



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:05 PM UTC

PDB ID : 4FA7 / pdb\_00004fa7  
Title : Structure of Recombinant Cytochrome ba3 Oxidase mutant A204F from *Thermus thermophilus*  
Authors : Li, Y.; Chen, Y.; Stout, C.D.  
Deposited on : 2012-05-21  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

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

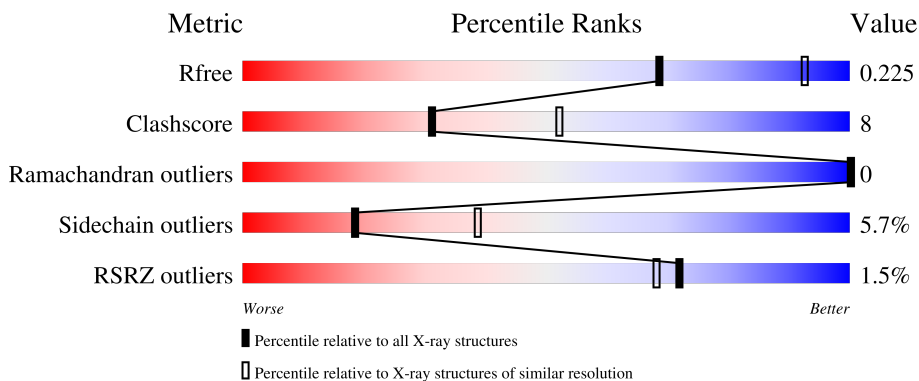
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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  $\geq 3$ , 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	-	-	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 6393 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	546	4298	2924	684	674	16	1	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	204	PHE	ALA	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	1289	838	213	234	4	0	0	0

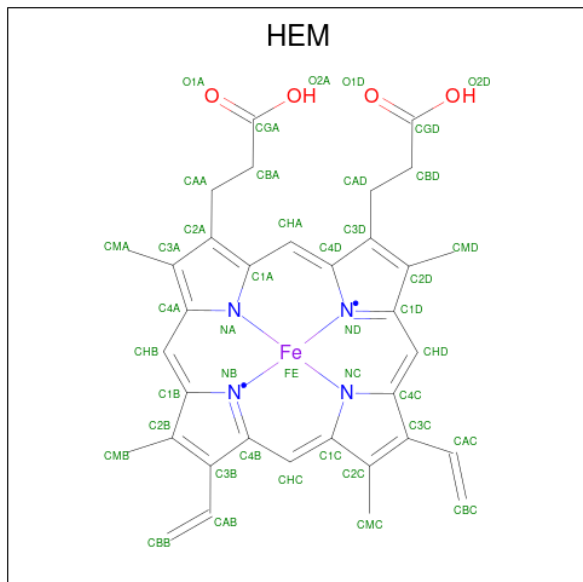
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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 (CCD ID: CU) (formula: Cu).

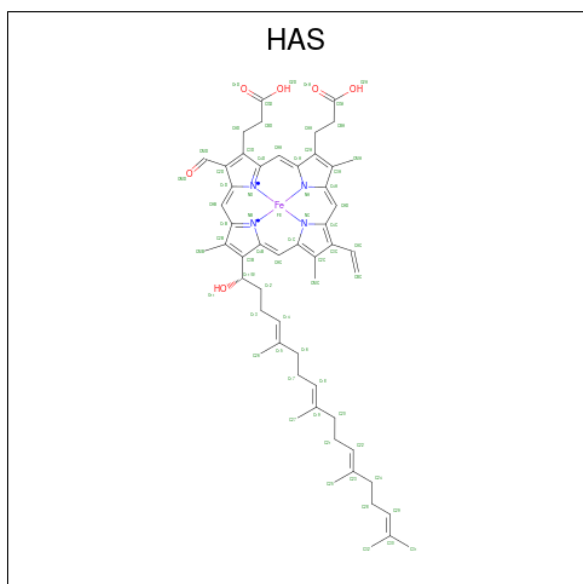
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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



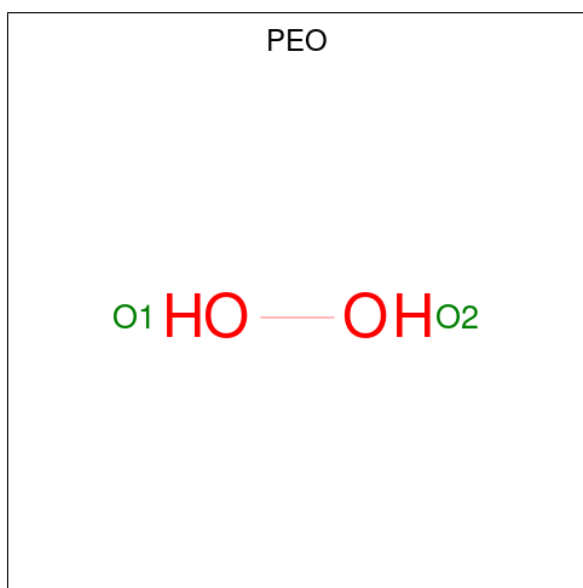
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
5	A	1	43	34	1	4	4	0	0

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



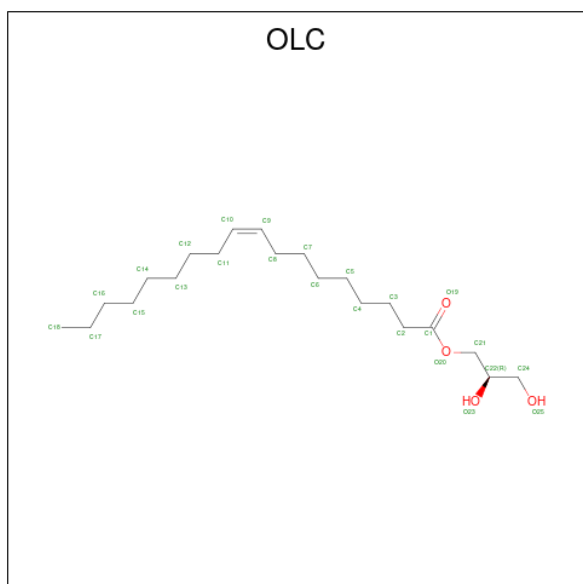
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
6	A	1	65	54	1	4	6	0	0

- Molecule 7 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H<sub>2</sub>O<sub>2</sub>).



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 (CCD ID: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



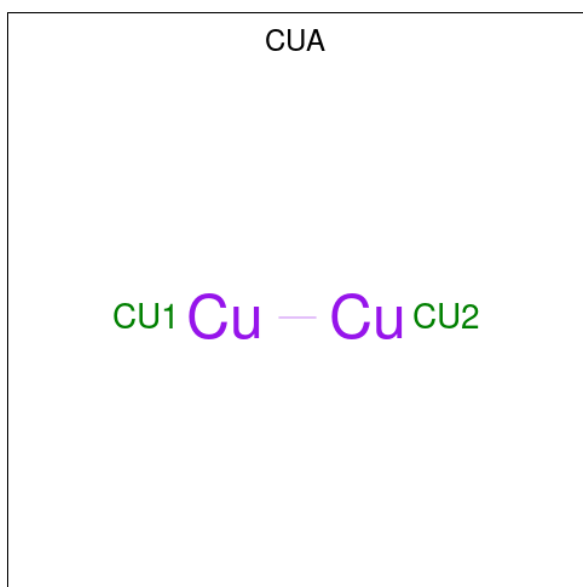
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 25 21 4	0	0

*Continued on next page...*

*Continued from previous page...*

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
			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		
8	C	1	Total	C	O	0	0
			25	21	4		

- Molecule 9 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>).



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	69	Total O 69 69	0	0
10	B	38	Total O 38 38	0	0
10	C	2	Total O 2 2	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.55Å 98.21Å 94.86Å 90.00° 127.92° 90.00°	Depositor
Resolution (Å)	74.83 – 2.50 74.83 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (74.83-2.50) 98.3 (74.83-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.50Å)	Xtrriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.169 , 0.220 0.173 , 0.225	Depositor DCC
$R_{free}$ test set	1796 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtrriage
Anisotropy	0.176	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6393	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OLC, PEO, CUA, HEM, CU, HAS

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	2.53	16/4453 (0.4%)	1.29	25/6115 (0.4%)
2	B	1.30	3/1325 (0.2%)	1.18	6/1810 (0.3%)
3	C	1.33	1/247 (0.4%)	1.20	0/335
All	All	2.28	20/6025 (0.3%)	1.27	31/8260 (0.4%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	330	ARG	CZ-NH1	103.26	2.77	1.32
1	A	330	ARG	NE-CZ	85.81	2.27	1.33
1	A	330	ARG	CZ-NH2	-57.58	0.58	1.33
1	A	475	ILE	CA-CB	9.13	1.67	1.54
1	A	368	SER	C-O	-7.02	1.15	1.24
1	A	131	VAL	N-CA	-6.23	1.38	1.46
1	A	347	VAL	CA-CB	6.08	1.61	1.54
1	A	370	THR	C-O	-6.08	1.16	1.24
1	A	223	VAL	CA-CB	5.75	1.61	1.54
2	B	111	ASP	N-CA	-5.70	1.38	1.46
1	A	204	PHE	CB-CG	-5.57	1.37	1.50
1	A	286	ALA	CA-CB	5.46	1.61	1.53
1	A	133	TYR	C-O	-5.38	1.17	1.24
2	B	110	PRO	C-O	-5.20	1.18	1.24
2	B	112	VAL	C-O	-5.19	1.16	1.23
1	A	131	VAL	C-N	-5.16	1.26	1.33
1	A	34	VAL	CA-CB	5.10	1.60	1.54
1	A	367	ALA	CA-CB	-5.07	1.44	1.53
1	A	482	LEU	N-CA	5.07	1.52	1.46
3	C	19	ILE	CA-CB	5.04	1.59	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ARG	CD-NE-CZ	-22.99	92.22	124.40
1	A	330	ARG	NE-CZ-NH2	18.25	135.62	119.20
1	A	330	ARG	NE-CZ-NH1	-14.91	106.58	121.50
1	A	131	VAL	CB-CA-C	8.93	125.94	111.29
1	A	369	PHE	N-CA-CB	-8.54	97.60	109.98
1	A	204	PHE	N-CA-C	7.54	119.58	111.36
1	A	131	VAL	N-CA-C	-6.62	95.58	109.34
1	A	233	HIS	N-CA-CB	6.59	116.65	110.39
2	B	97	VAL	N-CA-C	6.48	114.50	109.19
1	A	368	SER	N-CA-C	-6.08	100.09	109.76
1	A	108	LEU	N-CA-C	-6.08	104.58	111.14
1	A	367	ALA	N-CA-C	6.00	119.85	112.54
2	B	157	HIS	N-CA-C	5.93	118.25	111.02
1	A	475	ILE	N-CA-CB	5.53	119.79	110.56
1	A	369	PHE	CA-C-N	5.52	128.70	120.31
1	A	369	PHE	C-N-CA	5.52	128.70	120.31
1	A	156	THR	N-CA-C	5.50	118.20	111.82
1	A	392	LEU	N-CA-C	5.48	116.93	111.07
2	B	111	ASP	N-CA-C	5.42	122.35	110.80
2	B	58	VAL	N-CA-C	5.39	116.76	110.62
1	A	35	GLY	N-CA-C	-5.38	106.25	112.50
1	A	119	VAL	N-CA-C	5.33	115.54	110.42
1	A	195	LEU	CB-CA-C	-5.23	102.44	110.81
1	A	131	VAL	CA-C-N	-5.22	111.06	123.16
1	A	131	VAL	C-N-CA	-5.22	111.06	123.16
1	A	475	ILE	CA-CB-CG2	5.15	119.26	110.50
2	B	45	ILE	CA-C-N	-5.12	114.50	119.78
2	B	45	ILE	C-N-CA	-5.12	114.50	119.78
1	A	131	VAL	O-C-N	-5.12	116.18	122.57
1	A	100	ARG	CA-C-N	5.02	124.95	119.78
1	A	100	ARG	C-N-CA	5.02	124.95	119.78

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	4298	0	4391	76	0
2	B	1289	0	1264	12	0
3	C	241	0	267	6	0
4	A	1	0	0	0	0
5	A	43	0	30	4	0
6	A	65	0	62	2	0
7	A	2	0	0	0	0
8	A	243	0	353	23	0
8	B	75	0	120	3	0
8	C	25	0	40	2	0
9	B	2	0	0	0	0
10	A	69	0	0	3	0
10	B	38	0	0	4	1
10	C	2	0	0	0	0
All	All	6393	0	6527	105	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 8.

All (105) 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:CE2	1.70	1.56
1:A:233:HIS:NE2	1:A:237:TYR:HE2	0.77	1.25
1:A:233:HIS:CE1	1:A:237:TYR:HE2	1.83	0.96
1:A:233:HIS:CD2	1:A:237:TYR:HE2	1.86	0.92
1:A:168:ARG:HH22	8:A:612:OLC:H6A	1.32	0.92
5:A:602:HEM:HBC2	5:A:602:HEM:HMC1	1.57	0.84
1:A:233:HIS:CE1	1:A:237:TYR:CE2	2.63	0.82
8:A:606:OLC:C12	8:A:614:OLC:H14A	2.13	0.79
8:A:606:OLC:H12A	8:A:614:OLC:H14A	1.64	0.79
5:A:602:HEM:HBC2	5:A:602:HEM:CMC	2.14	0.77
1:A:161:TYR:CE2	8:A:611:OLC:H21	2.21	0.76
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.65	0.75
8:B:203:OLC:H6	3:C:33:ARG:HE	1.55	0.71
6:A:603:HAS:HMC1	6:A:603:HAS:HBC1	1.77	0.67
8:A:607:OLC:H13A	8:A:614:OLC:H12	1.79	0.65
2:B:6:LYS:C	10:B:338:HOH:O	2.39	0.65
1:A:465:VAL:HG22	8:A:613:OLC:H3A	1.77	0.65
2:B:6:LYS:O	10:B:338:HOH:O	2.14	0.65
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.33	0.64
1:A:236:VAL:HG12	1:A:239:TRP:CZ3	2.34	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:VAL:O	1:A:132:LEU:HD23	2.00	0.61
3:C:4:LYS:HG3	3:C:6:LYS:HG2	1.81	0.61
8:A:606:OLC:H12	8:A:614:OLC:H14A	1.83	0.61
1:A:168:ARG:NH2	8:A:612:OLC:H6A	2.12	0.61
1:A:241:LEU:N	1:A:242:PRO:CD	2.64	0.60
1:A:168:ARG:HH22	8:A:612:OLC:C6	2.11	0.58
2:B:9:LYS:N	10:B:338:HOH:O	2.35	0.58
1:A:146:TYR:HB3	1:A:204:PHE:CE1	2.37	0.58
1:A:400:SER:HA	1:A:403:TRP:NE1	2.19	0.57
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.87	0.56
5:A:602:HEM:HMC1	5:A:602:HEM:CBC	2.34	0.56
1:A:220:ASP:O	1:A:223:VAL:HG12	2.07	0.55
1:A:369:PHE:C	1:A:369:PHE:CD2	2.85	0.55
1:A:369:PHE:C	1:A:369:PHE:HD2	2.16	0.54
1:A:233:HIS:O	1:A:236:VAL:HG22	2.08	0.53
1:A:513:SER:HB3	10:A:739:HOH:O	2.07	0.53
1:A:34:VAL:HA	1:A:37:LEU:HD12	1.91	0.53
1:A:398:MET:O	1:A:401:LEU:HB2	2.09	0.53
8:A:607:OLC:H13	8:A:613:OLC:H12	1.91	0.53
8:A:607:OLC:H13A	8:A:614:OLC:C12	2.39	0.52
1:A:463:ALA:O	1:A:467:MET:HG3	2.09	0.52
1:A:300:VAL:HG22	2:B:30:ILE:HD13	1.93	0.51
8:A:607:OLC:H15	8:A:613:OLC:H12	1.94	0.50
1:A:174:ASN:N	1:A:175:PRO:HD3	2.26	0.50
1:A:405:LEU:HD23	1:A:491:VAL:HG11	1.93	0.50
1:A:174:ASN:HB3	1:A:177:LYS:HD2	1.93	0.49
1:A:516:GLU:O	1:A:517:ASP:C	2.55	0.49
8:A:607:OLC:H14A	8:A:614:OLC:H12A	1.95	0.49
1:A:341:TRP:HB3	8:A:607:OLC:H24A	1.95	0.48
1:A:147:LEU:O	1:A:150:SER:HB2	2.12	0.48
1:A:291:ASP:OD2	1:A:293:THR:HB	2.13	0.48
1:A:366:ASN:HB3	6:A:603:HAS:HBD2	1.95	0.48
1:A:341:TRP:CE2	8:A:616:OLC:H3	2.48	0.48
1:A:445:LEU:HD13	1:A:462:HIS:O	2.13	0.48
1:A:15:TYR:N	1:A:16:PRO:CD	2.77	0.48
1:A:233:HIS:CD2	1:A:233:HIS:C	2.92	0.48
1:A:341:TRP:CZ2	8:A:616:OLC:H3	2.48	0.48
5:A:602:HEM:CMC	5:A:602:HEM:CBC	2.91	0.47
1:A:146:TYR:O	1:A:204:PHE:HE1	1.98	0.47
1:A:168:ARG:HD2	8:A:611:OLC:O23	2.14	0.47
1:A:70:THR:OG1	1:A:131:VAL:O	2.25	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:GLN:O	2:B:152:TYR:C	2.58	0.47
1:A:168:ARG:HH11	8:A:611:OLC:C22	2.29	0.46
1:A:160:ILE:HG12	1:A:190:TRP:HB3	1.98	0.46
1:A:230:TRP:C	1:A:230:TRP:CD1	2.94	0.46
1:A:511:VAL:HG12	1:A:512:ILE:O	2.16	0.46
1:A:518:ARG:O	1:A:519:ARG:C	2.58	0.45
8:A:605:OLC:H10	8:C:101:OLC:H8	1.97	0.45
1:A:184:TYR:O	1:A:188:VAL:HG13	2.16	0.45
1:A:220:ASP:HB3	1:A:223:VAL:HG12	1.98	0.45
1:A:435:MET:HB2	1:A:473:ALA:HB1	1.99	0.45
2:B:18:TRP:CE3	3:C:12:ILE:HD13	2.52	0.45
1:A:146:TYR:O	1:A:204:PHE:CE1	2.69	0.45
1:A:220:ASP:OD1	1:A:220:ASP:C	2.61	0.44
1:A:405:LEU:HB3	1:A:406:PRO:HD3	1.99	0.44
1:A:136:TYR:O	1:A:139:LEU:HB2	2.18	0.44
1:A:450:ARG:O	2:B:157:HIS:CD2	2.70	0.44
1:A:472:LEU:HD22	8:A:614:OLC:H11	1.99	0.43
1:A:405:LEU:HD23	1:A:491:VAL:CG1	2.48	0.43
8:A:614:OLC:C9	8:A:614:OLC:H13A	2.47	0.43
1:A:471:VAL:HG11	8:A:614:OLC:H4	2.00	0.43
1:A:157:TRP:HA	1:A:160:ILE:HD12	2.00	0.43
1:A:272:PHE:CE1	1:A:308:PRO:HB2	2.54	0.43
1:A:460:TYR:N	1:A:461:PRO:CD	2.82	0.43
1:A:307:VAL:HA	1:A:310:LEU:HD12	2.01	0.43
1:A:371:LEU:HD21	3:C:27:TYR:HD1	1.83	0.43
2:B:114:HIS:CG	2:B:160:MET:HE1	2.53	0.43
1:A:225:ARG:HG3	10:A:752:HOH:O	2.18	0.42
8:B:203:OLC:C6	3:C:33:ARG:HE	2.27	0.42
1:A:330:ARG:O	1:A:334:GLY:HA3	2.19	0.42
2:B:141:ARG:HH12	8:B:203:OLC:H22	1.84	0.42
1:A:232:GLY:O	1:A:235:ILE:HG22	2.20	0.42
1:A:90:VAL:O	1:A:93:PRO:HG2	2.20	0.42
2:B:11:ILE:HA	3:C:5:PRO:HG3	2.01	0.41
1:A:34:VAL:HA	1:A:37:LEU:CD1	2.50	0.41
2:B:23:LEU:HD12	2:B:23:LEU:HA	1.91	0.41
1:A:134:THR:O	1:A:135:PHE:C	2.63	0.41
1:A:146:TYR:HB3	1:A:204:PHE:HE1	1.82	0.41
2:B:76:PRO:HD2	10:B:317:HOH:O	2.20	0.41
1:A:362:GLY:HA3	10:A:713:HOH:O	2.20	0.41
8:C:101:OLC:H7A	8:C:101:OLC:H4A	1.99	0.41
1:A:168:ARG:NH1	8:A:611:OLC:O20	2.54	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:HB3	1:A:346:PHE:CZ	2.56	0.40
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.93	0.40
1:A:290:ILE:HB	1:A:295:LYS:HE3	2.02	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:327:HOH:O	10:B:327:HOH:O[2_556]	2.00	0.20

## 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	542/568 (95%)	518 (96%)	24 (4%)	0	100	100
2	B	164/168 (98%)	161 (98%)	3 (2%)	0	100	100
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	735/770 (96%)	708 (96%)	27 (4%)	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	438/463 (95%)	418 (95%)	20 (5%)	24	48
2	B	134/138 (97%)	124 (92%)	10 (8%)	12	26
3	C	24/27 (89%)	20 (83%)	4 (17%)	2	4
All	All	596/628 (95%)	562 (94%)	34 (6%)	18	39

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	54	LEU
1	A	58	LEU
1	A	133	TYR
1	A	188	VAL
1	A	205	VAL
1	A	215	LEU
1	A	230	TRP
1	A	262	ASP
1	A	274	LEU
1	A	326	LEU
1	A	332	LEU
1	A	369	PHE
1	A	425	VAL
1	A	475	ILE
1	A	498	LYS
1	A	500	GLU
1	A	518	ARG
1	A	520	LEU
1	A	526	ARG
2	B	6	LYS
2	B	12	LEU
2	B	26	LEU
2	B	37	LEU
2	B	49	LYS
2	B	58	VAL
2	B	99	GLN
2	B	107	ILE
2	B	111	ASP
2	B	167	LYS
3	C	13	LEU
3	C	17	LEU
3	C	20	LEU
3	C	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	446	ASN
1	A	455	GLN
2	B	69	GLN
2	B	91	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 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	B	202	-	24,24,24	1.24	1 (4%)	25,25,25	1.11	2 (8%)
8	OLC	C	101	-	24,24,24	1.06	1 (4%)	25,25,25	1.15	2 (8%)
8	OLC	A	605	-	24,24,24	1.12	1 (4%)	25,25,25	1.02	2 (8%)
8	OLC	A	611	-	7,7,24	1.29	1 (14%)	6,7,25	0.88	0
7	PEO	A	604	6,4	1,1,1	0.48	0	-		
5	HEM	A	602	1	50,50,50	1.87	10 (20%)	67,82,82	1.55	11 (16%)
8	OLC	B	203	-	24,24,24	1.24	1 (4%)	25,25,25	1.22	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	OLC	A	615	-	20,20,24	1.25	1 (5%)	21,21,25	0.98	2 (9%)
8	OLC	A	613	-	19,19,24	1.20	1 (5%)	20,20,25	1.29	3 (15%)
8	OLC	B	204	-	24,24,24	1.03	1 (4%)	25,25,25	0.99	3 (12%)
9	CUA	B	201	2	0,1,1	-	-	-	-	-
8	OLC	A	607	-	22,22,24	1.05	1 (4%)	23,23,25	1.25	4 (17%)
8	OLC	A	616	-	24,24,24	1.06	1 (4%)	25,25,25	1.21	2 (8%)
8	OLC	A	606	-	24,24,24	1.02	1 (4%)	25,25,25	1.30	3 (12%)
8	OLC	A	614	-	24,24,24	1.13	1 (4%)	25,25,25	1.23	3 (12%)
6	HAS	A	603	7,1	72,72,72	2.55	28 (38%)	87,109,109	2.95	35 (40%)
8	OLC	A	609	-	17,17,24	1.26	1 (5%)	18,18,25	1.24	2 (11%)
8	OLC	A	608	-	20,20,24	1.27	1 (5%)	20,20,25	1.25	3 (15%)
8	OLC	A	610	-	16,16,24	1.43	1 (6%)	17,17,25	1.11	2 (11%)
8	OLC	A	612	-	14,14,24	1.29	1 (7%)	15,15,25	1.39	2 (13%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OLC	A	613	-	-	13/19/19/24	-
8	OLC	A	611	-	-	4/6/6/24	-
5	HEM	A	602	1	-	3/14/54/54	-
6	HAS	A	603	7,1	1/1/8/18	4/42/82/82	-
8	OLC	A	609	-	-	4/17/17/24	-
8	OLC	B	204	-	-	12/24/24/24	-
8	OLC	A	608	-	-	10/19/19/24	-
8	OLC	B	203	-	-	13/24/24/24	-
8	OLC	A	610	-	-	8/16/16/24	-
8	OLC	B	202	-	-	12/24/24/24	-
8	OLC	C	101	-	-	16/24/24/24	-
8	OLC	A	615	-	-	6/20/20/24	-
8	OLC	A	607	-	-	10/22/22/24	-
8	OLC	A	616	-	-	13/24/24/24	-
8	OLC	A	605	-	-	15/24/24/24	-
8	OLC	A	606	-	-	11/24/24/24	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OLC	A	612	-	-	4/14/14/24	-
8	OLC	A	614	-	-	10/24/24/24	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEM	C3D-C2D	7.59	1.53	1.36
6	A	603	HAS	C3B-C2B	6.87	1.50	1.34
8	B	203	OLC	O20-C1	5.52	1.49	1.33
6	A	603	HAS	CHB-C1D	5.35	1.49	1.38
8	B	202	OLC	O20-C1	5.28	1.48	1.33
6	A	603	HAS	C1D-ND	5.22	1.49	1.40
6	A	603	HAS	FE-NA	5.17	2.12	1.95
8	A	614	OLC	O20-C1	5.12	1.48	1.33
8	A	615	OLC	O20-C1	5.12	1.48	1.33
8	A	608	OLC	O20-C1	5.09	1.48	1.33
6	A	603	HAS	FE-NC	5.01	2.11	1.95
5	A	602	HEM	FE-ND	4.91	2.10	1.94
8	A	605	OLC	O20-C1	4.86	1.47	1.33
8	A	610	OLC	O20-C1	4.84	1.47	1.33
6	A	603	HAS	CHC-C4B	4.82	1.48	1.38
6	A	603	HAS	C4D-ND	4.78	1.48	1.38
8	A	616	OLC	O20-C1	4.76	1.47	1.33
8	C	101	OLC	O20-C1	4.75	1.47	1.33
8	A	606	OLC	O20-C1	4.70	1.47	1.33
8	A	609	OLC	O20-C1	4.65	1.46	1.33
8	A	613	OLC	O20-C1	4.64	1.46	1.33
6	A	603	HAS	FE-NB	4.61	2.09	1.94
5	A	602	HEM	FE-NB	4.53	2.08	1.94
8	A	612	OLC	O20-C1	4.49	1.46	1.33
8	B	204	OLC	O20-C1	4.40	1.46	1.33
6	A	603	HAS	C4C-NC	4.38	1.47	1.39
6	A	603	HAS	CHD-C4A	4.34	1.46	1.38
6	A	603	HAS	CBC-CAC	4.29	1.51	1.30
8	A	607	OLC	O20-C1	4.09	1.45	1.33
6	A	603	HAS	CHA-C4D	3.95	1.48	1.39
6	A	603	HAS	C4D-C3D	3.51	1.51	1.45
6	A	603	HAS	C2A-C3A	3.42	1.44	1.36
6	A	603	HAS	CHC-C1C	3.41	1.47	1.39
6	A	603	HAS	C2D-C1D	3.34	1.51	1.44
8	A	611	OLC	O20-C1	3.30	1.45	1.33
6	A	603	HAS	CHD-C4C	3.27	1.46	1.39

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	C1A-NA	-3.01	1.33	1.39
6	A	603	HAS	CHB-C1B	2.99	1.46	1.39
6	A	603	HAS	CMD-C2D	2.90	1.51	1.45
6	A	603	HAS	C2D-C3D	-2.90	1.30	1.37
6	A	603	HAS	CHA-C1A	2.89	1.44	1.38
5	A	602	HEM	CAB-C3B	2.76	1.54	1.47
6	A	603	HAS	C4A-C3A	2.63	1.50	1.45
6	A	603	HAS	C4B-C3B	2.56	1.49	1.44
5	A	602	HEM	FE-NC	2.53	2.03	1.95
6	A	603	HAS	C11-C3B	-2.49	1.48	1.51
6	A	603	HAS	C3C-C2C	2.45	1.49	1.41
6	A	603	HAS	C1C-C2C	2.27	1.48	1.43
5	A	602	HEM	O2A-CGA	-2.22	1.23	1.30
5	A	602	HEM	CAA-C2A	2.21	1.57	1.51
5	A	602	HEM	CAD-C3D	2.19	1.57	1.51
5	A	602	HEM	CMA-C3A	2.19	1.55	1.50
6	A	603	HAS	C4A-NA	-2.18	1.35	1.39
5	A	602	HEM	CMC-C2C	2.16	1.55	1.50

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	CHB-C1D-ND	-12.42	109.00	124.37
6	A	603	HAS	C2A-C1A-NA	8.92	118.93	110.32
6	A	603	HAS	C3C-C4C-NC	-7.92	103.13	109.80
5	A	602	HEM	C4D-ND-C1D	5.69	111.94	105.21
6	A	603	HAS	C3C-C2C-C1C	-5.11	101.14	107.17
6	A	603	HAS	CAA-CBA-CGA	-4.86	100.78	113.67
6	A	603	HAS	CHB-C1D-C2D	-4.66	110.24	125.91
6	A	603	HAS	C2B-C1B-NB	4.65	115.28	109.90
6	A	603	HAS	C3A-C4A-NA	4.64	118.23	109.64
6	A	603	HAS	CHA-C1A-C2A	-4.59	117.62	124.86
6	A	603	HAS	C4A-NA-C1A	-4.26	98.87	105.82
6	A	603	HAS	C4A-C3A-C2A	-4.25	100.67	106.97
8	A	606	OLC	O20-C1-C2	4.05	124.17	111.83
6	A	603	HAS	C1B-CHB-C1D	-4.04	116.94	125.69
6	A	603	HAS	C2D-C3D-C4D	3.96	109.29	106.43
6	A	603	HAS	C25-C23-C24	3.95	122.08	115.23
6	A	603	HAS	C27-C19-C20	3.84	121.90	115.23
8	C	101	OLC	O20-C1-C2	3.74	123.23	111.83
6	A	603	HAS	C4C-C3C-C2C	3.65	111.84	107.30
6	A	603	HAS	C3B-C4B-NB	3.64	114.02	109.84

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	CHD-C4A-C3A	-3.61	117.99	125.49
8	A	609	OLC	O20-C1-C2	3.58	122.75	111.83
8	A	612	OLC	O20-C1-C2	3.56	122.69	111.83
6	A	603	HAS	C1B-C2B-C3B	-3.39	102.87	106.80
6	A	603	HAS	C3D-C4D-ND	-3.35	107.11	110.35
8	A	612	OLC	O20-C1-O19	-3.32	115.33	123.63
6	A	603	HAS	C1A-C2A-C3A	-3.31	102.75	107.11
8	B	202	OLC	O20-C1-C2	3.27	121.82	111.83
8	B	203	OLC	O20-C1-C2	3.22	121.67	111.83
8	A	608	OLC	O20-C1-C2	3.15	124.04	112.14
8	A	608	OLC	C21-O20-C1	3.10	125.99	116.07
8	A	613	OLC	O20-C1-C2	3.08	121.23	111.83
8	A	616	OLC	O20-C1-C2	3.06	121.17	111.83
5	A	602	HEM	C4C-C3C-C2C	3.03	109.44	106.81
5	A	602	HEM	CMD-C2D-C1D	3.00	129.73	125.03
6	A	603	HAS	CMA-C3A-C4A	3.00	130.01	124.73
6	A	603	HAS	CHD-C4C-NC	2.99	129.28	123.86
5	A	602	HEM	CAD-C3D-C4D	2.97	129.87	124.70
8	B	202	OLC	O20-C21-C22	2.96	119.78	105.85
8	A	609	OLC	O20-C1-O19	-2.95	116.24	123.63
8	B	203	OLC	C21-O20-C1	2.88	127.64	117.12
6	A	603	HAS	C21-C22-C23	-2.87	121.05	127.62
8	A	607	OLC	O20-C1-O19	-2.85	116.49	123.63
8	C	101	OLC	O20-C1-O19	-2.85	116.49	123.63
5	A	602	HEM	C1B-NB-C4B	2.82	108.54	105.21
8	A	613	OLC	O20-C1-O19	-2.79	116.65	123.63
6	A	603	HAS	C4B-C3B-C2B	-2.76	102.80	107.44
6	A	603	HAS	C4C-NC-C1C	2.75	110.31	105.82
6	A	603	HAS	CMB-C2B-C1B	2.74	129.32	125.03
6	A	603	HAS	CHA-C4D-C3D	-2.74	120.78	124.77
8	A	616	OLC	C21-O20-C1	2.72	127.07	117.12
6	A	603	HAS	C26-C15-C16	2.68	119.89	115.23
8	A	614	OLC	O20-C21-C22	2.68	118.47	105.85
6	A	603	HAS	CHB-C1B-NB	-2.64	121.58	124.42
8	A	613	OLC	O20-C21-C22	2.58	117.97	105.85
8	A	614	OLC	C21-O20-C1	2.55	126.44	117.12
8	A	614	OLC	O20-C1-C2	2.54	119.59	111.83
8	B	203	OLC	O20-C21-C22	2.53	117.75	105.85
8	A	606	OLC	C21-O20-C1	2.53	126.36	117.12
8	A	610	OLC	O20-C1-C2	2.53	119.54	111.83
5	A	602	HEM	C3B-C4B-NB	-2.50	107.67	109.47
6	A	603	HAS	C1D-ND-C4D	-2.44	102.31	105.21

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	605	OLC	O20-C1-C2	2.44	119.26	111.83
8	A	610	OLC	O20-C1-O19	-2.42	117.57	123.63
8	A	608	OLC	O20-C1-O19	-2.40	116.04	123.20
8	B	204	OLC	C21-O20-C1	2.39	125.87	117.12
8	A	607	OLC	O20-C1-C2	2.29	118.82	111.83
8	A	607	OLC	C21-O20-C1	2.26	125.37	117.12
5	A	602	HEM	CAD-CBD-CGD	-2.25	107.70	113.67
8	A	615	OLC	O20-C1-C2	2.24	118.67	111.83
5	A	602	HEM	CHC-C4B-NB	2.23	126.83	124.42
5	A	602	HEM	O1D-CGD-CBD	-2.20	116.12	123.09
8	B	204	OLC	O20-C1-C2	2.19	118.51	111.83
8	A	615	OLC	C21-O20-C1	2.18	125.09	117.12
8	B	204	OLC	O20-C1-O19	-2.17	118.20	123.63
8	A	606	OLC	O20-C1-O19	-2.16	118.22	123.63
6	A	603	HAS	O1D-CGD-CBD	-2.16	116.24	123.09
8	A	607	OLC	C3-C2-C1	-2.14	105.86	113.69
5	A	602	HEM	CHA-C1A-NA	2.11	127.69	123.86
8	A	605	OLC	C21-O20-C1	2.07	124.70	117.12
6	A	603	HAS	CMC-C2C-C1C	2.06	128.56	125.42
6	A	603	HAS	CHC-C4B-C3B	-2.04	120.67	125.80
5	A	602	HEM	CBC-CAC-C3C	-2.01	117.49	127.53
6	A	603	HAS	O11-C11-C12	2.01	114.46	109.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	603	HAS	NA

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	606	OLC	O20-C21-C22-O23
8	A	607	OLC	C21-C22-C24-O25
8	A	607	OLC	O23-C22-C24-O25
8	A	610	OLC	O20-C21-C22-C24
8	A	611	OLC	O19-C1-O20-C21
8	A	612	OLC	O20-C21-C22-C24
8	A	613	OLC	C21-C22-C24-O25
8	A	615	OLC	C21-C22-C24-O25
8	B	202	OLC	C21-C22-C24-O25
8	B	202	OLC	O23-C22-C24-O25
8	B	204	OLC	C21-C22-C24-O25

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	A	608	OLC	C2-C1-O20-C21
8	A	610	OLC	O19-C1-O20-C21
8	A	610	OLC	C2-C1-O20-C21
8	A	613	OLC	O19-C1-O20-C21
8	A	608	OLC	O19-C1-O20-C21
8	A	613	OLC	C2-C1-O20-C21
8	A	612	OLC	O20-C21-C22-O23
8	A	616	OLC	O20-C21-C22-O23
8	A	616	OLC	C2-C1-O20-C21
8	A	610	OLC	O20-C21-C22-O23
8	A	616	OLC	O19-C1-O20-C21
8	A	614	OLC	C10-C11-C12-C13
8	B	203	OLC	C1-C2-C3-C4
8	A	614	OLC	C2-C3-C4-C5
8	A	616	OLC	C1-C2-C3-C4
8	B	204	OLC	C1-C2-C3-C4
8	B	202	OLC	C2-C1-O20-C21
8	A	609	OLC	C1-C2-C3-C4
8	A	607	OLC	O20-C21-C22-O23
8	A	613	OLC	O20-C21-C22-O23
8	C	101	OLC	O20-C21-C22-O23
8	C	101	OLC	C4-C5-C6-C7
8	A	607	OLC	O20-C21-C22-C24
8	C	101	OLC	O20-C21-C22-C24
8	B	202	OLC	O19-C1-O20-C21
8	A	609	OLC	C21-C22-C24-O25
8	A	610	OLC	C21-C22-C24-O25
8	A	616	OLC	C21-C22-C24-O25
8	B	203	OLC	C2-C1-O20-C21
8	A	605	OLC	C5-C6-C7-C8
8	C	101	OLC	C3-C4-C5-C6
8	A	605	OLC	C12-C13-C14-C15
8	B	202	OLC	C14-C15-C16-C17
8	A	610	OLC	O23-C22-C24-O25
8	A	615	OLC	O23-C22-C24-O25
8	A	605	OLC	C4-C5-C6-C7
8	A	607	OLC	C11-C12-C13-C14
8	A	605	OLC	C2-C3-C4-C5
8	C	101	OLC	C13-C14-C15-C16
8	A	614	OLC	C12-C13-C14-C15
8	B	202	OLC	C3-C4-C5-C6
8	B	203	OLC	O19-C1-O20-C21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	A	607	OLC	C12-C13-C14-C15
8	B	204	OLC	C13-C14-C15-C16
8	B	202	OLC	C6-C7-C8-C9
8	A	608	OLC	C11-C12-C13-C14
8	A	606	OLC	C14-C15-C16-C17
8	A	613	OLC	O20-C21-C22-C24
8	A	606	OLC	C3-C4-C5-C6
8	A	614	OLC	C4-C5-C6-C7
8	B	203	OLC	C2-C3-C4-C5
8	A	613	OLC	C6-C7-C8-C9
8	C	101	OLC	C6-C7-C8-C9
8	B	204	OLC	C5-C6-C7-C8
8	B	204	OLC	C3-C4-C5-C6
8	A	614	OLC	C14-C15-C16-C17
8	A	605	OLC	C10-C11-C12-C13
8	A	615	OLC	C10-C11-C12-C13
8	B	204	OLC	C10-C11-C12-C13
8	A	605	OLC	C11-C12-C13-C14
8	A	609	OLC	O23-C22-C24-O25
8	A	613	OLC	O23-C22-C24-O25
8	B	204	OLC	O23-C22-C24-O25
8	B	203	OLC	C6-C7-C8-C9
8	C	101	OLC	C10-C11-C12-C13
8	A	611	OLC	O20-C21-C22-O23
8	A	614	OLC	C5-C6-C7-C8
8	A	605	OLC	C2-C1-O20-C21
8	A	607	OLC	C2-C1-O20-C21
8	A	605	OLC	C6-C7-C8-C9
8	A	609	OLC	C6-C7-C8-C9
8	A	615	OLC	C3-C4-C5-C6
8	A	605	OLC	O19-C1-O20-C21
8	B	203	OLC	C12-C13-C14-C15
8	A	606	OLC	C10-C11-C12-C13
8	A	607	OLC	O19-C1-O20-C21
8	A	616	OLC	C13-C14-C15-C16
8	A	616	OLC	C11-C12-C13-C14
8	A	612	OLC	C4-C5-C6-C7
8	A	606	OLC	C6-C7-C8-C9
8	A	613	OLC	C3-C4-C5-C6
8	B	202	OLC	C12-C13-C14-C15
8	B	204	OLC	C15-C16-C17-C18
8	A	605	OLC	C13-C14-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	A	616	OLC	C15-C16-C17-C18
8	A	613	OLC	C4-C5-C6-C7
8	A	614	OLC	C13-C14-C15-C16
8	A	605	OLC	C15-C16-C17-C18
8	C	101	OLC	C2-C3-C4-C5
8	A	606	OLC	C4-C5-C6-C7
8	B	204	OLC	C12-C13-C14-C15
8	C	101	OLC	C14-C15-C16-C17
8	A	605	OLC	C14-C15-C16-C17
8	A	606	OLC	C12-C13-C14-C15
8	A	611	OLC	O20-C21-C22-C24
8	B	203	OLC	C10-C11-C12-C13
8	C	101	OLC	C11-C12-C13-C14
5	A	602	HEM	C2B-C3B-CAB-CBB
8	B	202	OLC	C11-C12-C13-C14
8	A	616	OLC	C6-C7-C8-C9
8	A	616	OLC	C14-C15-C16-C17
8	A	612	OLC	C5-C6-C7-C8
8	B	203	OLC	C11-C12-C13-C14
8	B	203	OLC	C5-C6-C7-C8
8	B	203	OLC	C13-C14-C15-C16
8	A	608	OLC	C15-C16-C17-C18
8	A	608	OLC	C10-C11-C12-C13
8	A	616	OLC	C12-C13-C14-C15
8	C	101	OLC	O19-C1-O20-C21
8	B	204	OLC	C11-C12-C13-C14
8	C	101	OLC	C2-C1-O20-C21
8	A	613	OLC	C2-C3-C4-C5
8	A	614	OLC	C7-C8-C9-C10
8	A	605	OLC	C1-C2-C3-C4
8	B	203	OLC	C4-C5-C6-C7
8	A	606	OLC	O20-C21-C22-C24
8	C	101	OLC	C9-C10-C11-C12
8	A	615	OLC	C5-C6-C7-C8
8	B	202	OLC	C1-C2-C3-C4
8	C	101	OLC	C7-C8-C9-C10
8	A	614	OLC	C15-C16-C17-C18
8	A	613	OLC	C10-C11-C12-C13
6	A	603	HAS	CAA-CBA-CGA-O1A
6	A	603	HAS	CAA-CBA-CGA-O2A
8	B	202	OLC	C7-C8-C9-C10
8	C	101	OLC	C12-C13-C14-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	A	603	HAS	CAD-CBD-CGD-O1D
8	A	606	OLC	C13-C14-C15-C16
8	B	203	OLC	C9-C10-C11-C12
8	B	204	OLC	O20-C21-C22-C24
8	A	607	OLC	C10-C11-C12-C13
8	B	202	OLC	C10-C11-C12-C13
8	A	608	OLC	C7-C8-C9-C10
8	A	613	OLC	C9-C10-C11-C12
8	A	616	OLC	C7-C8-C9-C10
8	A	606	OLC	C22-C21-O20-C1
8	A	607	OLC	C7-C8-C9-C10
8	A	616	OLC	C9-C10-C11-C12
5	A	602	HEM	C4B-C3B-CAB-CBB
8	A	611	OLC	C22-C21-O20-C1
8	A	610	OLC	O20-C1-C2-C3
8	A	605	OLC	C9-C10-C11-C12
8	B	203	OLC	C14-C15-C16-C17
8	A	605	OLC	O20-C21-C22-C24
8	A	608	OLC	C4-C5-C6-C7
8	A	615	OLC	C6-C7-C8-C9
6	A	603	HAS	CAD-CBD-CGD-O2D
8	A	613	OLC	C5-C6-C7-C8
8	C	101	OLC	C15-C16-C17-C18
8	A	608	OLC	O20-C1-C2-C3
8	A	610	OLC	O19-C1-C2-C3
5	A	602	HEM	CAD-CBD-CGD-O2D
8	A	614	OLC	O20-C1-C2-C3
8	A	608	OLC	C2-C3-C4-C5
8	A	606	OLC	O20-C1-C2-C3
8	A	608	OLC	O19-C1-C2-C3
8	B	204	OLC	C7-C8-C9-C10

There are no ring outliers.

12 monomers are involved in 33 short contacts:

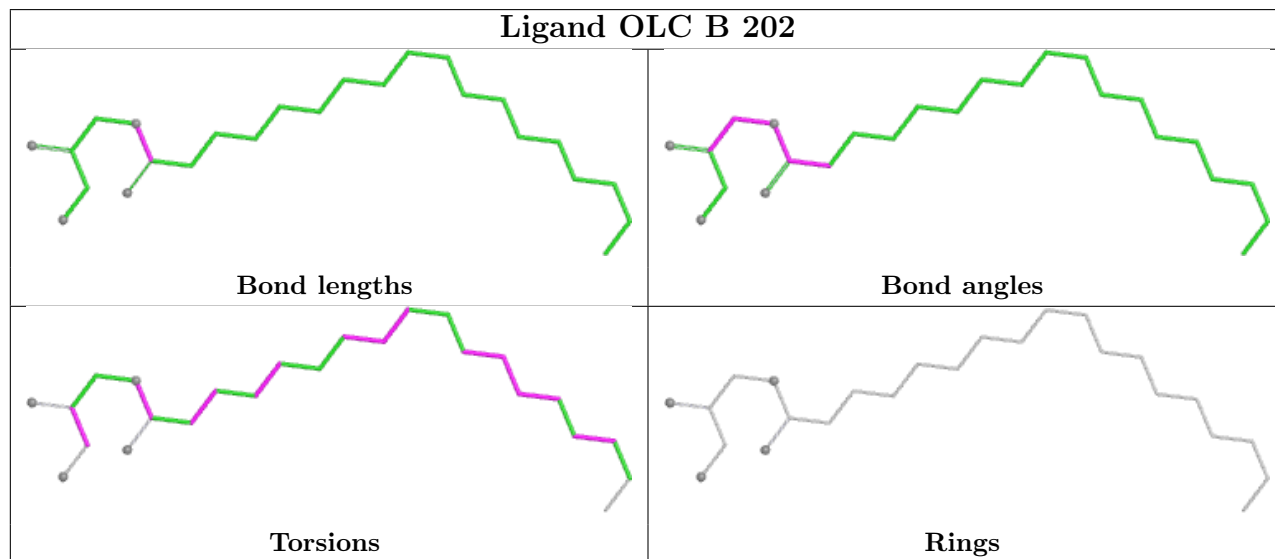
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	101	OLC	2	0
8	A	605	OLC	1	0
8	A	611	OLC	4	0
5	A	602	HEM	4	0
8	B	203	OLC	3	0
8	A	613	OLC	3	0

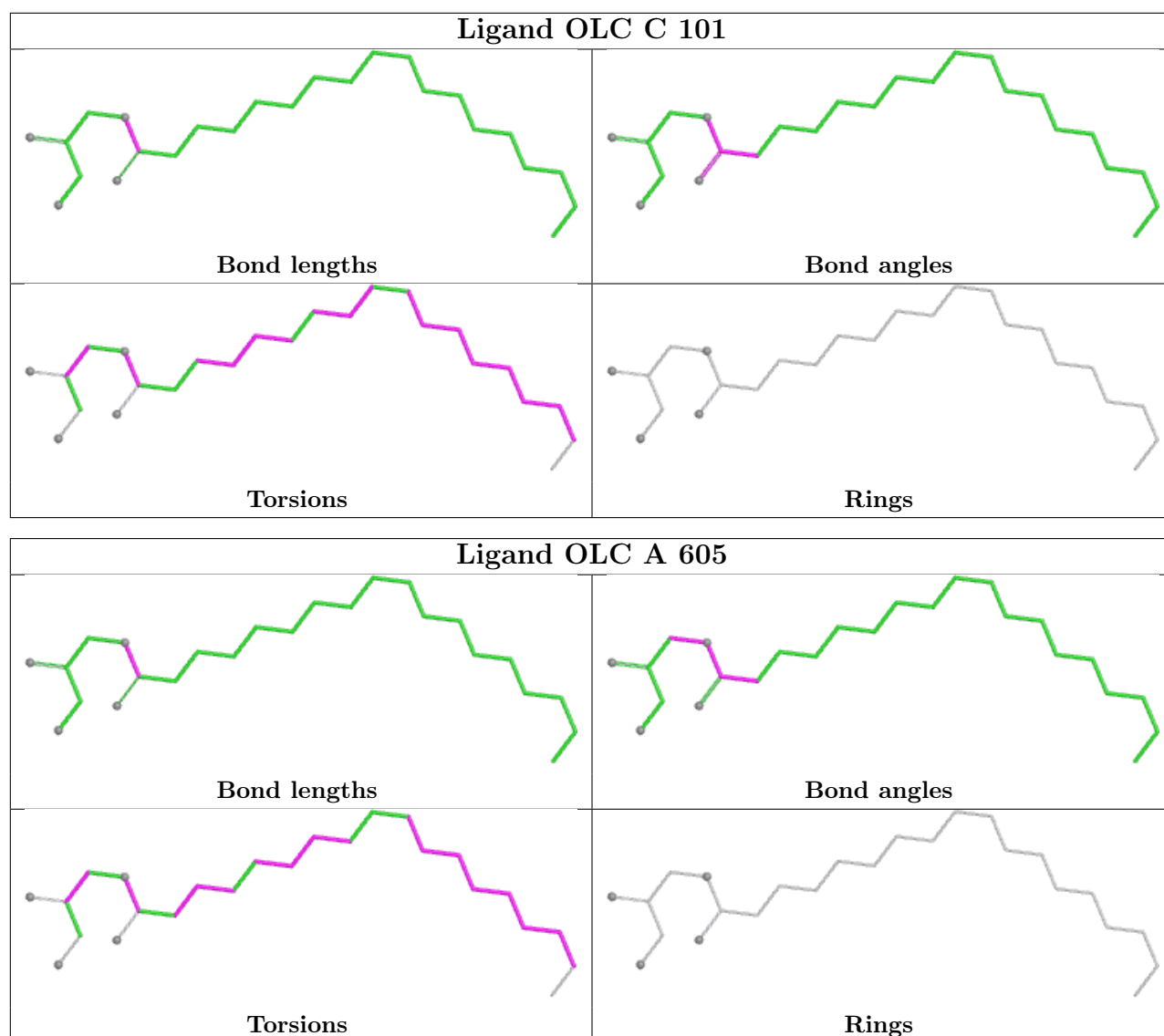
*Continued on next page...*

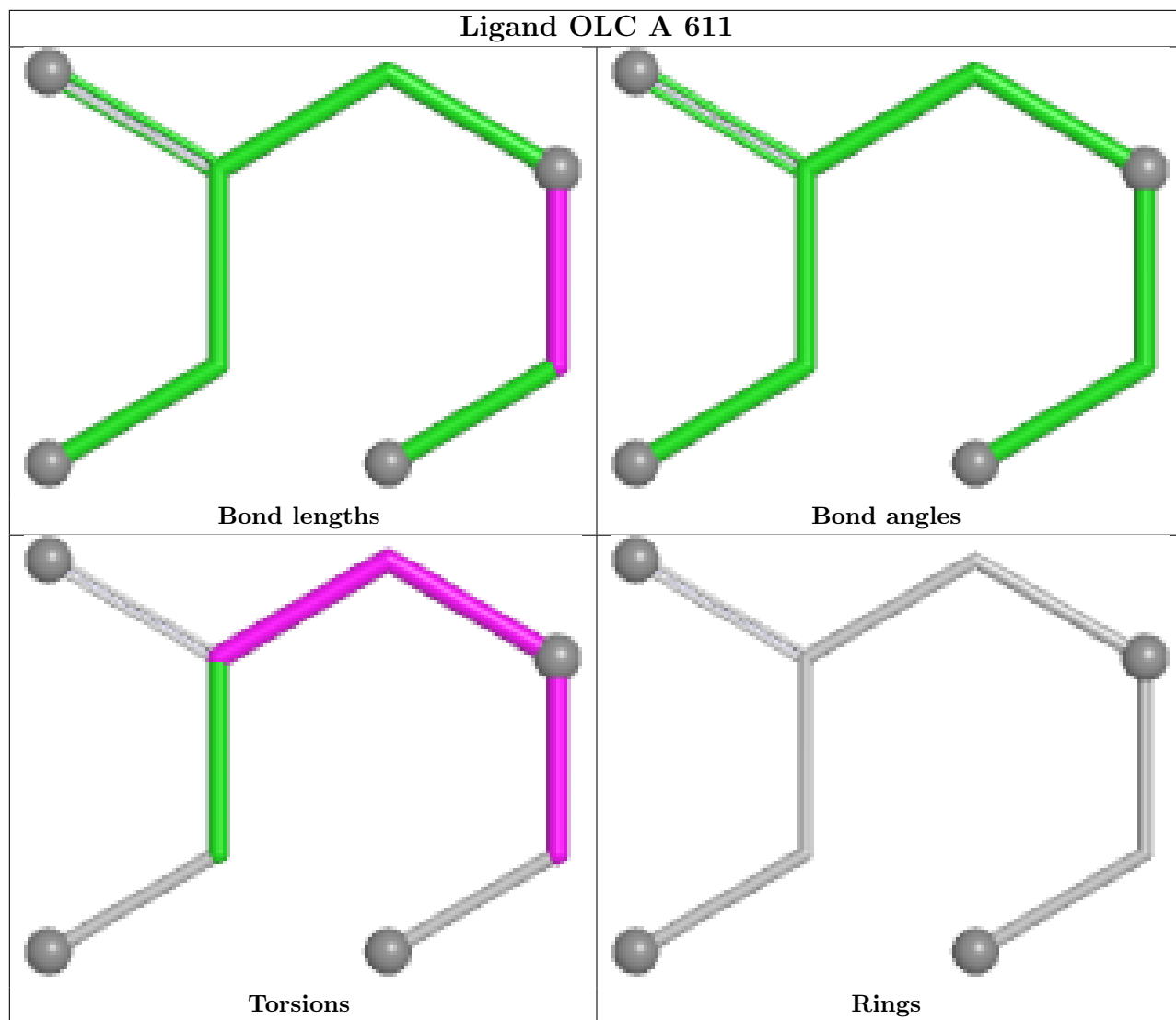
*Continued from previous page...*

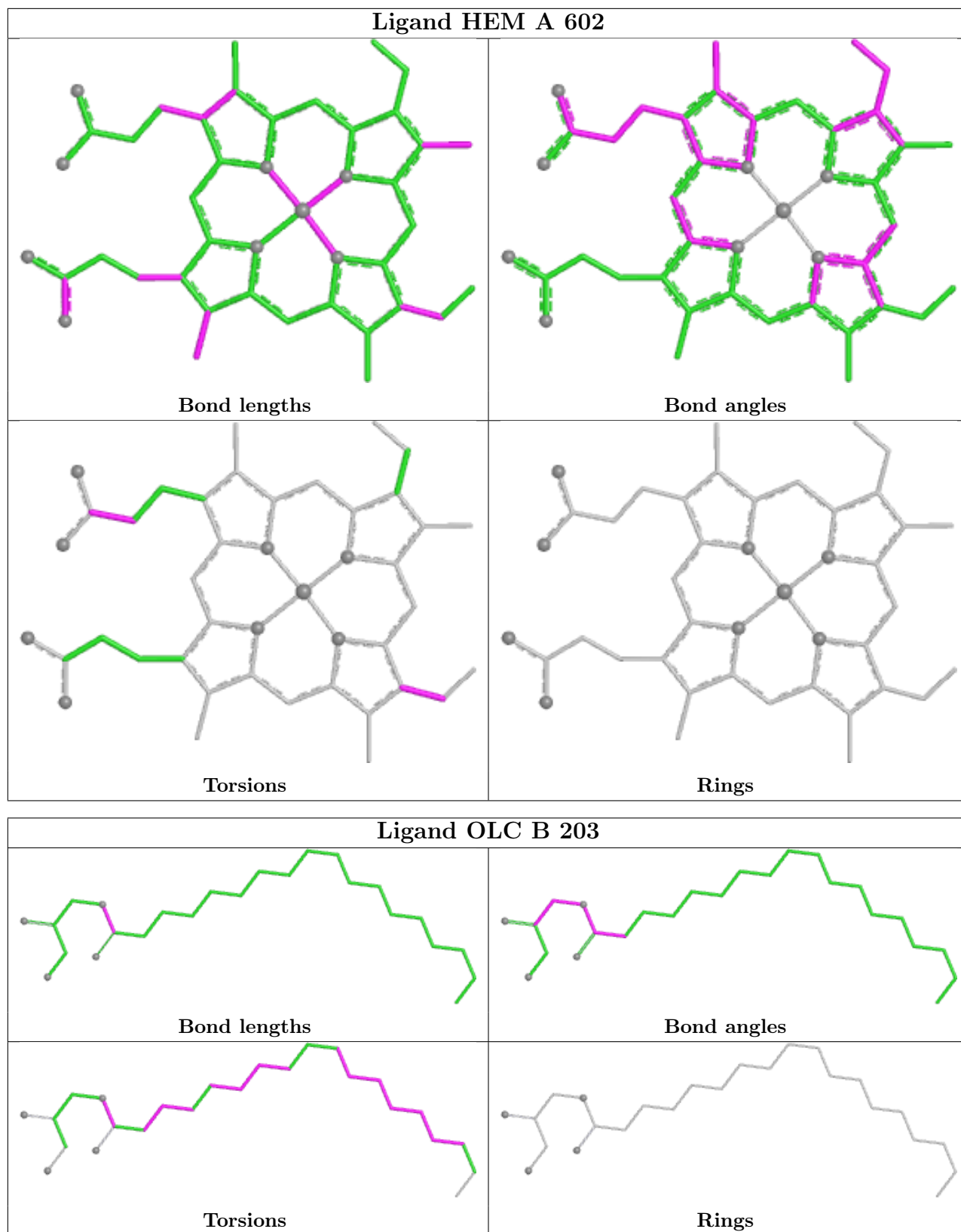
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	607	OLC	6	0
8	A	616	OLC	2	0
8	A	606	OLC	3	0
8	A	614	OLC	9	0
6	A	603	HAS	2	0
8	A	612	OLC	3	0

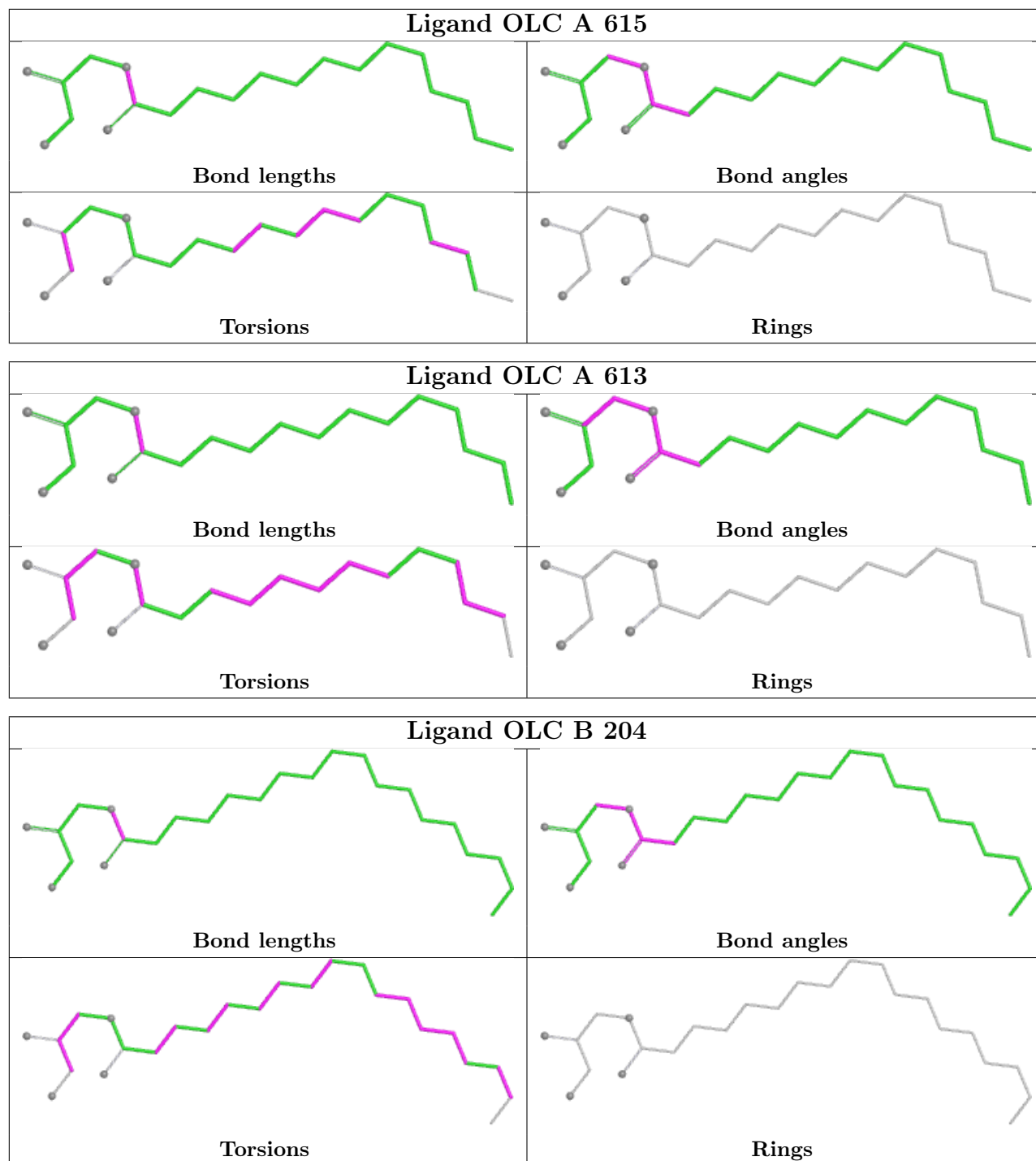
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

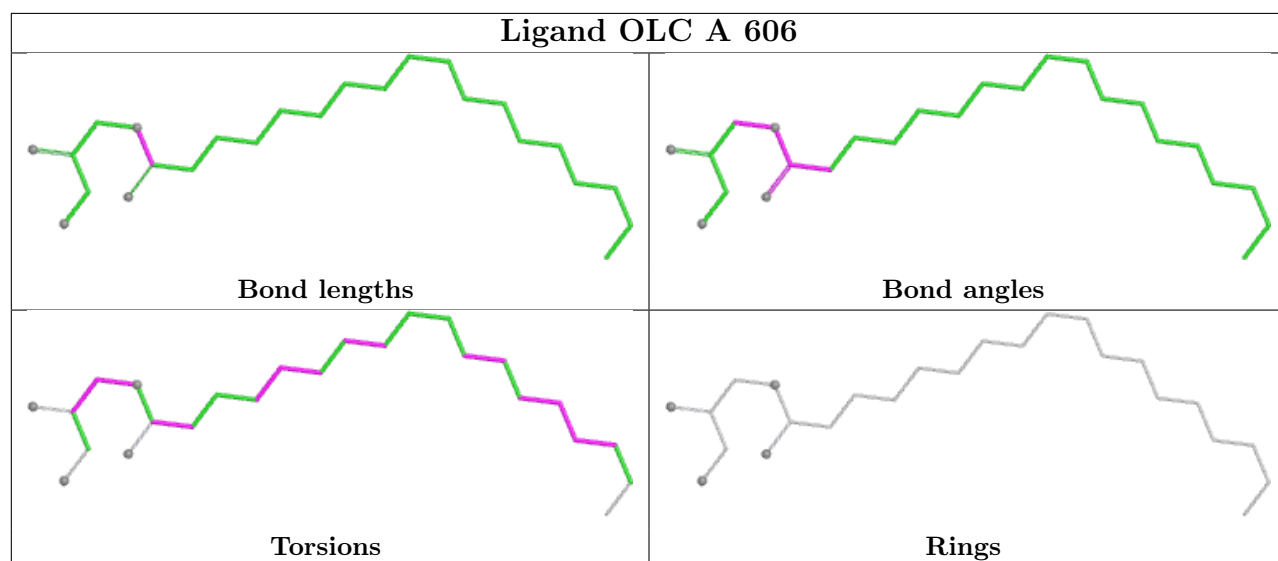
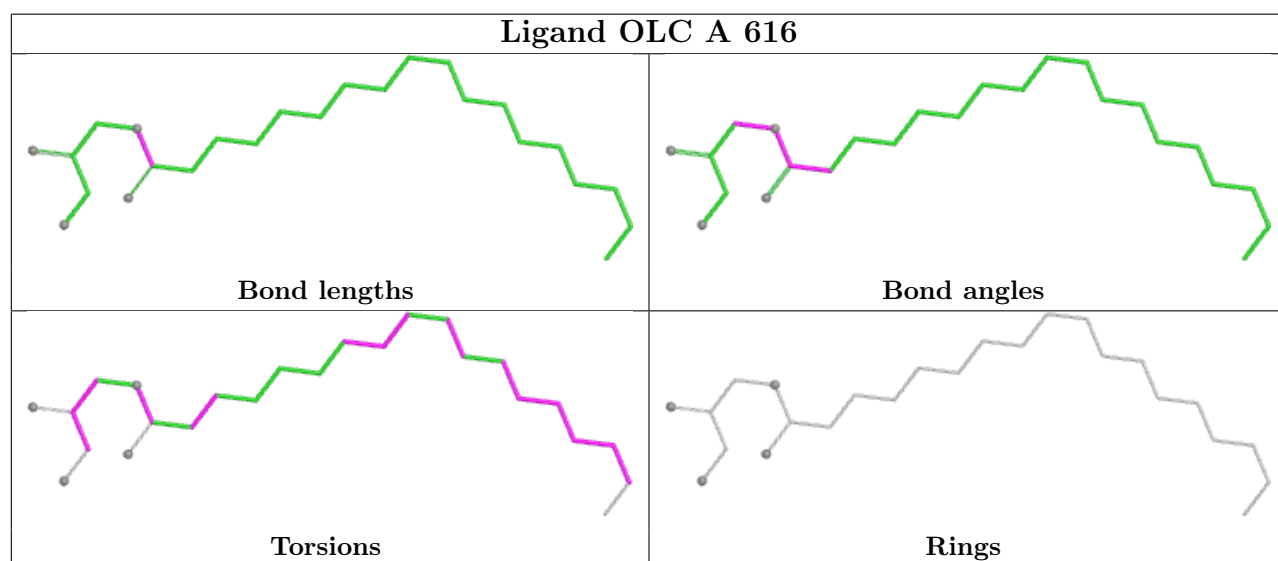
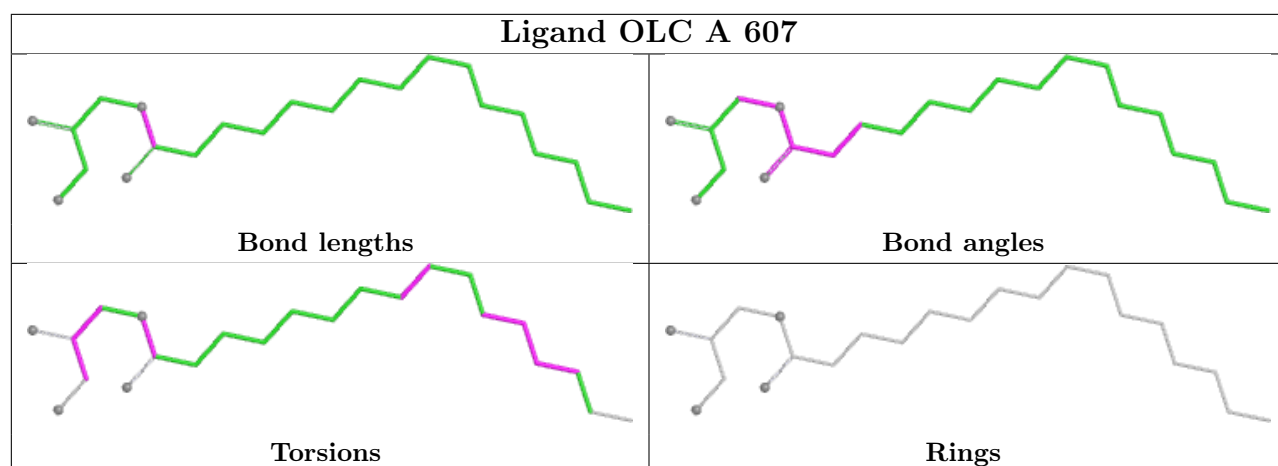


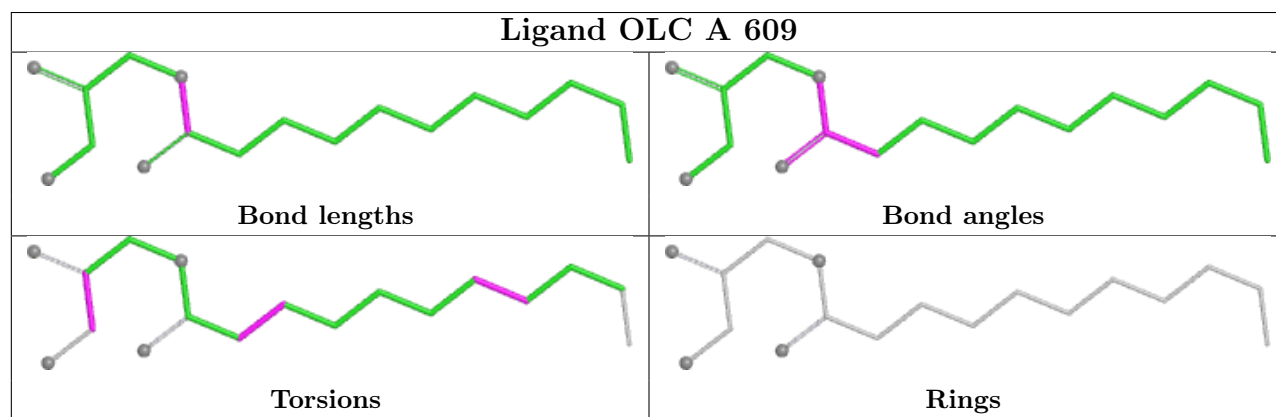
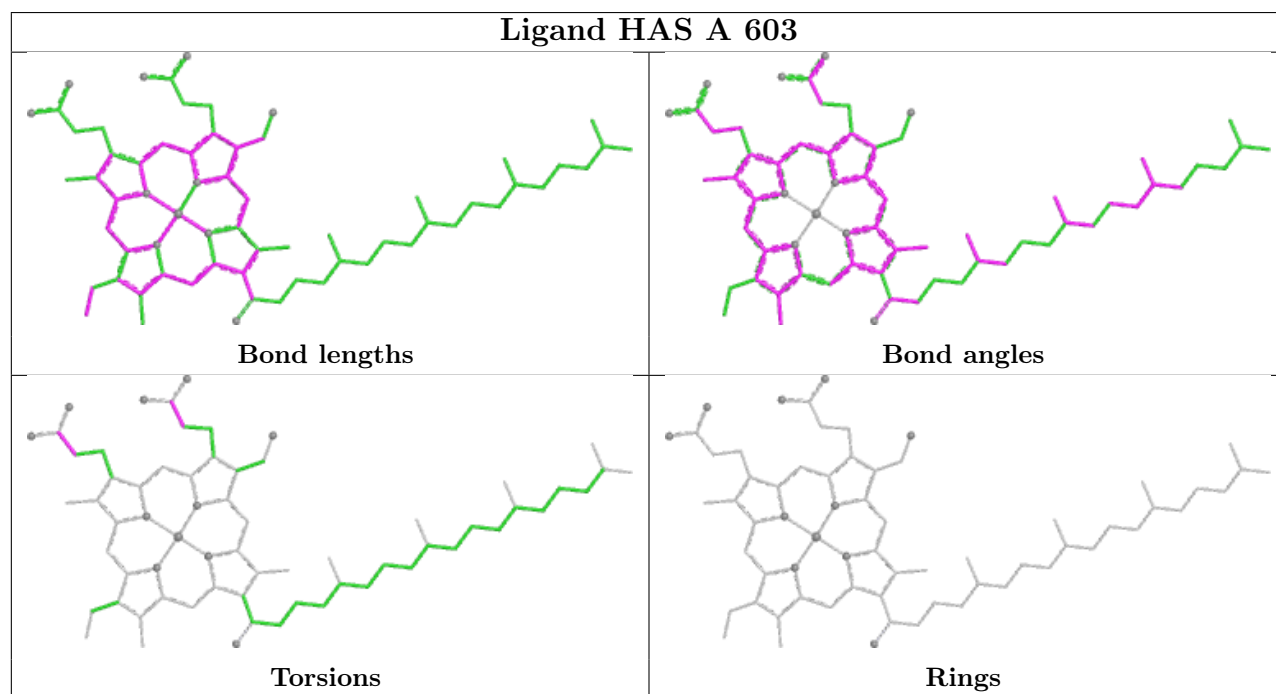
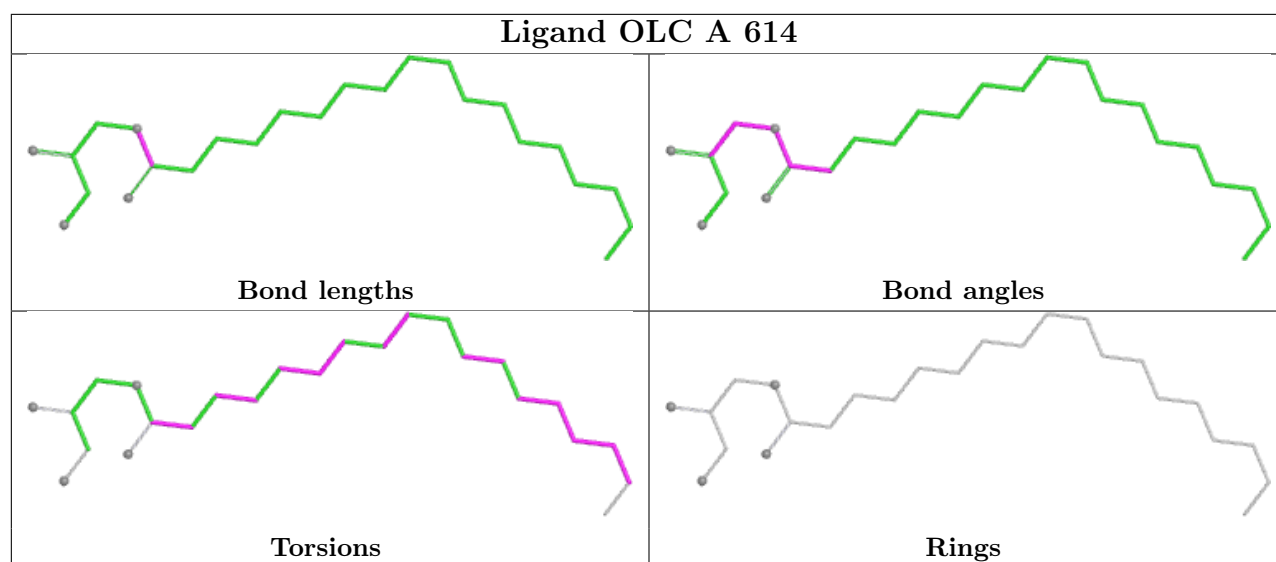


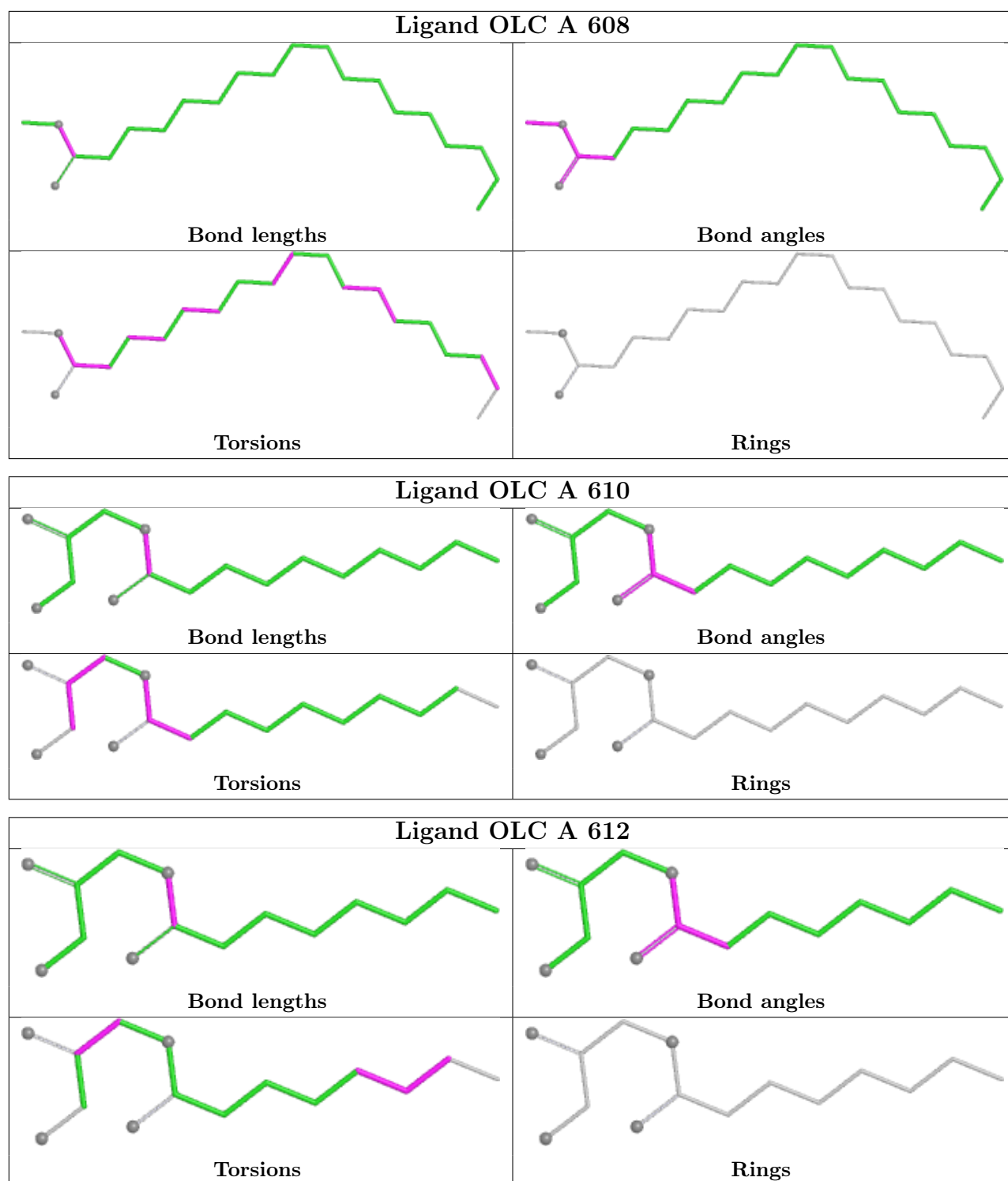












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	546/568 (96%)	-0.68	8 (1%) 72 68	10, 20, 43, 71	2 (0%)
2	B	166/168 (98%)	-0.62	3 (1%) 67 64	12, 22, 44, 87	0
3	C	31/34 (91%)	-0.78	0 100 100	15, 20, 37, 43	0
All	All	743/770 (96%)	-0.67	11 (1%) 72 68	10, 21, 43, 87	2 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	PHE	3.6
1	A	496	GLU	3.3
1	A	499	PRO	3.2
1	A	517	ASP	2.9
2	B	5	HIS	2.8
2	B	6	LYS	2.6
2	B	3	ASP	2.4
1	A	368	SER	2.3
1	A	497	ARG	2.2
1	A	504	ALA	2.2
1	A	494	SER	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands

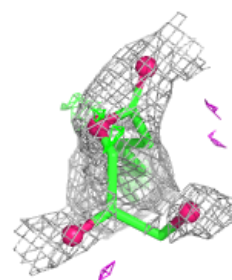
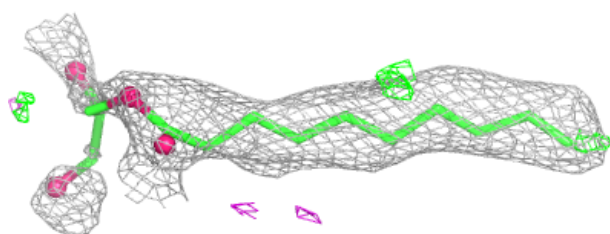
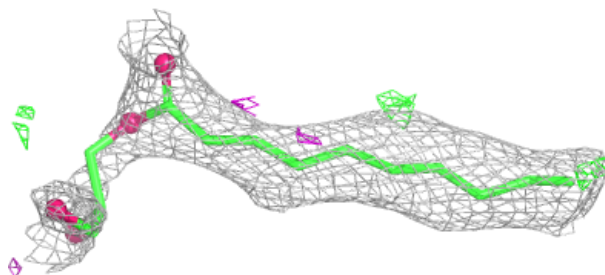
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	OLC	A	610	17/25	0.76	0.18	50,57,71,72	0
8	OLC	A	608	21/25	0.77	0.17	50,54,62,63	0
8	OLC	C	101	25/25	0.77	0.18	65,68,89,92	0
8	OLC	B	203	25/25	0.79	0.18	45,60,72,73	0
8	OLC	A	612	15/25	0.79	0.19	55,64,71,71	0
8	OLC	B	202	25/25	0.80	0.16	52,57,71,74	0
8	OLC	B	204	25/25	0.81	0.17	52,64,74,74	0
8	OLC	A	615	21/25	0.82	0.14	51,58,65,66	0
8	OLC	A	613	20/25	0.84	0.15	43,50,60,62	0
8	OLC	A	606	25/25	0.87	0.12	44,53,69,70	0
8	OLC	A	609	18/25	0.87	0.14	47,60,66,67	0
8	OLC	A	605	25/25	0.88	0.12	35,45,67,69	0
8	OLC	A	616	25/25	0.88	0.12	46,52,57,60	0
8	OLC	A	607	23/25	0.89	0.09	27,41,49,51	0
8	OLC	A	611	8/25	0.89	0.12	50,57,62,63	0
8	OLC	A	614	25/25	0.89	0.10	31,42,50,51	0
6	HAS	A	603	65/65	0.98	0.05	8,14,21,26	0
5	HEM	A	602	43/43	0.99	0.05	2,11,16,21	0
7	PEO	A	604	2/2	0.99	0.05	7,7,7,14	0
9	CUA	B	201	2/2	0.99	0.01	13,13,13,15	0
4	CU	A	601	1/1	1.00	0.01	15,15,15,15	0

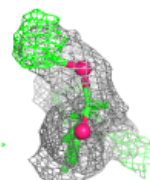
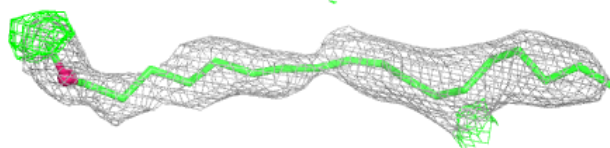
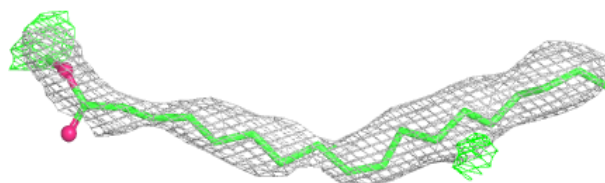
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

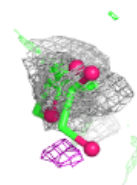
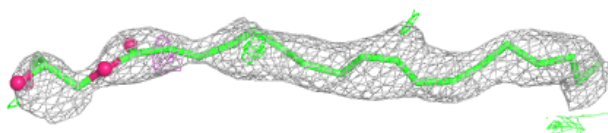
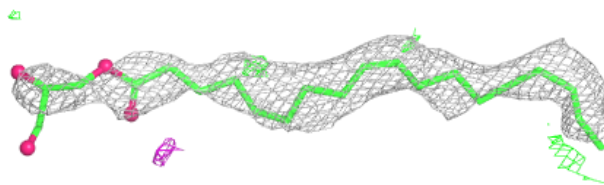
**Electron density around OLC A 608:**

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

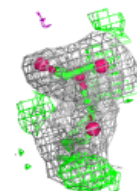
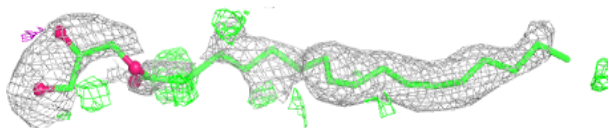
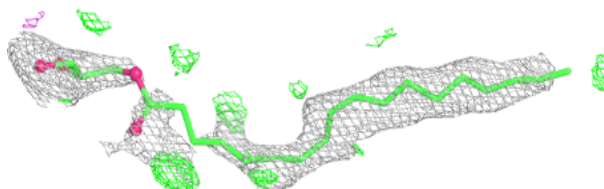


**Electron density around OLC C 101:**

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

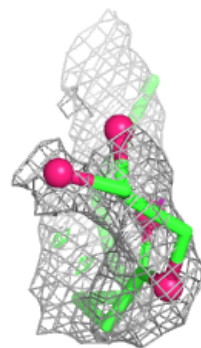
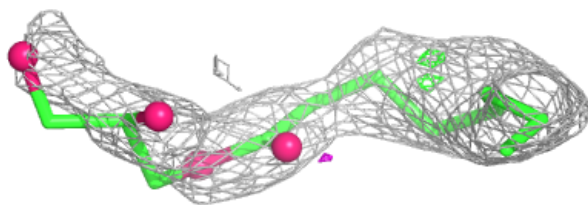
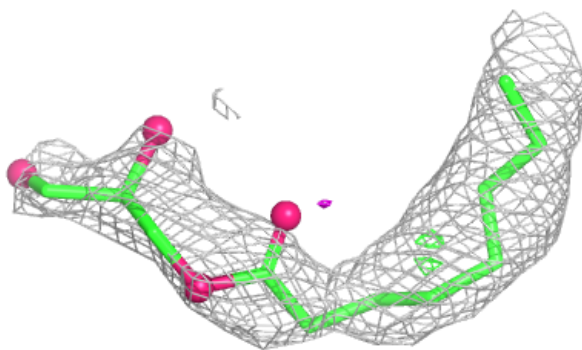
**Electron density around OLC B 203:**

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

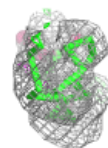
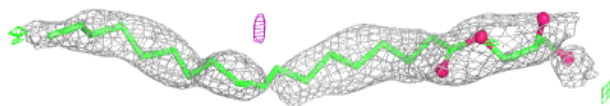
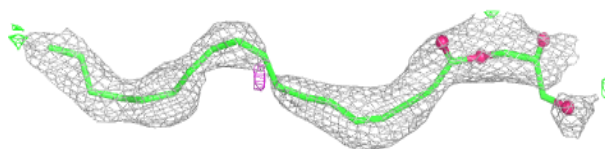


**Electron density around OLC A 612:**

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

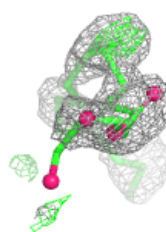
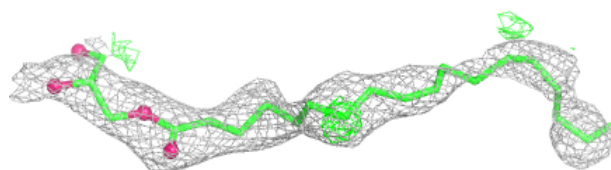
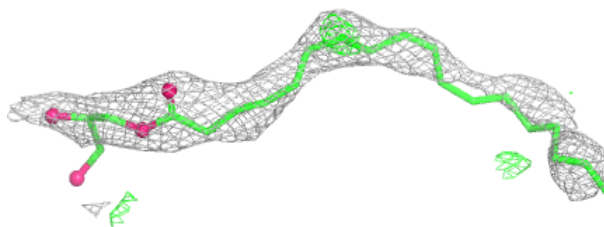
**Electron density around OLC B 202:**

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

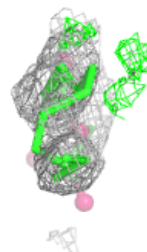
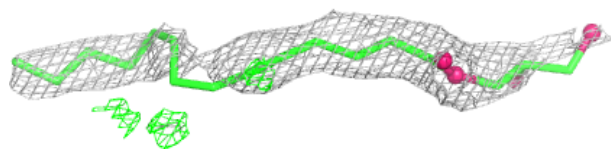
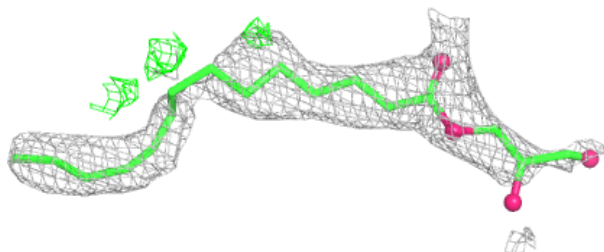


**Electron density around OLC B 204:**

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

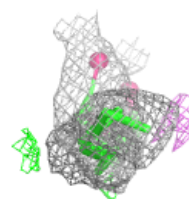
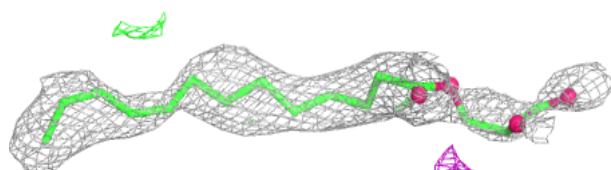
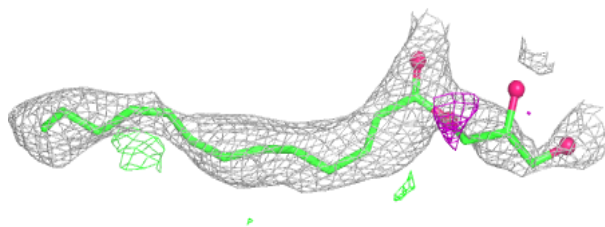
**Electron density around OLC A 615:**

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

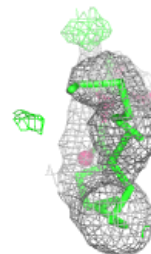
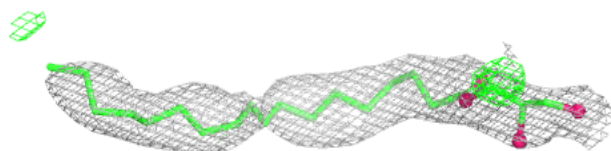
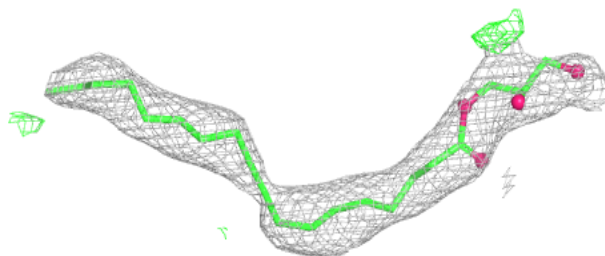


**Electron density around OLC A 613:**

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

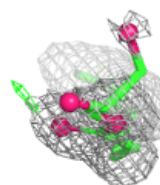
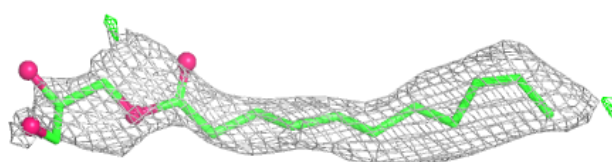
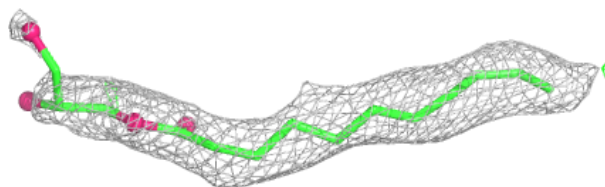
**Electron density around OLC A 606:**

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

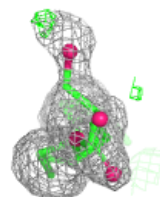
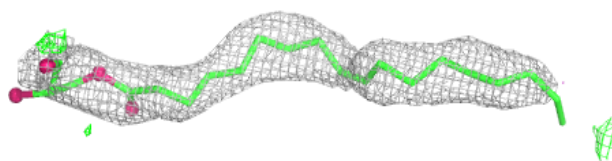
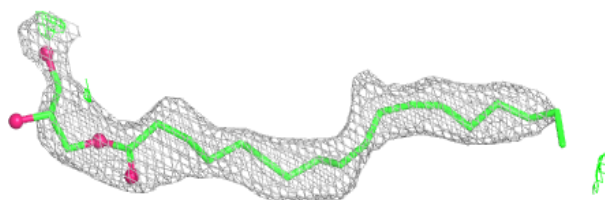


**Electron density around OLC A 609:**

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

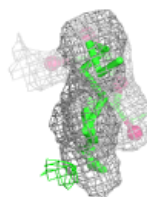
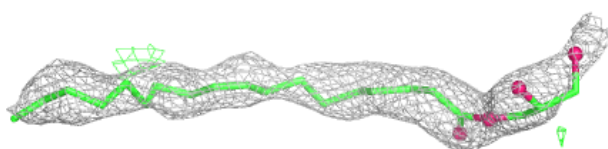
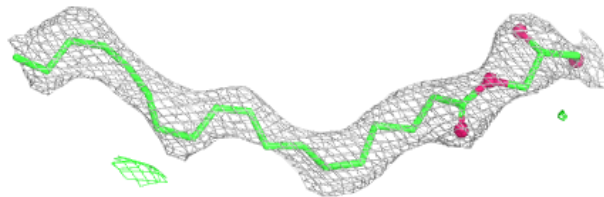
**Electron density around OLC A 605:**

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

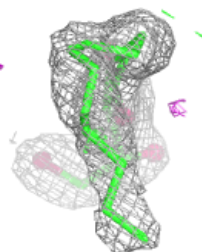
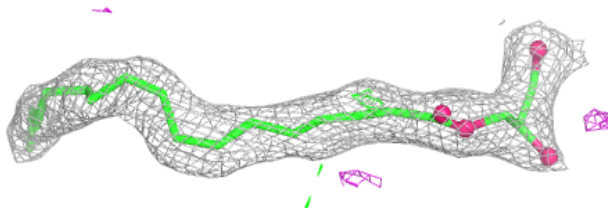
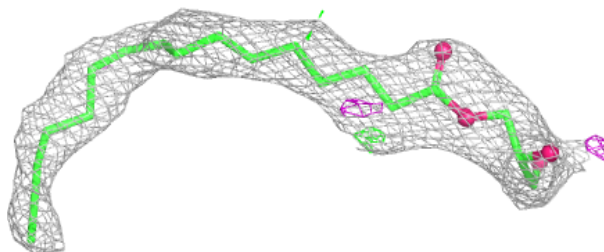


**Electron density around OLC A 616:**

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

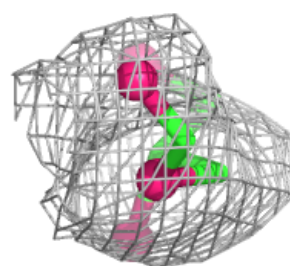
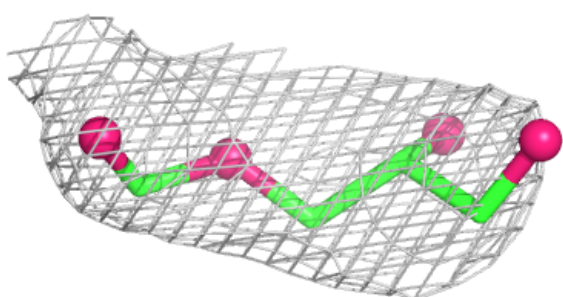
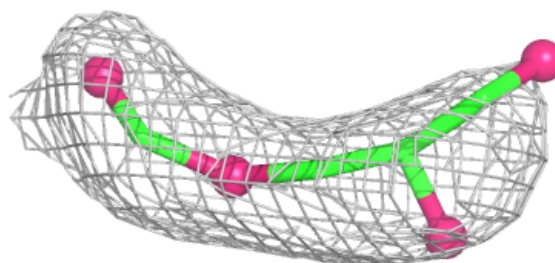
**Electron density around OLC A 607:**

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

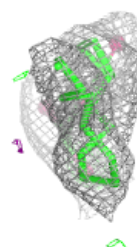
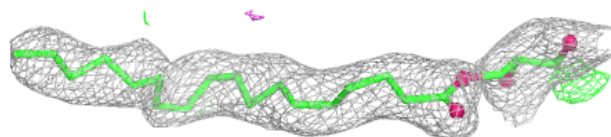
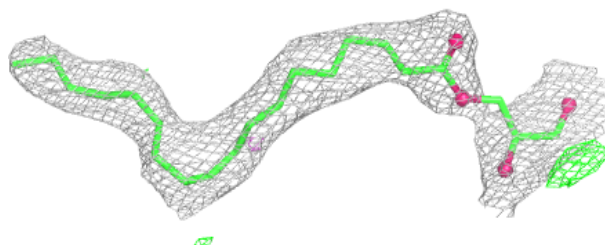


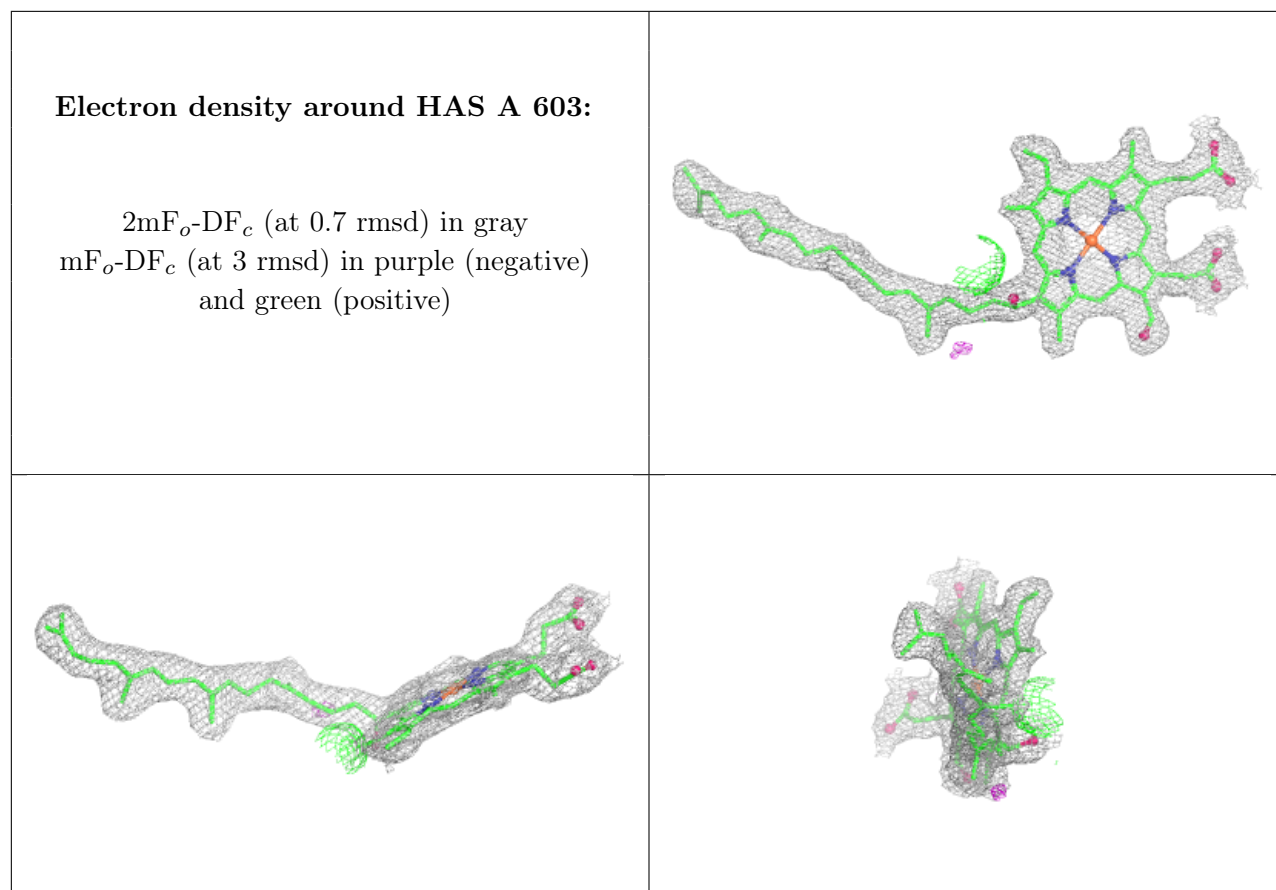
**Electron density around OLC A 611:**

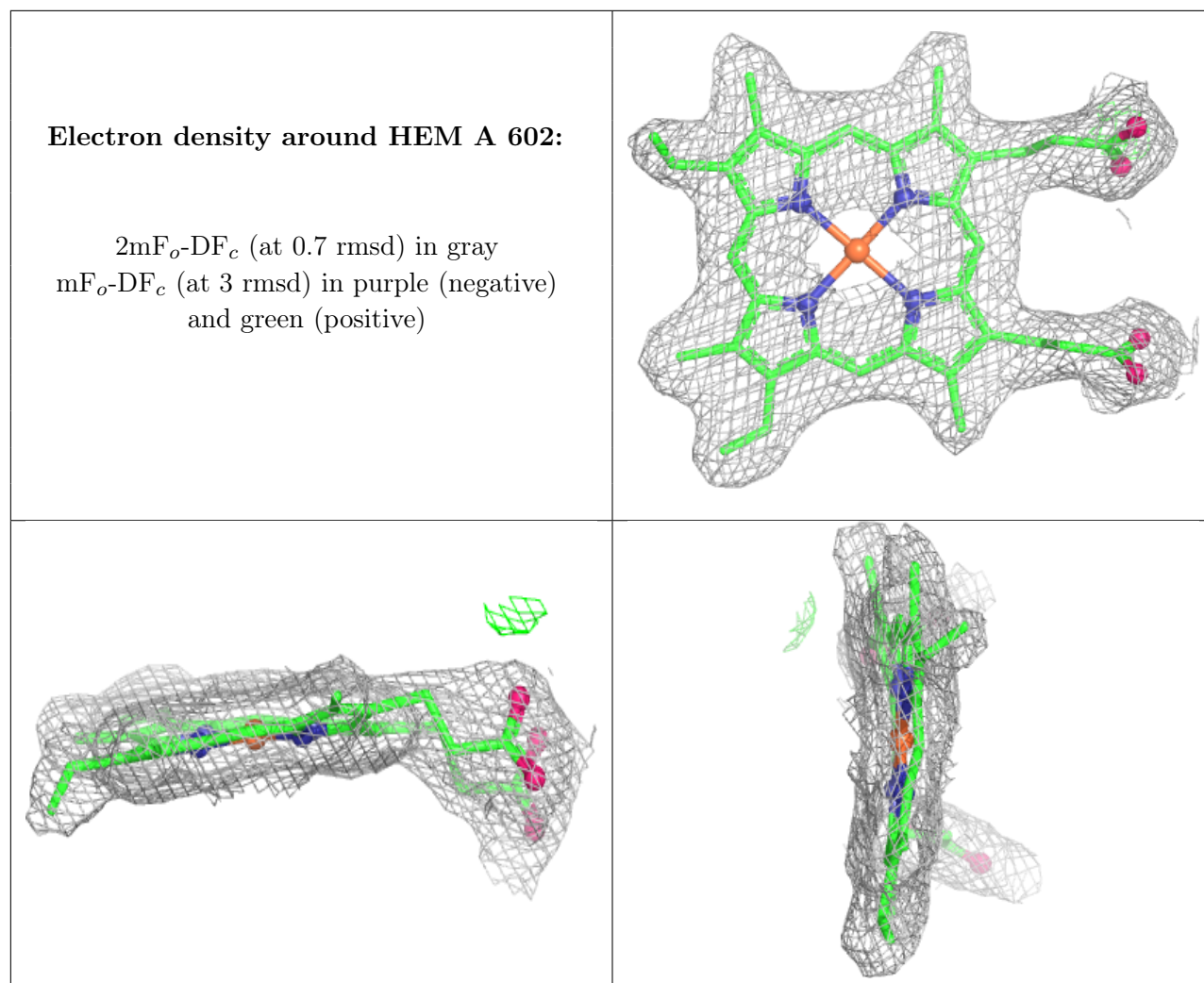
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around OLC A 614:**

$2mF_o-DF_c$  (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.