



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:05 AM UTC

PDB ID : 8K6Y / pdb_00008k6y
Title : Serial femtosecond crystallography structure of photo dissociated CO from ba3- type cytochrome c oxidase determined by extrapolation method
Authors : Safari, C.; Ghosh, S.; Andersson, R.; Johannesson, J.; Donoso, A.V.; Zoric, D.; Sandelin, E.; Iwata, S.; Neutze, R.; Branden, G.
Deposited on : 2023-07-25
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

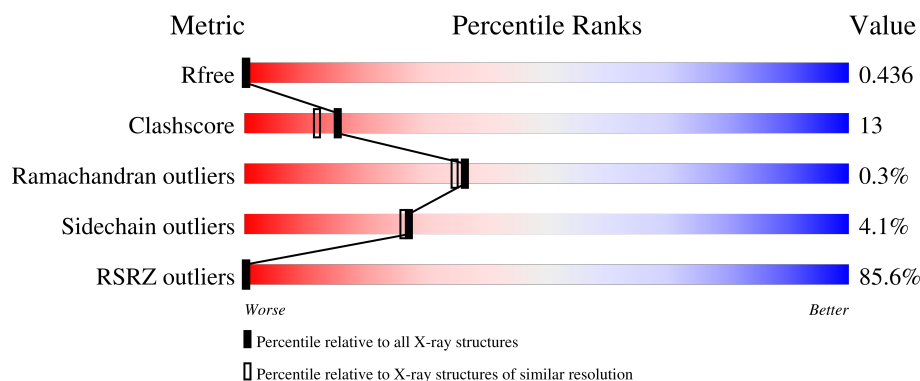
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	569	83% 68%26% . .
2	B	168	84% 73%24% . .
3	C	34	88% 76%12% . 9%

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
6	HAS	A	603	X	-	-	-
7	OLC	A	605	-	-	-	X
7	OLC	A	606	-	-	-	X
7	OLC	A	607	-	-	-	X
7	OLC	A	608	-	-	-	X
7	OLC	A	609	-	-	-	X
7	OLC	A	610	-	-	-	X
7	OLC	A	611	-	-	-	X
7	OLC	A	612	-	-	-	X
7	OLC	A	613	-	-	-	X
7	OLC	A	614	-	-	-	X
7	OLC	A	616	-	-	-	X
7	OLC	B	203	-	-	-	X
7	OLC	C	101	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6474 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	554	Total	C	N	O	S	0	0	0
			4368	2963	698	691	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q5SJ79
A	-5	HIS	-	expression tag	UNP Q5SJ79
A	-4	HIS	-	expression tag	UNP Q5SJ79
A	-3	HIS	-	expression tag	UNP Q5SJ79
A	-2	HIS	-	expression tag	UNP Q5SJ79
A	-1	HIS	-	expression tag	UNP Q5SJ79
A	0	HIS	-	expression tag	UNP Q5SJ79
A	1	HIS	-	expression tag	UNP Q5SJ79

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	0	0
			1301	846	216	235	4			

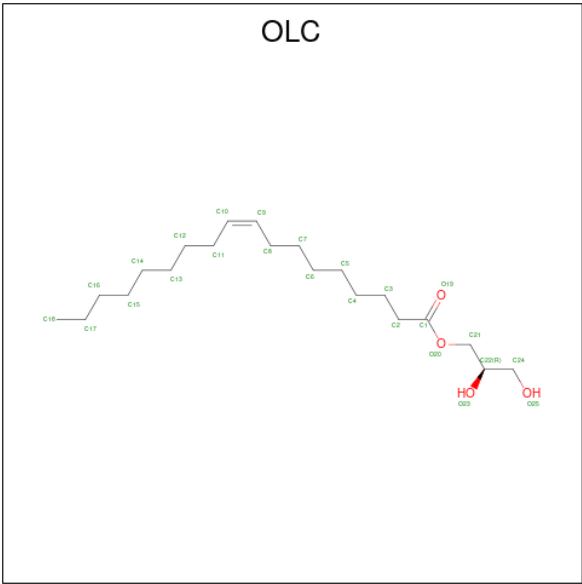
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	31	Total	C	N	O	0	0	0
			241	169	37	35			

- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



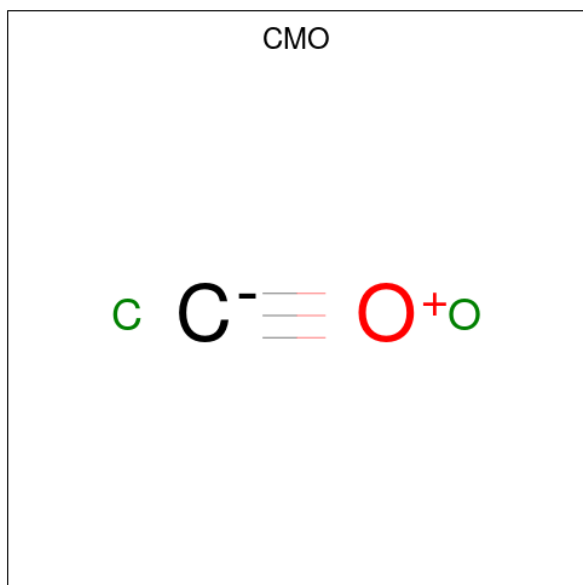
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			23	19	4		
7	A	1	Total	C	O	0	0
			18	14	4		
7	A	1	Total	C	O	0	0
			17	13	4		
7	A	1	Total	C	O	0	0
			15	11	4		
7	A	1	Total	C	O	0	0
			18	14	4		
7	A	1	Total	C	O	0	0
			15	11	4		
7	A	1	Total	C	O	0	0
			20	16	4		
7	A	1	Total	C	O	0	0
			21	17	4		
7	A	1	Total	C	O	0	0
			20	18	2		
7	A	1	Total	C		0	0
			9	9			
7	A	1	Total	C		0	0
			9	9			
7	A	1	Total	C	O	0	0
			15	11	4		

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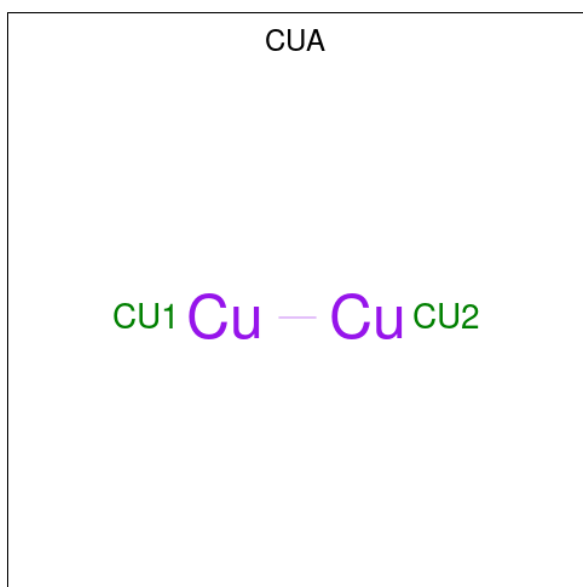
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			25	21	4		
7	B	1	Total	C	O	0	0
			24	20	4		
7	C	1	Total	C	O	0	0
			24	20	4		

- Molecule 8 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			2	1	1		

- Molecule 9 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



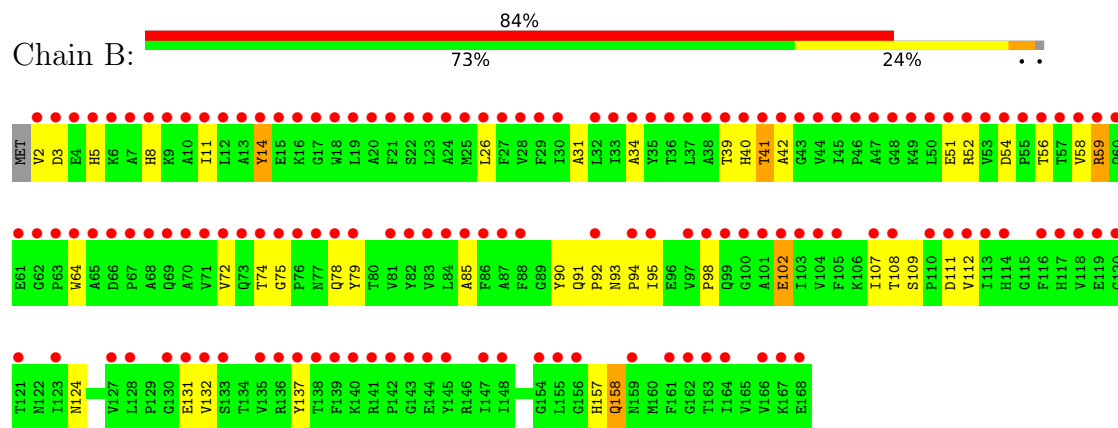
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Cu 2 2	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	97	Total O 97 97	0	0
10	B	76	Total O 76 76	0	0
10	C	5	Total O 5 5	0	0

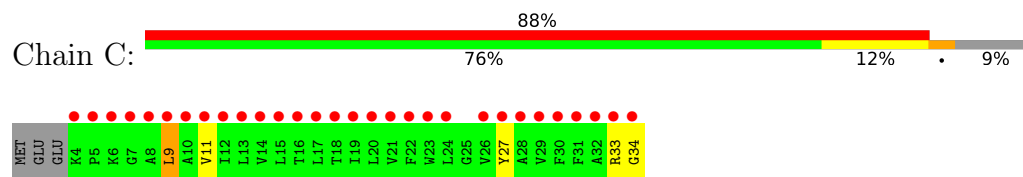
- Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



- Molecule 3: Cytochrome c oxidase polypeptide 2A

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.85Å 100.32Å 96.62Å 90.00° 126.76° 90.00°	Depositor
Resolution (Å)	37.15 – 2.00 37.15 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (37.15-2.00) 94.8 (37.15-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.48 (at 2.00Å)	Xtriage
Refinement program	REFMAC v8.0	Depositor
R, R_{free}	0.396 , 0.435 0.405 , 0.436	Depositor DCC
R_{free} test set	1877 reflections (2.63%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 79.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.58$, $\langle L^2 \rangle = 0.43$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	6474	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% 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: HAS, OLC, CUA, CMO, HEM, CU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.61	0/4525	1.28	20/6213 (0.3%)
2	B	0.63	0/1338	1.29	7/1828 (0.4%)
3	C	0.59	0/247	1.31	2/335 (0.6%)
All	All	0.61	0/6110	1.28	29/8376 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	HIS	CA-CB-CG	-12.09	101.71	113.80
2	B	124	ASN	CB-CA-C	-7.10	102.40	111.70
1	A	121	ALA	CA-C-N	6.36	128.78	120.26
1	A	121	ALA	C-N-CA	6.36	128.78	120.26
1	A	52	TYR	N-CA-CB	6.22	117.77	110.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ARG	Sidechain
2	B	59	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4368	0	4467	130	0
2	B	1301	0	1278	35	0
3	C	241	0	267	3	0
4	A	1	0	0	0	0
5	A	43	0	30	3	0
6	A	65	0	62	11	0
7	A	200	0	276	8	0
7	B	49	0	75	3	0
7	C	24	0	35	2	0
8	A	2	0	0	1	0
9	B	2	0	0	0	0
10	A	97	0	0	6	0
10	B	76	0	0	7	1
10	C	5	0	0	0	0
All	All	6474	0	6490	172	1

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 13.

The worst 5 of 172 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)
7:A:610:OLC:C13	7:A:610:OLC:C12	1.87	1.51
1:A:414:SER:OG	1:A:417:GLN:HG3	1.52	1.07
5:A:602:HEM:HMC2	5:A:602:HEM:HBC2	1.49	0.95
1:A:387:LEU:CD2	1:A:433:MET:CE	2.53	0.85
1:A:37:LEU:HD23	1:A:481:LEU:HD21	1.58	0.84

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:359:HOH:O	10:B:365:HOH:O[2_556]	1.95	0.25

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	552/569 (97%)	515 (93%)	36 (6%)	1 (0%)	43	42
2	B	165/168 (98%)	155 (94%)	9 (6%)	1 (1%)	21	17
3	C	29/34 (85%)	27 (93%)	2 (7%)	0	100	100
All	All	746/771 (97%)	697 (93%)	47 (6%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3	ASP
1	A	322	PHE

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	447/463 (96%)	428 (96%)	19 (4%)	26	25
2	B	136/138 (99%)	132 (97%)	4 (3%)	37	40
3	C	24/27 (89%)	22 (92%)	2 (8%)	10	7
All	All	607/628 (97%)	582 (96%)	25 (4%)	27	26

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	424	VAL
1	A	513	SER
3	C	11	VAL
1	A	498	LYS
1	A	548	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	158	GLN
2	B	159	ASN
1	A	552	HIS
2	B	60	GLN
2	B	91	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	CUA	B	201	2	0,1,1	-	-	-		
6	HAS	A	603	1	72,72,72	2.63	27 (37%)	87,109,109	3.01	43 (49%)
7	OLC	B	203	-	23,23,24	0.25	0	24,24,25	0.22	0
7	OLC	A	609	-	14,14,24	0.21	0	15,15,25	0.29	0
7	OLC	A	612	-	19,19,24	0.26	0	19,19,25	0.26	0
7	OLC	A	613	-	8,8,24	0.19	0	7,7,25	0.18	0
7	OLC	A	614	-	8,8,24	0.16	0	7,7,25	0.16	0
7	OLC	A	605	-	17,17,24	0.24	0	18,18,25	0.30	0
7	OLC	A	607	-	14,14,24	0.23	0	15,15,25	0.32	0
7	OLC	A	606	-	16,16,24	0.27	0	17,17,25	0.34	0
8	CMO	A	615	4	0,1,1	-	-	-		
7	OLC	C	101	-	23,23,24	0.48	1 (4%)	24,24,25	0.33	0
7	OLC	A	616	-	14,14,24	0.82	1 (7%)	15,15,25	0.67	0
5	HEM	A	602	1	50,50,50	1.59	7 (14%)	67,82,82	1.74	20 (29%)
7	OLC	A	604	-	22,22,24	0.23	0	23,23,25	0.44	0
7	OLC	A	611	-	20,20,24	0.72	1 (5%)	21,21,25	0.60	1 (4%)
7	OLC	A	610	-	19,19,24	1.23	1 (5%)	20,20,25	0.35	0
7	OLC	B	202	-	24,24,24	0.33	0	25,25,25	0.32	0
7	OLC	A	608	-	17,17,24	0.30	0	18,18,25	0.38	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
7	OLC	A	604	-	-	10/22/22/24	-
7	OLC	A	614	-	-	3/6/6/24	-
7	OLC	A	605	-	-	10/17/17/24	-
7	OLC	A	607	-	-	3/14/14/24	-
6	HAS	A	603	1	1/1/8/18	9/42/82/82	-
7	OLC	A	611	-	-	8/20/20/24	-
7	OLC	B	203	-	-	9/23/23/24	-
7	OLC	A	606	-	-	7/16/16/24	-
7	OLC	A	610	-	-	10/19/19/24	-
7	OLC	A	616	-	-	2/14/14/24	-
7	OLC	B	202	-	-	10/24/24/24	-
7	OLC	A	609	-	-	7/14/14/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OLC	A	608	-	-	9/17/17/24	-
7	OLC	A	612	-	-	9/18/18/24	-
5	HEM	A	602	1	-	2/14/54/54	-
7	OLC	A	613	-	-	5/6/6/24	-
7	OLC	C	101	-	-	16/23/23/24	-

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	C3B-C2B	6.22	1.48	1.34
6	A	603	HAS	FE-NA	5.92	2.14	1.95
6	A	603	HAS	CHD-C4A	5.73	1.49	1.38
6	A	603	HAS	FE-ND	5.64	2.12	1.94
5	A	602	HEM	FE-NB	5.36	2.11	1.94

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	C2D-C3D-C4D	-11.34	98.22	106.43
6	A	603	HAS	CAD-C3D-C4D	6.73	136.42	124.70
6	A	603	HAS	C3C-C4C-NC	6.55	115.31	109.80
6	A	603	HAS	C3D-C4D-ND	6.21	116.35	110.35
6	A	603	HAS	C2B-C1B-NB	5.89	116.71	109.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	603	HAS	NA

5 of 129 torsion outliers are listed below:

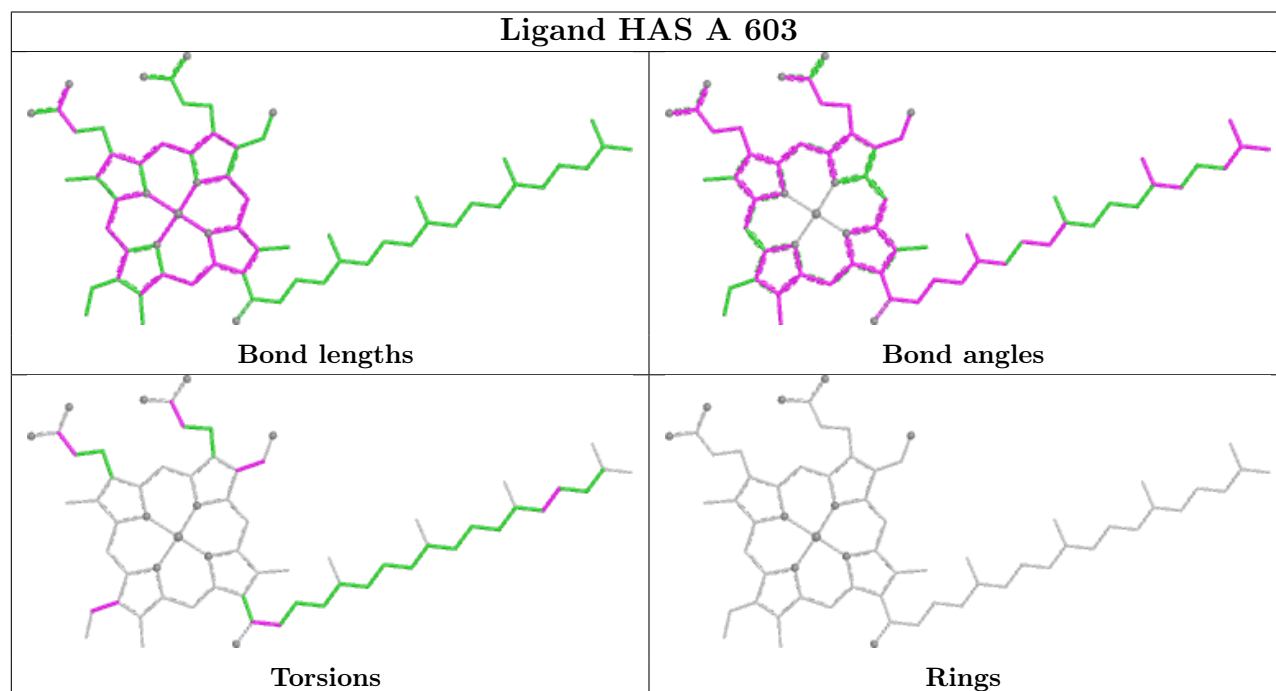
Mol	Chain	Res	Type	Atoms
6	A	603	HAS	C1D-C2D-CMD-OMD
6	A	603	HAS	C3D-C2D-CMD-OMD
7	A	604	OLC	C21-C22-C24-O25
7	A	608	OLC	C21-C22-C24-O25
7	A	610	OLC	C10-C11-C12-C13

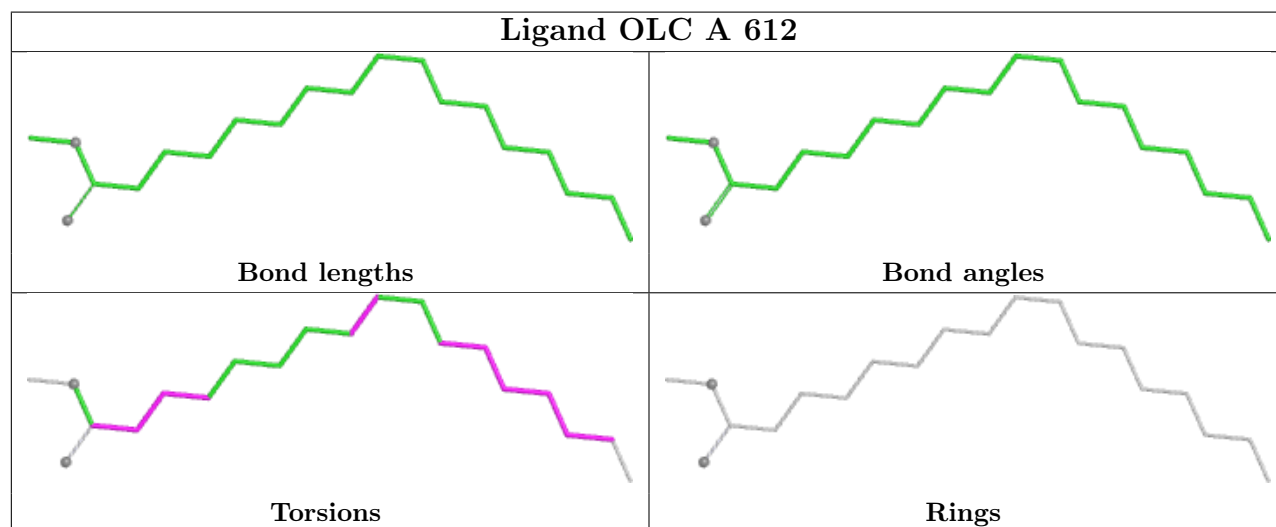
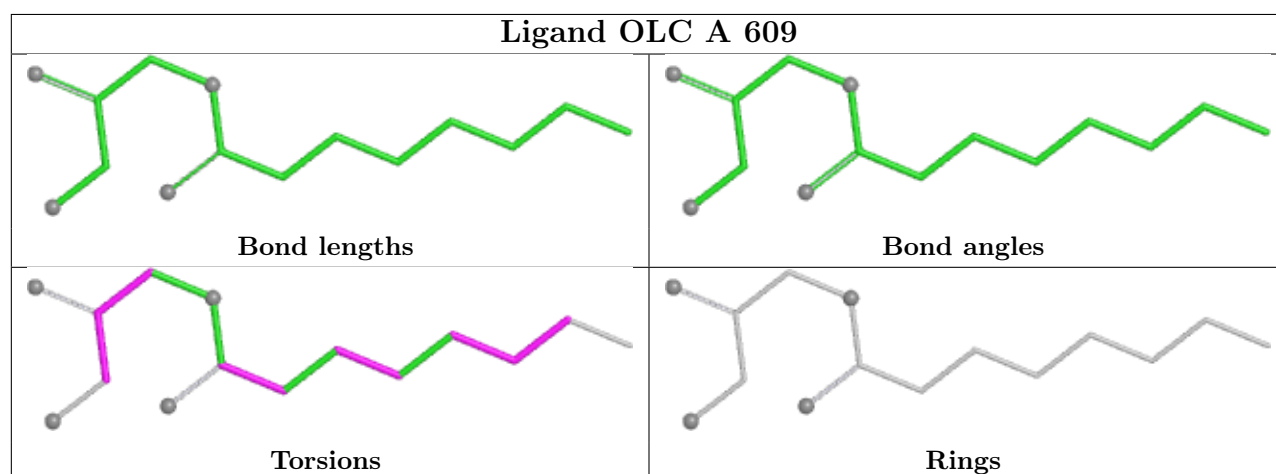
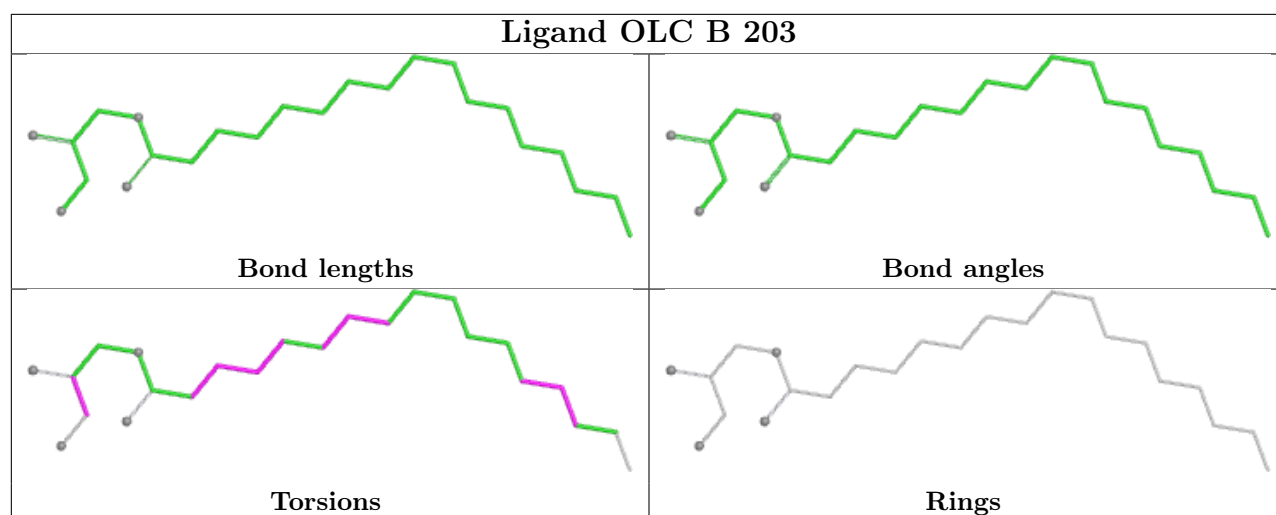
There are no ring outliers.

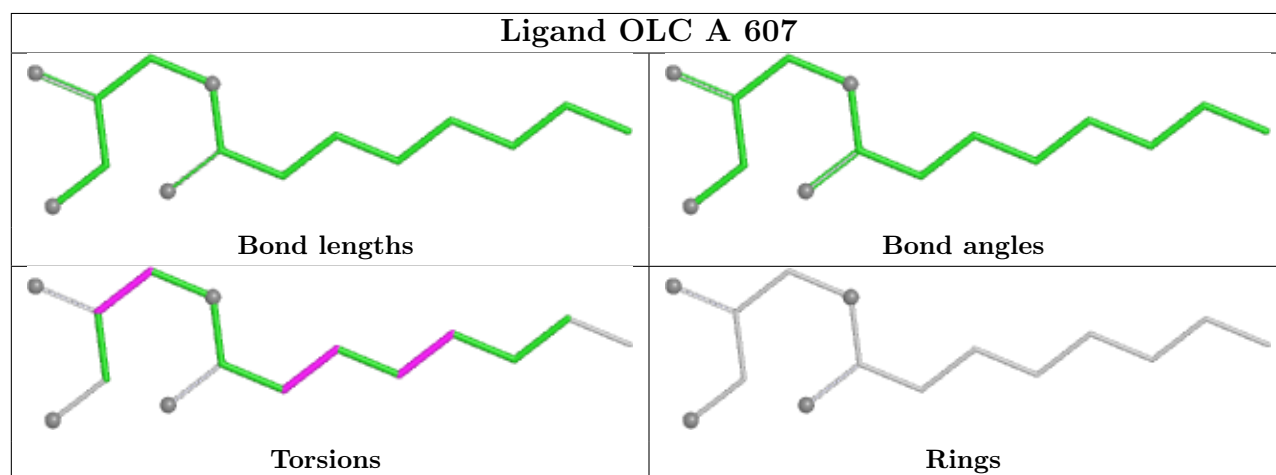
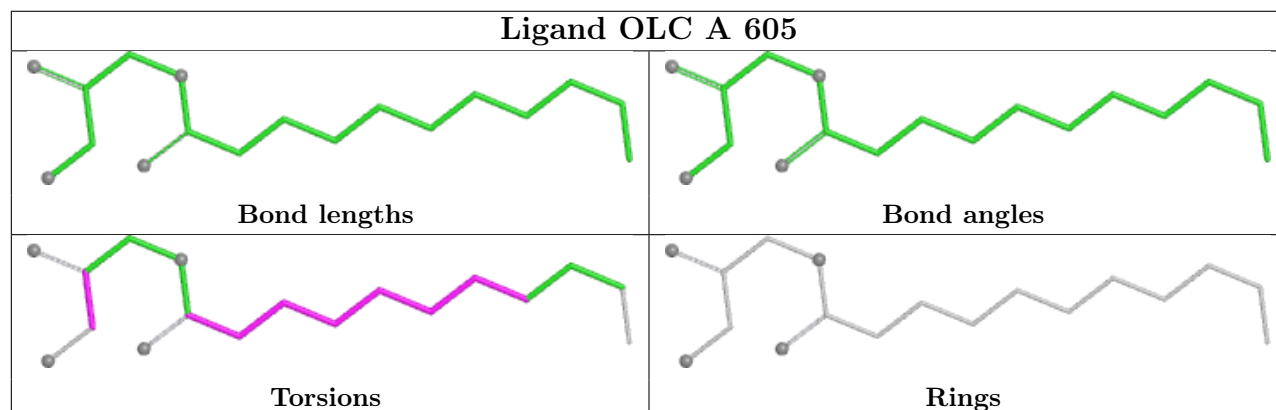
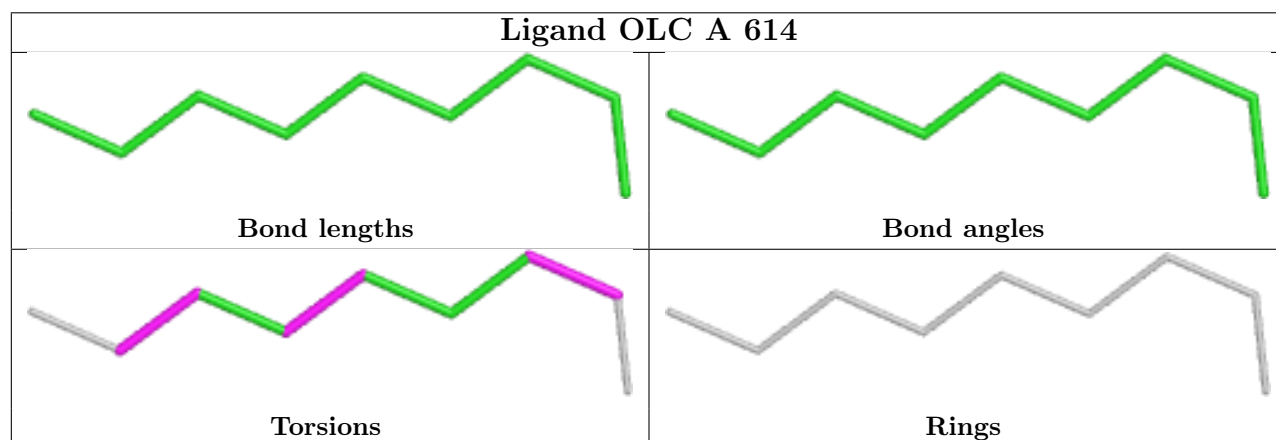
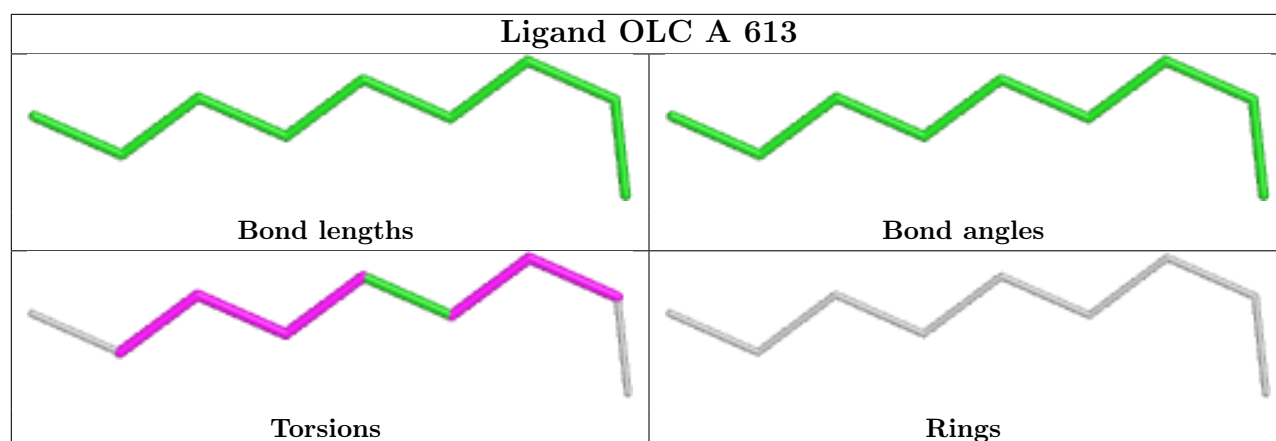
11 monomers are involved in 26 short contacts:

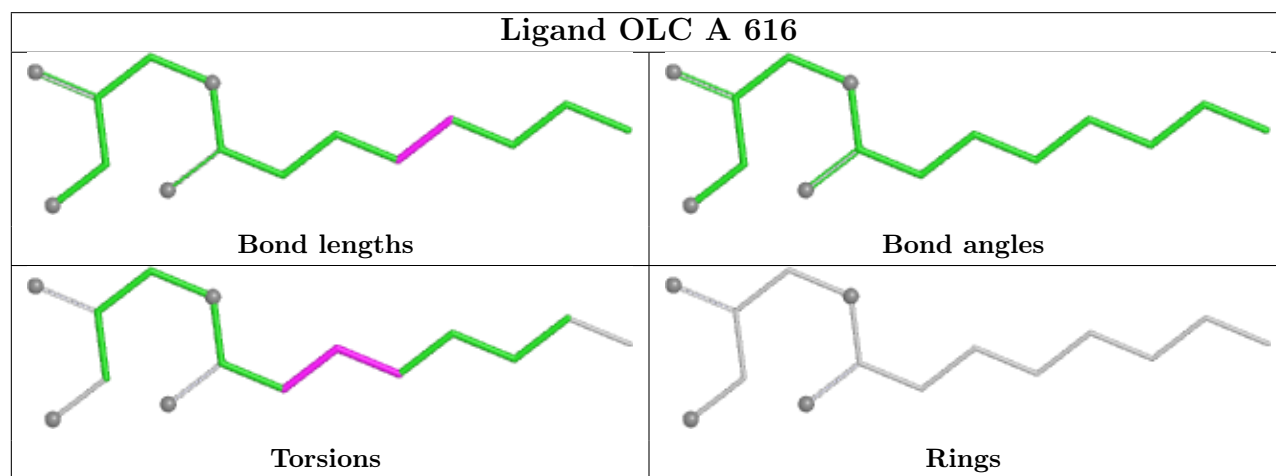
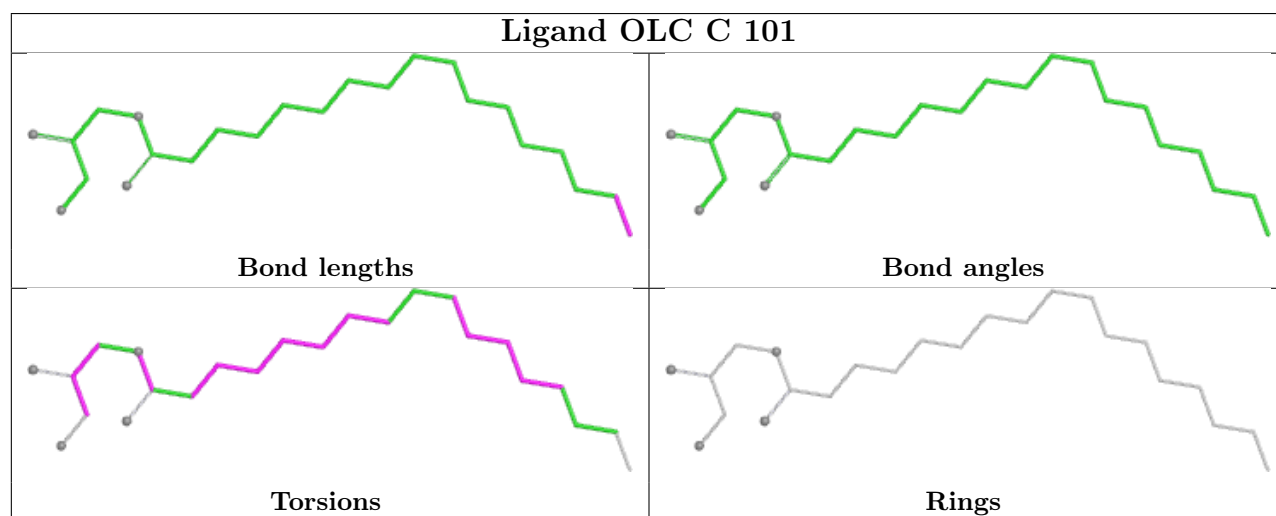
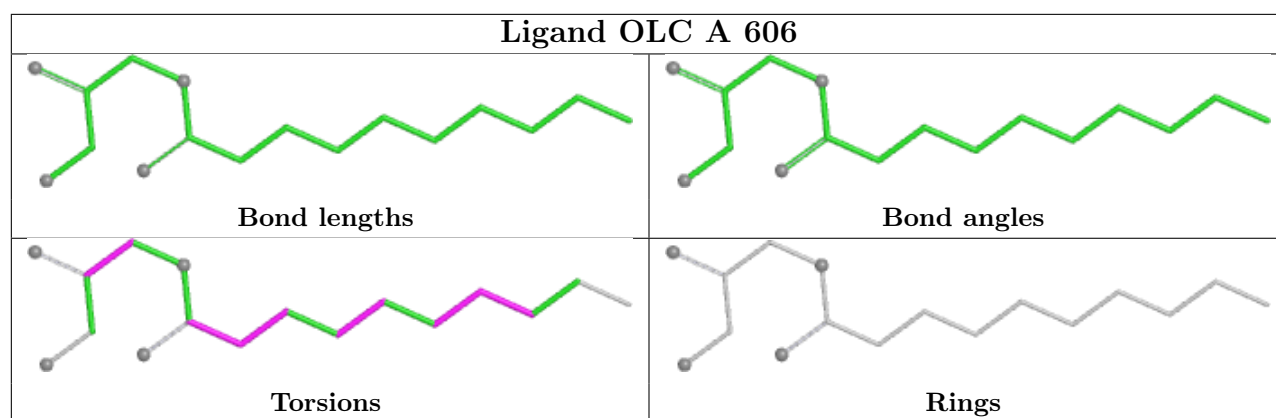
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	HAS	11	0
7	B	203	OLC	3	0
7	A	612	OLC	1	0
7	A	605	OLC	1	0
7	A	606	OLC	1	0
8	A	615	CMO	1	0
7	C	101	OLC	2	0
7	A	616	OLC	2	0
5	A	602	HEM	3	0
7	A	604	OLC	1	0
7	A	610	OLC	2	0

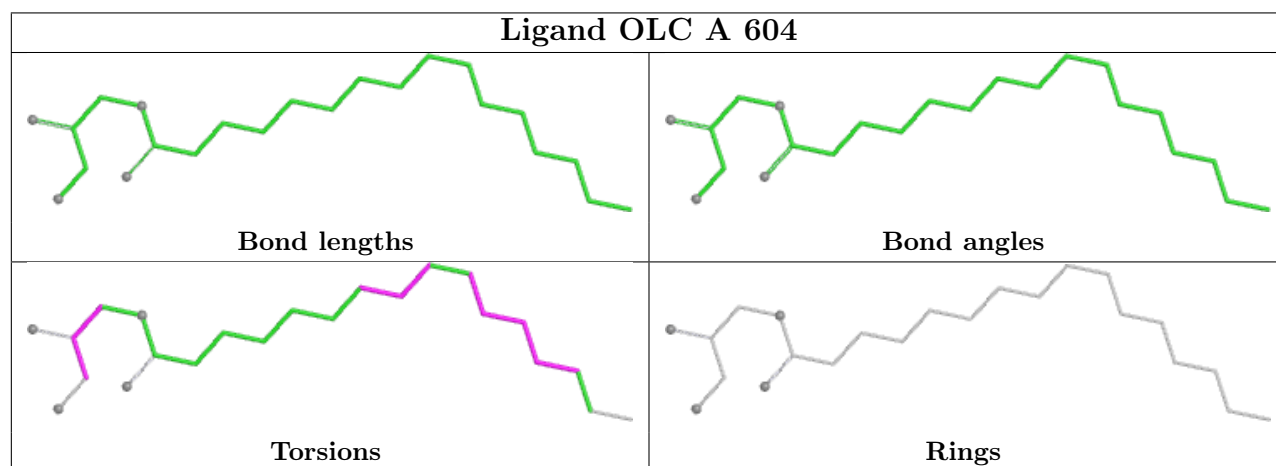
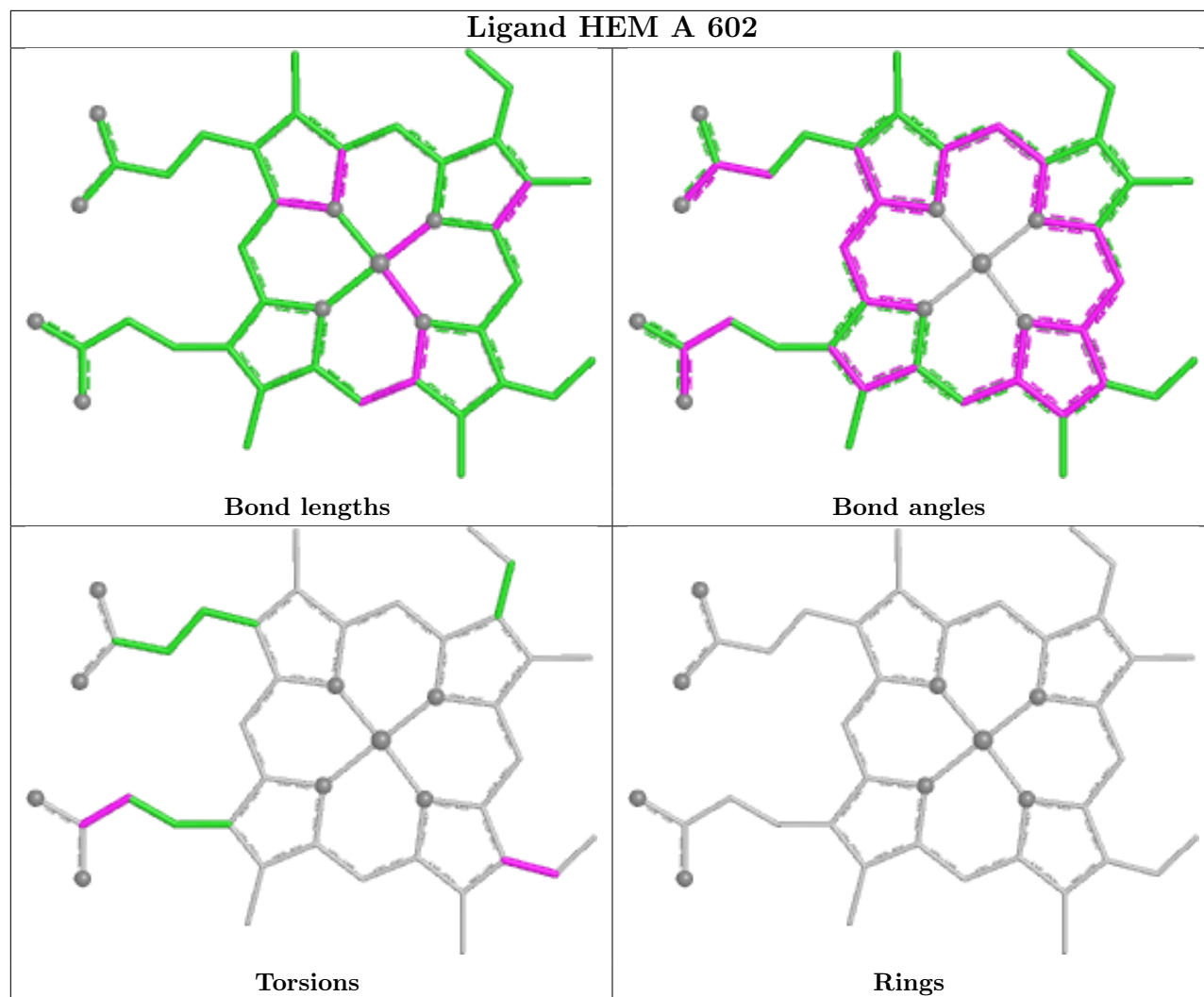
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

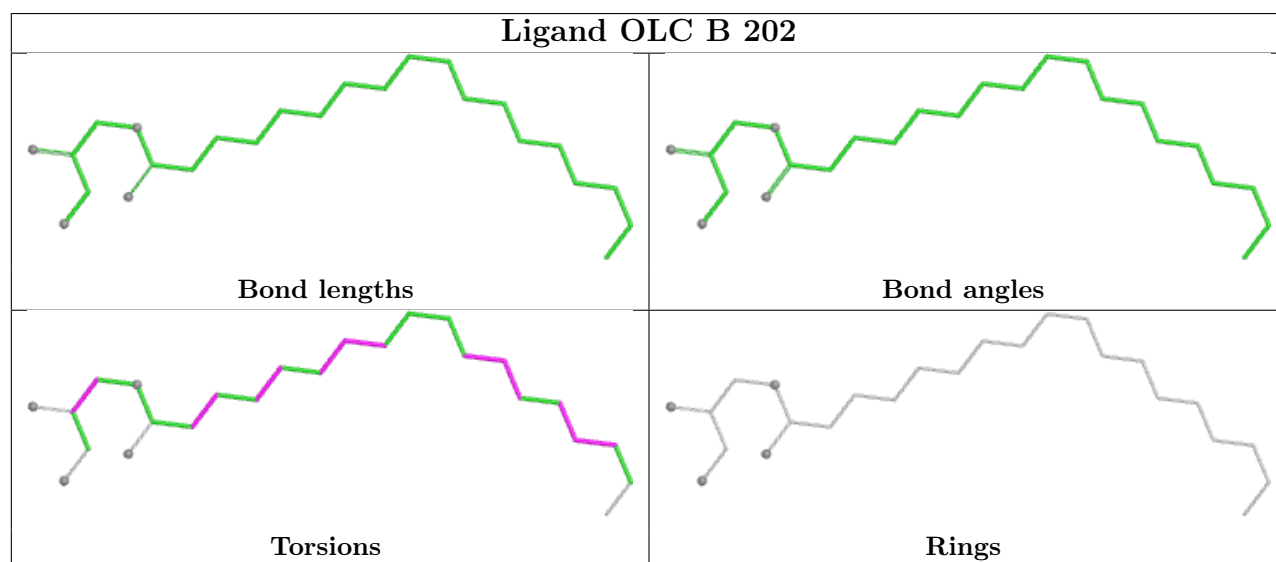
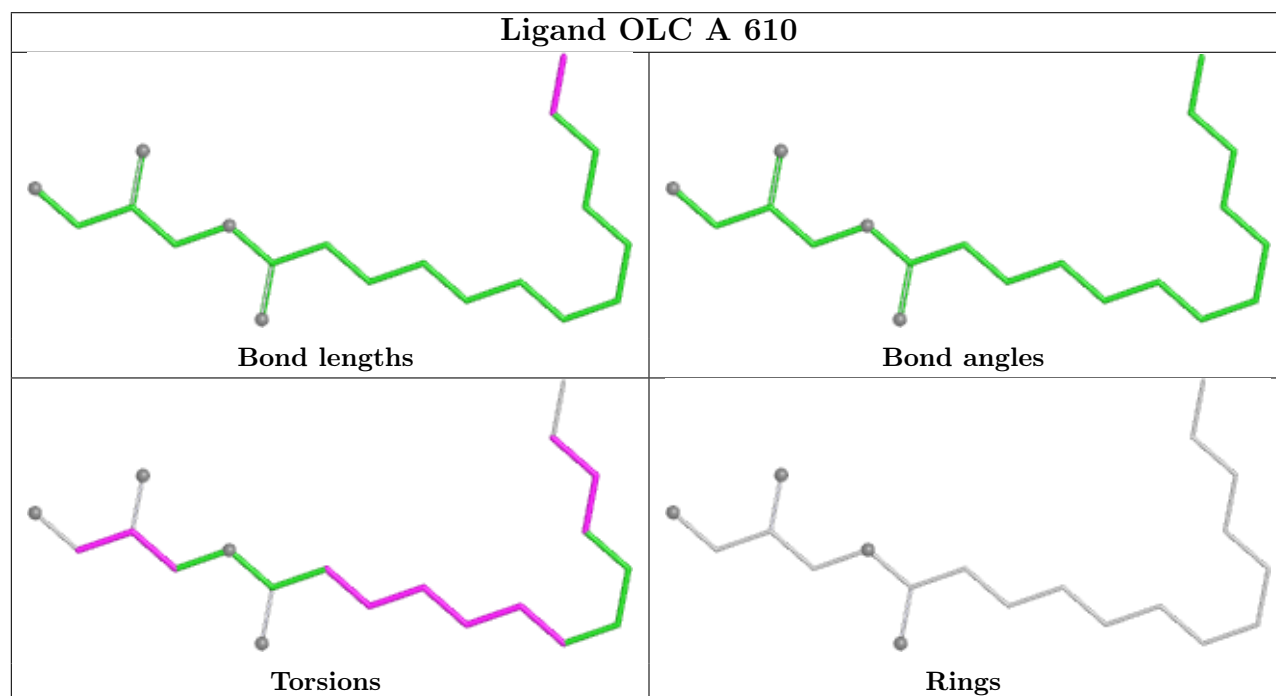
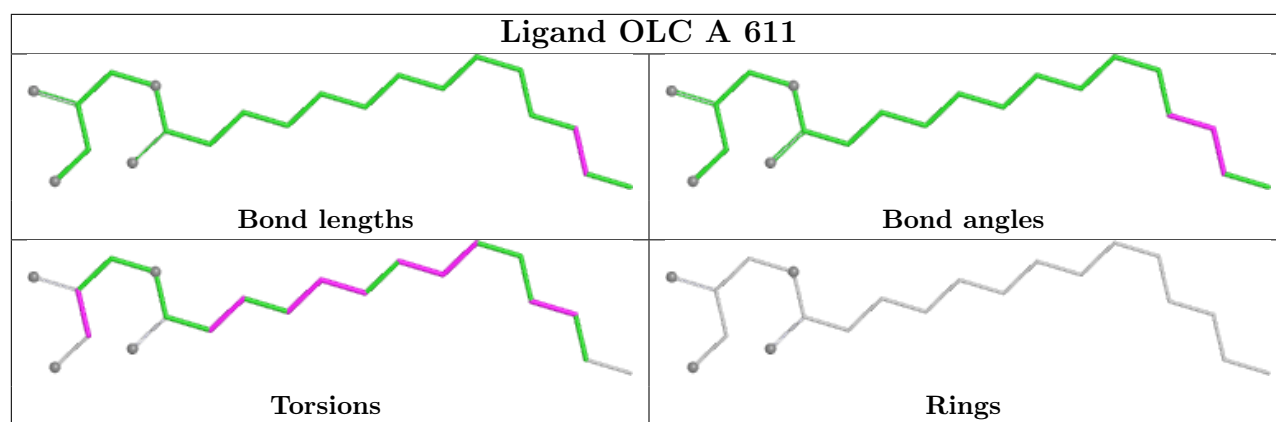


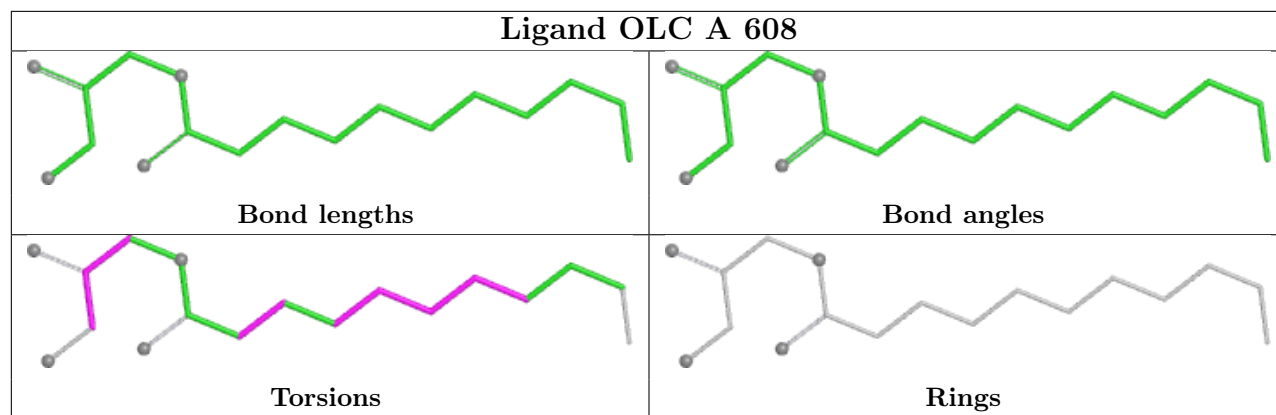












5.7 Other polymers [i](#)

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	554/569 (97%)	3.64	473 (85%) 0 0	21, 32, 59, 91	0
2	B	167/168 (99%)	3.46	141 (84%) 0 0	22, 32, 57, 104	0
3	C	31/34 (91%)	3.52	30 (96%) 0 0	27, 34, 42, 66	0
All	All	752/771 (97%)	3.60	644 (85%) 0 0	21, 32, 59, 104	0

The worst 5 of 644 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	VAL	11.9
1	A	58	LEU	11.4
1	A	322	PHE	10.1
1	A	491	VAL	10.0
1	A	494	SER	9.7

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](#)

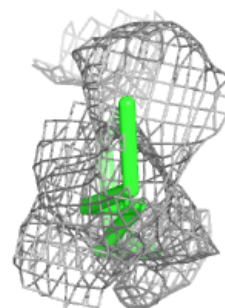
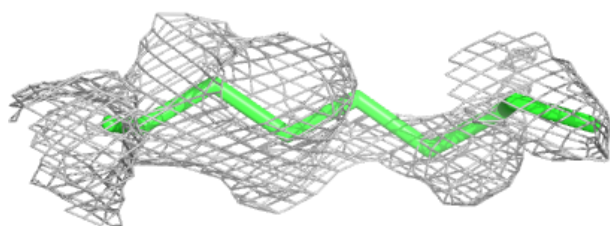
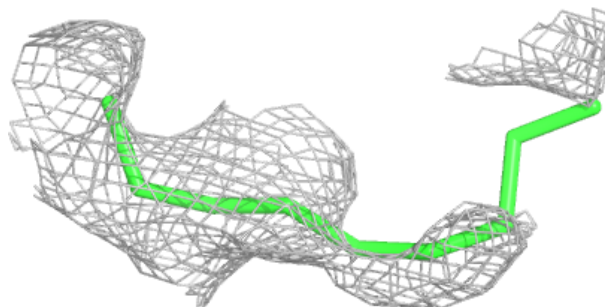
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
7	OLC	A	614	9/25	0.49	0.41	56,59,75,76	0
7	OLC	A	607	15/25	0.50	0.41	67,84,97,99	0
7	OLC	A	606	17/25	0.51	0.41	70,73,88,91	0
7	OLC	A	612	20/25	0.53	0.44	69,77,86,97	0
7	OLC	A	616	15/25	0.54	0.44	67,74,89,92	0
7	OLC	A	605	18/25	0.55	0.41	61,77,95,102	0
7	OLC	B	202	25/25	0.56	0.38	64,68,86,101	0
7	OLC	B	203	24/25	0.57	0.46	68,80,93,103	0
7	OLC	A	610	20/25	0.58	0.51	70,80,96,100	0
7	OLC	A	613	9/25	0.58	0.47	64,69,74,77	0
7	OLC	C	101	24/25	0.62	0.43	54,66,98,101	0
7	OLC	A	611	21/25	0.63	0.44	56,77,94,105	0
7	OLC	A	609	15/25	0.65	0.51	80,94,101,102	0
7	OLC	A	604	23/25	0.67	0.36	42,60,91,94	0
7	OLC	A	608	18/25	0.71	0.44	62,79,91,92	0
6	HAS	A	603	65/65	0.85	0.17	20,26,44,59	0
5	HEM	A	602	43/43	0.90	0.14	20,23,27,36	0
8	CMO	A	615	2/2	0.96	0.12	20,20,20,26	0
9	CUA	B	201	2/2	0.98	0.04	25,25,25,26	0
4	CU	A	601	1/1	0.99	0.05	29,29,29,29	0

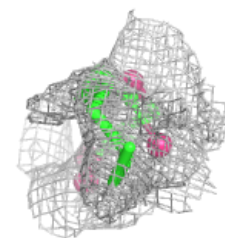
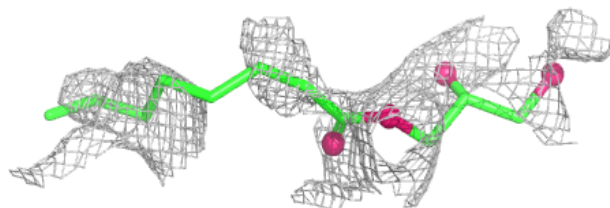
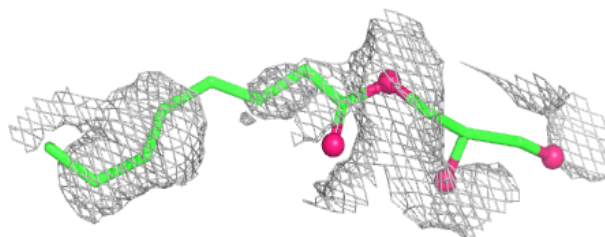
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 614:

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

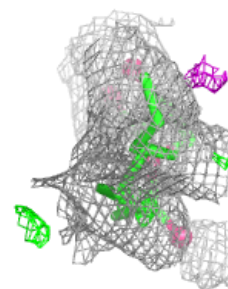
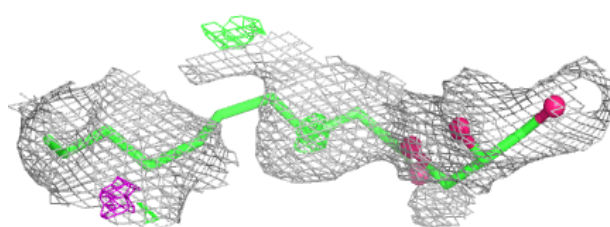
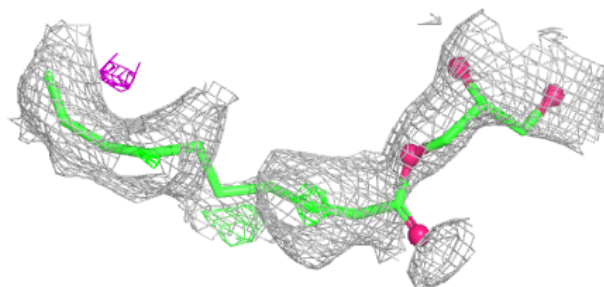
**Electron density around OLC A 607:**

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

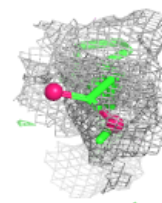
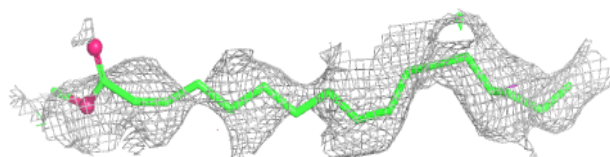
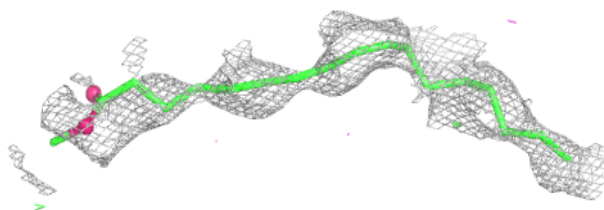


Electron density around OLC A 606:

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

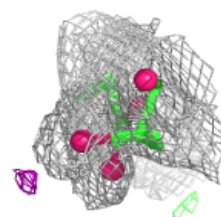
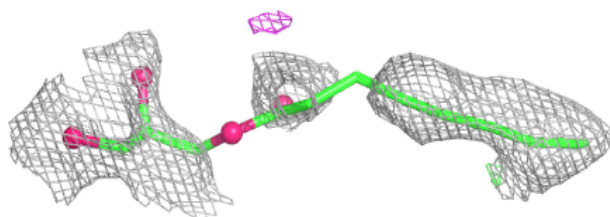
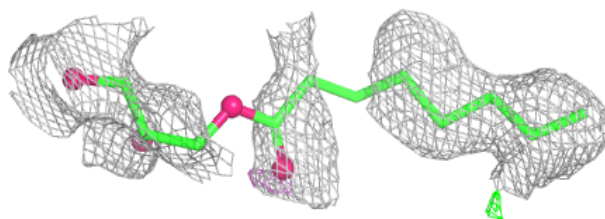
**Electron density around OLC A 612:**

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

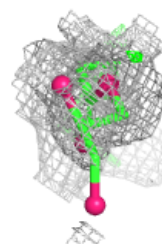
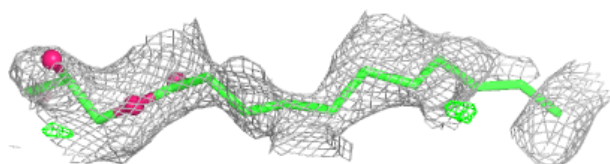
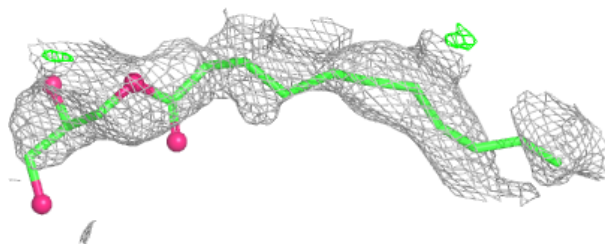


Electron density around OLC A 616:

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

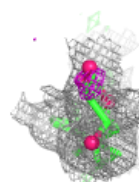
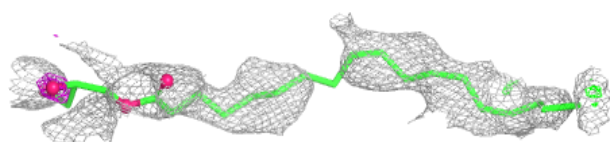
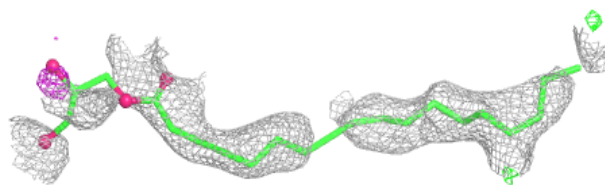
**Electron density around OLC A 605:**

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

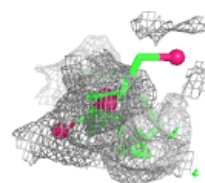
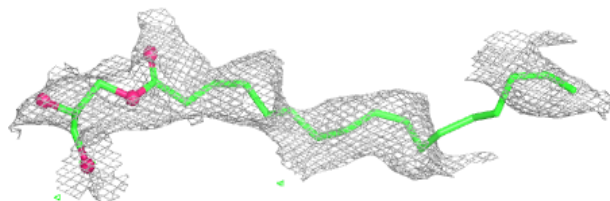
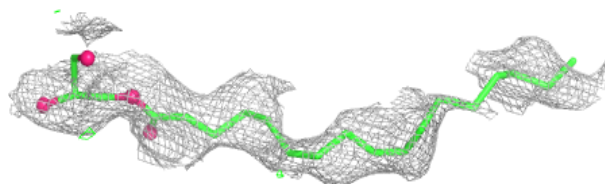


Electron density around OLC B 202:

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

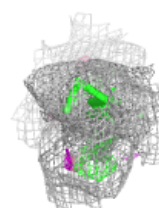
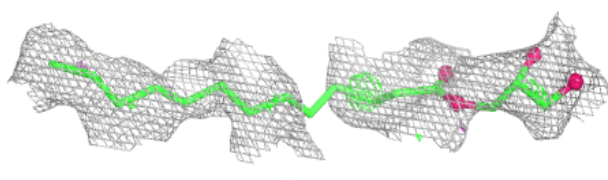
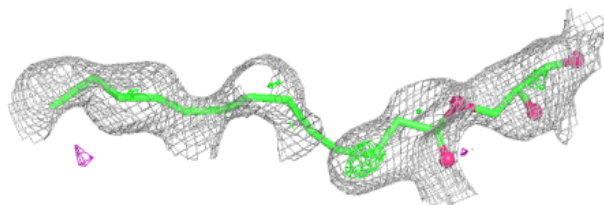
**Electron density around OLC B 203:**

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

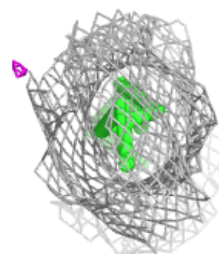
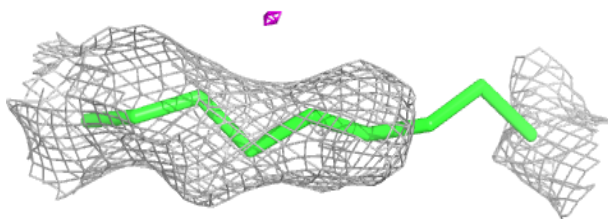
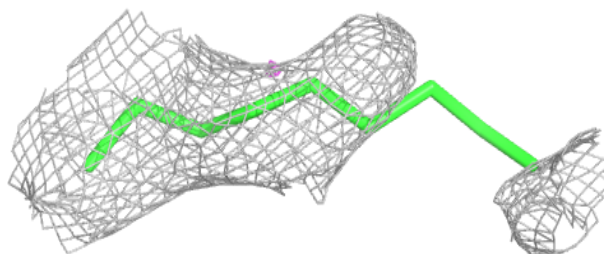


Electron density around OLC A 610:

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

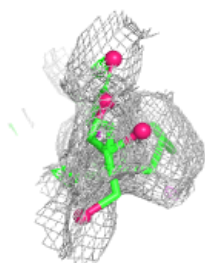
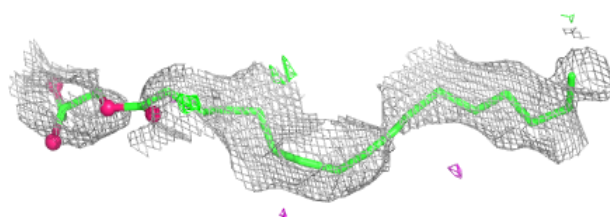
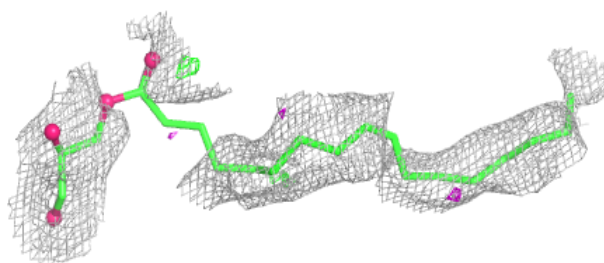
**Electron density around OLC A 613:**

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

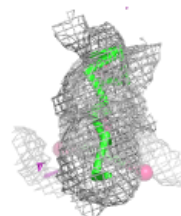
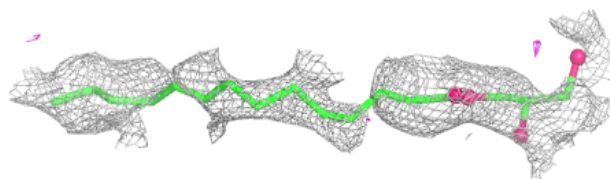
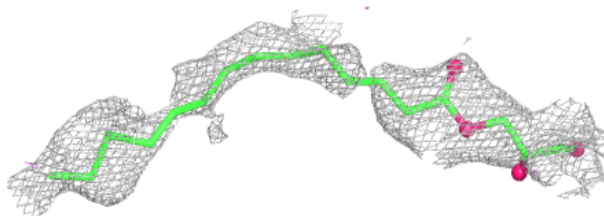


Electron density around OLC C 101:

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

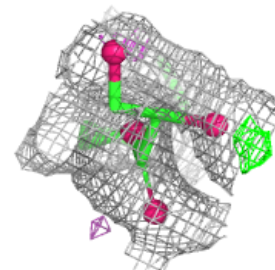
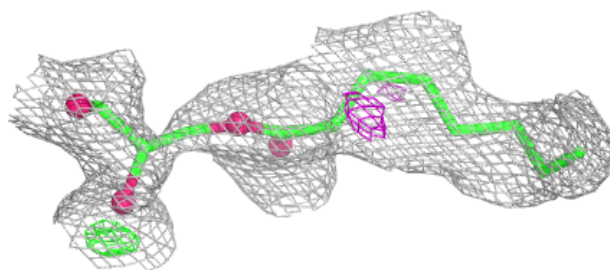
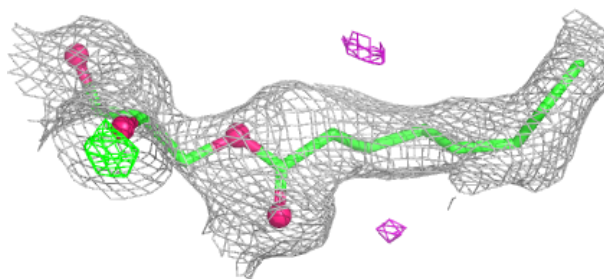
**Electron density around OLC A 611:**

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

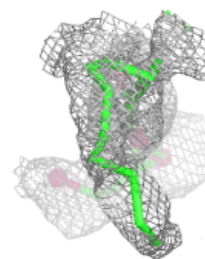
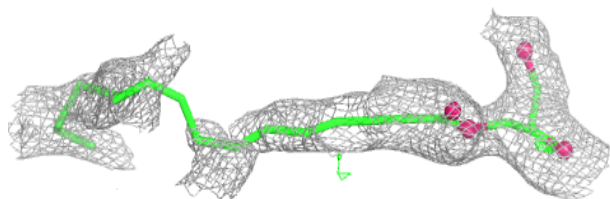
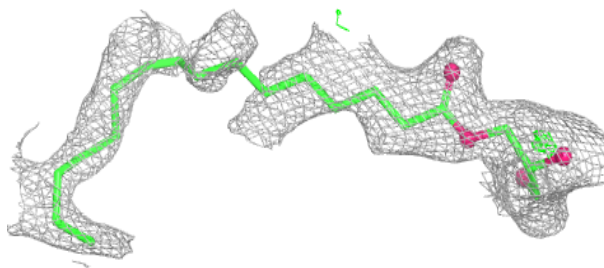


Electron density around OLC A 609:

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

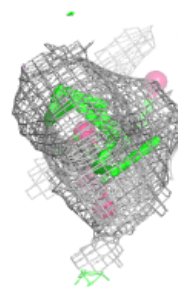
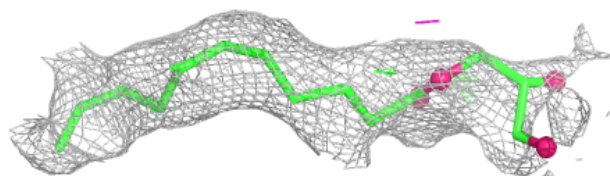
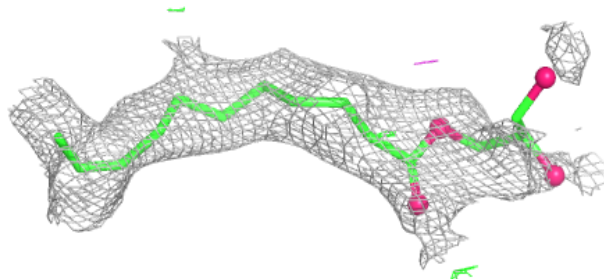
**Electron density around OLC A 604:**

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

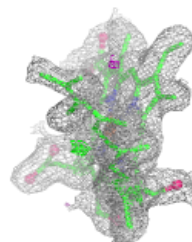
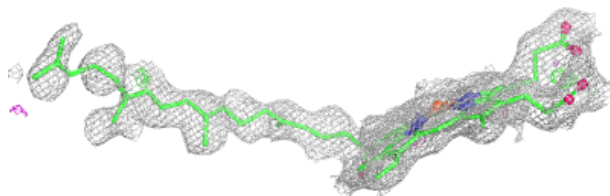
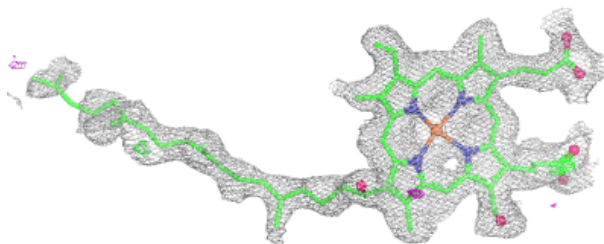


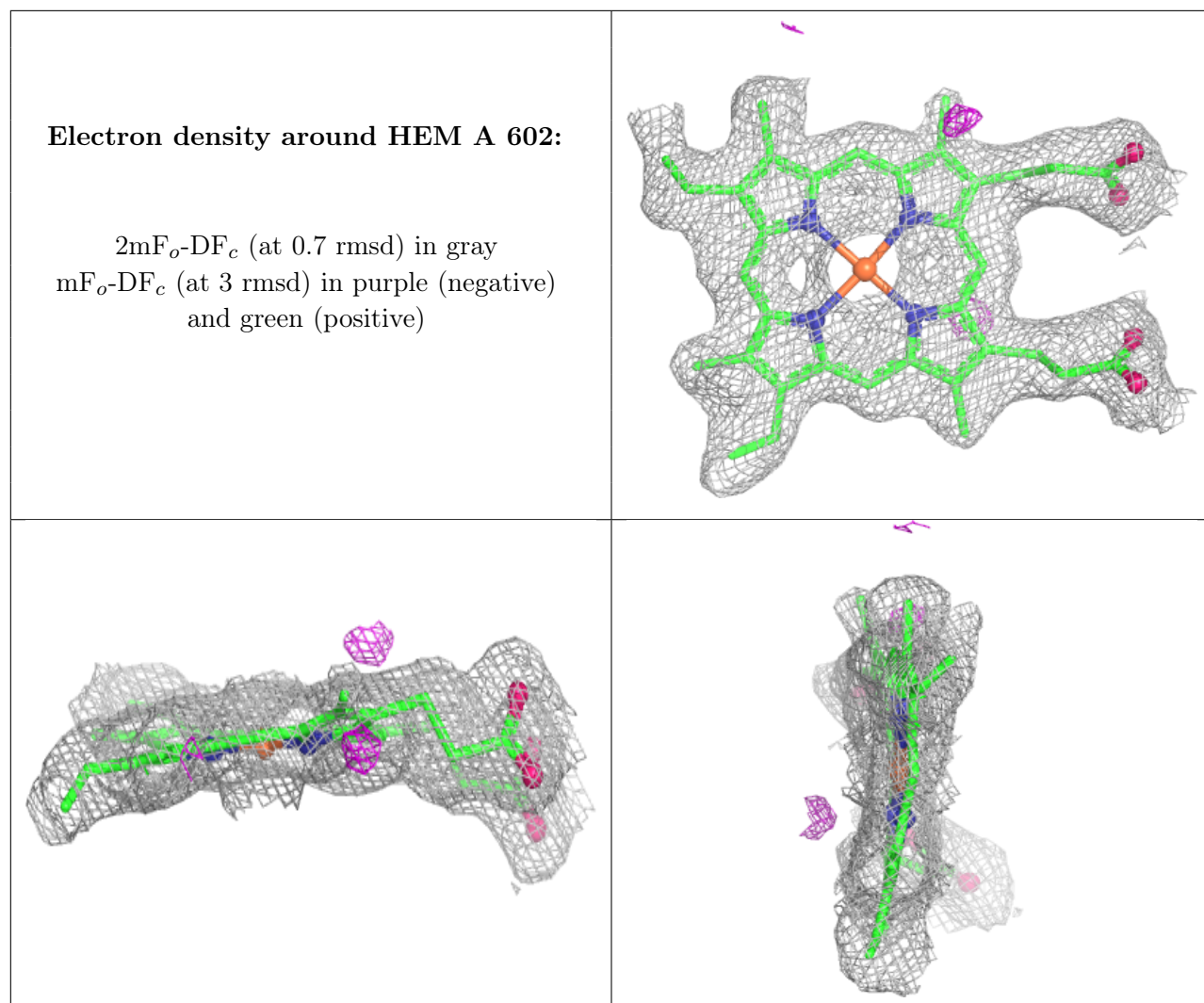
Electron density around OLC A 608:

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

**Electron density around HAS 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.