



Full wwPDB X-ray Structure Validation Report ⓘ

May 30, 2020 – 02:43 am BST

PDB ID : 4G71
Title : Structure of Recombinant Cytochrome ba3 Oxidase mutant V236N from *Thermus thermophilus*
Authors : Li, Y.; Chen, Y.; Stout, C.D.
Deposited on : 2012-07-19
Resolution : 2.90 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 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 : 2.11
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) : 2.11

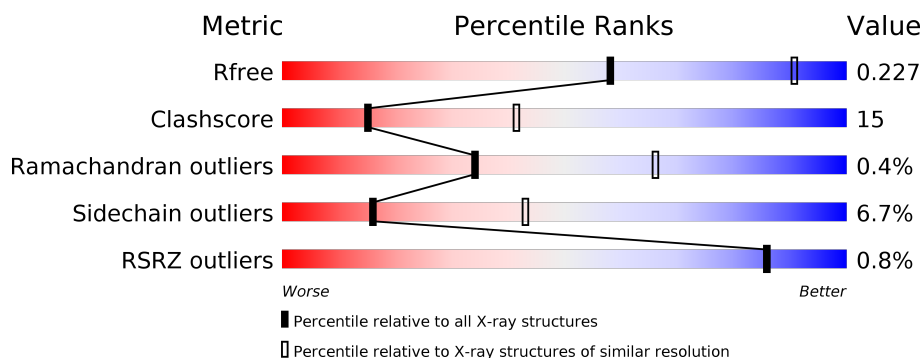
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	569	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 28%, green 66%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 66% 28% • • </div> </div>
2	B	168	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 32%, green 64%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 64% 32% • • </div> </div>
3	C	34	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 59%, yellow 26%, orange 6%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 59% 26% 6% 9% </div> </div>

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
7	PER	A	604	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6389 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	3	0
			4358	2962	688	692	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	EXPRESSION TAG	UNP Q5SJ79
A	-5	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-4	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-3	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-2	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-1	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	0	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	1	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	120	PHE	ALA	engineered mutation	UNP Q5SJ79
A	236	ASN	VAL	engineered mutation	UNP Q5SJ79

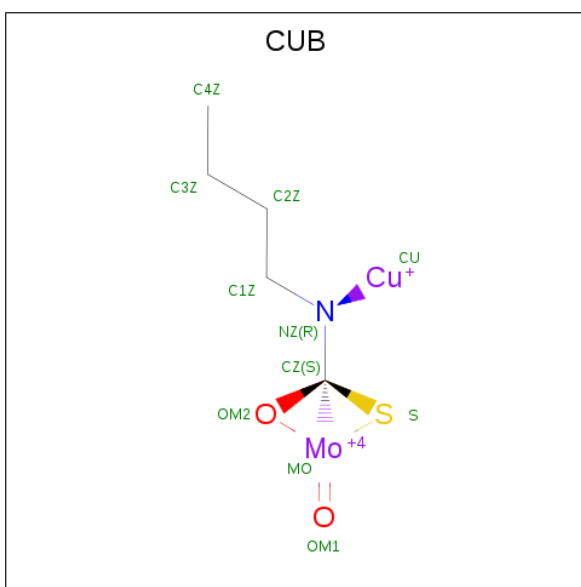
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	1	0
			1283	833	213	233	4			

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

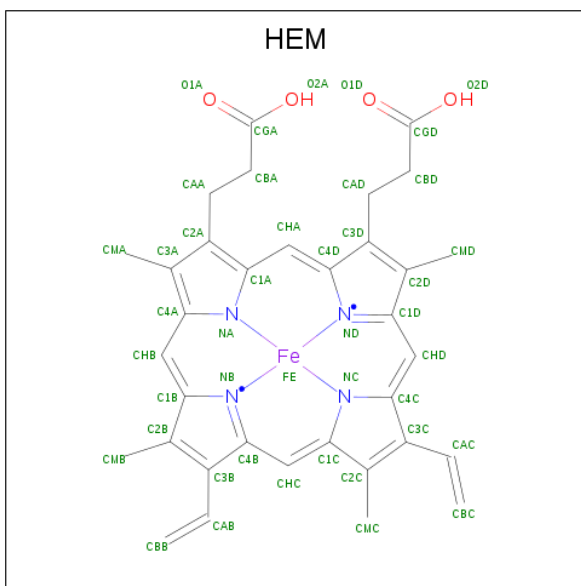
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	31	Total	C	N	O	0	0	0
			241	169	37	35			

- Molecule 4 is CU(I)-S-MO(IV)(=O)O-NBIC CLUSTER (three-letter code: CUB) (formula: C₅H₉CuMoNO₂S).



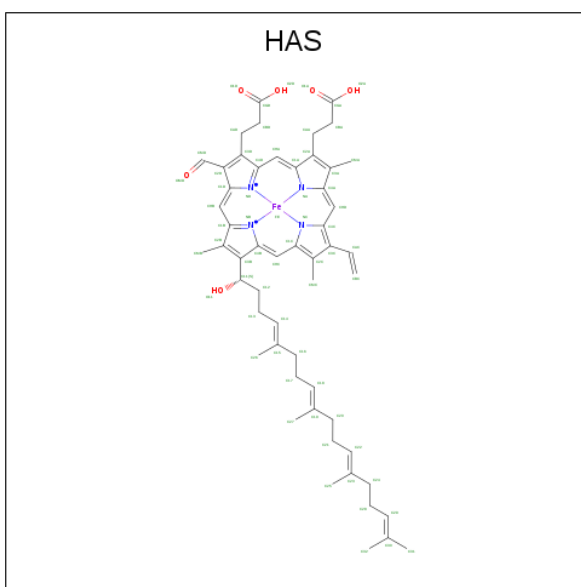
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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



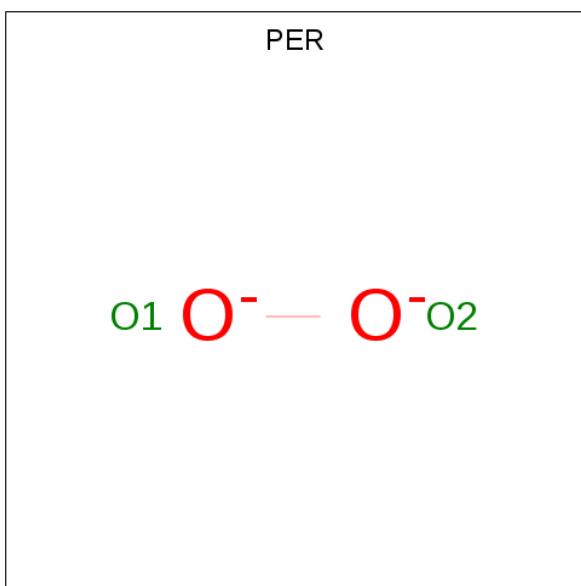
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



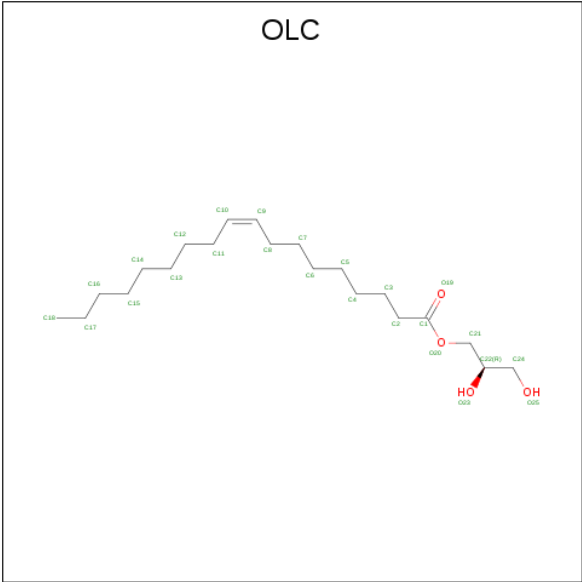
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	
			65	54	1	4	6	

- 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).



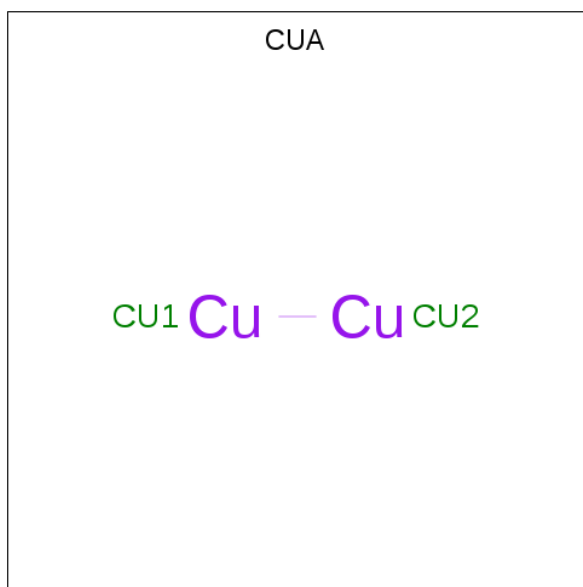
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			24	20	4		
8	A	1	Total	C	O	0	0
			22	18	4		
8	A	1	Total	C	O	0	0
			21	19	2		
8	A	1	Total	C	O	0	0
			18	14	4		
8	A	1	Total	C	O	0	0
			16	12	4		
8	A	1	Total	C	O	0	0
			8	4	4		
8	A	1	Total	C	O	0	0
			13	9	4		
8	A	1	Total	C	O	0	0
			20	16	4		
8	A	1	Total	C	O	0	0
			24	20	4		
8	A	1	Total	C	O	0	0
			20	16	4		
8	A	1	Total	C	O	0	0
			24	20	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			22	18	4		
8	C	1	Total	C	O	0	0
			23	19	4		

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



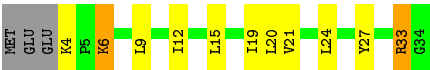
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Cu	0	0
			2	2		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	39	Total	O	0	0
			39	39		
10	B	23	Total	O	0	0
			23	23		
10	C	2	Total	O	0	0
			2	2		

- Molecule 1: Cytochrome c oxidase subunit 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.44Å 98.36Å 94.84Å 90.00° 127.81° 90.00°	Depositor
Resolution (Å)	74.93 – 2.90 19.72 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (74.93-2.90) 99.5 (19.72-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.180 , 0.224 0.183 , 0.227	Depositor DCC
R_{free} test set	1183 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6389	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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: OLC, PER, CUB, CUA, HEM, 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	0.90	9/4520 (0.2%)	0.87	6/6210 (0.1%)
2	B	0.81	1/1323 (0.1%)	0.84	1/1807 (0.1%)
3	C	0.85	0/247	0.86	1/335 (0.3%)
All	All	0.88	10/6090 (0.2%)	0.86	8/8352 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	TRP	CD2-CE2	7.63	1.50	1.41
1	A	167	TRP	CD2-CE2	6.97	1.49	1.41
1	A	335	TRP	CD2-CE2	5.87	1.48	1.41
1	A	230	TRP	CD2-CE2	5.72	1.48	1.41
1	A	426	TRP	CD2-CE2	5.63	1.48	1.41
1	A	380	TRP	CD2-CE2	5.63	1.48	1.41
1	A	157	TRP	CD2-CE2	5.33	1.47	1.41
2	B	18	TRP	CD2-CE2	5.12	1.47	1.41
1	A	403	TRP	CD2-CE2	5.04	1.47	1.41
1	A	107	TRP	CD2-CE2	5.03	1.47	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	ASP	CB-CG-OD2	6.39	124.05	118.30
2	B	84	LEU	CB-CG-CD1	-6.29	100.31	111.00
1	A	267	LEU	CB-CG-CD2	-6.00	100.81	111.00
1	A	274	LEU	CA-CB-CG	5.67	128.34	115.30
3	C	33	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	A	112	MET	CG-SD-CE	5.17	108.48	100.20
1	A	237	TYR	CZ-CE2-CD2	-5.06	115.25	119.80
1	A	514	GLY	N-CA-C	-5.06	100.45	113.10

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	4358	0	4422	139	0
2	B	1283	0	1245	45	0
3	C	241	0	267	14	0
4	A	1	0	0	0	0
5	A	43	0	30	3	0
6	A	65	0	62	4	0
7	A	2	0	0	3	0
8	A	210	0	289	16	0
8	B	75	0	120	10	0
8	C	45	0	64	6	0
9	B	2	0	0	0	0
10	A	39	0	0	4	0
10	B	23	0	0	6	1
10	C	2	0	0	1	0
All	All	6389	0	6499	192	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 15.

All (192) 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:475:ILE:HD11	8:A:605:OLC:H11	1.27	1.11
1:A:263:PRO:HG2	1:A:516:GLU:HG2	1.37	1.05
2:B:14:TYR:CD1	2:B:14:TYR:CD2	2.40	1.01
1:A:516:GLU:HG3	1:A:517:ASP:H	1.27	0.97
2:B:14:TYR:CB	2:B:14:TYR:CD2	2.49	0.95
2:B:14:TYR:CD1	2:B:14:TYR:CB	2.53	0.91
1:A:233:HIS:O	1:A:236:ASN:HB2	1.76	0.85
1:A:236:ASN:OD1	6:A:603:HAS:C4C	2.26	0.84
1:A:290:ILE:HG22	1:A:295:LYS:HE3	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ARG:NH2	8:A:611:OLC:H3A	1.94	0.83
1:A:236:ASN:OD1	6:A:603:HAS:CHD	2.28	0.82
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.16	0.80
1:A:475:ILE:CD1	8:A:605:OLC:H11	2.08	0.79
2:B:47:ALA:O	10:B:322:HOH:O	2.03	0.76
1:A:82:GLN:HB2	10:A:739:HOH:O	1.86	0.74
2:B:144:GLU:HG2	2:B:165:VAL:HG22	1.69	0.74
1:A:377:ASN:OD1	10:A:725:HOH:O	2.06	0.73
1:A:475:ILE:HD11	8:A:605:OLC:C11	2.15	0.71
1:A:516:GLU:HG3	1:A:517:ASP:N	2.06	0.70
1:A:381:VAL:HB	1:A:382:PRO:HD3	1.73	0.70
2:B:51:GLU:OE2	10:B:305:HOH:O	2.11	0.69
1:A:168:ARG:HH11	8:A:610:OLC:H22	1.58	0.69
8:B:203:OLC:H5A	3:C:33:ARG:HE	1.60	0.67
2:B:18:TRP:CE3	3:C:12:ILE:HD13	2.30	0.67
3:C:4:LYS:HG3	3:C:6:LYS:HG2	1.78	0.66
2:B:14:TYR:CD2	3:C:9:LEU:HD11	2.30	0.66
1:A:46:TYR:HA	1:A:453:ILE:HD11	1.78	0.66
1:A:236:ASN:ND2	7:A:604:PER:O2	2.29	0.65
1:A:280:GLY:HA3	1:A:542:TYR:OH	1.97	0.64
1:A:168:ARG:HH21	8:A:611:OLC:H3A	1.64	0.63
1:A:294:TRP:CH2	1:A:544:PRO:HG2	2.33	0.63
1:A:560:ARG:HG2	1:A:560:ARG:O	1.96	0.62
8:A:605:OLC:H2A	8:A:613:OLC:H3A	1.81	0.62
1:A:398:MET:O	1:A:401:LEU:HB2	2.00	0.62
1:A:216:VAL:HG12	8:A:614:OLC:H21A	1.82	0.61
1:A:332:LEU:HD13	1:A:333:PHE:CE1	2.35	0.61
1:A:400:SER:HA	1:A:403:TRP:NE1	2.15	0.61
1:A:59:LEU:HD22	1:A:61:PHE:HE1	1.65	0.61
1:A:165:ASP:OD1	10:A:721:HOH:O	2.17	0.61
8:B:203:OLC:H18A	8:C:102:OLC:H6	1.83	0.60
1:A:456:VAL:O	1:A:456:VAL:HG23	2.01	0.60
1:A:260:VAL:HG11	2:B:11:ILE:HD13	1.84	0.60
1:A:528:GLY:HA2	8:A:611:OLC:H2	1.84	0.60
1:A:341:TRP:CZ2	8:A:615:OLC:H3	2.36	0.60
1:A:445:LEU:HD12	1:A:463:ALA:HB2	1.84	0.59
1:A:521:VAL:HA	1:A:524:MET:HE2	1.85	0.59
1:A:286:ALA:HB1	2:B:125:VAL:HA	1.84	0.58
3:C:4:LYS:N	10:C:202:HOH:O	2.36	0.57
1:A:348:ALA:HA	1:A:425:VAL:HG11	1.87	0.57
1:A:341:TRP:CE2	8:A:615:OLC:H3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:GLY:O	1:A:358:PRO:HG2	2.05	0.56
1:A:520:LEU:O	1:A:521:VAL:C	2.43	0.56
1:A:357:ILE:HG23	3:C:15:LEU:HD13	1.88	0.55
8:B:203:OLC:H17	8:C:101:OLC:H11	1.89	0.55
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.42	0.55
2:B:78:GLN:NE2	2:B:102:GLU:OE2	2.38	0.55
2:B:120:GLY:HA2	8:B:203:OLC:H4	1.88	0.55
1:A:434:ILE:HG21	1:A:472:LEU:HD23	1.89	0.55
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.87	0.55
1:A:168:ARG:HH22	8:A:611:OLC:C6	2.20	0.55
1:A:78:ILE:HD11	1:A:133:TYR:HB2	1.89	0.55
2:B:93:ASN:ND2	10:B:316:HOH:O	2.39	0.55
1:A:348:ALA:HB1	1:A:395:LEU:O	2.08	0.54
2:B:76:PRO:HG2	10:B:318:HOH:O	2.07	0.54
1:A:35:GLY:HA3	1:A:76:ASN:OD1	2.08	0.54
1:A:405:LEU:HB3	1:A:406:PRO:HD3	1.91	0.53
1:A:562:TRP:HA	2:B:155:LEU:HG	1.91	0.52
1:A:52:TYR:N	1:A:53:PRO:CD	2.72	0.52
1:A:263:PRO:HG2	1:A:516:GLU:CG	2.25	0.52
1:A:357:ILE:HG23	3:C:15:LEU:CD1	2.41	0.51
1:A:161:TYR:CE2	8:A:610:OLC:H21	2.45	0.51
1:A:204:ALA:HA	1:A:208:LEU:HB2	1.93	0.51
1:A:430:LEU:O	1:A:434:ILE:HG13	2.10	0.51
3:C:21:VAL:HG11	8:C:102:OLC:H9	1.93	0.50
8:B:203:OLC:H12	8:C:102:OLC:H21A	1.93	0.50
1:A:310:LEU:HD13	2:B:22:SER:HB2	1.93	0.50
1:A:499:PRO:O	1:A:503:GLU:HG3	2.12	0.50
2:B:108:THR:OG1	2:B:109:SER:N	2.45	0.50
1:A:97:LEU:HD22	1:A:170:TRP:CD1	2.46	0.50
1:A:168:ARG:NH1	8:A:610:OLC:H22	2.25	0.50
1:A:193:TRP:CH2	1:A:235:ILE:HG13	2.46	0.50
1:A:140:LYS:HE3	1:A:211:TRP:NE1	2.27	0.50
1:A:332:LEU:HD13	1:A:333:PHE:HE1	1.74	0.50
2:B:125:VAL:HG22	2:B:126:GLU:O	2.12	0.49
1:A:220:ASP:HB3	1:A:223:VAL:HG12	1.94	0.49
1:A:23:TYR:HB3	1:A:110:TRP:NE1	2.28	0.49
1:A:52:TYR:N	1:A:53:PRO:HD2	2.26	0.49
1:A:332:LEU:CD1	1:A:333:PHE:HE1	2.26	0.49
1:A:517:ASP:OD2	1:A:520:LEU:HB2	2.12	0.49
2:B:92:PRO:HG3	10:B:323:HOH:O	2.11	0.48
1:A:377:ASN:O	1:A:449:ARG:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:VAL:N	1:A:308:PRO:HD2	2.28	0.48
1:A:556:VAL:HG12	2:B:55:PRO:HG3	1.96	0.48
2:B:142:PRO:HA	2:B:166:VAL:HG12	1.96	0.48
1:A:445:LEU:HD12	1:A:463:ALA:CB	2.44	0.48
2:B:12:LEU:O	2:B:16:LYS:HG3	2.13	0.47
1:A:377:ASN:HB2	2:B:150:ASN:ND2	2.30	0.47
2:B:95:ILE:HD12	2:B:164:ILE:HG12	1.95	0.47
8:B:203:OLC:H17	8:C:101:OLC:H12	1.95	0.47
2:B:93:ASN:HA	2:B:94:PRO:HA	1.75	0.47
1:A:258:LYS:HG2	1:A:510:GLU:HB3	1.95	0.47
2:B:113:ILE:HG23	2:B:128:LEU:HD12	1.96	0.47
1:A:277:THR:N	1:A:278:PRO:HD2	2.29	0.47
2:B:23:LEU:HD12	2:B:23:LEU:HA	1.59	0.46
2:B:35:TYR:OH	8:B:202:OLC:H24A	2.14	0.46
1:A:371:LEU:HD21	3:C:27:TYR:HD1	1.81	0.46
2:B:77:ASN:OD1	2:B:101:ALA:HA	2.15	0.46
1:A:341:TRP:HB3	8:A:606:OLC:H24A	1.96	0.46
1:A:67:GLN:HA	1:A:130:THR:HG23	1.97	0.46
1:A:401:LEU:O	1:A:405:LEU:HB2	2.15	0.46
2:B:63:PRO:HD2	2:B:64:TRP:CE3	2.50	0.46
2:B:85:ALA:O	2:B:110:PRO:HD2	2.16	0.46
3:C:20:LEU:HA	3:C:20:LEU:HD12	1.80	0.46
1:A:348:ALA:HA	1:A:425:VAL:CG1	2.45	0.46
1:A:140:LYS:HE3	1:A:211:TRP:CD1	2.51	0.46
1:A:277:THR:N	1:A:278:PRO:CD	2.79	0.46
1:A:172:ALA:O	1:A:175:PRO:HD3	2.16	0.45
1:A:236:ASN:OD1	6:A:603:HAS:C3C	2.64	0.45
1:A:247:ILE:HG21	1:A:316:VAL:HG21	1.97	0.45
1:A:354:LEU:HD13	8:A:615:OLC:H8	1.97	0.45
2:B:88:PHE:HB3	2:B:160:MET:HB2	1.98	0.45
1:A:186:ALA:O	1:A:190:TRP:CD1	2.70	0.45
1:A:203:GLU:O	1:A:207:PHE:HB2	2.17	0.45
1:A:232:GLY:O	1:A:235:ILE:HG22	2.17	0.45
1:A:247:ILE:CG2	1:A:316:VAL:HG21	2.47	0.45
1:A:290:ILE:CG2	1:A:295:LYS:HE3	2.41	0.45
1:A:76:ASN:HB3	5:A:602:HEM:CAC	2.46	0.45
1:A:254:GLN:H	1:A:254:GLN:HG2	1.63	0.45
1:A:386:HIS:CE1	5:A:602:HEM:C1A	3.05	0.44
2:B:87:ALA:HB1	2:B:88:PHE:CE1	2.52	0.44
1:A:59:LEU:HD22	1:A:61:PHE:CE1	2.48	0.44
6:A:603:HAS:C4A	7:A:604:PER:O2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ARG:HG2	1:A:101:PRO:O	2.17	0.44
1:A:211:TRP:CG	1:A:219:VAL:HG23	2.52	0.44
3:C:6:LYS:HB2	3:C:6:LYS:HZ3	1.83	0.44
1:A:251:LEU:N	1:A:252:PRO:CD	2.81	0.44
2:B:144:GLU:CG	2:B:165:VAL:HG22	2.43	0.44
1:A:326:LEU:HD12	1:A:326:LEU:HA	1.43	0.43
1:A:357:ILE:HB	1:A:358:PRO:CD	2.48	0.43
1:A:452:TYR:HB3	2:B:158[A]:GLN:OE1	2.17	0.43
1:A:44:LEU:HD12	1:A:471:VAL:HA	1.99	0.43
8:B:203:OLC:H17	8:C:101:OLC:C12	2.49	0.43
1:A:548:GLN:NE2	2:B:50:LEU:HD12	2.33	0.43
1:A:146:TYR:CD2	1:A:208:LEU:HD13	2.53	0.43
1:A:146:TYR:CE2	1:A:208:LEU:HD13	2.53	0.43
1:A:230:TRP:C	1:A:230:TRP:CD1	2.92	0.43
1:A:233:HIS:C	1:A:233:HIS:CD2	2.92	0.43
1:A:274:LEU:HD21	1:A:530:TRP:CE3	2.54	0.43
2:B:124:ASN:OD1	2:B:150:ASN:ND2	2.44	0.43
1:A:131:VAL:O	1:A:132:LEU:HB2	2.19	0.43
1:A:143:TRP:HB2	1:A:213:PHE:CE2	2.54	0.43
1:A:236:ASN:CG	7:A:604:PER:O2	2.57	0.43
1:A:154:LEU:HA	1:A:154:LEU:HD23	1.64	0.43
1:A:139:LEU:HA	1:A:559:TRP:O	2.19	0.43
1:A:516:GLU:HA	1:A:516:GLU:OE1	2.19	0.42
2:B:109:SER:OG	2:B:111:ASP:OD2	2.38	0.42
1:A:378:THR:HG22	10:B:315:HOH:O	2.19	0.42
1:A:380:TRP:H	1:A:443:GLY:HA3	1.85	0.42
1:A:516:GLU:CG	1:A:517:ASP:N	2.76	0.42
2:B:32:LEU:HD21	8:B:202:OLC:H7A	2.01	0.42
1:A:339:LEU:HB3	1:A:346:PHE:CZ	2.54	0.42
1:A:364:ILE:HD12	3:C:19:ILE:HG12	2.02	0.42
2:B:19:LEU:HA	2:B:19:LEU:HD23	1.95	0.42
2:B:32:LEU:HA	2:B:32:LEU:HD23	1.82	0.42
3:C:6:LYS:NZ	3:C:6:LYS:HB2	2.35	0.42
1:A:355:GLY:HA3	1:A:433:MET:HE1	2.00	0.41
1:A:460:TYR:N	1:A:461:PRO:CD	2.83	0.41
1:A:28:GLY:HA2	1:A:83:LEU:HD12	2.01	0.41
2:B:72:VAL:O	2:B:79:TYR:HA	2.19	0.41
1:A:21:THR:OG1	1:A:91:TYR:HB2	2.21	0.41
1:A:220:ASP:HA	1:A:221:PRO:HD3	1.79	0.41
1:A:48:ASN:HB2	1:A:467:MET:SD	2.61	0.41
5:A:602:HEM:HBC2	5:A:602:HEM:HMC2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ILE:CG2	1:A:236:ASN:N	2.84	0.41
1:A:330:ARG:O	1:A:334:GLY:HA3	2.20	0.41
1:A:308:PRO:O	1:A:311:MET:HB3	2.21	0.41
2:B:6:LYS:O	2:B:9:LYS:N	2.54	0.41
1:A:355:GLY:CA	1:A:433:MET:HE1	2.51	0.41
1:A:522:LEU:HA	1:A:522:LEU:HD23	1.91	0.41
1:A:377:ASN:N	10:A:716:HOH:O	2.41	0.40
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.78	0.40
1:A:420:LEU:O	1:A:423:ALA:HB3	2.20	0.40
1:A:55:LEU:HD11	1:A:59:LEU:HD12	2.03	0.40
1:A:95:ARG:HD2	1:A:95:ARG:HA	1.92	0.40
1:A:258:LYS:HE2	1:A:510:GLU:HB3	2.02	0.40
2:B:147:ILE:HD11	2:B:164:ILE:HG13	2.02	0.40
1:A:235:ILE:HA	1:A:238:PHE:HB3	2.04	0.40
2:B:75:GLY:HA3	2:B:78:GLN:HB3	2.03	0.40
1:A:332:LEU:HD13	1:A:333:PHE:CD1	2.57	0.40
8:B:204:OLC:H9	3:C:12:ILE:CD1	2.52	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:319:HOH:O[2_556]	2.15	0.05

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	554/569 (97%)	497 (90%)	54 (10%)	3 (0%)	29	61
2	B	165/168 (98%)	154 (93%)	11 (7%)	0	100	100
3	C	29/34 (85%)	27 (93%)	2 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	748/771 (97%)	678 (91%)	67 (9%)	3 (0%)	34 66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	537	LEU
1	A	369	PHE
1	A	557	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	442/464 (95%)	413 (93%)	29 (7%)	16 44
2	B	132/138 (96%)	122 (92%)	10 (8%)	13 36
3	C	24/27 (89%)	22 (92%)	2 (8%)	11 32
All	All	598/629 (95%)	557 (93%)	41 (7%)	16 41

All (41) 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	134	THR
1	A	158	VAL
1	A	201	VAL
1	A	215	LEU
1	A	230	TRP
1	A	235	ILE
1	A	261	SER
1	A	262	ASP
1	A	274	LEU

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Mol	Chain	Res	Type
1	A	287	ASP
1	A	309	SER
1	A	332	LEU
1	A	356	PHE
1	A	369	PHE
1	A	400	SER
1	A	401	LEU
1	A	405	LEU
1	A	475	ILE
1	A	490	SER
1	A	493	LEU
1	A	500	GLU
1	A	510	GLU
1	A	516	GLU
1	A	518	ARG
1	A	520	LEU
2	B	4	GLU
2	B	12	LEU
2	B	15	GLU
2	B	26	LEU
2	B	37	LEU
2	B	58	VAL
2	B	111	ASP
2	B	128	LEU
2	B	158[A]	GLN
2	B	158[B]	GLN
3	C	6	LYS
3	C	24	LEU

Some 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	548	GLN
2	B	69	GLN
2	B	93	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 1 is modelled with single atom - 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	615	-	23,23,24	0.61	1 (4%)	24,24,25	1.13	2 (8%)
5	HEM	A	602	1	27,50,50	3.07	12 (44%)	17,82,82	2.45	7 (41%)
8	OLC	A	612	-	19,19,24	0.58	0	20,20,25	0.70	0
7	PER	A	604	6	0,1,1	0.00	-	-	-	-
8	OLC	B	204	-	24,24,24	0.56	0	25,25,25	0.58	0
8	OLC	A	609	-	15,15,24	0.70	1 (6%)	16,16,25	0.67	0
8	OLC	C	101	-	21,21,24	0.66	1 (4%)	22,22,25	0.69	0
6	HAS	A	603	1,7	56,72,72	4.35	17 (30%)	50,109,109	2.72	13 (26%)
8	OLC	A	607	-	20,20,24	0.55	0	20,20,25	0.69	1 (5%)
8	OLC	C	102	-	22,22,24	0.56	1 (4%)	23,23,25	0.63	0
9	CUA	B	201	2	0,1,1	0.00	-	-	-	-
8	OLC	A	613	-	23,23,24	0.54	1 (4%)	24,24,25	0.81	2 (8%)
8	OLC	A	606	-	21,21,24	0.62	0	22,22,25	0.78	1 (4%)
8	OLC	A	610	-	7,7,24	0.49	0	6,7,25	0.46	0
8	OLC	A	608	-	17,17,24	0.52	0	18,18,25	0.66	0
8	OLC	B	203	-	24,24,24	0.75	1 (4%)	25,25,25	0.99	2 (8%)
8	OLC	A	614	-	19,19,24	0.67	1 (5%)	20,20,25	0.83	1 (5%)
8	OLC	B	202	-	24,24,24	0.59	0	25,25,25	0.55	0
8	OLC	A	605	-	23,23,24	0.63	1 (4%)	24,24,25	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	OLC	A	611	-	12,12,24	0.67	0	13,13,25	0.81	1 (7%)

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	615	-	-	10/23/23/24	-
5	HEM	A	602	1	-	0/6/54/54	-
8	OLC	A	612	-	-	7/19/19/24	-
8	OLC	B	204	-	-	8/24/24/24	-
8	OLC	A	609	-	-	10/15/15/24	-
6	HAS	A	603	1,7	-	6/35/122/122	-
8	OLC	A	607	-	-	8/19/19/24	-
8	OLC	C	102	-	-	13/22/22/24	-
8	OLC	B	203	-	-	12/24/24/24	-
8	OLC	A	613	-	-	11/23/23/24	-
8	OLC	A	606	-	-	8/21/21/24	-
8	OLC	A	610	-	-	3/6/6/24	-
8	OLC	A	608	-	-	9/17/17/24	-
8	OLC	A	611	-	-	6/12/12/24	-
8	OLC	A	614	-	-	9/19/19/24	-
8	OLC	B	202	-	-	8/24/24/24	-
8	OLC	A	605	-	-	10/23/23/24	-
8	OLC	C	101	-	-	6/21/21/24	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	CHD-C4A	-15.57	1.35	1.51
6	A	603	HAS	CHC-C4B	-12.26	1.32	1.53
6	A	603	HAS	C1B-NB	-11.65	1.33	1.49
6	A	603	HAS	C4B-NB	-11.27	1.34	1.49
6	A	603	HAS	C4A-C3A	8.82	1.50	1.38
6	A	603	HAS	CHA-C1A	-8.00	1.31	1.51
6	A	603	HAS	C3C-CAC	-7.77	1.32	1.47
6	A	603	HAS	C1A-C2A	7.68	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEM	C3B-CAB	-7.23	1.33	1.47
5	A	602	HEM	C3C-C2C	6.53	1.49	1.40
6	A	603	HAS	C3C-C2C	6.46	1.49	1.40
5	A	602	HEM	C3B-C2B	6.43	1.49	1.40
6	A	603	HAS	CHB-C1B	-5.77	1.31	1.53
5	A	602	HEM	C1B-C2B	-5.22	1.30	1.42
5	A	602	HEM	C1A-NA	3.43	1.43	1.36
5	A	602	HEM	C4A-CHB	-3.40	1.31	1.41
5	A	602	HEM	C1C-C2C	-3.31	1.35	1.42
5	A	602	HEM	CBB-CAB	3.30	1.51	1.29
6	A	603	HAS	CBC-CAC	3.30	1.51	1.29
5	A	602	HEM	C1A-CHA	3.22	1.49	1.41
5	A	602	HEM	C4B-CHC	-3.03	1.32	1.41
6	A	603	HAS	CHA-C4D	-2.98	1.48	1.53
5	A	602	HEM	C4D-C3D	2.75	1.48	1.42
6	A	603	HAS	CMD-C2D	2.73	1.49	1.44
6	A	603	HAS	C1D-ND	-2.67	1.46	1.49
8	B	203	OLC	O20-C1	2.54	1.40	1.33
5	A	602	HEM	C1D-CHD	-2.41	1.34	1.41
8	A	614	OLC	O20-C1	2.36	1.40	1.33
6	A	603	HAS	C2A-C3A	-2.32	1.30	1.37
8	A	605	OLC	O20-C1	2.30	1.40	1.33
6	A	603	HAS	C4D-ND	-2.30	1.46	1.49
8	A	615	OLC	O20-C1	2.22	1.39	1.33
8	C	101	OLC	O20-C1	2.14	1.39	1.33
8	A	609	OLC	O20-C1	2.08	1.39	1.33
8	C	102	OLC	O20-C1	2.02	1.39	1.33
8	A	613	OLC	O20-C1	2.02	1.39	1.33
6	A	603	HAS	C1C-C2C	-2.01	1.35	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	CHB-C1B-NB	9.24	122.43	110.94
6	A	603	HAS	CHB-C1D-ND	6.61	119.16	110.94
6	A	603	HAS	CHC-C4B-NB	6.43	122.87	110.75
6	A	603	HAS	CHA-C4D-ND	5.65	121.40	110.75
5	A	602	HEM	CMD-C2D-C1D	-5.04	120.71	128.46
6	A	603	HAS	C4C-CHD-C4A	4.81	124.61	112.87
6	A	603	HAS	CHD-C4A-C3A	-4.43	122.11	129.53
6	A	603	HAS	CHC-C1C-C2C	-4.27	122.06	129.45
6	A	603	HAS	CAA-CBA-CGA	-4.06	105.86	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	HEM	C4C-C3C-C2C	-4.01	104.10	106.90
6	A	603	HAS	C25-C23-C24	3.95	121.92	115.27
5	A	602	HEM	CBA-CAA-C2A	-3.86	105.36	112.49
5	A	602	HEM	C3B-C4B-NB	-3.77	104.34	109.21
5	A	602	HEM	CMA-C3A-C4A	-3.49	123.09	128.46
8	A	615	OLC	C3-C2-C1	-3.17	102.08	113.62
8	B	203	OLC	O20-C21-C22	3.17	121.08	105.77
6	A	603	HAS	CAA-C2A-C1A	-3.08	125.13	127.30
6	A	603	HAS	CHB-C1B-C2B	2.90	123.75	114.70
6	A	603	HAS	C1D-CHB-C1B	2.49	123.35	116.15
8	A	606	OLC	C21-O20-C1	2.27	125.52	117.12
8	A	614	OLC	C21-O20-C1	2.20	125.26	117.12
5	A	602	HEM	CMC-C2C-C3C	2.14	128.68	124.68
5	A	602	HEM	C4A-C3A-C2A	2.12	108.47	107.00
8	A	615	OLC	C21-O20-C1	2.09	124.84	117.12
8	A	613	OLC	C21-O20-C1	2.08	124.81	117.12
8	B	203	OLC	C21-O20-C1	2.05	124.72	117.12
6	A	603	HAS	C12-C13-C14	2.05	117.65	112.23
8	A	613	OLC	O20-C1-O19	2.05	128.76	123.59
8	A	607	OLC	C21-O20-C1	2.03	122.81	116.11
8	A	611	OLC	C21-O20-C1	2.01	124.56	117.12

There are no chirality outliers.

All (144) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	603	HAS	C4D-C3D-CAD-CBD
8	C	102	OLC	C21-C22-C24-O25
8	A	613	OLC	C21-C22-C24-O25
8	A	613	OLC	O23-C22-C24-O25
8	A	613	OLC	O20-C21-C22-C24
8	A	606	OLC	C21-C22-C24-O25
8	A	610	OLC	O20-C21-C22-C24
8	A	610	OLC	O19-C1-O20-C21
8	A	614	OLC	C10-C11-C12-C13
8	A	614	OLC	C21-C22-C24-O25
8	A	605	OLC	C21-C22-C24-O25
8	A	611	OLC	C21-C22-C24-O25
8	A	611	OLC	O20-C21-C22-C24
8	B	204	OLC	O19-C1-O20-C21
8	A	609	OLC	O19-C1-O20-C21
8	A	614	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
8	A	605	OLC	O19-C1-O20-C21
8	A	614	OLC	C2-C1-O20-C21
6	A	603	HAS	C25-C23-C24-C28
8	B	204	OLC	C2-C1-O20-C21
8	A	609	OLC	C2-C1-O20-C21
8	A	605	OLC	C2-C1-O20-C21
8	B	203	OLC	O19-C1-O20-C21
8	B	202	OLC	C2-C1-O20-C21
8	B	202	OLC	O19-C1-O20-C21
8	A	613	OLC	O20-C21-C22-O23
8	A	610	OLC	O20-C21-C22-O23
8	A	607	OLC	C2-C1-O20-C21
8	B	203	OLC	C2-C1-O20-C21
8	A	615	OLC	C2-C1-O20-C21
8	A	612	OLC	C2-C1-O20-C21
8	C	101	OLC	C2-C1-O20-C21
8	A	609	OLC	O20-C21-C22-C24
8	A	607	OLC	O19-C1-O20-C21
6	A	603	HAS	C22-C23-C24-C28
8	A	609	OLC	O20-C21-C22-O23
8	A	611	OLC	O20-C21-C22-O23
8	A	615	OLC	C1-C2-C3-C4
8	C	101	OLC	O19-C1-O20-C21
8	A	615	OLC	O19-C1-O20-C21
8	A	612	OLC	O19-C1-O20-C21
8	B	203	OLC	C6-C7-C8-C9
8	A	608	OLC	C2-C1-O20-C21
8	A	613	OLC	C11-C12-C13-C14
8	C	102	OLC	C2-C3-C4-C5
8	C	102	OLC	C2-C1-O20-C21
8	C	102	OLC	C11-C12-C13-C14
8	A	614	OLC	C1-C2-C3-C4
8	A	607	OLC	C10-C11-C12-C13
8	A	606	OLC	C11-C12-C13-C14
6	A	603	HAS	C3D-CAD-CBD-CGD
8	B	202	OLC	C3-C4-C5-C6
8	C	102	OLC	O23-C22-C24-O25
8	A	606	OLC	O23-C22-C24-O25
8	A	614	OLC	O23-C22-C24-O25
8	A	605	OLC	O23-C22-C24-O25
8	A	611	OLC	O23-C22-C24-O25
8	B	204	OLC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
8	A	615	OLC	C12-C13-C14-C15
8	A	614	OLC	C3-C4-C5-C6
8	B	202	OLC	C14-C15-C16-C17
8	C	102	OLC	O19-C1-O20-C21
8	A	608	OLC	O19-C1-O20-C21
8	C	101	OLC	C5-C6-C7-C8
8	A	615	OLC	C6-C7-C8-C9
8	A	608	OLC	C6-C7-C8-C9
8	C	102	OLC	C4-C5-C6-C7
8	A	612	OLC	C3-C4-C5-C6
8	B	202	OLC	C12-C13-C14-C15
8	A	613	OLC	C12-C13-C14-C15
8	A	612	OLC	C6-C7-C8-C9
8	A	611	OLC	C3-C4-C5-C6
8	A	608	OLC	C4-C5-C6-C7
8	A	605	OLC	C4-C5-C6-C7
8	A	613	OLC	C2-C1-O20-C21
8	A	611	OLC	C1-C2-C3-C4
8	A	609	OLC	C2-C3-C4-C5
8	B	203	OLC	C3-C4-C5-C6
8	A	607	OLC	C2-C3-C4-C5
8	C	102	OLC	C3-C4-C5-C6
8	A	613	OLC	C13-C14-C15-C16
6	A	603	HAS	C1D-C2D-CMD-OMD
8	B	204	OLC	C15-C16-C17-C18
8	A	613	OLC	O19-C1-O20-C21
8	B	204	OLC	C12-C13-C14-C15
8	A	608	OLC	C2-C3-C4-C5
8	C	102	OLC	C13-C14-C15-C16
8	A	607	OLC	C6-C7-C8-C9
8	C	102	OLC	C1-C2-C3-C4
8	A	609	OLC	C3-C4-C5-C6
8	B	204	OLC	O20-C21-C22-C24
8	A	605	OLC	C14-C15-C16-C17
8	C	101	OLC	C3-C4-C5-C6
8	A	613	OLC	C4-C5-C6-C7
8	B	203	OLC	C4-C5-C6-C7
8	B	202	OLC	O20-C21-C22-C24
8	A	605	OLC	C13-C14-C15-C16
8	A	615	OLC	C10-C11-C12-C13
8	B	204	OLC	C6-C7-C8-C9
8	B	204	OLC	O20-C21-C22-O23

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Mol	Chain	Res	Type	Atoms
8	A	606	OLC	O20-C21-C22-O23
8	A	606	OLC	O19-C1-O20-C21
8	A	607	OLC	C3-C4-C5-C6
8	A	606	OLC	C2-C1-O20-C21
8	A	612	OLC	C2-C3-C4-C5
8	A	605	OLC	C5-C6-C7-C8
6	A	603	HAS	C11-C12-C13-C14
8	A	609	OLC	C1-C2-C3-C4
8	B	203	OLC	C11-C12-C13-C14
8	A	615	OLC	C11-C12-C13-C14
8	A	614	OLC	O20-C21-C22-O23
8	B	203	OLC	C10-C11-C12-C13
8	A	614	OLC	C6-C7-C8-C9
8	A	605	OLC	C1-C2-C3-C4
8	A	615	OLC	C9-C10-C11-C12
8	C	101	OLC	C9-C10-C11-C12
8	A	606	OLC	C2-C3-C4-C5
8	C	101	OLC	C10-C11-C12-C13
8	A	608	OLC	O20-C21-C22-C24
8	B	202	OLC	O20-C21-C22-O23
8	A	607	OLC	C13-C14-C15-C16
8	A	609	OLC	C21-C22-C24-O25
8	A	608	OLC	O20-C21-C22-O23
8	A	612	OLC	O20-C1-C2-C3
8	A	615	OLC	C7-C8-C9-C10
8	A	613	OLC	C7-C8-C9-C10
8	B	203	OLC	C5-C6-C7-C8
8	B	202	OLC	C7-C8-C9-C10
8	B	203	OLC	O20-C21-C22-O23
8	A	608	OLC	C1-C2-C3-C4
8	A	609	OLC	O20-C1-C2-C3
8	A	612	OLC	C9-C10-C11-C12
8	A	607	OLC	C7-C8-C9-C10
8	B	203	OLC	C9-C10-C11-C12
8	A	606	OLC	C7-C8-C9-C10
8	A	608	OLC	C7-C8-C9-C10
8	C	102	OLC	C7-C8-C9-C10
8	B	203	OLC	C7-C8-C9-C10
8	B	203	OLC	O20-C21-C22-C24
8	A	609	OLC	O19-C1-C2-C3
8	A	615	OLC	C4-C5-C6-C7
8	C	102	OLC	O20-C1-C2-C3

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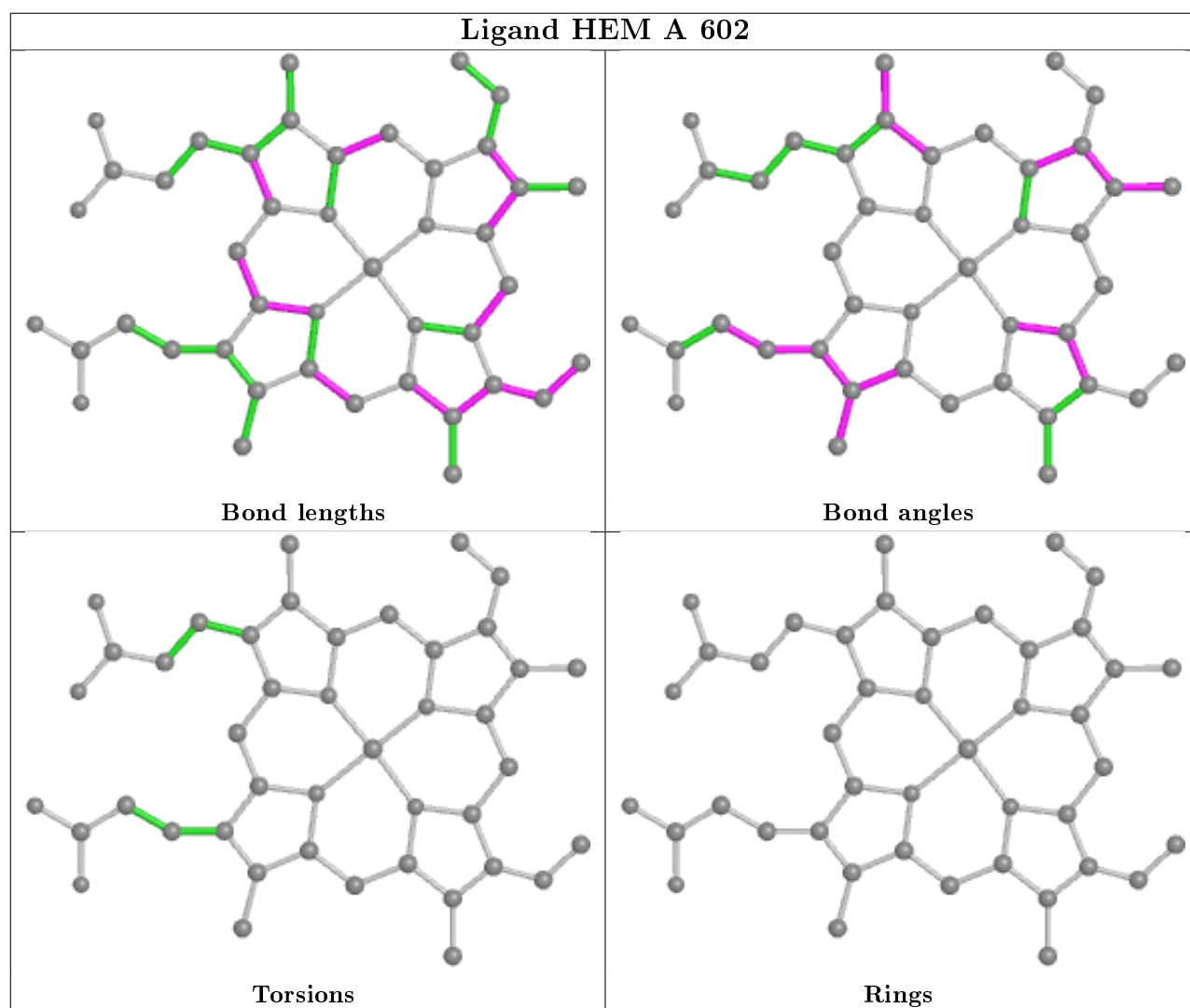
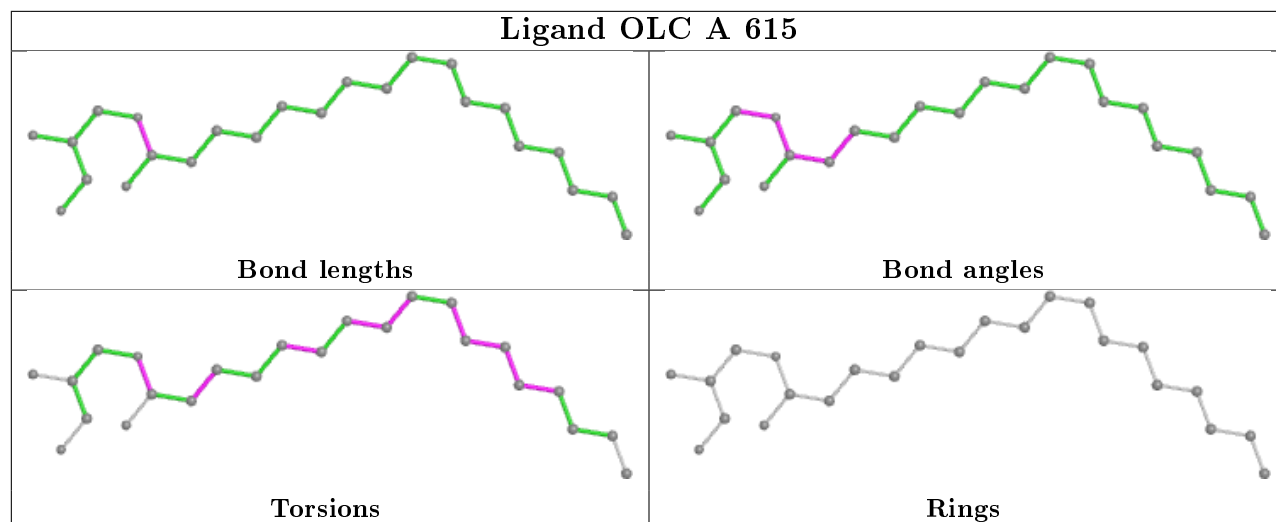
Mol	Chain	Res	Type	Atoms
8	A	605	OLC	C7-C8-C9-C10
8	C	102	OLC	O19-C1-C2-C3

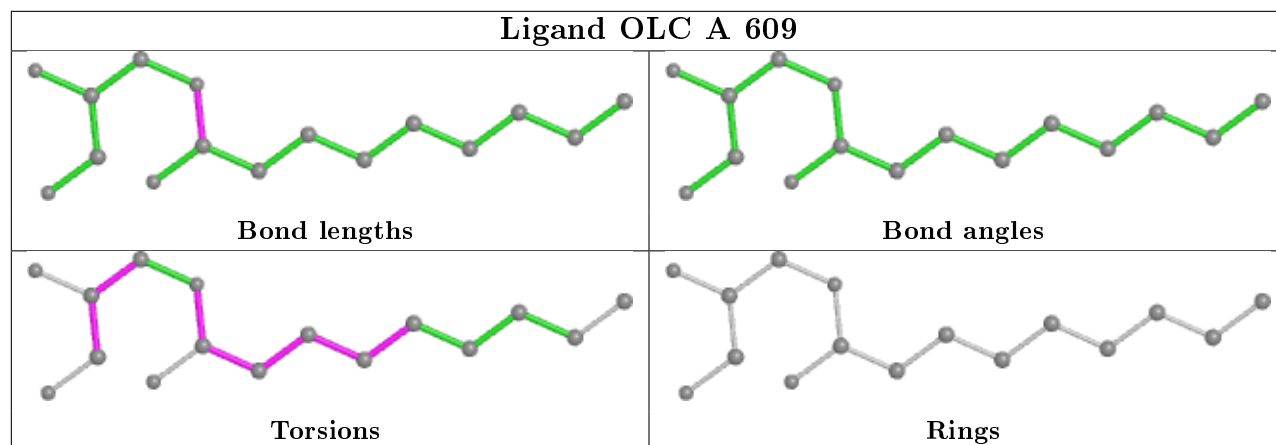
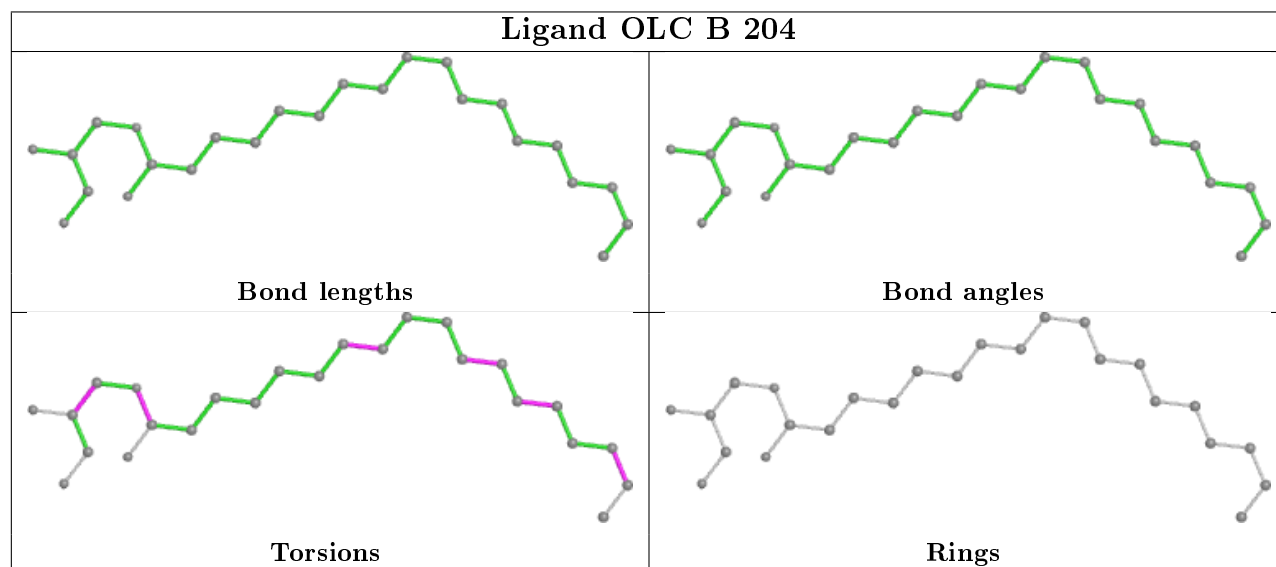
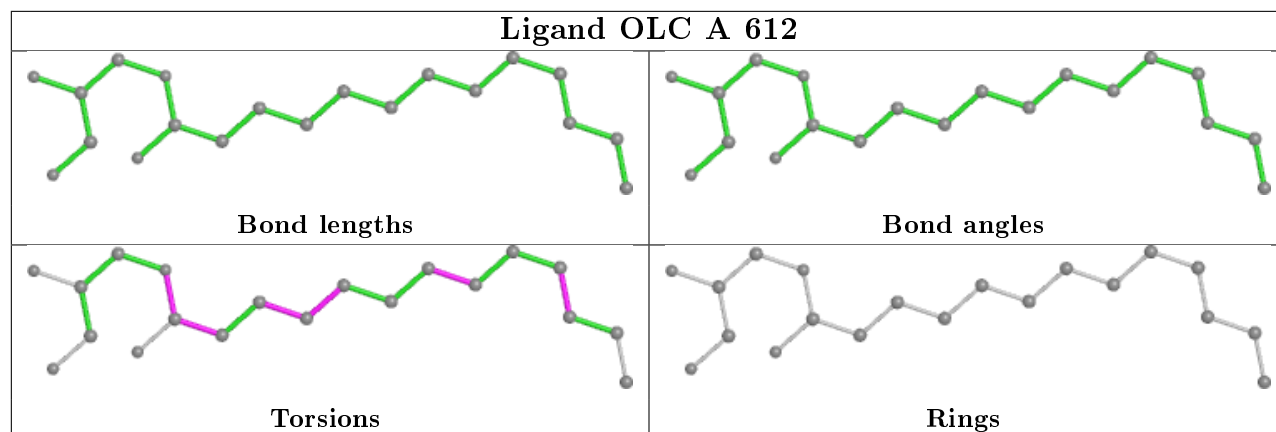
There are no ring outliers.

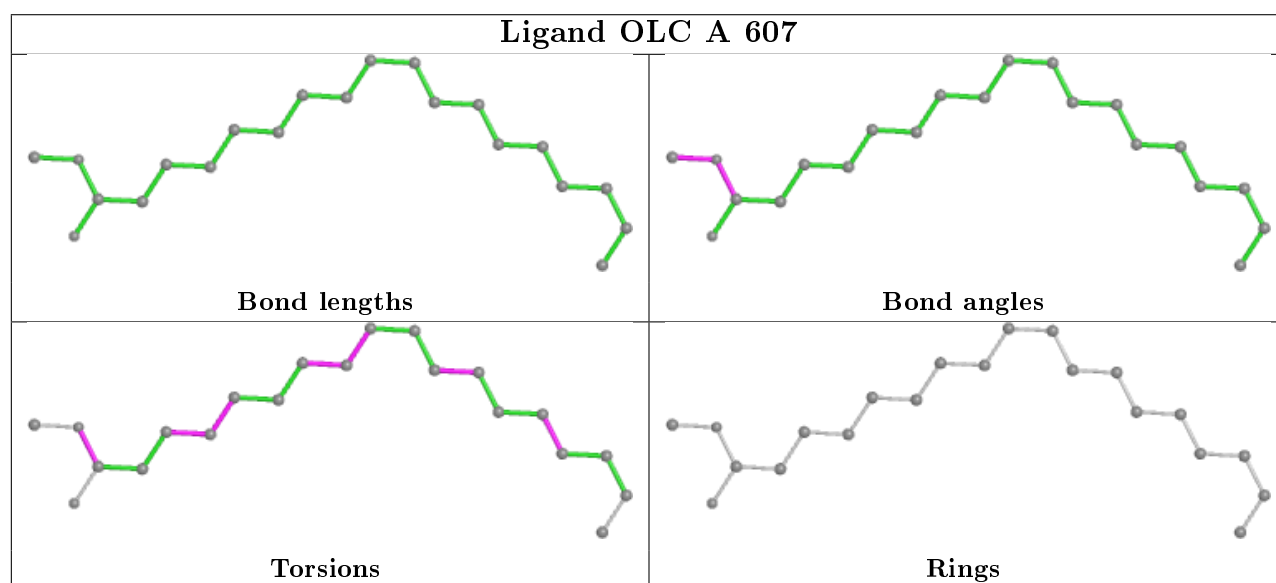
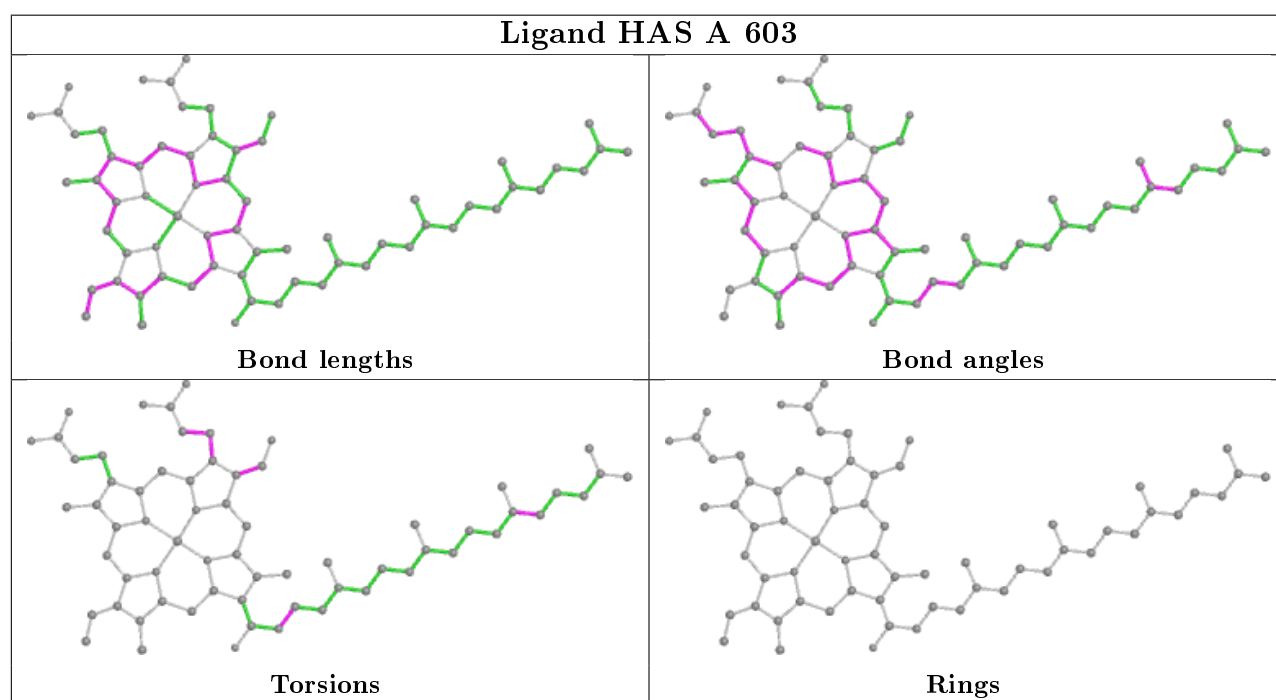
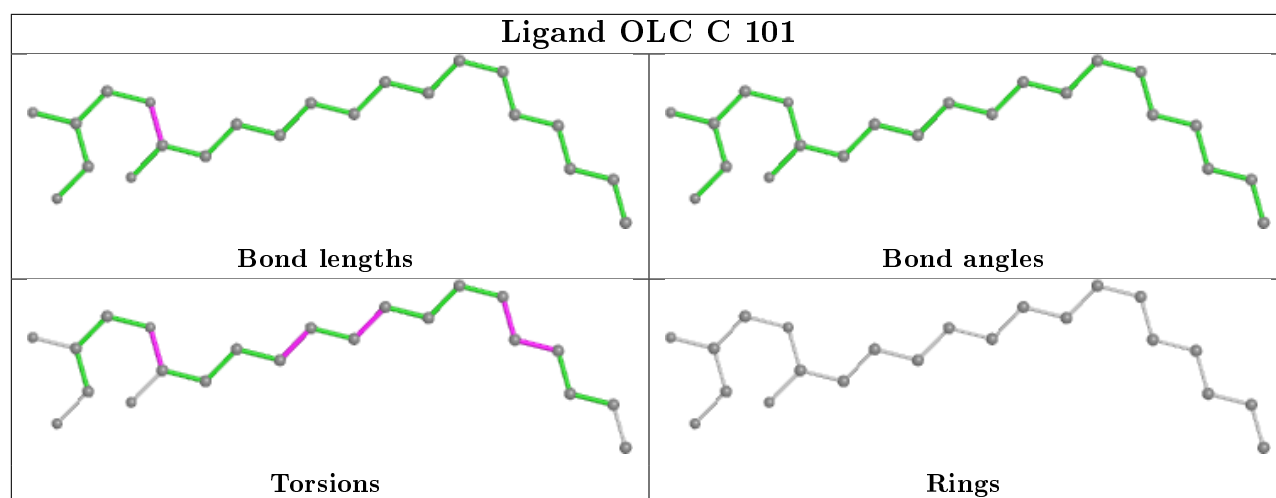
15 monomers are involved in 36 short contacts:

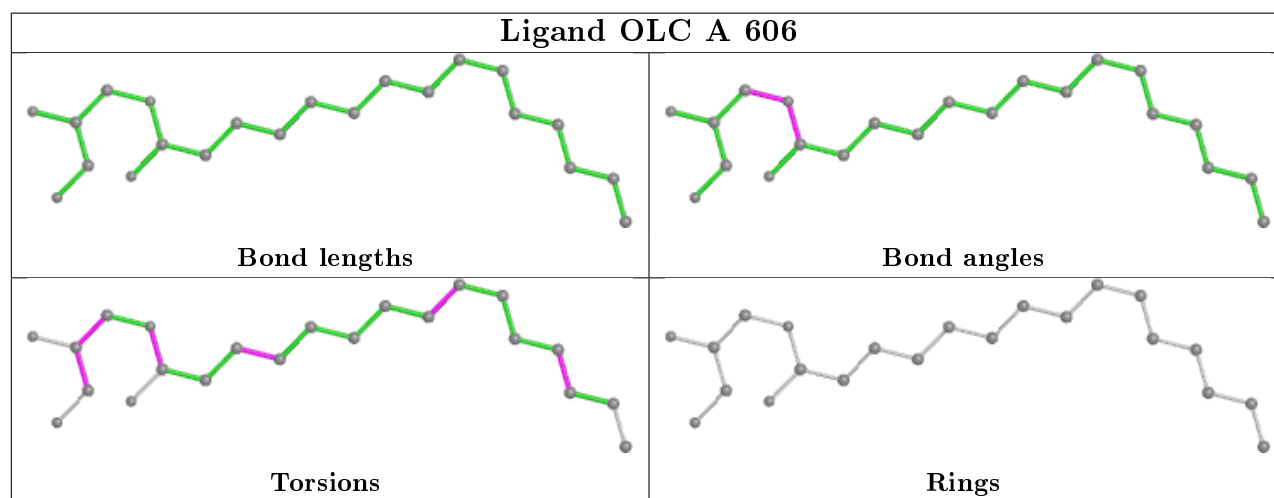
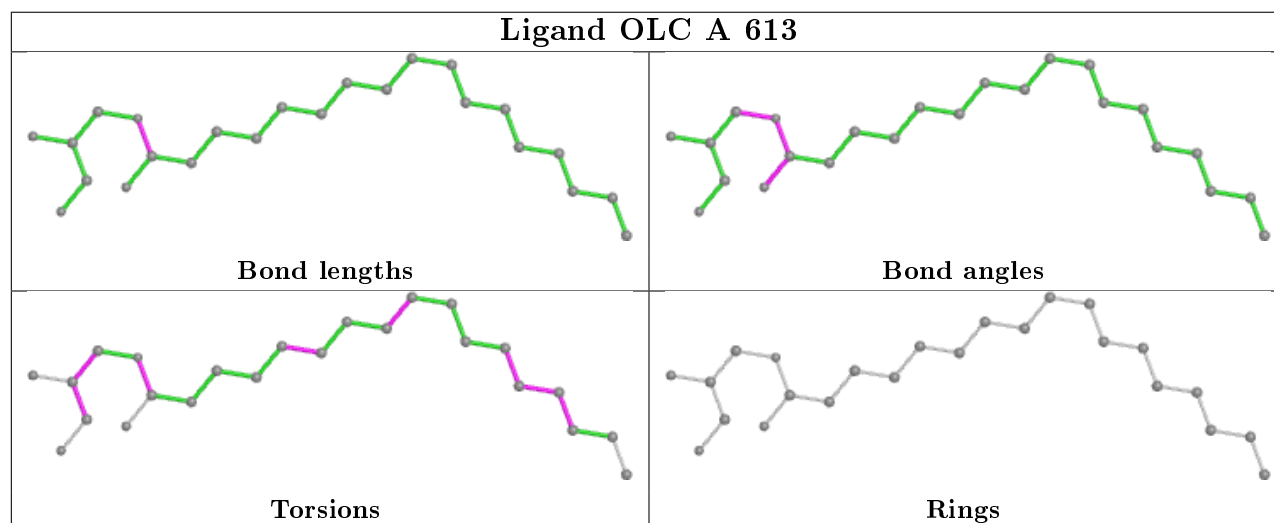
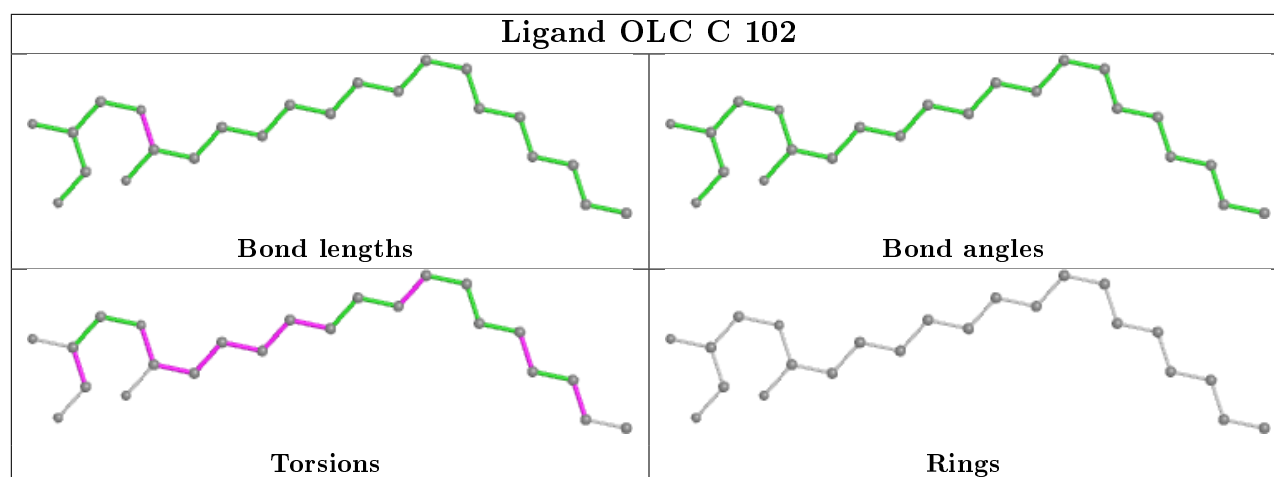
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	615	OLC	3	0
5	A	602	HEM	3	0
7	A	604	PER	3	0
8	B	204	OLC	1	0
8	C	101	OLC	3	0
6	A	603	HAS	4	0
8	C	102	OLC	3	0
8	A	613	OLC	1	0
8	A	606	OLC	1	0
8	A	610	OLC	3	0
8	B	203	OLC	7	0
8	A	614	OLC	1	0
8	B	202	OLC	2	0
8	A	605	OLC	4	0
8	A	611	OLC	4	0

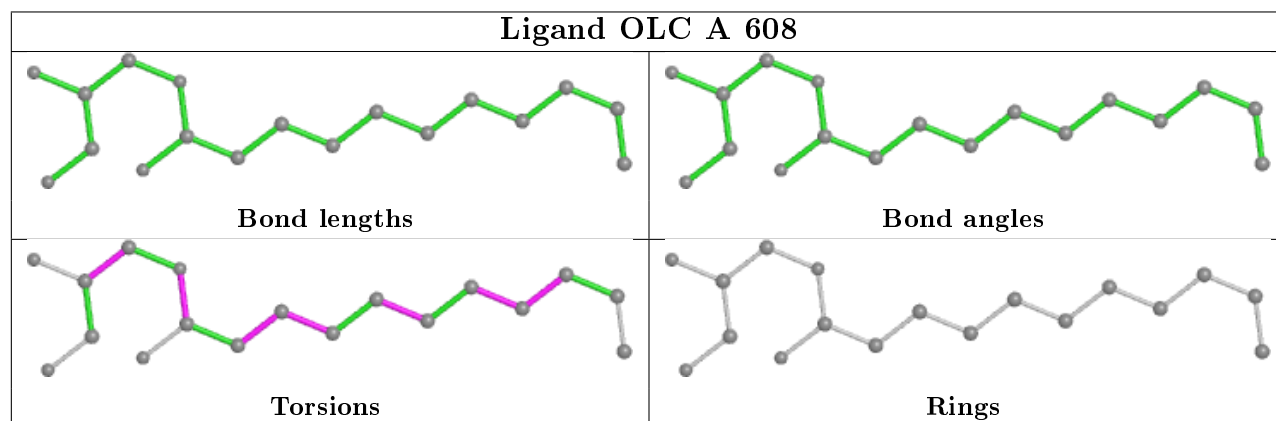
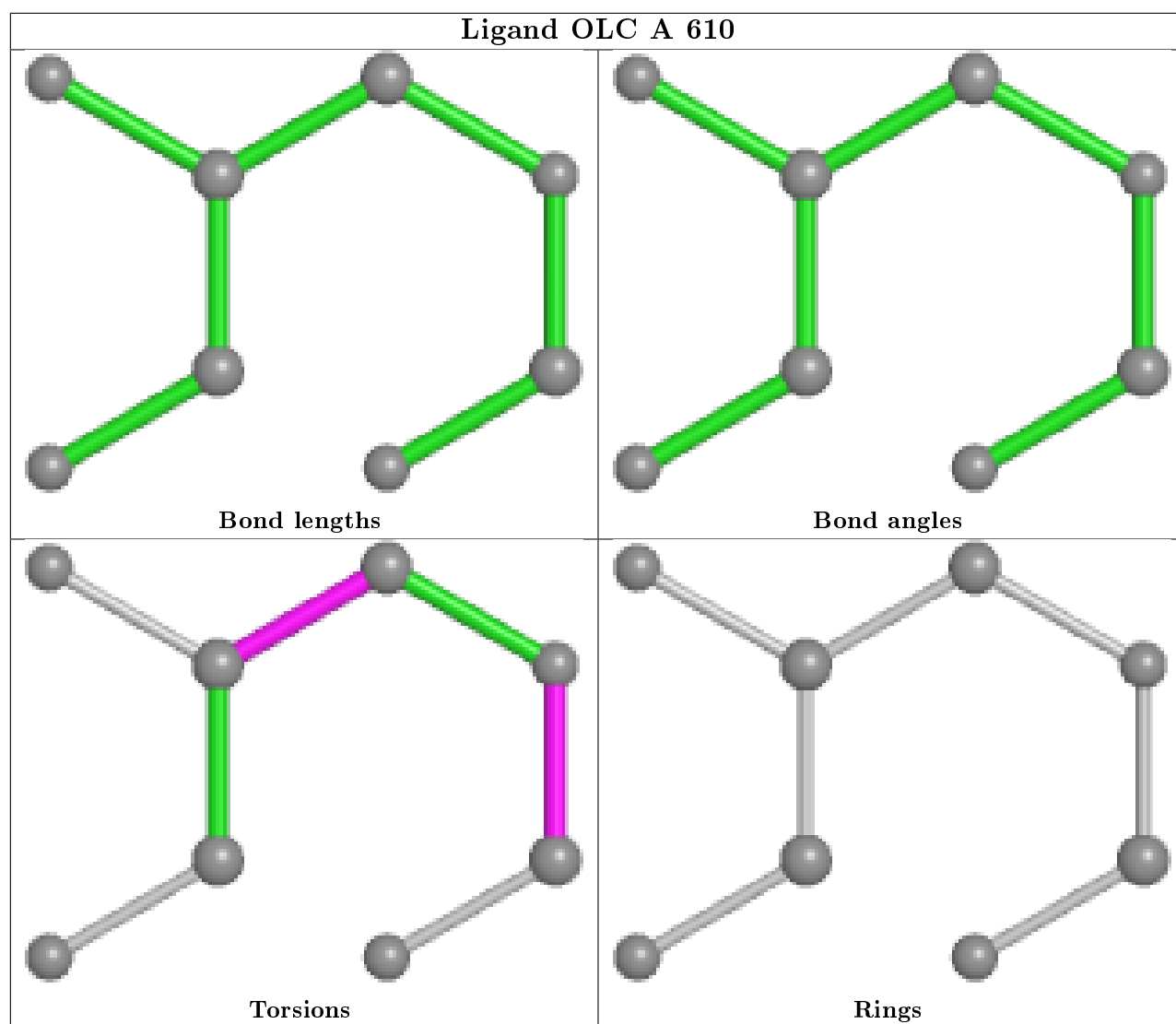
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

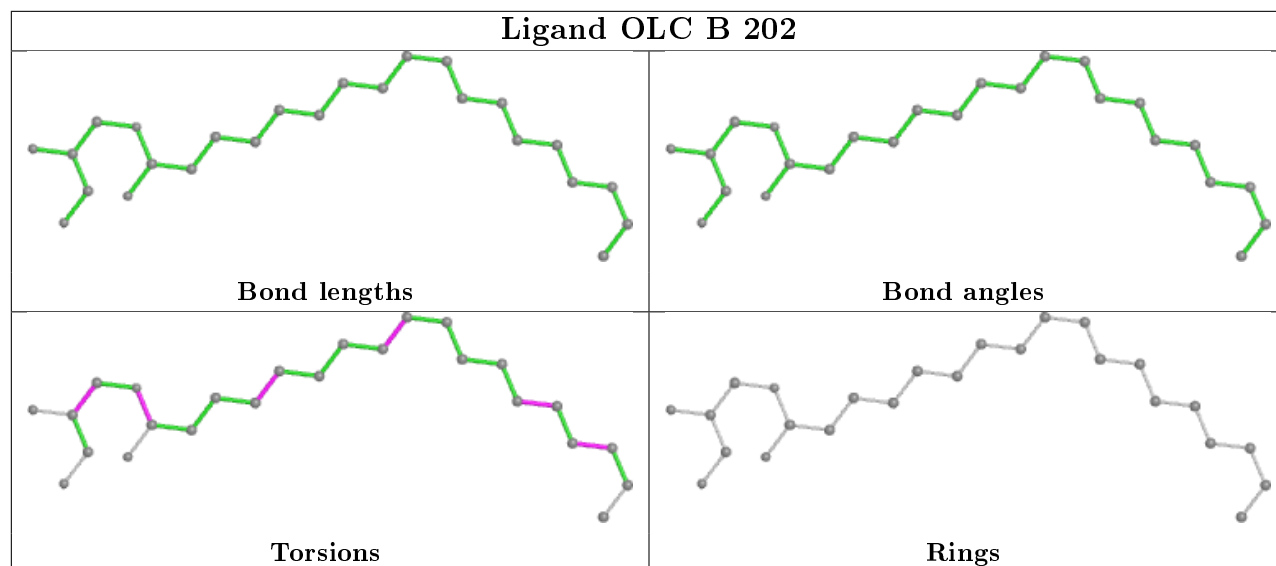
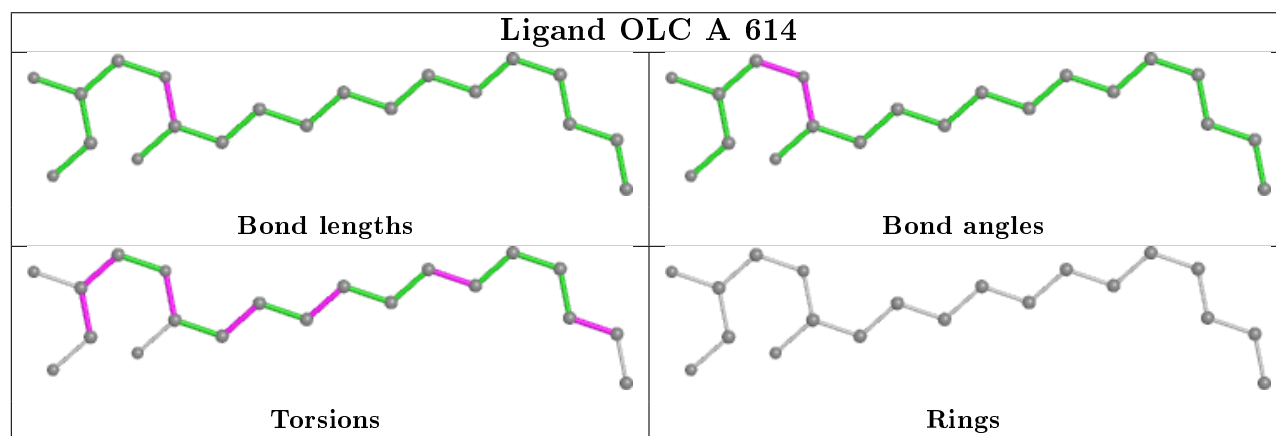
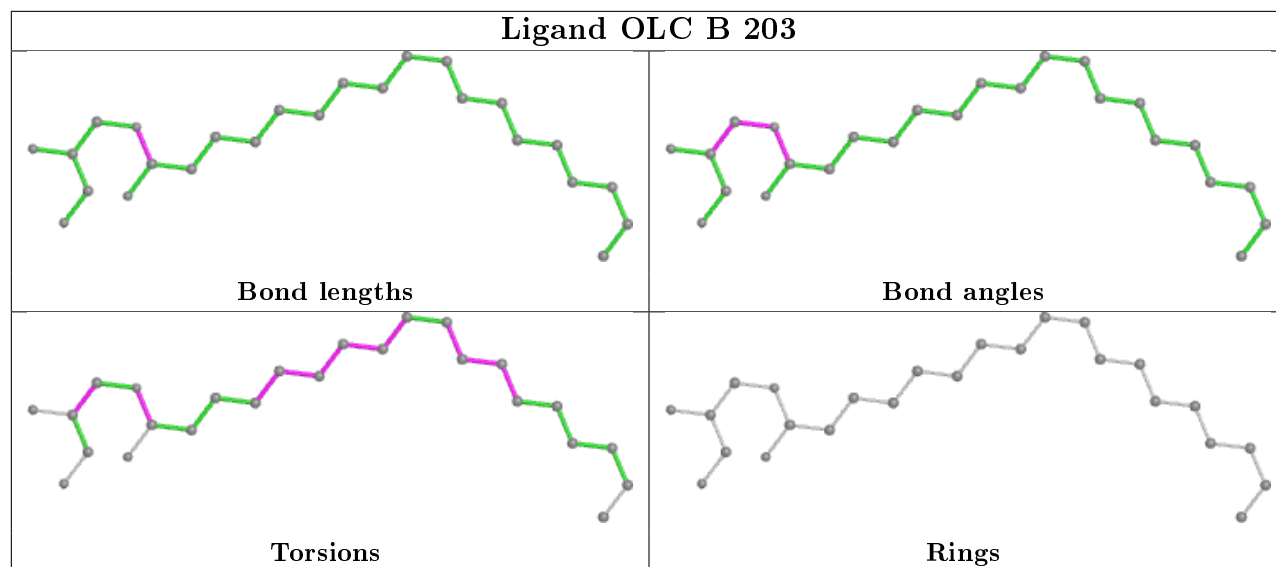


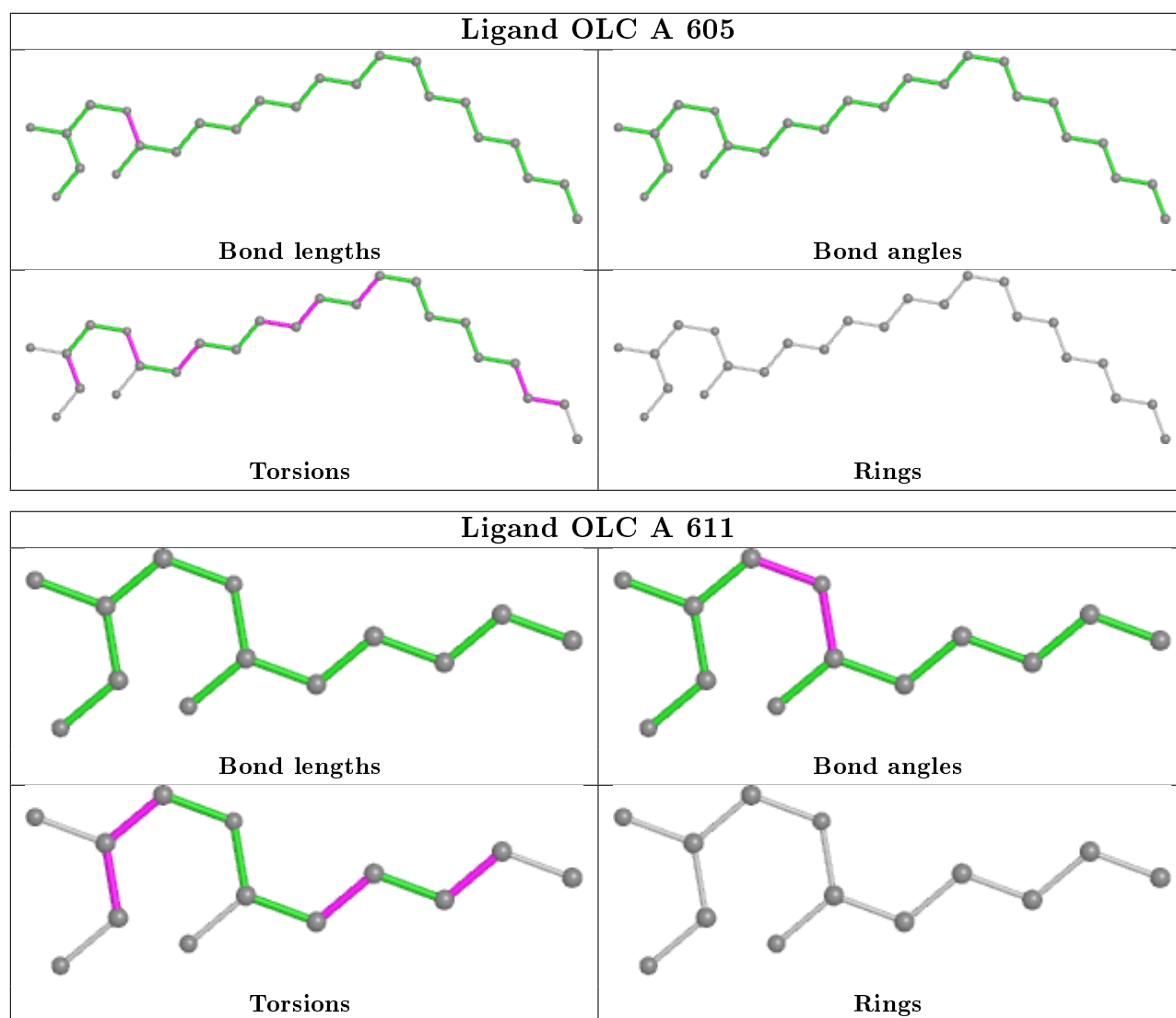












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	554/569 (97%)	-0.65	5 (0%) 84 84	18, 32, 57, 86	0
2	B	166/168 (98%)	-0.66	1 (0%) 89 89	21, 32, 49, 73	0
3	C	31/34 (91%)	-0.89	0 100 100	25, 30, 43, 50	0
All	All	751/771 (97%)	-0.66	6 (0%) 86 86	18, 32, 54, 86	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	SER	4.0
1	A	495	ARG	2.6
2	B	168	GLU	2.4
1	A	10	ARG	2.1
1	A	499	PRO	2.1
1	A	494	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

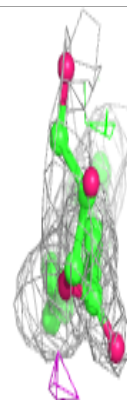
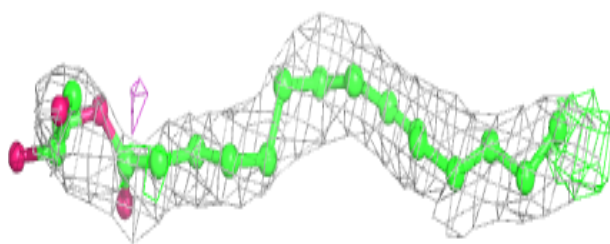
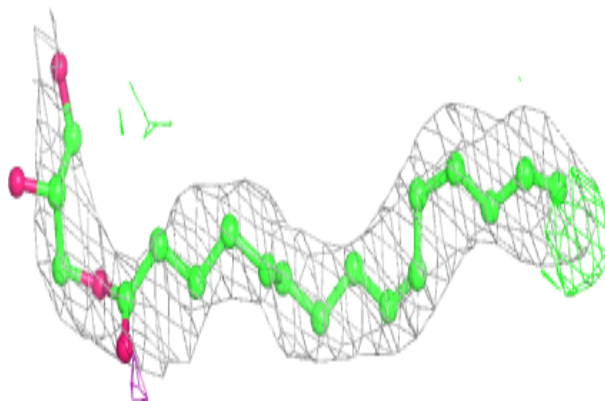
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	OLC	C	101	22/25	0.74	0.33	39,52,84,101	0
8	OLC	A	609	16/25	0.75	0.35	36,64,100,105	0
8	OLC	A	614	20/25	0.77	0.29	41,46,81,82	0
8	OLC	A	605	24/25	0.77	0.26	45,59,71,71	0
8	OLC	B	204	25/25	0.79	0.32	40,58,74,75	0
8	OLC	A	612	20/25	0.80	0.27	45,60,68,69	0
8	OLC	A	611	13/25	0.80	0.35	50,67,74,83	0
8	OLC	B	202	25/25	0.81	0.28	37,56,68,82	0
8	OLC	C	102	23/25	0.83	0.44	50,65,91,92	0
8	OLC	B	203	25/25	0.86	0.20	37,53,84,91	0
8	OLC	A	613	24/25	0.87	0.22	43,58,68,70	0
8	OLC	A	615	24/25	0.88	0.32	43,59,75,81	0
8	OLC	A	610	8/25	0.88	0.33	57,60,64,66	0
8	OLC	A	606	22/25	0.89	0.21	38,51,60,66	0
8	OLC	A	607	21/25	0.91	0.33	41,51,53,54	0
8	OLC	A	608	18/25	0.92	0.16	31,55,68,76	0
7	PER	A	604	2/2	0.95	0.17	36,36,36,38	0
6	HAS	A	603	65/65	0.97	0.12	25,28,35,40	0
5	HEM	A	602	43/43	0.98	0.10	19,22,27,31	0
9	CUA	B	201	2/2	0.99	0.06	22,22,22,25	0
4	CUB	A	601	1/11	0.99	0.08	29,29,29,29	0

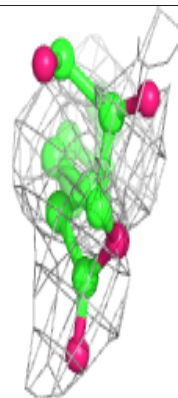
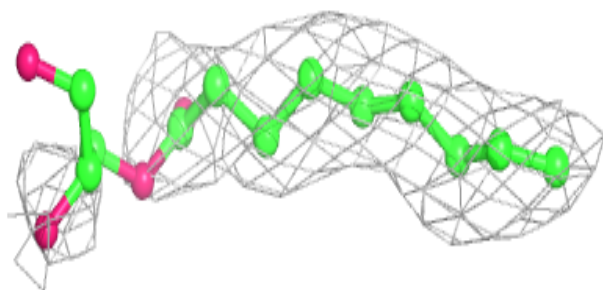
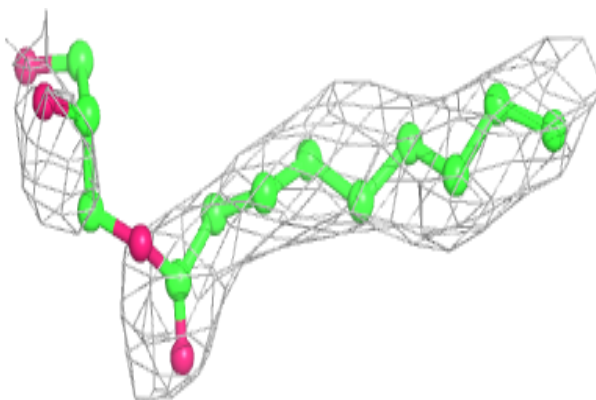
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC C 101:

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

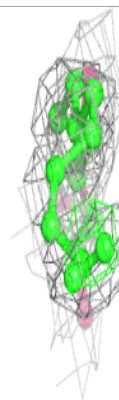
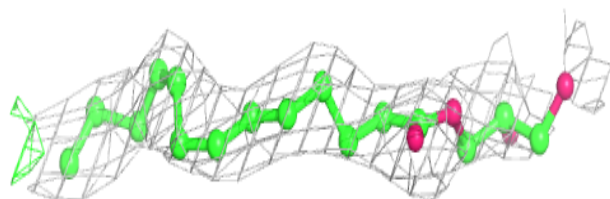
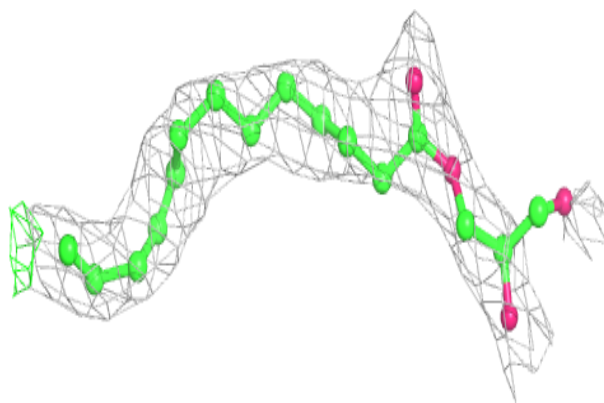
**Electron density around OLC A 609:**

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

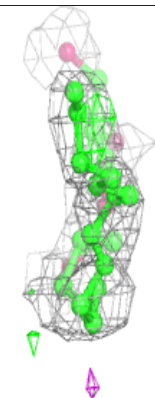
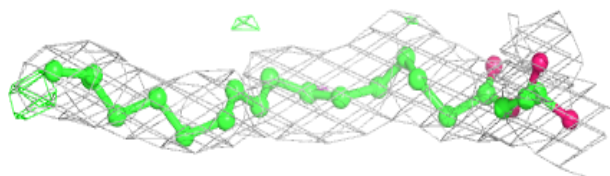
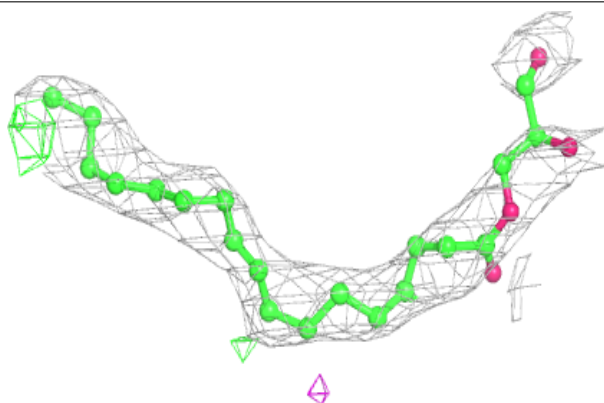


Electron density around OLC A 614:

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

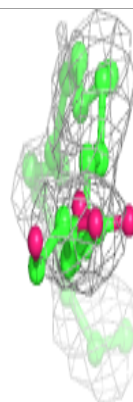
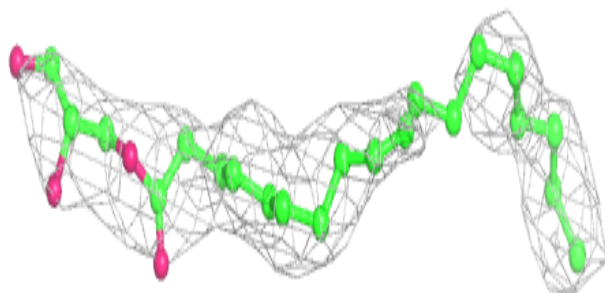
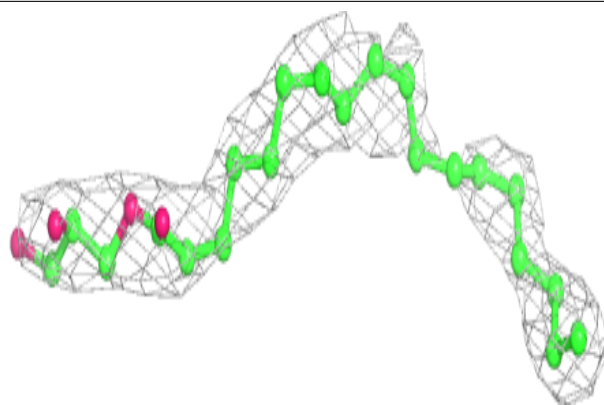
**Electron density around OLC A 605:**

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

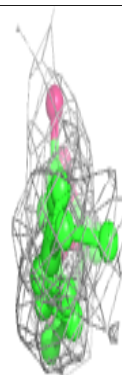
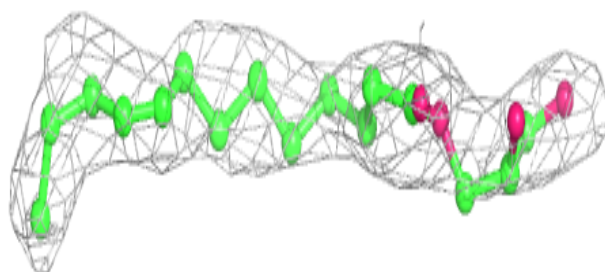
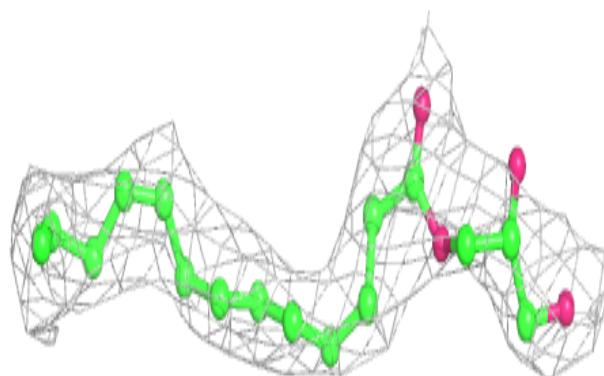


Electron density around OLC B 204:

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

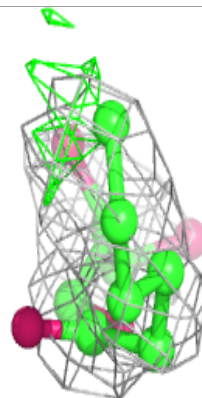
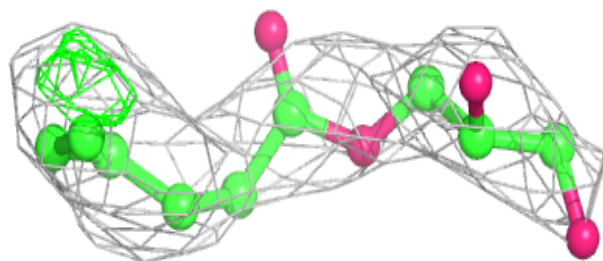
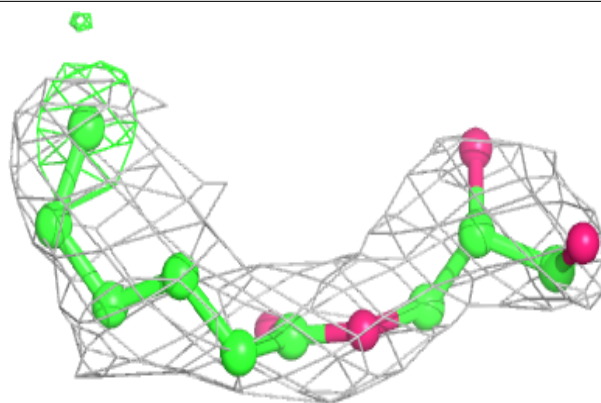
**Electron density around OLC A 612:**

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

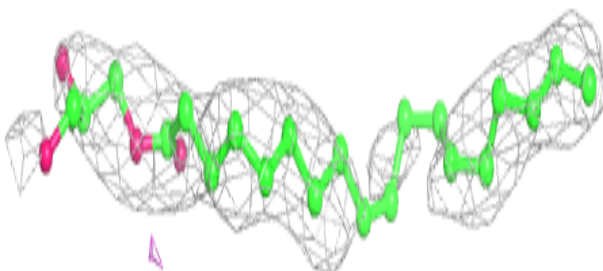
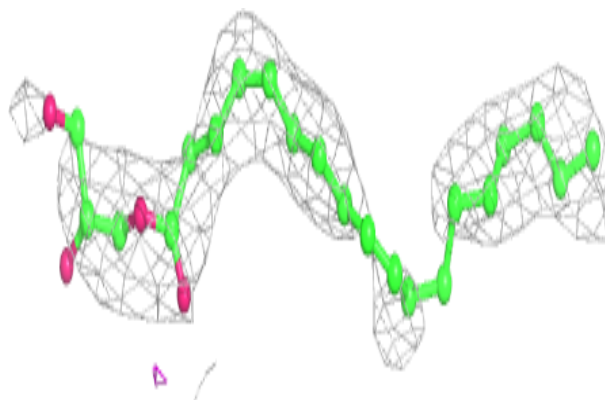


Electron density around OLC A 611:

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

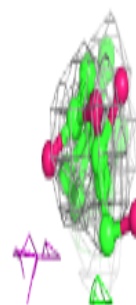
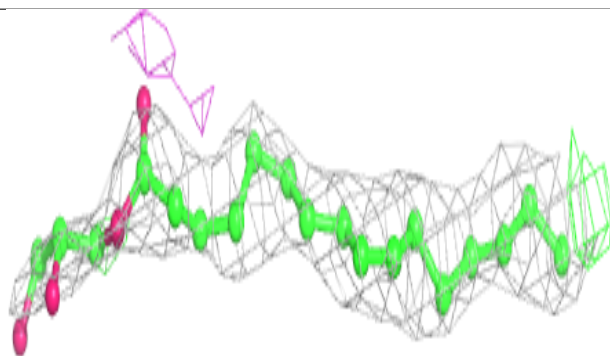
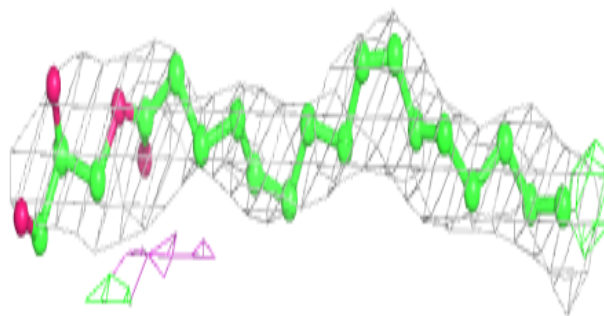
**Electron density around OLC B 202:**

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

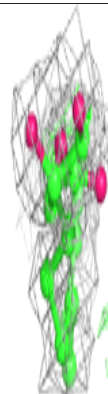
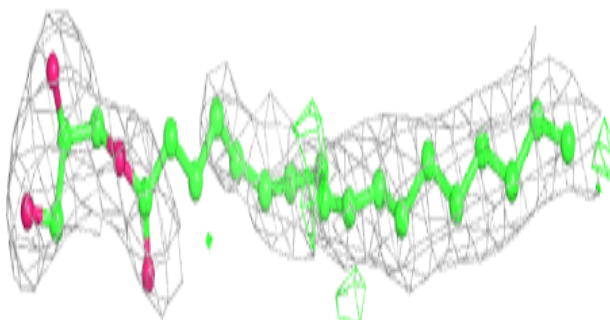
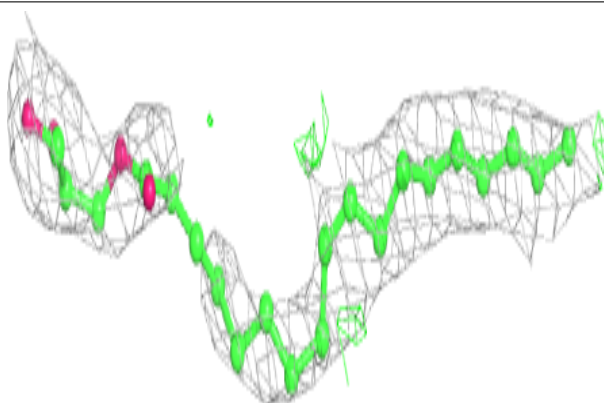


Electron density around OLC C 102:

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

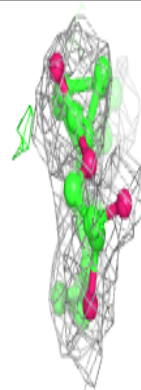
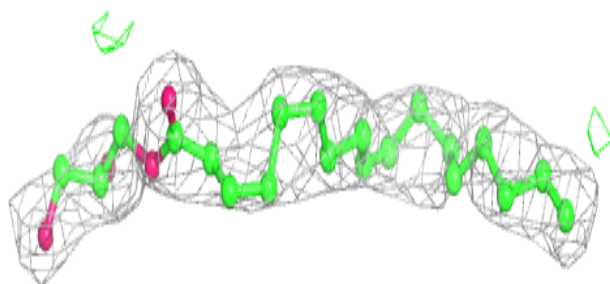
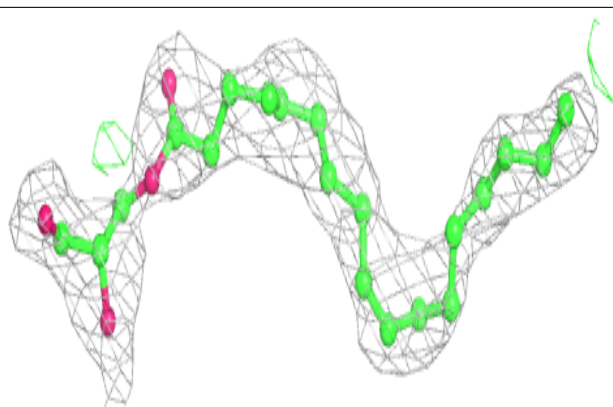
**Electron density around OLC B 203:**

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

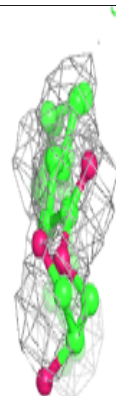
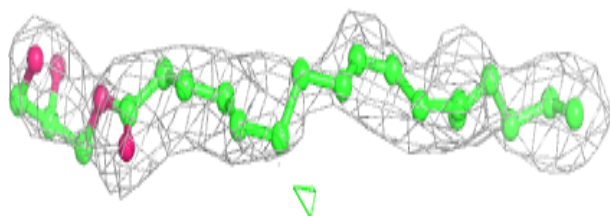
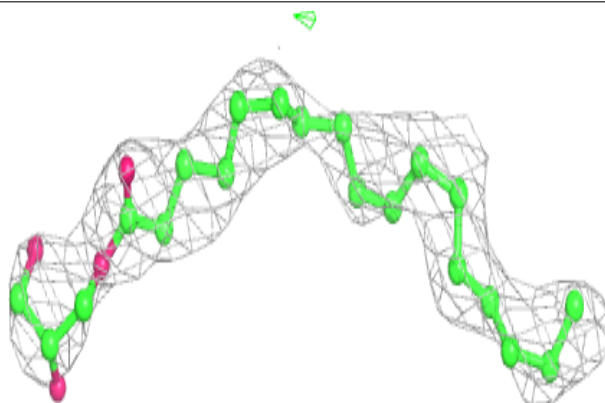


Electron density around OLC A 613:

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

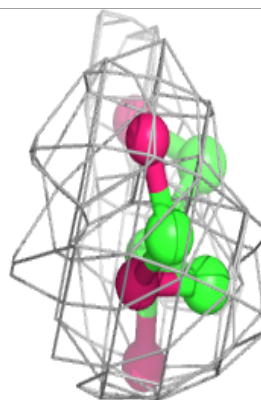
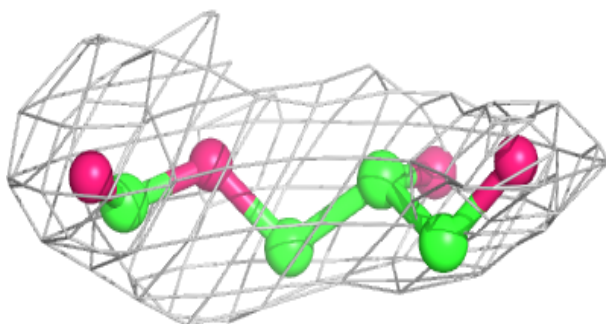
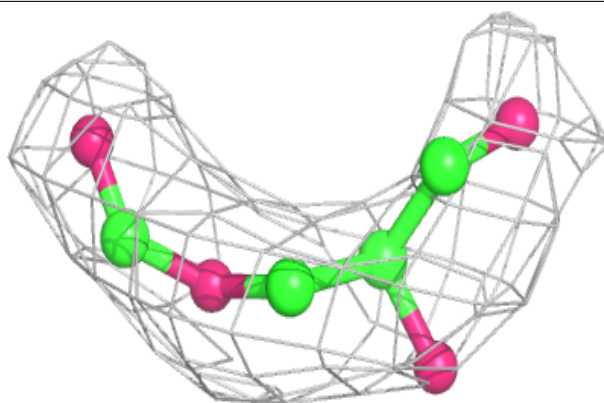
**Electron density around OLC A 615:**

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

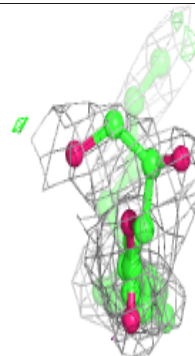
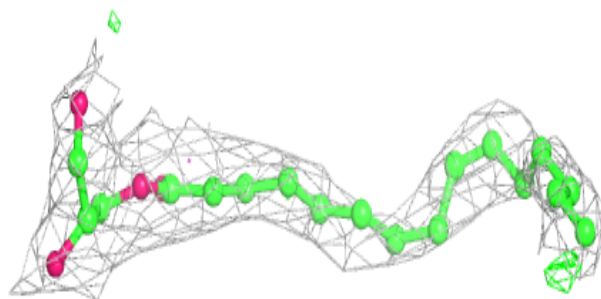
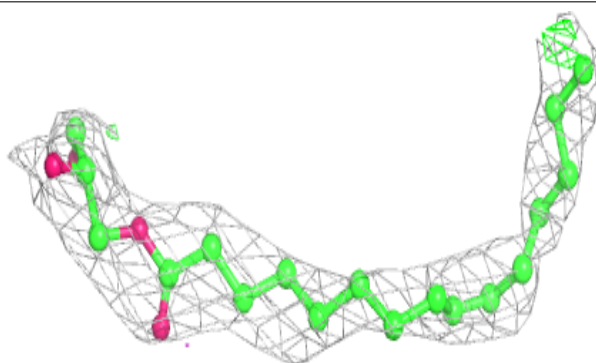


Electron density around OLC A 610:

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

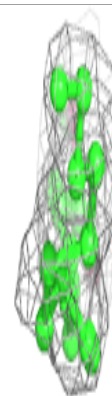
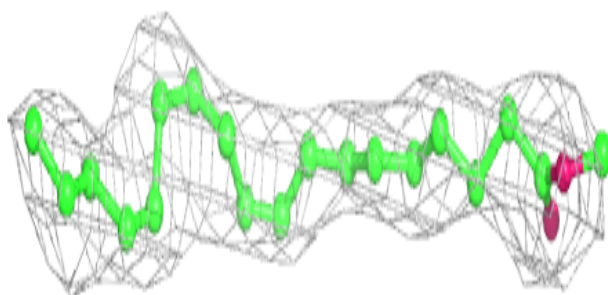
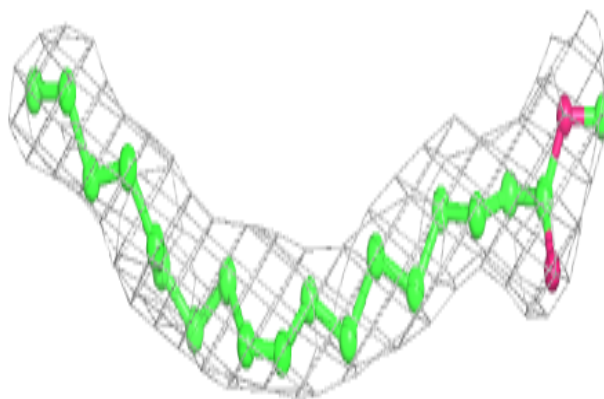
**Electron density around OLC A 606:**

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

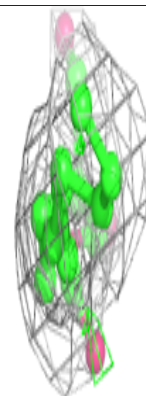
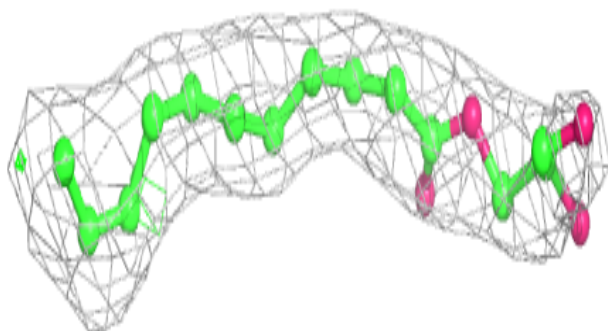
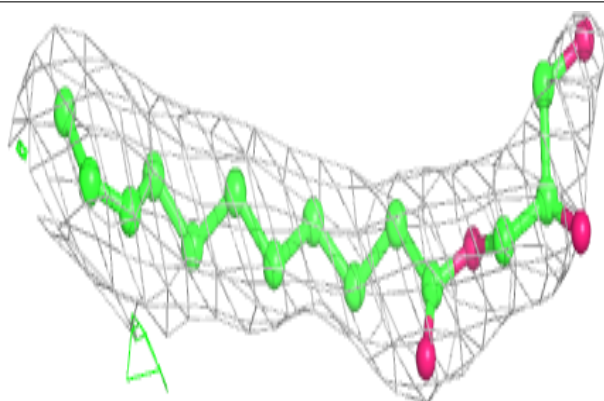


Electron density around OLC A 607:

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

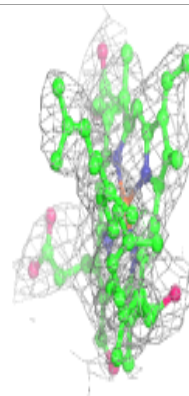
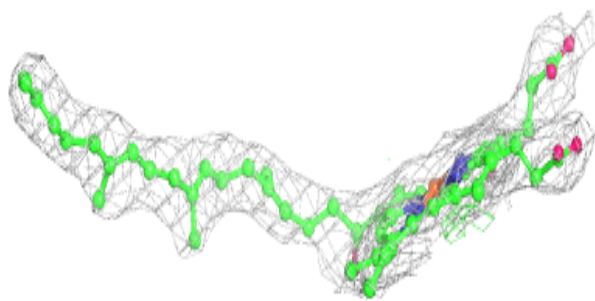
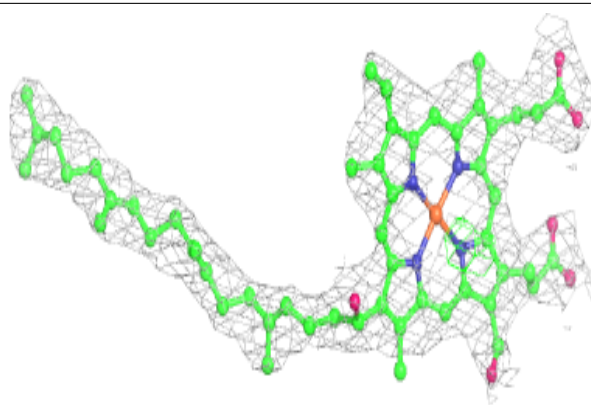
**Electron density around OLC A 608:**

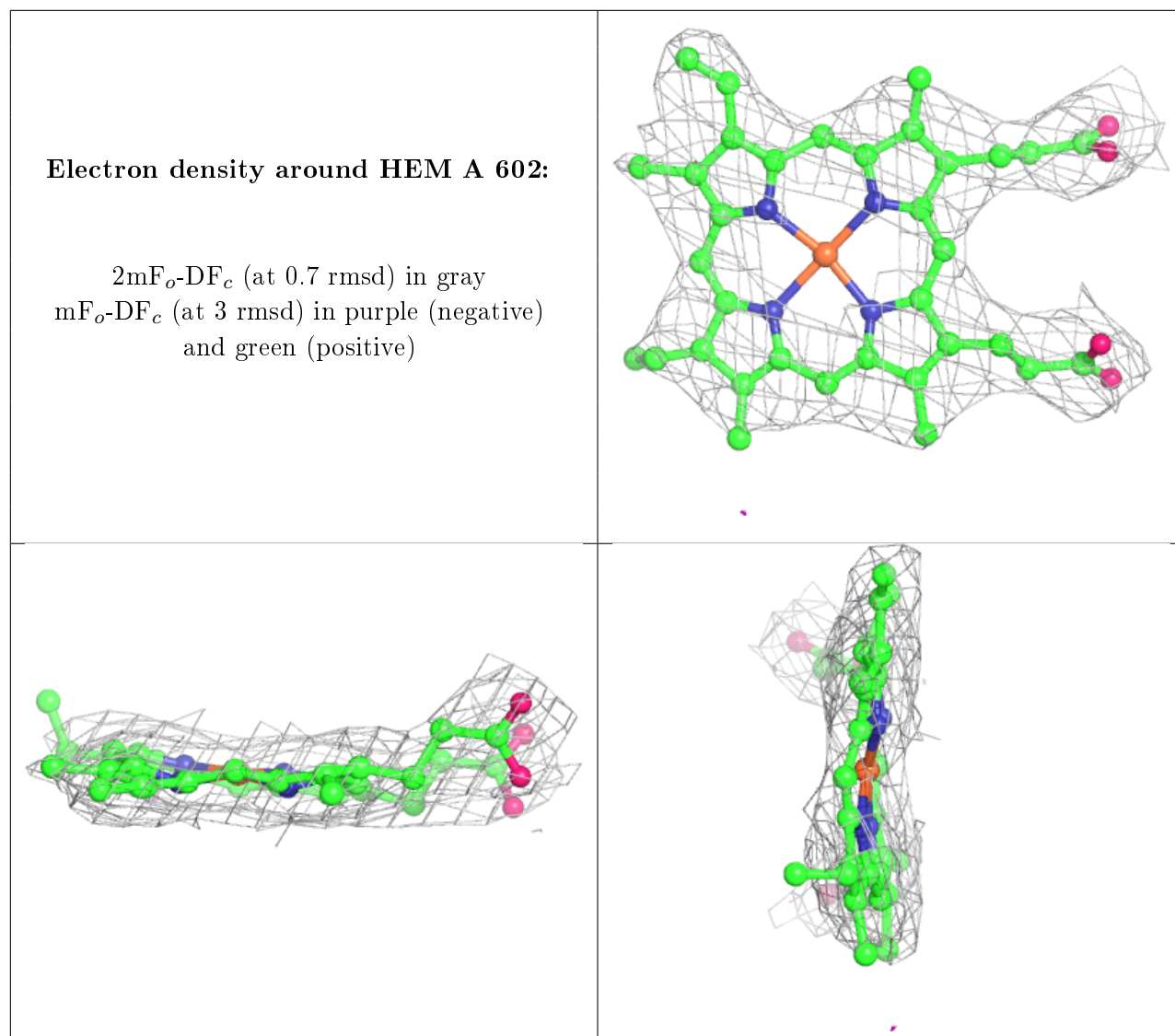
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HAS A 603:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.