



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 08:20 am BST

PDB ID : 3FYI
Title : Catalytic core subunits (I and II) of cytochrome C oxidase from Rhodobacter sphaeroides in the reduced state bound with cyanide
Authors : Qin, L.; Mills, D.A.; Proshlyakov, D.A.; Hiser, C.; Ferguson-Miller, S.
Deposited on : 2009-01-22
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

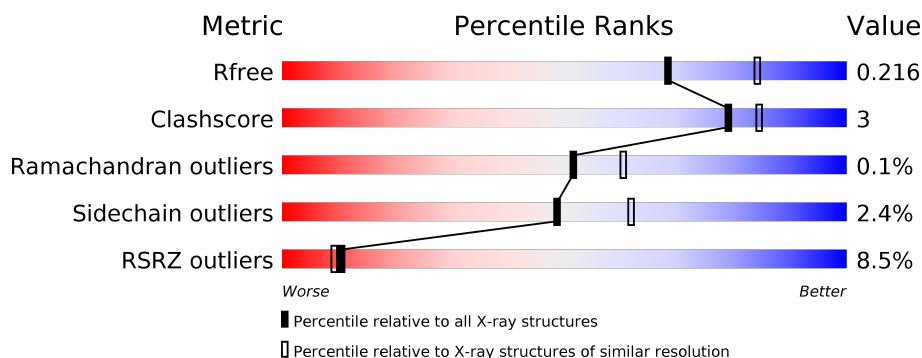
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	566	<div> <div>6%</div> <div>87%</div> <div>7%</div> <div>5%</div> </div>
1	C	566	<div> <div>14%</div> <div>85%</div> <div>9%</div> <div>6%</div> </div>
2	B	262	<div> <div>2%</div> <div>92%</div> <div>5%</div> <div>•</div> </div>
2	D	262	<div> <div>5%</div> <div>90%</div> <div>8%</div> <div>•</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	HTO	B	1	X	-	-	-
3	HEA	A	567	X	-	-	-
3	HEA	A	568	X	-	-	-
3	HEA	C	567	X	-	-	-
3	HEA	C	568	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 13601 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	22	0	0
			4212	2822	663	696	31			
1	C	531	Total	C	N	O	S	26	0	0
			4172	2794	656	691	31			

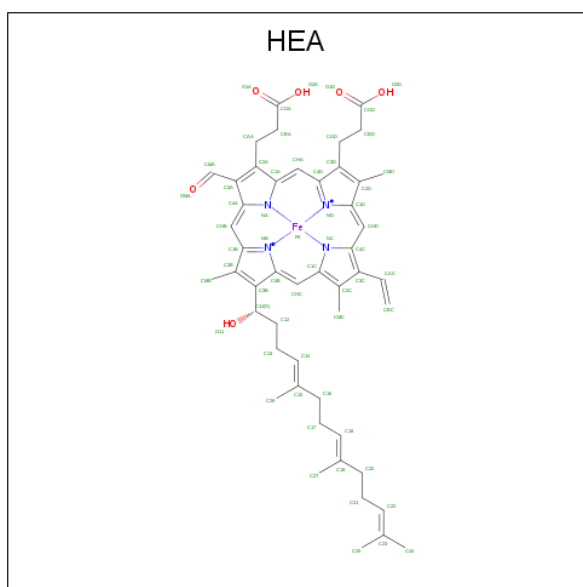
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	4	1	0
			2031	1325	333	367	6			
2	D	256	Total	C	N	O	S	9	1	0
			2031	1325	333	367	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 HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

- Molecule 4 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

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

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

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

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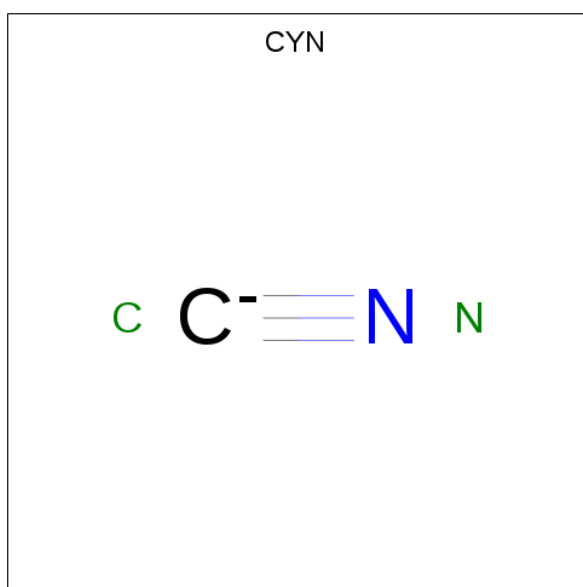
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mg	0	0
			1	1		

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

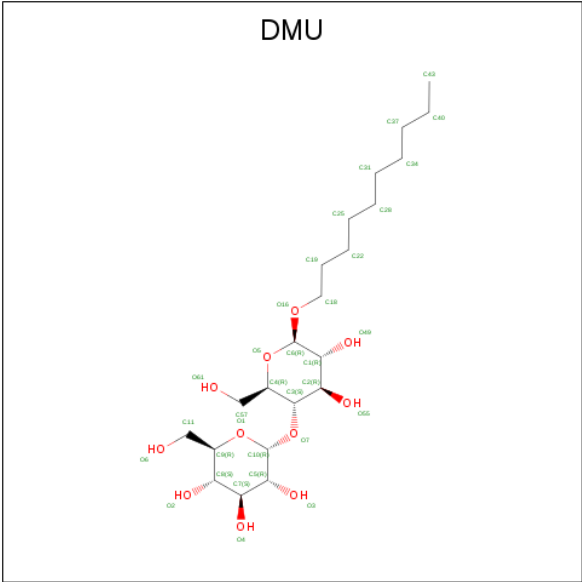
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		

- Molecule 7 is CYANIDE ION (three-letter code: CYN) (formula: CN).



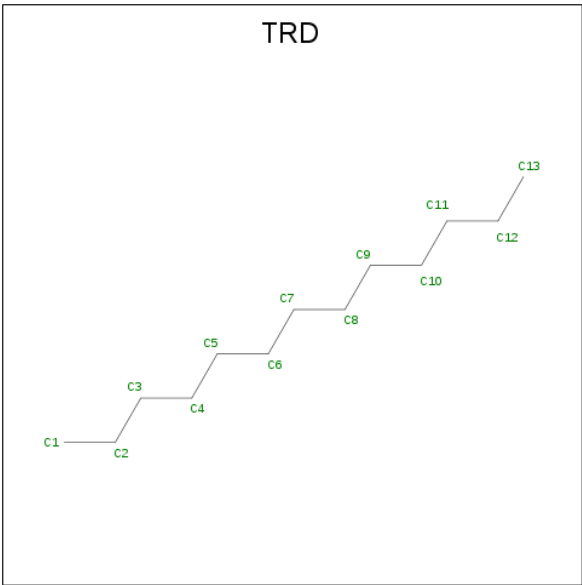
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	N	0	0
			2	1	1		
7	C	1	Total	C	N	0	0
			2	1	1		

- Molecule 8 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



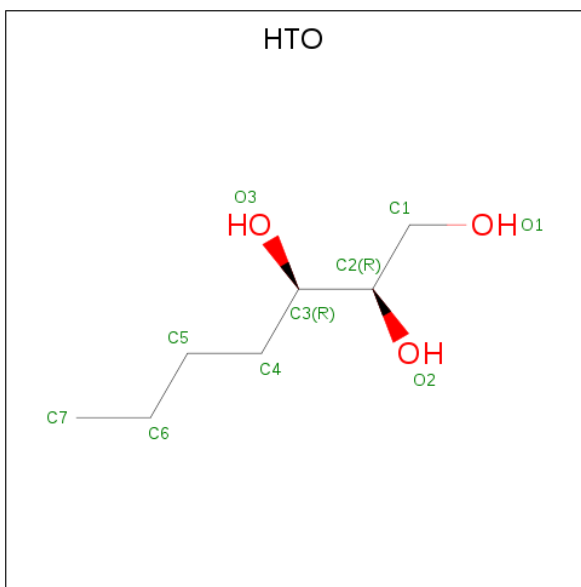
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			33	22	11		
8	A	1	Total	C	O	0	0
			33	22	11		
8	A	1	Total	C	O	0	0
			22	16	6		
8	A	1	Total	C	O	0	0
			33	22	11		
8	B	1	Total	C	O	0	0
			33	22	11		
8	B	1	Total	C	O	0	0
			23	12	11		
8	C	1	Total	C	O	0	0
			23	12	11		
8	C	1	Total	C	O	0	0
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

- Molecule 9 is TRIDECANE (three-letter code: TRD) (formula: C₁₃H₂₈).



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

- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C₇H₁₆O₃).



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

- Molecule 11 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

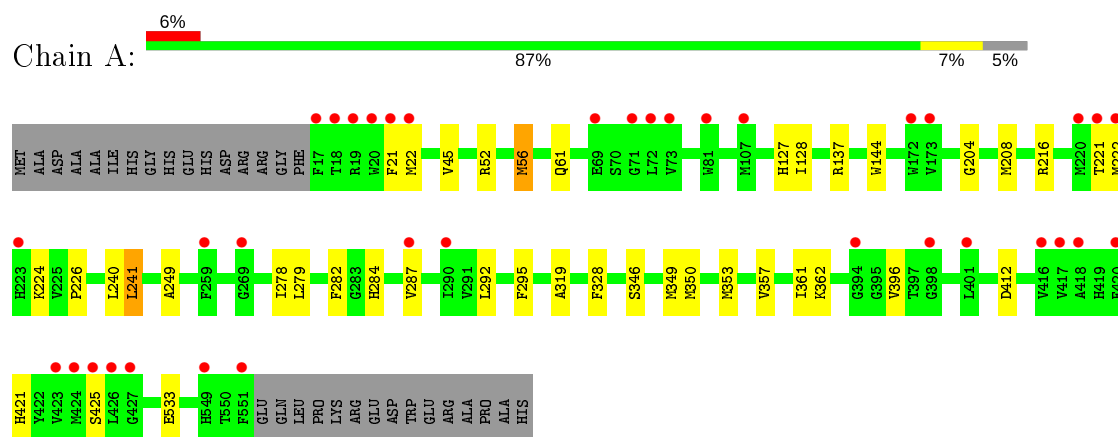
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	126	Total	O	0	0
			126	126		
12	B	133	Total	O	0	0
			133	133		
12	C	102	Total	O	0	0
			102	102		
12	D	109	Total	O	0	0
			109	109		

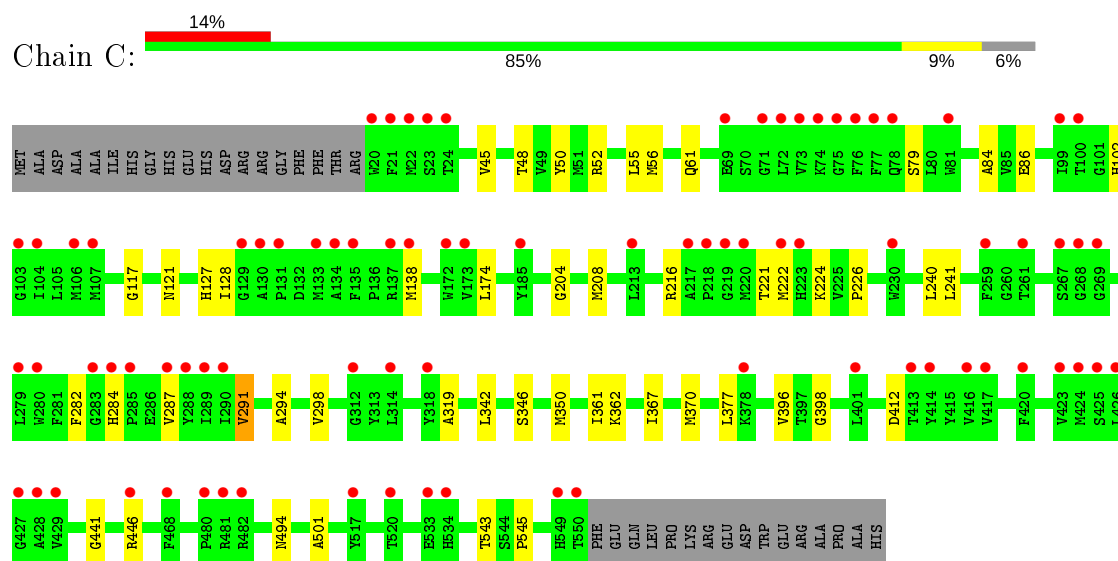
3 Residue-property plots [i](#)

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

• Molecule 1: Cytochrome c oxidase subunit 1

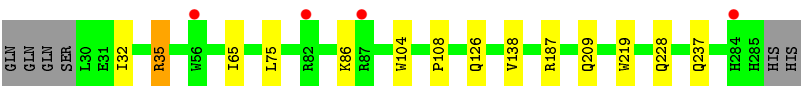


• Molecule 1: Cytochrome c oxidase subunit 1

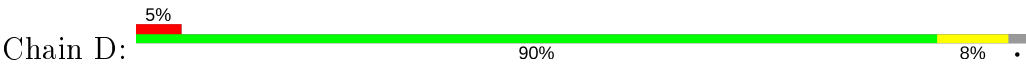


• Molecule 2: Cytochrome c oxidase subunit 2





● Molecule 2: Cytochrome c oxidase subunit 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	124.34Å 131.88Å 176.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 41.77 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-2.20) 96.2 (41.77-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.219 0.193 , 0.216	Depositor DCC
R_{free} test set	3933 reflections (2.78%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13601	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: MG, CU1, HTO, CA, TRD, CD, DMU, CYN, HEA

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	0.54	0/4368	0.54	0/5961
1	C	0.46	0/4326	0.51	0/5905
2	B	0.51	0/2096	0.55	0/2869
2	D	0.46	0/2096	0.53	0/2869
All	All	0.50	0/12886	0.53	0/17604

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	4212	0	4134	26	0
1	C	4172	0	4097	29	0
2	B	2031	0	1988	8	0
2	D	2031	0	1988	8	0
3	A	120	0	108	5	0
3	C	120	0	108	8	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0	0	0	0
7	C	2	0	0	0	0
8	A	121	0	157	1	0
8	B	56	0	63	1	0
8	C	56	0	63	2	0
8	D	56	0	63	1	0
9	A	66	0	138	0	0
9	C	42	0	86	2	0
9	D	20	0	41	0	0
10	B	10	0	16	0	0
11	B	2	0	0	0	0
11	D	2	0	0	0	0
12	A	126	0	0	0	0
12	B	133	0	0	2	0
12	C	102	0	0	0	0
12	D	109	0	0	0	0
All	All	13601	0	13050	74	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 74 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:B:228:GLN:NE2	12:B:389:HOH:O	1.96	0.95
2:B:32:ILE:HG22	2:B:35:ARG:HD3	1.58	0.86
3:C:568:HEA:HBD2	3:C:568:HEA:HMD1	1.61	0.81
1:A:21:PHE:HB3	1:A:144:TRP:HZ2	1.45	0.81
3:C:567:HEA:HMC1	3:C:567:HEA:HBC1	1.62	0.79

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	533/566 (94%)	523 (98%)	10 (2%)	0	100	100
1	C	529/566 (94%)	524 (99%)	5 (1%)	0	100	100
2	B	255/262 (97%)	249 (98%)	6 (2%)	0	100	100
2	D	255/262 (97%)	249 (98%)	5 (2%)	1 (0%)	34	37
All	All	1572/1656 (95%)	1545 (98%)	26 (2%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	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	435/459 (95%)	425 (98%)	10 (2%)	50	63
1	C	431/459 (94%)	422 (98%)	9 (2%)	53	67
2	B	216/221 (98%)	211 (98%)	5 (2%)	50	63
2	D	216/221 (98%)	209 (97%)	7 (3%)	39	50
All	All	1298/1360 (95%)	1267 (98%)	31 (2%)	49	62

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	187	ARG
1	C	174	LEU
2	D	131	GLU
1	C	61	GLN
1	C	222	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	534	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 14 are monoatomic - leaving 29 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	$\# Z > 2$
9	TRD	C	1010	-	8,8,12	0.27	0	7,7,11	0.40	0
9	TRD	D	1007	-	12,12,12	0.24	0	11,11,11	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	DMU	C	1005	-	34,34,34	0.60	1 (2%)	45,45,45	0.83	0
9	TRD	A	579	-	6,6,12	0.26	0	5,5,11	0.36	0
9	TRD	A	578	-	12,12,12	0.28	0	11,11,11	0.52	0
9	TRD	C	1001	-	12,12,12	0.25	0	11,11,11	0.52	0
9	TRD	C	1006	-	12,12,12	0.27	0	11,11,11	0.49	0
8	DMU	A	573	-	34,34,34	0.51	0	45,45,45	0.94	3 (6%)
8	DMU	D	1003	-	34,34,34	0.53	0	45,45,45	0.62	0
9	TRD	A	577	-	12,12,12	0.26	0	11,11,11	0.48	0
9	TRD	A	582	-	12,12,12	0.29	0	11,11,11	0.51	0
3	HEA	A	567	1	44,67,67	1.67	7 (15%)	37,103,103	1.36	7 (18%)
8	DMU	C	1002	-	24,24,34	0.52	0	35,35,45	0.65	0
9	TRD	D	1008	-	6,6,12	0.26	0	5,5,11	0.41	0
3	HEA	C	567	1	44,67,67	1.65	8 (18%)	37,103,103	1.35	6 (16%)
10	HTO	B	1	-	9,9,9	0.36	0	10,10,10	0.93	1 (10%)
8	DMU	B	11	-	24,24,34	0.50	0	35,35,45	0.70	0
9	TRD	A	580	-	6,6,12	0.25	0	5,5,11	0.39	0
9	TRD	A	581	-	12,12,12	0.27	0	11,11,11	0.53	0
7	CYN	C	572	4	0,1,1	0.00	-	-	-	-
9	TRD	C	1009	-	6,6,12	0.27	0	5,5,11	0.34	0
8	DMU	D	1011	-	24,24,34	0.51	0	35,35,45	0.84	0
8	DMU	A	574	-	34,34,34	0.57	1 (2%)	45,45,45	0.83	2 (4%)
3	HEA	C	568	1	44,67,67	1.51	5 (11%)	37,103,103	1.88	12 (32%)
8	DMU	B	288	-	34,34,34	0.54	0	45,45,45	0.71	0
7	CYN	A	572	4	0,1,1	0.00	-	-	-	-
8	DMU	A	576	-	34,34,34	0.59	0	45,45,45	0.73	0
8	DMU	A	575	-	22,22,34	0.60	1 (4%)	27,27,45	0.86	1 (3%)
3	HEA	A	568	1	44,67,67	1.47	8 (18%)	37,103,103	1.85	12 (32%)

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
9	TRD	C	1010	-	-	3/6/6/10	-
9	TRD	D	1007	-	-	6/10/10/10	-
8	DMU	C	1005	-	-	11/19/59/59	0/2/2/2
9	TRD	A	579	-	-	2/4/4/10	-
9	TRD	A	578	-	-	5/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	TRD	C	1001	-	-	2/10/10/10	-
9	TRD	C	1006	-	-	0/10/10/10	-
8	DMU	A	573	-	-	2/19/59/59	0/2/2/2
8	DMU	D	1003	-	-	6/19/59/59	0/2/2/2
9	TRD	A	577	-	-	5/10/10/10	-
9	TRD	A	582	-	-	4/10/10/10	-
8	DMU	A	574	-	-	9/19/59/59	0/2/2/2
8	DMU	C	1002	-	-	3/8/48/59	0/2/2/2
9	TRD	D	1008	-	-	1/4/4/10	-
3	HEA	C	567	1	3/3/7/16	0/24/76/76	-
10	HTO	B	1	-	1/1/2/2	6/10/10/10	-
8	DMU	B	11	-	-	1/8/48/59	0/2/2/2
9	TRD	A	580	-	-	2/4/4/10	-
9	TRD	A	581	-	-	6/10/10/10	-
9	TRD	C	1009	-	-	3/4/4/10	-
8	DMU	D	1011	-	-	4/8/48/59	0/2/2/2
3	HEA	A	567	1	2/2/7/16	0/24/76/76	-
3	HEA	C	568	1	2/2/7/16	5/24/76/76	-
8	DMU	B	288	-	-	5/19/59/59	0/2/2/2
8	DMU	A	576	-	-	11/19/59/59	0/2/2/2
8	DMU	A	575	-	-	4/13/33/59	0/1/1/2
3	HEA	A	568	1	2/2/7/16	3/24/76/76	-

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	568	HEA	C3B-C11	5.76	1.57	1.52
3	A	567	HEA	C3A-C2A	-5.60	1.32	1.40
3	C	567	HEA	C3A-C2A	-4.95	1.33	1.40
3	A	568	HEA	C3B-C11	4.89	1.56	1.52
3	C	567	HEA	C3C-C2C	-4.43	1.34	1.40

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	568	HEA	CBA-CAA-C2A	-3.93	105.24	112.48
3	C	568	HEA	C1B-C2B-C3B	3.77	109.62	107.00
3	C	568	HEA	C3C-C4C-NC	-3.60	104.56	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	568	HEA	C3C-C4C-NC	-3.60	104.56	109.21
3	C	568	HEA	CBA-CAA-C2A	-3.57	105.91	112.48

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	567	HEA	ND
3	A	567	HEA	NB
3	C	567	HEA	ND
3	C	567	HEA	NA
3	C	567	HEA	NB

5 of 109 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1005	DMU	C19-C18-O16-C6
10	B	1	HTO	O1-C1-C2-O2
10	B	1	HTO	O1-C1-C2-C3
10	B	1	HTO	C2-C3-C4-C5
10	B	1	HTO	O3-C3-C4-C5

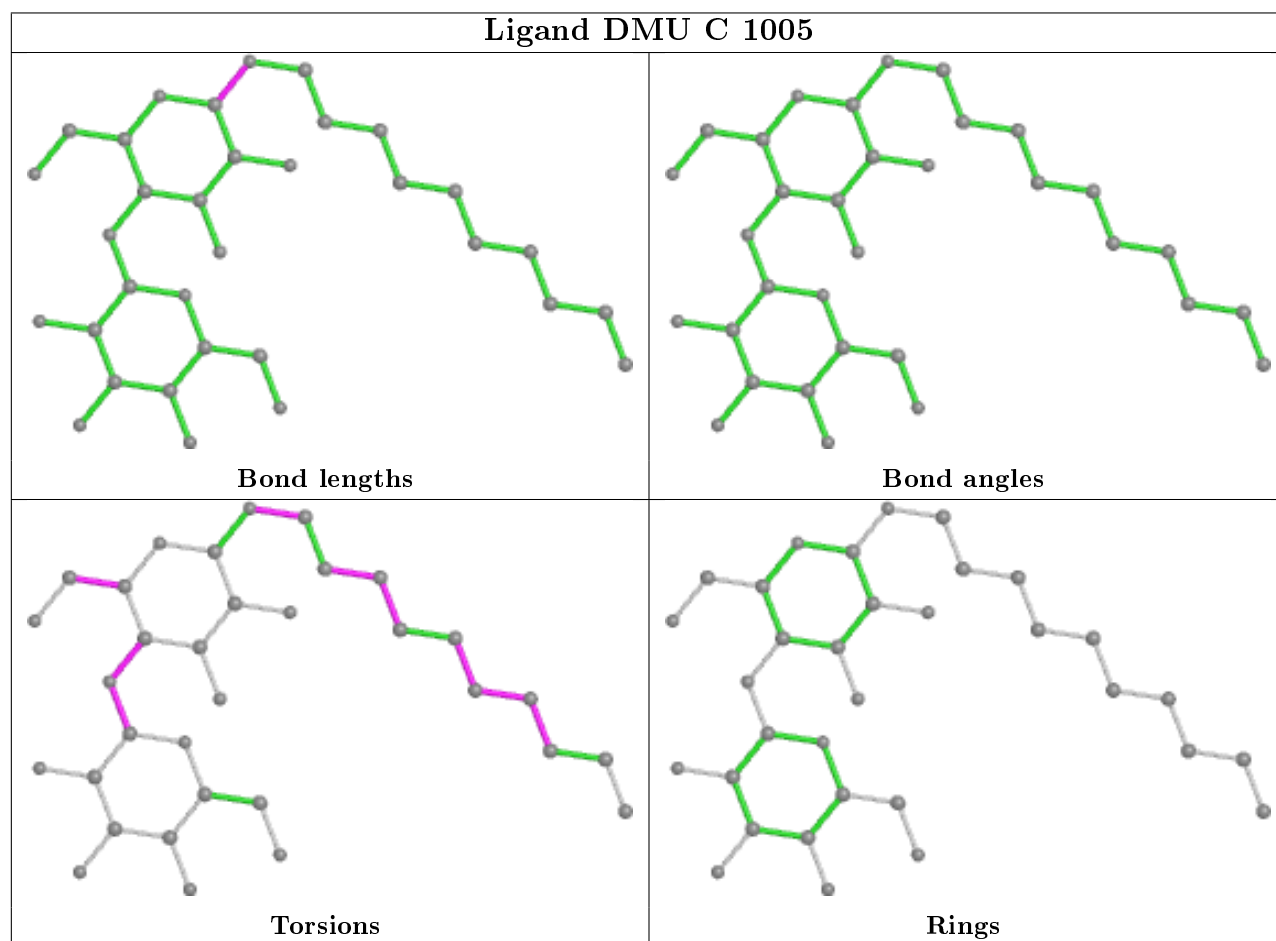
There are no ring outliers.

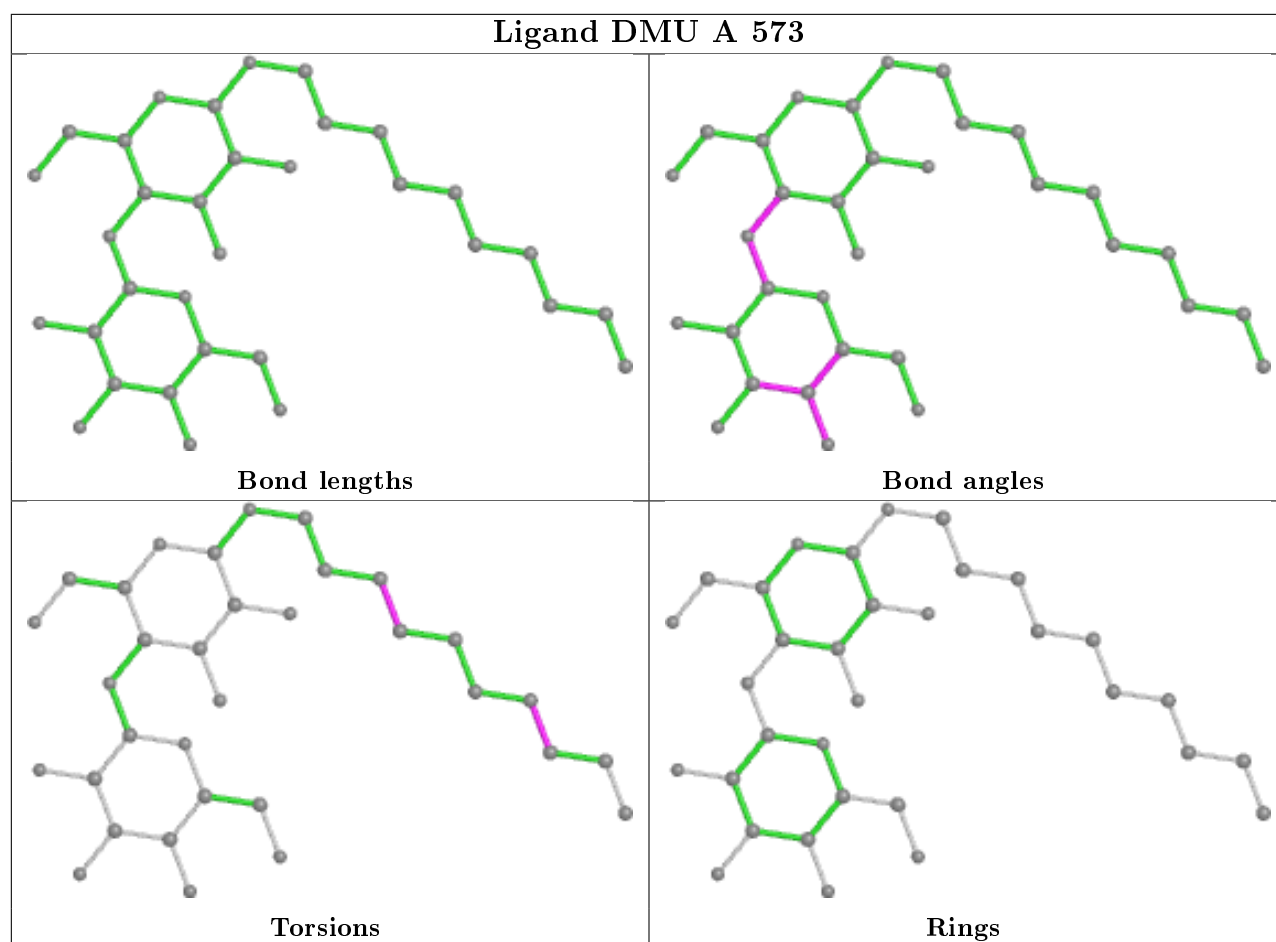
10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1010	TRD	1	0
8	C	1005	DMU	2	0
9	C	1006	TRD	1	0
8	D	1003	DMU	1	0
3	A	567	HEA	2	0
3	C	567	HEA	2	0
3	C	568	HEA	6	0
8	B	288	DMU	1	0
8	A	576	DMU	1	0
3	A	568	HEA	3	0

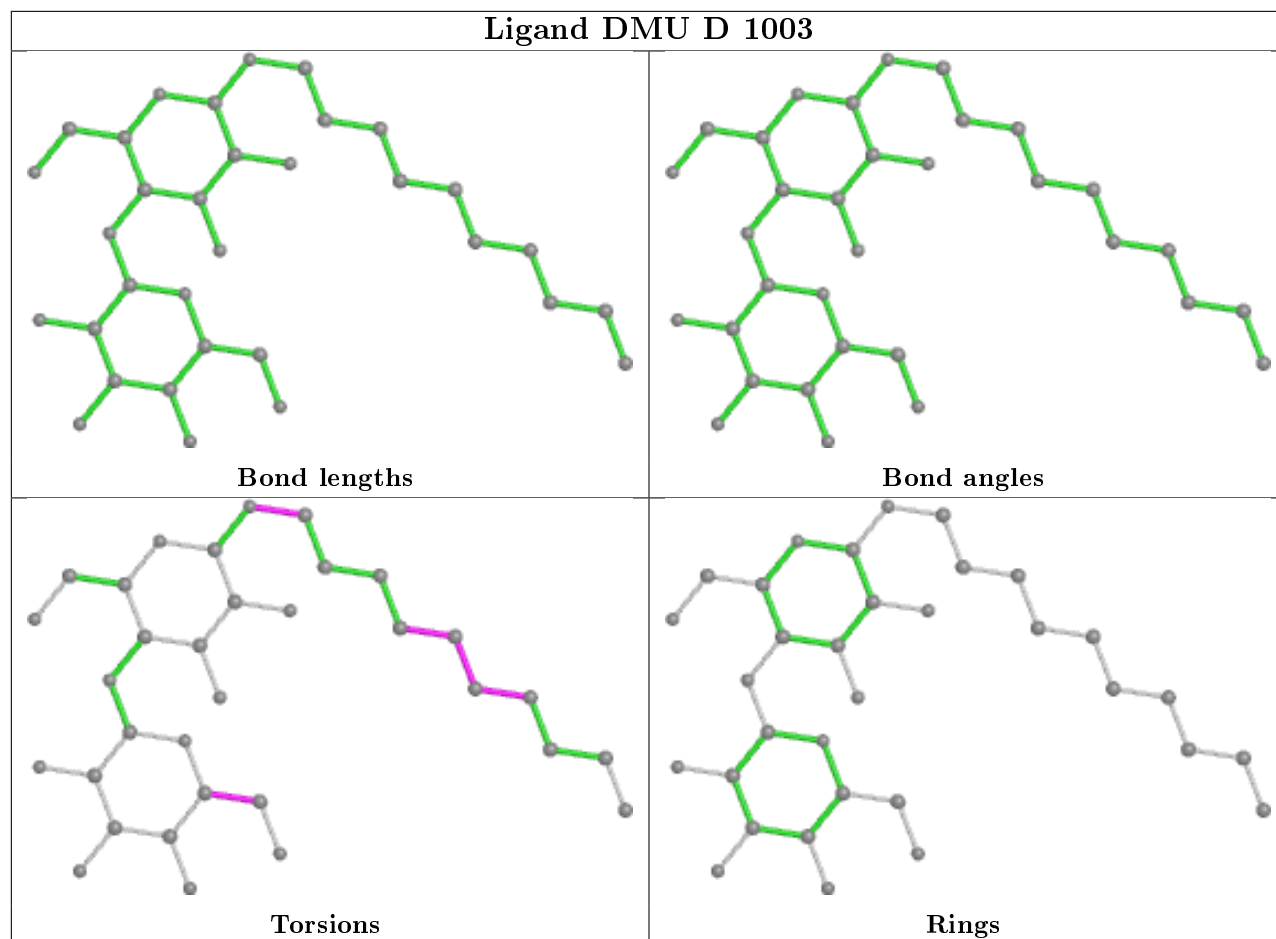
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

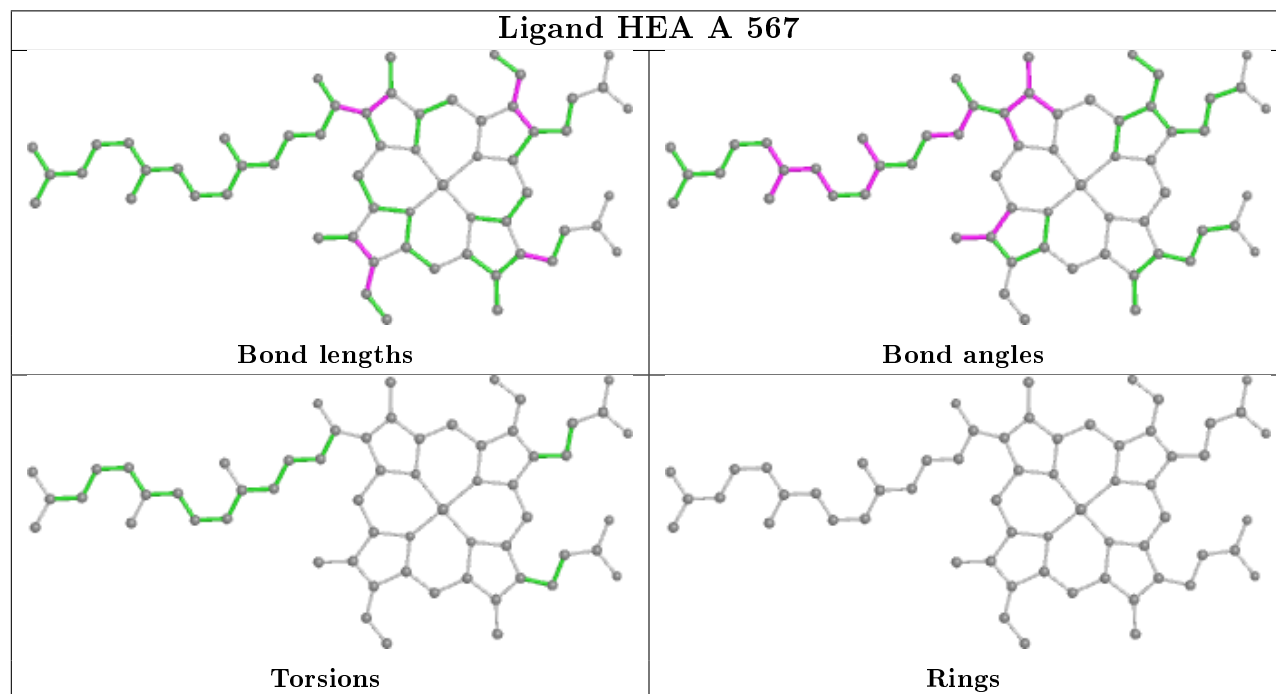




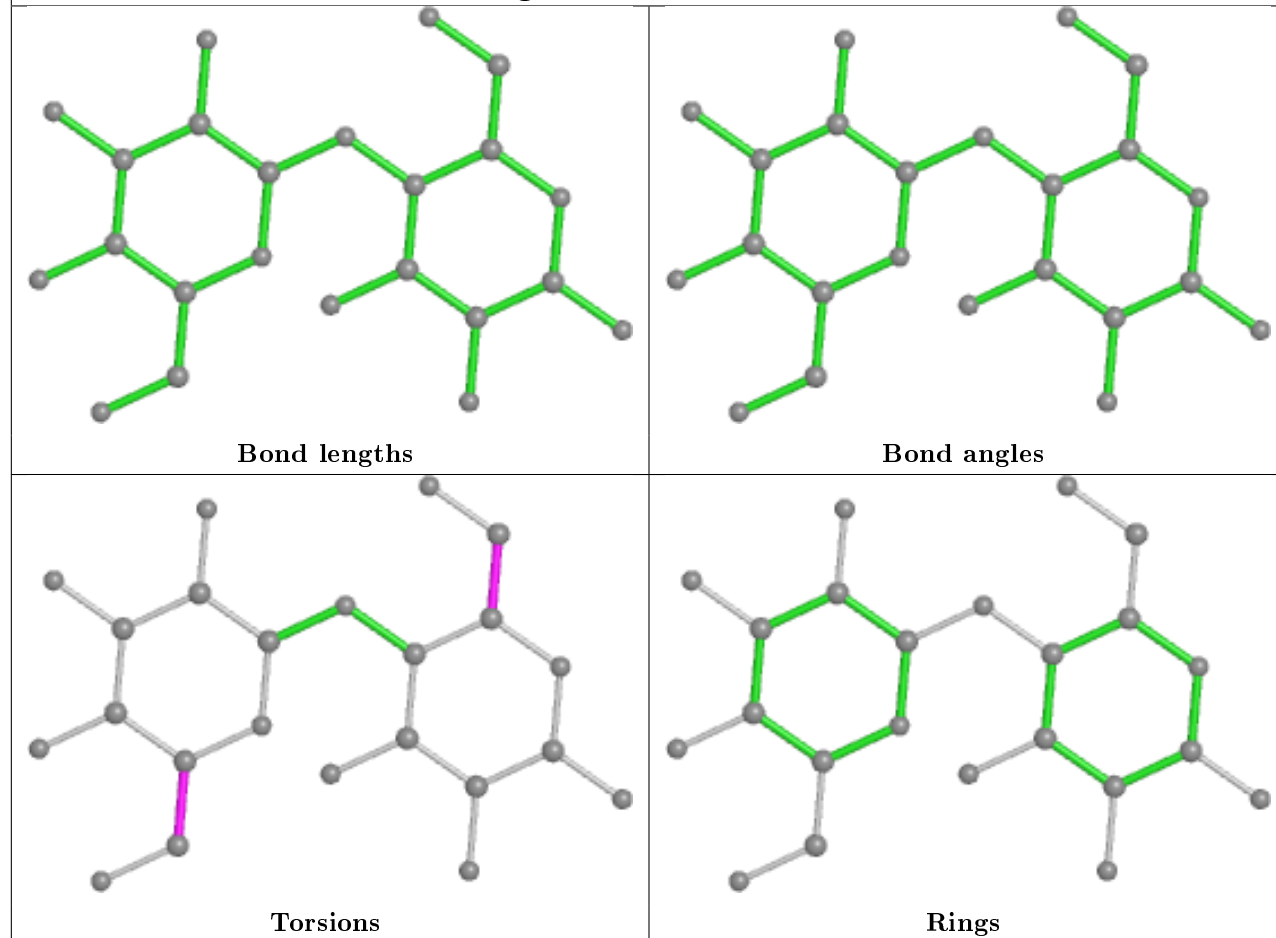
Ligand DMU D 1003



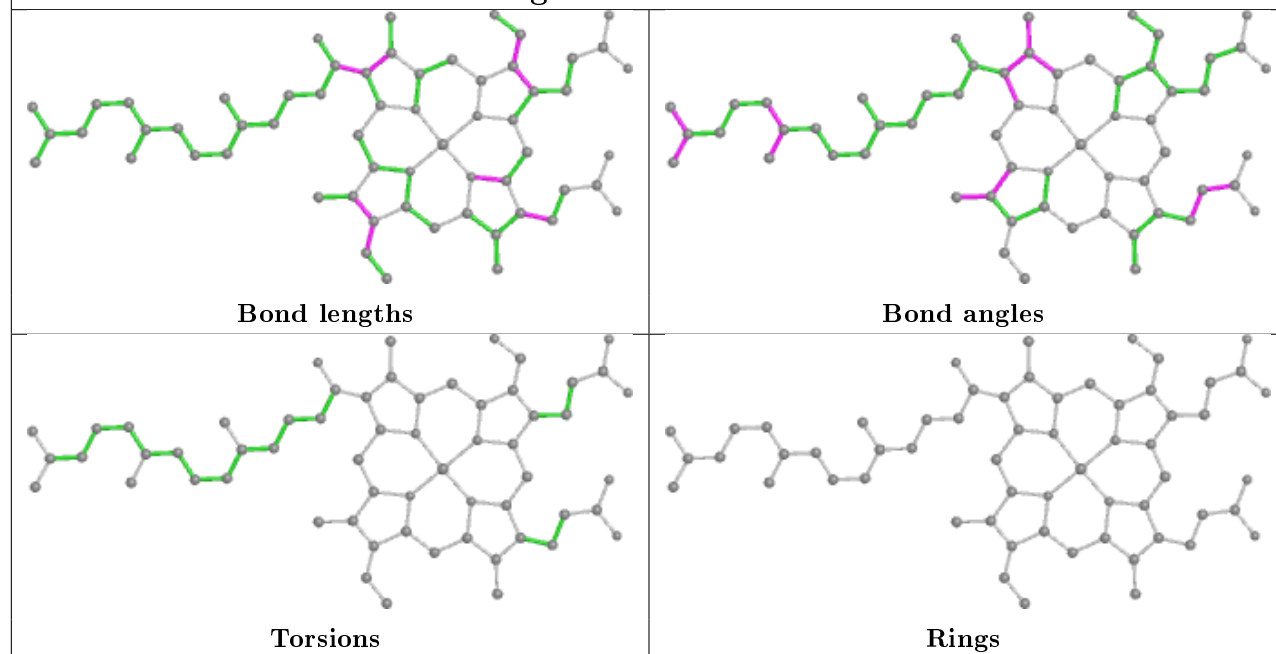
Ligand HEA A 567



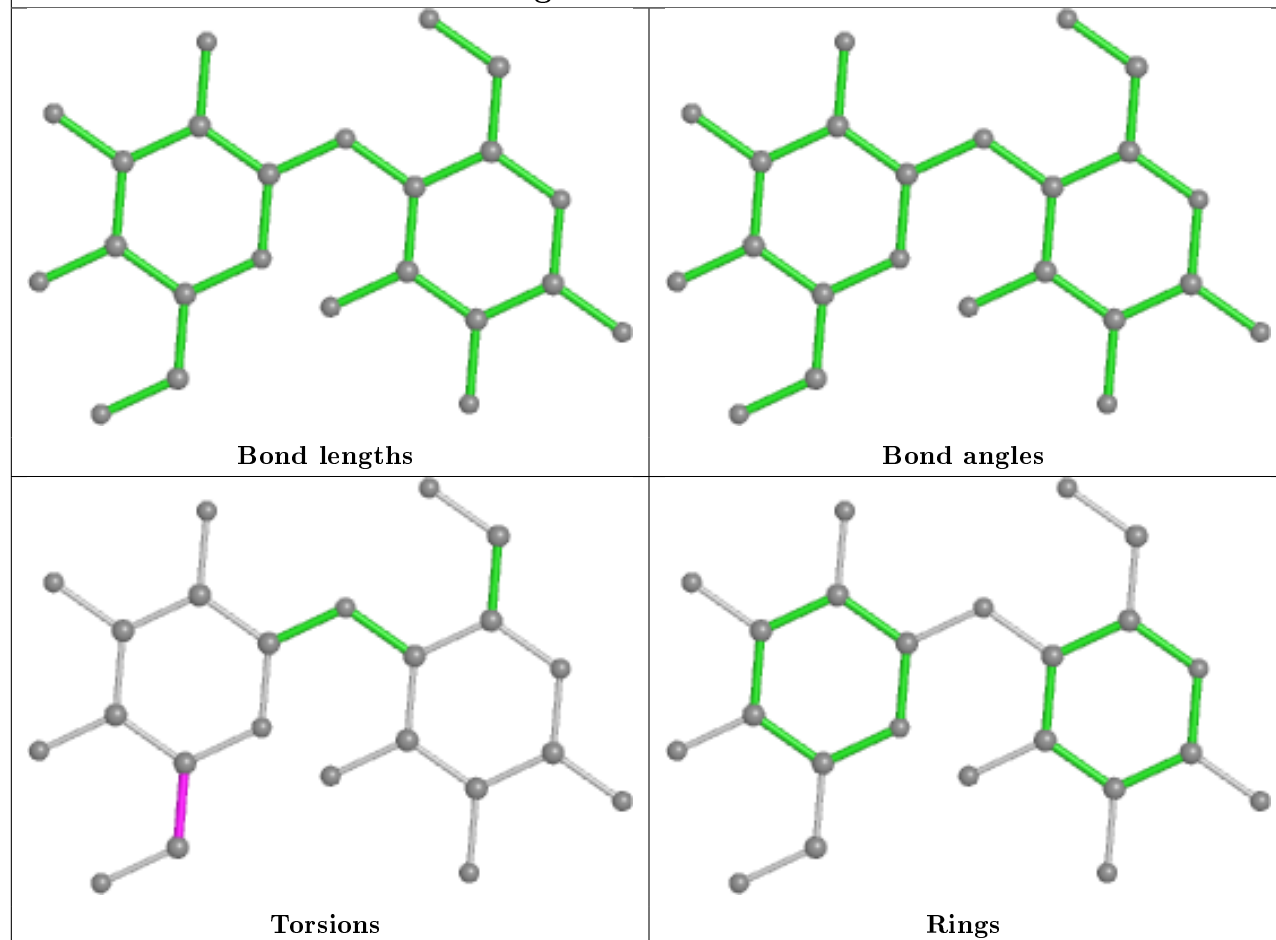
Ligand DMU C 1002



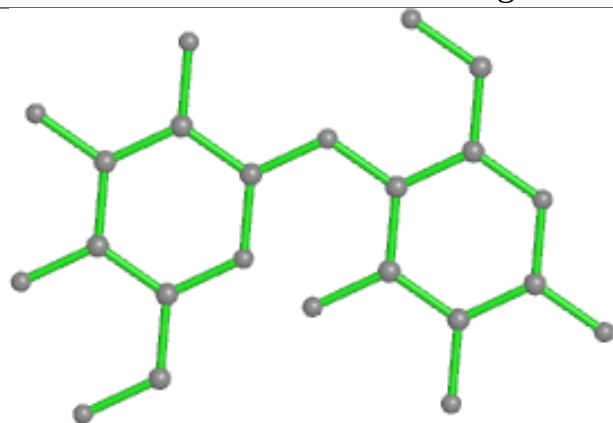
Ligand HEA C 567



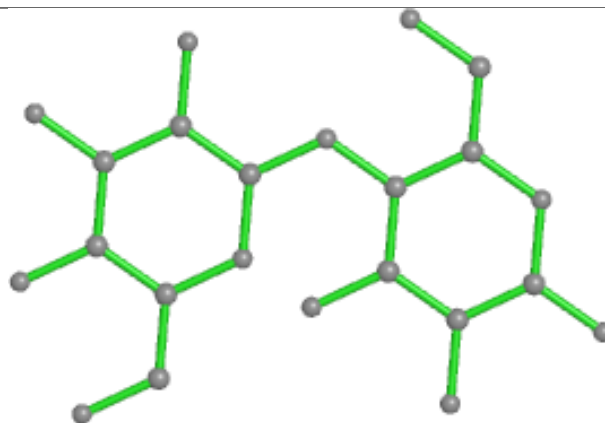
Ligand DMU B 11



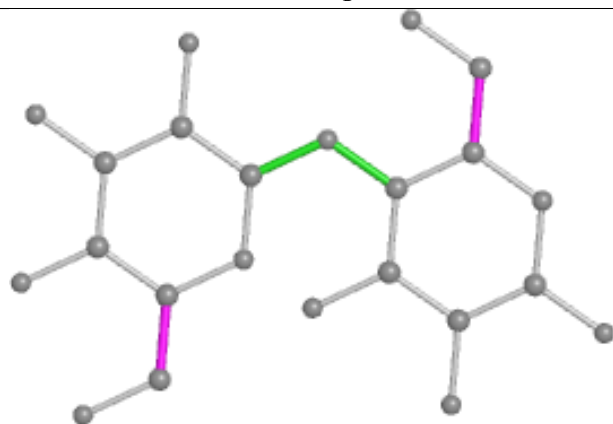
Ligand DMU D 1011



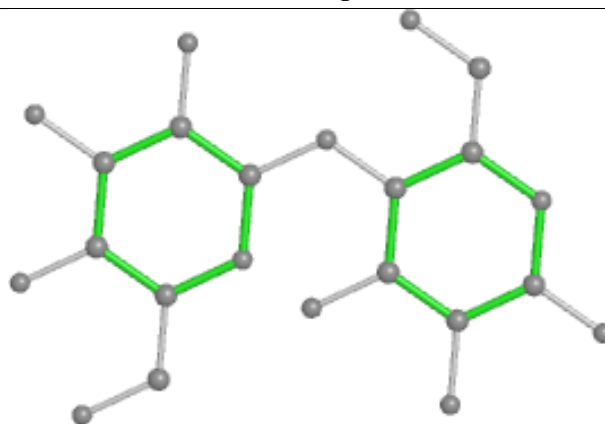
Bond lengths



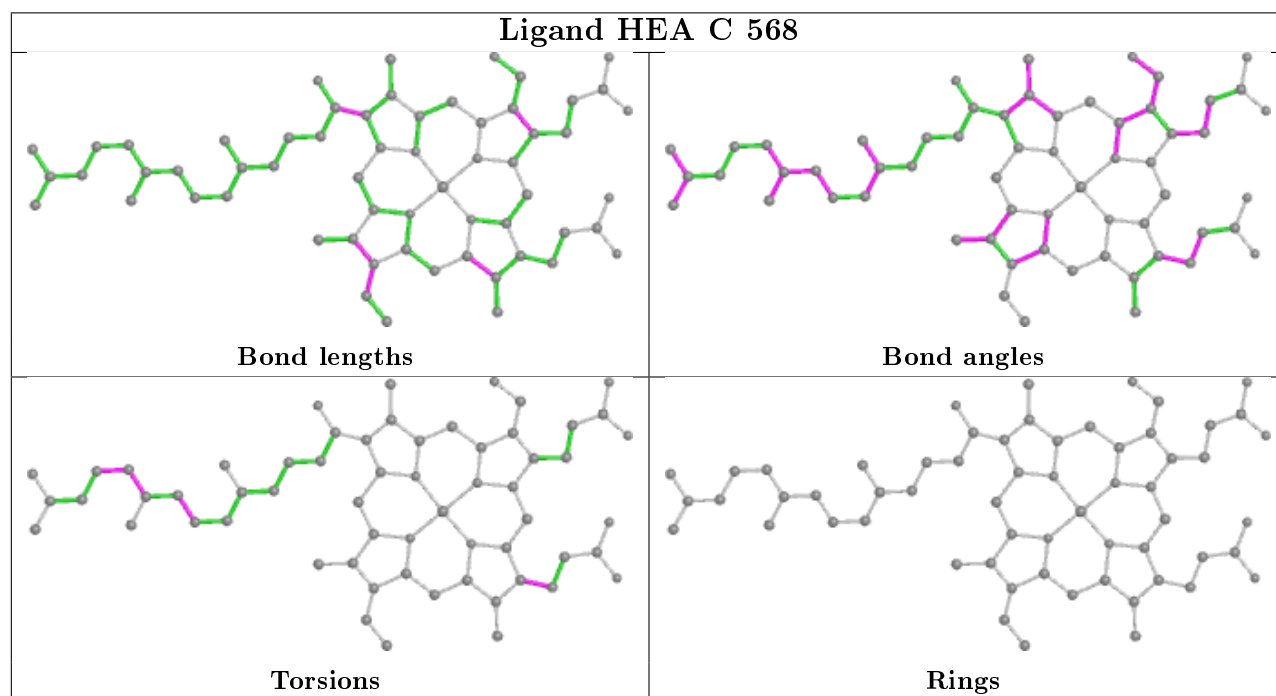
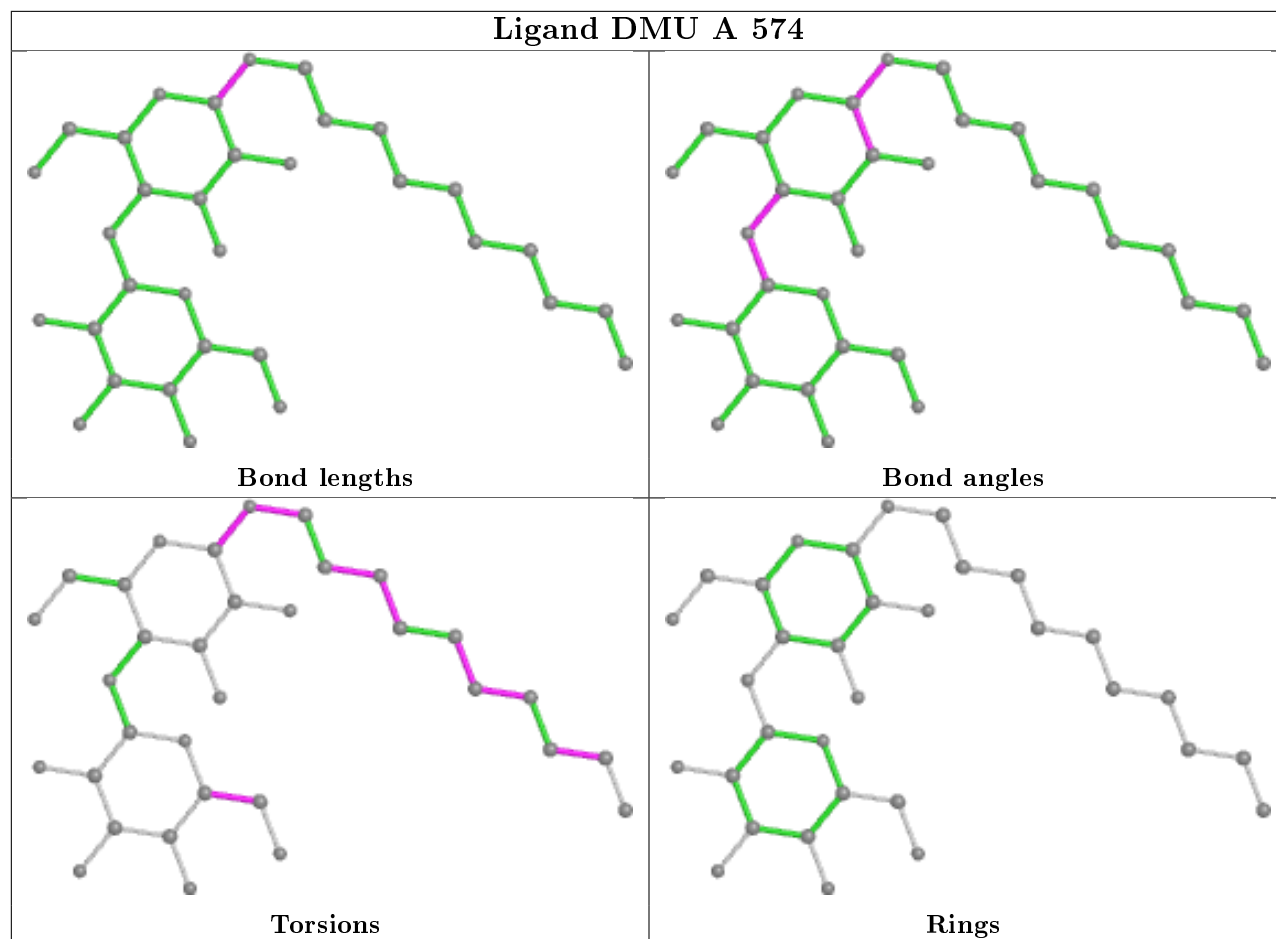
Bond angles

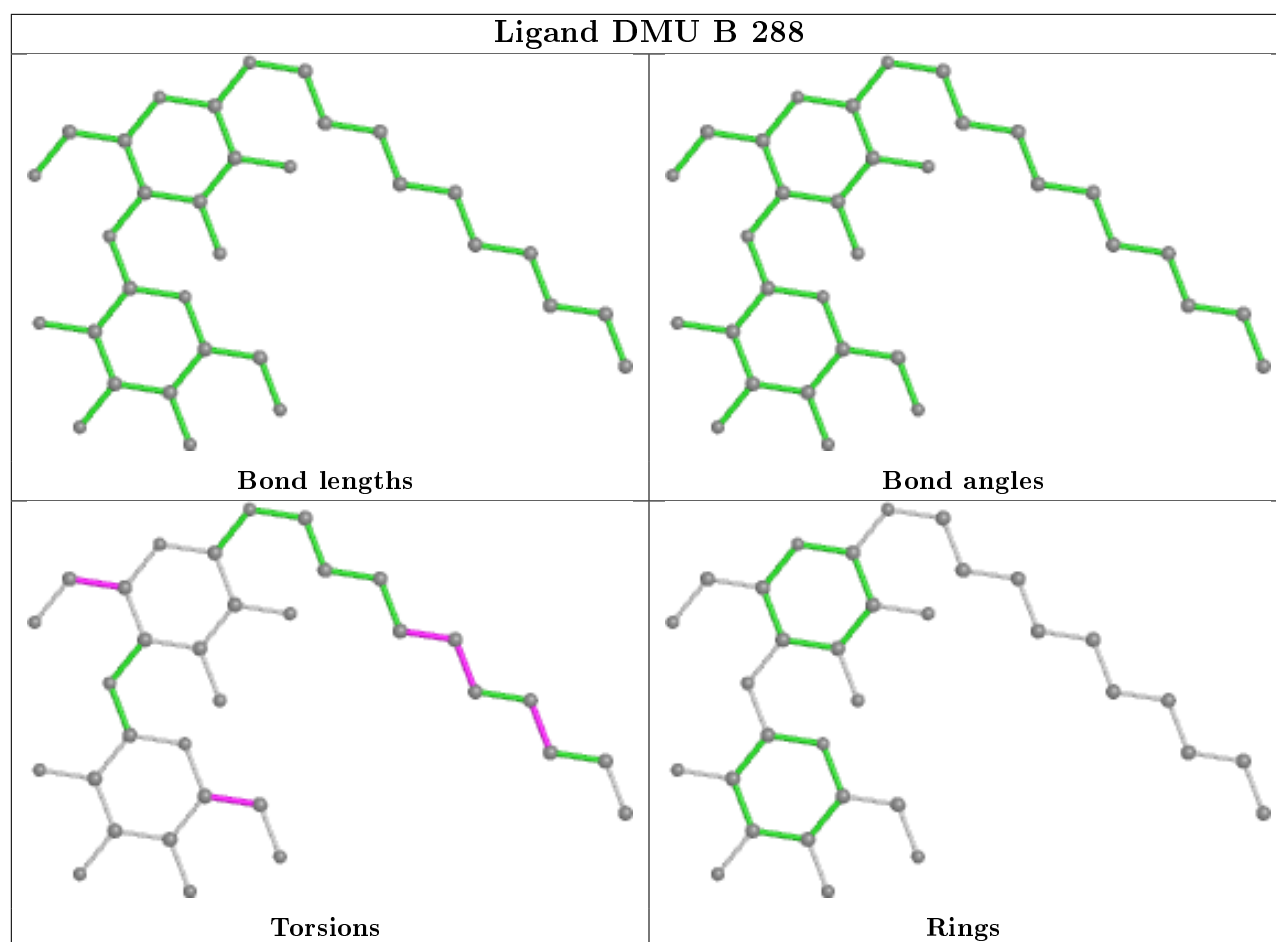


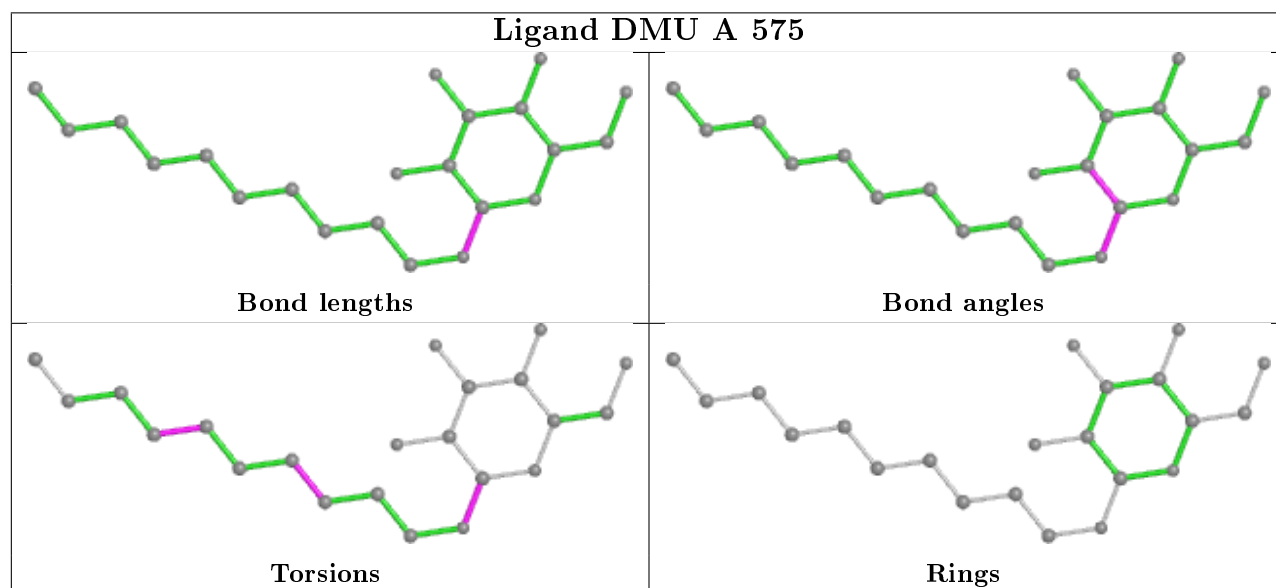
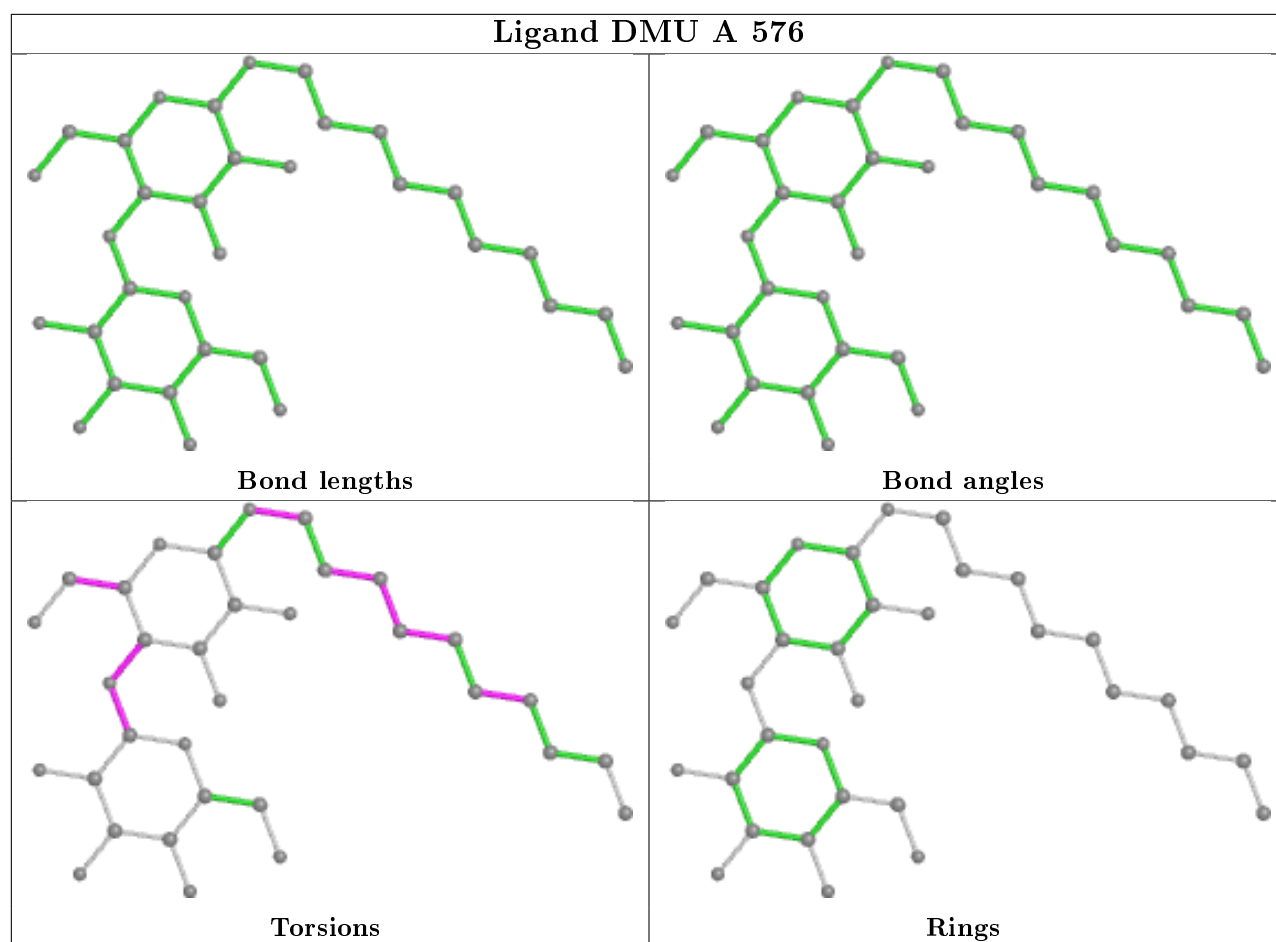
Torsions

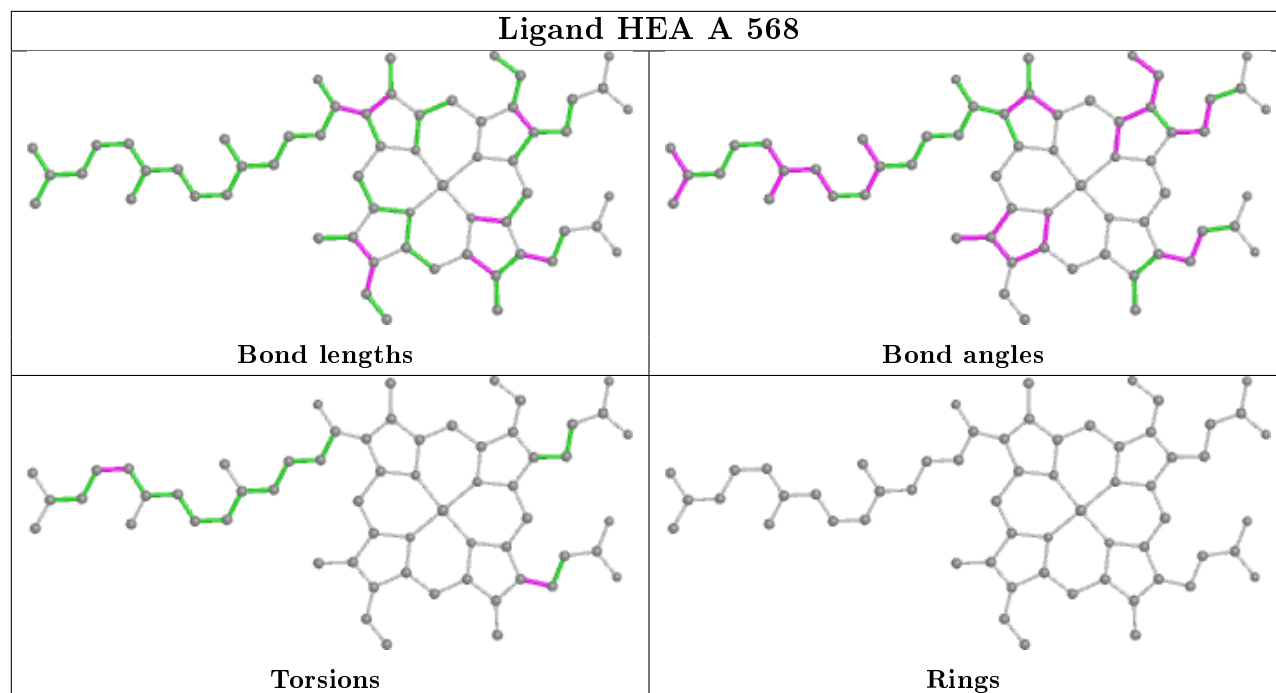


Rings









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%)	-0.00	36 (6%) 17 16	23, 34, 57, 72	5 (0%)
1	C	531/566 (93%)	0.64	82 (15%) 2 1	29, 51, 76, 95	5 (0%)
2	B	256/262 (97%)	-0.37	4 (1%) 72 70	22, 37, 55, 60	1 (0%)
2	D	256/262 (97%)	-0.17	12 (4%) 31 30	29, 42, 62, 71	2 (0%)
All	All	1578/1656 (95%)	0.13	134 (8%) 10 9	22, 41, 68, 95	13 (0%)

The worst 5 of 134 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	TRP	9.1
1	A	20	TRP	6.6
1	C	222	MET	6.0
2	B	56	TRP	5.2
1	C	22	MET	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](#)

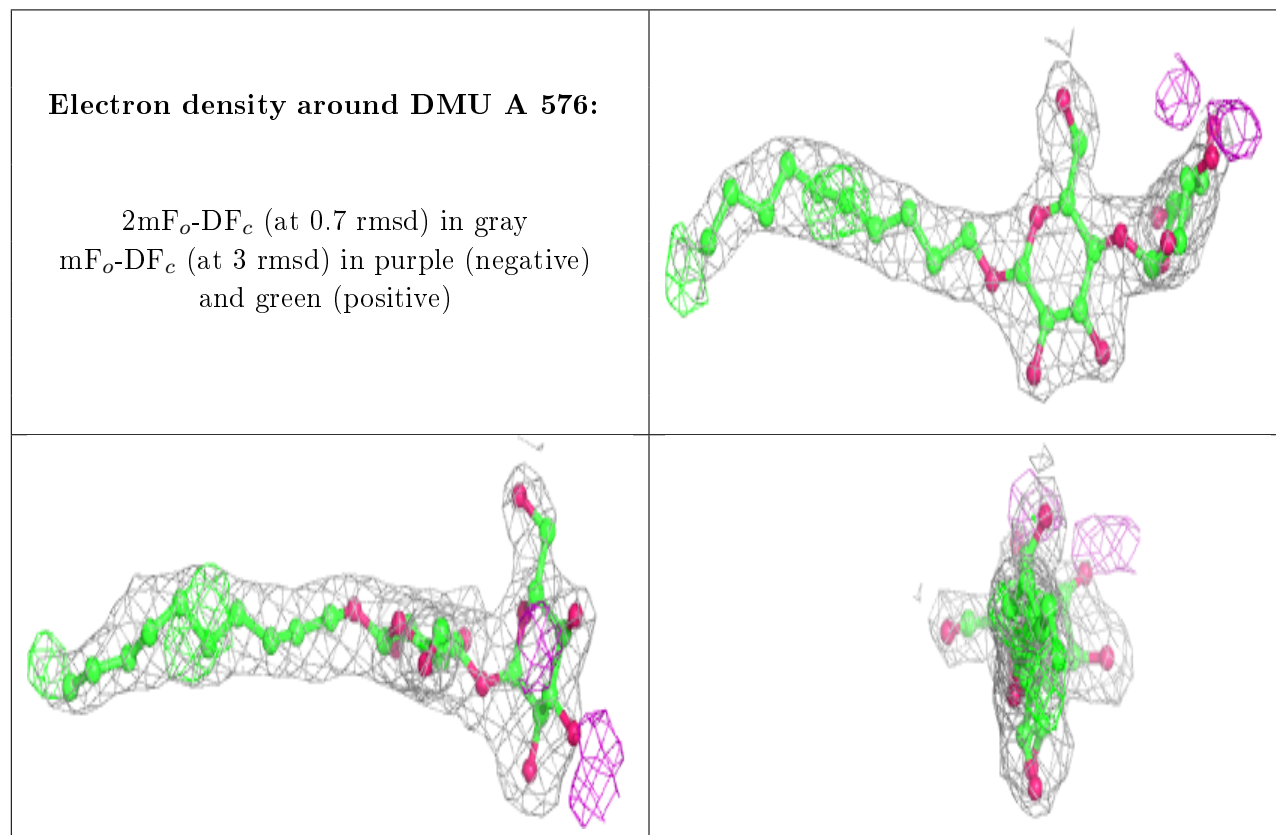
There are no carbohydrates in this entry.

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.

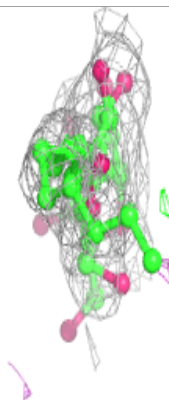
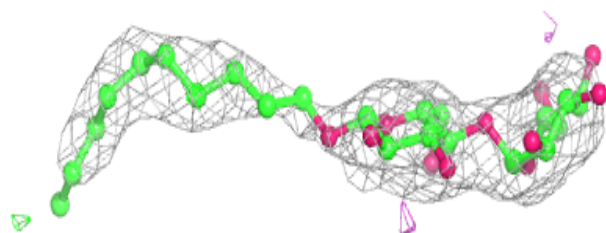
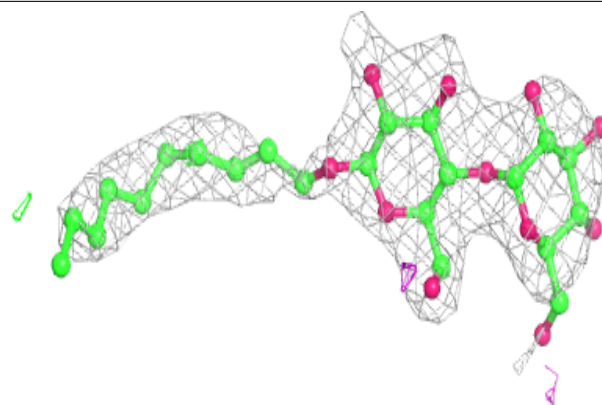
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	TRD	C	1001	13/13	0.56	0.23	78,79,79,79	0
9	TRD	C	1010	9/13	0.64	0.22	68,69,70,70	0
9	TRD	A	581	13/13	0.64	0.20	53,60,67,68	0
9	TRD	A	577	13/13	0.74	0.24	66,67,71,71	0
9	TRD	C	1006	13/13	0.75	0.25	72,74,76,76	0
9	TRD	A	582	13/13	0.75	0.20	63,66,67,68	0
9	TRD	C	1009	7/13	0.77	0.21	64,65,65,65	0
9	TRD	A	579	7/13	0.77	0.22	59,59,60,60	0
8	DMU	A	576	33/33	0.79	0.24	41,50,51,52	33
8	DMU	D	1003	33/33	0.80	0.28	93,99,103,103	0
8	DMU	C	1002	23/33	0.80	0.23	97,98,99,99	23
8	DMU	A	575	22/33	0.80	0.18	41,61,68,70	0
9	TRD	A	580	7/13	0.81	0.17	59,59,60,60	0
10	HTO	B	1	10/10	0.82	0.36	54,57,58,59	0
8	DMU	B	11	23/33	0.83	0.16	72,73,75,75	23
8	DMU	D	1011	23/33	0.83	0.16	68,69,70,70	23
8	DMU	C	1005	33/33	0.84	0.16	59,61,62,63	33
9	TRD	D	1008	7/13	0.85	0.16	61,62,62,63	0
8	DMU	B	288	33/33	0.86	0.24	77,82,86,86	0
9	TRD	D	1007	13/13	0.88	0.23	51,53,56,57	0
8	DMU	A	574	33/33	0.89	0.20	66,72,74,75	0
9	TRD	A	578	13/13	0.90	0.24	43,45,48,50	0
11	CD	D	9	1/1	0.92	0.14	45,45,45,45	1
3	HEA	C	568	60/60	0.95	0.21	30,37,49,50	0
3	HEA	C	567	60/60	0.96	0.22	30,33,45,46	0
8	DMU	A	573	33/33	0.96	0.09	24,35,51,53	0
3	HEA	A	568	60/60	0.96	0.23	26,31,46,47	0
5	MG	C	570	1/1	0.97	0.24	20,20,20,20	0
4	CU1	C	569	1/1	0.98	0.14	42,42,42,42	0
7	CYN	C	572	2/2	0.98	0.22	36,36,36,37	0
6	CA	C	571	1/1	0.98	0.04	40,40,40,40	0
3	HEA	A	567	60/60	0.98	0.20	20,23,29,30	0
11	CD	D	8	1/1	0.99	0.07	40,40,40,40	0
11	CD	B	9	1/1	0.99	0.10	47,47,47,47	1
11	CD	B	8	1/1	0.99	0.07	40,40,40,40	0
5	MG	A	570	1/1	0.99	0.26	17,17,17,17	0
7	CYN	A	572	2/2	0.99	0.25	31,31,31,32	0
6	CA	A	571	1/1	1.00	0.11	27,27,27,27	0
4	CU1	A	569	1/1	1.00	0.16	35,35,35,35	0
4	CU1	D	4	1/1	1.00	0.12	33,33,33,33	0
4	CU1	B	4	1/1	1.00	0.13	25,25,25,25	0
4	CU1	B	3	1/1	1.00	0.12	25,25,25,25	0
4	CU1	D	3	1/1	1.00	0.13	33,33,33,33	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.



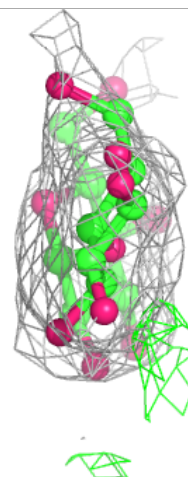
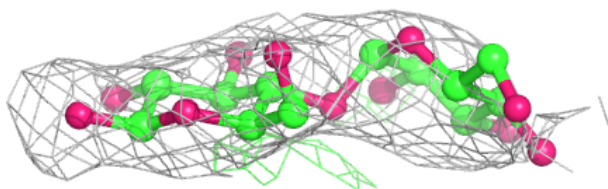
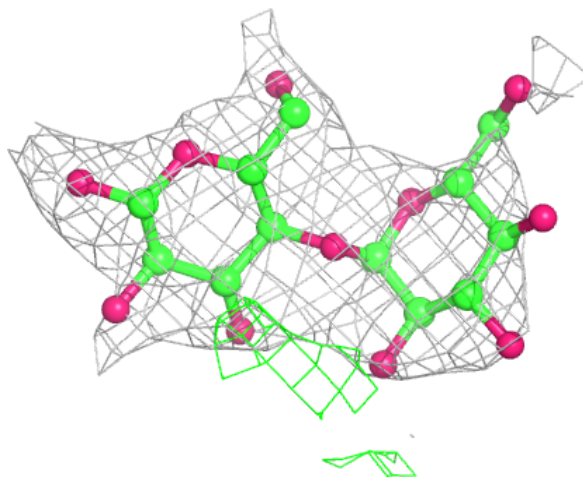
Electron density around DMU D 1003:

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



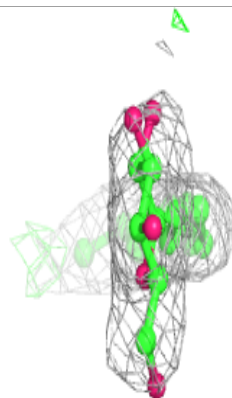
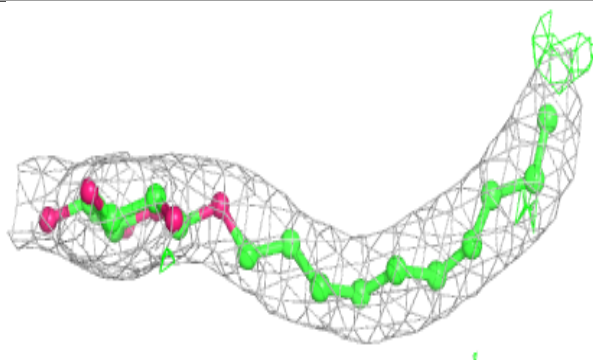
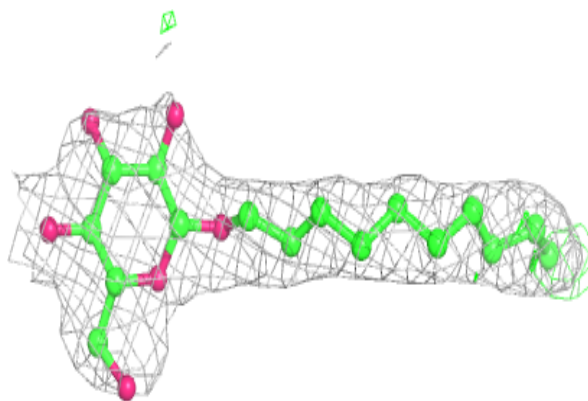
Electron density around DMU C 1002:

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and green (positive)

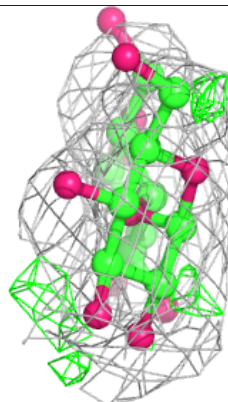
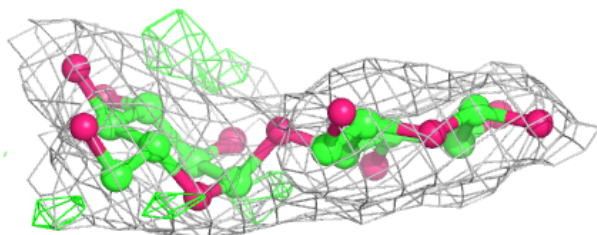
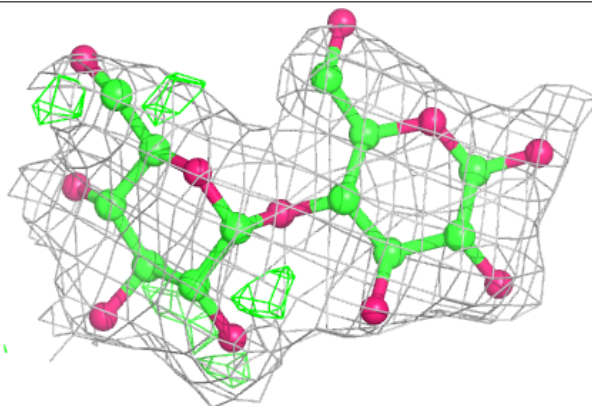


Electron density around DMU A 575:

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and green (positive)

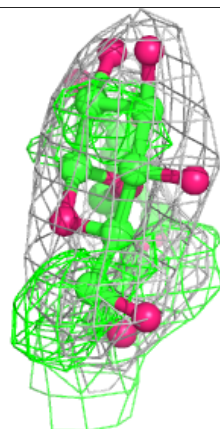
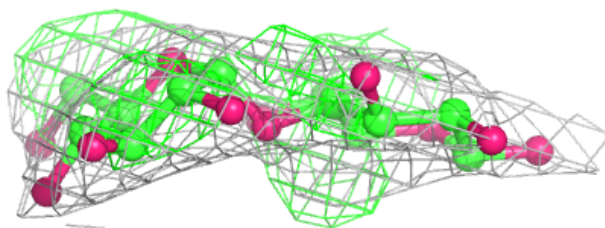
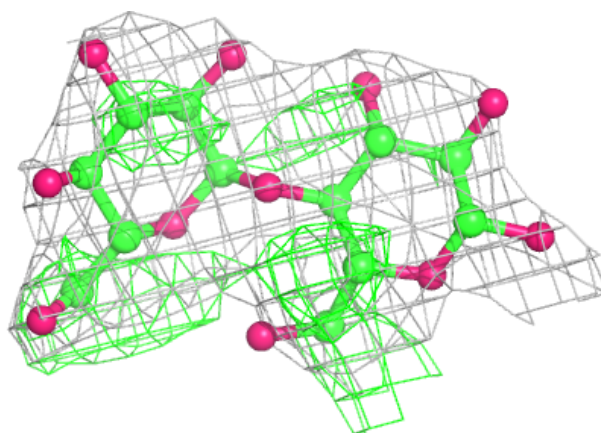
**Electron density around DMU B 11:**

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and green (positive)

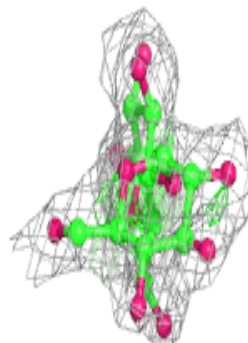
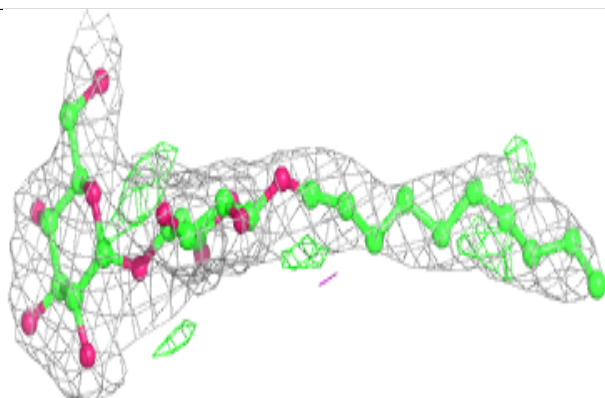
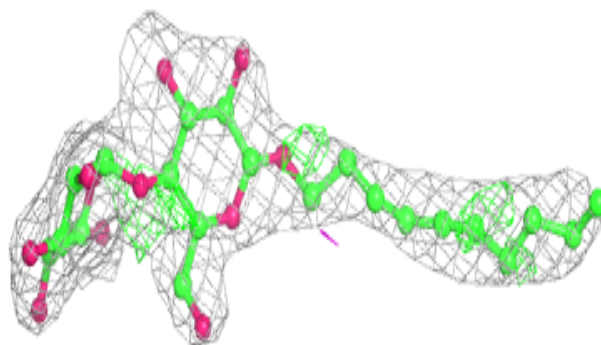


Electron density around DMU D 1011:

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

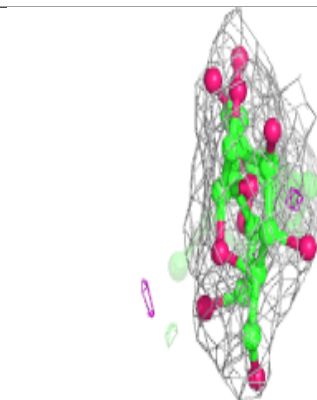
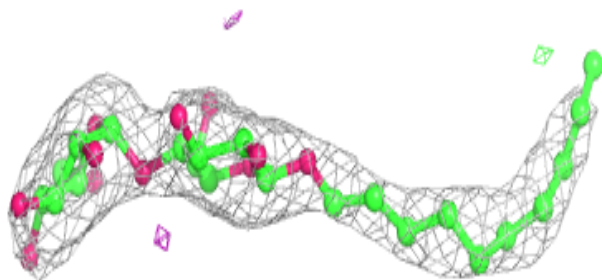
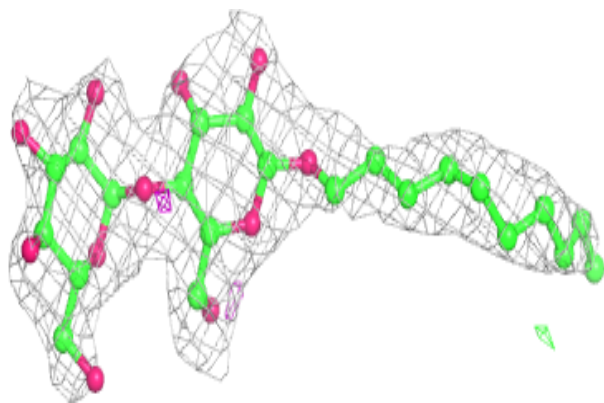
**Electron density around DMU C 1005:**

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and green (positive)

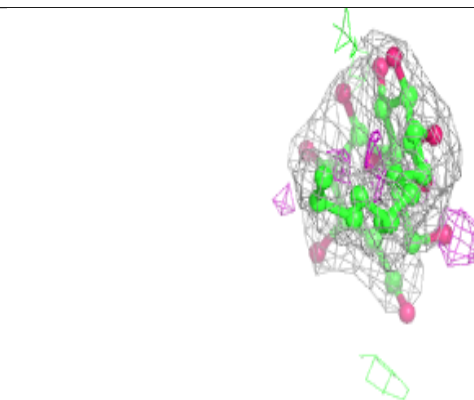
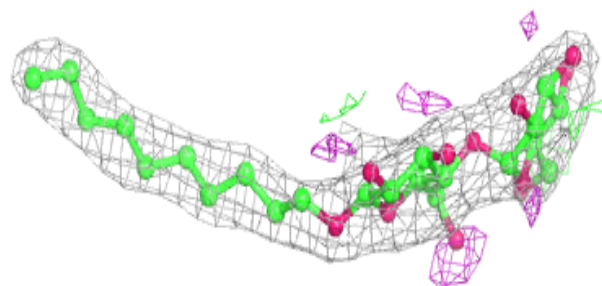
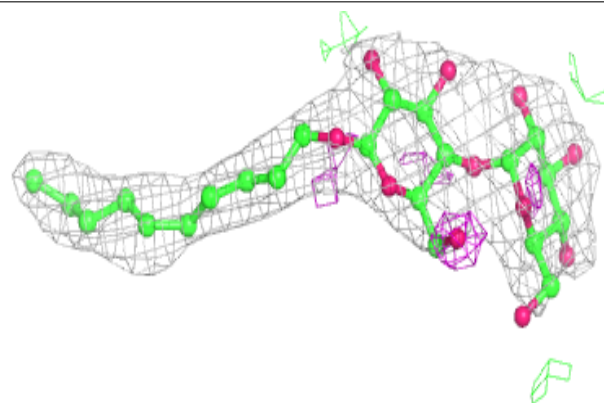


Electron density around DMU B 288:

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

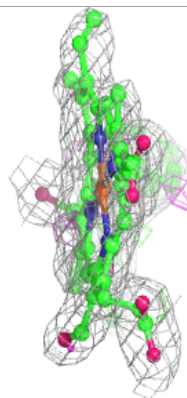
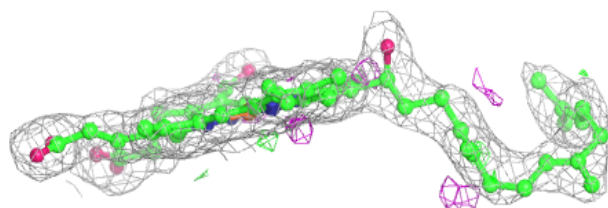
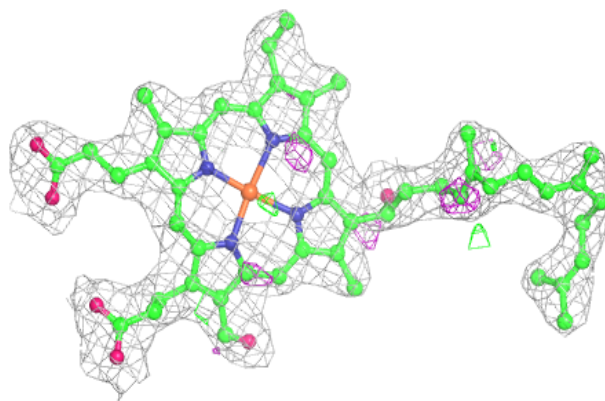
**Electron density around DMU A 574:**

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

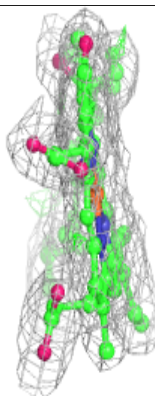
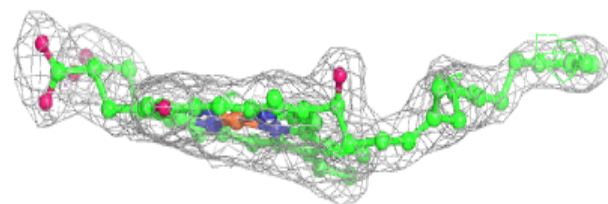
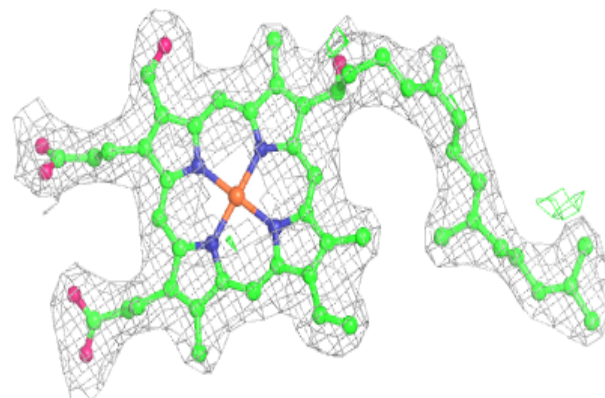


Electron density around HEA C 568:

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

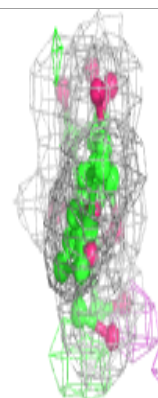
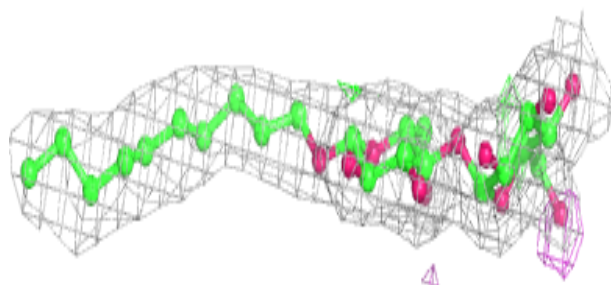
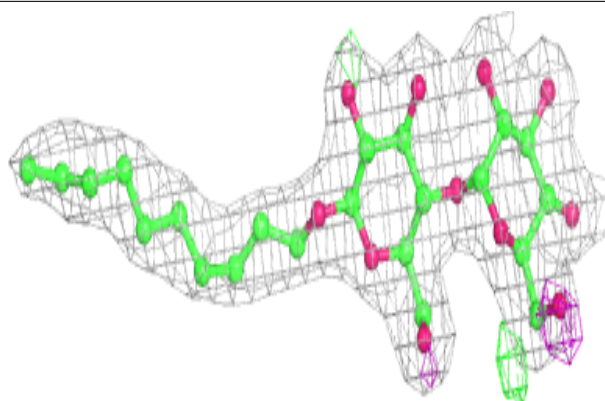
**Electron density around HEA C 567:**

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

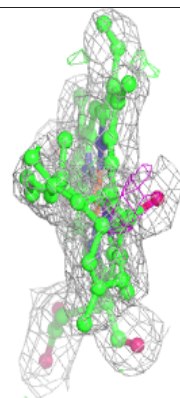
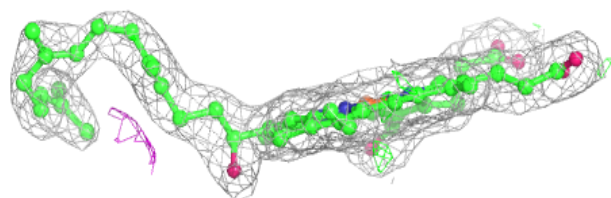
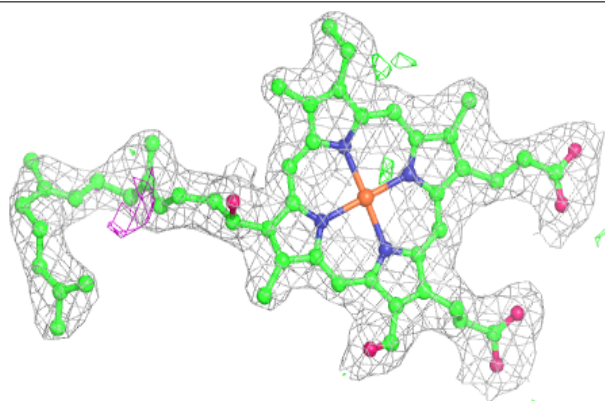


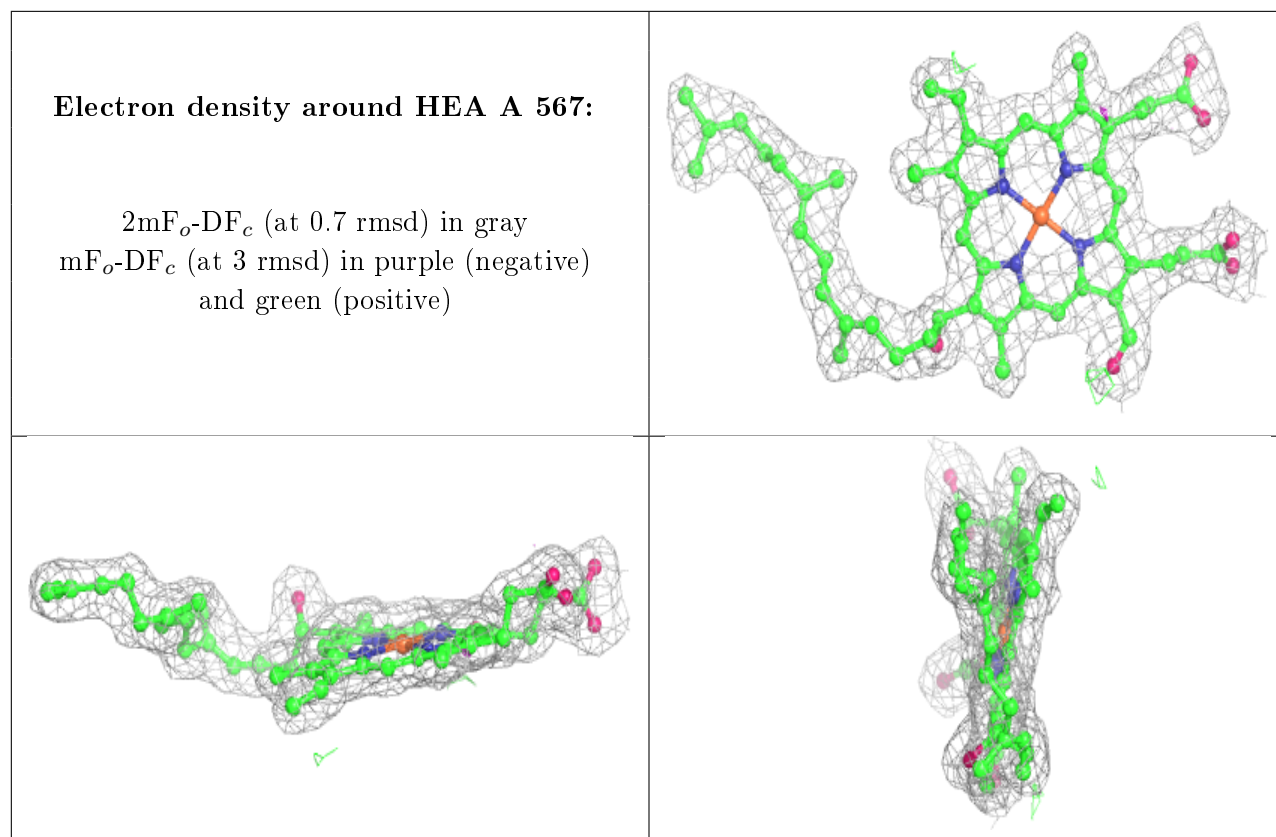
Electron density around DMU A 573:

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

**Electron density around HEA A 568:**

$2mF_o-DF_c$ (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.