



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:39 PM UTC

PDB ID : 5NDC / pdb_00005ndc
Title : Structure of ba3-type cytochrome c oxidase from *Thermus thermophilus* by serial femtosecond crystallography
Authors : Andersson, R.; Safari, C.; Dods, R.; Nango, E.; Tanaka, R.; Nakane, T.; Tono, K.; Joti, Y.; Bath, P.; Dunevall, E.; Bosman, E.; Nureki, O.; Iwata, S.; Neutze, R.; Branden, G.
Deposited on : 2017-03-08
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) 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

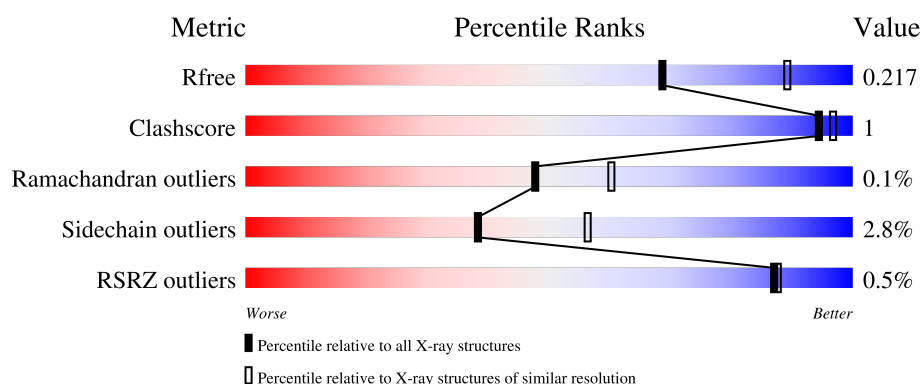
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	569	% 92% 5% .
2	B	168	% 95% . ..
3	C	34	88% . 9%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6386 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			

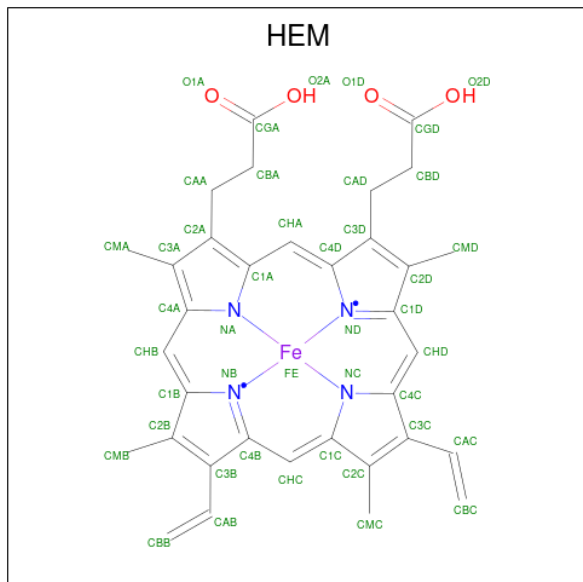
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide IIA.

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).

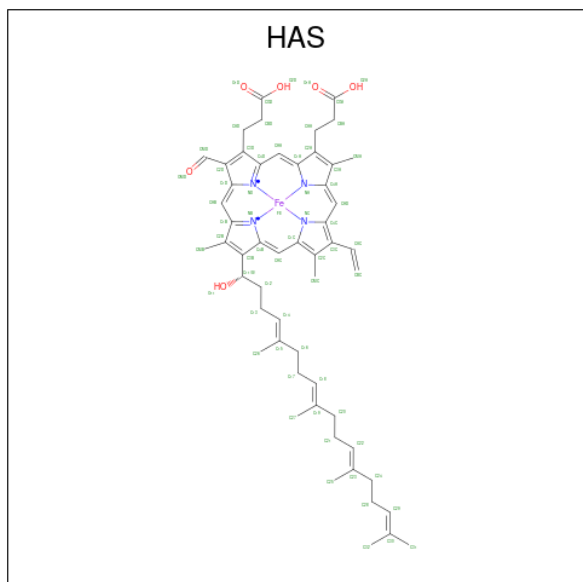
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



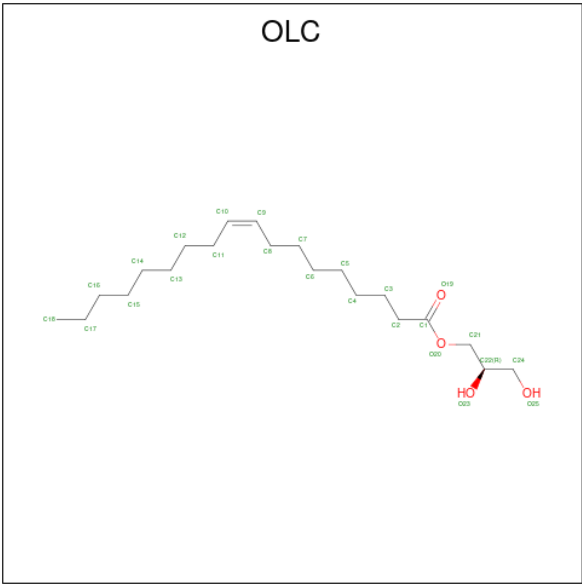
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is HEME-AS (CCD ID: HAS) (formula: $C_{54}H_{64}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

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



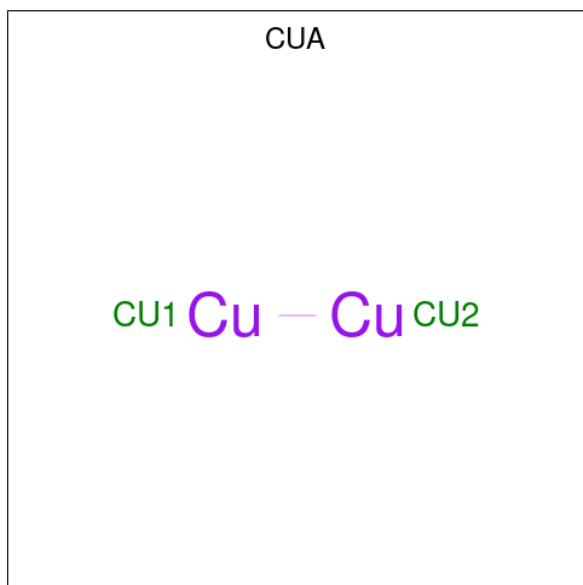
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			23	19	4		
7	A	1	Total	C	O	0	0
			18	14	4		
7	A	1	Total	C	O	0	0
			17	13	4		
7	A	1	Total	C	O	0	0
			15	11	4		
7	A	1	Total	C	O	0	0
			18	14	4		
7	A	1	Total	C	O	0	0
			15	11	4		
7	A	1	Total	C	O	0	0
			20	16	4		
7	A	1	Total	C	O	0	0
			21	17	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	B	1	Total	C	O	0	0
			25	21	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			24	20	4		
7	C	1	Total	C	O	0	0
			15	11	4		
7	C	1	Total	C	O	0	0
			24	20	4		

- Molecule 8 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

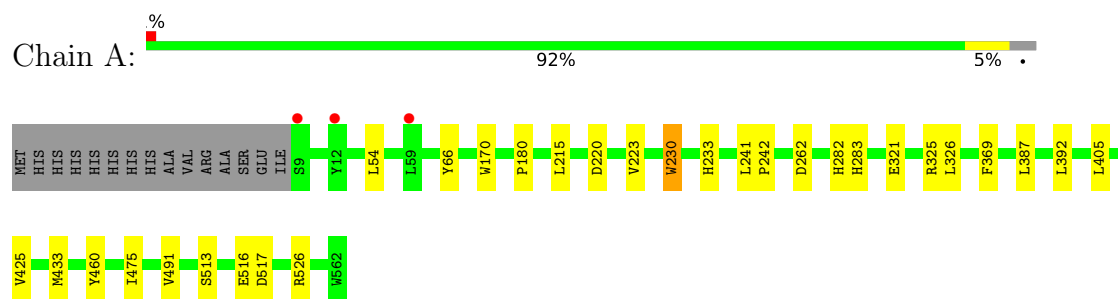
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	58	Total	O	0	0
			58	58		
9	B	34	Total	O	0	0
			34	34		

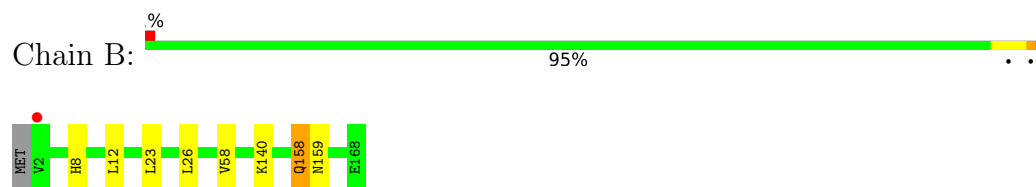
3 Residue-property plots [i](#)

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.

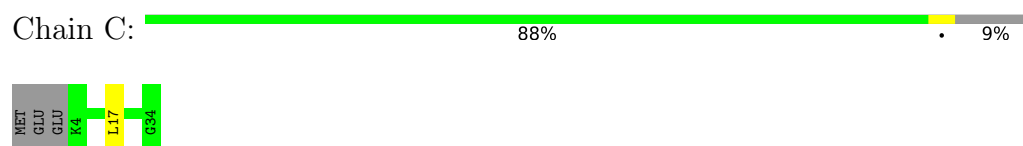
- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 3: Cytochrome c oxidase polypeptide IIA



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)	36.40 – 2.30 36.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.40-2.30) 99.9 (36.40-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.162 , 0.197 (Not available) , 0.217	Depositor DCC
R_{free} test set	2511 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 71.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6386	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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: HEM, HAS, CUA, CU, OLC

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	0.83	0/4525	0.99	3/6213 (0.0%)
2	B	0.80	0/1338	0.87	0/1828
3	C	0.81	0/247	1.02	0/335
All	All	0.83	0/6110	0.96	3/8376 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	HIS	N-CA-CB	8.41	118.38	110.39
1	A	460	TYR	CA-C-N	5.02	124.63	119.05
1	A	460	TYR	C-N-CA	5.02	124.63	119.05

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	4368	0	4467	13	0
2	B	1301	0	1278	2	0
3	C	241	0	267	0	0
4	A	1	0	0	0	0
5	A	43	0	30	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	65	0	62	1	0
7	A	185	0	257	0	0
7	B	25	0	40	0	0
7	C	63	0	89	0	0
8	B	2	0	0	0	0
9	A	58	0	0	1	1
9	B	34	0	0	0	0
All	All	6386	0	6490	16	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 1.

All (16) 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:516:GLU:OE2	2:B:8:HIS:NE2	2.01	0.94
1:A:516:GLU:OE2	1:A:517:ASP:OD1	1.88	0.91
5:A:602:HEM:HBC2	5:A:602:HEM:HMC2	1.72	0.71
6:A:603:HAS:HBC1	6:A:603:HAS:HMC1	1.75	0.67
1:A:321:GLU:OE1	1:A:325:ARG:NH1	2.40	0.52
1:A:516:GLU:CD	1:A:517:ASP:OD1	2.51	0.52
5:A:602:HEM:HBC2	5:A:602:HEM:CMC	2.40	0.50
1:A:387:LEU:HD22	1:A:433:MET:HE1	1.94	0.49
1:A:282:HIS:CD2	1:A:283:HIS:CD2	3.00	0.49
1:A:220:ASP:HB3	1:A:223:VAL:HG12	1.96	0.47
1:A:66:TYR:OH	2:B:158:GLN:NE2	2.50	0.43
1:A:526:ARG:NH2	9:A:703:HOH:O	2.51	0.43
1:A:405:LEU:HD23	1:A:491:VAL:HG11	2.02	0.41
1:A:230:TRP:C	1:A:230:TRP:CD1	2.99	0.41
1:A:170:TRP:CH2	1:A:180:PRO:HD3	2.56	0.40
1:A:241:LEU:N	1:A:242:PRO:CD	2.85	0.40

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)
9:A:706:HOH:O	9:A:706:HOH:O[2_656]	2.06	0.14

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	527/569 (93%)	509 (97%)	17 (3%)	1 (0%)	43	55
2	B	165/168 (98%)	162 (98%)	3 (2%)	0	100	100
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	721/771 (94%)	700 (97%)	20 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	PHE

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	447/463 (96%)	438 (98%)	9 (2%)	48	67
2	B	136/138 (99%)	129 (95%)	7 (5%)	21	32
3	C	24/27 (89%)	23 (96%)	1 (4%)	26	40
All	All	607/628 (97%)	590 (97%)	17 (3%)	38	56

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	215	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	230	TRP
1	A	262	ASP
1	A	326	LEU
1	A	392	LEU
1	A	425	VAL
1	A	475	ILE
1	A	513	SER
2	B	12	LEU
2	B	23	LEU
2	B	26	LEU
2	B	58	VAL
2	B	140	LYS
2	B	158	GLN
2	B	159	ASN
3	C	17	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	455	GLN
1	A	462	HIS
2	B	78	GLN
2	B	91	GLN
2	B	158	GLN

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 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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$
7	OLC	A	614	-	8,8,24	0.33	0	7,7,25	0.34	0
7	OLC	C	101	-	23,23,24	1.00	1 (4%)	24,24,25	0.78	1 (4%)
8	CUA	B	201	2	0,1,1	-	-	-	-	-
7	OLC	A	612	-	19,19,24	1.23	1 (5%)	19,19,25	1.04	2 (10%)
7	OLC	A	613	-	8,8,24	0.26	0	7,7,25	0.46	0
7	OLC	A	607	-	14,14,24	1.36	1 (7%)	15,15,25	1.17	2 (13%)
7	OLC	A	611	-	20,20,24	1.07	1 (5%)	21,21,25	0.84	1 (4%)
6	HAS	A	603	1	72,72,72	2.23	25 (34%)	87,109,109	2.49	28 (32%)
7	OLC	A	610	-	19,19,24	1.20	1 (5%)	20,20,25	1.14	2 (10%)
7	OLC	B	202	-	24,24,24	1.08	1 (4%)	25,25,25	0.89	1 (4%)
7	OLC	A	605	-	17,17,24	1.14	1 (5%)	18,18,25	1.15	2 (11%)
7	OLC	C	102	-	14,14,24	1.36	1 (7%)	15,15,25	1.18	2 (13%)
7	OLC	C	103	-	23,23,24	0.99	1 (4%)	24,24,25	0.98	1 (4%)
7	OLC	A	606	-	16,16,24	1.27	1 (6%)	17,17,25	1.11	3 (17%)
7	OLC	A	608	-	17,17,24	1.22	1 (5%)	18,18,25	1.02	1 (5%)
7	OLC	A	609	-	14,14,24	1.30	1 (7%)	15,15,25	1.02	1 (6%)
7	OLC	A	604	-	22,22,24	1.07	1 (4%)	23,23,25	1.11	2 (8%)
5	HEM	A	602	1	50,50,50	1.58	7 (14%)	67,82,82	1.58	11 (16%)

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	614	-	-	3/6/6/24	-
7	OLC	C	101	-	-	12/23/23/24	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OLC	A	612	-	-	8/18/18/24	-
7	OLC	A	613	-	-	2/6/6/24	-
7	OLC	A	607	-	-	7/14/14/24	-
7	OLC	A	611	-	-	6/20/20/24	-
6	HAS	A	603	1	-	6/42/82/82	-
7	OLC	A	610	-	-	9/19/19/24	-
7	OLC	B	202	-	-	7/24/24/24	-
7	OLC	A	605	-	-	7/17/17/24	-
7	OLC	C	102	-	-	7/14/14/24	-
7	OLC	C	103	-	-	7/23/23/24	-
7	OLC	A	606	-	-	4/16/16/24	-
7	OLC	A	608	-	-	8/17/17/24	-
7	OLC	A	609	-	-	6/14/14/24	-
7	OLC	A	604	-	-	5/22/22/24	-
5	HEM	A	602	1	-	1/14/54/54	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	C3B-C2B	5.46	1.47	1.34
7	A	612	OLC	O20-C1	5.04	1.48	1.33
5	A	602	HEM	FE-NB	4.98	2.10	1.94
6	A	603	HAS	CHB-C1D	4.88	1.48	1.38
6	A	603	HAS	FE-NB	4.87	2.09	1.94
7	C	102	OLC	O20-C1	4.83	1.47	1.33
7	B	202	OLC	O20-C1	4.81	1.47	1.33
7	A	607	OLC	O20-C1	4.74	1.47	1.33
7	A	606	OLC	O20-C1	4.69	1.47	1.33
7	A	610	OLC	O20-C1	4.69	1.47	1.33
7	A	609	OLC	O20-C1	4.62	1.46	1.33
6	A	603	HAS	CHD-C4A	4.58	1.47	1.38
7	A	608	OLC	O20-C1	4.57	1.46	1.33
7	A	604	OLC	O20-C1	4.56	1.46	1.33
7	A	611	OLC	O20-C1	4.55	1.46	1.33
5	A	602	HEM	FE-NC	4.48	2.10	1.95
7	C	103	OLC	O20-C1	4.47	1.46	1.33
7	C	101	OLC	O20-C1	4.41	1.46	1.33
6	A	603	HAS	FE-NC	4.37	2.09	1.95
7	A	605	OLC	O20-C1	4.33	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEM	C1B-NB	-4.31	1.32	1.40
6	A	603	HAS	C4B-NB	-4.16	1.33	1.40
6	A	603	HAS	FE-NA	4.13	2.08	1.95
6	A	603	HAS	CHC-C1C	3.92	1.48	1.39
6	A	603	HAS	FE-ND	3.91	2.07	1.94
6	A	603	HAS	C2A-C3A	3.84	1.45	1.36
6	A	603	HAS	CHD-C4C	3.49	1.47	1.39
6	A	603	HAS	CHA-C1A	3.38	1.45	1.38
6	A	603	HAS	C2D-C3D	3.22	1.44	1.37
6	A	603	HAS	CHC-C4B	3.17	1.44	1.38
6	A	603	HAS	C4B-C3B	2.96	1.49	1.44
6	A	603	HAS	C4A-NA	-2.95	1.34	1.39
6	A	603	HAS	CHB-C1B	2.82	1.45	1.39
5	A	602	HEM	C4B-NB	-2.80	1.33	1.38
6	A	603	HAS	CHA-C4D	2.70	1.45	1.39
6	A	603	HAS	C1D-ND	-2.62	1.35	1.40
6	A	603	HAS	C11-C3B	-2.59	1.48	1.51
6	A	603	HAS	C1A-NA	-2.54	1.34	1.39
5	A	602	HEM	C4D-C3D	2.47	1.49	1.45
6	A	603	HAS	C1C-C2C	2.44	1.48	1.43
6	A	603	HAS	C4C-NC	-2.40	1.35	1.39
6	A	603	HAS	C1C-NC	-2.38	1.35	1.39
5	A	602	HEM	O1D-CGD	2.17	1.29	1.22
5	A	602	HEM	C4D-ND	-2.07	1.36	1.40
6	A	603	HAS	C1B-C2B	2.07	1.48	1.44

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	C2D-C3D-C4D	-8.09	100.57	106.43
6	A	603	HAS	C2B-C1B-NB	6.18	117.05	109.90
6	A	603	HAS	C2A-C1A-NA	5.96	116.08	110.32
6	A	603	HAS	C3D-C4D-ND	5.81	115.96	110.35
6	A	603	HAS	C3B-C4B-NB	5.64	116.33	109.84
6	A	603	HAS	C3C-C4C-NC	5.52	114.45	109.80
5	A	602	HEM	CHC-C4B-NB	5.10	129.91	124.42
6	A	603	HAS	C3C-C2C-C1C	-4.99	101.29	107.17
6	A	603	HAS	C1B-C2B-C3B	-4.68	101.38	106.80
5	A	602	HEM	C1B-NB-C4B	4.55	110.60	105.21
6	A	603	HAS	CAD-C3D-C4D	4.54	132.60	124.70
5	A	602	HEM	CHD-C1D-ND	4.03	128.76	124.42
6	A	603	HAS	OMD-CMD-C2D	-3.71	117.25	125.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	610	OLC	O20-C1-C2	3.70	123.13	111.83
6	A	603	HAS	C1A-C2A-C3A	-3.61	102.35	107.11
5	A	602	HEM	O2A-CGA-CBA	3.53	125.17	114.00
7	A	604	OLC	O20-C1-C2	3.53	122.61	111.83
6	A	603	HAS	CAA-CBA-CGA	-3.51	104.35	113.67
7	A	612	OLC	C21-O20-C1	3.44	127.09	116.07
6	A	603	HAS	C2C-C1C-NC	3.38	115.56	110.14
6	A	603	HAS	CMB-C2B-C1B	3.36	130.28	125.03
7	A	605	OLC	O20-C1-C2	3.33	122.00	111.83
6	A	603	HAS	C3A-C4A-NA	3.23	115.61	109.64
7	A	607	OLC	O20-C1-C2	3.07	121.19	111.83
7	C	103	OLC	O20-C1-C2	3.04	121.09	111.83
6	A	603	HAS	C4B-C3B-C2B	-3.01	102.38	107.44
6	A	603	HAS	CMA-C3A-C4A	2.96	129.95	124.73
7	B	202	OLC	O20-C1-C2	2.96	120.85	111.83
7	A	610	OLC	O20-C1-O19	-2.94	116.28	123.63
7	C	102	OLC	O20-C1-C2	2.89	120.66	111.83
7	A	606	OLC	O20-C1-C2	2.86	120.55	111.83
6	A	603	HAS	CAA-C2A-C1A	2.85	130.65	124.85
6	A	603	HAS	CHB-C1B-C2B	-2.85	120.53	125.03
6	A	603	HAS	C4A-C3A-C2A	-2.79	102.84	106.97
7	A	608	OLC	O20-C1-C2	2.69	120.05	111.83
7	A	605	OLC	O20-C1-O19	-2.67	116.94	123.63
6	A	603	HAS	C32-C30-C31	2.64	120.67	114.59
6	A	603	HAS	CHA-C1A-C2A	-2.63	120.72	124.86
7	A	604	OLC	O20-C1-O19	-2.61	117.11	123.63
6	A	603	HAS	CHA-C4D-C3D	-2.58	121.01	124.77
5	A	602	HEM	CHD-C1D-C2D	-2.58	120.95	125.03
5	A	602	HEM	C3B-C4B-NB	-2.58	107.61	109.47
7	A	611	OLC	O20-C1-C2	2.56	119.64	111.83
5	A	602	HEM	CAD-C3D-C4D	2.55	129.14	124.70
6	A	603	HAS	C4B-NB-C1B	-2.51	102.23	105.21
7	A	607	OLC	O20-C1-O19	-2.51	117.34	123.63
5	A	602	HEM	C1A-CHA-C4D	-2.46	120.45	126.25
5	A	602	HEM	CHA-C4D-C3D	-2.46	120.69	125.23
7	A	609	OLC	O20-C1-C2	2.46	119.34	111.83
6	A	603	HAS	C4C-C3C-C2C	-2.42	104.29	107.30
5	A	602	HEM	CHA-C4D-ND	2.38	127.31	124.37
6	A	603	HAS	CMC-C2C-C1C	2.30	128.93	125.42
5	A	602	HEM	O1A-CGA-CBA	-2.21	116.08	123.09
7	A	612	OLC	O20-C1-C2	2.20	120.46	112.14
6	A	603	HAS	CHD-C4A-C3A	-2.18	120.96	125.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	C27-C19-C20	2.10	118.87	115.23
7	A	606	OLC	O20-C1-O19	-2.05	118.49	123.63
7	A	606	OLC	C21-O20-C1	2.05	124.62	117.12
7	C	102	OLC	C21-O20-C1	2.05	124.61	117.12
7	C	101	OLC	O20-C1-C2	2.04	118.07	111.83

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	603	HAS	C3D-C2D-CMD-OMD
7	A	605	OLC	C21-C22-C24-O25
7	A	608	OLC	C21-C22-C24-O25
7	A	609	OLC	O20-C21-C22-O23
7	A	611	OLC	O20-C21-C22-C24
7	B	202	OLC	C21-C22-C24-O25
7	A	608	OLC	C2-C1-O20-C21
7	A	611	OLC	O20-C21-C22-O23
7	C	102	OLC	C2-C1-O20-C21
7	A	608	OLC	O19-C1-O20-C21
7	C	102	OLC	O19-C1-O20-C21
7	A	612	OLC	C2-C1-O20-C21
7	C	103	OLC	O20-C21-C22-C24
7	C	102	OLC	O20-C21-C22-O23
7	C	103	OLC	O20-C21-C22-O23
7	C	103	OLC	C2-C1-O20-C21
7	A	605	OLC	O23-C22-C24-O25
7	A	609	OLC	O23-C22-C24-O25
7	A	611	OLC	C1-C2-C3-C4
7	C	103	OLC	O19-C1-O20-C21
7	C	101	OLC	C1-C2-C3-C4
7	A	610	OLC	O20-C21-C22-O23
7	C	102	OLC	C1-C2-C3-C4
7	A	612	OLC	O19-C1-O20-C21
7	A	607	OLC	C21-C22-C24-O25
7	A	609	OLC	C21-C22-C24-O25
7	C	102	OLC	C21-C22-C24-O25
7	C	102	OLC	O23-C22-C24-O25
7	A	610	OLC	C2-C3-C4-C5
7	A	605	OLC	C2-C3-C4-C5
7	A	610	OLC	C2-C1-O20-C21
7	A	605	OLC	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	610	OLC	O20-C21-C22-C24
7	A	610	OLC	C5-C6-C7-C8
7	A	606	OLC	C5-C6-C7-C8
7	A	610	OLC	O19-C1-O20-C21
7	A	608	OLC	C2-C3-C4-C5
7	A	614	OLC	C14-C15-C16-C17
7	A	608	OLC	O23-C22-C24-O25
7	B	202	OLC	O23-C22-C24-O25
7	B	202	OLC	C6-C7-C8-C9
7	C	101	OLC	C2-C1-O20-C21
7	A	604	OLC	C12-C13-C14-C15
7	C	101	OLC	C5-C6-C7-C8
7	A	604	OLC	C2-C3-C4-C5
7	C	103	OLC	C10-C11-C12-C13
7	A	612	OLC	C14-C15-C16-C17
7	A	612	OLC	C11-C12-C13-C14
7	A	608	OLC	C3-C4-C5-C6
7	A	607	OLC	O23-C22-C24-O25
7	A	613	OLC	C10-C11-C12-C13
7	C	101	OLC	O19-C1-O20-C21
7	A	609	OLC	C5-C6-C7-C8
7	A	610	OLC	C3-C4-C5-C6
7	C	101	OLC	C11-C12-C13-C14
7	A	607	OLC	C2-C3-C4-C5
7	A	606	OLC	C3-C4-C5-C6
7	B	202	OLC	C3-C4-C5-C6
7	A	612	OLC	C3-C4-C5-C6
7	A	605	OLC	C1-C2-C3-C4
7	A	611	OLC	C11-C12-C13-C14
7	A	609	OLC	O20-C21-C22-C24
7	A	612	OLC	C2-C3-C4-C5
7	A	606	OLC	O19-C1-O20-C21
7	A	606	OLC	C2-C1-O20-C21
7	C	101	OLC	C13-C14-C15-C16
7	A	607	OLC	C1-C2-C3-C4
7	A	614	OLC	C10-C11-C12-C13
7	C	102	OLC	O20-C21-C22-C24
7	C	101	OLC	O20-C21-C22-O23
7	A	608	OLC	C4-C5-C6-C7
7	C	103	OLC	C13-C14-C15-C16
7	A	604	OLC	C13-C14-C15-C16
7	A	610	OLC	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	609	OLC	C1-C2-C3-C4
7	A	612	OLC	C1-C2-C3-C4
7	A	612	OLC	C4-C5-C6-C7
7	A	604	OLC	C10-C11-C12-C13
7	B	202	OLC	C9-C10-C11-C12
7	A	613	OLC	C14-C15-C16-C17
7	A	605	OLC	O20-C21-C22-O23
6	A	603	HAS	C23-C24-C28-C29
7	C	101	OLC	C9-C10-C11-C12
7	C	101	OLC	O20-C21-C22-C24
7	C	101	OLC	C14-C15-C16-C17
6	A	603	HAS	CAA-CBA-CGA-O1A
7	C	103	OLC	C7-C8-C9-C10
6	A	603	HAS	CAA-CBA-CGA-O2A
6	A	603	HAS	CAD-CBD-CGD-O1D
6	A	603	HAS	CAD-CBD-CGD-O2D
7	B	202	OLC	O19-C1-O20-C21
7	C	101	OLC	C6-C7-C8-C9
7	A	608	OLC	C7-C8-C9-C10
7	A	611	OLC	C7-C8-C9-C10
7	A	607	OLC	C2-C1-O20-C21
7	B	202	OLC	C2-C1-O20-C21
7	C	101	OLC	C7-C8-C9-C10
7	A	604	OLC	C7-C8-C9-C10
7	A	605	OLC	C7-C8-C9-C10
7	A	610	OLC	C9-C10-C11-C12
7	A	614	OLC	C11-C12-C13-C14
7	A	607	OLC	O19-C1-O20-C21
7	A	607	OLC	O20-C1-C2-C3
5	A	602	HEM	CAD-CBD-CGD-O2D
7	A	611	OLC	C4-C5-C6-C7

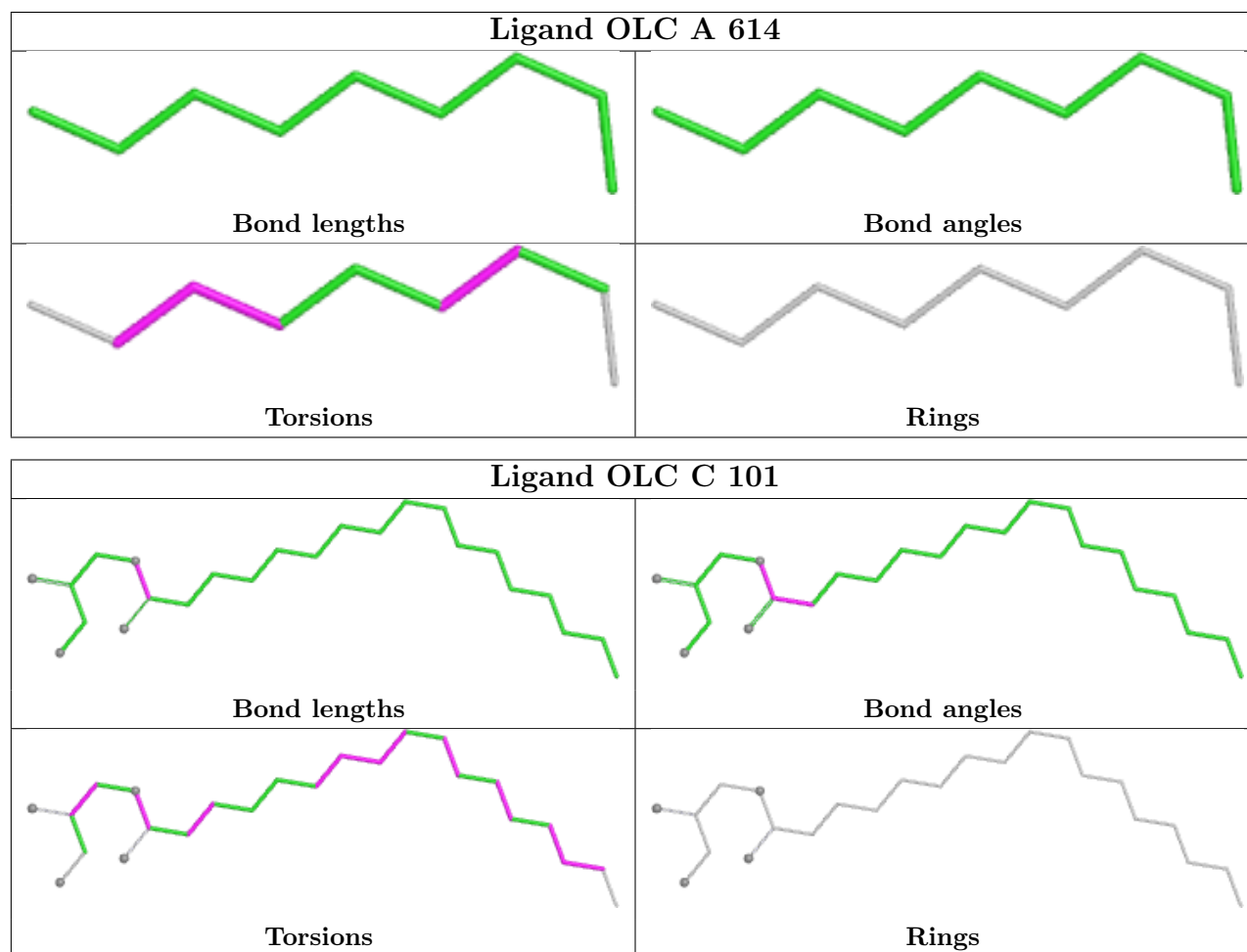
There are no ring outliers.

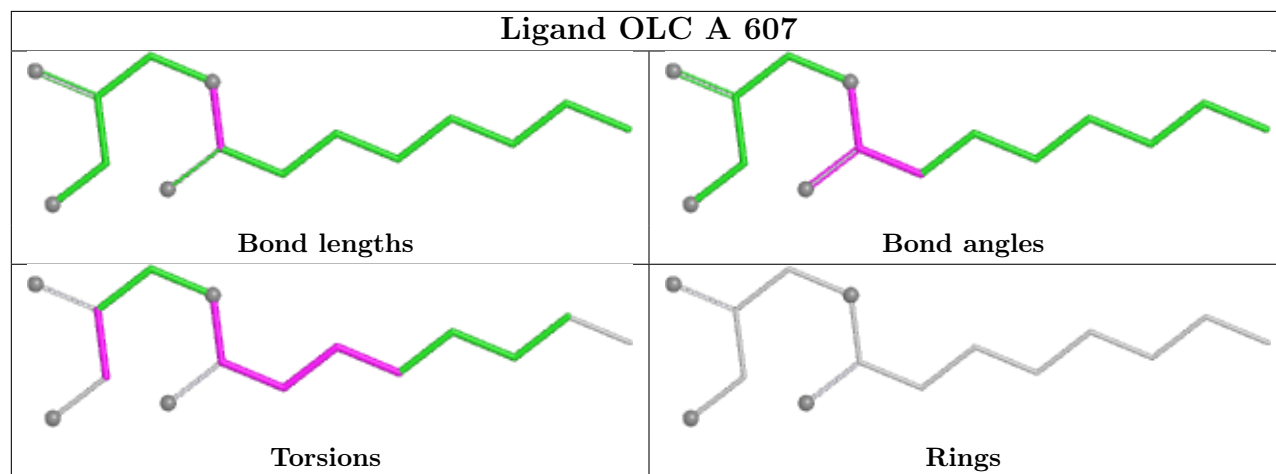
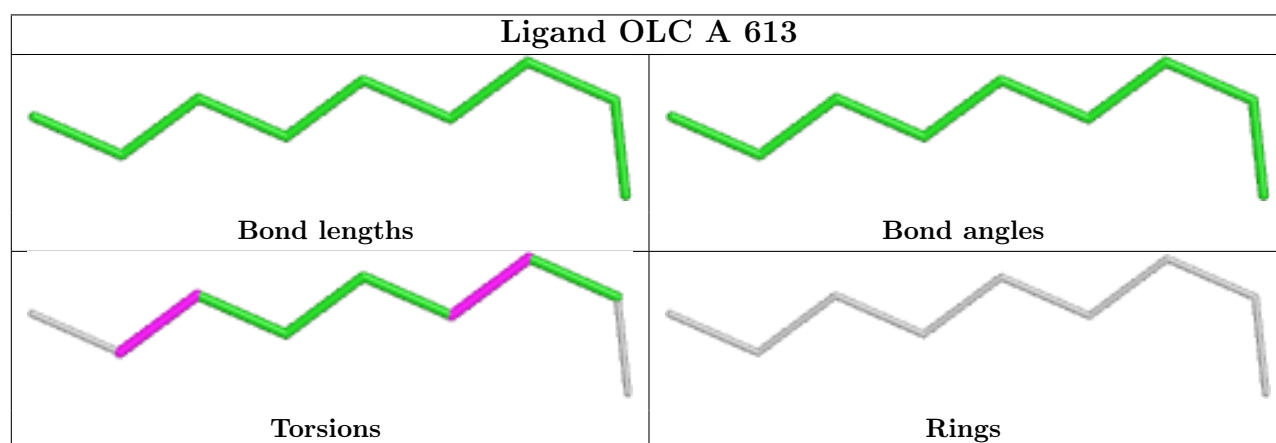
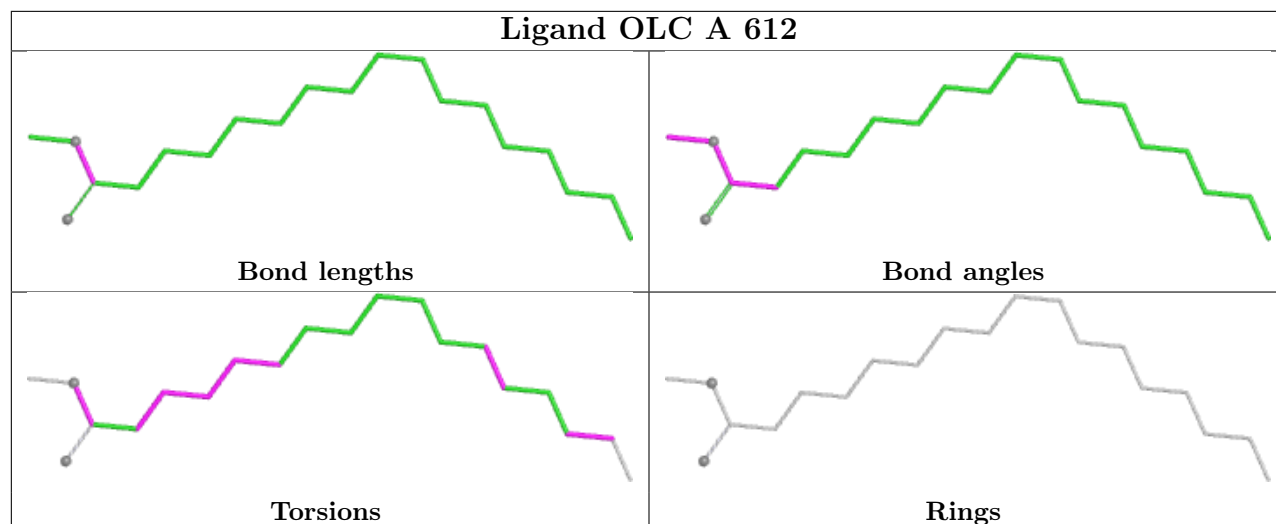
2 monomers are involved in 3 short contacts:

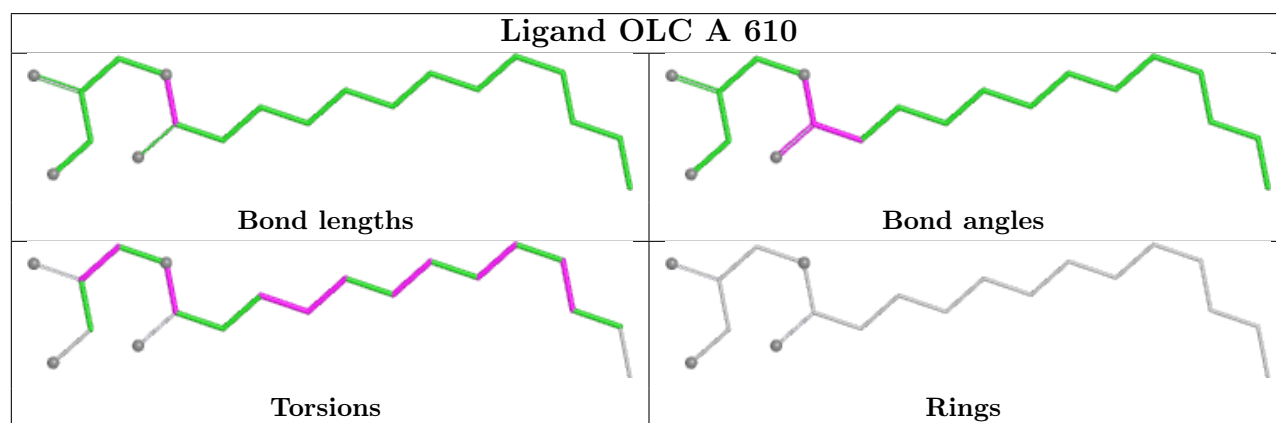
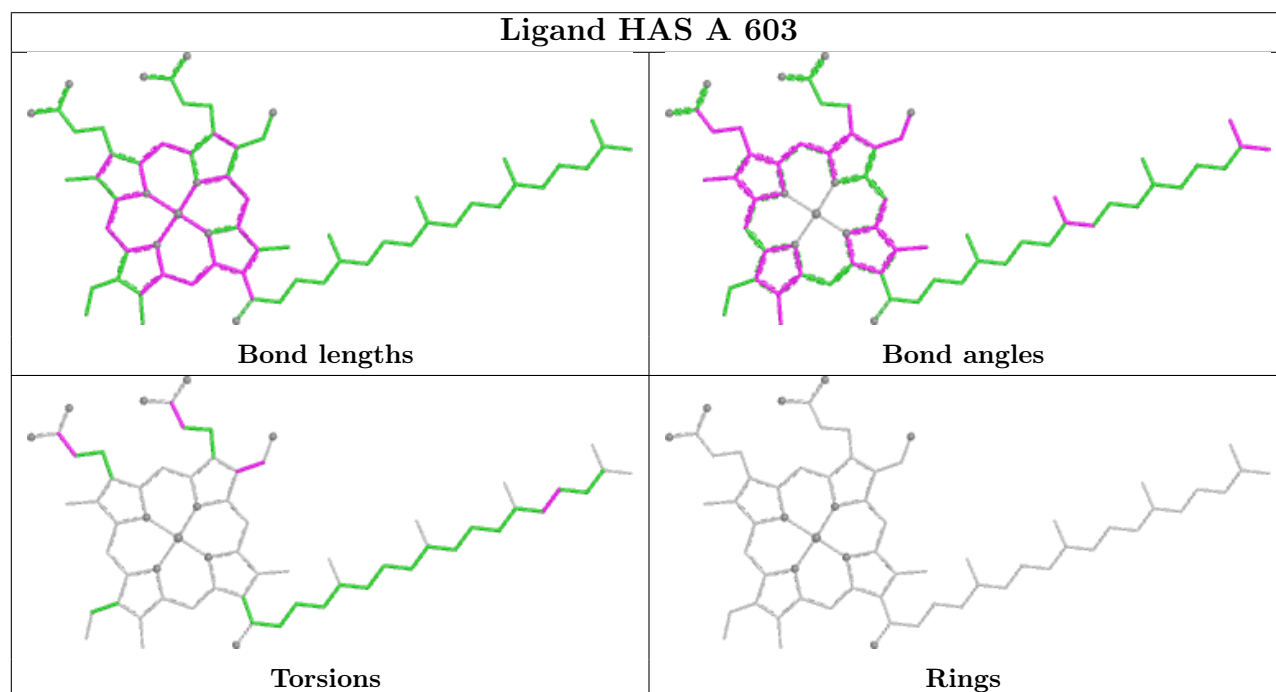
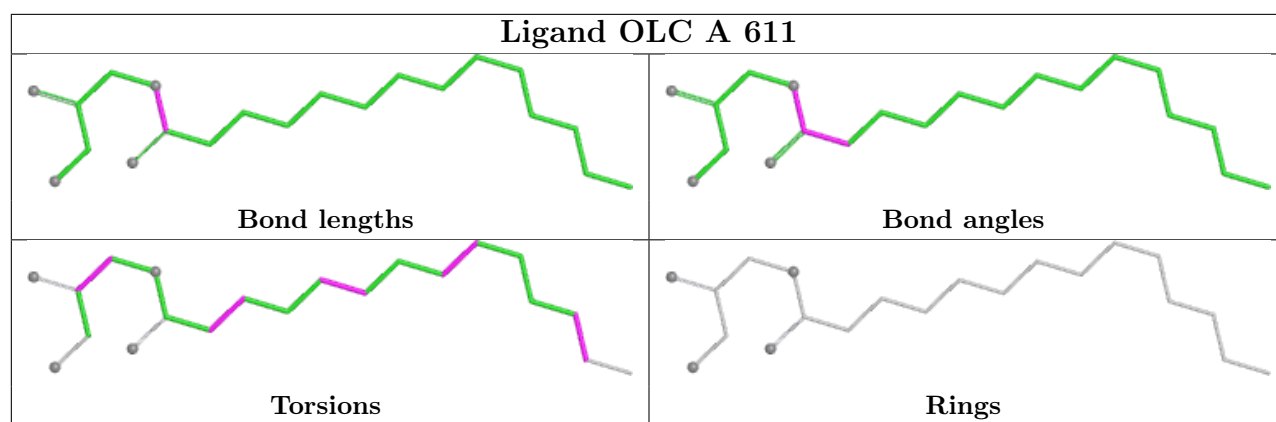
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	HAS	1	0
5	A	602	HEM	2	0

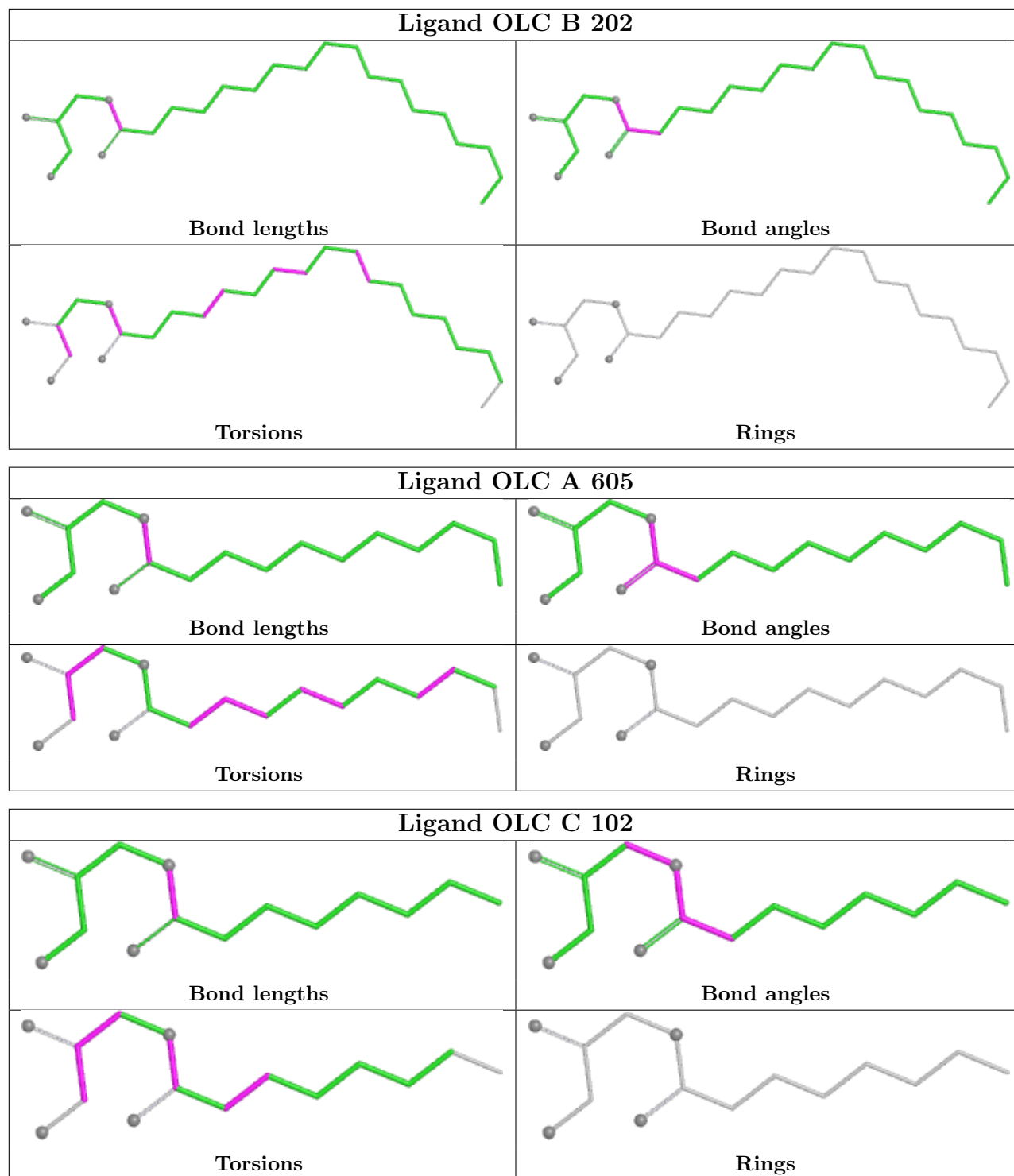
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

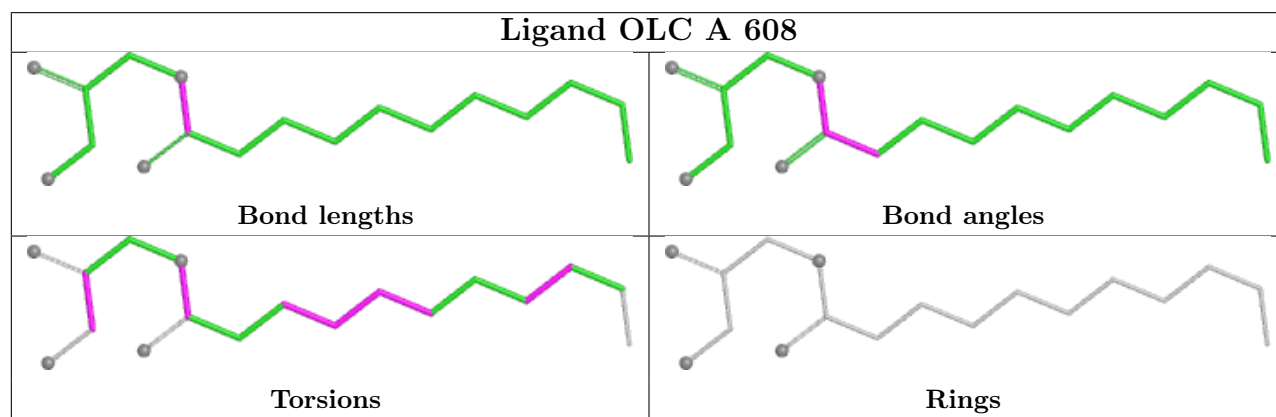
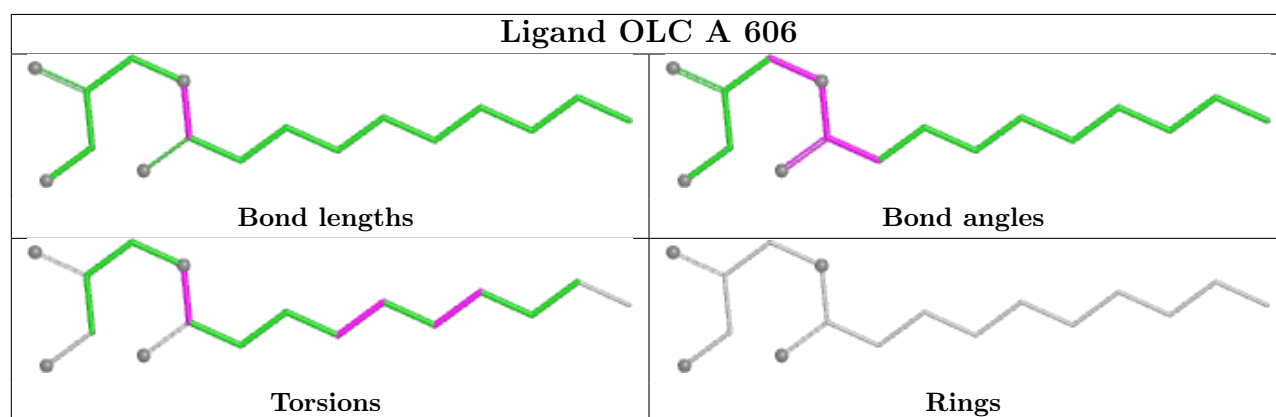
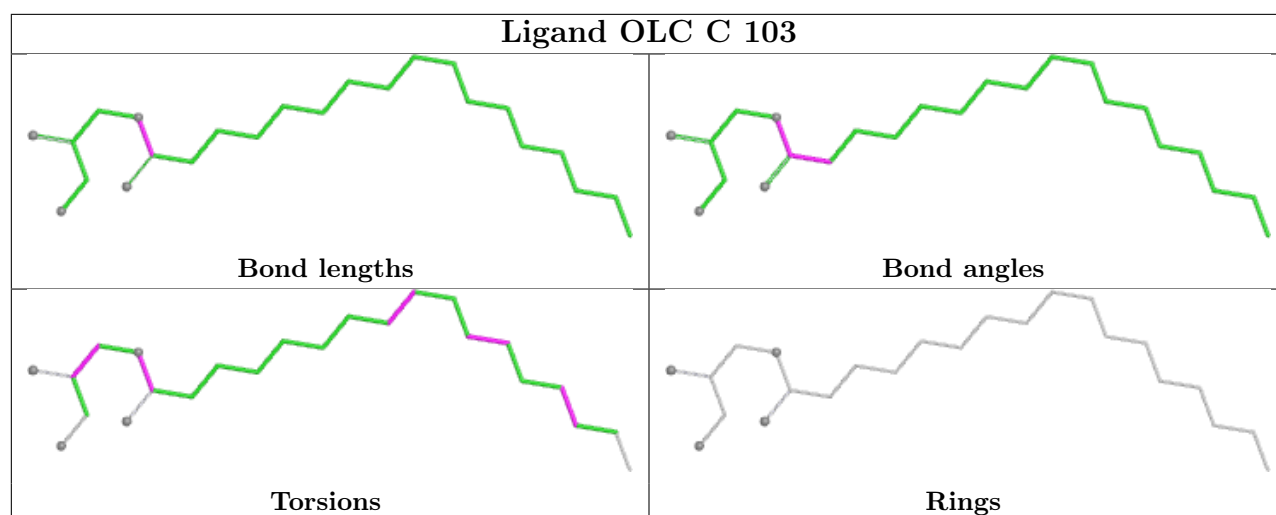
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

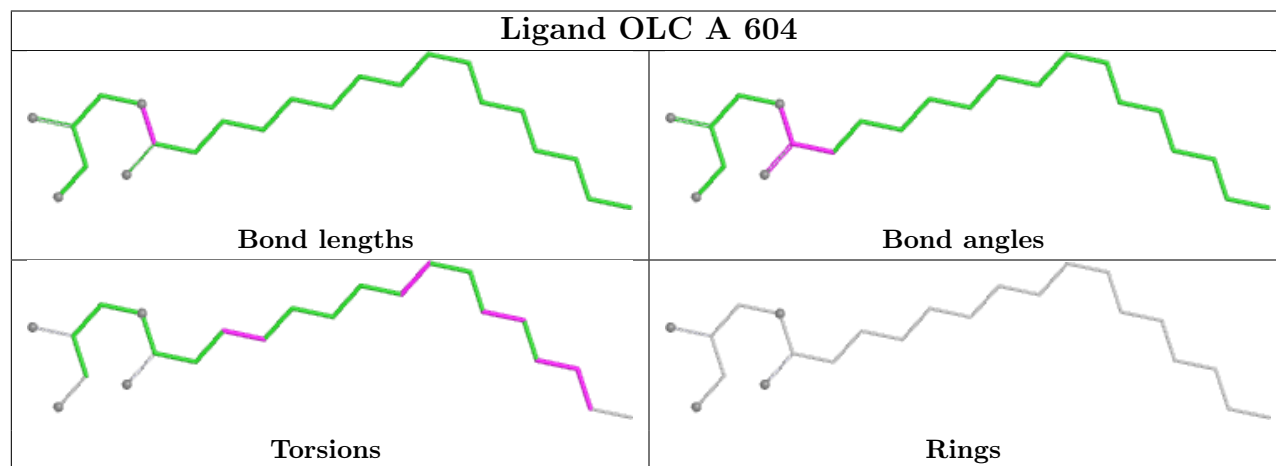
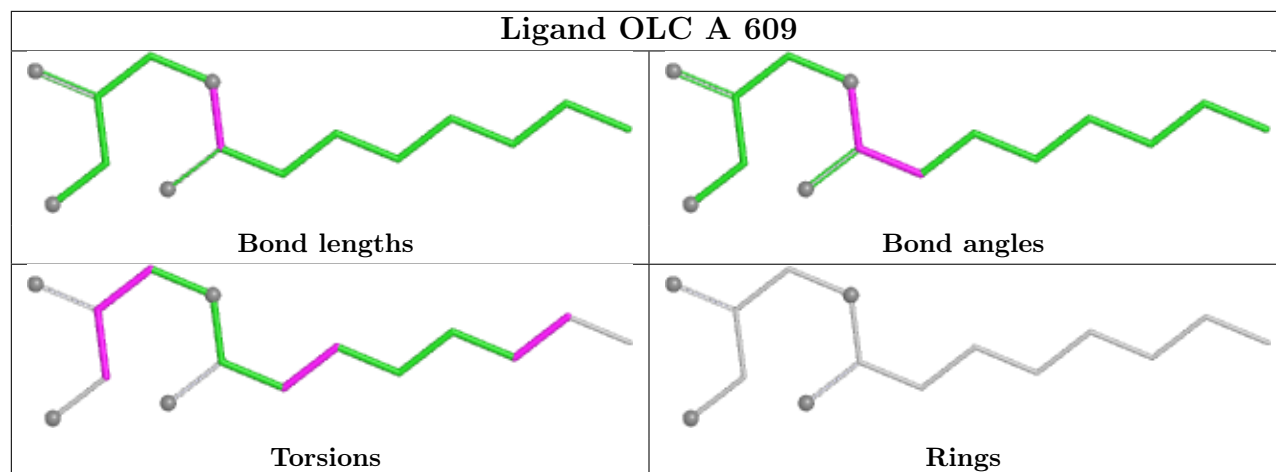


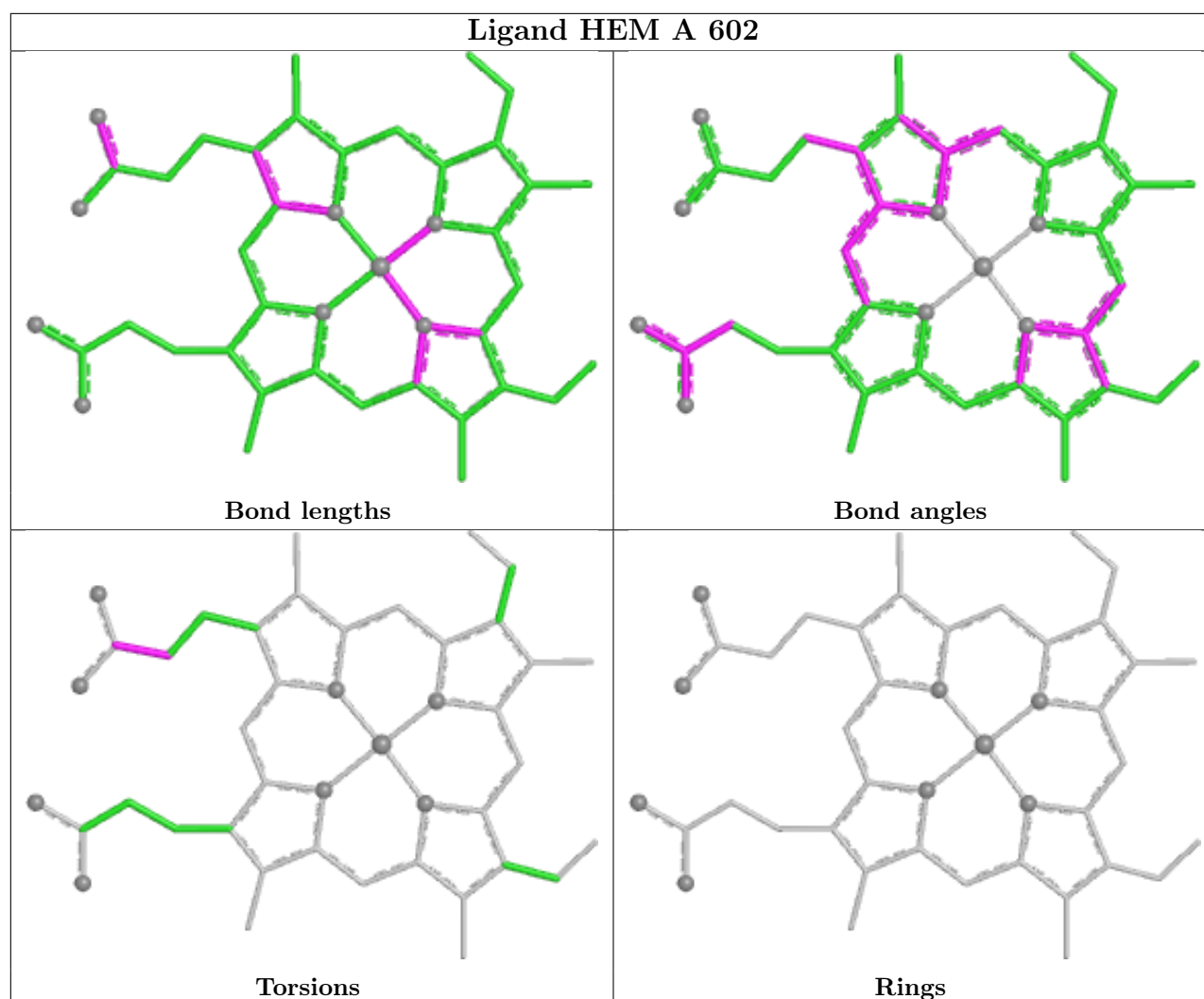












5.7 Other polymers [i](#)

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%)	-0.07	3 (0%) 87 87	35, 47, 77, 114	0
2	B	167/168 (99%)	-0.22	1 (0%) 85 86	35, 47, 70, 110	0
3	C	31/34 (91%)	-0.23	0 100 100	42, 47, 61, 76	0
All	All	752/771 (97%)	-0.11	4 (0%) 87 87	35, 47, 75, 114	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	VAL	5.9
1	A	9	SER	2.9
1	A	59	LEU	2.7
1	A	12	TYR	2.7

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](#)

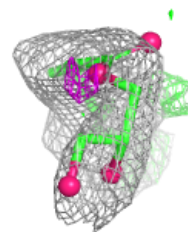
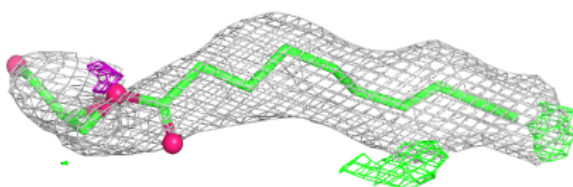
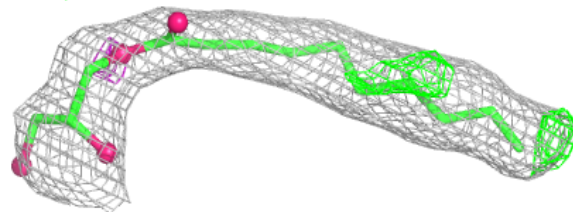
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	606	17/25	0.77	0.20	77,85,100,102	0
7	OLC	A	610	20/25	0.77	0.19	75,81,90,91	0
7	OLC	A	607	15/25	0.78	0.19	69,79,84,85	0
7	OLC	C	102	15/25	0.79	0.22	90,95,99,103	0
7	OLC	A	612	20/25	0.80	0.17	72,76,87,87	0
7	OLC	A	605	18/25	0.82	0.17	74,79,84,90	0
7	OLC	A	611	21/25	0.83	0.17	75,82,87,88	0
7	OLC	A	609	15/25	0.84	0.16	77,80,89,90	0
7	OLC	B	202	25/25	0.85	0.15	66,69,90,93	0
7	OLC	A	608	18/25	0.85	0.16	65,72,94,94	0
7	OLC	C	101	24/25	0.86	0.18	79,87,103,105	0
7	OLC	C	103	24/25	0.87	0.16	74,83,86,87	0
7	OLC	A	614	9/25	0.88	0.19	73,75,82,82	0
7	OLC	A	604	23/25	0.89	0.14	49,61,87,88	0
7	OLC	A	613	9/25	0.94	0.17	79,81,85,86	0
6	HAS	A	603	65/65	0.98	0.07	29,35,49,53	0
5	HEM	A	602	43/43	0.98	0.06	28,33,37,42	0
8	CUA	B	201	2/2	0.99	0.04	32,32,32,33	0
4	CU	A	601	1/1	1.00	0.02	35,35,35,35	0

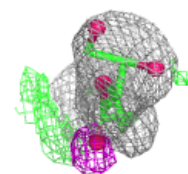
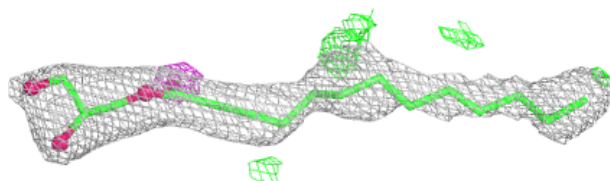
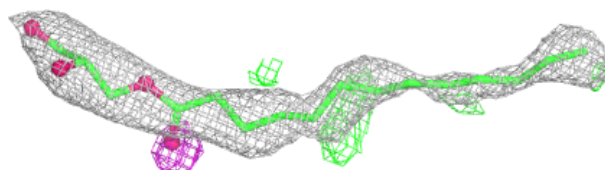
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 606:

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

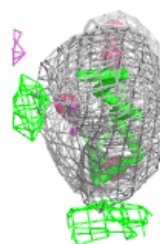
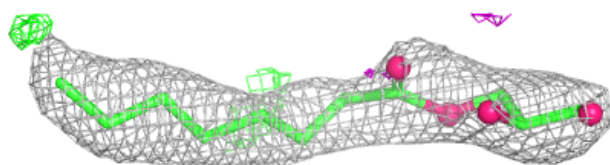
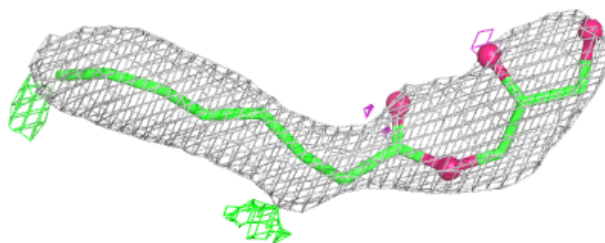
**Electron density around OLC A 610:**

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

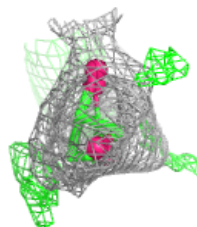
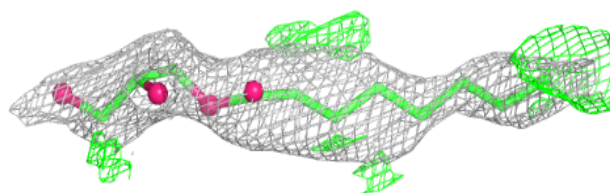
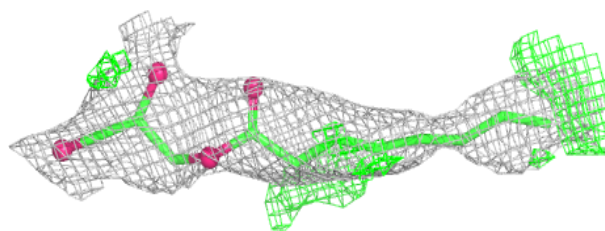


Electron density around OLC A 607:

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

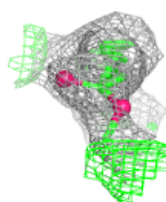
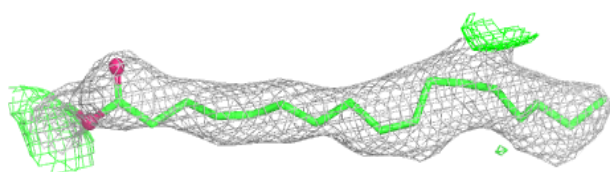
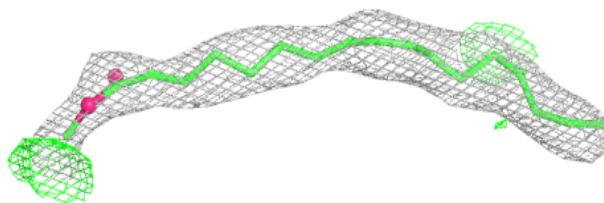
**Electron density around OLC C 102:**

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

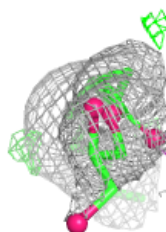
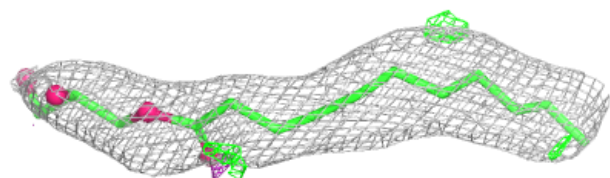
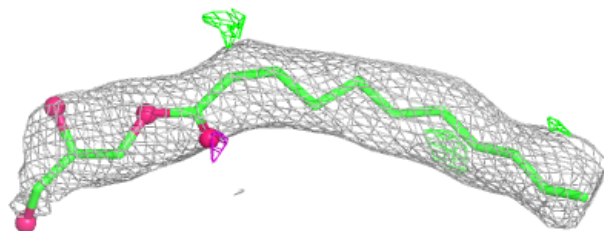


Electron density around OLC A 612:

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

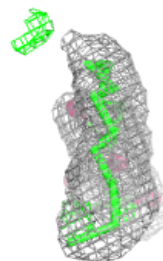
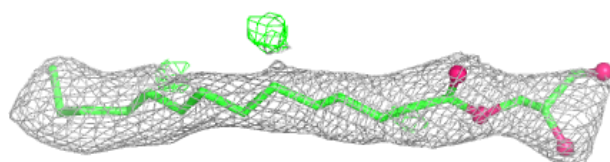
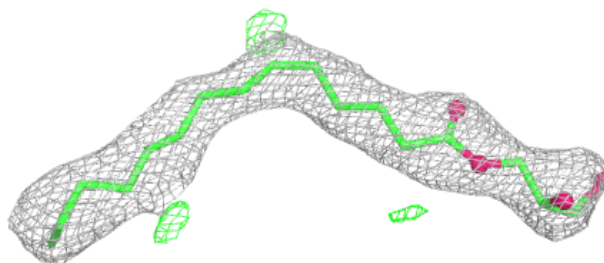
**Electron density around OLC A 605:**

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

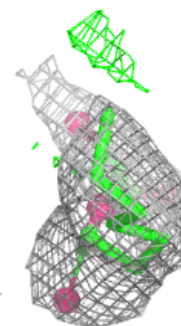
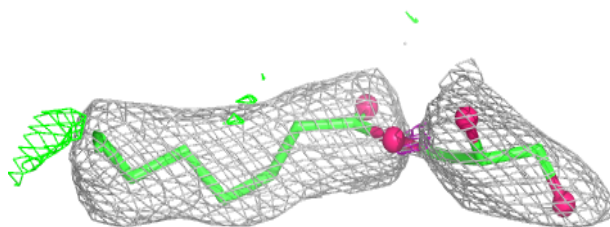
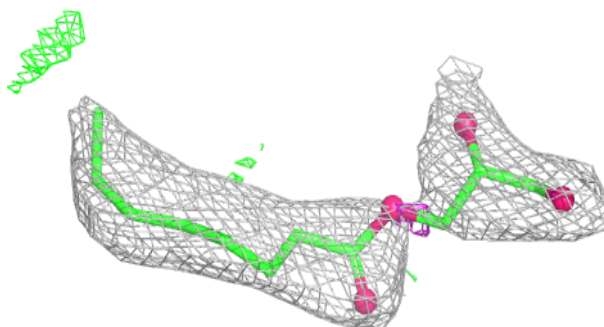


Electron density around OLC A 611:

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

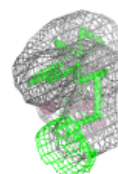
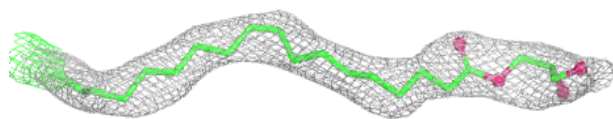
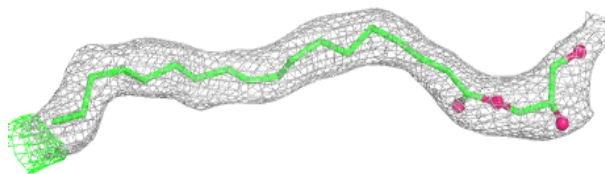
**Electron density around OLC A 609:**

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

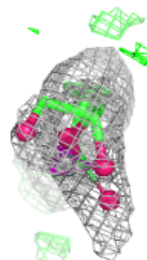
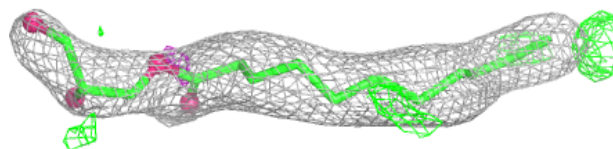
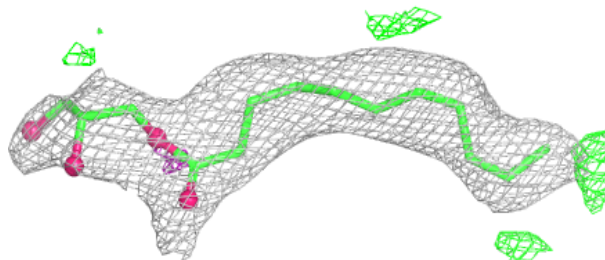


Electron density around OLC B 202:

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

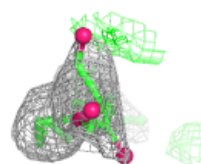
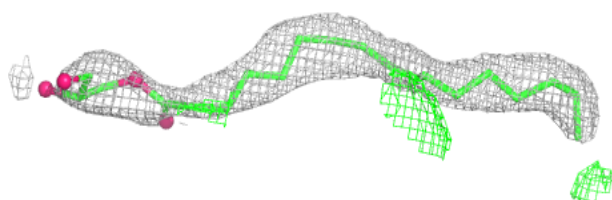
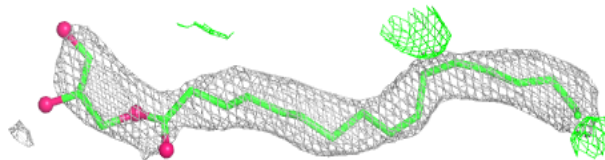
**Electron density around OLC A 608:**

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

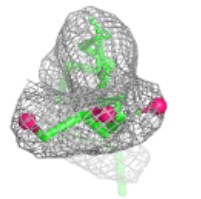
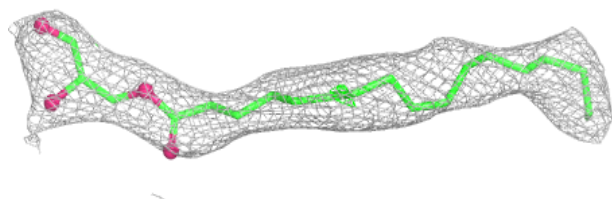
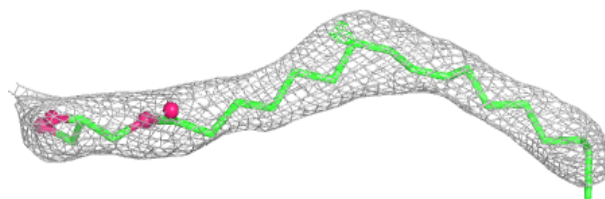


Electron density around OLC C 101:

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

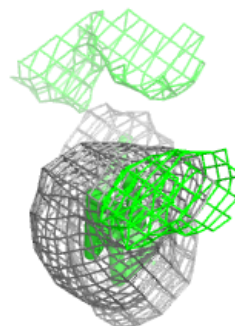
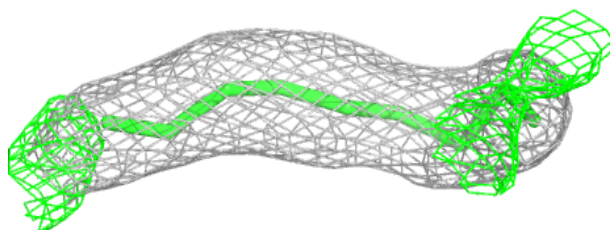
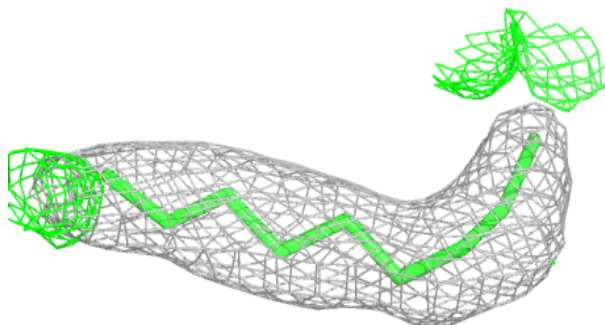
**Electron density around OLC C 103:**

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

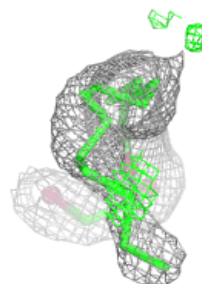
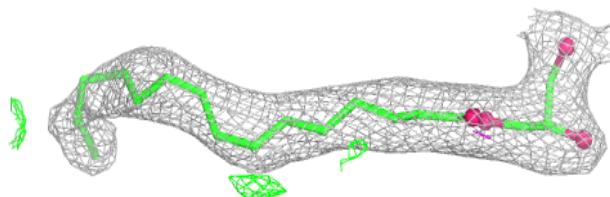
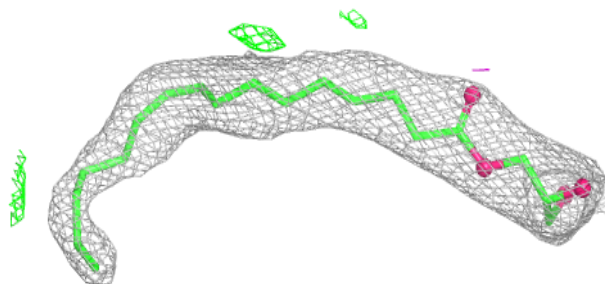


Electron density around OLC A 614:

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

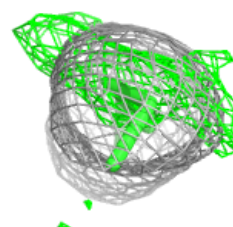
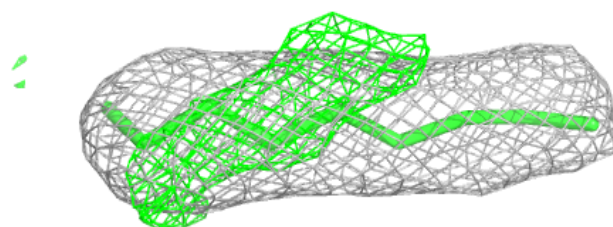
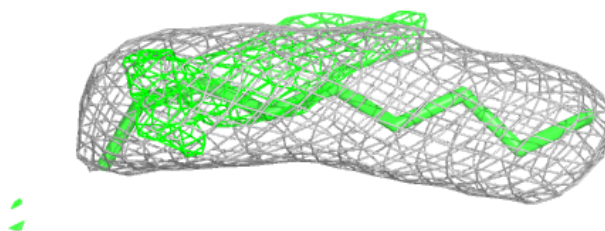
**Electron density around OLC A 604:**

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

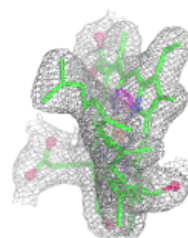
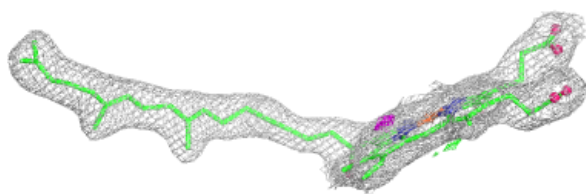
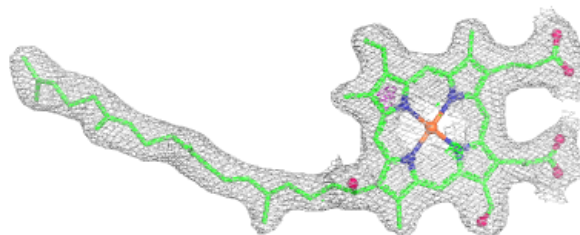


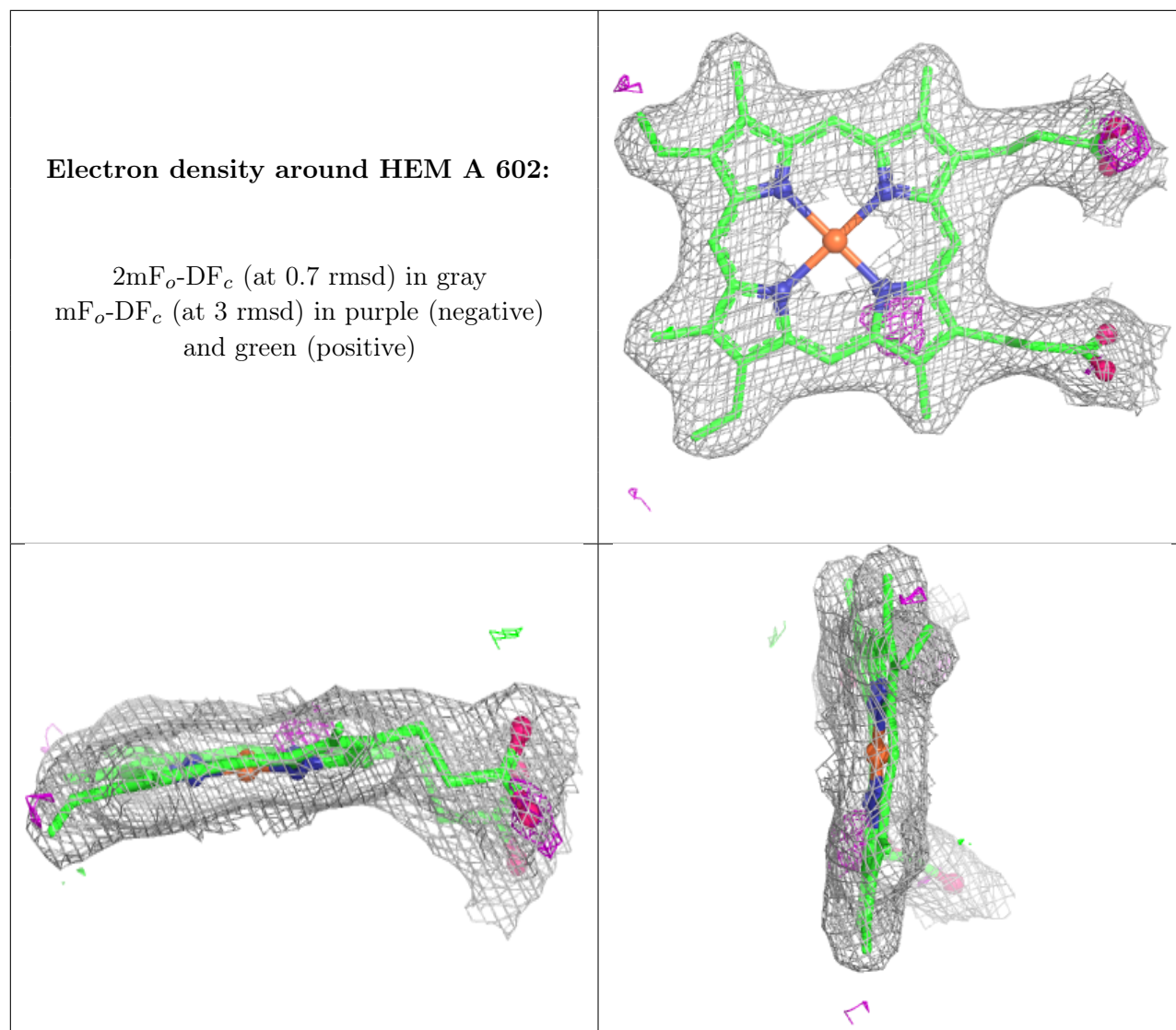
Electron density around OLC A 613:

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

**Electron density around 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.