



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 12:39 AM EST

PDB ID : 4GP4
Title : Structure of Recombinant Cytochrome ba3 Oxidase mutant Y133F from *Thermus thermophilus*
Authors : Li, Y.; Chen, Y.; Stout, C.D.
Deposited on : 2012-08-20
Resolution : 2.80 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

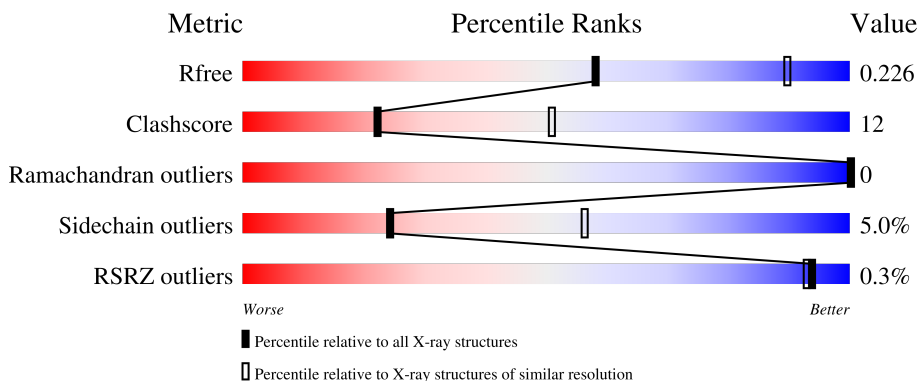
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	568	
2	B	168	
3	C	34	

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	-	-	-
8	OLC	A	613	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 6458 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
			Total	C	N	O	S			
1	A	554	4361	2960	695	690	16	2	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	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
A	133	PHE	TYR	engineered mutation	UNP Q5SJ79

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	166	1285	836	213	232	4	0	0	0

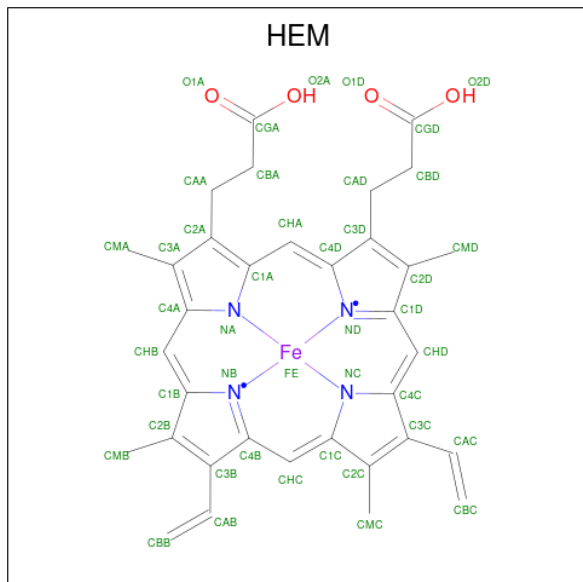
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

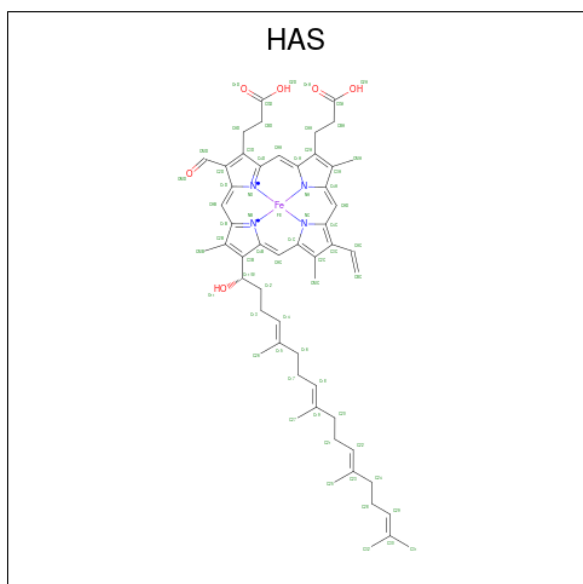
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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



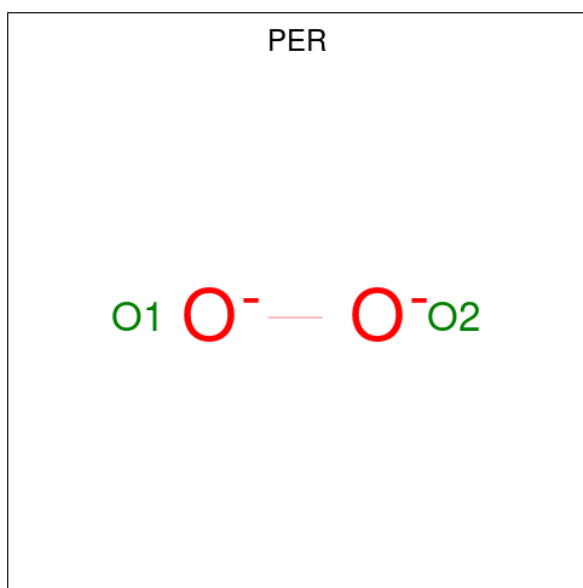
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
5	A	1	43	34	1	4	4	0	0

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



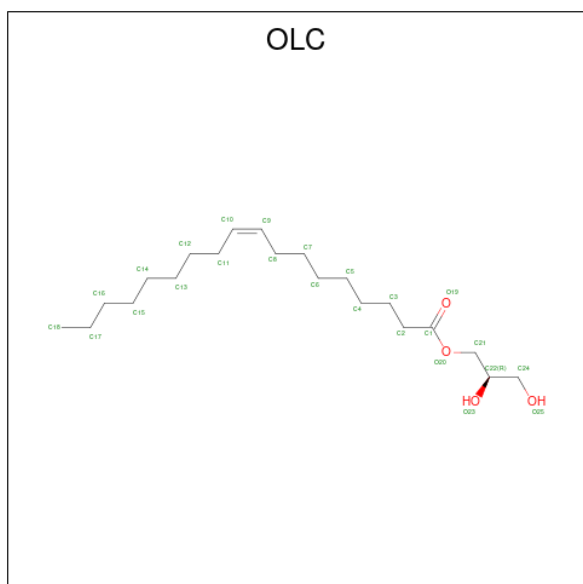
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
6	A	1	65	54	1	4	6	0	0

- Molecule 7 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



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

- Molecule 8 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



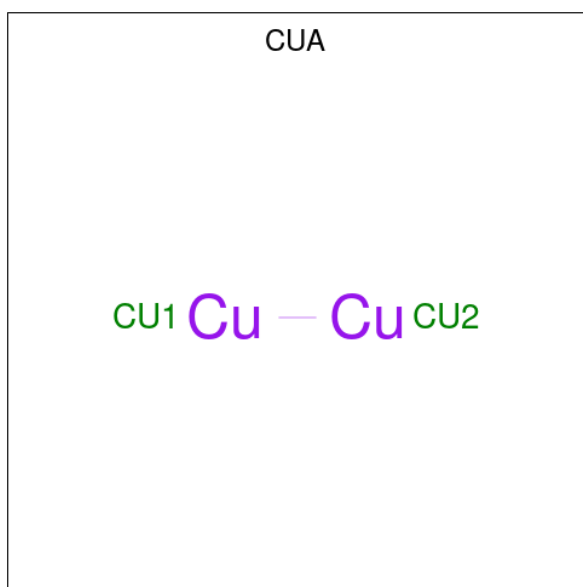
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 25 21 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			25	21	4		
8	A	1	Total	C	O	0	0
			25	21	4		
8	A	1	Total	C	O	0	0
			23	19	4		
8	A	1	Total	C	O	0	0
			21	19	2		
8	A	1	Total	C	O	0	0
			18	14	4		
8	A	1	Total	C	O	0	0
			17	13	4		
8	A	1	Total	C	O	0	0
			8	4	4		
8	A	1	Total	C	O	0	0
			15	11	4		
8	A	1	Total	C	O	0	0
			20	16	4		
8	A	1	Total	C	O	0	0
			25	21	4		
8	A	1	Total	C	O	0	0
			21	17	4		
8	A	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		

- Molecule 9 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

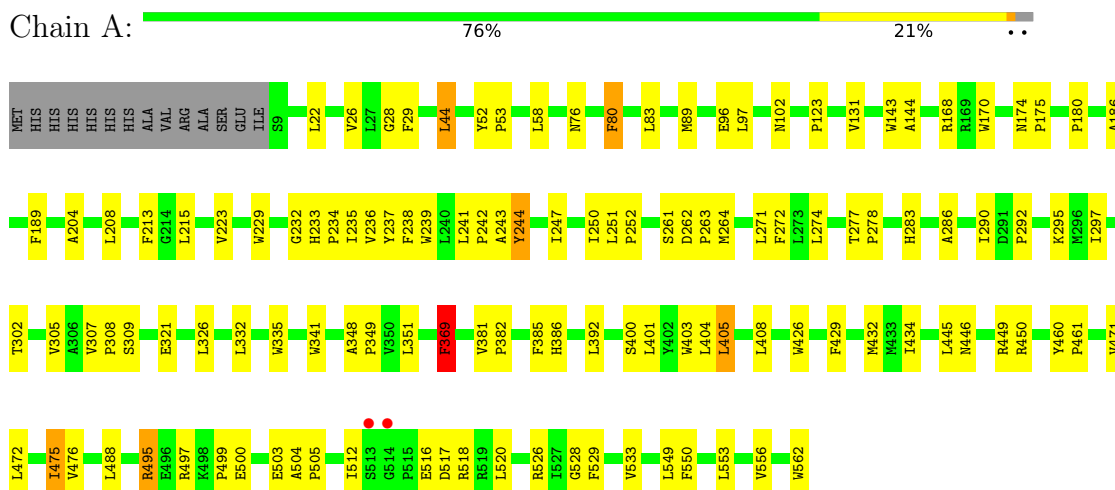
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	74	Total O 74 74	0	0
10	B	40	Total O 40 40	0	0
10	C	1	Total O 1 1	0	0

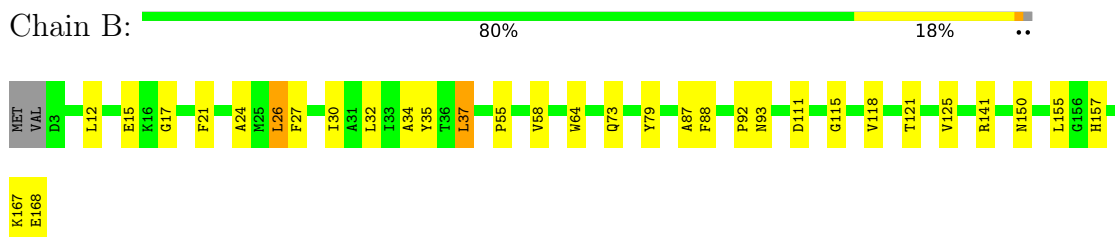
3 Residue-property plots [i](#)

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	144.14Å 98.58Å 94.80Å 90.00° 127.89° 90.00°	Depositor
Resolution (Å)	74.82 – 2.80 74.50 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (74.82-2.80) 99.4 (74.50-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.82Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.179 , 0.227 0.178 , 0.226	Depositor DCC
R_{free} test set	1312 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtrriage
Anisotropy	0.256	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6458	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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: CU, HEM, HAS, OLC, PER, CUA

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	0.44	0/4517	0.57	2/6201 (0.0%)
2	B	0.44	0/1321	0.55	0/1805
3	C	0.45	0/247	0.51	0/335
All	All	0.44	0/6085	0.56	2/8341 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	VAL	N-CA-C	-5.79	95.35	111.00
1	A	369	PHE	N-CA-CB	-5.09	101.43	110.60

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	4361	0	4455	110	0
2	B	1285	0	1260	27	0
3	C	241	0	267	9	0
4	A	1	0	0	0	0
5	A	43	0	30	7	0
6	A	65	0	62	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	2	0	0	0	0
8	A	268	0	393	24	0
8	B	75	0	120	15	0
9	B	2	0	0	0	0
10	A	74	0	0	1	0
10	B	40	0	0	2	1
10	C	1	0	0	0	0
All	All	6458	0	6587	151	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 12.

All (151) 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:233:HIS:NE2	1:A:237:TYR:HE2	1.19	1.37
1:A:233:HIS:NE2	1:A:237:TYR:CE2	2.10	1.19
1:A:263:PRO:HG2	1:A:516:GLU:HG2	1.36	1.07
1:A:263:PRO:HG2	1:A:516:GLU:CG	1.88	1.02
1:A:168:ARG:HH11	8:A:612:OLC:H22	1.24	1.00
1:A:168:ARG:HH22	8:A:613:OLC:H6A	1.27	0.97
1:A:516:GLU:HG3	1:A:517:ASP:H	1.27	0.97
1:A:168:ARG:NH1	8:A:612:OLC:H22	1.91	0.83
1:A:263:PRO:CG	1:A:516:GLU:HG2	2.10	0.81
1:A:168:ARG:NH2	8:A:613:OLC:H6A	1.94	0.80
1:A:476:VAL:HG22	8:A:607:OLC:H16A	1.63	0.79
1:A:341:TRP:CZ2	8:A:617:OLC:H3	2.17	0.79
1:A:233:HIS:O	1:A:236:VAL:HG22	1.85	0.77
2:B:21:PHE:CE2	8:B:204:OLC:H10	2.21	0.74
1:A:341:TRP:CE2	8:A:617:OLC:H3	2.23	0.74
1:A:516:GLU:CG	1:A:517:ASP:H	2.01	0.74
1:A:495:ARG:HH21	1:A:495:ARG:HA	1.55	0.70
1:A:516:GLU:HG3	1:A:517:ASP:N	2.02	0.70
2:B:21:PHE:CZ	8:B:204:OLC:H10	2.26	0.70
1:A:262:ASP:HB3	1:A:263:PRO:HD3	1.76	0.68
1:A:400:SER:HA	1:A:403:TRP:NE1	2.08	0.68
1:A:233:HIS:CD2	1:A:237:TYR:HE2	2.10	0.67
2:B:35:TYR:CE2	8:B:202:OLC:H2A	2.30	0.67
8:B:203:OLC:H6	3:C:33:ARG:HE	1.59	0.66
1:A:297:ILE:HG12	8:A:609:OLC:H14A	1.78	0.66
2:B:32:LEU:HD21	8:B:202:OLC:H7A	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:VAL:HB	1:A:382:PRO:HD3	1.79	0.65
8:A:606:OLC:H6	8:B:203:OLC:H18A	1.78	0.64
8:A:605:OLC:H6	3:C:25:GLY:HA3	1.80	0.64
1:A:305:VAL:O	1:A:308:PRO:HD2	1.98	0.64
2:B:93:ASN:ND2	10:B:320:HOH:O	2.30	0.64
6:A:603:HAS:HMC1	6:A:603:HAS:HBC1	1.81	0.62
2:B:35:TYR:CZ	8:B:202:OLC:H2A	2.35	0.61
1:A:263:PRO:HG2	1:A:516:GLU:HG3	1.83	0.60
1:A:233:HIS:CE1	1:A:237:TYR:HE2	2.09	0.60
1:A:401:LEU:HG	1:A:405:LEU:HD22	1.82	0.60
1:A:168:ARG:HH11	8:A:612:OLC:C22	2.05	0.59
1:A:401:LEU:HD21	1:A:488:LEU:HD13	1.84	0.59
1:A:497:ARG:O	1:A:499:PRO:HD3	2.03	0.59
2:B:17:GLY:HA3	8:B:204:OLC:H3	1.85	0.58
1:A:348:ALA:HB3	1:A:349:PRO:HD3	1.85	0.58
1:A:277:THR:N	1:A:278:PRO:HD2	2.19	0.57
1:A:495:ARG:HA	1:A:495:ARG:NH2	2.20	0.57
1:A:232:GLY:O	1:A:235:ILE:HG22	2.05	0.57
1:A:29:PHE:CE1	1:A:401:LEU:HD11	2.40	0.56
2:B:141:ARG:NH2	8:B:203:OLC:O19	2.39	0.56
8:A:607:OLC:H12	8:A:615:OLC:H14A	1.87	0.56
1:A:401:LEU:O	1:A:405:LEU:HB2	2.05	0.55
1:A:277:THR:N	1:A:278:PRO:CD	2.70	0.55
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.92	0.55
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.42	0.54
1:A:475:ILE:HD11	8:A:607:OLC:H13A	1.90	0.53
1:A:204:ALA:HA	1:A:208:LEU:HB2	1.89	0.53
1:A:369:PHE:C	1:A:369:PHE:CD2	2.81	0.53
1:A:529:PHE:O	1:A:533:VAL:HG23	2.10	0.51
1:A:241:LEU:N	1:A:242:PRO:CD	2.74	0.51
2:B:26:LEU:O	2:B:30:ILE:HG13	2.11	0.51
1:A:52:TYR:N	1:A:53:PRO:CD	2.75	0.50
1:A:236:VAL:HG12	1:A:239:TRP:CZ3	2.46	0.50
1:A:123:PRO:HG3	1:A:144:ALA:HB3	1.93	0.50
3:C:4:LYS:HE3	3:C:6:LYS:HG2	1.94	0.50
1:A:550:PHE:HA	1:A:553:LEU:HD21	1.93	0.50
2:B:34:ALA:O	2:B:37:LEU:HB2	2.12	0.50
1:A:250:ILE:HD13	1:A:403:TRP:CH2	2.47	0.50
1:A:400:SER:HA	1:A:403:TRP:CD1	2.45	0.49
1:A:277:THR:H	1:A:278:PRO:HD2	1.76	0.49
1:A:277:THR:H	1:A:278:PRO:CD	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ARG:NH1	8:A:612:OLC:C22	2.71	0.49
1:A:404:LEU:O	1:A:408:LEU:HG	2.13	0.49
2:B:21:PHE:CD2	8:B:204:OLC:H9	2.47	0.49
2:B:141:ARG:HH12	8:B:203:OLC:H24A	1.77	0.48
1:A:89:MET:HG3	1:A:189:PHE:CE2	2.48	0.48
1:A:369:PHE:C	1:A:369:PHE:HD2	2.17	0.48
1:A:28:GLY:HA2	1:A:83:LEU:HD12	1.96	0.48
1:A:229:TRP:CE3	1:A:283:HIS:CD2	3.01	0.48
1:A:236:VAL:HB	6:A:603:HAS:C3C	2.45	0.47
1:A:271:LEU:HB3	1:A:308:PRO:HG3	1.96	0.47
1:A:272:PHE:CZ	1:A:308:PRO:HB2	2.50	0.47
1:A:386:HIS:CE1	5:A:602:HEM:C1A	3.02	0.47
1:A:233:HIS:N	1:A:234:PRO:HD2	2.30	0.47
1:A:382:PRO:HA	1:A:385:PHE:CZ	2.50	0.47
2:B:118:VAL:HB	2:B:121:THR:OG1	2.14	0.47
1:A:143:TRP:HB2	1:A:213:PHE:CE2	2.50	0.47
1:A:434:ILE:HG21	1:A:472:LEU:HD23	1.97	0.47
1:A:286:ALA:HB1	2:B:125:VAL:HA	1.96	0.47
1:A:235:ILE:O	1:A:238:PHE:HB3	2.15	0.46
1:A:392:LEU:HD22	1:A:392:LEU:O	2.14	0.46
1:A:243:ALA:O	1:A:247:ILE:HD12	2.15	0.46
2:B:35:TYR:OH	8:B:202:OLC:H24A	2.15	0.46
1:A:76:ASN:HB3	5:A:602:HEM:CAC	2.45	0.46
1:A:251:LEU:HD13	1:A:349:PRO:HG2	1.98	0.46
1:A:449:ARG:HG3	1:A:450:ARG:HG3	1.96	0.46
1:A:52:TYR:N	1:A:53:PRO:HD2	2.30	0.46
8:A:606:OLC:H9	3:C:21:VAL:HG11	1.97	0.46
1:A:28:GLY:O	1:A:80:PHE:HB2	2.16	0.45
8:A:617:OLC:H13	8:A:617:OLC:H10	1.32	0.45
1:A:97:LEU:HD22	1:A:170:TRP:CD1	2.52	0.45
5:A:602:HEM:CMC	5:A:602:HEM:HBC2	2.47	0.45
1:A:562:TRP:HA	2:B:155:LEU:HG	1.97	0.45
8:B:203:OLC:H6	3:C:33:ARG:HH11	1.81	0.45
8:A:605:OLC:O25	8:B:203:OLC:H7	2.16	0.44
1:A:445:LEU:O	1:A:446:ASN:HB2	2.17	0.44
1:A:556:VAL:HG12	2:B:55:PRO:HG3	1.99	0.44
1:A:264:MET:HG3	2:B:15:GLU:OE2	2.18	0.44
1:A:44:LEU:HD12	1:A:471:VAL:HA	2.00	0.44
1:A:292:PRO:HB2	8:A:609:OLC:H3A	2.00	0.44
1:A:22:LEU:O	1:A:26:VAL:HG23	2.17	0.44
2:B:32:LEU:HD21	8:B:202:OLC:C7	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4:LYS:HG3	3:C:6:LYS:HG2	2.00	0.44
1:A:386:HIS:CE1	5:A:602:HEM:NA	2.86	0.43
2:B:87:ALA:HA	2:B:88:PHE:HA	1.68	0.43
2:B:73:GLN:HB2	2:B:79:TYR:CE1	2.54	0.43
8:A:607:OLC:H12	8:A:615:OLC:C14	2.48	0.43
1:A:186:ALA:O	1:A:189:PHE:HB3	2.19	0.43
1:A:450:ARG:O	2:B:157:HIS:CD2	2.71	0.43
1:A:445:LEU:HD23	1:A:445:LEU:HA	1.79	0.43
1:A:504:ALA:HA	1:A:505:PRO:HD3	1.88	0.43
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.84	0.42
1:A:302:THR:O	1:A:305:VAL:HG12	2.18	0.42
1:A:386:HIS:HE1	5:A:602:HEM:C1A	2.38	0.42
1:A:241:LEU:HA	1:A:244:TYR:HB2	2.02	0.42
1:A:168:ARG:HH22	8:A:613:OLC:C6	2.14	0.42
1:A:290:ILE:HB	1:A:295:LYS:HE3	2.01	0.42
1:A:400:SER:HB3	10:A:704:HOH:O	2.20	0.42
8:A:607:OLC:H2	8:A:607:OLC:H5A	1.88	0.42
3:C:16:THR:HG22	3:C:20:LEU:HD22	2.00	0.42
1:A:432:MET:CE	5:A:602:HEM:HAB	2.50	0.42
5:A:602:HEM:HBC2	5:A:602:HEM:HMC2	2.02	0.42
1:A:174:ASN:N	1:A:175:PRO:CD	2.82	0.42
1:A:516:GLU:CG	1:A:517:ASP:N	2.67	0.42
1:A:307:VAL:N	1:A:308:PRO:CD	2.82	0.42
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.55	0.41
2:B:21:PHE:O	2:B:24:ALA:HB3	2.19	0.41
1:A:475:ILE:HG13	1:A:476:VAL:N	2.35	0.41
3:C:24:LEU:HD12	3:C:24:LEU:HA	1.84	0.41
1:A:233:HIS:CE1	1:A:237:TYR:CE2	2.94	0.41
2:B:92:PRO:HG3	10:B:339:HOH:O	2.21	0.41
2:B:115:GLY:HA3	2:B:150:ASN:H	1.85	0.41
1:A:460:TYR:N	1:A:461:PRO:CD	2.83	0.41
2:B:58:VAL:HG22	2:B:64:TRP:HB2	2.03	0.41
1:A:351:LEU:HB3	1:A:429:PHE:CD2	2.56	0.41
1:A:528:GLY:HA2	8:A:613:OLC:H2	2.02	0.41
8:A:608:OLC:H11	8:A:615:OLC:H14	2.03	0.41
1:A:426:TRP:NE1	8:A:608:OLC:H21	2.36	0.40
1:A:102:ASN:OD1	1:A:102:ASN:C	2.60	0.40
1:A:261:SER:HB3	1:A:264:MET:HB2	2.04	0.40
3:C:9:LEU:O	3:C:12:ILE:HG13	2.21	0.40
1:A:96:GLU:OE2	1:A:180:PRO:HB2	2.20	0.40
2:B:27:PHE:HD1	2:B:27:PHE:HA	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.89	0.40
1:A:247:ILE:O	1:A:252:PRO:HD3	2.22	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)
10:B:308:HOH:O	10:B:324:HOH:O[2_556]	1.72	0.48

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	552/568 (97%)	520 (94%)	32 (6%)	0	100	100
2	B	164/168 (98%)	160 (98%)	4 (2%)	0	100	100
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	745/770 (97%)	709 (95%)	36 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	445/462 (96%)	424 (95%)	21 (5%)	26	59
2	B	133/138 (96%)	127 (96%)	6 (4%)	27	60
3	C	24/27 (89%)	21 (88%)	3 (12%)	4	14
All	All	602/627 (96%)	572 (95%)	30 (5%)	24	56

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	58	LEU
1	A	80	PHE
1	A	215	LEU
1	A	223	VAL
1	A	244	TYR
1	A	274	LEU
1	A	309	SER
1	A	326	LEU
1	A	332	LEU
1	A	369	PHE
1	A	405	LEU
1	A	475	ILE
1	A	495	ARG
1	A	500	GLU
1	A	503	GLU
1	A	512	ILE
1	A	518	ARG
1	A	520	LEU
1	A	526	ARG
1	A	549	LEU
2	B	12	LEU
2	B	26	LEU
2	B	37	LEU
2	B	111	ASP
2	B	167	LYS
2	B	168	GLU
3	C	13	LEU
3	C	20	LEU
3	C	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	$\# Z > 2$
8	OLC	A	605	-	24,24,24	0.51	0	25,25,25	0.66	0
8	OLC	A	616	-	20,20,24	0.50	0	21,21,25	0.72	0
8	OLC	A	606	-	24,24,24	0.44	0	25,25,25	0.58	0
8	OLC	A	613	-	14,14,24	0.49	0	15,15,25	0.58	0
8	OLC	A	615	-	24,24,24	0.43	0	25,25,25	0.75	0
8	OLC	A	611	-	16,16,24	0.54	0	17,17,25	0.68	0
8	OLC	B	202	-	24,24,24	0.50	0	25,25,25	0.58	0
8	OLC	B	204	-	24,24,24	0.46	0	25,25,25	0.51	0
8	OLC	A	607	-	24,24,24	0.53	0	25,25,25	0.64	0
8	OLC	A	617	-	24,24,24	0.44	0	25,25,25	0.80	1 (4%)
8	OLC	A	608	-	22,22,24	0.47	0	23,23,25	0.48	0
5	HEM	A	602	1	41,50,50	2.88	18 (43%)	45,82,82	1.95	7 (15%)
7	PER	A	604	6,4	0,1,1	-	-	-	-	-
8	OLC	A	612	-	7,7,24	0.44	0	6,7,25	0.29	0
8	OLC	B	203	-	24,24,24	0.57	0	25,25,25	0.67	0
8	OLC	A	610	-	17,17,24	0.55	0	18,18,25	0.55	0
8	OLC	A	609	-	20,20,24	0.50	0	20,20,25	0.55	0

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	1,7	69,72,72	2.40	23 (33%)	73,109,109	1.48	13 (17%)
8	OLC	A	614	-	19,19,24	0.49	0	20,20,25	0.57	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
8	OLC	A	605	-	-	11/24/24/24	-
8	OLC	A	608	-	-	10/22/22/24	-
5	HEM	A	602	1	-	3/12/54/54	-
8	OLC	A	616	-	-	7/20/20/24	-
8	OLC	A	606	-	-	11/24/24/24	-
8	OLC	B	204	-	-	10/24/24/24	-
8	OLC	A	613	-	-	7/14/14/24	-
8	OLC	A	607	-	-	17/24/24/24	-
8	OLC	A	612	-	-	3/6/6/24	-
6	HAS	A	603	1,7	1/1/8/18	7/40/82/82	-
8	OLC	A	614	-	-	9/19/19/24	-
8	OLC	A	615	-	-	16/24/24/24	-
8	OLC	A	617	-	-	11/24/24/24	-
8	OLC	B	203	-	-	10/24/24/24	-
8	OLC	A	611	-	-	10/16/16/24	-
8	OLC	A	610	-	-	6/17/17/24	-
8	OLC	A	609	-	-	9/19/19/24	-
8	OLC	B	202	-	-	7/24/24/24	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	C3C-C2C	7.71	1.51	1.40
6	A	603	HAS	C3C-CAC	-7.27	1.33	1.47
5	A	602	HEM	C3B-C2B	6.24	1.49	1.37
5	A	602	HEM	CHB-C1B	6.18	1.50	1.35
6	A	603	HAS	CHB-C1D	5.87	1.50	1.38
5	A	602	HEM	C3C-C2C	5.69	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEM	C1B-C2B	-5.49	1.33	1.44
5	A	602	HEM	CAB-C3B	-5.26	1.33	1.47
6	A	603	HAS	CHA-C4D	5.25	1.51	1.39
5	A	602	HEM	C1A-NA	4.89	1.46	1.36
5	A	602	HEM	FE-NB	4.67	2.20	1.96
6	A	603	HAS	C4D-ND	4.45	1.48	1.38
6	A	603	HAS	C1D-ND	4.27	1.47	1.40
5	A	602	HEM	CBB-CAB	4.20	1.51	1.30
5	A	602	HEM	C2C-C1C	-4.19	1.33	1.42
6	A	603	HAS	C4D-C3D	4.07	1.52	1.45
6	A	603	HAS	C4B-C3B	3.90	1.51	1.44
5	A	602	HEM	C1A-CHA	3.68	1.51	1.41
6	A	603	HAS	C4C-NC	3.68	1.43	1.36
6	A	603	HAS	C2D-C1D	3.63	1.52	1.44
6	A	603	HAS	C1C-CHC	3.43	1.50	1.41
6	A	603	HAS	CBC-CAC	3.29	1.51	1.29
6	A	603	HAS	O1D-CGD	3.22	1.32	1.22
5	A	602	HEM	C1D-C2D	3.17	1.50	1.44
6	A	603	HAS	C4C-CHD	3.08	1.49	1.41
6	A	603	HAS	CHB-C1B	-3.07	1.32	1.39
5	A	602	HEM	CHC-C4B	-3.01	1.32	1.41
5	A	602	HEM	CHD-C1D	-2.92	1.32	1.41
6	A	603	HAS	C1A-C2A	2.90	1.50	1.45
5	A	602	HEM	C4D-ND	-2.87	1.35	1.40
5	A	602	HEM	C4A-CHB	-2.80	1.33	1.41
5	A	602	HEM	C4D-C3D	2.74	1.49	1.45
6	A	603	HAS	O2D-CGD	-2.70	1.21	1.30
6	A	603	HAS	C1B-C2B	2.55	1.49	1.44
6	A	603	HAS	CHD-C4A	-2.38	1.32	1.35
5	A	602	HEM	C1B-NB	-2.23	1.36	1.40
6	A	603	HAS	CHA-C1A	-2.21	1.34	1.38
6	A	603	HAS	CMD-C2D	2.16	1.49	1.45
6	A	603	HAS	FE-NA	2.15	2.04	1.95
5	A	602	HEM	C3B-C4B	2.14	1.49	1.44
6	A	603	HAS	C2A-C3A	-2.13	1.32	1.36

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	HEM	C1B-NB-C4B	5.96	111.23	105.07
5	A	602	HEM	CHC-C4B-NB	5.80	130.74	124.43
5	A	602	HEM	C4B-C3B-C2B	-4.74	103.35	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	C1D-ND-C4D	-4.05	100.89	105.07
6	A	603	HAS	CAA-CBA-CGA	-3.92	105.16	113.60
5	A	602	HEM	C4D-ND-C1D	3.50	108.69	105.07
6	A	603	HAS	CMB-C2B-C3B	-3.49	123.69	130.34
6	A	603	HAS	CMC-C2C-C1C	-3.17	123.59	128.46
6	A	603	HAS	CHB-C1D-ND	-2.95	120.74	124.37
6	A	603	HAS	CHA-C4D-ND	-2.86	121.31	124.42
6	A	603	HAS	CHA-C1A-C2A	-2.86	120.31	124.94
6	A	603	HAS	CHA-C1A-NA	2.69	127.35	124.44
5	A	602	HEM	C4A-C3A-C2A	2.64	108.83	107.00
5	A	602	HEM	CHA-C4D-ND	2.53	127.51	124.38
8	A	617	OLC	C3-C2-C1	-2.49	104.55	113.62
6	A	603	HAS	O1A-CGA-CBA	-2.28	115.75	123.08
5	A	602	HEM	CMA-C3A-C4A	-2.25	125.00	128.46
6	A	603	HAS	CHA-C4D-C3D	2.10	127.93	124.84
6	A	603	HAS	C2D-C3D-C4D	2.05	107.95	106.49
6	A	603	HAS	C2B-C1B-NB	2.04	112.33	109.88
6	A	603	HAS	C3B-C4B-NB	2.02	112.24	109.84

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	603	HAS	NA

All (164) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	603	HAS	C3D-C2D-CMD-OMD
8	A	607	OLC	O20-C21-C22-O23
8	A	608	OLC	O20-C21-C22-C24
8	A	612	OLC	O20-C21-C22-C24
8	A	612	OLC	O19-C1-O20-C21
8	A	614	OLC	C10-C11-C12-C13
8	A	615	OLC	C21-C22-C24-O25
8	A	605	OLC	C2-C1-O20-C21
8	B	203	OLC	C2-C1-O20-C21
8	A	605	OLC	O19-C1-O20-C21
8	A	611	OLC	O19-C1-O20-C21
8	B	203	OLC	O19-C1-O20-C21
8	A	607	OLC	C2-C1-O20-C21
8	A	608	OLC	O20-C21-C22-O23
8	A	612	OLC	O20-C21-C22-O23

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Mol	Chain	Res	Type	Atoms
6	A	603	HAS	C28-C29-C30-C31
8	A	607	OLC	C2-C3-C4-C5
8	A	611	OLC	C2-C1-O20-C21
8	A	607	OLC	O19-C1-O20-C21
6	A	603	HAS	C28-C29-C30-C32
8	A	614	OLC	C2-C1-O20-C21
8	A	607	OLC	O20-C21-C22-C24
8	A	611	OLC	O20-C21-C22-C24
8	A	613	OLC	O20-C21-C22-C24
8	B	202	OLC	O20-C21-C22-C24
8	A	610	OLC	C1-C2-C3-C4
8	A	611	OLC	O20-C21-C22-O23
8	B	203	OLC	C1-C2-C3-C4
8	A	614	OLC	O19-C1-O20-C21
8	A	615	OLC	C1-C2-C3-C4
8	B	202	OLC	C1-C2-C3-C4
8	B	204	OLC	C1-C2-C3-C4
8	A	606	OLC	O20-C21-C22-O23
8	A	610	OLC	O20-C21-C22-O23
8	B	202	OLC	O20-C21-C22-O23
8	A	608	OLC	C2-C1-O20-C21
8	A	606	OLC	C3-C4-C5-C6
8	A	613	OLC	C4-C5-C6-C7
8	A	606	OLC	O20-C21-C22-C24
8	A	610	OLC	O20-C21-C22-C24
8	A	615	OLC	C2-C3-C4-C5
8	A	615	OLC	C14-C15-C16-C17
8	A	615	OLC	C11-C12-C13-C14
8	A	608	OLC	C12-C13-C14-C15
8	A	616	OLC	C3-C4-C5-C6
8	A	607	OLC	C4-C5-C6-C7
8	A	614	OLC	C2-C3-C4-C5
8	B	202	OLC	C3-C4-C5-C6
8	A	606	OLC	C5-C6-C7-C8
8	A	607	OLC	C3-C4-C5-C6
8	A	608	OLC	C21-C22-C24-O25
8	A	610	OLC	C21-C22-C24-O25
8	A	611	OLC	C21-C22-C24-O25
8	A	613	OLC	C21-C22-C24-O25
8	A	616	OLC	C21-C22-C24-O25
8	A	615	OLC	O20-C21-C22-O23
8	A	607	OLC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
8	A	614	OLC	C6-C7-C8-C9
8	A	616	OLC	C10-C11-C12-C13
8	A	617	OLC	C1-C2-C3-C4
8	B	203	OLC	C5-C6-C7-C8
8	A	608	OLC	O19-C1-O20-C21
8	A	606	OLC	C13-C14-C15-C16
8	A	606	OLC	C12-C13-C14-C15
8	A	609	OLC	C14-C15-C16-C17
8	A	605	OLC	C11-C12-C13-C14
8	A	607	OLC	C1-C2-C3-C4
8	A	613	OLC	O23-C22-C24-O25
8	A	616	OLC	O23-C22-C24-O25
8	A	606	OLC	C6-C7-C8-C9
8	B	204	OLC	C10-C11-C12-C13
8	A	605	OLC	C4-C5-C6-C7
8	B	204	OLC	C5-C6-C7-C8
8	A	607	OLC	C6-C7-C8-C9
8	A	615	OLC	C10-C11-C12-C13
8	A	611	OLC	C5-C6-C7-C8
8	A	615	OLC	C12-C13-C14-C15
8	A	607	OLC	C14-C15-C16-C17
8	A	607	OLC	C11-C12-C13-C14
5	A	602	HEM	C2B-C3B-CAB-CBB
8	A	605	OLC	C10-C11-C12-C13
8	A	609	OLC	C10-C11-C12-C13
8	A	609	OLC	C3-C4-C5-C6
8	A	605	OLC	C12-C13-C14-C15
8	A	609	OLC	C12-C13-C14-C15
8	A	617	OLC	C15-C16-C17-C18
8	A	615	OLC	O23-C22-C24-O25
8	A	617	OLC	C4-C5-C6-C7
8	B	202	OLC	C6-C7-C8-C9
8	A	609	OLC	C15-C16-C17-C18
8	B	204	OLC	C3-C4-C5-C6
8	A	615	OLC	O20-C21-C22-C24
8	A	609	OLC	C2-C3-C4-C5
8	A	607	OLC	C9-C10-C11-C12
8	A	617	OLC	C2-C1-O20-C21
8	A	615	OLC	C5-C6-C7-C8
8	B	202	OLC	C4-C5-C6-C7
8	A	611	OLC	C3-C4-C5-C6
8	B	203	OLC	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
8	A	615	OLC	C4-C5-C6-C7
8	A	617	OLC	O19-C1-O20-C21
8	A	615	OLC	C13-C14-C15-C16
8	A	613	OLC	O20-C21-C22-O23
8	A	613	OLC	C1-C2-C3-C4
8	A	616	OLC	C1-C2-C3-C4
8	B	204	OLC	C15-C16-C17-C18
8	A	617	OLC	C10-C11-C12-C13
8	A	615	OLC	C3-C4-C5-C6
8	A	606	OLC	C2-C3-C4-C5
8	A	607	OLC	C13-C14-C15-C16
8	A	608	OLC	O23-C22-C24-O25
8	A	610	OLC	O23-C22-C24-O25
8	A	611	OLC	O23-C22-C24-O25
8	B	203	OLC	C10-C11-C12-C13
8	A	607	OLC	C5-C6-C7-C8
8	B	204	OLC	C13-C14-C15-C16
8	A	607	OLC	C7-C8-C9-C10
8	B	204	OLC	C2-C1-O20-C21
8	A	613	OLC	C5-C6-C7-C8
8	A	617	OLC	C11-C12-C13-C14
8	A	605	OLC	C5-C6-C7-C8
6	A	603	HAS	C1D-C2D-CMD-OMD
8	B	204	OLC	O19-C1-O20-C21
6	A	603	HAS	C23-C24-C28-C29
8	A	605	OLC	C14-C15-C16-C17
8	A	605	OLC	C2-C3-C4-C5
8	A	615	OLC	C15-C16-C17-C18
8	A	609	OLC	C7-C8-C9-C10
8	A	606	OLC	C10-C11-C12-C13
8	A	610	OLC	C6-C7-C8-C9
8	B	203	OLC	O23-C22-C24-O25
8	B	203	OLC	C6-C7-C8-C9
8	A	617	OLC	C13-C14-C15-C16
8	A	617	OLC	C2-C3-C4-C5
8	A	606	OLC	C11-C12-C13-C14
8	A	608	OLC	C7-C8-C9-C10
8	B	203	OLC	C7-C8-C9-C10
6	A	603	HAS	CAA-CBA-CGA-O2A
8	A	616	OLC	C5-C6-C7-C8
8	A	615	OLC	C7-C8-C9-C10
8	A	609	OLC	C6-C7-C8-C9

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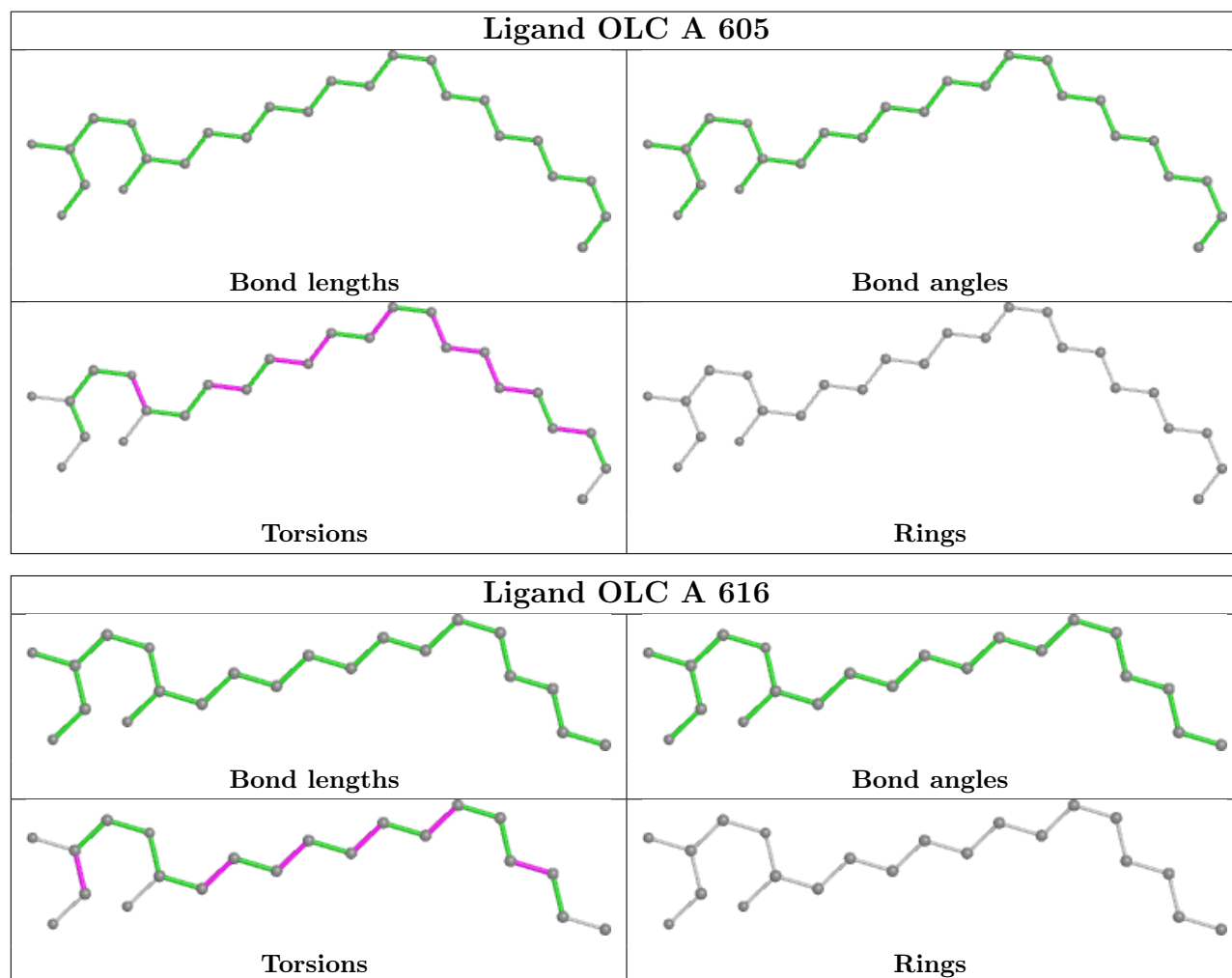
Mol	Chain	Res	Type	Atoms
8	A	609	OLC	C13-C14-C15-C16
8	B	204	OLC	C14-C15-C16-C17
8	A	605	OLC	C9-C10-C11-C12
8	A	605	OLC	C7-C8-C9-C10
8	A	614	OLC	C9-C10-C11-C12
8	A	617	OLC	C9-C10-C11-C12
8	B	202	OLC	C7-C8-C9-C10
8	B	203	OLC	C9-C10-C11-C12
8	B	204	OLC	C7-C8-C9-C10
8	A	614	OLC	O20-C1-C2-C3
8	A	614	OLC	C4-C5-C6-C7
8	A	617	OLC	C12-C13-C14-C15
8	A	611	OLC	O20-C1-C2-C3
6	A	603	HAS	CAA-CBA-CGA-O1A
8	A	608	OLC	C6-C7-C8-C9
8	A	607	OLC	C15-C16-C17-C18
8	A	616	OLC	C7-C8-C9-C10
8	A	614	OLC	O19-C1-C2-C3
8	A	606	OLC	C9-C10-C11-C12
8	A	611	OLC	O19-C1-C2-C3
8	A	608	OLC	C11-C12-C13-C14
5	A	602	HEM	CAA-CBA-CGA-O2A
5	A	602	HEM	CAD-CBD-CGD-O2D

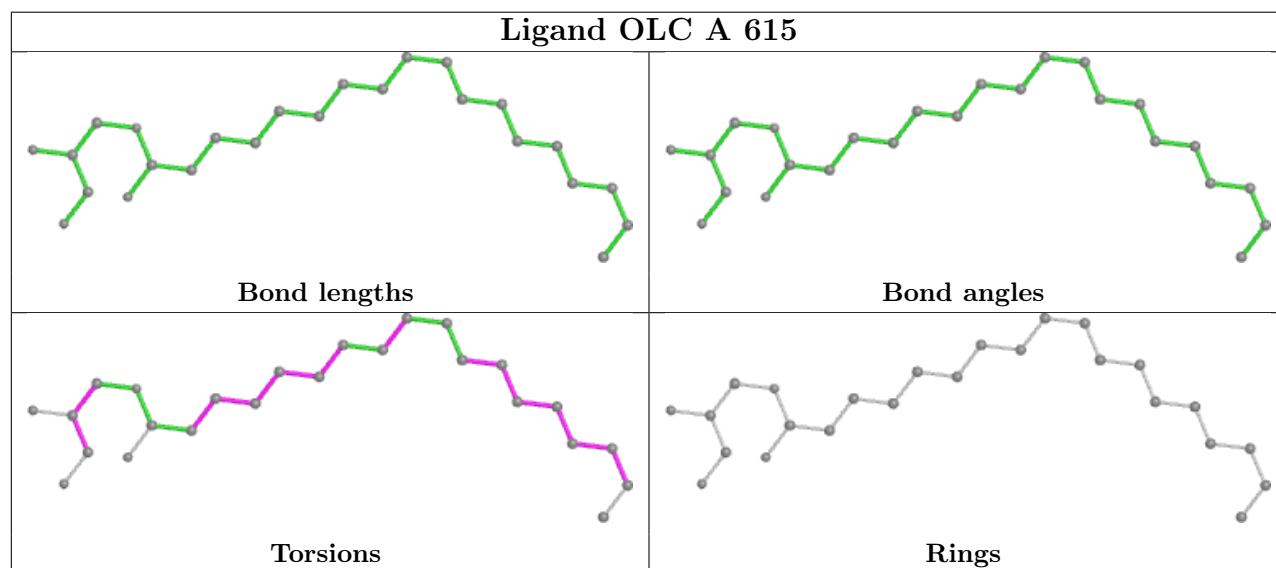
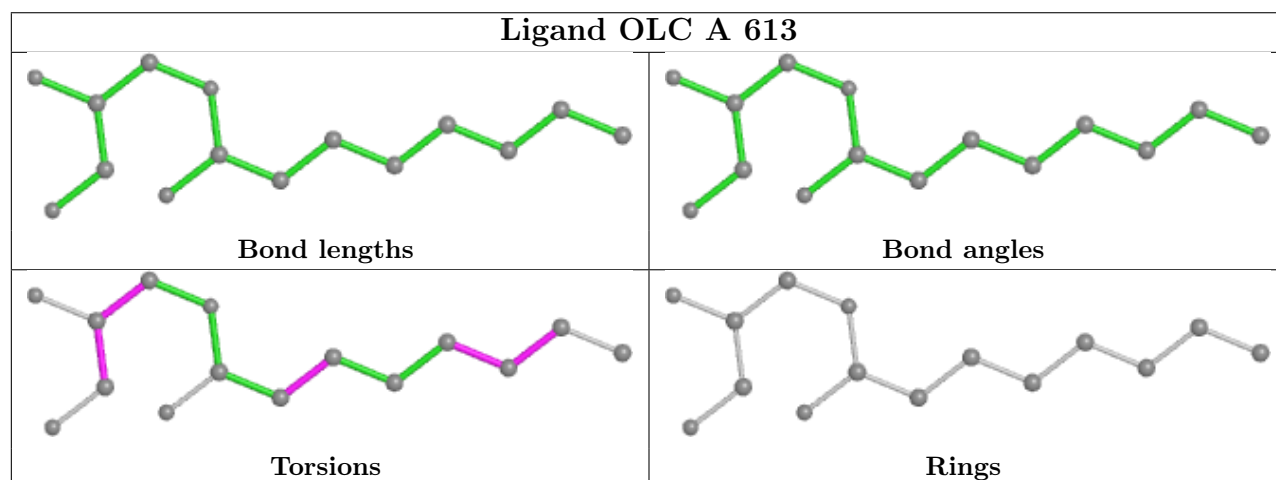
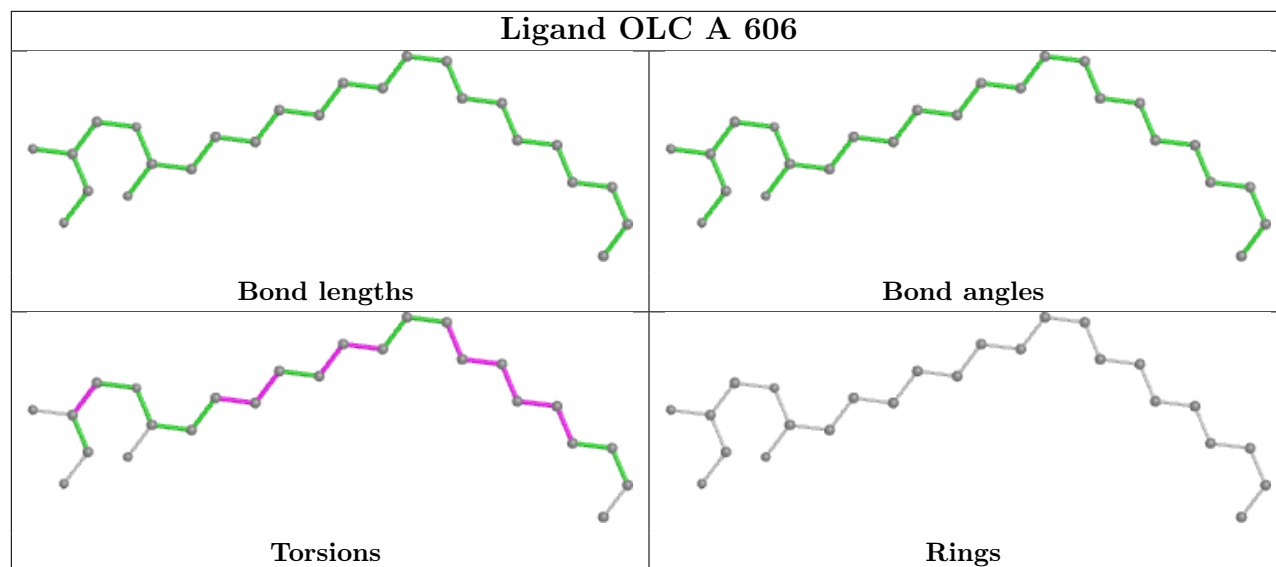
There are no ring outliers.

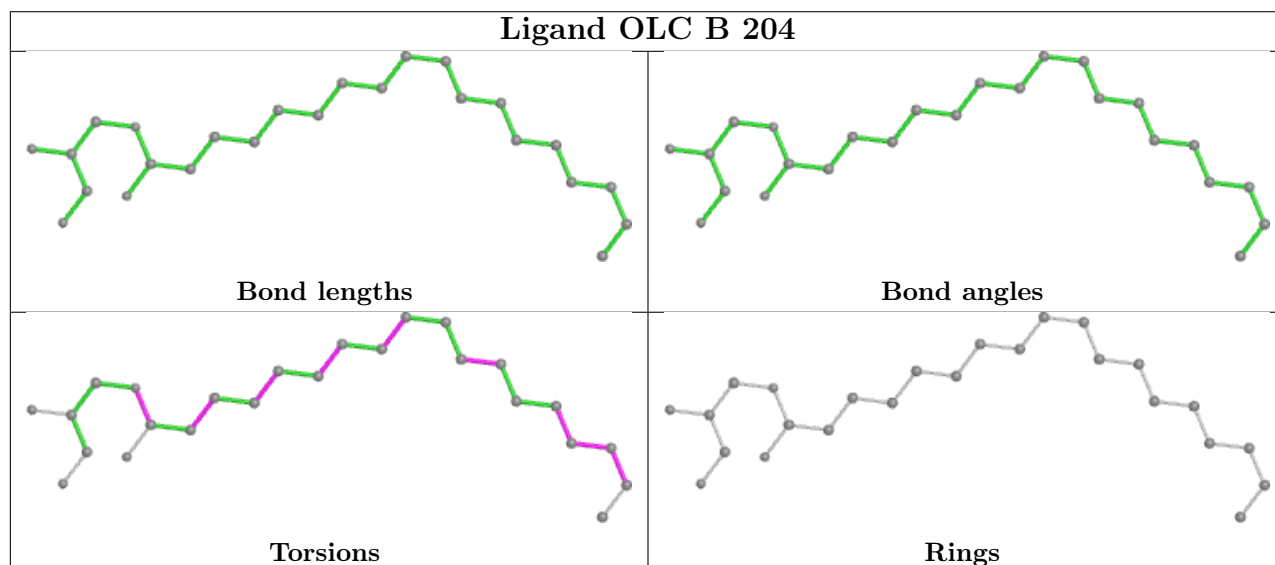
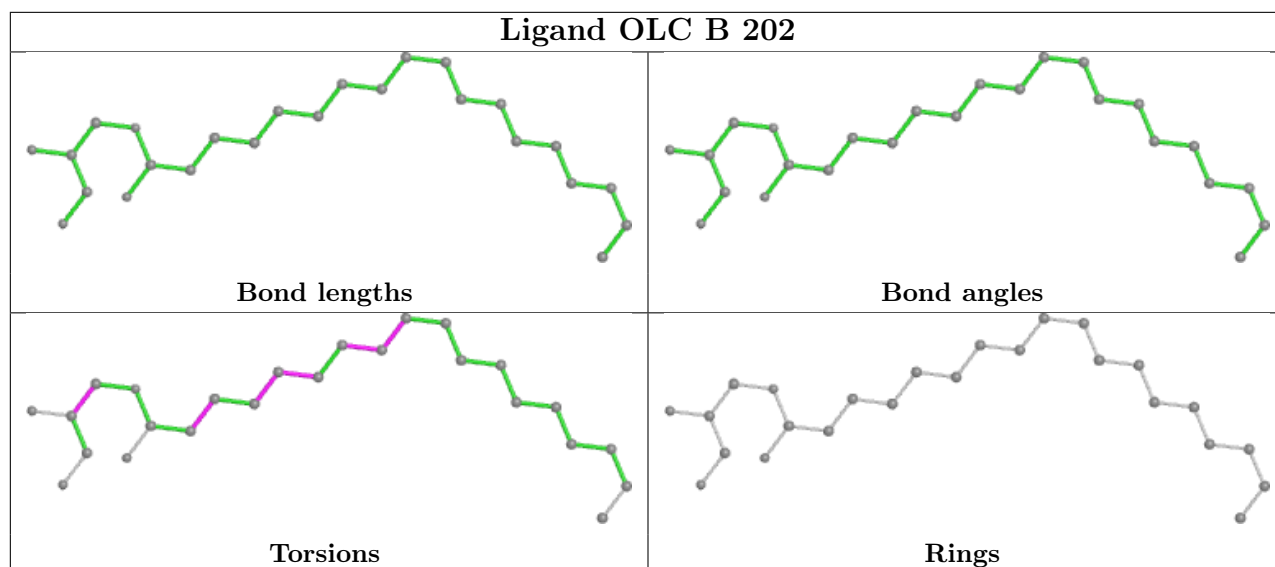
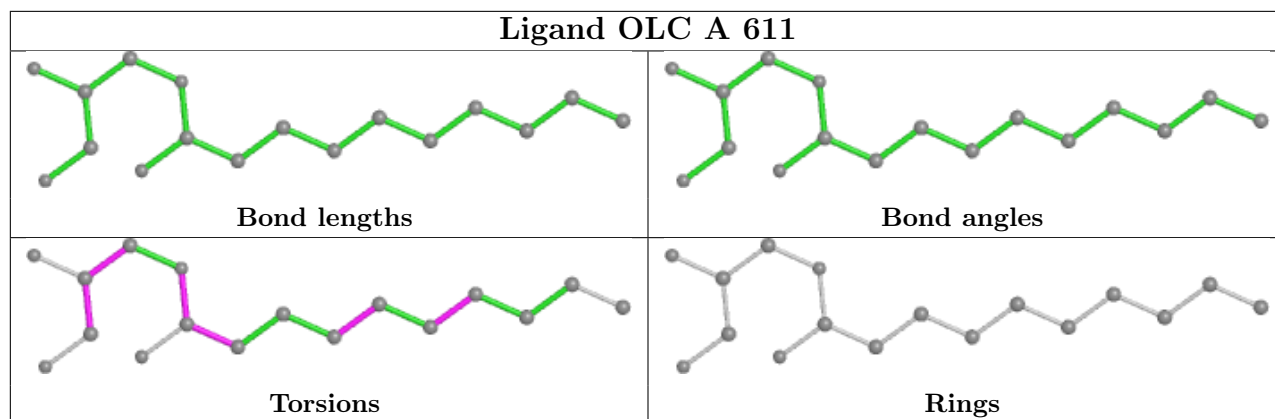
14 monomers are involved in 46 short contacts:

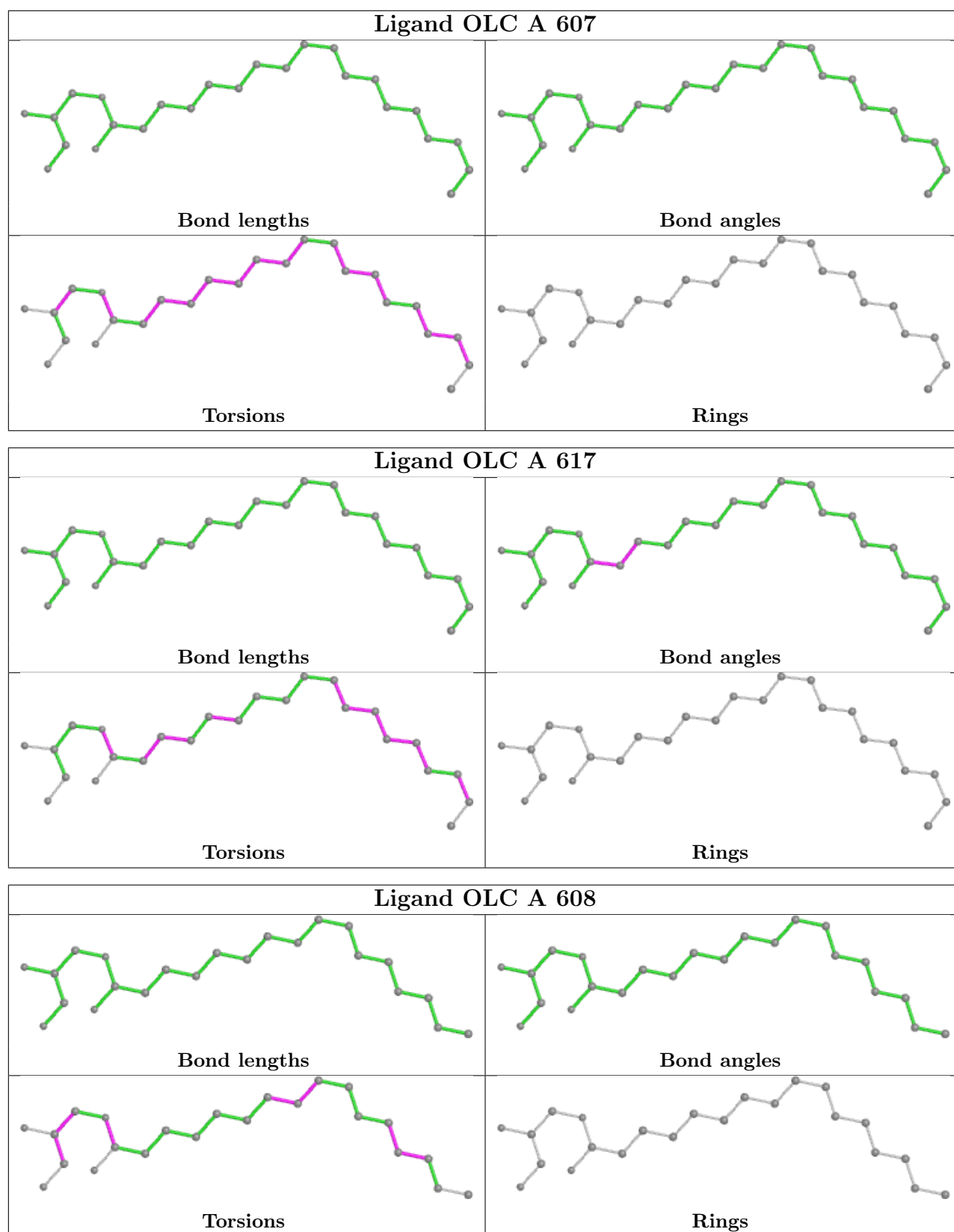
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	605	OLC	2	0
8	A	606	OLC	2	0
8	A	613	OLC	4	0
8	A	615	OLC	3	0
8	B	202	OLC	5	0
8	B	204	OLC	4	0
8	A	607	OLC	5	0
8	A	617	OLC	3	0
8	A	608	OLC	2	0
5	A	602	HEM	7	0
8	A	612	OLC	4	0
8	B	203	OLC	6	0
8	A	609	OLC	2	0
6	A	603	HAS	2	0

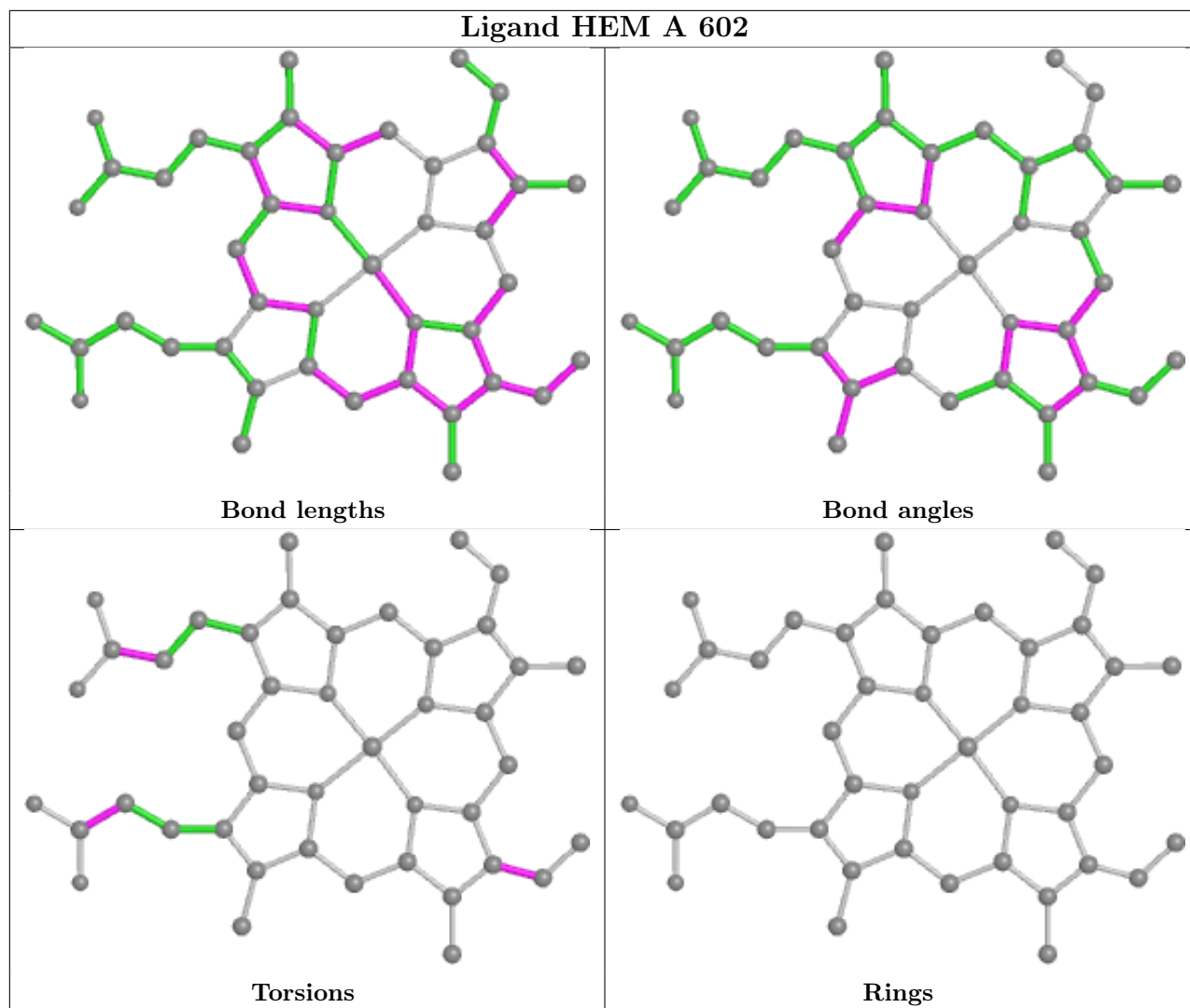
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

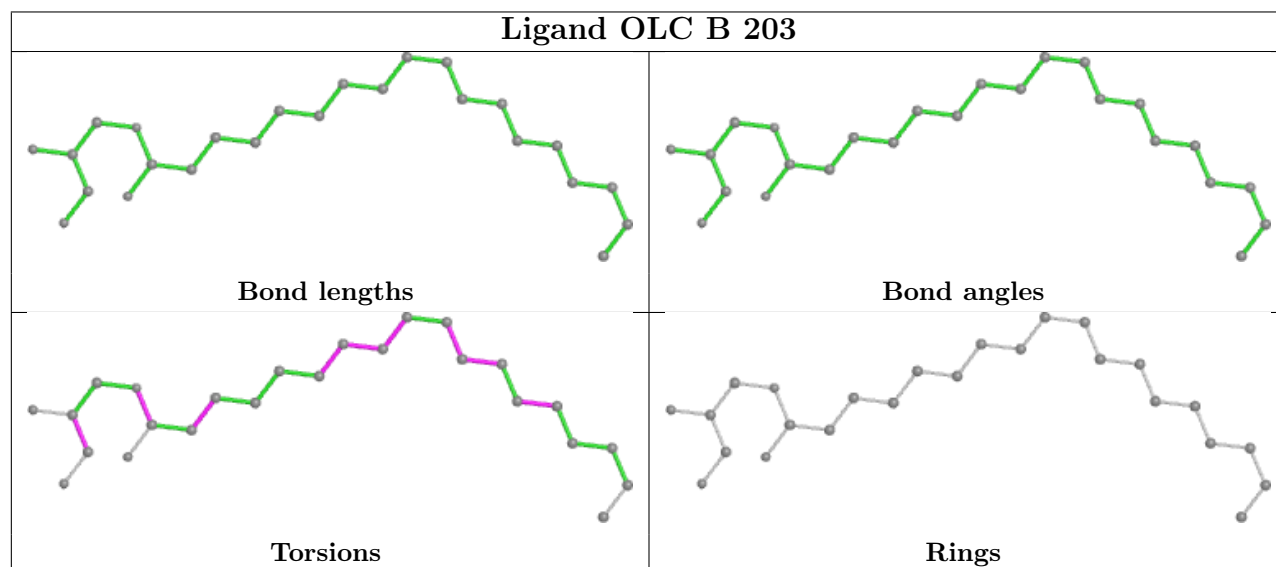
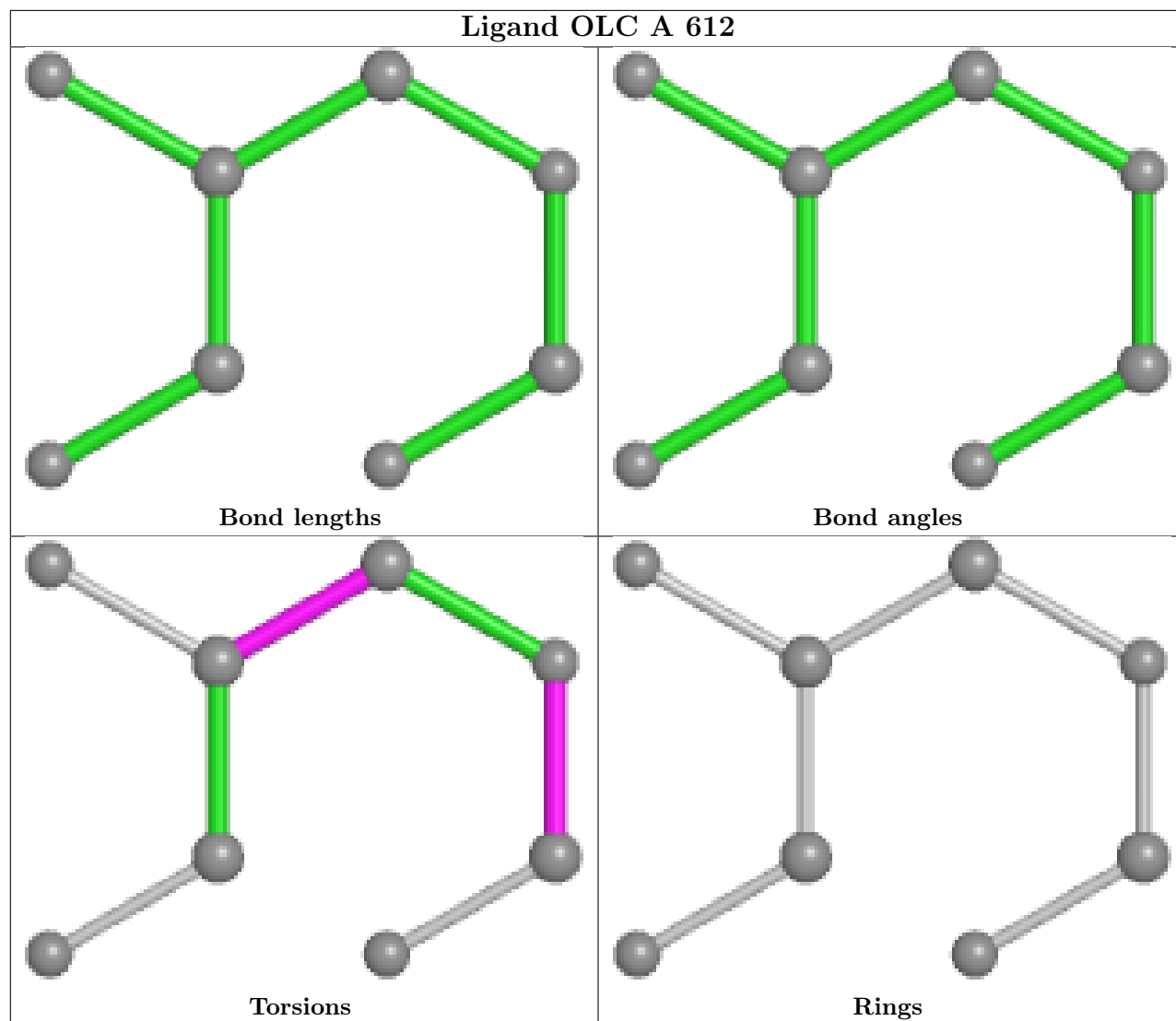


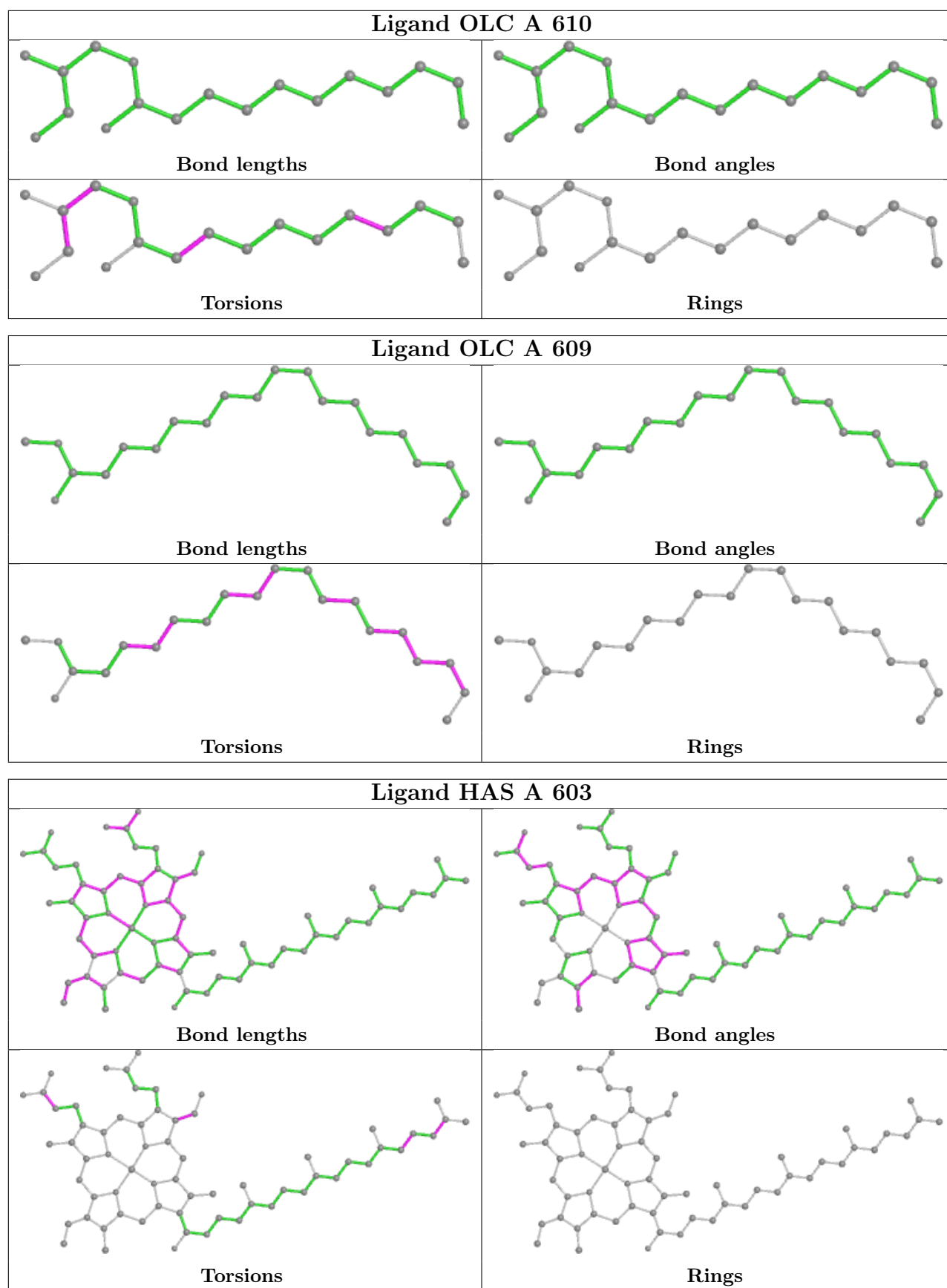


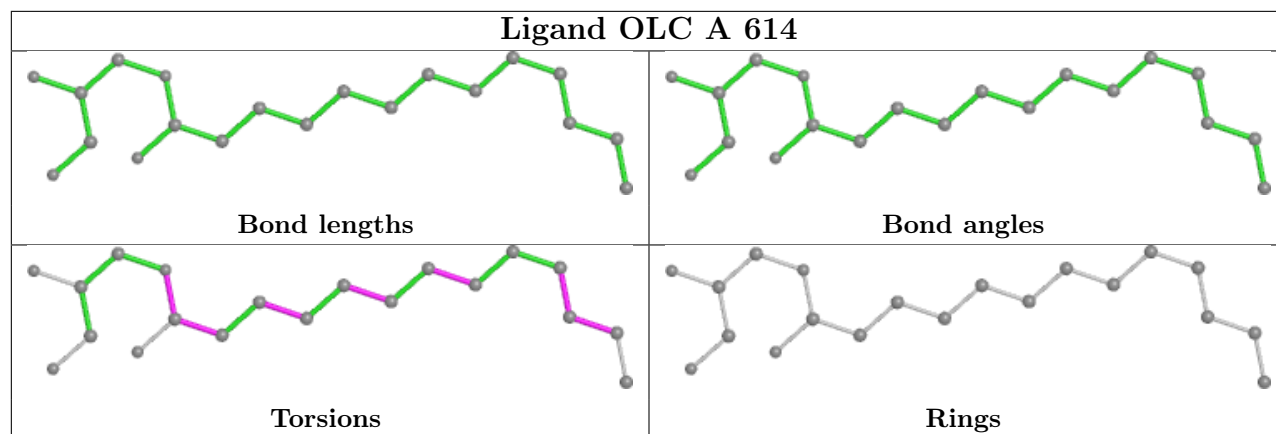












5.7 Other polymers [i](#)

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	554/568 (97%)	-0.44	2 (0%) 92 91	15, 25, 45, 87	3 (0%)
2	B	166/168 (98%)	-0.41	0 100 100	16, 25, 43, 61	1 (0%)
3	C	31/34 (91%)	-0.48	0 100 100	17, 24, 37, 48	0
All	All	751/770 (97%)	-0.43	2 (0%) 94 93	15, 25, 45, 87	4 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	SER	5.4
1	A	514	GLY	2.8

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 monosaccharides 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(Å ²)	Q<0.9
8	OLC	A	613	15/25	0.76	0.40	41,48,71,73	0

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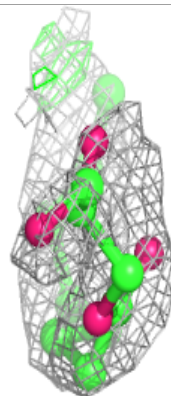
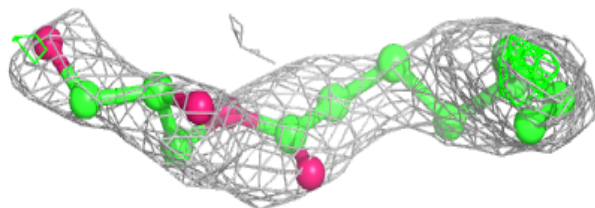
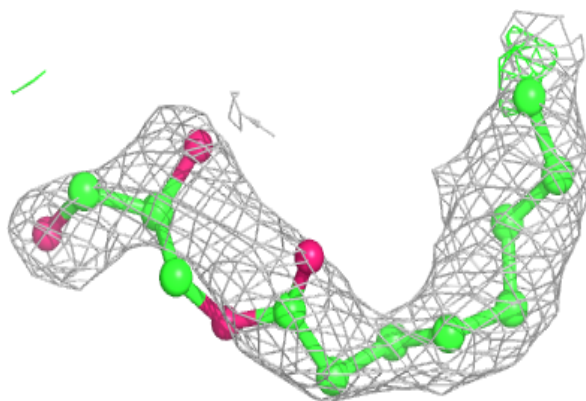
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	OLC	A	611	17/25	0.79	0.27	35,47,97,98	0
8	OLC	B	203	25/25	0.79	0.23	36,53,75,82	0
8	OLC	A	609	21/25	0.82	0.32	37,43,63,71	0
8	OLC	A	614	20/25	0.82	0.26	32,50,64,65	0
8	OLC	A	607	25/25	0.82	0.24	40,44,65,79	0
8	OLC	A	616	21/25	0.85	0.23	35,45,61,72	0
8	OLC	A	606	25/25	0.86	0.27	35,58,90,105	0
8	OLC	A	617	25/25	0.88	0.23	35,47,62,70	0
8	OLC	A	610	18/25	0.89	0.20	32,43,62,65	0
8	OLC	B	204	25/25	0.89	0.38	38,50,66,77	0
8	OLC	A	605	25/25	0.90	0.32	26,45,69,79	0
8	OLC	B	202	25/25	0.90	0.31	32,44,52,55	0
8	OLC	A	608	23/25	0.91	0.21	27,39,49,55	0
8	OLC	A	615	25/25	0.92	0.20	31,44,58,69	0
8	OLC	A	612	8/25	0.93	0.26	39,44,48,49	0
6	HAS	A	603	65/65	0.97	0.20	14,19,24,27	0
5	HEM	A	602	43/43	0.98	0.15	13,17,20,21	0
7	PER	A	604	2/2	0.99	0.17	23,23,23,24	0
4	CU	A	601	1/1	1.00	0.09	17,17,17,17	0
9	CUA	B	201	2/2	1.00	0.13	17,17,17,17	0

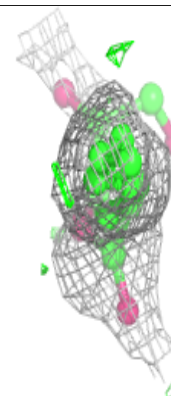
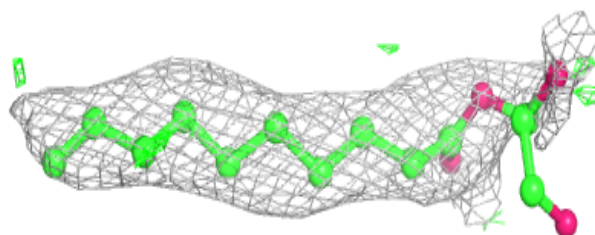
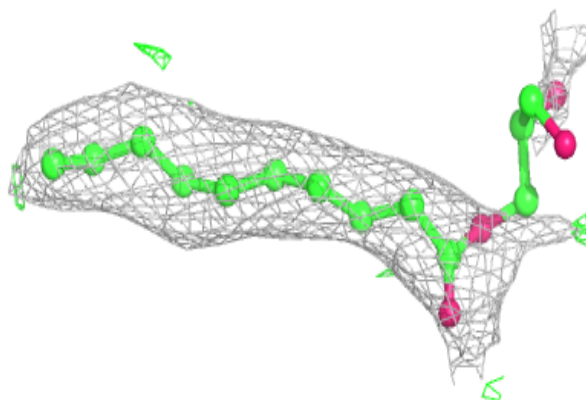
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 613:

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

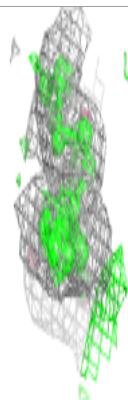
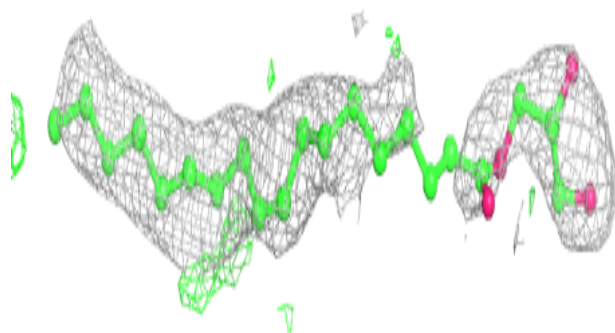
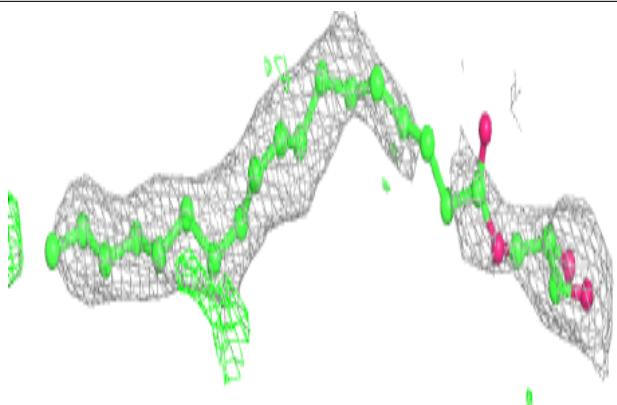
**Electron density around OLC A 611:**

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

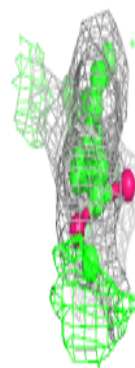
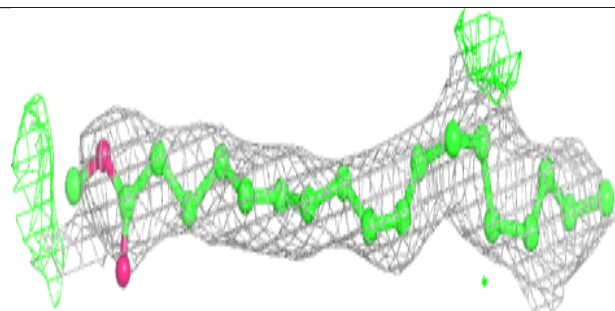
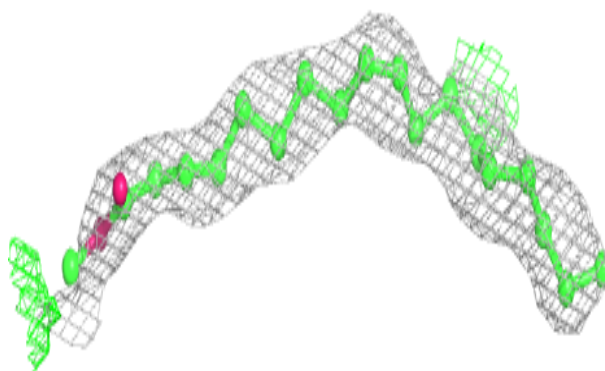


Electron density around OLC B 203:

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

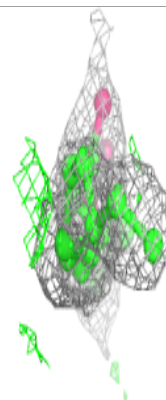
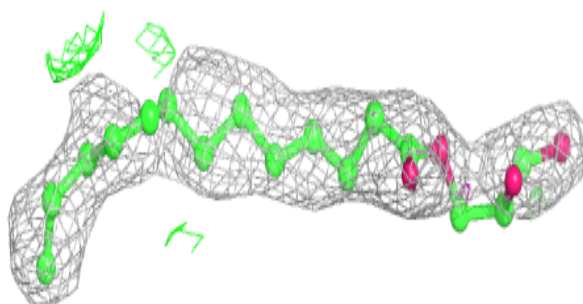
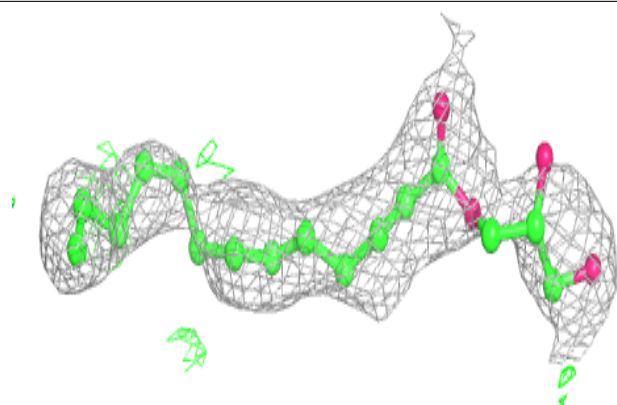
**Electron density around OLC A 609:**

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

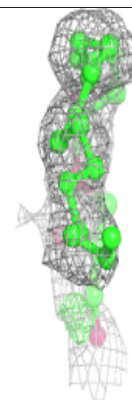
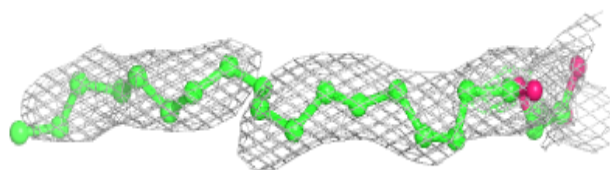
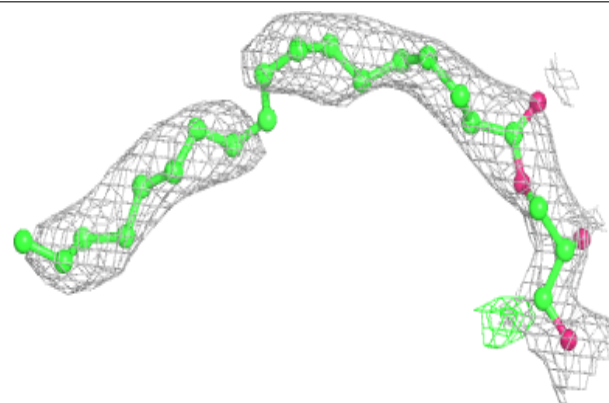


Electron density around OLC A 614:

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

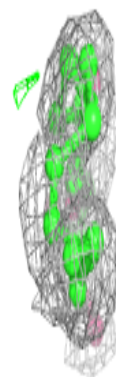
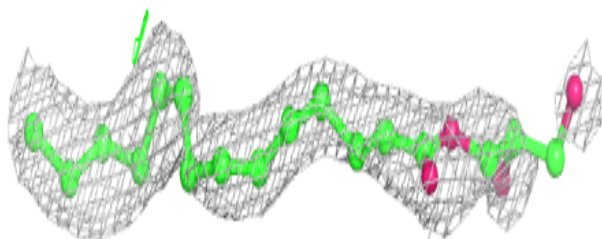
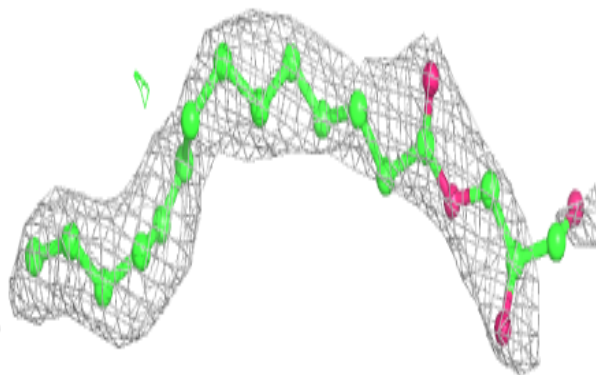
**Electron density around OLC A 607:**

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

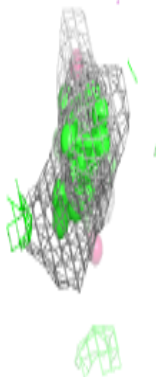
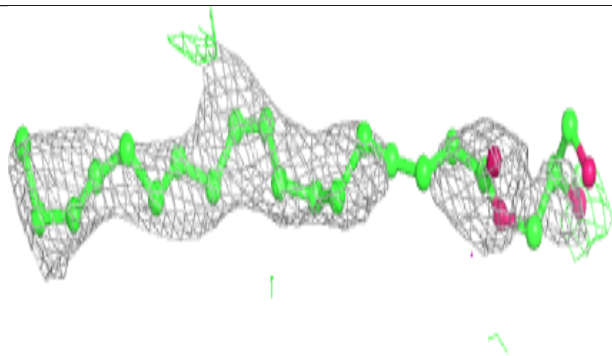
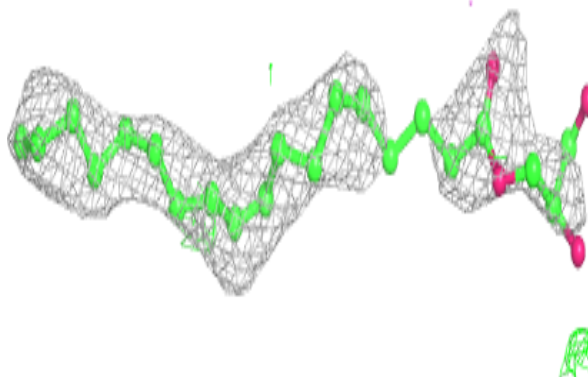


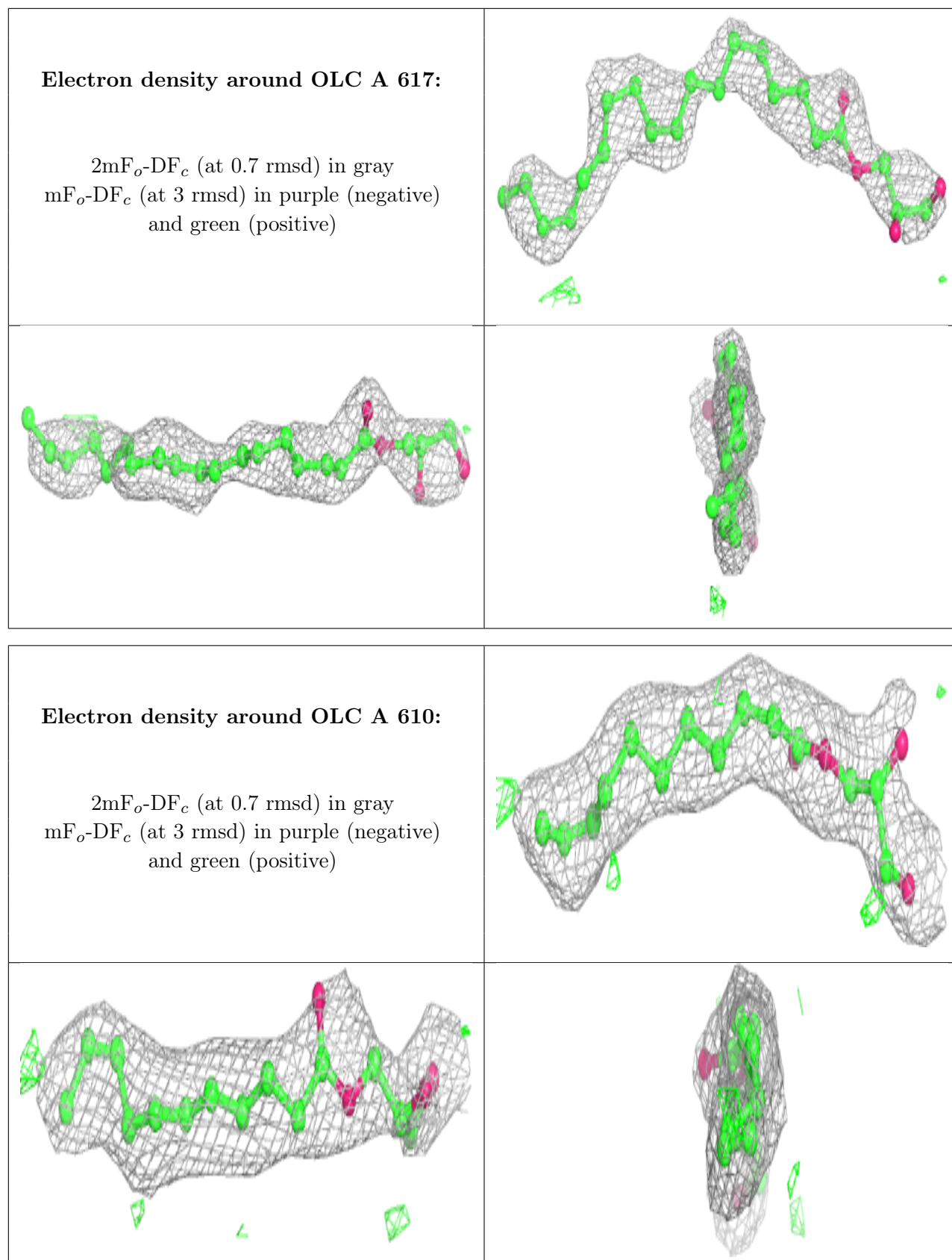
Electron density around OLC A 616:

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

**Electron density around OLC A 606:**

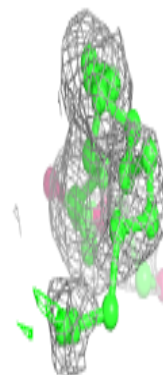
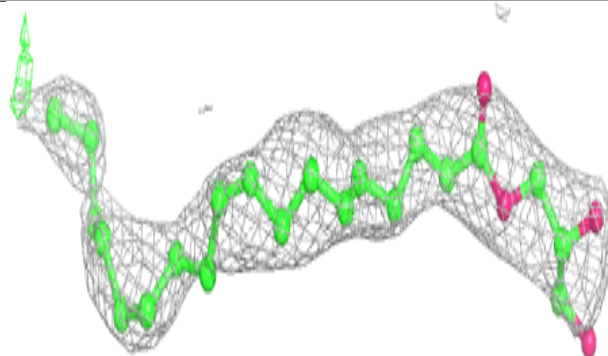
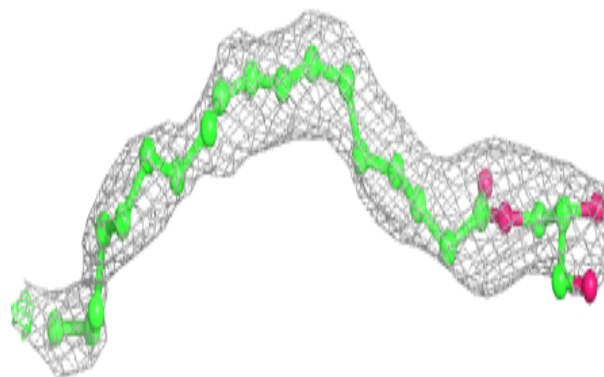
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



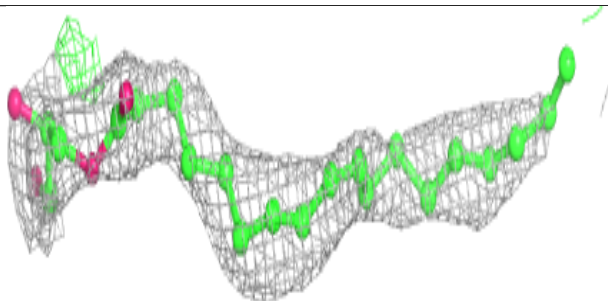
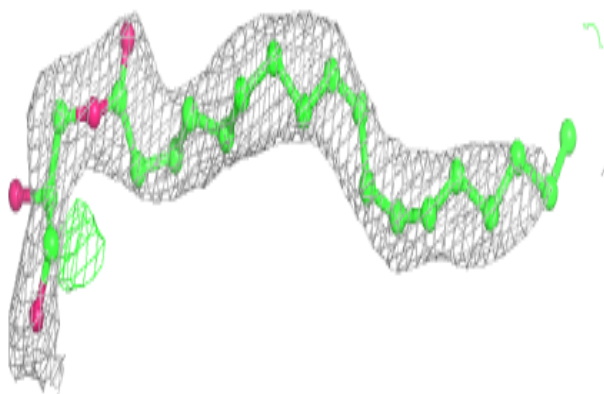


Electron density around OLC B 204:

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

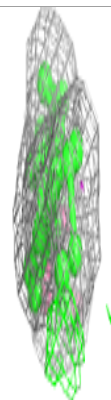
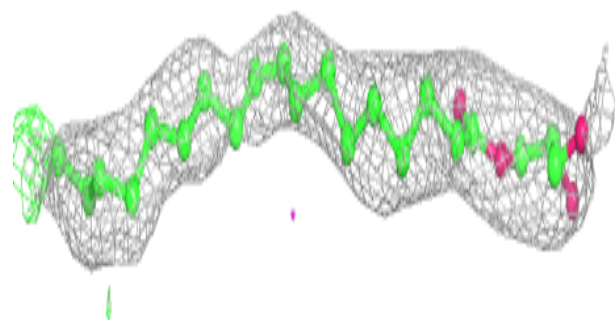
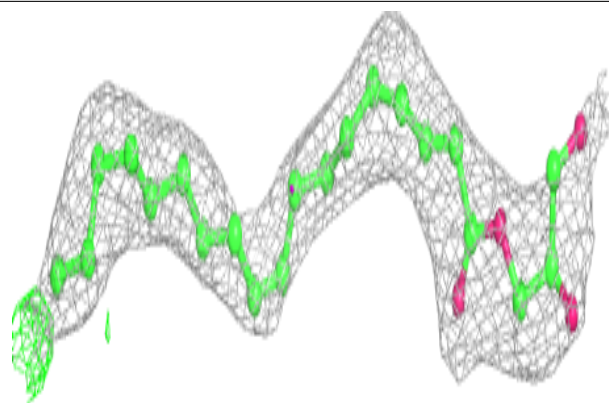
**Electron density around OLC A 605:**

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

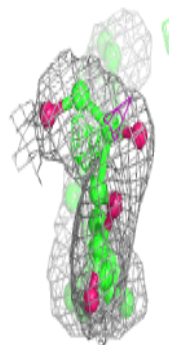
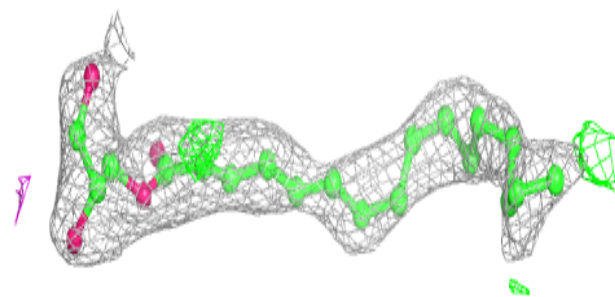
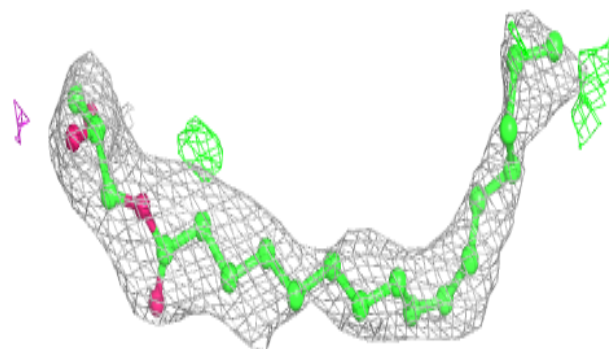


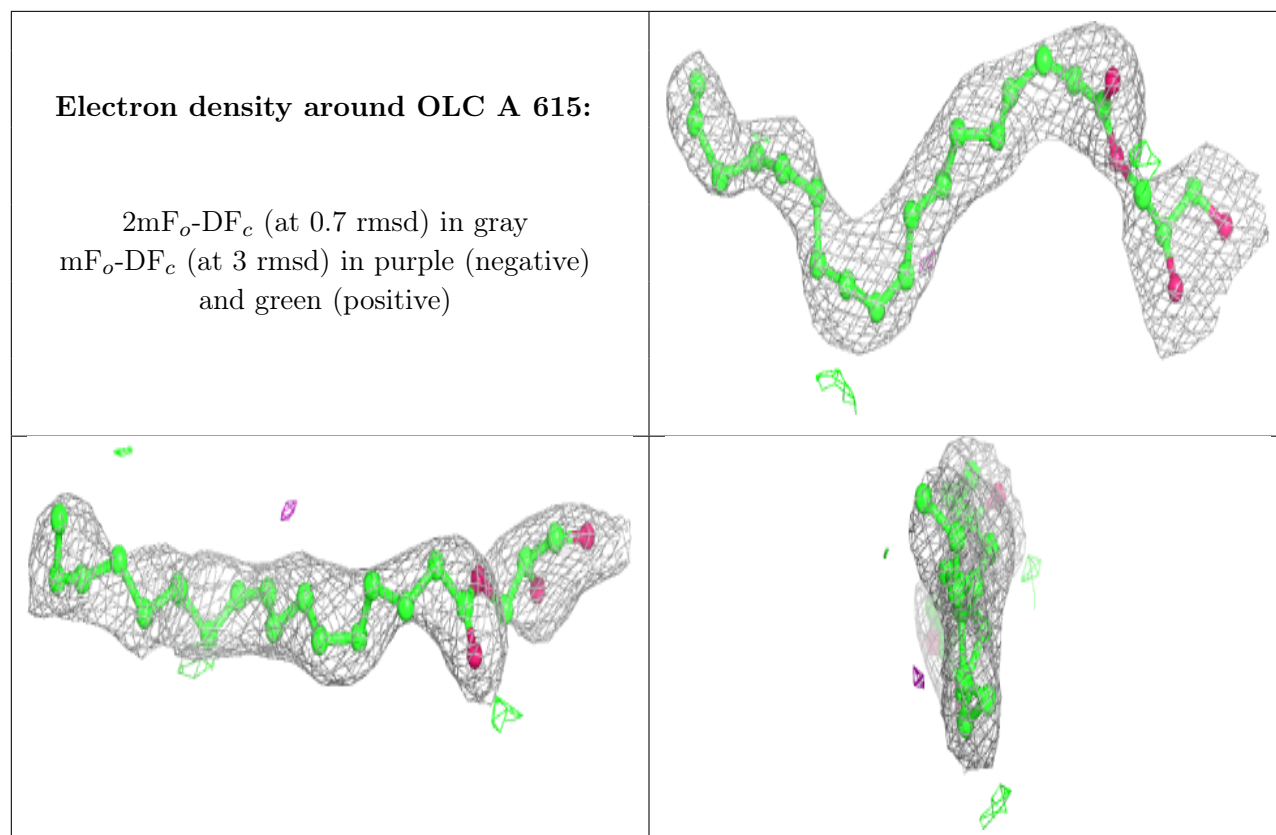
Electron density around OLC B 202:

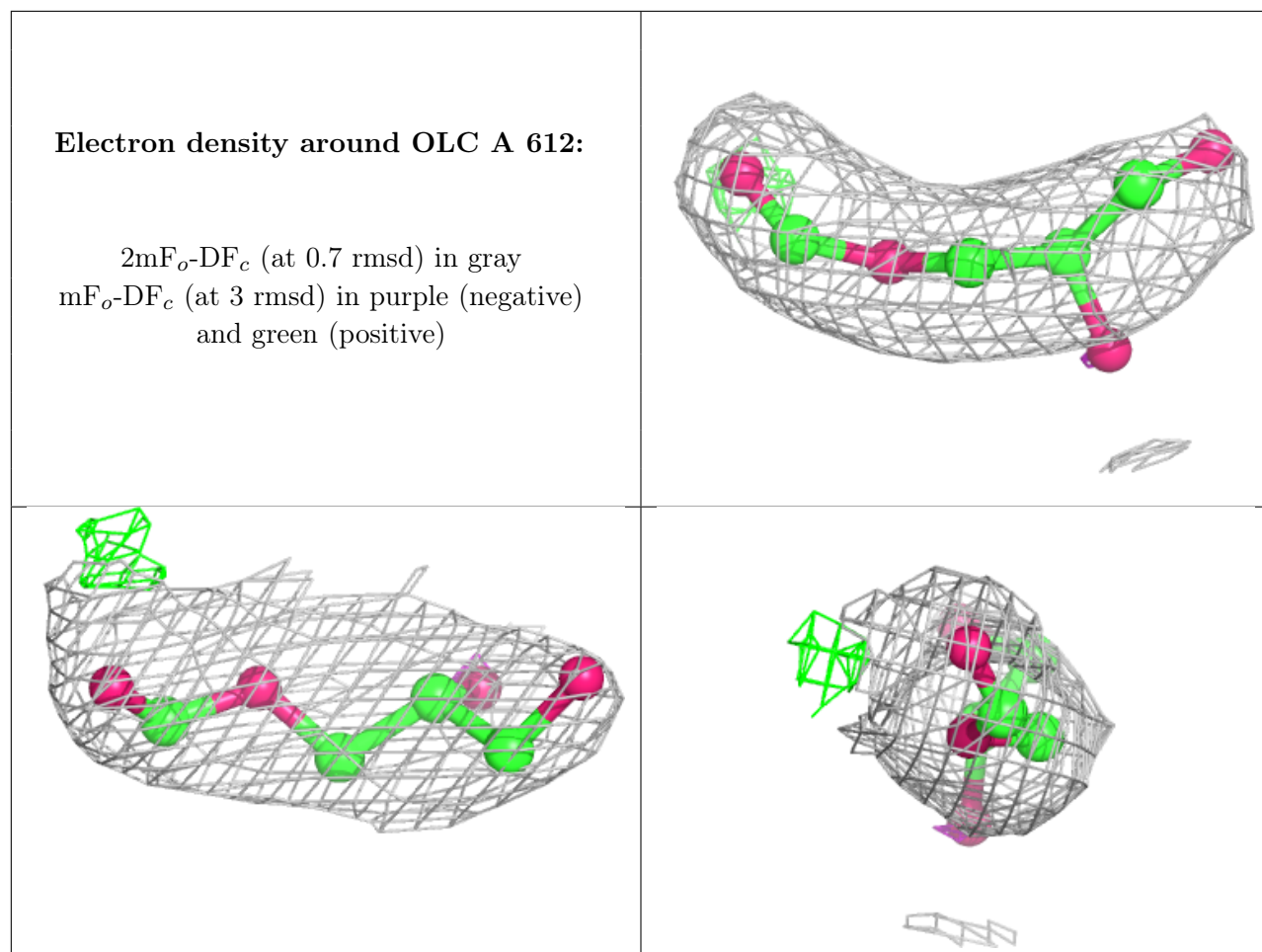
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around OLC 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)

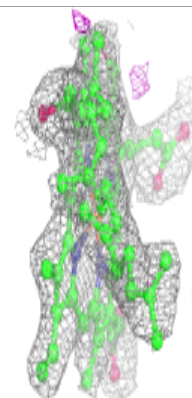
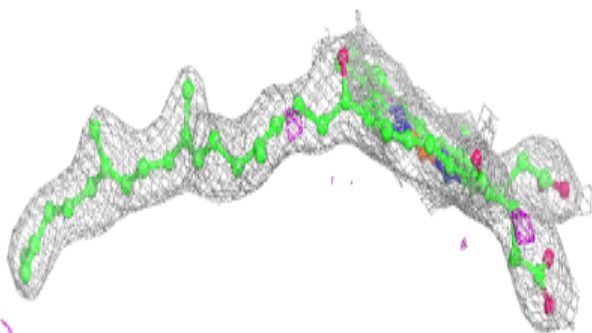
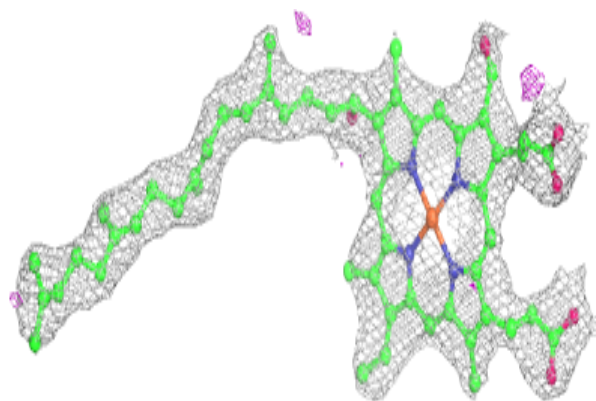




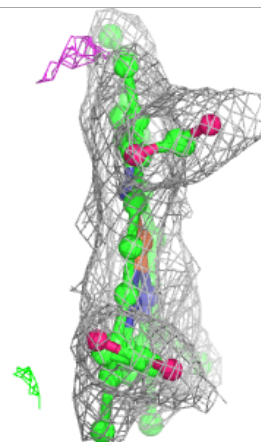
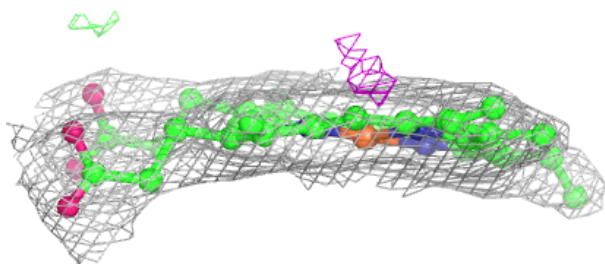
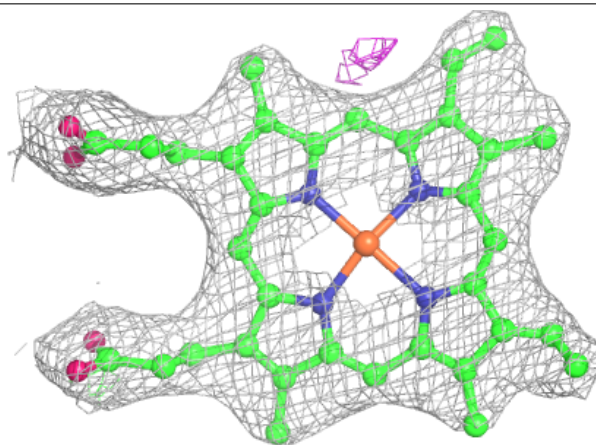


Electron density around HAS A 603:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.