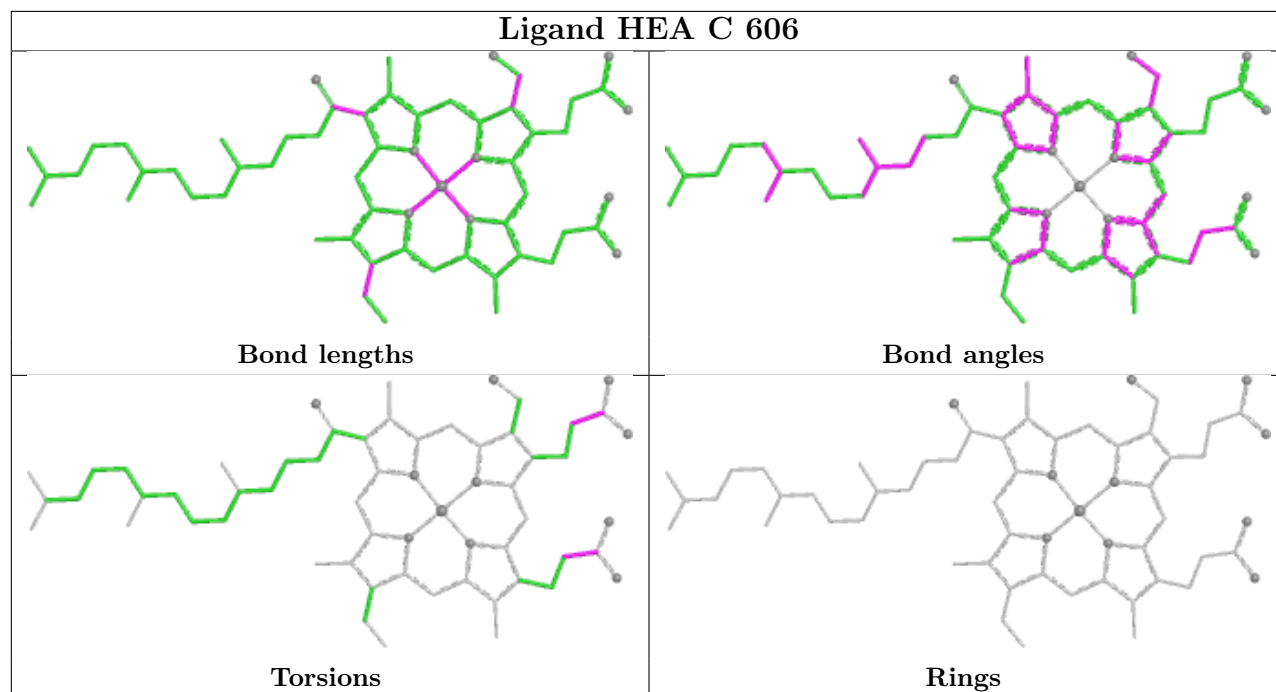
There are no ring outliers.

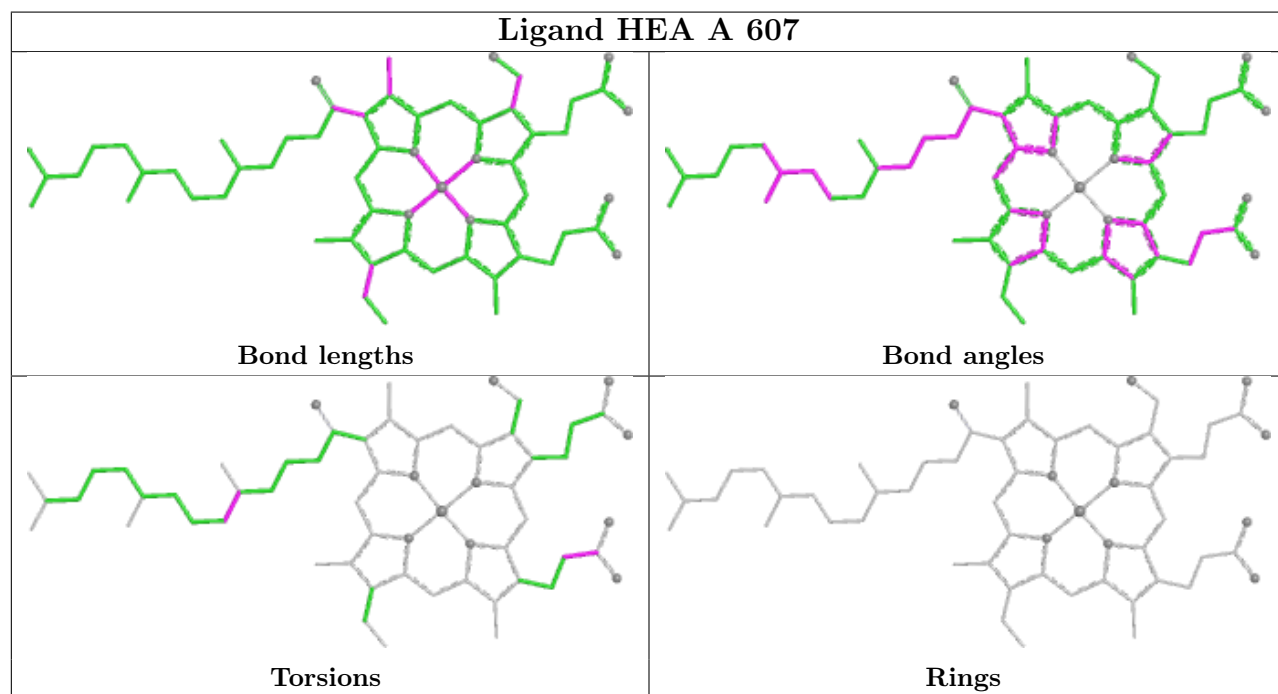
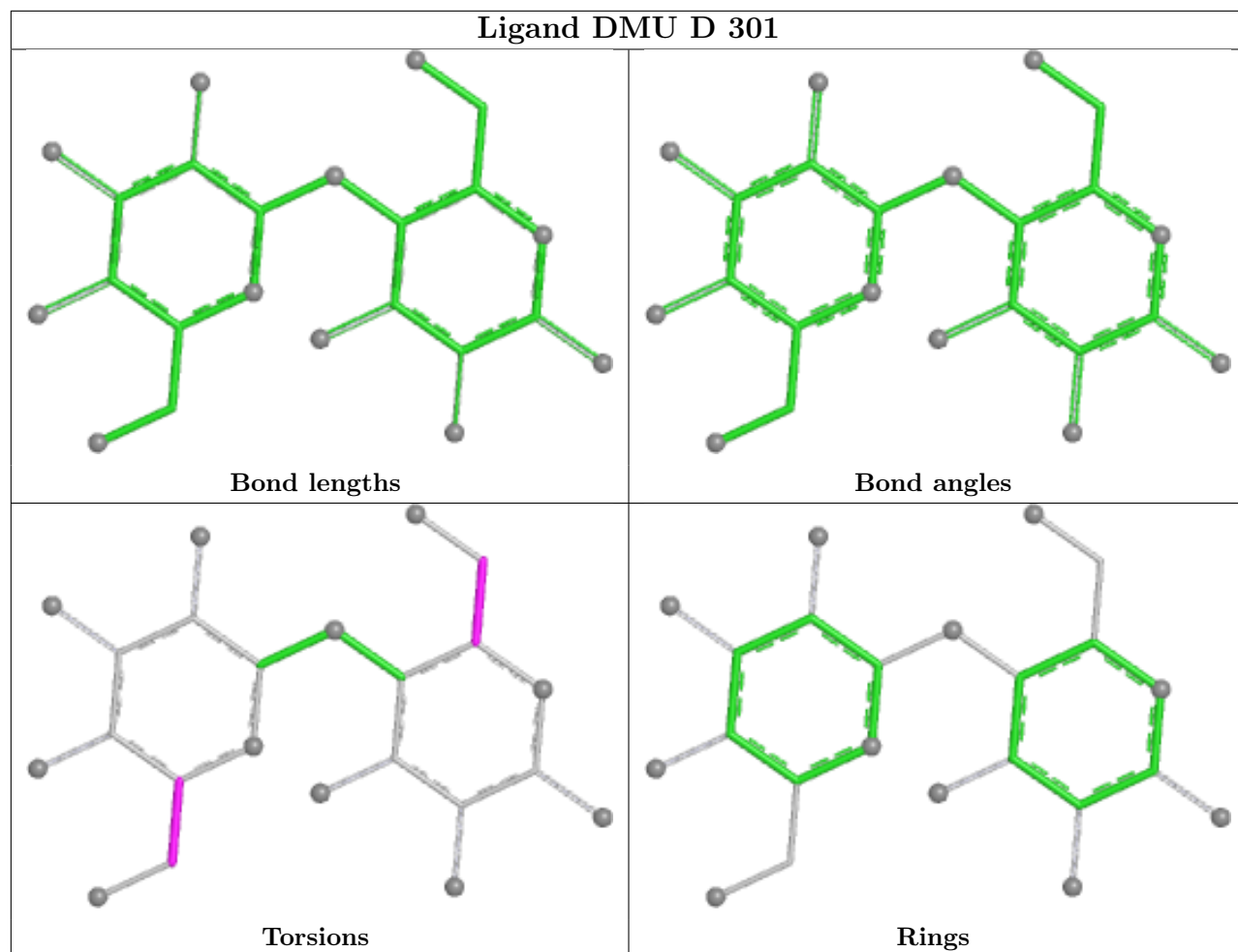
13 monomers are involved in 18 short contacts:

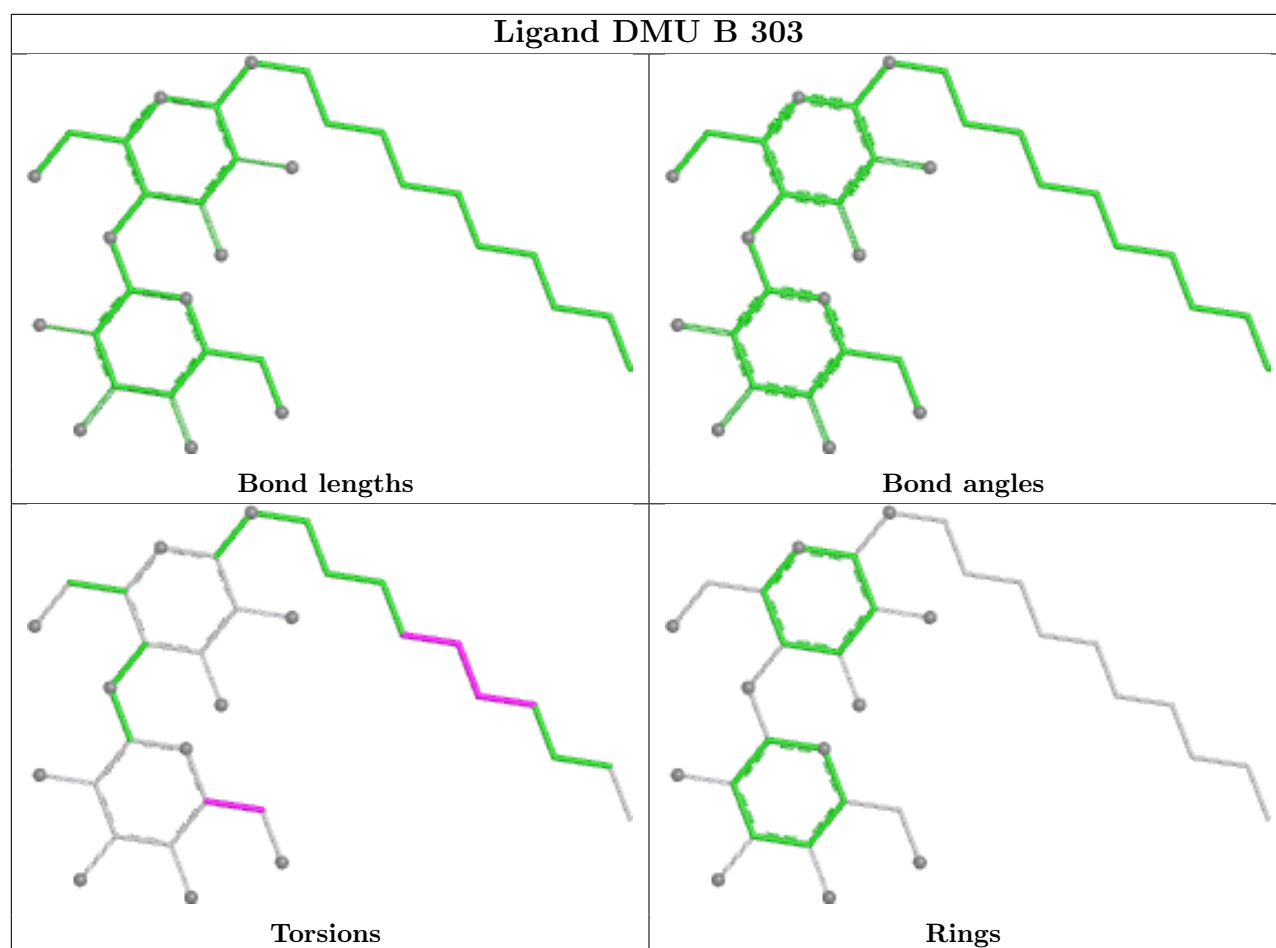
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	606	HEA	2	0
4	D	301	DMU	1	0
6	A	607	HEA	2	0
5	D	303	TRD	1	0
4	C	604	DMU	1	0
5	B	305	TRD	2	0
4	D	302	DMU	1	0
6	A	608	HEA	2	0
6	C	605	HEA	1	0
4	C	602	DMU	2	0
5	A	610	TRD	1	0
4	A	603	DMU	1	0
5	A	609	TRD	1	0

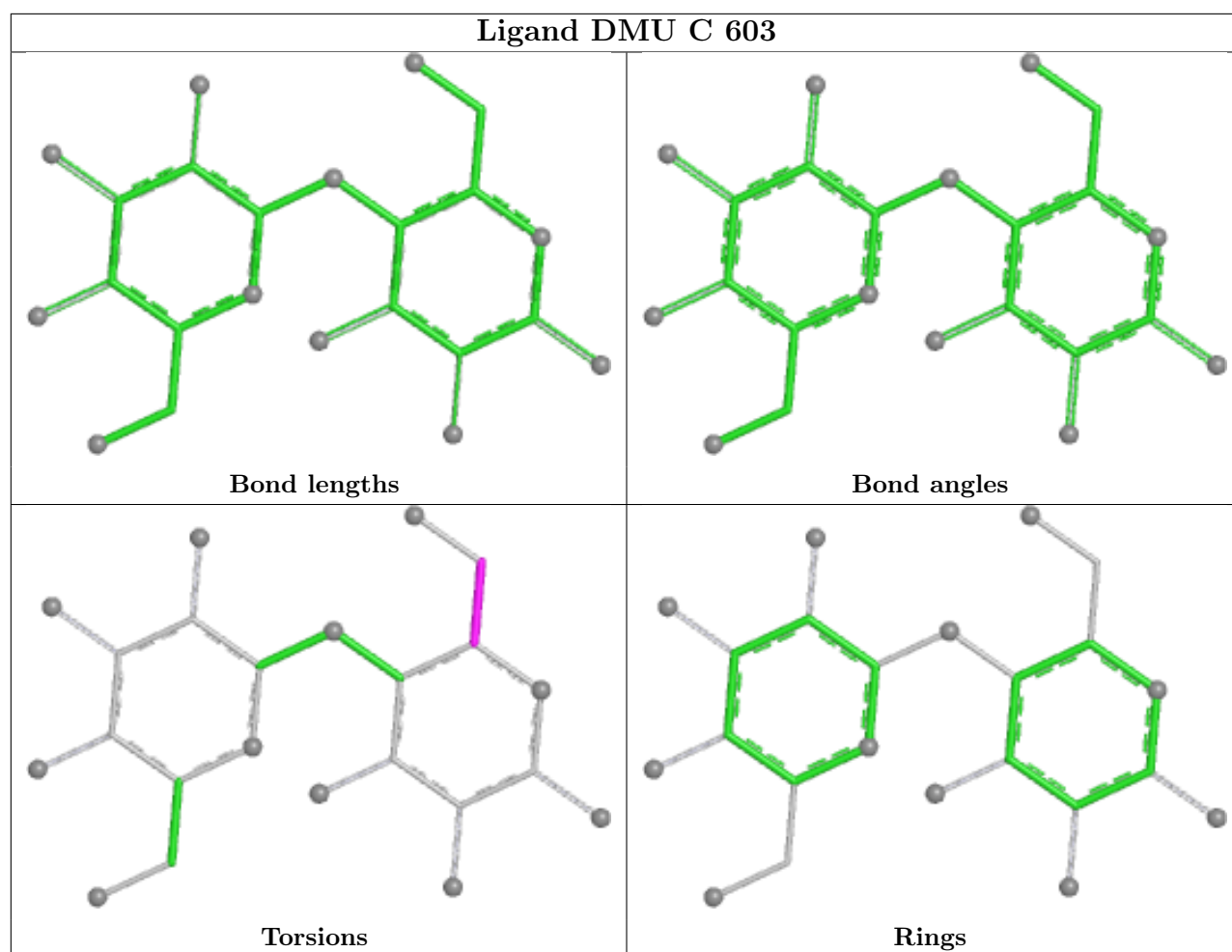
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

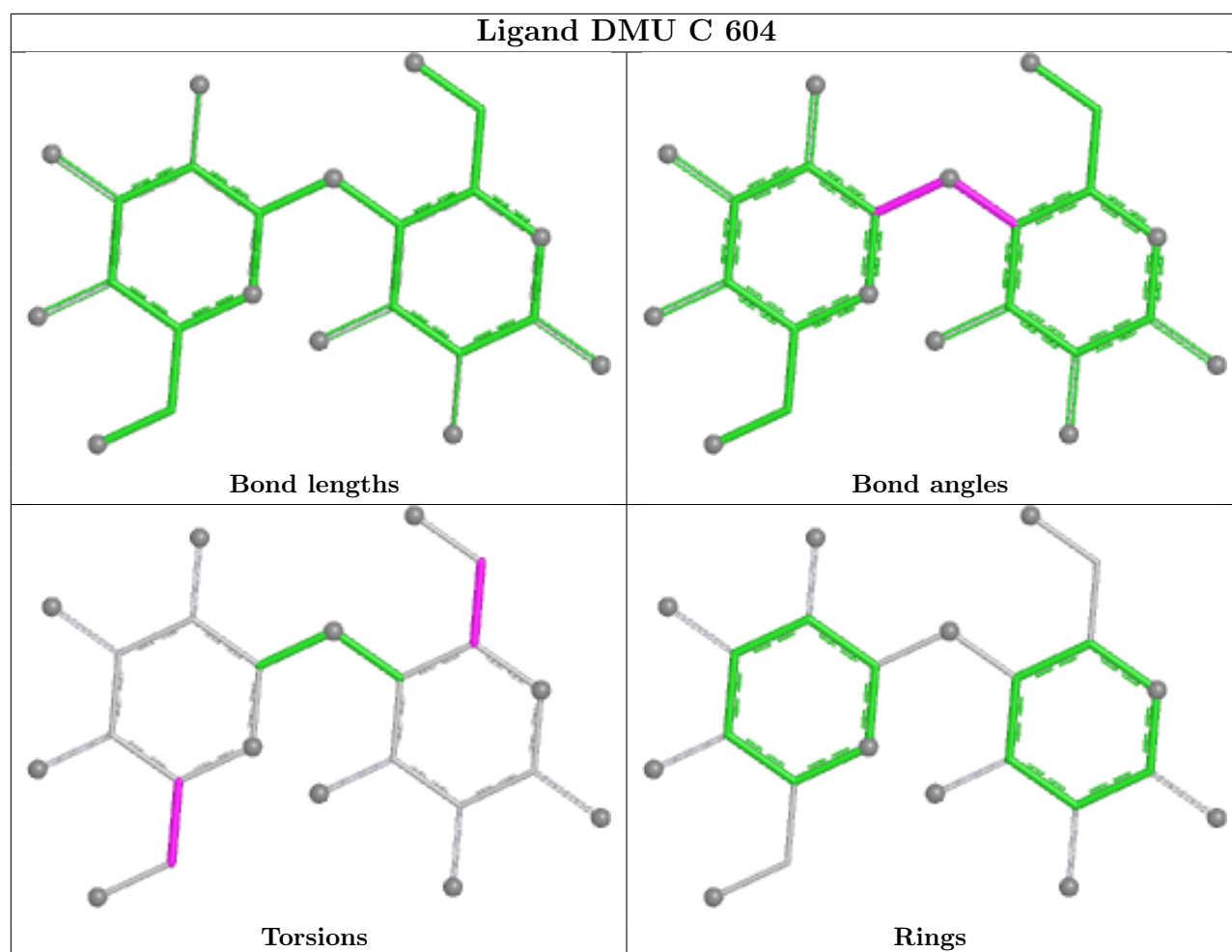
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

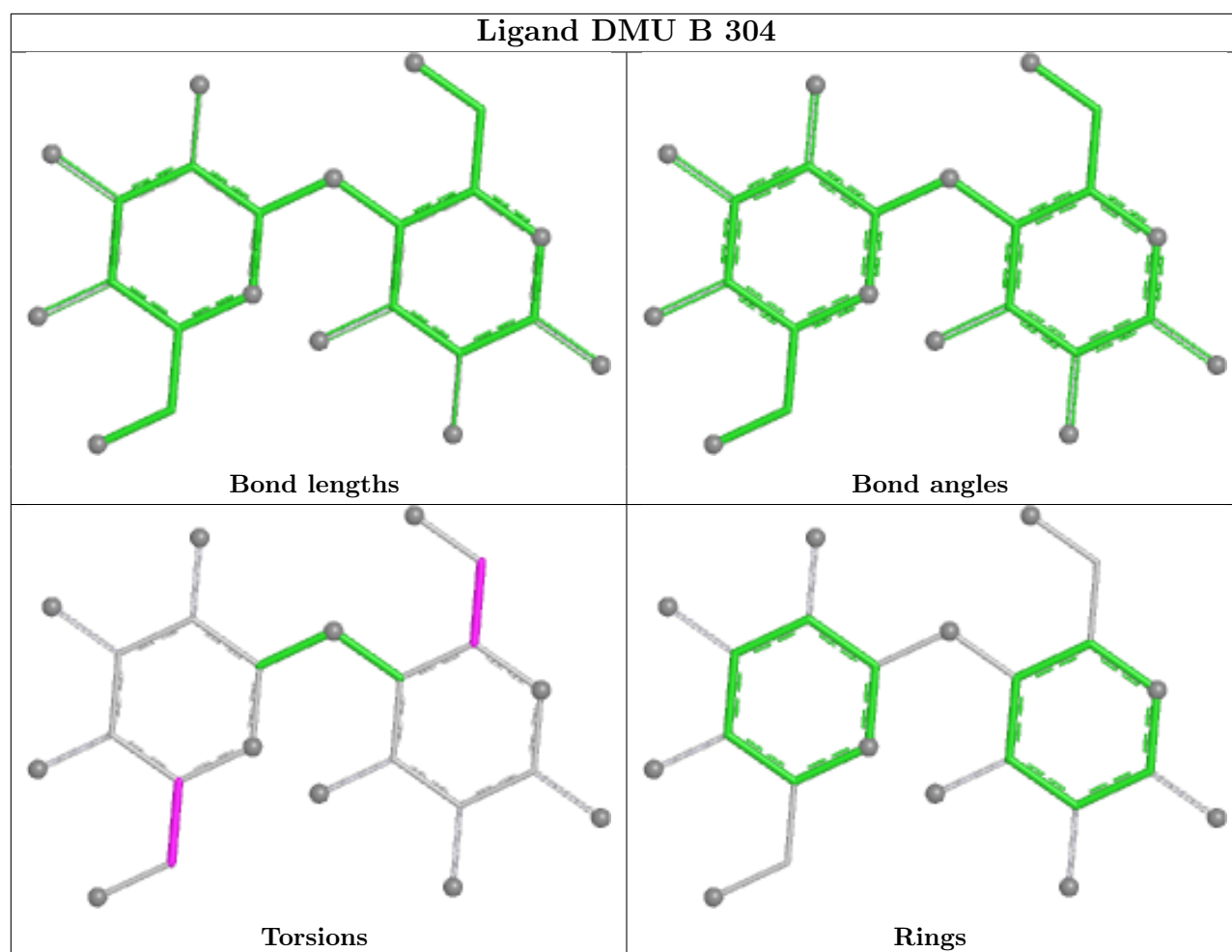


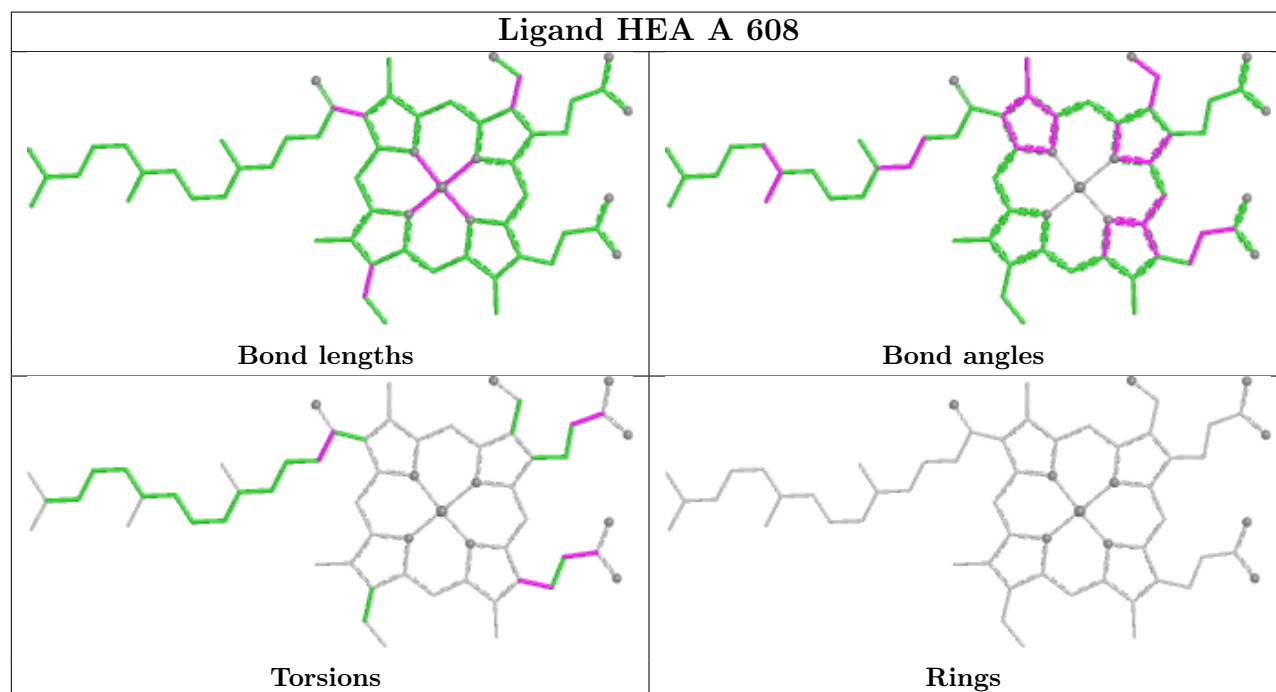
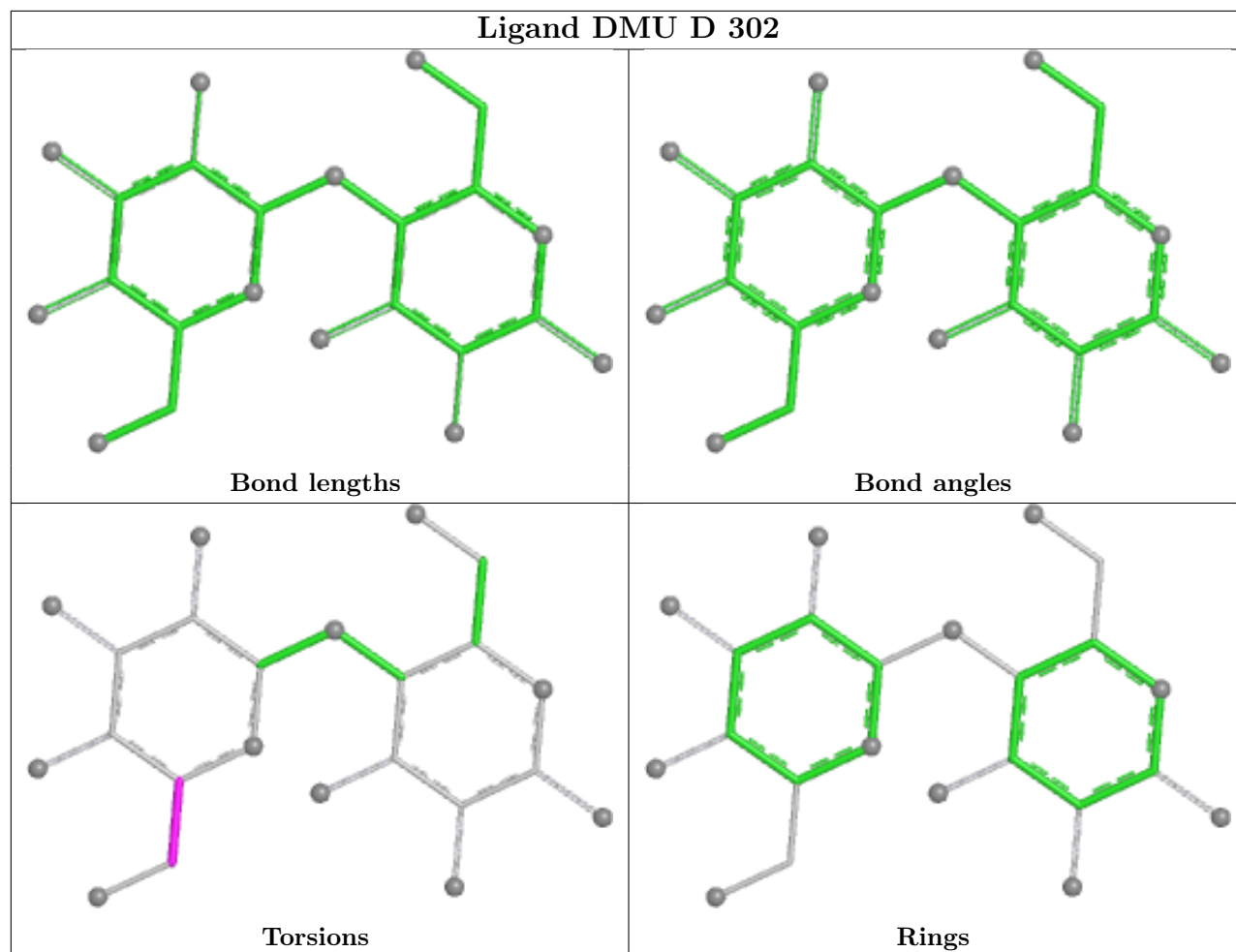


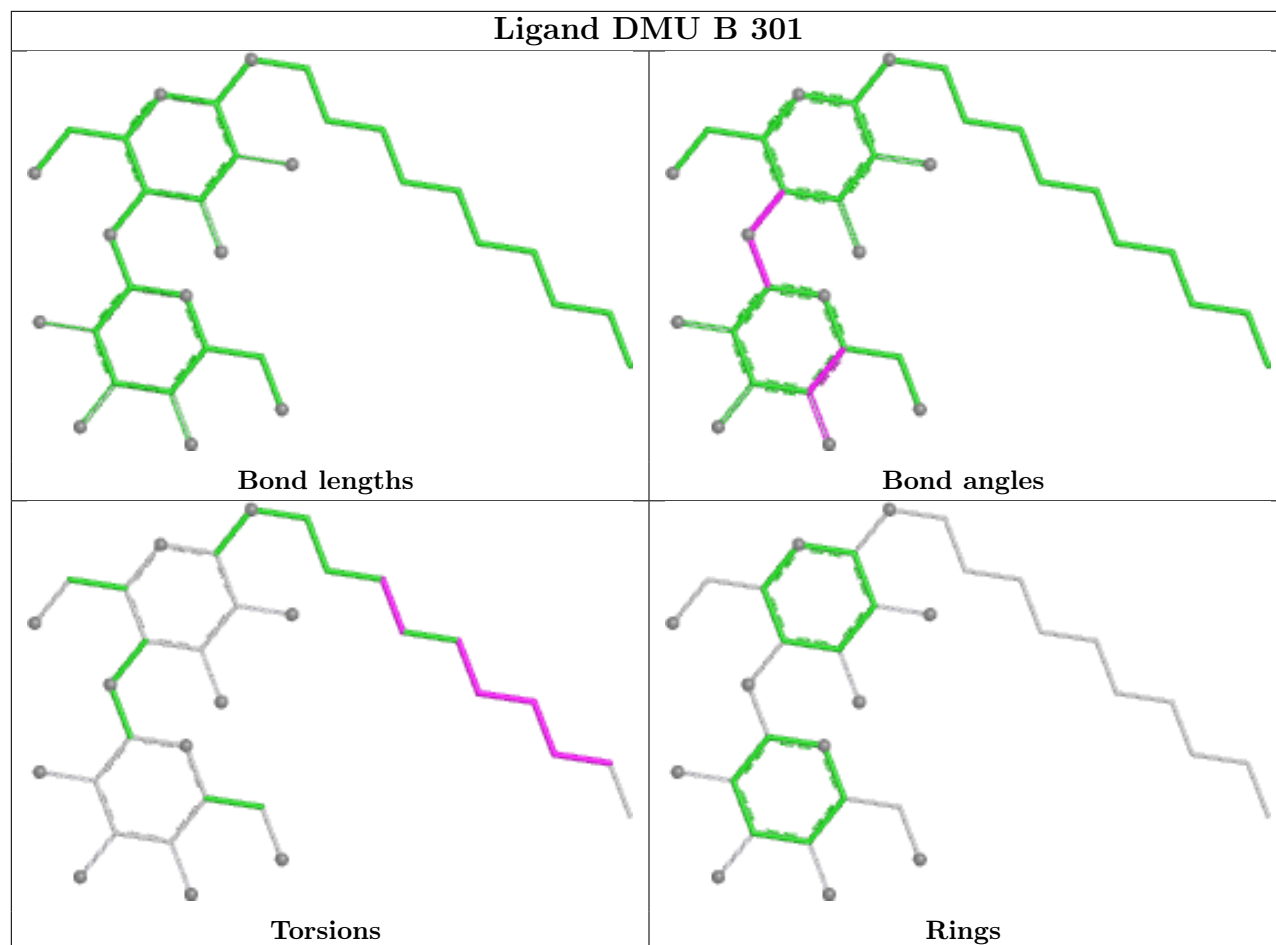


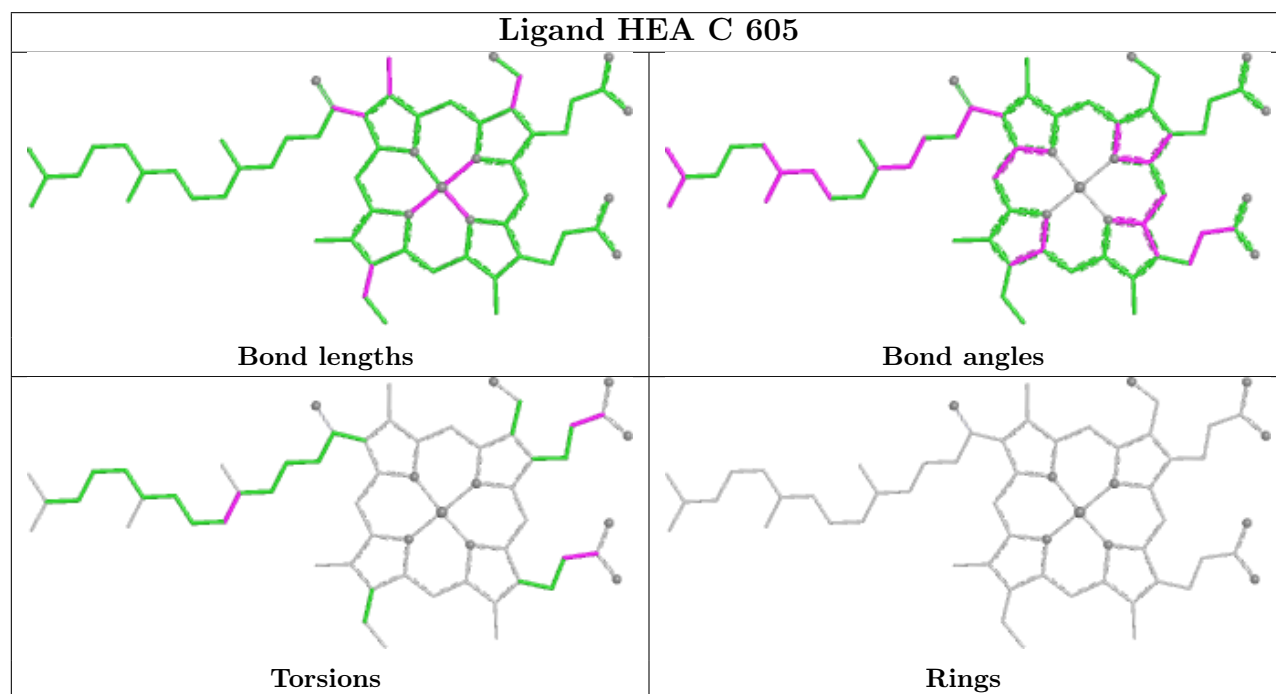
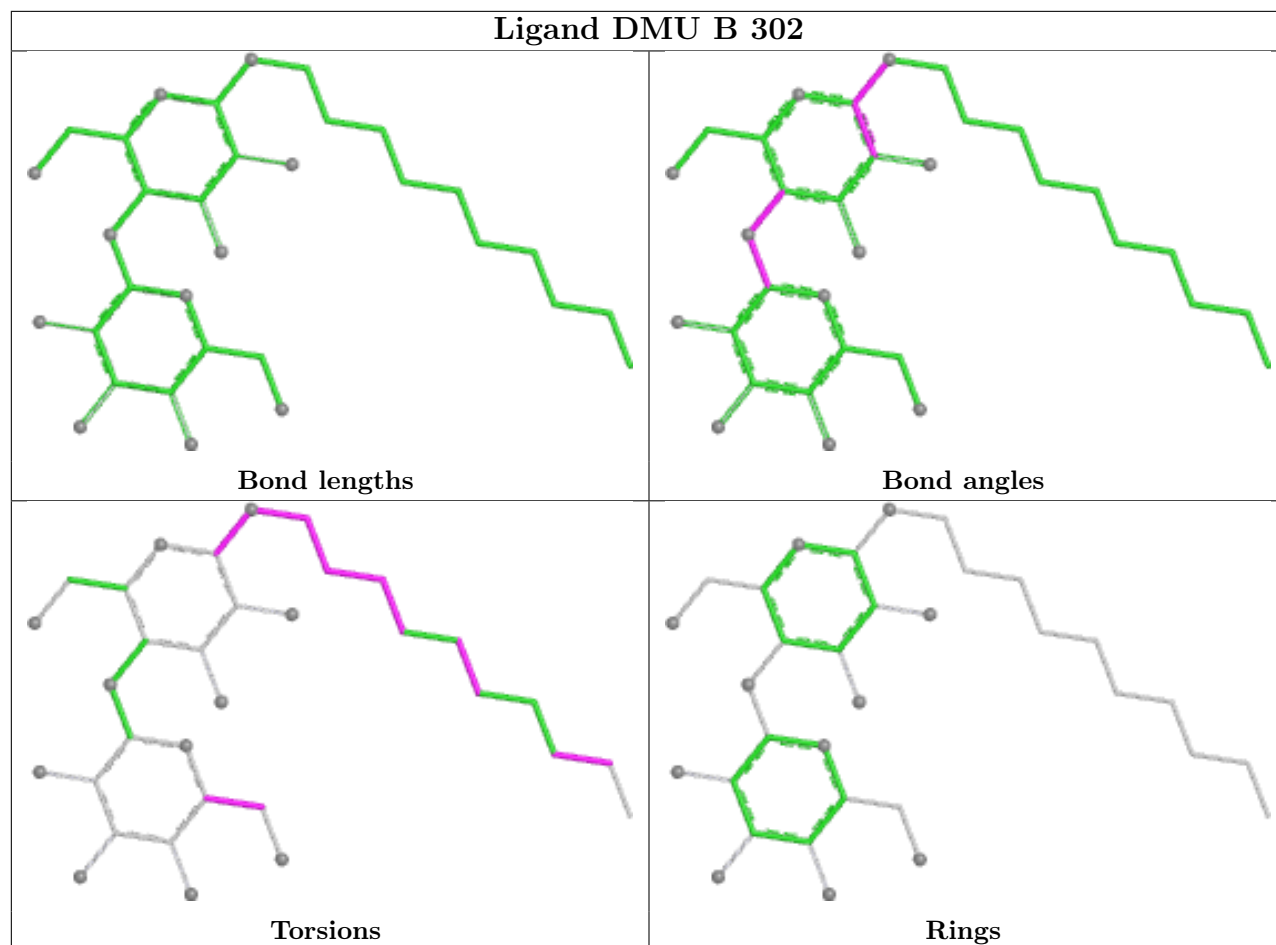


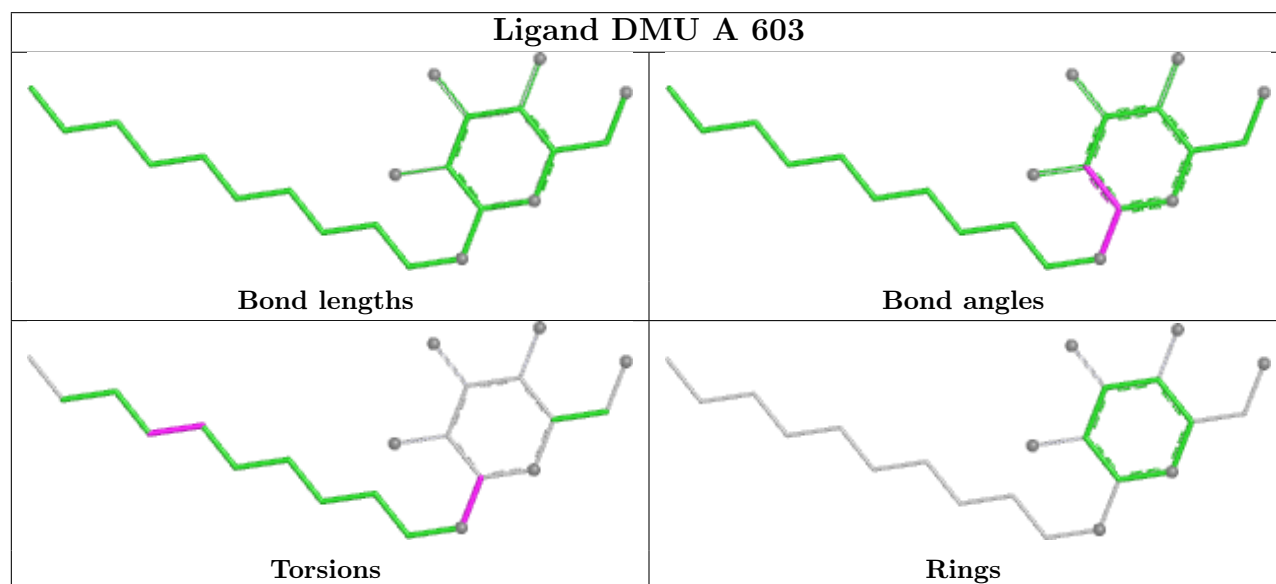
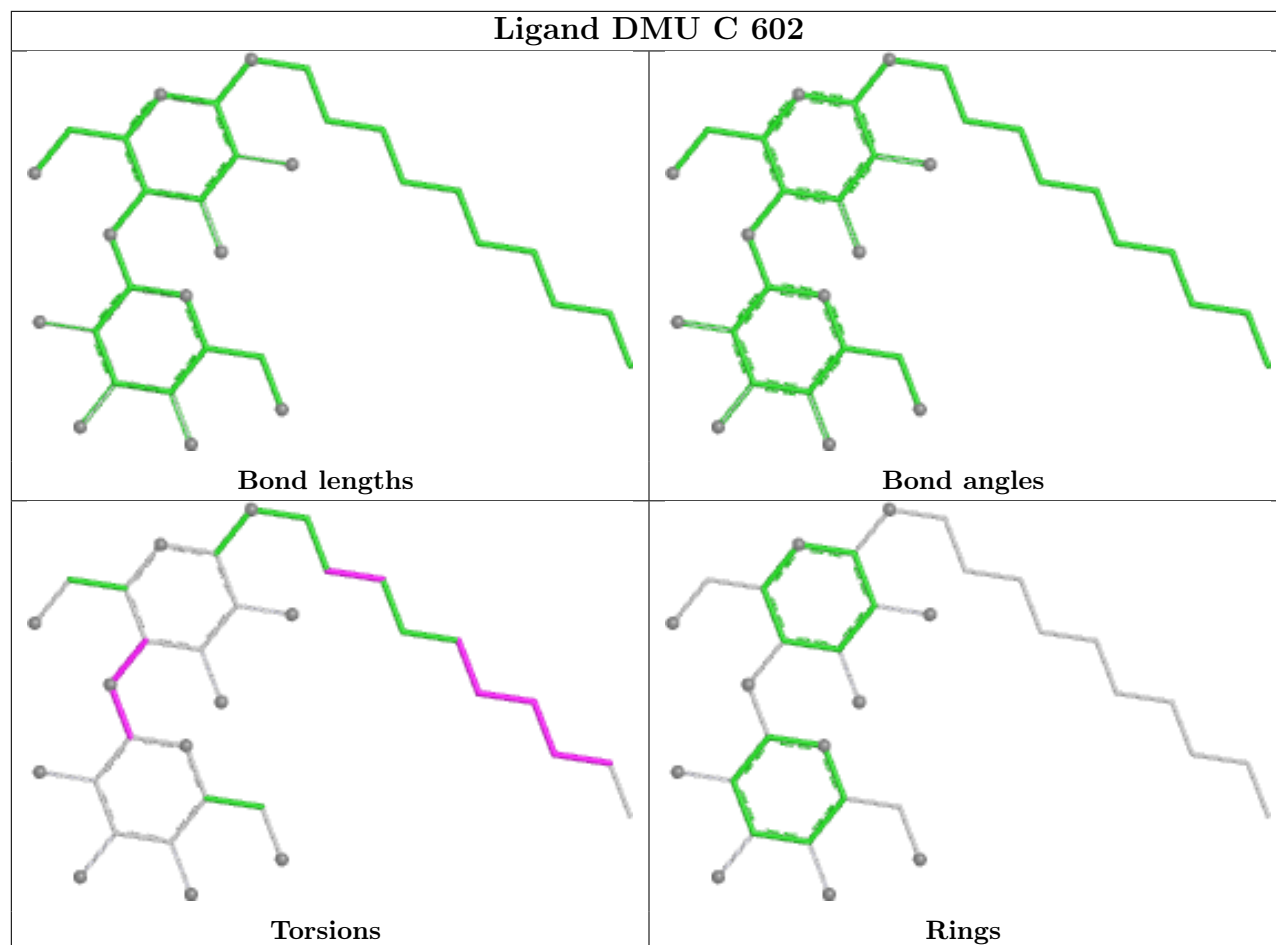


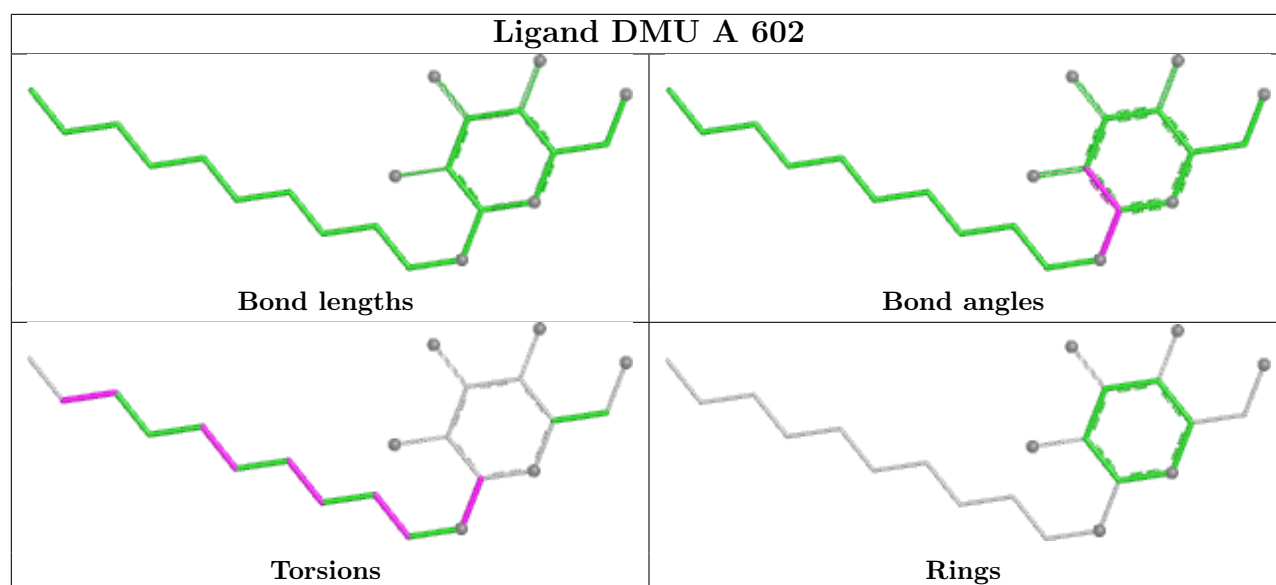












5.7 Other polymers [i](#)

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	535/535 (100%)	0.19	35 (6%) 25 28	18, 30, 53, 75	0
1	C	530/535 (99%)	1.11	91 (17%) 4 4	25, 45, 68, 81	0
2	B	256/256 (100%)	0.29	11 (4%) 40 45	18, 34, 47, 54	0
2	D	256/256 (100%)	0.60	27 (10%) 11 13	24, 38, 58, 67	0
All	All	1577/1582 (99%)	0.58	164 (10%) 11 13	18, 36, 61, 81	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	TRP	7.1
1	C	549	HIS	6.5
1	A	20	TRP	5.7
1	C	72	LEU	5.5
1	A	217	ALA	5.1

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](#)

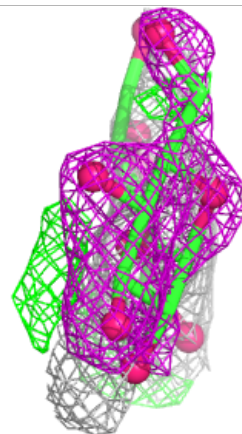
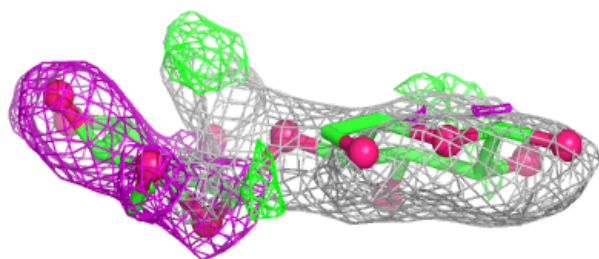
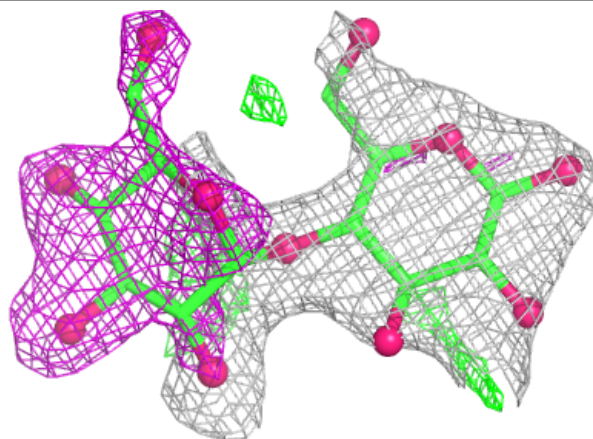
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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
4	DMU	C	604	23/33	0.31	0.24	39,43,51,51	23
4	DMU	C	602	33/33	0.72	0.17	40,44,46,47	0
4	DMU	D	302	23/33	0.72	0.20	70,72,76,76	23
4	DMU	C	603	23/33	0.73	0.21	85,85,86,86	23
5	TRD	A	605	7/13	0.74	0.24	50,52,52,52	0
4	DMU	D	301	23/33	0.78	0.39	64,64,65,65	23
5	TRD	C	607	11/13	0.78	0.31	70,71,72,72	0
5	TRD	A	609	13/13	0.80	0.25	64,65,68,68	0
5	TRD	A	606	7/13	0.81	0.22	60,61,62,62	0
5	TRD	A	610	13/13	0.82	0.17	37,41,46,46	0
4	DMU	B	302	33/33	0.82	0.22	43,49,51,54	33
5	TRD	A	604	7/13	0.83	0.20	52,55,57,57	0
4	DMU	B	304	23/33	0.84	0.20	69,69,70,70	23
4	DMU	A	602	22/33	0.84	0.16	38,59,66,66	0
5	TRD	D	304	7/13	0.84	0.19	54,54,55,55	0
5	TRD	D	303	13/13	0.85	0.19	48,49,55,55	0
4	DMU	A	603	22/33	0.85	0.16	35,44,50,51	22
5	TRD	B	305	9/13	0.86	0.22	39,40,41,43	9
10	CL	C	611	1/1	0.87	0.15	66,66,66,66	0
4	DMU	B	303	33/33	0.88	0.17	46,51,57,59	33
11	HTH	B	306	10/10	0.89	0.20	51,57,60,60	0
4	DMU	B	301	33/33	0.94	0.09	20,31,51,53	0
6	HEA	C	606	60/60	0.97	0.08	25,31,41,42	0
3	OH	C	601	1/1	0.98	0.09	27,27,27,27	0
10	CL	A	614	1/1	0.98	0.07	39,39,39,39	0
6	HEA	A	608	60/60	0.98	0.07	19,24,36,39	0
6	HEA	C	605	60/60	0.98	0.07	25,29,42,43	0
7	CU	C	608	1/1	0.99	0.02	35,35,35,35	0
9	CA	C	610	1/1	0.99	0.03	34,34,34,34	0
6	HEA	A	607	60/60	0.99	0.05	16,19,27,28	0
3	OH	A	601	1/1	0.99	0.04	17,17,17,17	0
7	CU	A	611	1/1	0.99	0.03	28,28,28,28	0
13	CD	B	309	1/1	0.99	0.02	37,37,37,37	0
13	CD	B	310	1/1	0.99	0.08	35,35,35,35	1
13	CD	D	307	1/1	0.99	0.02	36,36,36,36	0
13	CD	D	308	1/1	0.99	0.08	47,47,47,47	1
8	MG	C	609	1/1	1.00	0.06	20,20,20,20	0
12	CU1	B	308	1/1	1.00	0.02	21,21,21,21	0
12	CU1	D	306	1/1	1.00	0.01	26,26,26,26	0
9	CA	A	613	1/1	1.00	0.03	23,23,23,23	0
7	CU	B	307	1/1	1.00	0.01	21,21,21,21	0
7	CU	D	305	1/1	1.00	0.01	27,27,27,27	0
8	MG	A	612	1/1	1.00	0.09	16,16,16,16	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.

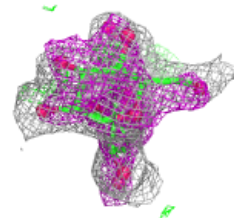
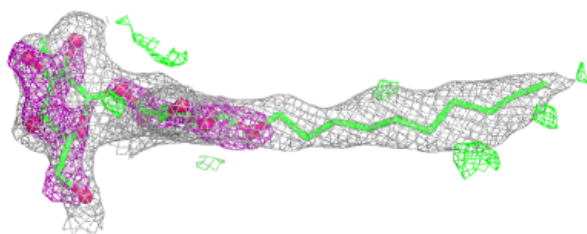
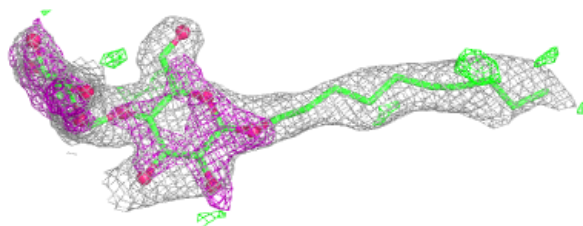
Electron density around DMU C 604:

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

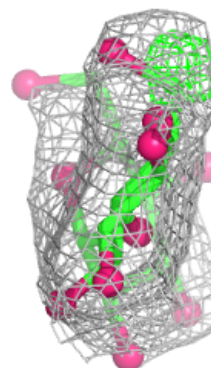
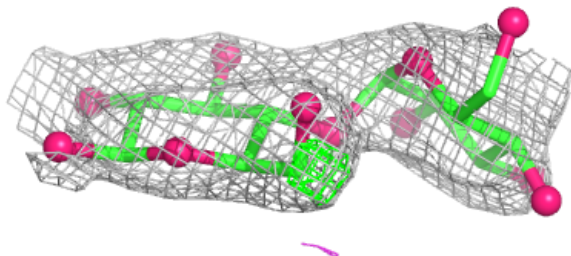
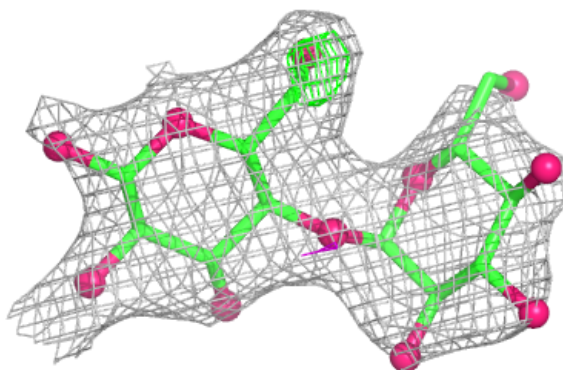


Electron density around DMU C 602:

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and green (positive)

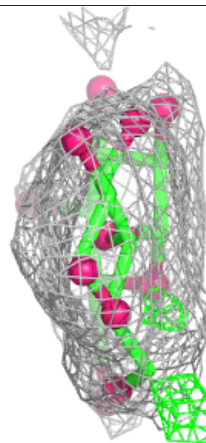
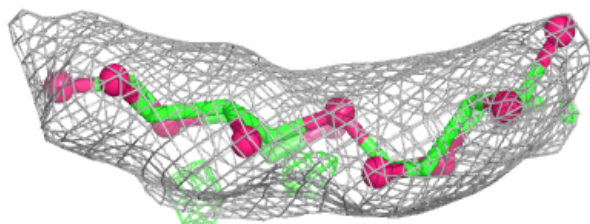
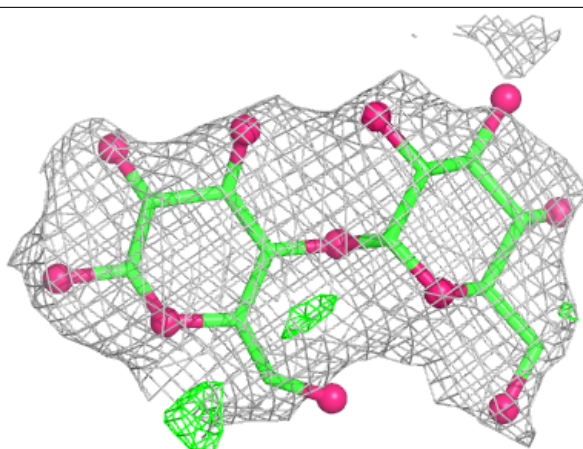
**Electron density around DMU D 302:**

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



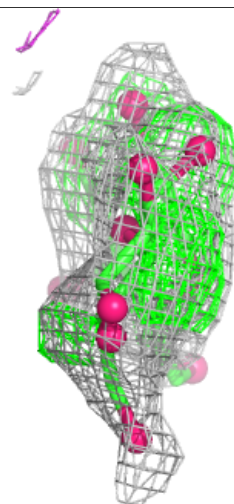
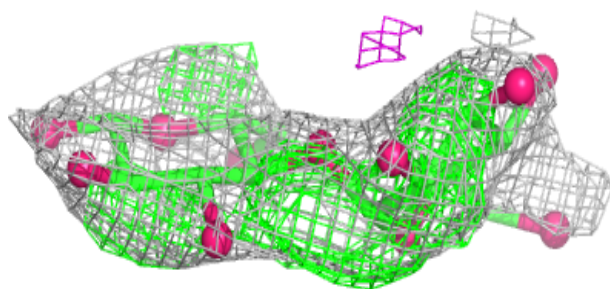
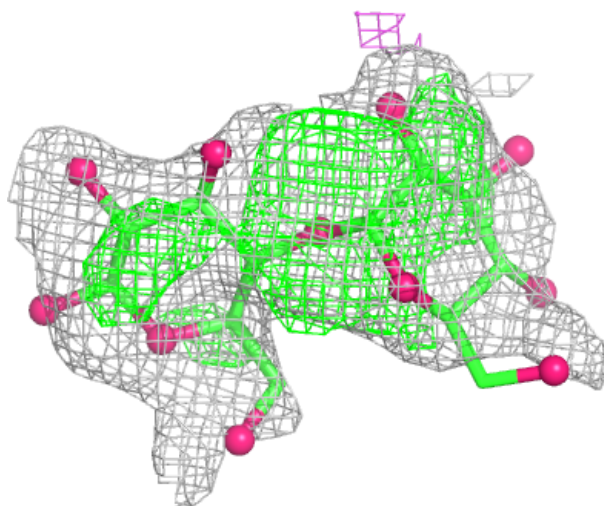
Electron density around DMU C 603:

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and green (positive)



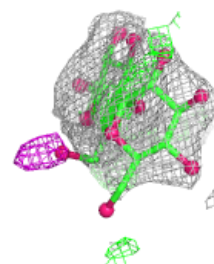
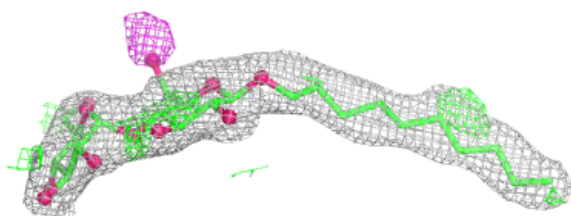
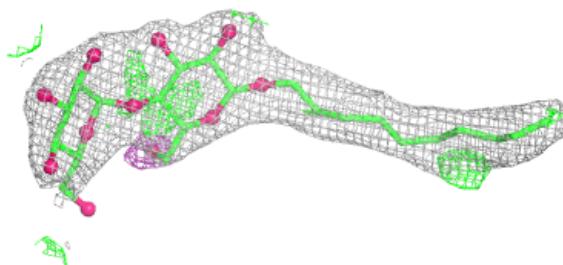
Electron density around DMU D 301:

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and green (positive)

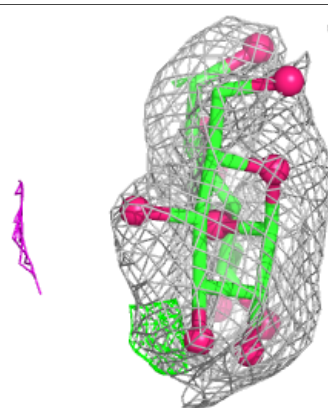
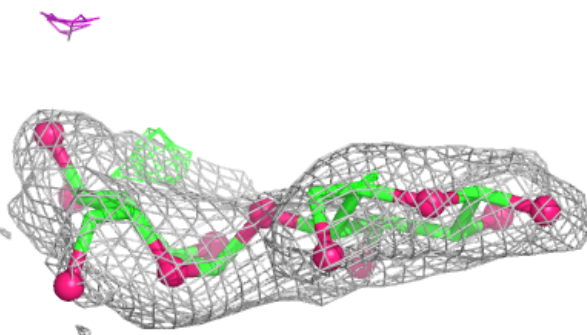
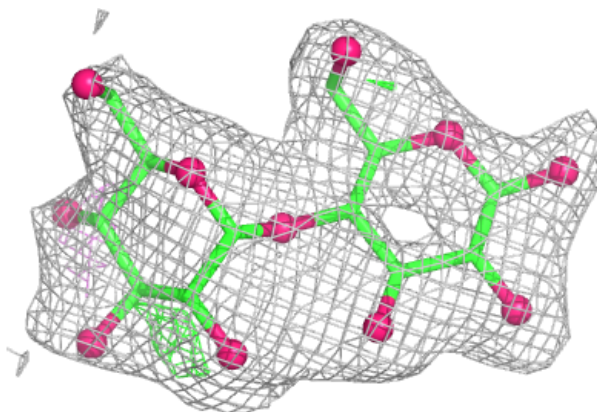


Electron density around DMU B 302:

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and green (positive)

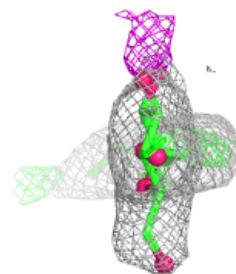
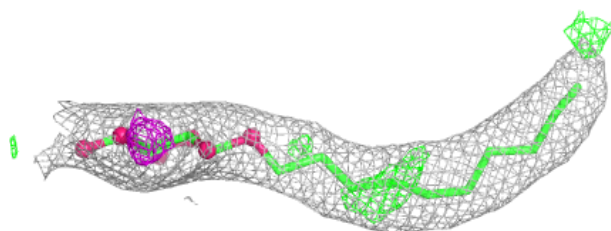
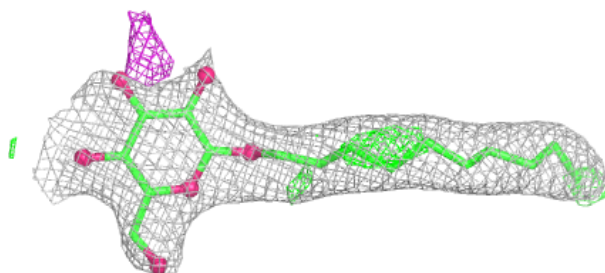
**Electron density around DMU B 304:**

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and green (positive)

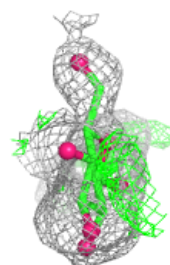
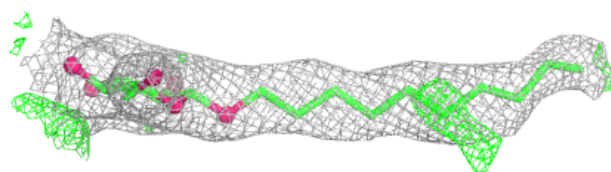
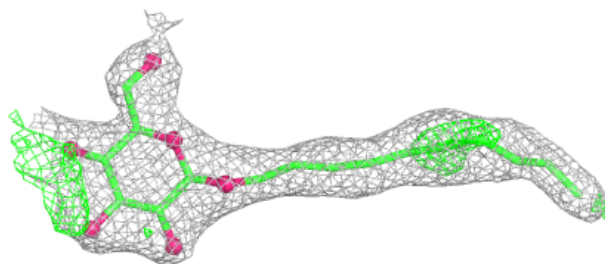


Electron density around DMU A 602:

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

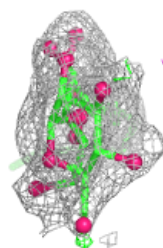
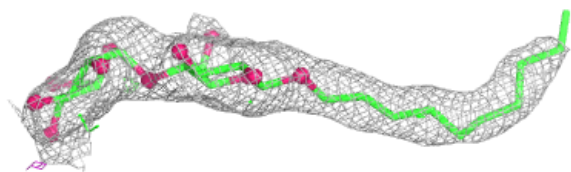
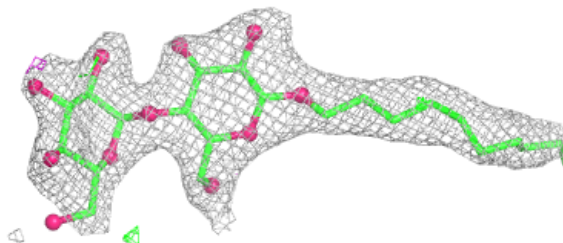
**Electron density around DMU A 603:**

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

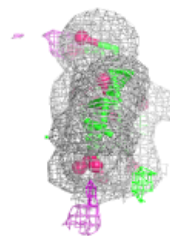
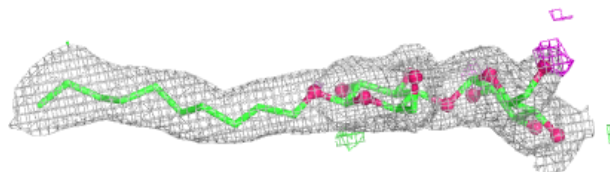
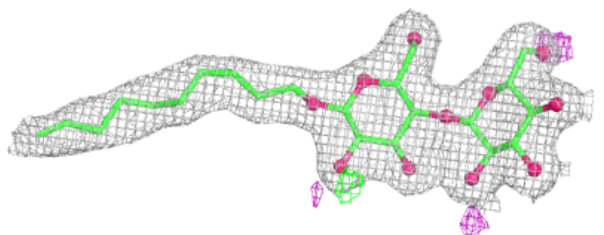


Electron density around DMU B 303:

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

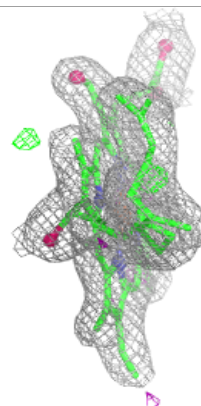
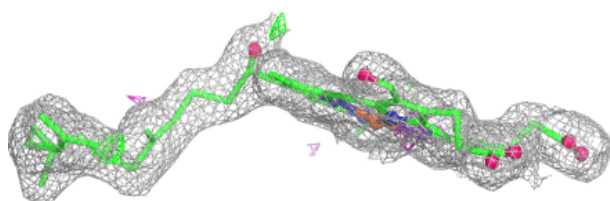
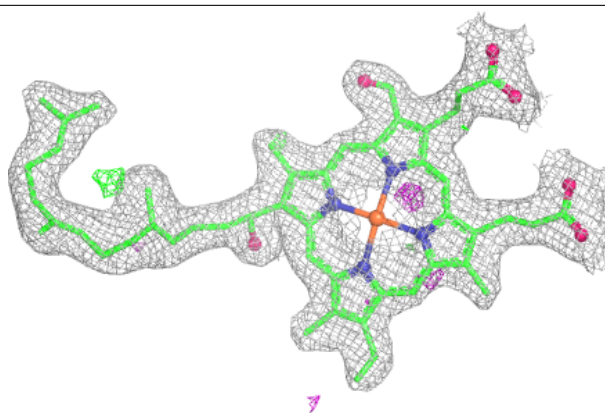
**Electron density around DMU B 301:**

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

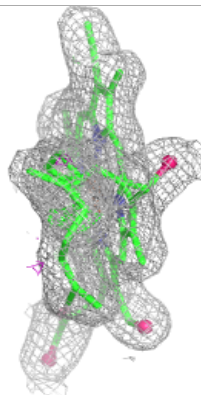
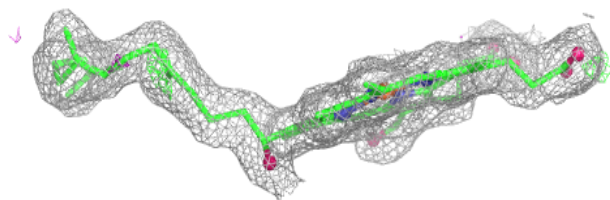
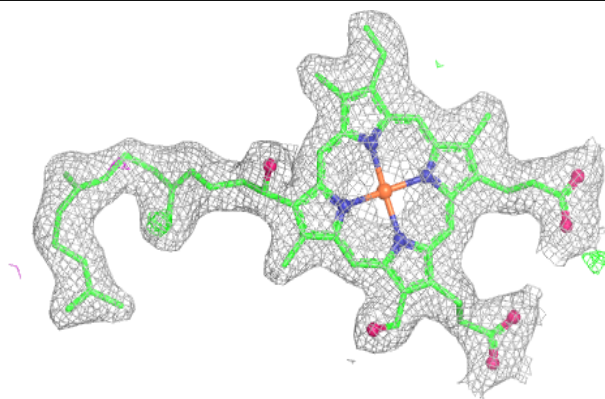


Electron density around HEA C 606:

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

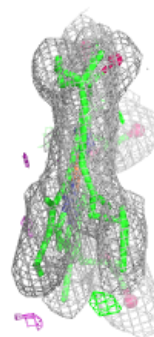
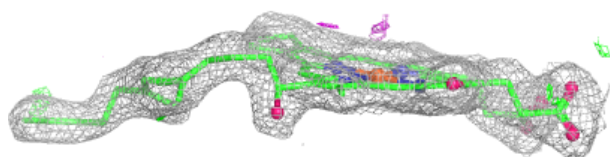
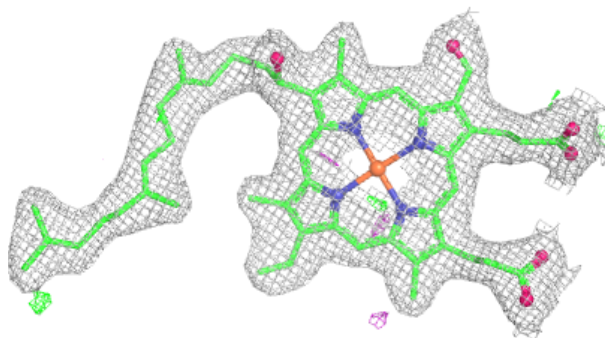
**Electron density around HEA A 608:**

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

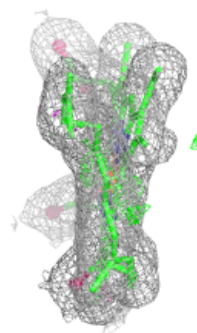
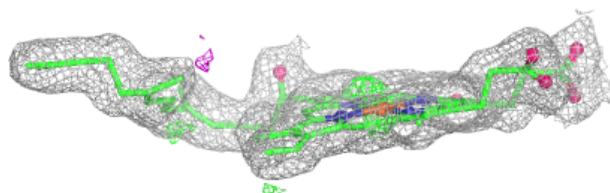
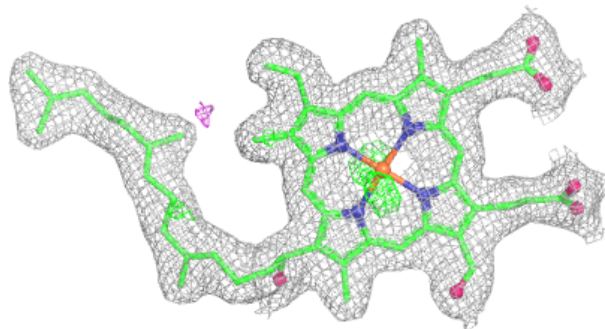


Electron density around HEA C 605:

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

**Electron density around HEA A 607:**

$2mF_o-DF_c$ (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.