



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:45 AM UTC

PDB ID : 8K65 / pdb_00008k65
Title : Serial femtosecond crystallography structure of CO bound ba3- type cytochrome c oxidase without pump laser irradiation
Authors : Safari, C.; Ghosh, S.; Andersson, R.; Johannesson, J.; Donoso, A.V.; Bath, P.; Zoric, D.; Sandelin, E.; Nango, E.; Tanaka, R.; Iwata, S.; Neutze, R.; Branden, G.
Deposited on : 2023-07-25
Resolution : 2.00 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

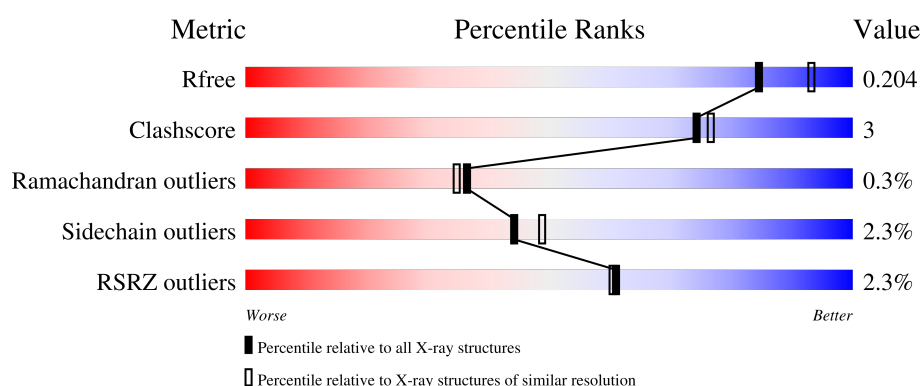
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	2% 90% 7% ••
2	B	168	2% 90% 9% •
3	C	34	3% 82% 9% 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	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6487 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			

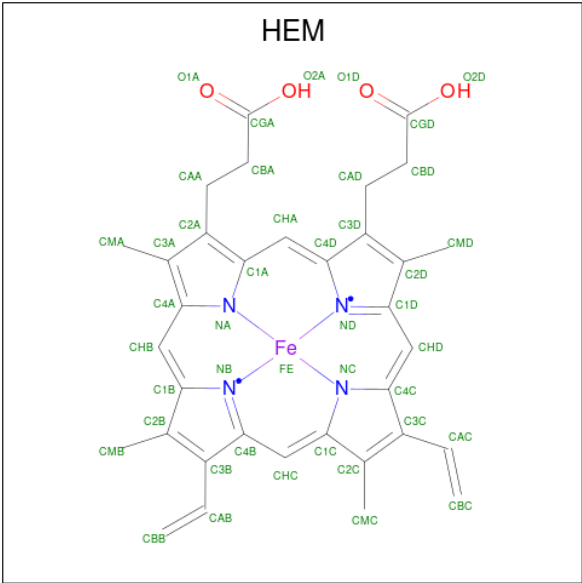
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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) (labeled as "Ligand of Interest" by depositor).

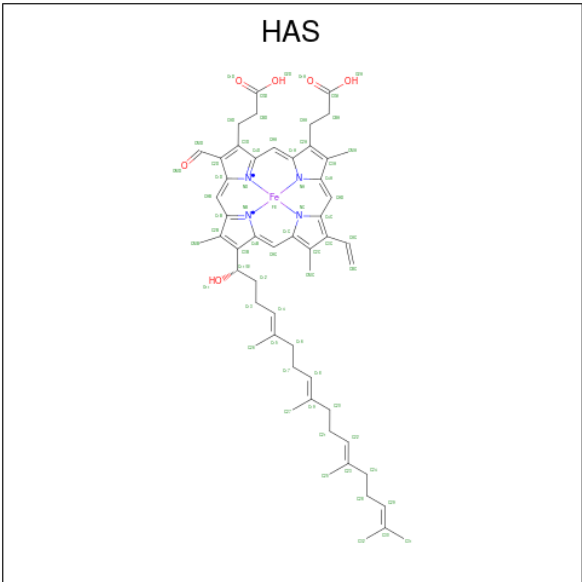
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



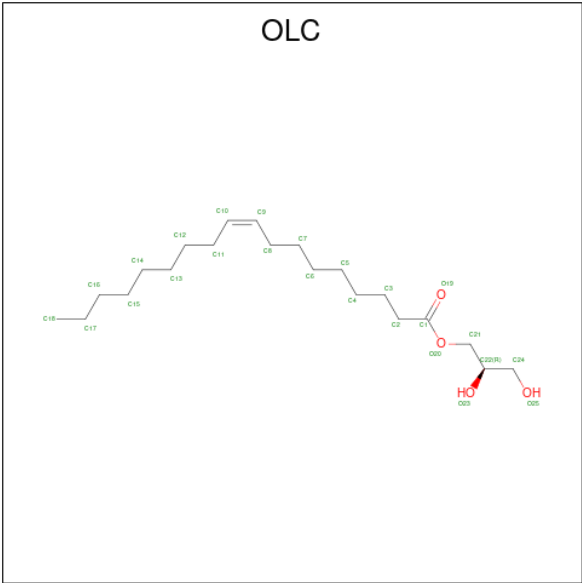
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is HEME-AS (CCD ID: HAS) (formula: $C_{54}H_{64}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄) (labeled as "Ligand of Interest" by depositor).



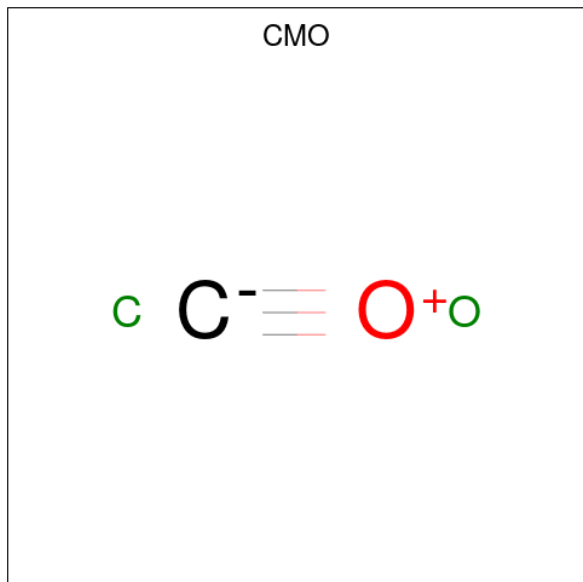
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			23	19	4		
7	A	1	Total	C	O	0	0
			18	14	4		
7	A	1	Total	C	O	0	0
			17	13	4		
7	A	1	Total	C	O	0	0
			15	11	4		
7	A	1	Total	C	O	0	0
			18	14	4		
7	A	1	Total	C	O	0	0
			15	11	4		
7	A	1	Total	C	O	0	0
			20	16	4		
7	A	1	Total	C	O	0	0
			21	17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

Continued on next page...

Continued from previous page...

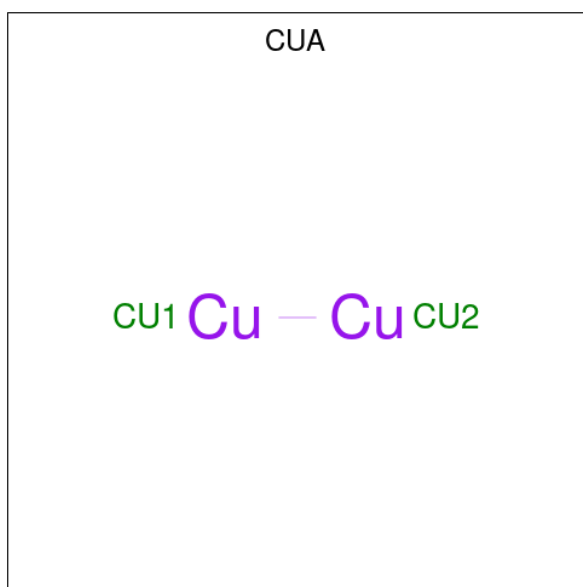
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			20	18	2		
7	B	1	Total	C	O	0	0
			25	21	4		
7	B	1	Total	C	O	0	0
			24	20	4		
7	C	1	Total	C	O	0	0
			24	20	4		
7	C	1	Total	C	O	0	0
			15	11	4		

- Molecule 8 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO) (labeled as "Ligand of Interest" by depositor).



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) (labeled as "Ligand of Interest" by depositor).



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

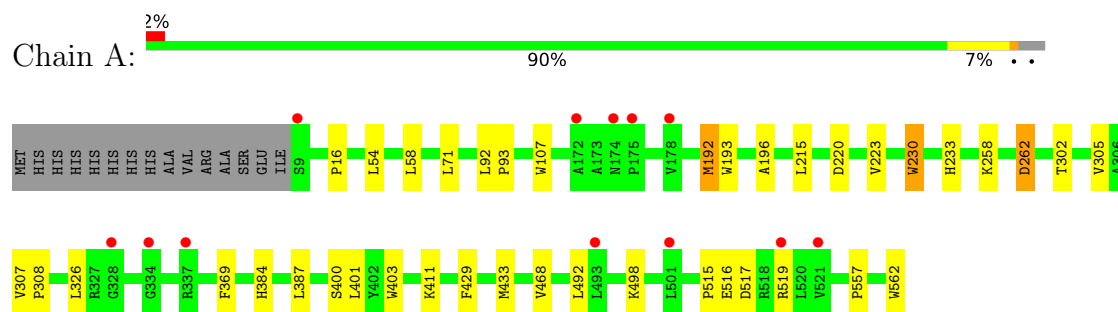
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	99	Total O 100 100	0	1
10	B	88	Total O 88 88	0	0
10	C	3	Total O 3 3	0	0

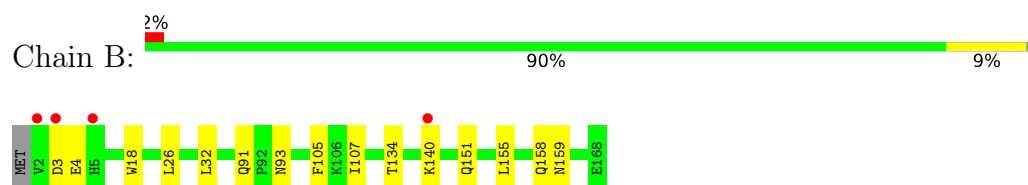
3 Residue-property plots [i](#)

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

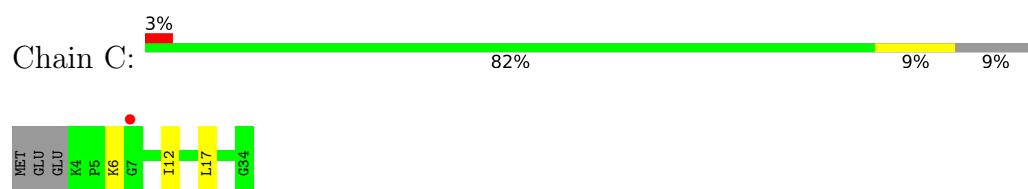
- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 3: Cytochrome c oxidase polypeptide 2A



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)	37.20 – 2.00 37.20 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.20-2.00) 100.0 (37.20-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.00Å)	Xtriage
Refinement program	REFMAC v8.0	Depositor
R, R_{free}	0.170 , 0.196 0.179 , 0.204	Depositor DCC
R_{free} test set	3773 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6487	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 3.83% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CMO, HAS, HEM, 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	1.12	4/4525 (0.1%)	1.37	6/6213 (0.1%)
2	B	1.16	1/1338 (0.1%)	1.20	0/1828
3	C	1.07	0/247	1.44	2/335 (0.6%)
All	All	1.13	5/6110 (0.1%)	1.34	8/8376 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	151	GLN	C-O	8.01	1.33	1.24
1	A	233	HIS	CE1-NE2	6.74	1.39	1.32
1	A	71	LEU	C-O	5.64	1.30	1.24
1	A	16	PRO	C-O	-5.44	1.17	1.24
1	A	384	HIS	CE1-NE2	5.27	1.37	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	HIS	N-CA-CB	9.23	119.16	110.39
1	A	233	HIS	CA-CB-CG	-8.19	105.61	113.80
1	A	557	PRO	CA-C-N	5.82	126.48	120.60
1	A	557	PRO	C-N-CA	5.82	126.48	120.60
1	A	515	PRO	CA-C-N	5.77	128.28	120.38
1	A	515	PRO	C-N-CA	5.77	128.28	120.38
3	C	6	LYS	CA-C-N	5.19	125.70	119.94
3	C	6	LYS	C-N-CA	5.19	125.70	119.94

There are no chirality outliers.

There are no planarity outliers.

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	29	0
2	B	1301	0	1278	10	0
3	C	241	0	267	1	0
4	A	1	0	0	0	0
5	A	43	0	30	1	0
6	A	65	0	62	1	0
7	A	165	0	229	2	0
7	B	69	0	103	2	0
7	C	39	0	54	0	0
8	A	2	0	0	0	0
9	B	2	0	0	0	0
10	A	100	0	0	1	0
10	B	88	0	0	4	0
10	C	3	0	0	0	0
All	All	6487	0	6490	39	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.

All (39) 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:192:MET:CE	1:A:196:ALA:HB2	1.82	1.10
1:A:192:MET:HE3	1:A:196:ALA:HB2	1.49	0.94
1:A:192:MET:CE	1:A:196:ALA:CB	2.55	0.85
1:A:192:MET:HE2	1:A:192:MET:O	1.78	0.83
1:A:220:ASP:HB3	1:A:223:VAL:HG12	1.64	0.80
1:A:192:MET:HE2	1:A:192:MET:C	2.19	0.66
1:A:258:LYS:NZ	2:B:4:GLU:OE1	2.27	0.64
1:A:220:ASP:HB3	1:A:223:VAL:CG1	2.29	0.62
2:B:93:ASN:CG	10:B:311:HOH:O	2.43	0.61
1:A:192:MET:HE1	1:A:196:ALA:CB	2.30	0.60
1:A:387:LEU:HD22	1:A:433:MET:HE1	1.87	0.57
5:A:602:HEM:HBC2	5:A:602:HEM:HMC1	1.88	0.55
2:B:32:LEU:HD21	7:B:203:OLC:H7A	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:LYS:NZ	1:A:492:LEU:O	2.40	0.54
1:A:519:ARG:N	1:A:519:ARG:HD3	2.26	0.50
2:B:91:GLN:NE2	10:B:301:HOH:O	2.19	0.50
1:A:107:TRP:CE3	7:A:606:OLC:H21	2.47	0.50
2:B:159:ASN:HB2	10:B:343:HOH:O	2.11	0.49
1:A:220:ASP:CB	1:A:223:VAL:HG12	2.40	0.49
1:A:519:ARG:HD3	1:A:519:ARG:H	1.79	0.47
1:A:307:VAL:N	1:A:308:PRO:HD2	2.30	0.46
2:B:18:TRP:CE3	3:C:12:ILE:HD13	2.52	0.45
1:A:516:GLU:OE2	1:A:517:ASP:OD1	2.36	0.44
1:A:192:MET:HE2	1:A:193:TRP:HA	2.01	0.43
1:A:516:GLU:HG2	1:A:517:ASP:N	2.34	0.43
6:A:603:HAS:HBC1	6:A:603:HAS:HMC3	2.00	0.43
1:A:429:PHE:CE1	1:A:433:MET:HE3	2.55	0.42
1:A:230:TRP:CD1	1:A:230:TRP:C	2.96	0.42
1:A:400:SER:HA	1:A:403:TRP:NE1	2.34	0.42
1:A:468:VAL:HG21	7:A:608:OLC:H2	2.01	0.42
1:A:516:GLU:HG2	1:A:517:ASP:OD1	2.20	0.42
1:A:562:TRP:HA	2:B:155:LEU:HG	2.02	0.41
1:A:302:THR:O	1:A:305:VAL:HG12	2.20	0.41
1:A:262:ASP:OD1	1:A:262:ASP:C	2.64	0.41
2:B:105:PHE:O	2:B:134:THR:HA	2.20	0.41
2:B:32:LEU:CD2	7:B:203:OLC:H7A	2.51	0.41
1:A:92:LEU:HB2	1:A:93:PRO:HD3	2.03	0.40
1:A:400:SER:CA	10:A:719:HOH:O	2.69	0.40
2:B:91:GLN:HG3	10:B:386:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	552/569 (97%)	537 (97%)	14 (2%)	1 (0%)	43	42
2	B	165/168 (98%)	162 (98%)	2 (1%)	1 (1%)	21	17
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	746/771 (97%)	728 (98%)	16 (2%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3	ASP
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	54
2	B	136/138 (99%)	132 (97%)	4 (3%)	37	40
3	C	24/27 (89%)	23 (96%)	1 (4%)	26	25
All	All	607/628 (97%)	593 (98%)	14 (2%)	44	49

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	58	LEU
1	A	192	MET
1	A	215	LEU
1	A	230	TRP
1	A	262	ASP
1	A	326	LEU
1	A	401	LEU
1	A	498	LYS
2	B	26	LEU
2	B	107	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	140	LYS
2	B	158	GLN
3	C	17	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	455	GLN
2	B	91	GLN
2	B	158	GLN
2	B	159	ASN

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	$\# Z > 2$
7	OLC	A	607	-	14,14,24	0.25	0	15,15,25	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	OLC	B	203	-	24,24,24	0.27	0	25,25,25	0.23	0
9	CUA	B	202	2	0,1,1	-	-	-		
7	OLC	C	101	-	23,23,24	0.27	0	24,24,25	0.32	0
7	OLC	A	612	-	8,8,24	0.15	0	7,7,25	0.13	0
7	OLC	A	606	-	16,16,24	0.33	0	17,17,25	0.34	0
8	CMO	A	614	4	0,1,1	-	-	-		
7	OLC	A	604	-	22,22,24	0.25	0	23,23,25	0.40	0
7	OLC	B	204	-	23,23,24	0.26	0	24,24,25	0.24	0
7	OLC	A	608	-	17,17,24	0.34	0	18,18,25	0.41	0
7	OLC	A	609	-	14,14,24	0.27	0	15,15,25	0.26	0
7	OLC	A	611	-	20,20,24	0.26	0	21,21,25	0.25	0
7	OLC	A	613	-	8,8,24	0.20	0	7,7,25	0.20	0
7	OLC	A	605	-	17,17,24	0.28	0	18,18,25	0.28	0
7	OLC	C	102	-	14,14,24	0.26	0	15,15,25	0.33	0
5	HEM	A	602	1	50,50,50	1.57	6 (12%)	67,82,82	1.67	16 (23%)
6	HAS	A	603	1	72,72,72	2.31	24 (33%)	87,109,109	2.15	24 (27%)
7	OLC	B	201	-	19,19,24	0.23	0	19,19,25	0.21	0
7	OLC	A	610	-	19,19,24	0.27	0	20,20,25	0.33	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	607	-	-	9/14/14/24	-
7	OLC	A	611	-	-	6/20/20/24	-
7	OLC	A	606	-	-	8/16/16/24	-
7	OLC	A	604	-	-	4/22/22/24	-
5	HEM	A	602	1	-	0/14/54/54	-
7	OLC	B	204	-	-	10/23/23/24	-
7	OLC	A	608	-	-	8/17/17/24	-
7	OLC	A	605	-	-	6/17/17/24	-
6	HAS	A	603	1	1/1/8/18	5/42/82/82	-
7	OLC	A	613	-	-	2/6/6/24	-
7	OLC	A	609	-	-	3/14/14/24	-
7	OLC	B	201	-	-	11/18/18/24	-
7	OLC	C	101	-	-	9/23/23/24	-
7	OLC	C	102	-	-	6/14/14/24	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OLC	B	203	-	-	10/24/24/24	-
7	OLC	A	610	-	-	6/19/19/24	-
7	OLC	A	612	-	-	3/6/6/24	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	FE-NB	5.42	2.11	1.94
5	A	602	HEM	FE-NB	5.02	2.10	1.94
6	A	603	HAS	FE-NC	4.96	2.11	1.95
6	A	603	HAS	FE-NA	4.89	2.11	1.95
6	A	603	HAS	C3B-C2B	4.36	1.44	1.34
6	A	603	HAS	C4B-NB	-4.30	1.32	1.40
6	A	603	HAS	FE-ND	4.29	2.08	1.94
6	A	603	HAS	CHC-C1C	4.29	1.49	1.39
6	A	603	HAS	C1B-NB	-4.12	1.30	1.38
5	A	602	HEM	C1B-NB	-4.02	1.33	1.40
6	A	603	HAS	C1D-ND	-3.97	1.33	1.40
6	A	603	HAS	CHC-C4B	3.88	1.46	1.38
6	A	603	HAS	C11-C3B	-3.71	1.46	1.51
6	A	603	HAS	C2A-C3A	3.70	1.44	1.36
6	A	603	HAS	C4A-NA	-3.63	1.32	1.39
6	A	603	HAS	CHB-C1D	3.55	1.45	1.38
6	A	603	HAS	C4C-NC	-3.52	1.33	1.39
6	A	603	HAS	CHD-C4A	3.43	1.45	1.38
5	A	602	HEM	FE-NC	3.21	2.05	1.95
5	A	602	HEM	C4B-NB	-3.13	1.32	1.38
6	A	603	HAS	CHB-C1B	3.06	1.46	1.39
6	A	603	HAS	CHA-C4D	2.95	1.45	1.39
6	A	603	HAS	CHA-C1A	2.79	1.43	1.38
5	A	602	HEM	CMD-C2D	2.78	1.56	1.50
6	A	603	HAS	C4A-C3A	2.68	1.50	1.45
5	A	602	HEM	C4D-ND	-2.48	1.35	1.40
6	A	603	HAS	C1C-NC	-2.36	1.35	1.39
6	A	603	HAS	C4D-ND	-2.34	1.34	1.38
6	A	603	HAS	C1A-NA	-2.19	1.35	1.39
6	A	603	HAS	C1C-C2C	2.15	1.48	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	C2D-C3D-C4D	-5.97	102.11	106.43
5	A	602	HEM	CHC-C4B-NB	5.83	130.70	124.42
6	A	603	HAS	C3C-C4C-NC	5.29	114.26	109.80
6	A	603	HAS	C3C-C2C-C1C	-5.19	101.05	107.17
6	A	603	HAS	C2A-C1A-NA	5.09	115.24	110.32
6	A	603	HAS	CAD-C3D-C4D	4.79	133.04	124.70
6	A	603	HAS	C3B-C4B-NB	4.55	115.07	109.84
6	A	603	HAS	C13-C12-C11	-4.36	107.43	114.39
6	A	603	HAS	C3D-C4D-ND	4.07	114.29	110.35
5	A	602	HEM	CHD-C1D-ND	4.00	128.73	124.42
6	A	603	HAS	C2B-C1B-NB	3.99	114.52	109.90
5	A	602	HEM	C1B-NB-C4B	3.69	109.57	105.21
6	A	603	HAS	OMD-CMD-C2D	-3.36	118.05	125.62
6	A	603	HAS	CAA-CBA-CGA	-3.32	104.86	113.67
6	A	603	HAS	CMC-C2C-C3C	3.25	134.20	126.55
6	A	603	HAS	C1B-C2B-C3B	-3.17	103.12	106.80
6	A	603	HAS	C4B-C3B-C2B	-3.15	102.14	107.44
5	A	602	HEM	CHD-C4C-NC	3.11	127.84	124.45
6	A	603	HAS	C2C-C1C-NC	2.97	114.91	110.14
6	A	603	HAS	C4A-C3A-C2A	-2.96	102.58	106.97
6	A	603	HAS	CMA-C3A-C4A	2.83	129.71	124.73
6	A	603	HAS	C1A-C2A-C3A	-2.81	103.41	107.11
6	A	603	HAS	C3A-C4A-NA	2.60	114.44	109.64
5	A	602	HEM	O2A-CGA-CBA	2.53	122.00	114.00
5	A	602	HEM	CAB-C3B-C2B	2.50	136.56	128.43
6	A	603	HAS	CMB-C2B-C1B	2.42	128.82	125.03
5	A	602	HEM	CHA-C4D-ND	2.42	127.37	124.37
5	A	602	HEM	O1A-CGA-CBA	-2.39	115.51	123.09
6	A	603	HAS	CHA-C4D-ND	-2.39	121.85	124.42
5	A	602	HEM	C1A-CHA-C4D	-2.35	120.72	126.25
5	A	602	HEM	C4C-CHD-C1D	-2.33	121.06	126.02
5	A	602	HEM	O2D-CGD-O1D	-2.29	117.45	123.33
6	A	603	HAS	O1D-CGD-CBD	-2.27	115.88	123.09
5	A	602	HEM	CHA-C4D-C3D	-2.27	121.04	125.23
5	A	602	HEM	CHD-C1D-C2D	-2.24	121.49	125.03
6	A	603	HAS	C32-C30-C31	2.23	119.72	114.59
5	A	602	HEM	CHC-C4B-C3B	-2.19	120.69	125.07
5	A	602	HEM	O2D-CGD-CBD	2.18	120.90	114.00
5	A	602	HEM	CAC-C3C-C4C	-2.11	119.78	124.82
6	A	603	HAS	C12-C11-C3B	-2.09	108.86	112.12

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	603	HAS	NA

All (106) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	605	OLC	O20-C21-C22-O23
7	A	607	OLC	C21-C22-C24-O25
7	A	607	OLC	O20-C21-C22-C24
7	A	607	OLC	O20-C21-C22-O23
7	A	610	OLC	C10-C11-C12-C13
7	C	101	OLC	O19-C1-O20-C21
7	C	101	OLC	C2-C1-O20-C21
7	A	608	OLC	C2-C1-O20-C21
7	C	102	OLC	C2-C1-O20-C21
7	C	102	OLC	O19-C1-O20-C21
7	A	608	OLC	O19-C1-O20-C21
7	A	613	OLC	C11-C12-C13-C14
7	A	607	OLC	C2-C1-O20-C21
7	B	204	OLC	C2-C1-O20-C21
7	A	607	OLC	O19-C1-O20-C21
7	B	204	OLC	O19-C1-O20-C21
7	A	610	OLC	O20-C21-C22-O23
7	B	204	OLC	O20-C21-C22-O23
7	A	610	OLC	O20-C21-C22-C24
7	B	204	OLC	O20-C21-C22-C24
7	A	606	OLC	C1-C2-C3-C4
7	A	605	OLC	C21-C22-C24-O25
7	A	611	OLC	C21-C22-C24-O25
7	C	102	OLC	C21-C22-C24-O25
7	B	204	OLC	C11-C12-C13-C14
7	C	102	OLC	O23-C22-C24-O25
7	A	612	OLC	C12-C13-C14-C15
7	A	606	OLC	O20-C21-C22-O23
7	C	101	OLC	C1-C2-C3-C4
7	A	606	OLC	C3-C4-C5-C6
7	A	610	OLC	C2-C3-C4-C5
7	B	203	OLC	C4-C5-C6-C7
7	A	604	OLC	C11-C12-C13-C14
7	C	101	OLC	C3-C4-C5-C6
7	B	201	OLC	C1-C2-C3-C4
7	B	203	OLC	C13-C14-C15-C16
7	A	610	OLC	C5-C6-C7-C8
7	C	102	OLC	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	203	OLC	C11-C12-C13-C14
7	B	204	OLC	C12-C13-C14-C15
7	A	607	OLC	O23-C22-C24-O25
7	A	606	OLC	C6-C7-C8-C9
7	A	613	OLC	C14-C15-C16-C17
7	B	204	OLC	C2-C3-C4-C5
7	A	608	OLC	C3-C4-C5-C6
7	B	201	OLC	C6-C7-C8-C9
7	C	101	OLC	C6-C7-C8-C9
7	B	201	OLC	C11-C12-C13-C14
7	B	201	OLC	C13-C14-C15-C16
7	A	611	OLC	C3-C4-C5-C6
7	B	203	OLC	C2-C1-O20-C21
7	A	604	OLC	C6-C7-C8-C9
7	A	611	OLC	C5-C6-C7-C8
7	B	201	OLC	C2-C1-O20-C21
7	A	612	OLC	C14-C15-C16-C17
7	B	201	OLC	C2-C3-C4-C5
7	B	203	OLC	C3-C4-C5-C6
7	A	605	OLC	O20-C21-C22-C24
7	A	609	OLC	C4-C5-C6-C7
7	A	607	OLC	C5-C6-C7-C8
7	B	203	OLC	O19-C1-O20-C21
7	A	604	OLC	C10-C11-C12-C13
7	B	204	OLC	C10-C11-C12-C13
7	C	101	OLC	C5-C6-C7-C8
7	A	606	OLC	C5-C6-C7-C8
7	B	203	OLC	C5-C6-C7-C8
7	C	101	OLC	C10-C11-C12-C13
7	B	203	OLC	C9-C10-C11-C12
7	A	606	OLC	O20-C21-C22-C24
7	A	611	OLC	O23-C22-C24-O25
7	B	201	OLC	O19-C1-O20-C21
7	A	608	OLC	C4-C5-C6-C7
7	A	608	OLC	C7-C8-C9-C10
7	B	204	OLC	C7-C8-C9-C10
7	A	605	OLC	C1-C2-C3-C4
7	B	201	OLC	C10-C11-C12-C13
7	A	608	OLC	O20-C21-C22-O23
7	A	607	OLC	C2-C3-C4-C5
7	B	201	OLC	C14-C15-C16-C17
7	B	201	OLC	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	609	OLC	C2-C3-C4-C5
6	A	603	HAS	CAA-CBA-CGA-O1A
6	A	603	HAS	CAA-CBA-CGA-O2A
7	B	203	OLC	C12-C13-C14-C15
7	A	611	OLC	C9-C10-C11-C12
7	A	611	OLC	C11-C12-C13-C14
7	A	605	OLC	C3-C4-C5-C6
6	A	603	HAS	CAD-CBD-CGD-O1D
7	A	605	OLC	O23-C22-C24-O25
6	A	603	HAS	C23-C24-C28-C29
7	B	203	OLC	O20-C21-C22-C24
7	A	608	OLC	O20-C21-C22-C24
7	A	610	OLC	C9-C10-C11-C12
7	B	201	OLC	C9-C10-C11-C12
7	A	606	OLC	O20-C1-C2-C3
7	A	608	OLC	O20-C1-C2-C3
7	A	604	OLC	C7-C8-C9-C10
7	C	101	OLC	C9-C10-C11-C12
7	C	101	OLC	C7-C8-C9-C10
7	C	102	OLC	C5-C6-C7-C8
6	A	603	HAS	CAD-CBD-CGD-O2D
7	A	606	OLC	O19-C1-C2-C3
7	A	612	OLC	C13-C14-C15-C16
7	B	204	OLC	C3-C4-C5-C6
7	A	609	OLC	O20-C1-C2-C3
7	A	607	OLC	O20-C1-C2-C3

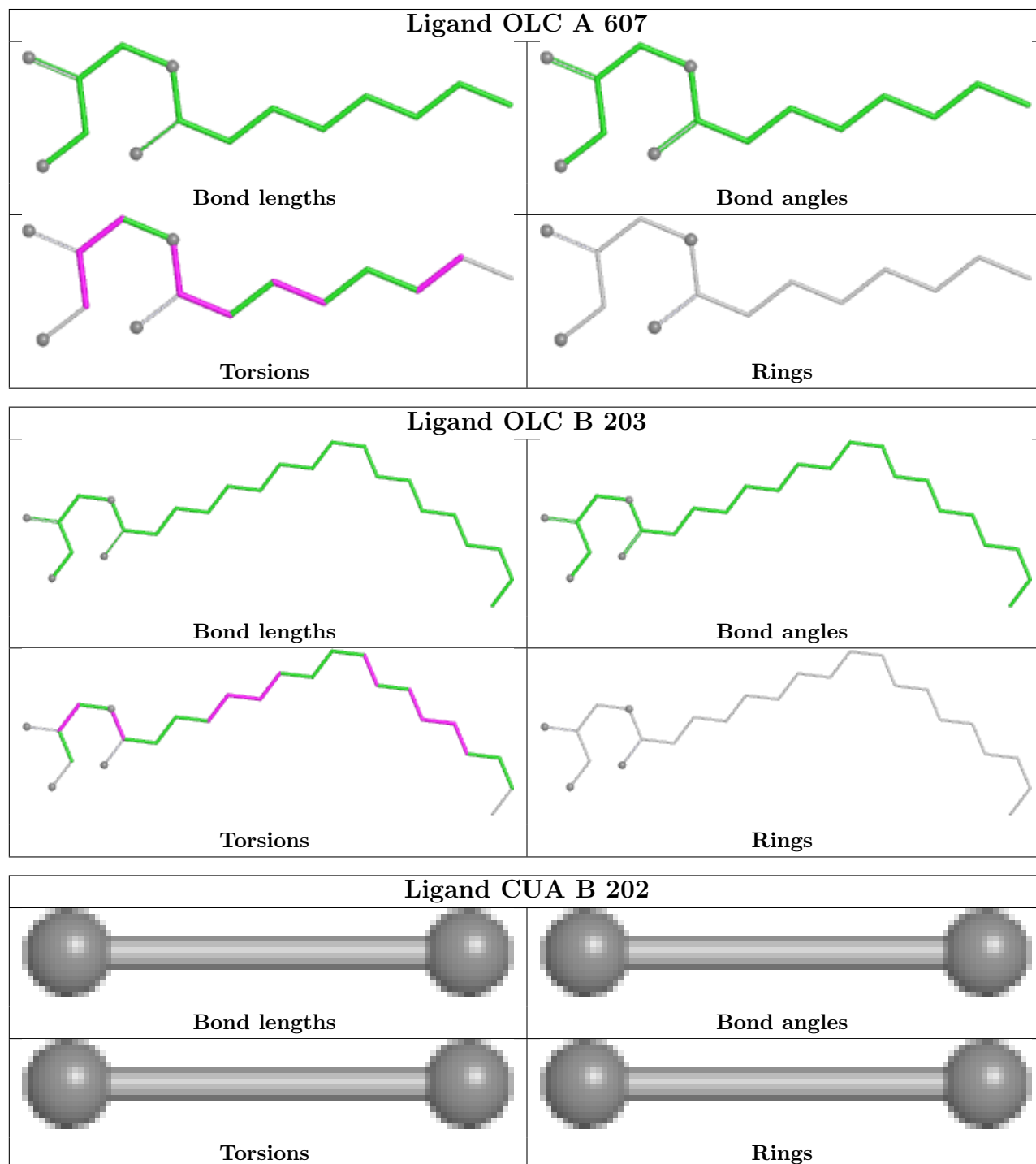
There are no ring outliers.

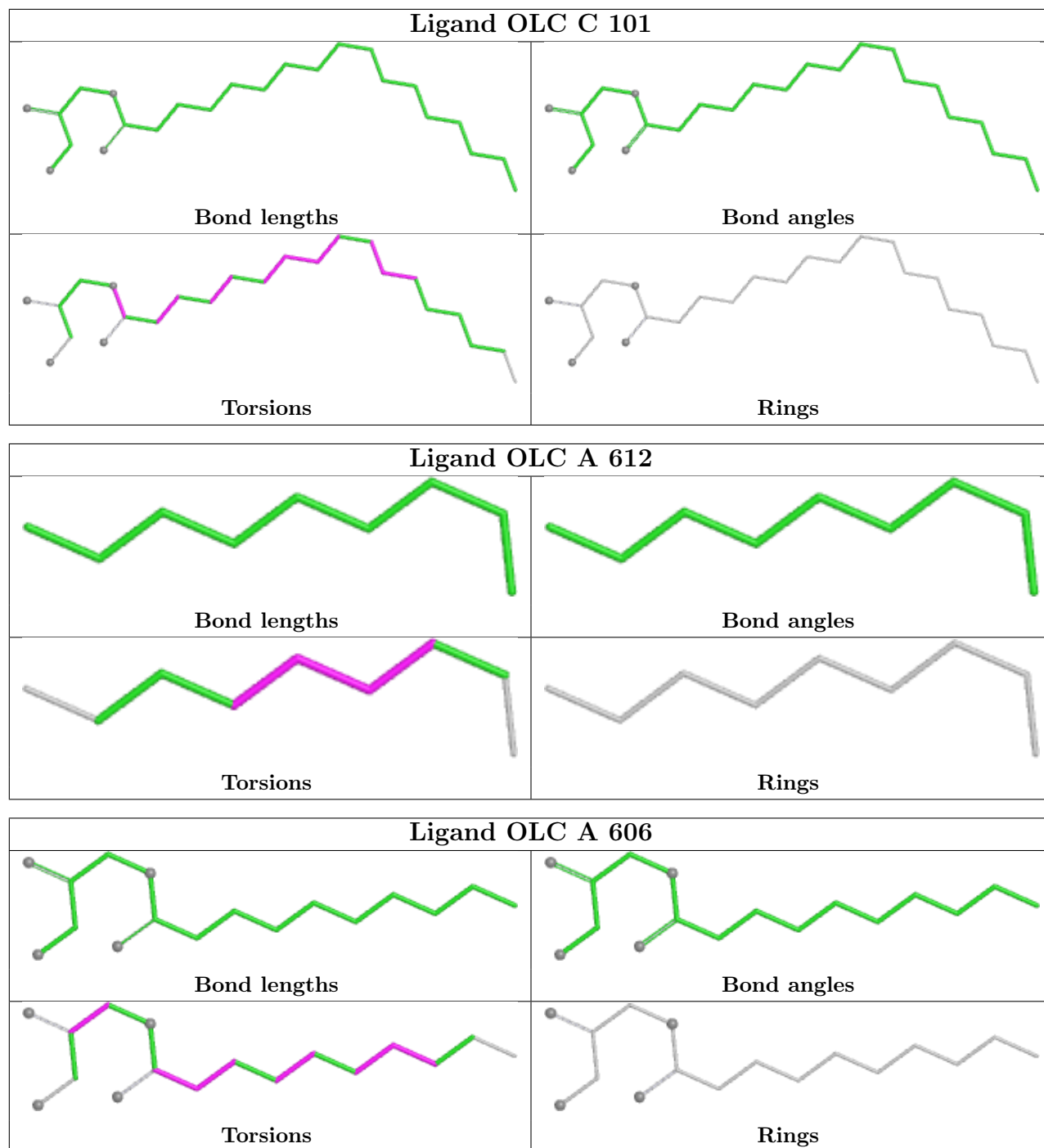
5 monomers are involved in 6 short contacts:

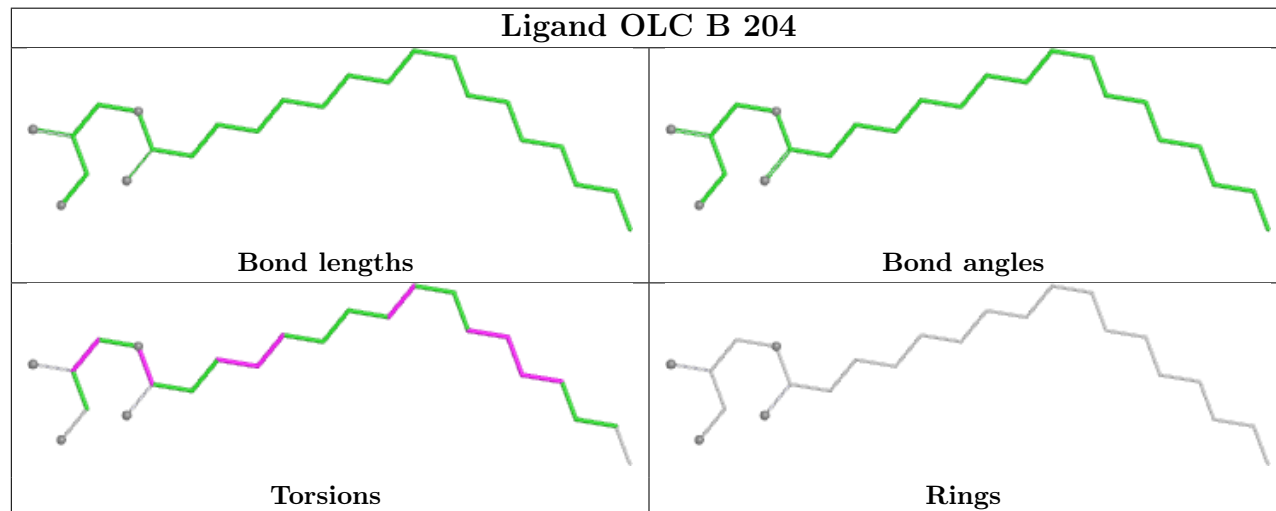
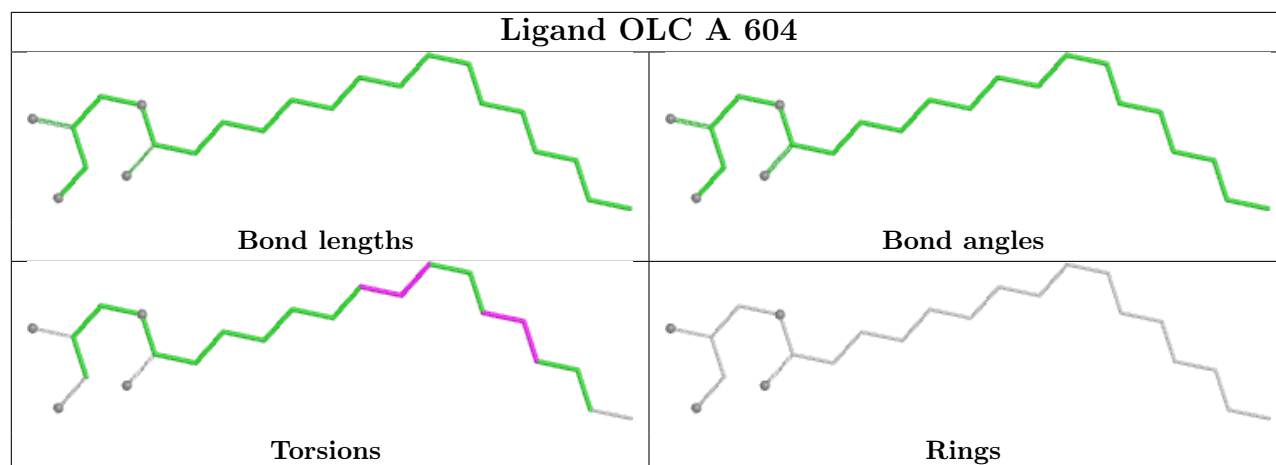
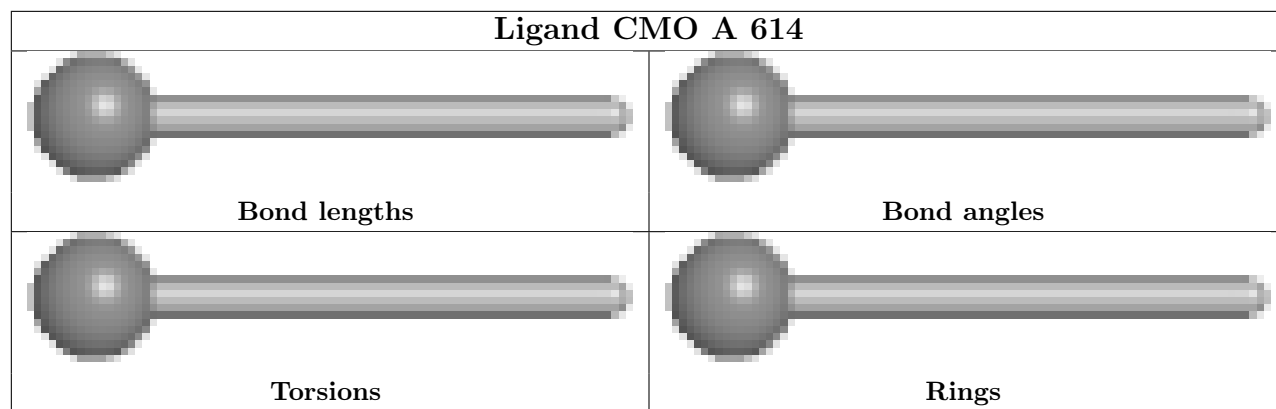
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	203	OLC	2	0
7	A	606	OLC	1	0
7	A	608	OLC	1	0
5	A	602	HEM	1	0
6	A	603	HAS	1	0

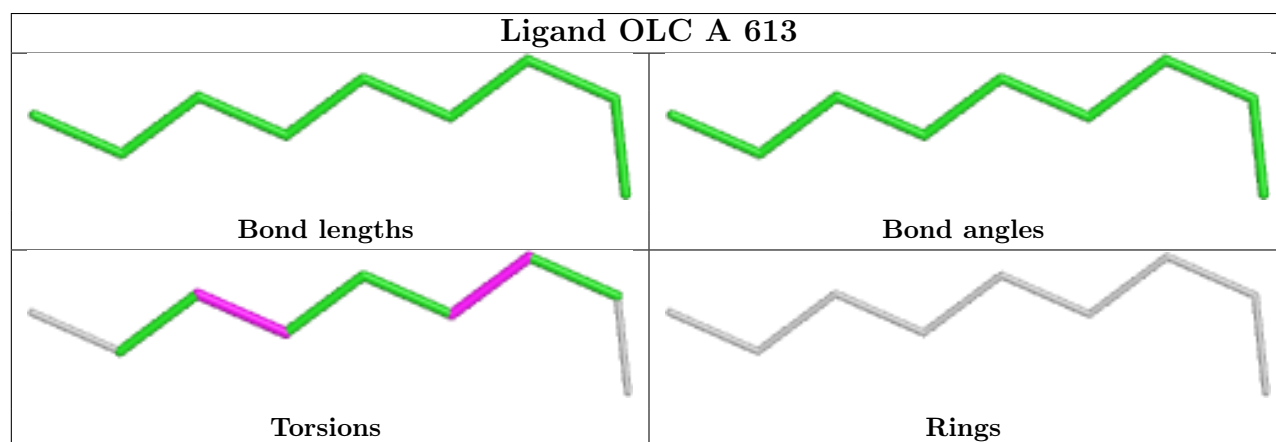
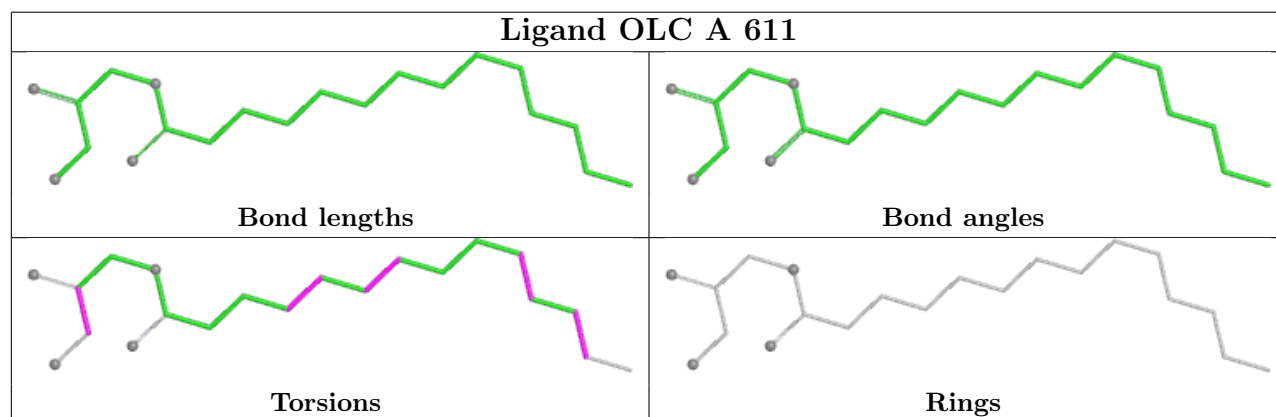
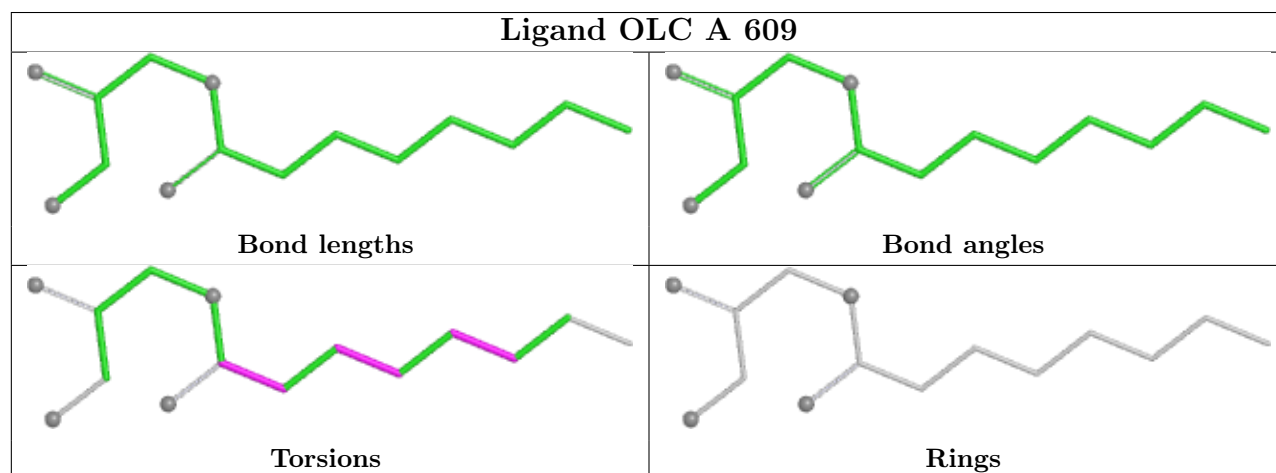
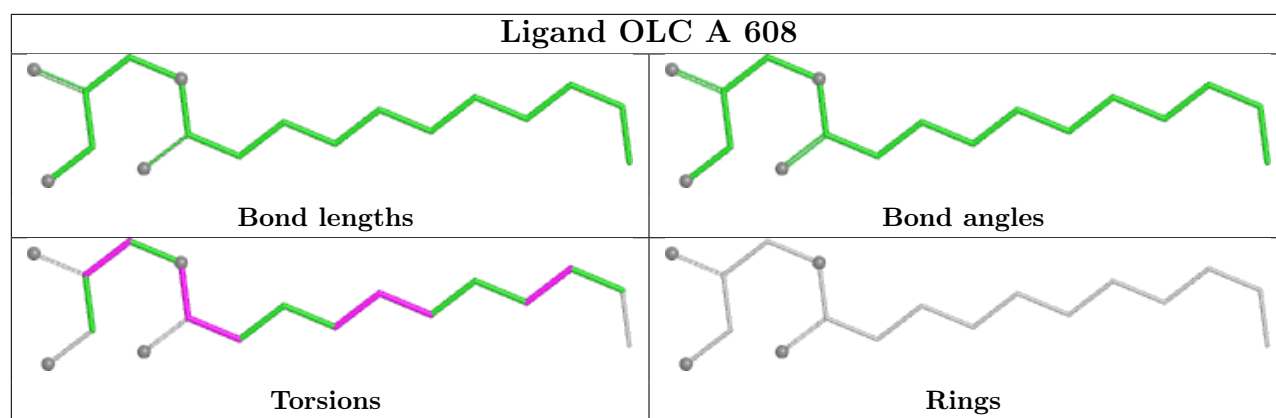
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

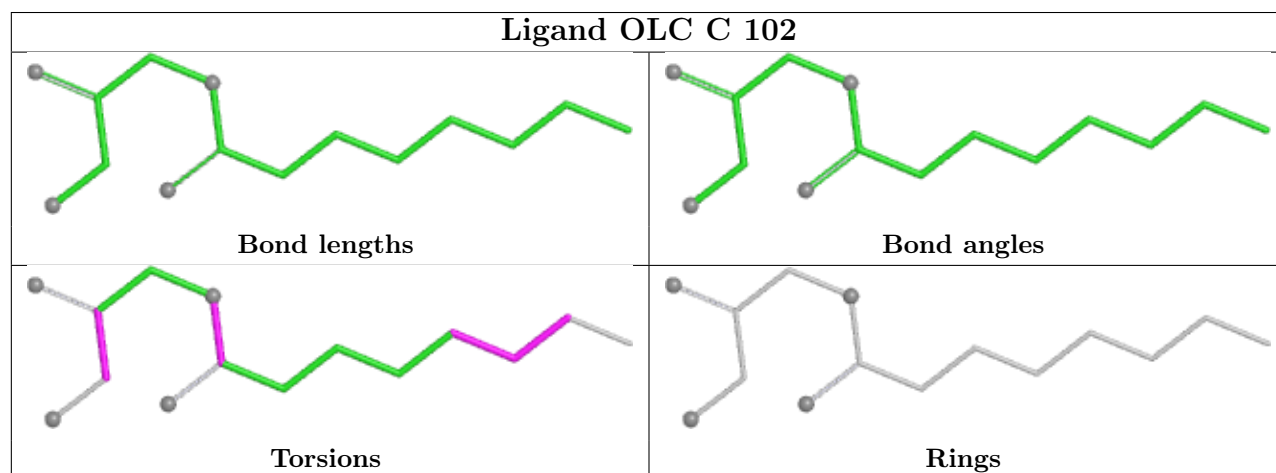
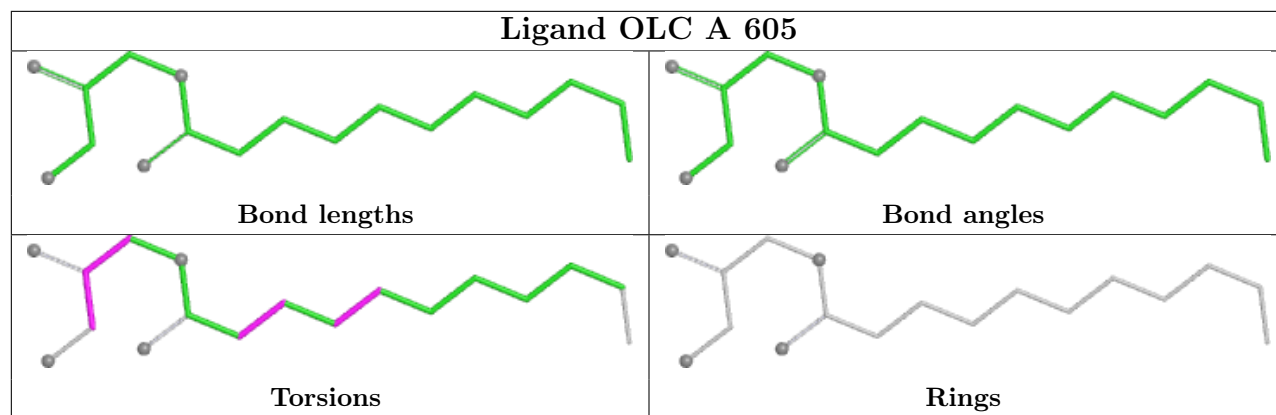
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD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

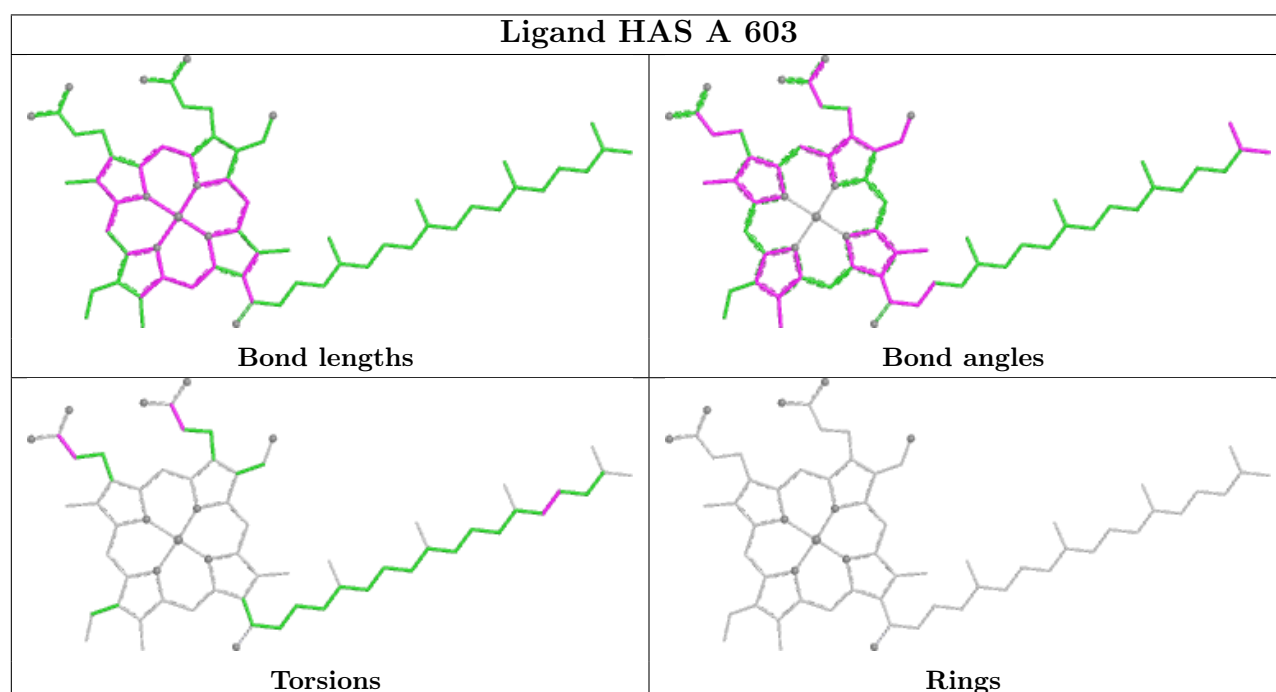
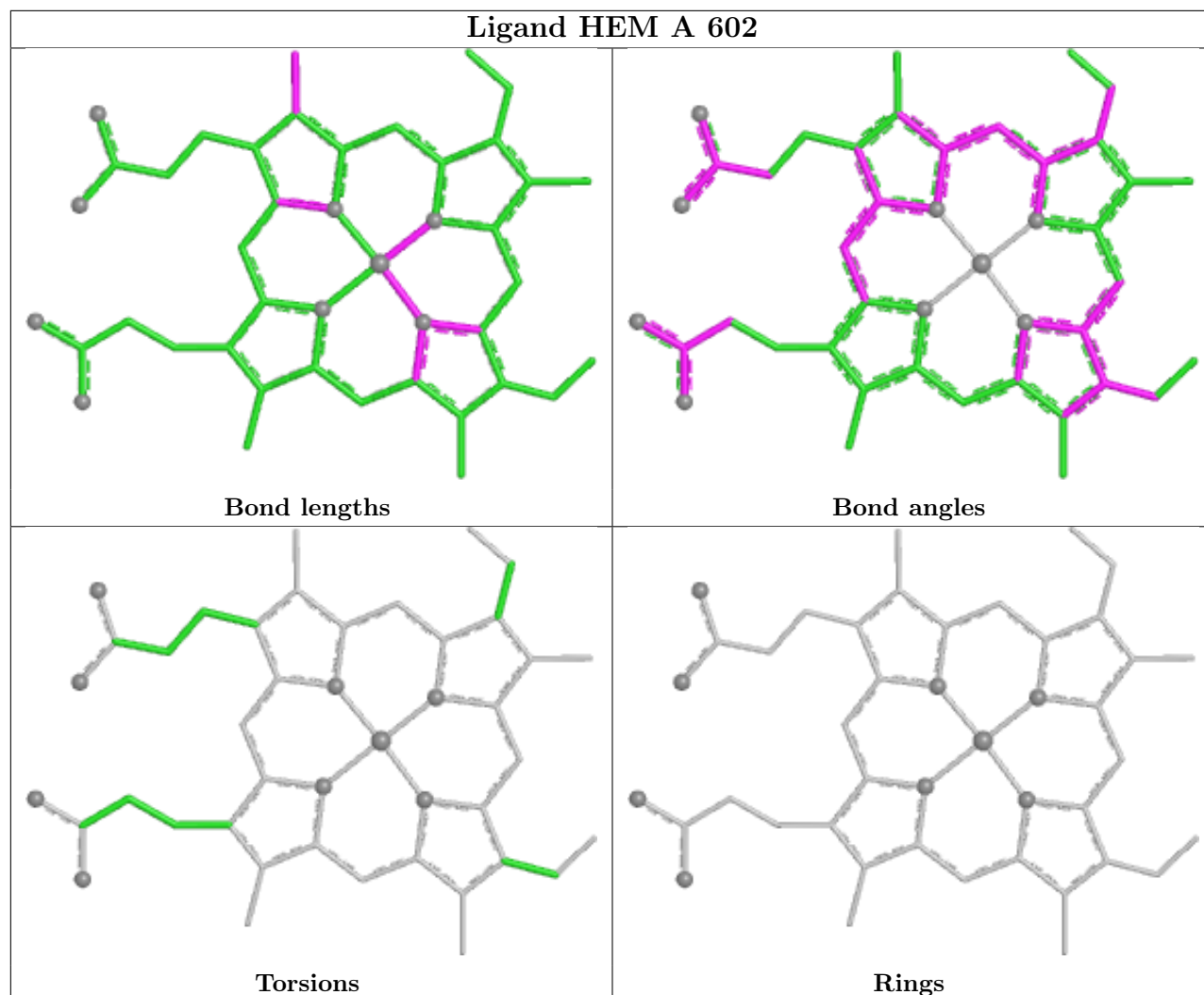


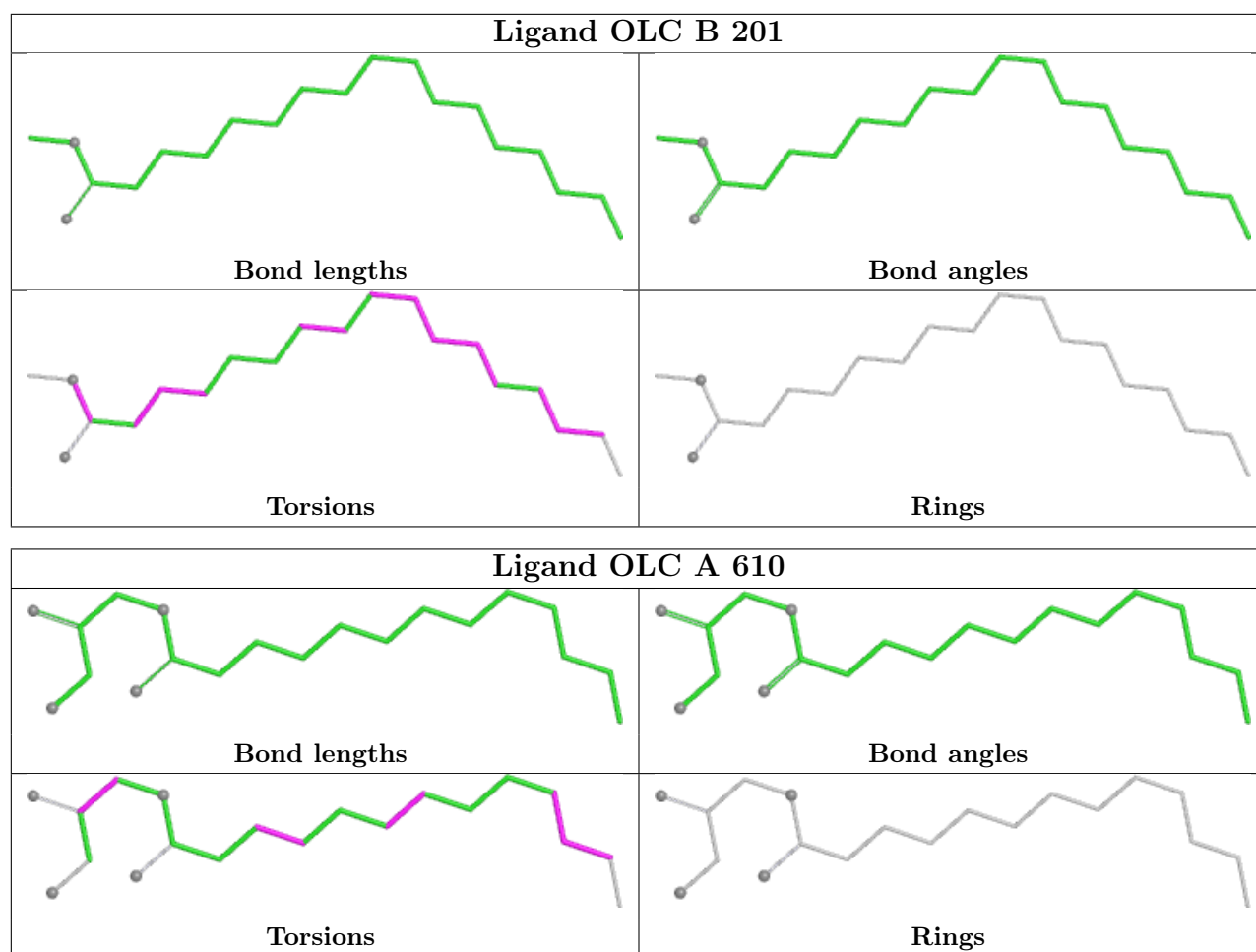












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	554/569 (97%)	0.18	12 (2%) 62 61	21, 32, 59, 91	0
2	B	167/168 (99%)	0.17	4 (2%) 59 59	22, 32, 57, 104	0
3	C	31/34 (91%)	0.23	1 (3%) 50 49	27, 34, 42, 66	0
All	All	752/771 (97%)	0.18	17 (2%) 61 60	21, 32, 59, 104	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	VAL	4.7
2	B	5	HIS	3.2
1	A	493	LEU	3.0
1	A	519	ARG	2.9
1	A	175	PRO	2.8
1	A	178	VAL	2.7
2	B	140	LYS	2.6
1	A	328	GLY	2.5
1	A	334	GLY	2.5
1	A	172	ALA	2.5
3	C	7	GLY	2.3
1	A	9	SER	2.3
1	A	337	ARG	2.2
1	A	174	ASN	2.1
1	A	521	VAL	2.1
1	A	501	LEU	2.1
2	B	3	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

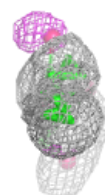
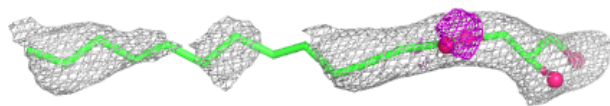
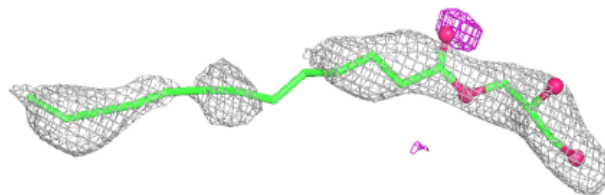
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	610	20/25	0.75	0.19	70,80,96,100	0
7	OLC	A	607	15/25	0.77	0.21	67,84,97,99	0
7	OLC	A	611	21/25	0.79	0.19	56,77,94,105	0
7	OLC	A	609	15/25	0.80	0.22	80,94,101,102	0
7	OLC	C	102	15/25	0.80	0.19	67,74,89,92	0
7	OLC	A	606	17/25	0.81	0.19	70,73,88,91	0
7	OLC	A	613	9/25	0.81	0.19	56,59,75,76	0
7	OLC	A	608	18/25	0.81	0.21	62,79,91,92	0
7	OLC	B	201	20/25	0.84	0.19	69,77,86,97	0
7	OLC	B	203	25/25	0.86	0.16	64,68,86,101	0
7	OLC	B	204	24/25	0.87	0.17	68,80,93,103	0
7	OLC	C	101	24/25	0.87	0.16	54,66,98,101	0
7	OLC	A	605	18/25	0.87	0.20	61,77,95,102	0
7	OLC	A	604	23/25	0.88	0.16	42,60,91,94	0
7	OLC	A	612	9/25	0.88	0.17	64,69,74,77	0
8	CMO	A	614	2/2	0.93	0.10	20,20,20,26	0
6	HAS	A	603	65/65	0.97	0.07	20,26,44,59	0
5	HEM	A	602	43/43	0.98	0.06	20,23,27,36	0
4	CU	A	601	1/1	1.00	0.02	29,29,29,29	0
9	CUA	B	202	2/2	1.00	0.02	25,25,25,26	0

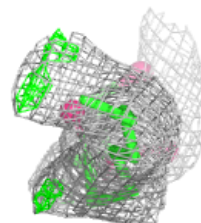
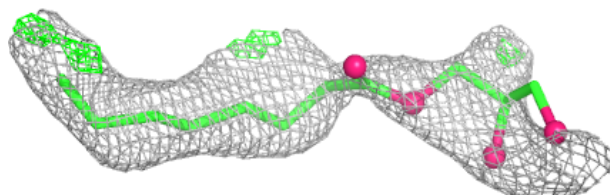
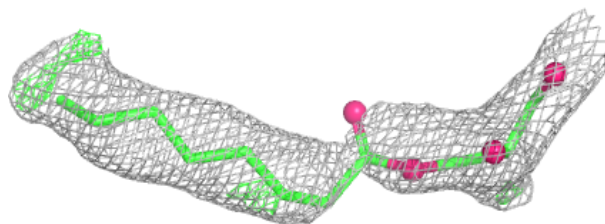
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 610:

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

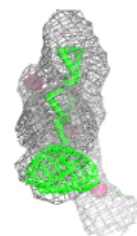
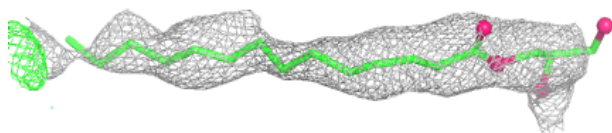
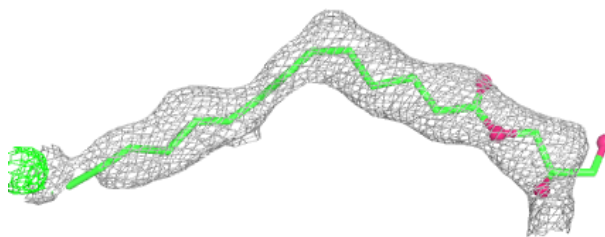
**Electron density around OLC A 607:**

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

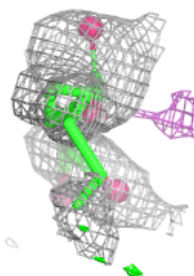
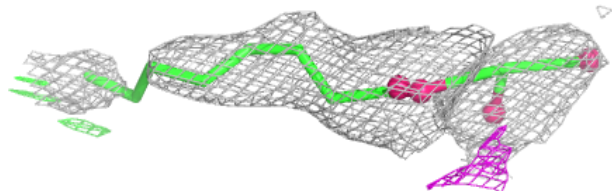
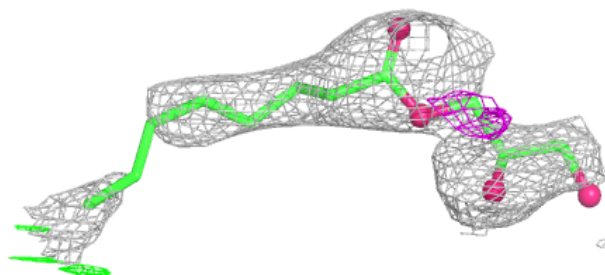


Electron density around OLC A 611:

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

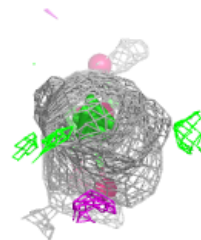
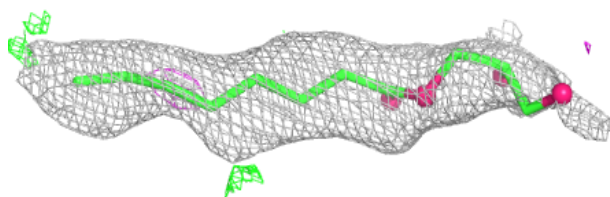
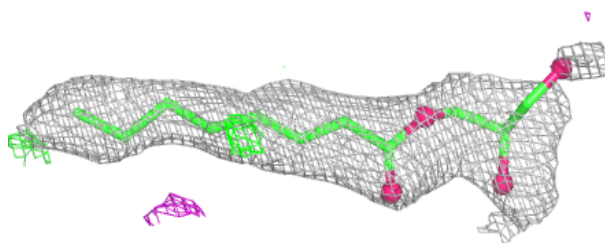
**Electron density around OLC A 609:**

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

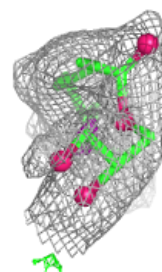
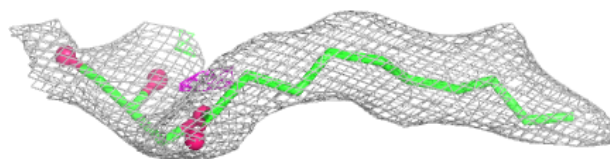
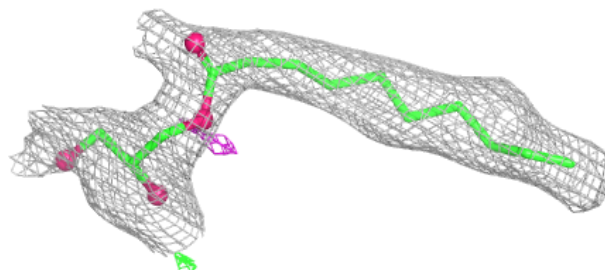


Electron density around OLC C 102:

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

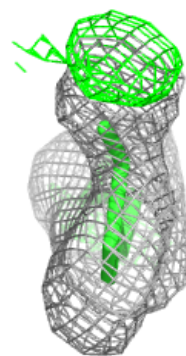
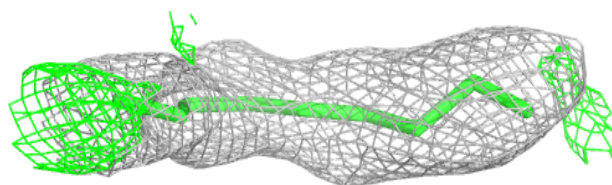
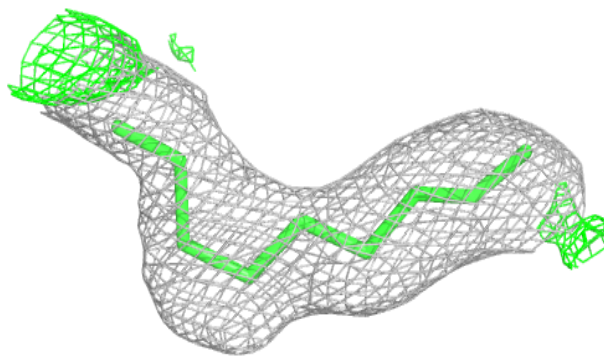
**Electron density around OLC A 606:**

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

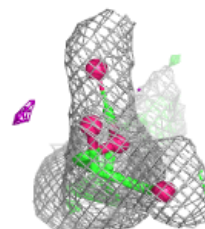
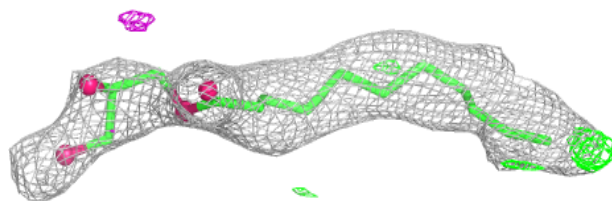
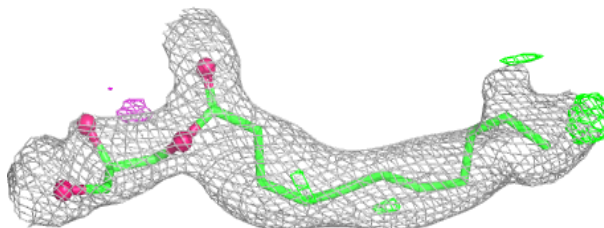


Electron density around OLC A 613:

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

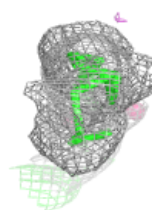
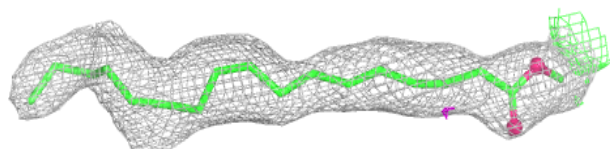
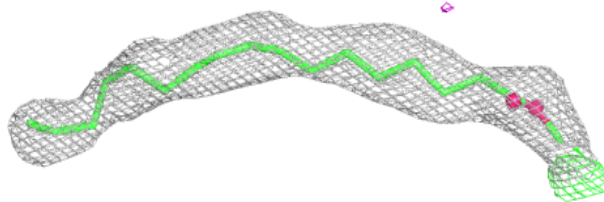
**Electron density around OLC A 608:**

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

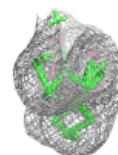
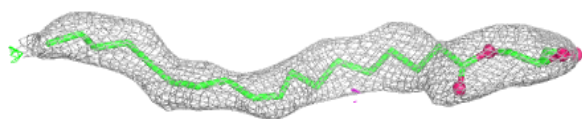
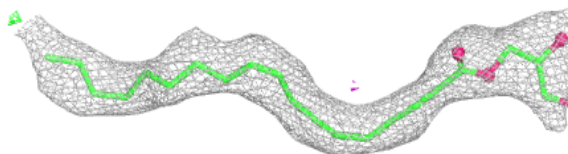


Electron density around OLC B 201:

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

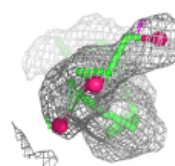
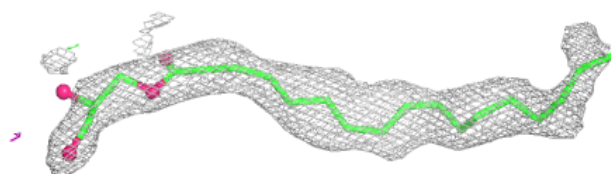
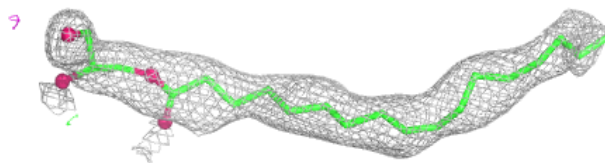
**Electron density around OLC B 203:**

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

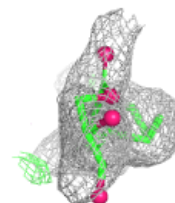
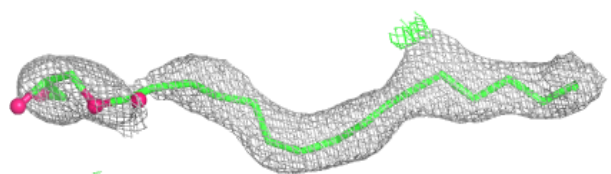
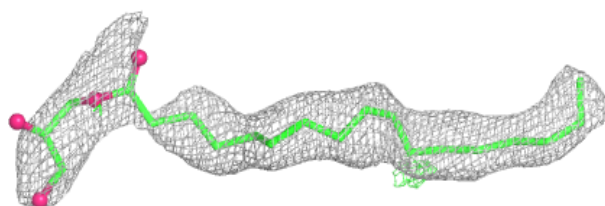


Electron density around OLC B 204:

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

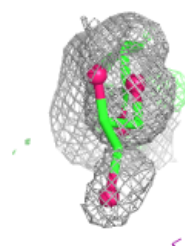
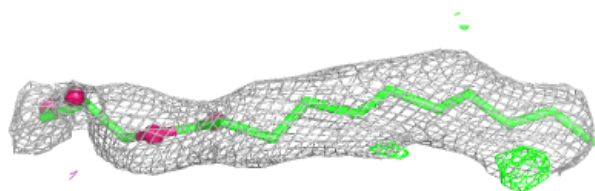
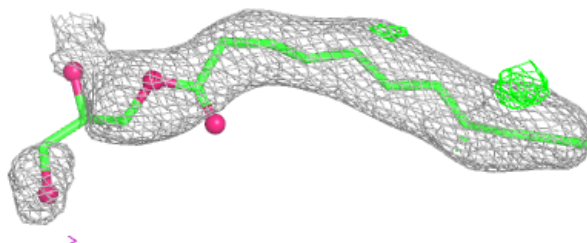
**Electron density around OLC C 101:**

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

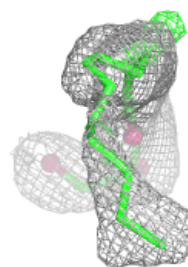
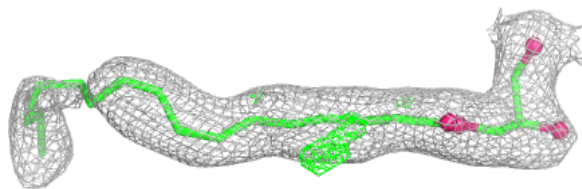
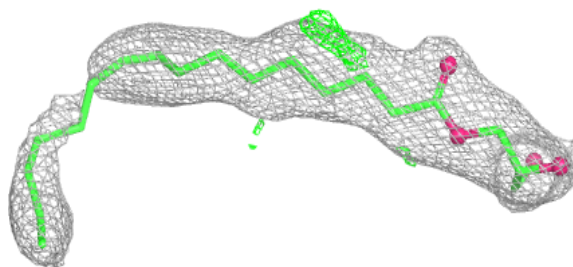


Electron density around OLC A 605:

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

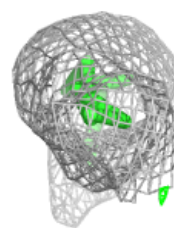
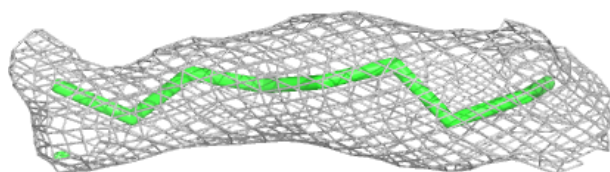
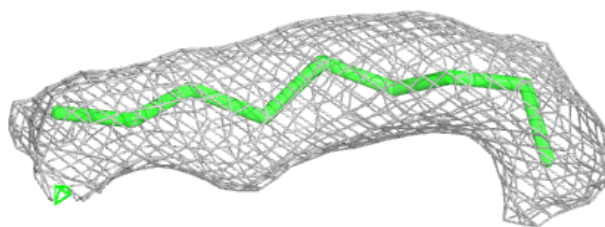
**Electron density around OLC A 604:**

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



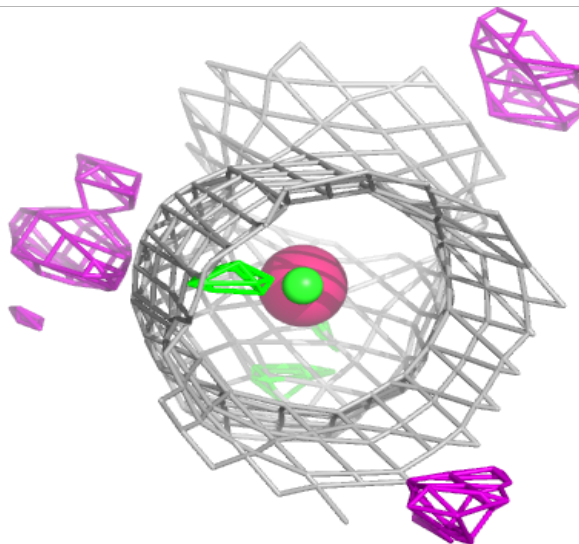
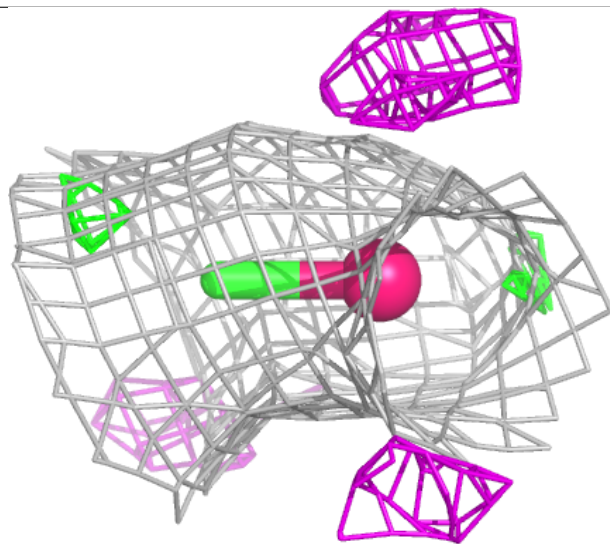
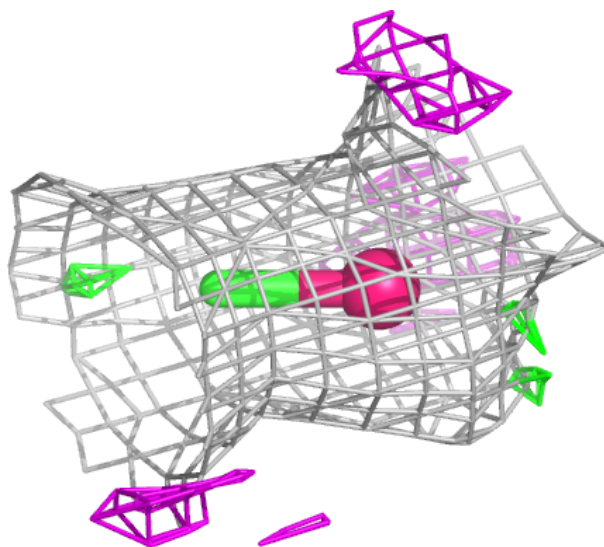
Electron density around OLC A 612:

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



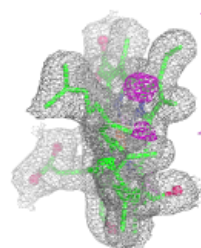
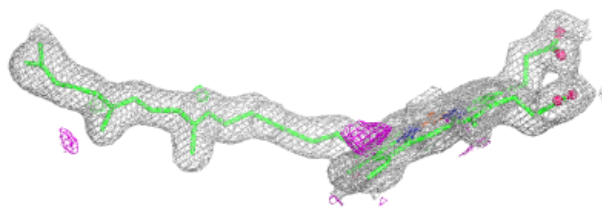
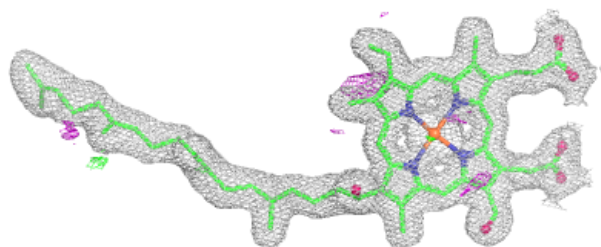
Electron density around CMO A 614:

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



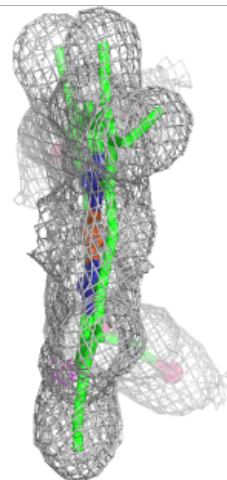
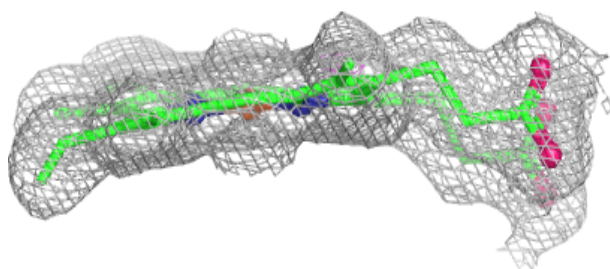
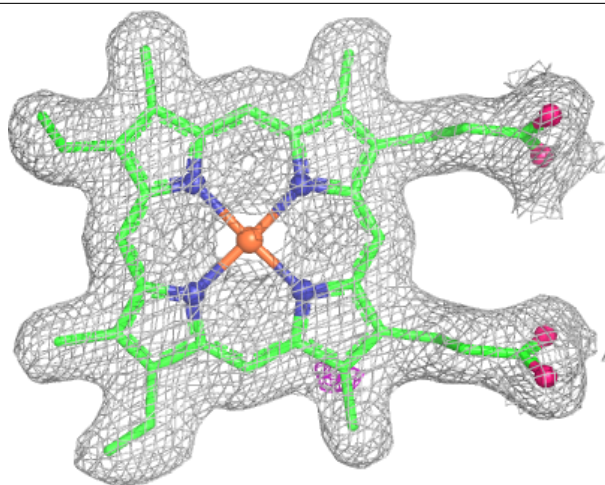
Electron density around HAS A 603:

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



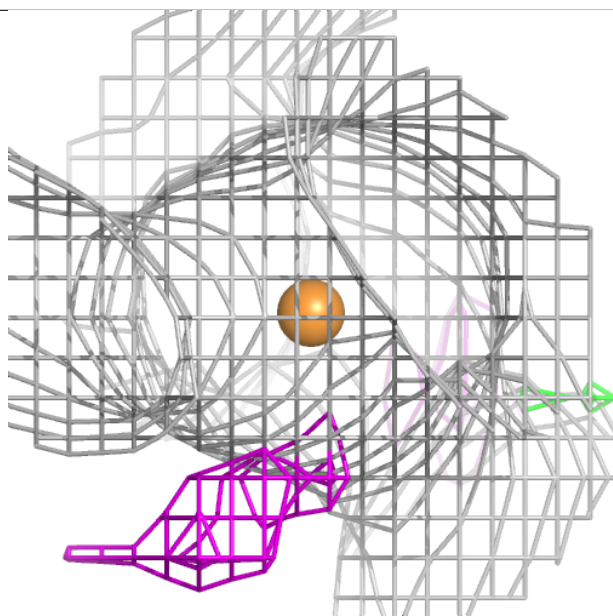
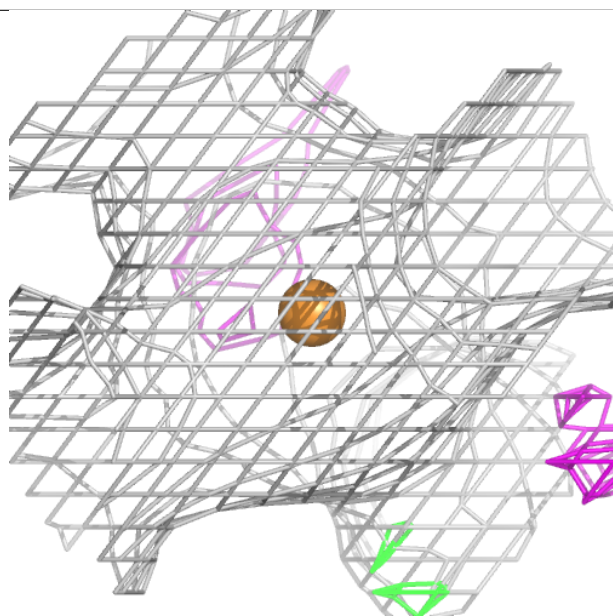
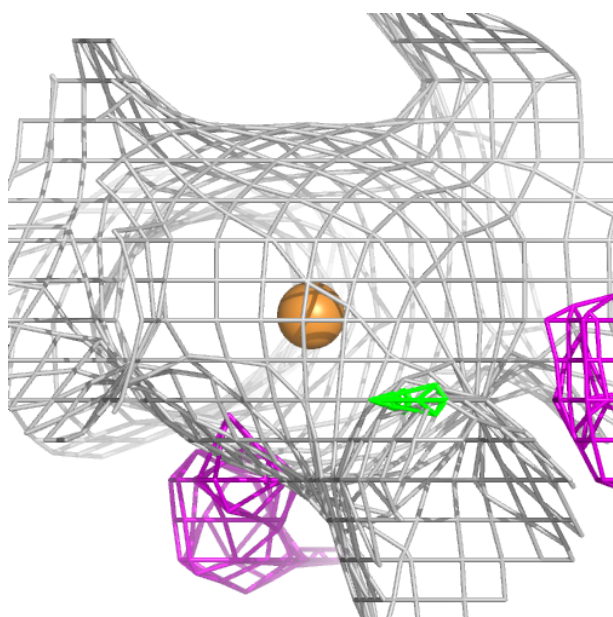
Electron density around HEM A 602:

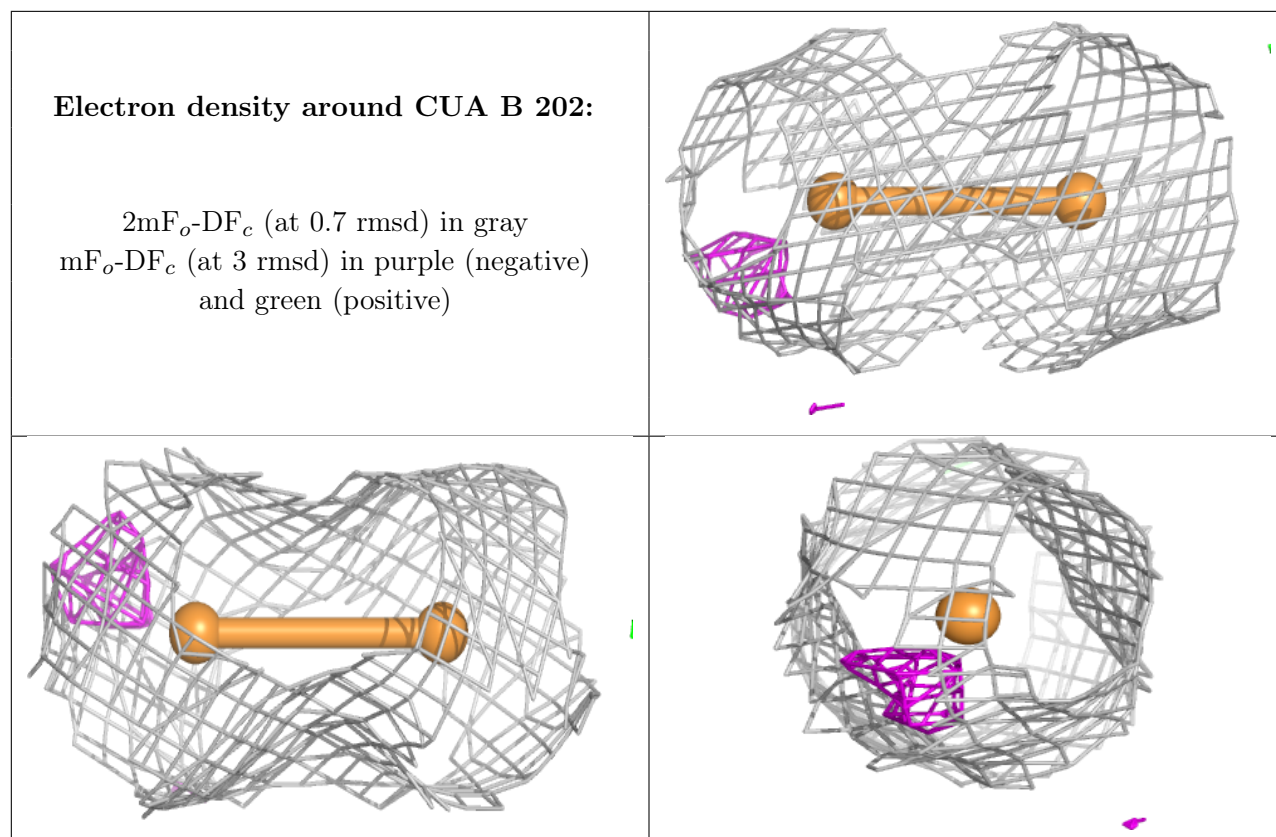
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CU A 601:

$2mF_o-DF_c$ (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.