



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:14 AM EDT

PDB ID : 4FAA / pdb_00004faa
Title : Structure of Recombinant Cytochrome ba3 Oxidase mutant A120F+A204F from *Thermus thermophilus*
Authors : Li, Y.; Chen, Y.; Stout, C.D.
Deposited on : 2012-05-21
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

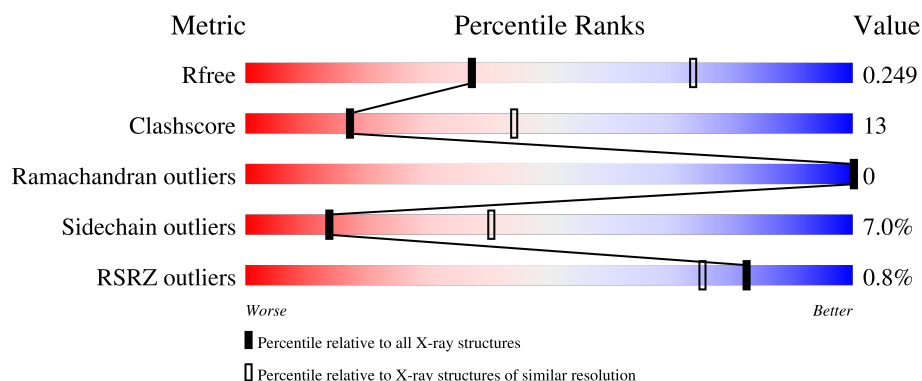
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	568	
2	B	168	
3	C	34	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	HAS	A	603	X	-	-	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 6278 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	535	Total	C	N	O	S	0	0	0
			4203	2863	663	661	16			

There are 9 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	120	PHE	ALA	engineered mutation	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
2	B	166	Total	C	N	O	S	0	0	0
			1281	833	212	232	4			

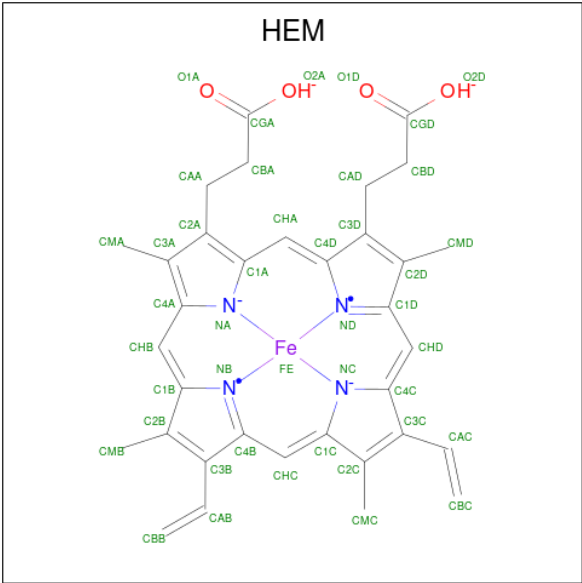
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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

- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

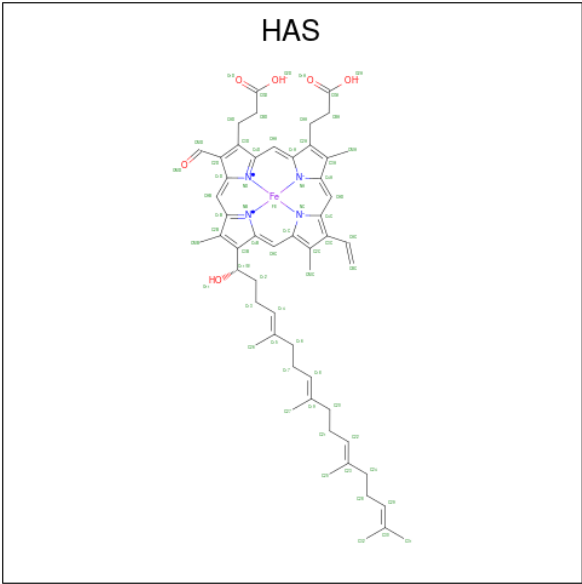
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Cu			0	0
			1	1				

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



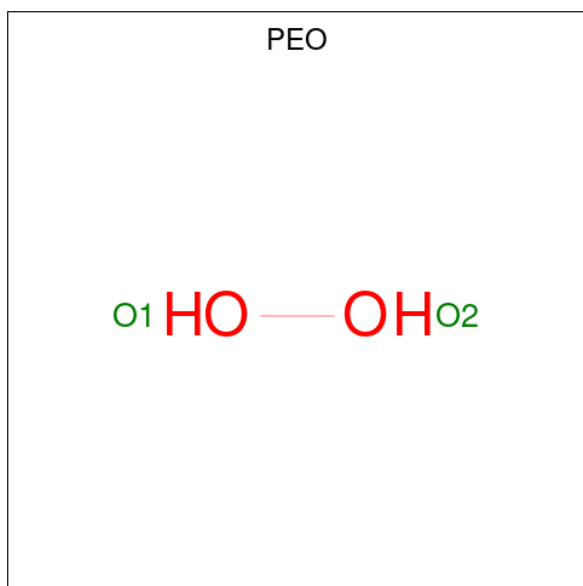
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

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



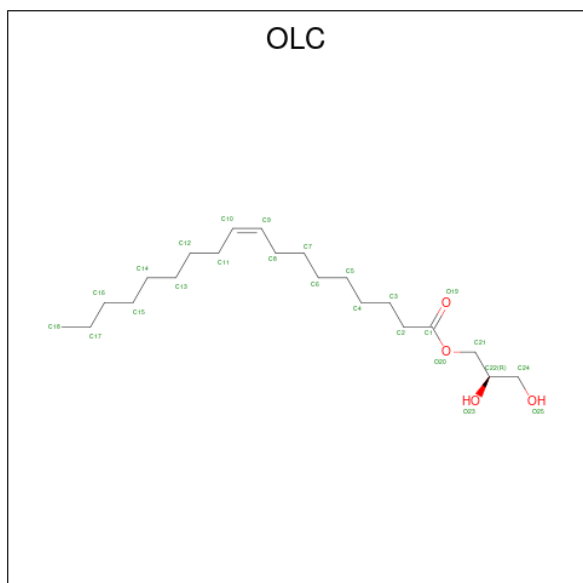
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	
			65	54	1	4	6	
							0	0

- Molecule 7 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H_2O_2).



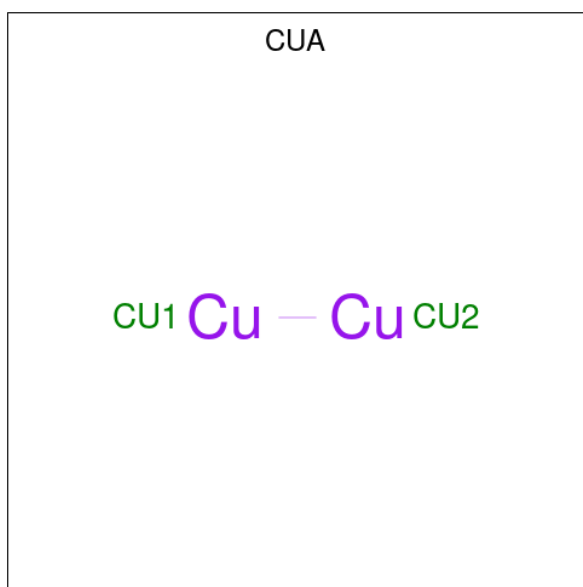
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O		
			2	2	0	0

- Molecule 8 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $\text{C}_{21}\text{H}_{40}\text{O}_4$).



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

- Molecule 9 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

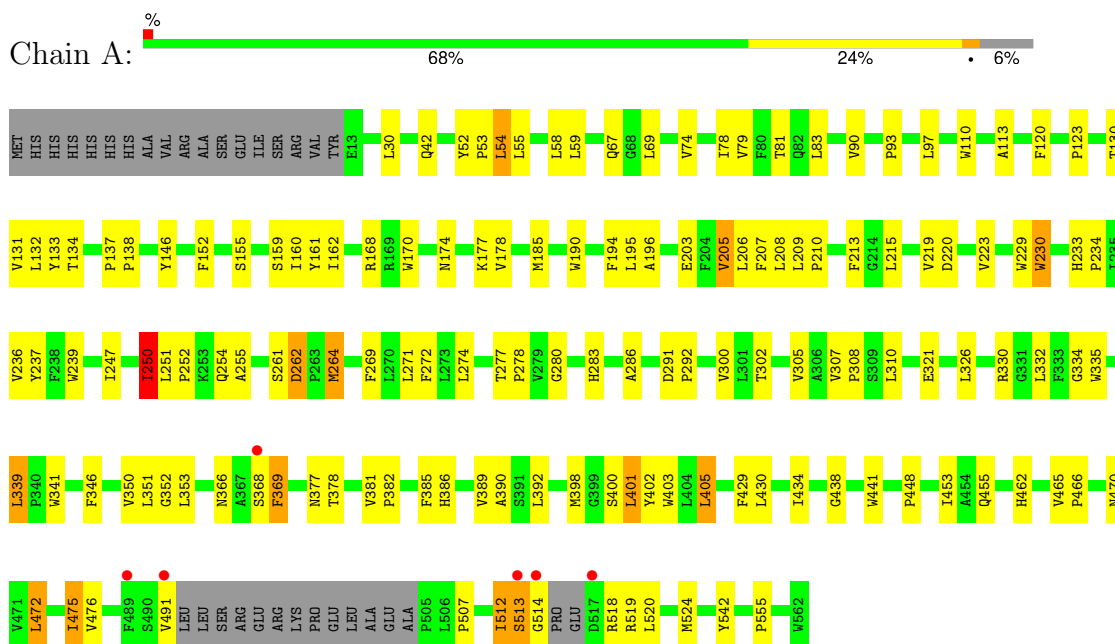
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	51	Total O 51 51	0	0
10	B	44	Total O 44 44	0	0
10	C	2	Total O 2 2	0	0

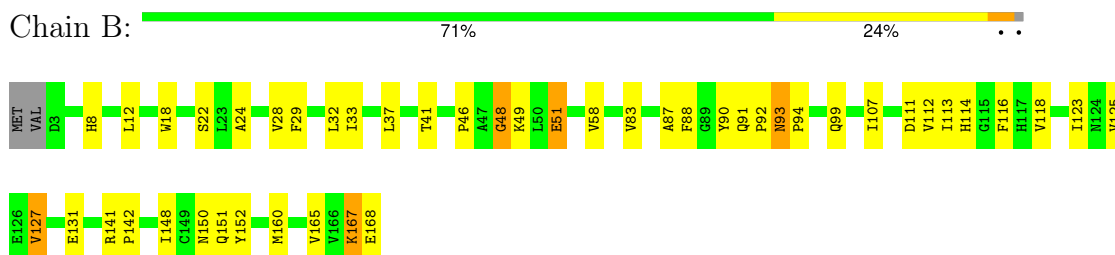
3 Residue-property plots [i](#)

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

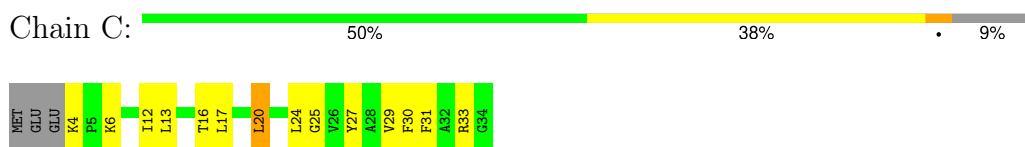
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 3: Cytochrome c oxidase polypeptide 2A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.28Å 98.29Å 95.05Å 90.00° 127.50° 90.00°	Depositor
Resolution (Å)	56.84 – 2.80 56.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.2 (56.84-2.80) 97.3 (56.84-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 2011_01_25_1225)	Depositor
R, R_{free}	0.194 , 0.254 0.192 , 0.249	Depositor DCC
R_{free} test set	1290 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.7	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	6278	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HAS, PEO, HEM, OLC, CUA, CU

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	0.63	2/4356 (0.0%)	0.90	8/5982 (0.1%)
2	B	0.64	0/1317	0.86	0/1801
3	C	0.60	0/247	0.77	0/335
All	All	0.63	2/5920 (0.0%)	0.88	8/8118 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	PRO	CA-C	7.58	1.56	1.51
1	A	368	SER	C-O	-5.71	1.17	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	518	ARG	N-CA-C	-11.13	100.42	114.56
1	A	513	SER	N-CA-C	7.61	121.38	107.99
1	A	131	VAL	N-CA-C	-6.77	95.26	109.34
1	A	369	PHE	N-CA-CB	-6.23	100.98	110.01
1	A	519	ARG	N-CA-C	5.52	117.11	111.14
1	A	369	PHE	CA-C-N	5.13	129.40	120.68
1	A	369	PHE	C-N-CA	5.13	129.40	120.68
1	A	250	ILE	N-CA-C	-5.11	107.59	111.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	48	GLY	Peptide

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	4203	0	4278	114	0
2	B	1281	0	1249	29	0
3	C	241	0	267	9	0
4	A	1	0	0	0	0
5	A	43	0	30	0	0
6	A	65	0	62	2	0
7	A	2	0	0	0	0
8	A	243	0	353	28	0
8	B	75	0	120	10	0
8	C	25	0	40	3	0
9	B	2	0	0	0	0
10	A	51	0	0	4	0
10	B	44	0	0	2	2
10	C	2	0	0	0	0
All	All	6278	0	6399	158	2

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 13.

All (158) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:HIS:NE2	1:A:237:TYR:HE2	1.26	1.30
1:A:233:HIS:NE2	1:A:237:TYR:CE2	2.10	1.19
1:A:233:HIS:CD2	1:A:237:TYR:HE2	1.76	1.04
1:A:174:ASN:HB3	1:A:177:LYS:HD2	1.49	0.94
2:B:51:GLU:OE2	10:B:309:HOH:O	1.89	0.90
8:A:605:OLC:H11	8:B:203:OLC:H17	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ARG:HH22	8:A:612:OLC:H6A	1.40	0.86
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.60	0.85
8:A:605:OLC:H12	8:B:203:OLC:H18	1.62	0.82
1:A:261:SER:HB3	1:A:264:MET:HB2	1.69	0.74
1:A:161:TYR:CZ	8:A:611:OLC:H24A	2.27	0.69
1:A:310:LEU:HD13	2:B:22:SER:HB2	1.75	0.69
8:B:203:OLC:H18A	8:C:101:OLC:H7A	1.74	0.69
1:A:229:TRP:CE3	1:A:283:HIS:CD2	2.81	0.68
8:A:605:OLC:H2A	8:C:101:OLC:H21A	1.76	0.68
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.76	0.66
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.31	0.65
1:A:381:VAL:HB	1:A:382:PRO:HD3	1.78	0.63
1:A:434:ILE:HG12	8:A:616:OLC:H18A	1.80	0.62
1:A:514:GLY:HA3	2:B:8:HIS:CD2	2.35	0.61
2:B:46:PRO:O	10:B:340:HOH:O	2.16	0.61
8:B:203:OLC:H7A	3:C:29:VAL:HG13	1.81	0.61
1:A:280:GLY:HA3	1:A:542:TYR:OH	2.00	0.61
1:A:74:VAL:O	1:A:79:VAL:HG23	2.02	0.59
1:A:160:ILE:HG12	1:A:190:TRP:HB3	1.86	0.58
8:A:605:OLC:H12	8:B:203:OLC:C18	2.34	0.57
1:A:230:TRP:C	1:A:230:TRP:CD1	2.82	0.57
1:A:67:GLN:HA	1:A:130:THR:HG23	1.87	0.56
2:B:29:PHE:O	2:B:33:ILE:HG13	2.05	0.56
1:A:209:LEU:HB2	1:A:210:PRO:HD3	1.88	0.56
2:B:32:LEU:HD21	8:B:202:OLC:H7A	1.85	0.56
1:A:462:HIS:HB2	10:A:725:HOH:O	2.06	0.56
1:A:250:ILE:HG23	1:A:507:PRO:HG2	1.88	0.56
8:B:203:OLC:H5A	3:C:33:ARG:HE	1.71	0.55
8:A:605:OLC:H6	3:C:25:GLY:HA3	1.88	0.55
3:C:16:THR:HG22	3:C:20:LEU:HD22	1.87	0.55
1:A:366:ASN:HB3	6:A:603:HAS:HBD2	1.89	0.55
1:A:278:PRO:HD3	10:A:718:HOH:O	2.05	0.55
8:A:605:OLC:C11	8:B:203:OLC:H17	2.34	0.55
1:A:152:PHE:O	1:A:155:SER:HB3	2.06	0.54
1:A:251:LEU:HB3	1:A:252:PRO:HD3	1.89	0.54
1:A:398:MET:O	1:A:401:LEU:HB2	2.07	0.54
8:A:606:OLC:H13A	8:A:614:OLC:H14A	1.90	0.54
1:A:261:SER:CB	1:A:264:MET:HB2	2.38	0.53
1:A:352:GLY:HA3	1:A:392:LEU:HA	1.90	0.53
1:A:291:ASP:HB2	10:A:730:HOH:O	2.08	0.53
1:A:378:THR:HA	1:A:448:PRO:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:TRP:CE2	8:A:616:OLC:H3A	2.44	0.53
1:A:205:VAL:HG12	1:A:206:LEU:HD23	1.91	0.52
2:B:18:TRP:CE3	3:C:12:ILE:HD13	2.45	0.52
1:A:233:HIS:O	1:A:236:VAL:HG22	2.10	0.52
1:A:161:TYR:CE2	8:A:611:OLC:H21	2.45	0.52
1:A:352:GLY:C	1:A:392:LEU:HD23	2.35	0.51
1:A:475:ILE:HD11	8:A:606:OLC:H12A	1.92	0.51
1:A:52:TYR:N	1:A:53:PRO:HD2	2.26	0.51
1:A:280:GLY:HA3	1:A:542:TYR:HH	1.74	0.51
2:B:107:ILE:HG22	2:B:127:VAL:HG11	1.92	0.51
1:A:55:LEU:HD11	1:A:59:LEU:HD12	1.93	0.50
1:A:400:SER:HA	1:A:403:TRP:NE1	2.26	0.50
1:A:233:HIS:HB3	1:A:234:PRO:CD	2.42	0.50
1:A:351:LEU:HB3	1:A:429:PHE:CD2	2.47	0.49
2:B:165:VAL:HG12	2:B:167:LYS:HD3	1.95	0.49
1:A:97:LEU:HD22	1:A:170:TRP:CD1	2.48	0.49
1:A:291:ASP:CB	10:A:730:HOH:O	2.60	0.49
1:A:330:ARG:O	1:A:334:GLY:HA3	2.13	0.49
1:A:353:LEU:N	1:A:392:LEU:HD23	2.27	0.49
1:A:369:PHE:C	1:A:369:PHE:CD2	2.90	0.49
1:A:196:ALA:HB1	1:A:234:PRO:CG	2.43	0.49
1:A:401:LEU:O	1:A:405:LEU:HB2	2.12	0.49
1:A:213:PHE:CD2	8:A:609:OLC:H4	2.48	0.49
2:B:32:LEU:CD2	8:B:202:OLC:H7A	2.43	0.49
1:A:254:GLN:NE2	1:A:507:PRO:HG3	2.28	0.48
1:A:386:HIS:HA	1:A:390:ALA:HB3	1.96	0.48
1:A:302:THR:HA	1:A:305:VAL:HG12	1.95	0.48
1:A:74:VAL:HA	1:A:78:ILE:HD12	1.95	0.48
1:A:476:VAL:HG22	8:A:606:OLC:H16A	1.96	0.47
1:A:262:ASP:C	1:A:262:ASP:OD2	2.57	0.47
1:A:254:GLN:HE22	1:A:507:PRO:HG3	1.79	0.47
1:A:159:SER:HA	1:A:162:ILE:HD12	1.96	0.47
8:A:605:OLC:O25	8:B:203:OLC:H7	2.15	0.46
2:B:113:ILE:HA	2:B:127:VAL:O	2.15	0.46
1:A:453:ILE:C	1:A:455:GLN:N	2.73	0.46
2:B:118:VAL:HB	2:B:123:ILE:HB	1.97	0.46
2:B:93:ASN:HA	2:B:94:PRO:HA	1.64	0.46
1:A:168:ARG:NH2	8:A:612:OLC:H6A	2.21	0.46
1:A:90:VAL:O	1:A:93:PRO:HG2	2.16	0.46
1:A:230:TRP:C	1:A:230:TRP:HD1	2.22	0.46
8:A:614:OLC:H2A	8:A:614:OLC:H5	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:ASP:OD2	2:B:112:VAL:N	2.37	0.45
1:A:341:TRP:CZ2	8:A:616:OLC:H3A	2.51	0.45
1:A:438:GLY:HA3	1:A:470:ASN:OD1	2.16	0.45
8:A:605:OLC:H24A	3:C:29:VAL:HG22	1.99	0.45
8:A:607:OLC:H15A	8:A:613:OLC:H12	1.99	0.45
2:B:114:HIS:O	2:B:127:VAL:HG23	2.16	0.45
1:A:247:ILE:O	1:A:252:PRO:HD3	2.16	0.45
1:A:300:VAL:HG11	8:A:608:OLC:H16A	1.98	0.45
1:A:441:TRP:HB3	1:A:466:PRO:HB3	1.99	0.45
2:B:151:GLN:O	2:B:152:TYR:C	2.59	0.45
8:C:101:OLC:H18A	8:C:101:OLC:H15	1.56	0.45
1:A:277:THR:N	1:A:278:PRO:HD2	2.32	0.45
1:A:346:PHE:CE1	1:A:350:VAL:HG21	2.52	0.44
1:A:520:LEU:O	1:A:524:MET:HG3	2.18	0.44
1:A:292:PRO:HD3	2:B:48:GLY:CA	2.47	0.44
1:A:161:TYR:CE2	8:A:611:OLC:H24A	2.53	0.44
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.71	0.44
1:A:382:PRO:HA	1:A:385:PHE:CZ	2.52	0.43
1:A:52:TYR:N	1:A:53:PRO:CD	2.81	0.43
1:A:120:PHE:O	1:A:123:PRO:HG2	2.18	0.43
1:A:277:THR:H	1:A:278:PRO:HD2	1.84	0.43
1:A:392:LEU:C	1:A:392:LEU:HD13	2.43	0.43
2:B:87:ALA:HA	2:B:88:PHE:HA	1.60	0.43
8:A:606:OLC:H18B	8:A:606:OLC:H15A	1.65	0.43
1:A:110:TRP:O	1:A:113:ALA:HB3	2.19	0.43
8:A:616:OLC:H4A	8:A:616:OLC:H7	1.77	0.43
1:A:472:LEU:HD23	8:A:614:OLC:H8	2.00	0.43
1:A:203:GLU:O	1:A:207:PHE:HB2	2.19	0.43
1:A:254:GLN:NE2	1:A:507:PRO:CG	2.81	0.43
1:A:255:ALA:HB1	1:A:339:LEU:HD12	2.01	0.43
8:A:613:OLC:H2	8:A:613:OLC:H5A	1.74	0.43
2:B:24:ALA:O	2:B:28:VAL:HG23	2.19	0.43
1:A:138:PRO:HG2	2:B:111:ASP:O	2.19	0.42
2:B:99:GLN:OE1	2:B:142:PRO:HD3	2.19	0.42
1:A:220:ASP:O	1:A:223:VAL:HG12	2.20	0.42
1:A:400:SER:C	1:A:402:TYR:H	2.27	0.42
1:A:185:MET:HG2	1:A:269:PHE:CG	2.55	0.42
1:A:465:VAL:N	1:A:466:PRO:HD2	2.35	0.42
1:A:512:ILE:HG23	2:B:8:HIS:HB2	2.00	0.42
1:A:54:LEU:HD22	1:A:54:LEU:O	2.20	0.42
1:A:286:ALA:HB1	2:B:125:VAL:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:TYR:CD2	1:A:208:LEU:HB3	2.55	0.42
2:B:91:GLN:HA	2:B:92:PRO:C	2.45	0.42
3:C:20:LEU:HD12	3:C:20:LEU:HA	1.89	0.42
1:A:81:THR:HB	1:A:239:TRP:CD1	2.55	0.42
1:A:307:VAL:N	1:A:308:PRO:HD2	2.34	0.42
3:C:27:TYR:CE2	3:C:31:PHE:HE2	2.37	0.42
1:A:236:VAL:HG12	1:A:239:TRP:CZ3	2.54	0.42
1:A:272:PHE:CE1	1:A:308:PRO:HB2	2.55	0.41
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.55	0.41
1:A:185:MET:HG2	1:A:269:PHE:CD1	2.55	0.41
1:A:389:VAL:HB	6:A:603:HAS:HBC2	2.01	0.41
2:B:83:VAL:HG11	2:B:116:PHE:CE1	2.55	0.41
1:A:219:VAL:C	1:A:555:PRO:HA	2.45	0.41
1:A:377:ASN:O	2:B:150:ASN:HB2	2.20	0.41
8:A:613:OLC:H9	8:A:613:OLC:H6	1.76	0.41
1:A:233:HIS:NE2	1:A:237:TYR:CZ	2.73	0.41
1:A:277:THR:N	1:A:278:PRO:CD	2.83	0.41
2:B:41:THR:HG1	3:C:30:PHE:HE2	1.67	0.41
1:A:250:ILE:HD12	1:A:403:TRP:CH2	2.55	0.41
1:A:42:GLN:HE22	1:A:69:LEU:HA	1.85	0.41
1:A:132:LEU:C	1:A:134:THR:H	2.29	0.41
1:A:369:PHE:C	1:A:369:PHE:HD2	2.28	0.41
1:A:42:GLN:NE2	1:A:69:LEU:HA	2.35	0.41
2:B:51:GLU:N	2:B:131:GLU:OE2	2.52	0.41
1:A:83:LEU:HD23	1:A:83:LEU:HA	1.86	0.40
1:A:207:PHE:CD1	1:A:219:VAL:HG13	2.56	0.40
1:A:385:PHE:C	1:A:385:PHE:CD1	2.99	0.40
1:A:453:ILE:C	1:A:455:GLN:H	2.28	0.40
2:B:90:TYR:CZ	2:B:160:MET:HE2	2.57	0.40

All (2) 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:330:HOH:O	10:B:330:HOH:O[2_554]	1.94	0.26
10:B:308:HOH:O	10:B:324:HOH:O[2_554]	2.08	0.12

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	529/568 (93%)	489 (92%)	40 (8%)	0	100	100
2	B	164/168 (98%)	154 (94%)	10 (6%)	0	100	100
3	C	29/34 (85%)	24 (83%)	5 (17%)	0	100	100
All	All	722/770 (94%)	667 (92%)	55 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	428/464 (92%)	404 (94%)	24 (6%)	19	50
2	B	132/138 (96%)	121 (92%)	11 (8%)	10	32
3	C	24/27 (89%)	18 (75%)	6 (25%)	0	2
All	All	584/629 (93%)	543 (93%)	41 (7%)	14	40

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	54	LEU
1	A	58	LEU
1	A	133	TYR
1	A	178	VAL

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Mol	Chain	Res	Type
1	A	195	LEU
1	A	205	VAL
1	A	215	LEU
1	A	230	TRP
1	A	250	ILE
1	A	262	ASP
1	A	264	MET
1	A	274	LEU
1	A	326	LEU
1	A	332	LEU
1	A	339	LEU
1	A	401	LEU
1	A	405	LEU
1	A	430	LEU
1	A	472	LEU
1	A	475	ILE
1	A	491	VAL
1	A	512	ILE
1	A	513	SER
2	B	12	LEU
2	B	37	LEU
2	B	49	LYS
2	B	51	GLU
2	B	58	VAL
2	B	93	ASN
2	B	127	VAL
2	B	141	ARG
2	B	148	ILE
2	B	167	LYS
2	B	168	GLU
3	C	4	LYS
3	C	6	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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	455	GLN
2	B	157	HIS

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Mol	Chain	Res	Type
2	B	159	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
6	HAS	A	603	1,7	72,72,72	2.35	29 (40%)	87,109,109	1.44	11 (12%)
8	OLC	A	608	-	20,20,24	0.58	1 (5%)	20,20,25	0.63	0
8	OLC	A	612	-	14,14,24	0.56	0	15,15,25	0.74	0
8	OLC	B	203	-	24,24,24	0.57	1 (4%)	25,25,25	0.84	2 (8%)
8	OLC	A	613	-	19,19,24	0.68	1 (5%)	20,20,25	0.70	0
8	OLC	C	101	-	24,24,24	0.53	0	25,25,25	0.58	0
9	CUA	B	201	2	0,1,1	-	-	-	-	-
5	HEM	A	602	1	50,50,50	3.68	30 (60%)	67,82,82	2.02	15 (22%)
8	OLC	A	605	-	24,24,24	0.48	0	25,25,25	0.77	0
8	OLC	A	616	-	24,24,24	0.56	1 (4%)	25,25,25	0.61	0
8	OLC	A	606	-	24,24,24	0.49	0	25,25,25	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	OLC	A	607	-	22,22,24	0.54	0	23,23,25	0.51	0
8	OLC	A	609	-	17,17,24	0.65	1 (5%)	18,18,25	0.77	0
7	PEO	A	604	6,4	1,1,1	0.37	0	-		
8	OLC	B	202	-	24,24,24	0.62	1 (4%)	25,25,25	0.69	0
8	OLC	B	204	-	24,24,24	0.49	0	25,25,25	0.65	0
8	OLC	A	611	-	7,7,24	0.38	0	6,7,25	0.25	0
8	OLC	A	615	-	20,20,24	0.52	0	21,21,25	0.70	0
8	OLC	A	610	-	16,16,24	0.77	1 (6%)	17,17,25	0.86	0
8	OLC	A	614	-	24,24,24	0.57	1 (4%)	25,25,25	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OLC	C	101	-	-	19/24/24/24	-
6	HAS	A	603	1,7	1/1/8/18	16/42/82/82	-
5	HEM	A	602	1	-	4/14/54/54	-
8	OLC	A	608	-	-	8/19/19/24	-
8	OLC	A	615	-	-	8/20/20/24	-
8	OLC	A	609	-	-	7/17/17/24	-
8	OLC	A	605	-	-	10/24/24/24	-
8	OLC	A	612	-	-	5/14/14/24	-
8	OLC	A	610	-	-	9/16/16/24	-
8	OLC	A	616	-	-	11/24/24/24	-
8	OLC	B	203	-	-	9/24/24/24	-
8	OLC	B	202	-	-	9/24/24/24	-
8	OLC	A	613	-	-	8/19/19/24	-
8	OLC	A	614	-	-	12/24/24/24	-
8	OLC	A	606	-	-	13/24/24/24	-
8	OLC	B	204	-	-	12/24/24/24	-
8	OLC	A	611	-	-	1/6/6/24	-
8	OLC	A	607	-	-	6/22/22/24	-

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEM	FE-NB	12.33	2.32	1.94
5	A	602	HEM	C3C-C4C	-7.18	1.33	1.46
5	A	602	HEM	C3B-C2B	6.44	1.50	1.37
5	A	602	HEM	C1C-C2C	-6.25	1.33	1.45
6	A	603	HAS	CHB-C1D	5.95	1.50	1.38
5	A	602	HEM	CHD-C4C	5.84	1.49	1.38
5	A	602	HEM	C3C-C2C	5.77	1.48	1.37
5	A	602	HEM	CAB-C3B	-5.75	1.32	1.47
5	A	602	HEM	CHC-C1C	5.64	1.49	1.38
6	A	603	HAS	CAC-C3C	-5.47	1.32	1.47
5	A	602	HEM	CHA-C1A	5.31	1.51	1.39
5	A	602	HEM	CHB-C1B	5.29	1.49	1.38
5	A	602	HEM	C1B-C2B	-5.03	1.34	1.44
6	A	603	HAS	CHC-C1C	5.02	1.50	1.39
6	A	603	HAS	CHA-C4D	4.82	1.50	1.39
6	A	603	HAS	C2D-C1D	4.62	1.53	1.44
6	A	603	HAS	CHD-C4C	4.62	1.49	1.39
6	A	603	HAS	C4D-ND	4.55	1.47	1.38
5	A	602	HEM	CBB-CAB	4.44	1.51	1.30
6	A	603	HAS	CBC-CAC	4.37	1.51	1.30
6	A	603	HAS	C1D-ND	4.14	1.47	1.40
6	A	603	HAS	O1D-CGD	3.59	1.33	1.22
5	A	602	HEM	C1A-NA	3.58	1.46	1.39
6	A	603	HAS	C4D-C3D	3.51	1.51	1.45
5	A	602	HEM	C4A-C3A	3.41	1.51	1.43
6	A	603	HAS	C1C-C2C	-3.35	1.35	1.43
6	A	603	HAS	FE-NA	3.33	2.06	1.95
6	A	603	HAS	CHB-C1B	-3.21	1.31	1.39
6	A	603	HAS	C4C-NC	3.19	1.45	1.39
6	A	603	HAS	C4B-C3B	3.18	1.50	1.44
5	A	602	HEM	FE-NC	3.17	2.05	1.95
5	A	602	HEM	C1D-C2D	3.11	1.50	1.44
5	A	602	HEM	C1A-C2A	3.10	1.50	1.44
5	A	602	HEM	CHA-C4D	-3.09	1.32	1.38
5	A	602	HEM	CHB-C4A	-3.09	1.32	1.39
6	A	603	HAS	C3C-C2C	2.99	1.51	1.41
5	A	602	HEM	C1B-NB	-2.97	1.35	1.40
6	A	603	HAS	CHA-C1A	-2.92	1.32	1.38
6	A	603	HAS	FE-NB	2.88	2.03	1.94
5	A	602	HEM	FE-ND	2.84	2.03	1.94
6	A	603	HAS	CHD-C4A	-2.82	1.32	1.38
5	A	602	HEM	C4D-ND	-2.76	1.35	1.40
5	A	602	HEM	C4A-NA	-2.67	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEM	CHC-C4B	-2.65	1.33	1.39
6	A	603	HAS	FE-NC	2.59	2.03	1.95
5	A	602	HEM	C4D-C3D	2.59	1.49	1.45
6	A	603	HAS	C2A-C3A	-2.55	1.31	1.36
5	A	602	HEM	CHD-C1D	-2.51	1.33	1.39
6	A	603	HAS	C1A-C2A	2.45	1.49	1.45
6	A	603	HAS	C1B-C2B	2.33	1.49	1.44
8	B	202	OLC	O20-C1	2.24	1.39	1.33
6	A	603	HAS	O2D-CGD	-2.22	1.23	1.30
8	A	614	OLC	O20-C1	2.21	1.39	1.33
8	A	613	OLC	O20-C1	2.20	1.39	1.33
8	A	610	OLC	O20-C1	2.18	1.39	1.33
8	B	203	OLC	O20-C1	2.16	1.39	1.33
5	A	602	HEM	C3B-C4B	2.13	1.49	1.44
5	A	602	HEM	FE-NA	2.11	2.02	1.95
5	A	602	HEM	C1D-ND	-2.10	1.34	1.38
6	A	603	HAS	C3C-C4C	2.08	1.48	1.42
6	A	603	HAS	C1A-NA	-2.06	1.35	1.39
6	A	603	HAS	C1B-NB	-2.05	1.34	1.38
8	A	616	OLC	O20-C1	2.05	1.39	1.33
5	A	602	HEM	C1C-NC	-2.04	1.35	1.39
6	A	603	HAS	C4A-C3A	2.03	1.49	1.45
8	A	608	OLC	O20-C1	2.01	1.39	1.33
8	A	609	OLC	O20-C1	2.01	1.39	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	HEM	C1B-NB-C4B	6.48	112.88	105.21
5	A	602	HEM	C3B-C4B-NB	-6.36	104.90	109.47
5	A	602	HEM	CHC-C4B-NB	5.44	130.27	124.42
6	A	603	HAS	C4C-C3C-C2C	-5.22	100.82	107.30
5	A	602	HEM	C2A-C1A-NA	-4.65	104.99	110.15
6	A	603	HAS	C1D-ND-C4D	-4.41	99.99	105.21
6	A	603	HAS	CHB-C1D-ND	-3.60	119.92	124.37
5	A	602	HEM	C4B-C3B-C2B	-3.43	104.13	107.28
6	A	603	HAS	CHA-C1A-C2A	-3.22	119.78	124.86
5	A	602	HEM	C4D-ND-C1D	3.18	108.98	105.21
6	A	603	HAS	C2C-C1C-NC	3.09	115.09	110.14
6	A	603	HAS	CHB-C1B-C2B	-3.05	120.22	125.03
5	A	602	HEM	CHA-C1A-NA	2.76	128.87	123.86
5	A	602	HEM	CHD-C1D-ND	2.74	127.38	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	HEM	CHA-C4D-ND	2.59	127.57	124.37
5	A	602	HEM	C4C-NC-C1C	2.51	109.92	105.82
6	A	603	HAS	CMB-C2B-C3B	-2.47	125.51	130.28
5	A	602	HEM	C4A-C3A-C2A	2.46	109.63	106.82
5	A	602	HEM	C1A-CHA-C4D	-2.35	120.72	126.25
5	A	602	HEM	CHD-C4C-NC	2.34	127.00	124.45
6	A	603	HAS	CAD-CBD-CGD	-2.30	107.57	113.67
6	A	603	HAS	CHA-C1A-NA	2.23	126.88	124.45
8	B	203	OLC	C21-O20-C1	2.21	125.19	117.12
5	A	602	HEM	O2A-CGA-CBA	2.15	120.81	114.00
8	B	203	OLC	C3-C2-C1	-2.06	106.15	113.69
5	A	602	HEM	CMC-C2C-C1C	2.03	128.31	124.73
6	A	603	HAS	CHD-C4A-C3A	-2.02	121.29	125.49
6	A	603	HAS	C21-C22-C23	-2.02	123.01	127.62

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	603	HAS	NA

All (167) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	HEM	C2B-C3B-CAB-CBB
6	A	603	HAS	C1D-C2D-CMD-OMD
6	A	603	HAS	C3D-C2D-CMD-OMD
8	A	606	OLC	C21-C22-C24-O25
8	A	609	OLC	C21-C22-C24-O25
8	A	609	OLC	O23-C22-C24-O25
8	A	610	OLC	O20-C21-C22-C24
8	A	611	OLC	O19-C1-O20-C21
8	A	613	OLC	C10-C11-C12-C13
8	A	615	OLC	C21-C22-C24-O25
8	C	101	OLC	C21-C22-C24-O25
8	B	203	OLC	O19-C1-O20-C21
8	A	608	OLC	C2-C1-O20-C21
6	A	603	HAS	C28-C29-C30-C31
6	A	603	HAS	C28-C29-C30-C32
8	B	202	OLC	C2-C1-O20-C21
8	B	203	OLC	C2-C1-O20-C21
8	B	202	OLC	O19-C1-O20-C21
8	A	613	OLC	C2-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
8	A	608	OLC	O19-C1-O20-C21
8	A	615	OLC	C2-C1-O20-C21
8	C	101	OLC	C2-C1-O20-C21
6	A	603	HAS	C21-C22-C23-C25
8	A	613	OLC	O19-C1-O20-C21
8	A	610	OLC	C2-C1-O20-C21
8	A	610	OLC	O20-C21-C22-O23
8	A	610	OLC	O19-C1-O20-C21
8	A	615	OLC	O19-C1-O20-C21
8	C	101	OLC	O19-C1-O20-C21
8	A	609	OLC	O19-C1-O20-C21
8	A	606	OLC	C2-C1-O20-C21
8	A	609	OLC	C2-C1-O20-C21
8	A	612	OLC	C2-C1-O20-C21
8	C	101	OLC	C13-C14-C15-C16
8	A	609	OLC	O20-C21-C22-C24
8	A	606	OLC	O19-C1-O20-C21
8	A	612	OLC	O19-C1-O20-C21
8	A	605	OLC	C1-C2-C3-C4
8	A	614	OLC	C1-C2-C3-C4
8	A	612	OLC	C1-C2-C3-C4
8	A	607	OLC	O20-C21-C22-O23
8	A	614	OLC	C2-C3-C4-C5
6	A	603	HAS	C27-C19-C20-C21
8	A	607	OLC	O20-C21-C22-C24
8	A	613	OLC	C2-C3-C4-C5
8	A	609	OLC	O20-C21-C22-O23
8	C	101	OLC	O20-C21-C22-O23
8	A	610	OLC	C21-C22-C24-O25
8	B	204	OLC	C21-C22-C24-O25
8	A	612	OLC	C3-C4-C5-C6
8	A	616	OLC	C12-C13-C14-C15
8	A	615	OLC	O23-C22-C24-O25
8	C	101	OLC	O23-C22-C24-O25
8	A	614	OLC	C12-C13-C14-C15
8	C	101	OLC	C3-C4-C5-C6
8	A	605	OLC	C10-C11-C12-C13
8	B	204	OLC	C1-C2-C3-C4
8	A	607	OLC	C11-C12-C13-C14
8	A	616	OLC	C14-C15-C16-C17
8	B	203	OLC	C1-C2-C3-C4
8	A	614	OLC	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
8	A	616	OLC	C10-C11-C12-C13
8	A	606	OLC	C3-C4-C5-C6
8	B	204	OLC	C5-C6-C7-C8
6	A	603	HAS	C21-C22-C23-C24
6	A	603	HAS	C18-C19-C20-C21
8	B	203	OLC	C4-C5-C6-C7
8	B	203	OLC	C12-C13-C14-C15
8	C	101	OLC	C11-C12-C13-C14
8	A	605	OLC	C11-C12-C13-C14
8	A	616	OLC	C3-C4-C5-C6
8	A	606	OLC	C6-C7-C8-C9
8	A	614	OLC	C3-C4-C5-C6
8	C	101	OLC	C5-C6-C7-C8
8	A	606	OLC	C1-C2-C3-C4
8	A	615	OLC	C10-C11-C12-C13
8	A	608	OLC	C11-C12-C13-C14
8	A	605	OLC	C3-C4-C5-C6
8	A	605	OLC	C2-C3-C4-C5
8	C	101	OLC	C15-C16-C17-C18
8	A	606	OLC	C15-C16-C17-C18
8	C	101	OLC	C2-C3-C4-C5
8	B	204	OLC	O23-C22-C24-O25
8	B	202	OLC	C3-C4-C5-C6
8	A	605	OLC	C4-C5-C6-C7
8	A	605	OLC	C14-C15-C16-C17
8	B	204	OLC	C12-C13-C14-C15
8	A	614	OLC	C10-C11-C12-C13
8	B	202	OLC	C6-C7-C8-C9
8	A	616	OLC	C2-C1-O20-C21
8	A	616	OLC	O19-C1-O20-C21
8	A	606	OLC	C13-C14-C15-C16
8	A	613	OLC	C4-C5-C6-C7
8	A	614	OLC	C15-C16-C17-C18
8	A	616	OLC	C6-C7-C8-C9
8	B	202	OLC	C14-C15-C16-C17
8	A	606	OLC	C12-C13-C14-C15
8	A	614	OLC	C11-C12-C13-C14
8	A	615	OLC	C2-C3-C4-C5
8	C	101	OLC	C12-C13-C14-C15
8	A	608	OLC	C12-C13-C14-C15
8	B	203	OLC	C3-C4-C5-C6
8	B	202	OLC	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
8	A	608	OLC	C14-C15-C16-C17
8	A	615	OLC	O20-C21-C22-O23
8	A	609	OLC	C6-C7-C8-C9
8	A	605	OLC	C15-C16-C17-C18
8	A	616	OLC	C4-C5-C6-C7
8	A	607	OLC	C12-C13-C14-C15
8	A	614	OLC	O20-C21-C22-C24
8	A	606	OLC	O23-C22-C24-O25
8	A	613	OLC	O23-C22-C24-O25
8	A	606	OLC	C10-C11-C12-C13
8	A	614	OLC	C14-C15-C16-C17
8	C	101	OLC	O20-C21-C22-C24
8	A	614	OLC	C13-C14-C15-C16
8	B	203	OLC	C13-C14-C15-C16
8	A	613	OLC	O20-C1-C2-C3
8	B	204	OLC	C15-C16-C17-C18
8	C	101	OLC	C1-C2-C3-C4
8	B	204	OLC	C3-C4-C5-C6
8	A	610	OLC	C4-C5-C6-C7
8	B	203	OLC	C9-C10-C11-C12
8	A	615	OLC	O20-C21-C22-C24
8	C	101	OLC	C4-C5-C6-C7
6	A	603	HAS	C3A-C2A-CAA-CBA
8	A	610	OLC	O23-C22-C24-O25
8	B	202	OLC	C13-C14-C15-C16
8	B	204	OLC	C7-C8-C9-C10
8	C	101	OLC	C14-C15-C16-C17
8	C	101	OLC	C10-C11-C12-C13
8	A	608	OLC	C7-C8-C9-C10
8	B	204	OLC	C13-C14-C15-C16
8	A	613	OLC	C9-C10-C11-C12
6	A	603	HAS	C2C-C3C-CAC-CBC
8	A	614	OLC	O20-C21-C22-O23
8	B	203	OLC	C7-C8-C9-C10
6	A	603	HAS	CAA-CBA-CGA-O2A
6	A	603	HAS	CAD-CBD-CGD-O1D
6	A	603	HAS	C26-C15-C16-C17
6	A	603	HAS	CAA-CBA-CGA-O1A
8	B	202	OLC	C1-C2-C3-C4
6	A	603	HAS	CAD-CBD-CGD-O2D
8	A	616	OLC	C7-C8-C9-C10
8	A	607	OLC	C7-C8-C9-C10

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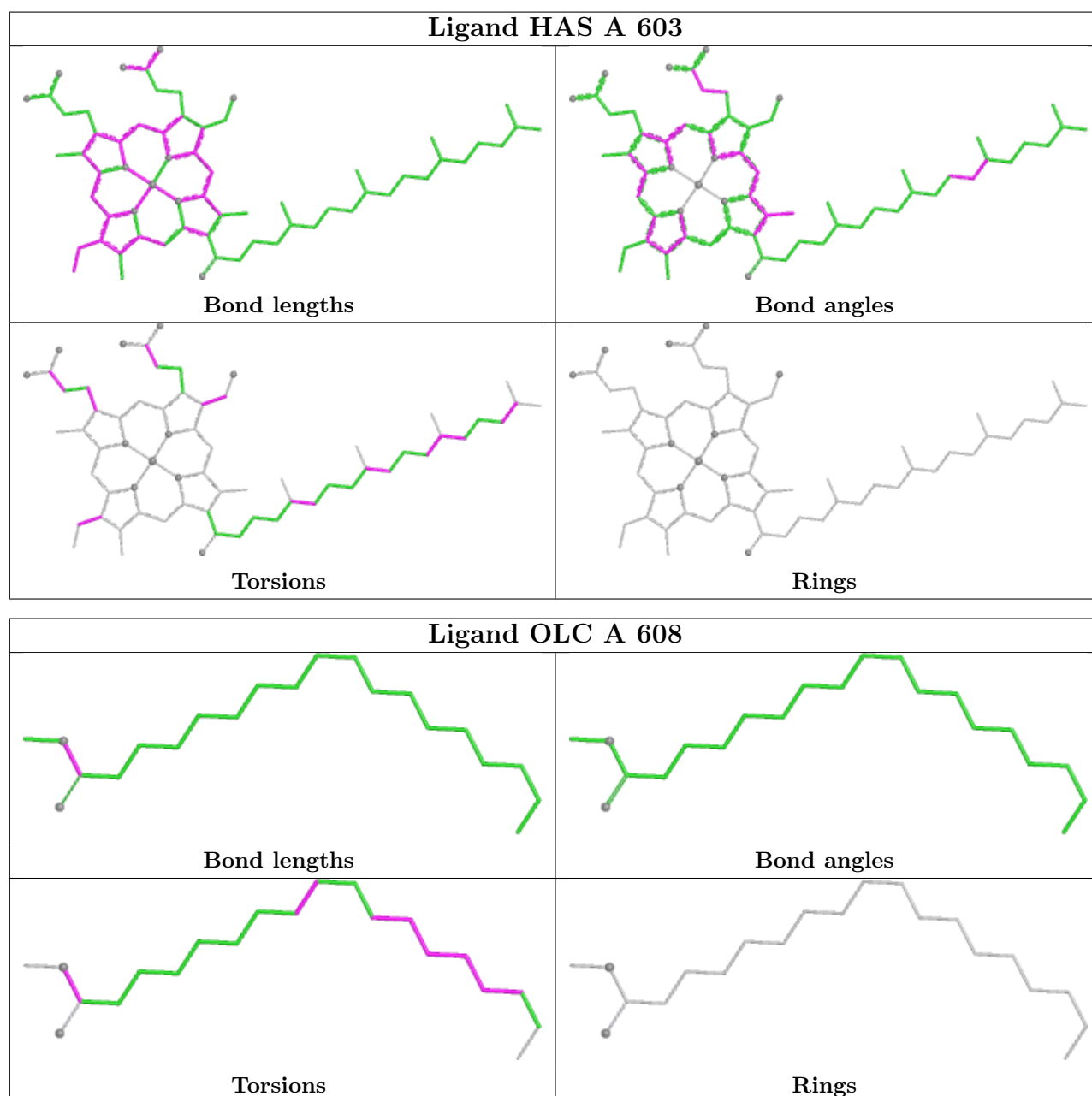
Mol	Chain	Res	Type	Atoms
8	A	616	OLC	C9-C10-C11-C12
8	C	101	OLC	C7-C8-C9-C10
8	A	606	OLC	C4-C5-C6-C7
8	A	606	OLC	C11-C12-C13-C14
8	B	204	OLC	C2-C3-C4-C5
8	B	202	OLC	C7-C8-C9-C10
8	A	608	OLC	C10-C11-C12-C13
8	A	605	OLC	C7-C8-C9-C10
8	A	612	OLC	C2-C3-C4-C5
8	A	610	OLC	O20-C1-C2-C3
8	A	616	OLC	C11-C12-C13-C14
8	A	605	OLC	C9-C10-C11-C12
8	C	101	OLC	C9-C10-C11-C12
8	A	607	OLC	C6-C7-C8-C9
8	B	204	OLC	C11-C12-C13-C14
8	A	608	OLC	C13-C14-C15-C16
6	A	603	HAS	C25-C23-C24-C28
5	A	602	HEM	CAD-CBD-CGD-O2D
8	A	610	OLC	O19-C1-C2-C3
5	A	602	HEM	C2C-C3C-CAC-CBC
8	B	204	OLC	C6-C7-C8-C9
5	A	602	HEM	CAD-CBD-CGD-O1D

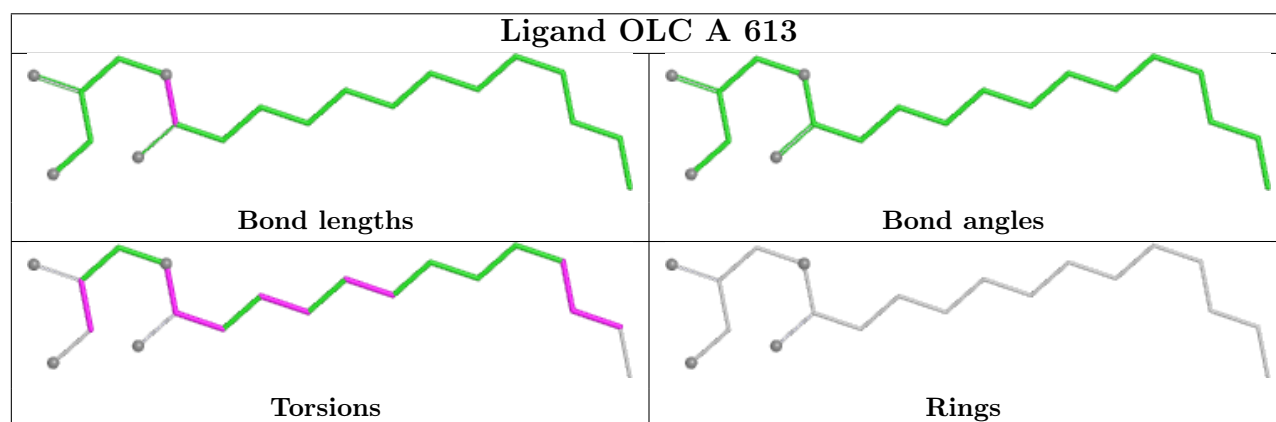
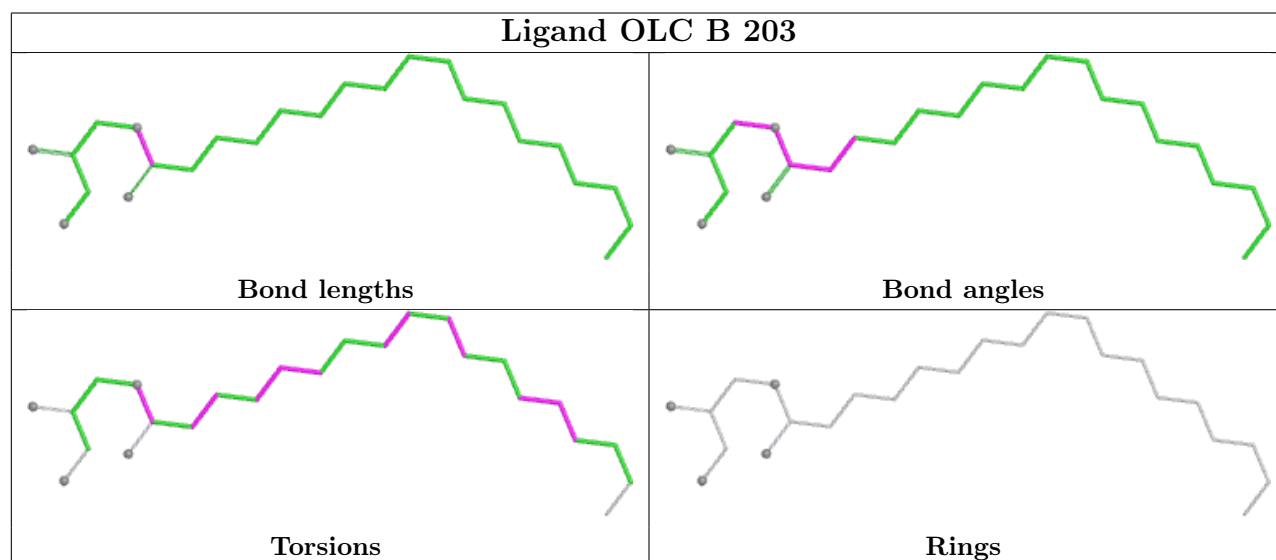
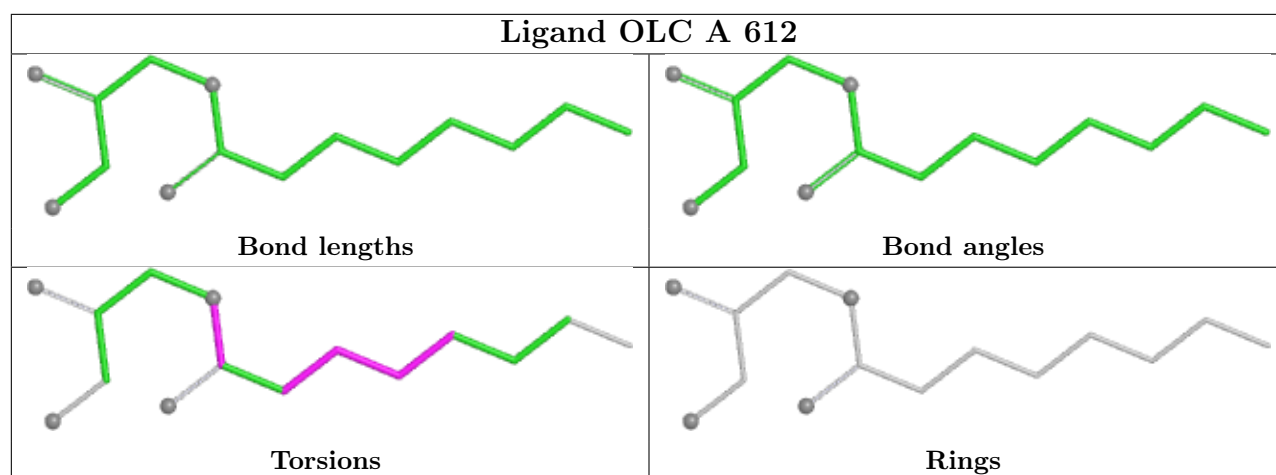
There are no ring outliers.

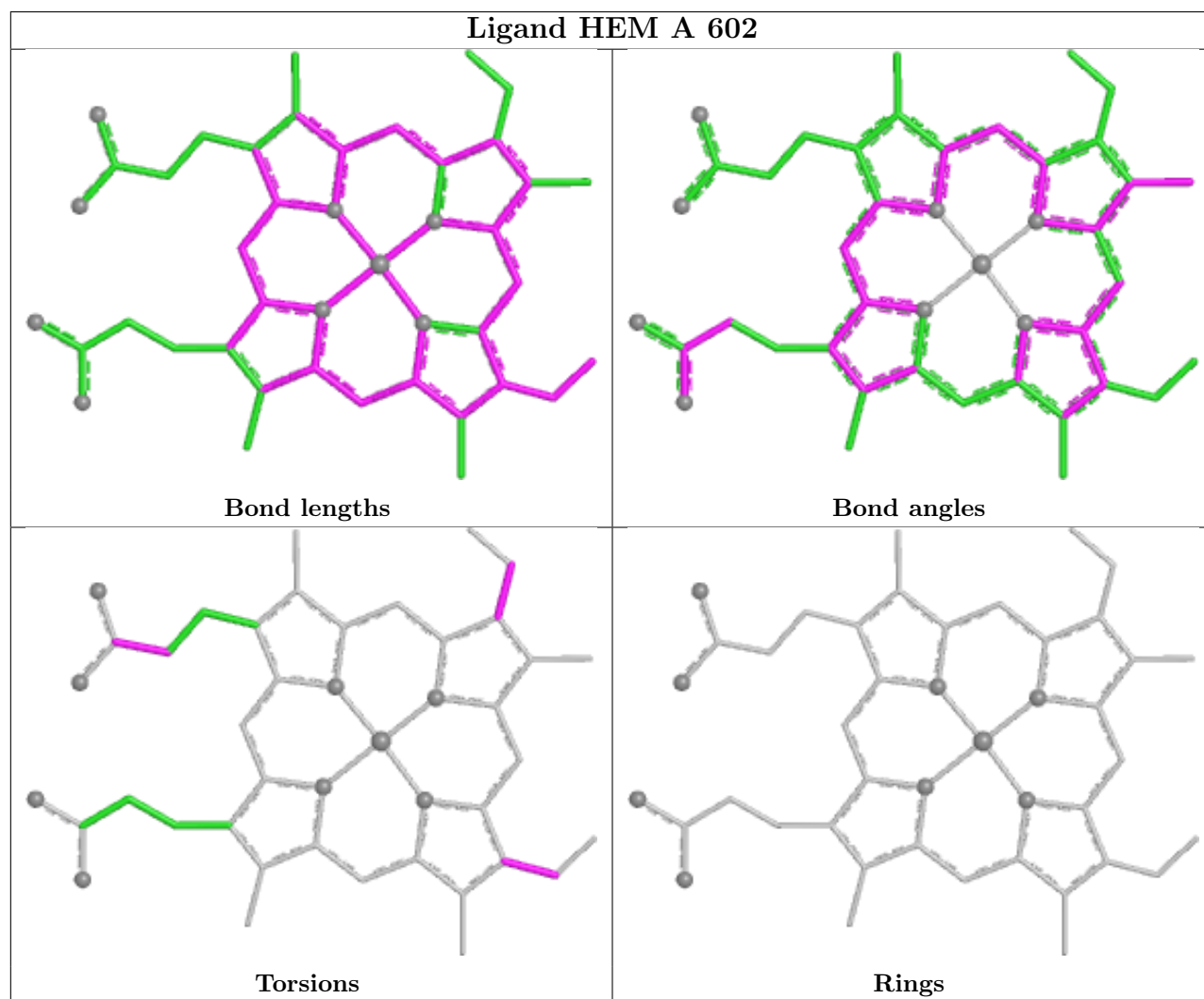
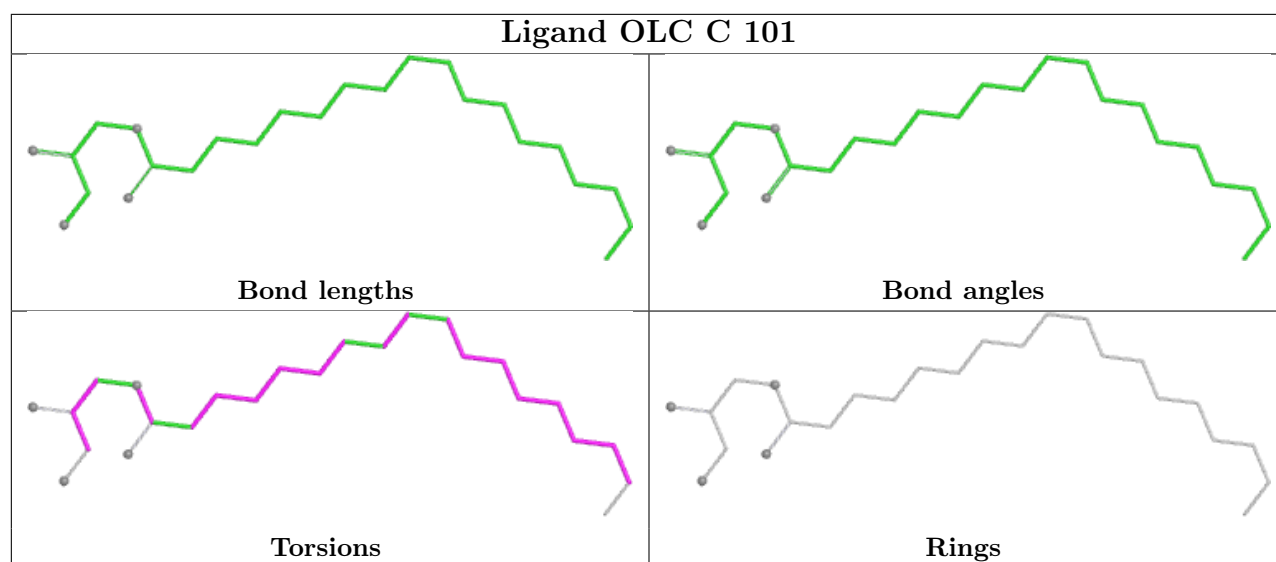
14 monomers are involved in 36 short contacts:

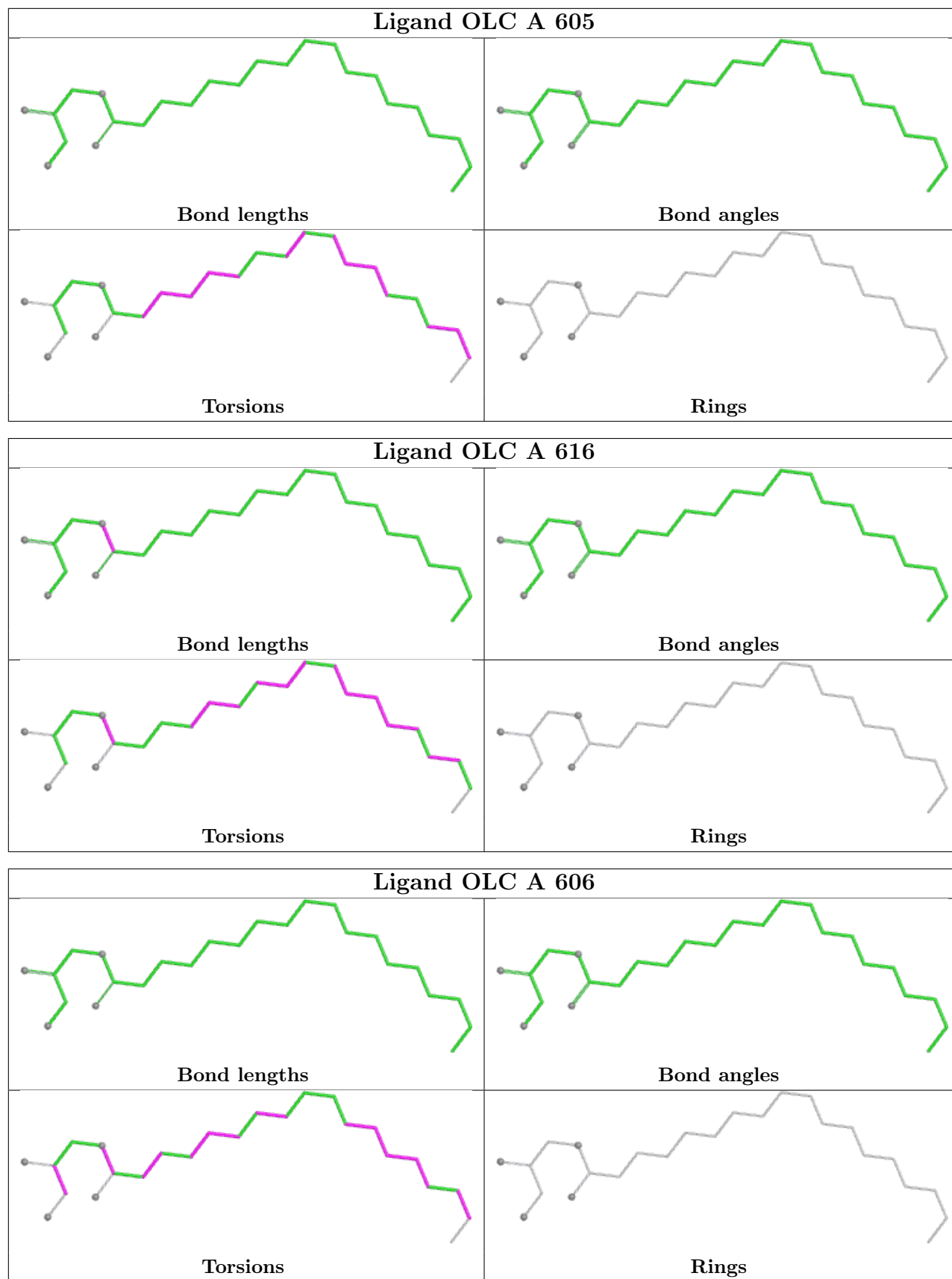
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	HAS	2	0
8	A	608	OLC	1	0
8	A	612	OLC	2	0
8	B	203	OLC	8	0
8	A	613	OLC	3	0
8	C	101	OLC	3	0
8	A	605	OLC	8	0
8	A	616	OLC	4	0
8	A	606	OLC	4	0
8	A	607	OLC	1	0
8	A	609	OLC	1	0
8	B	202	OLC	2	0
8	A	611	OLC	3	0
8	A	614	OLC	3	0

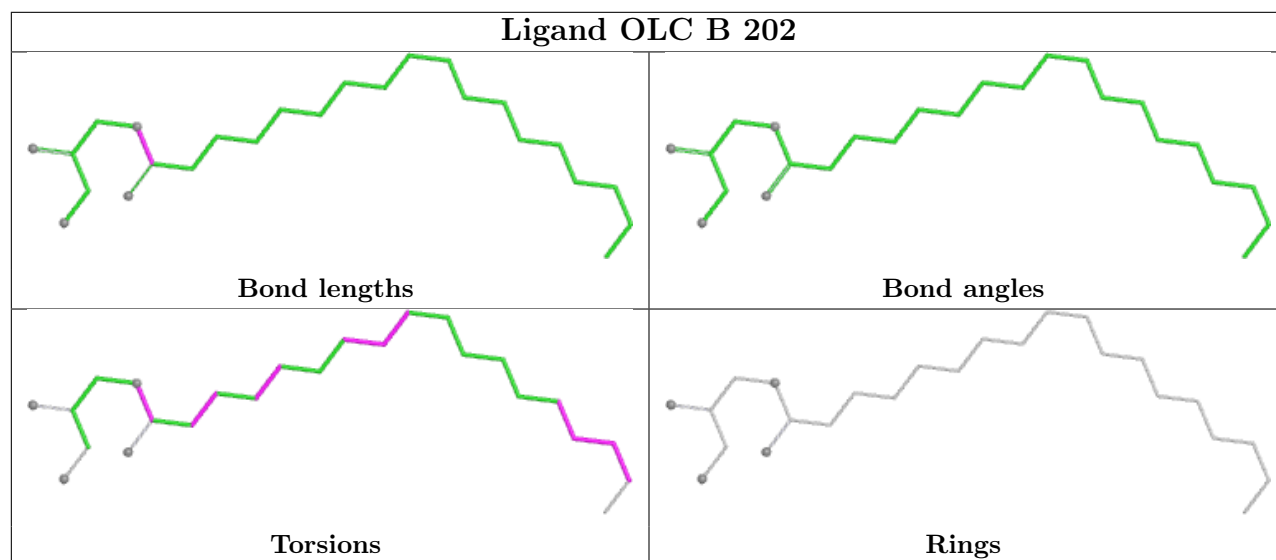
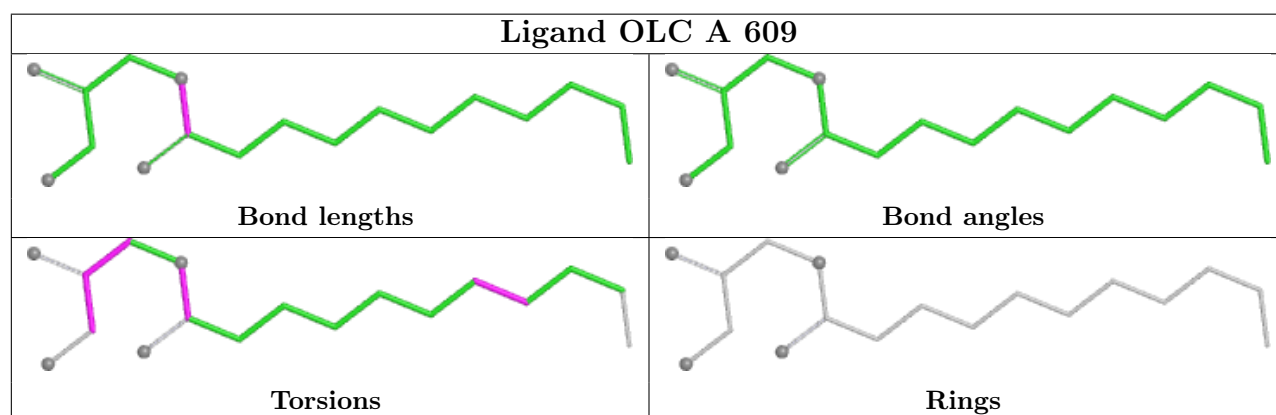
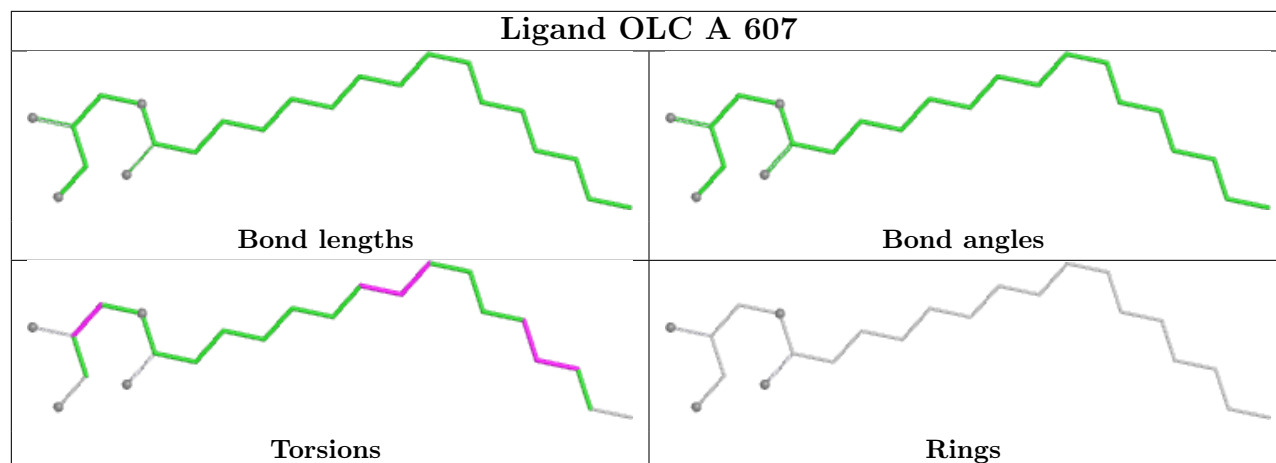
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

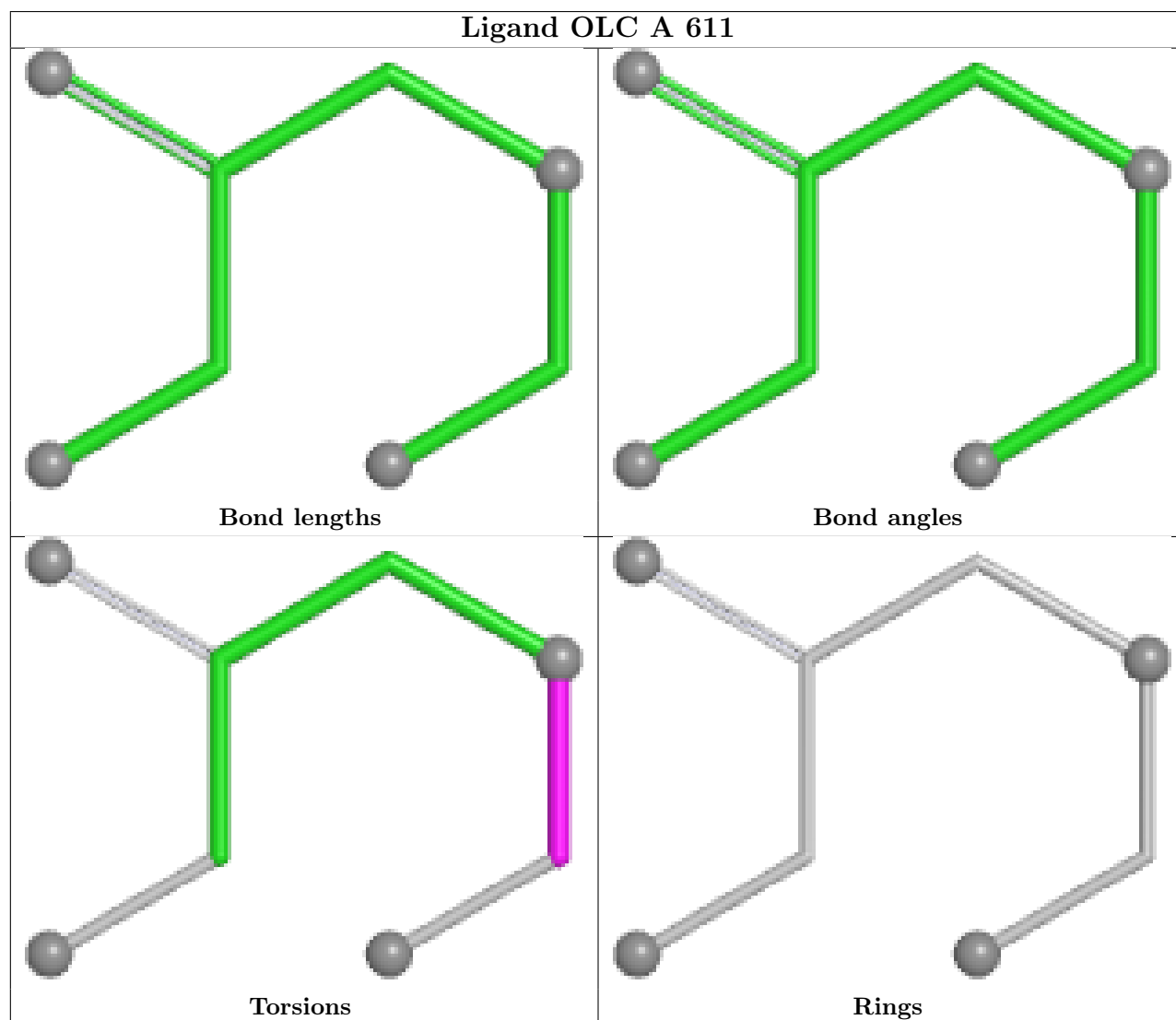
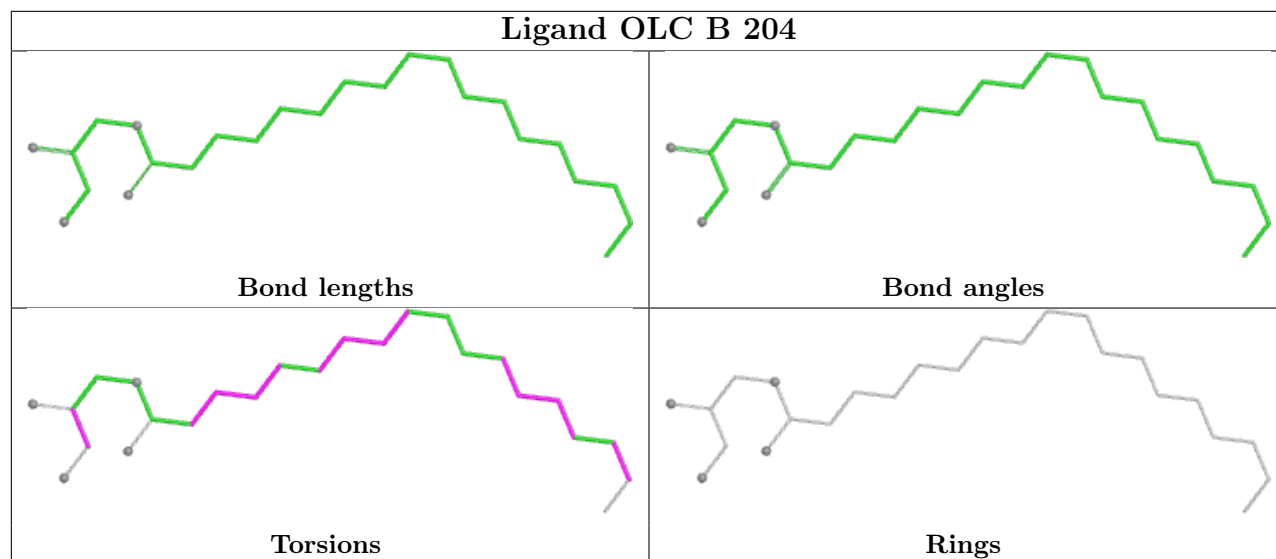


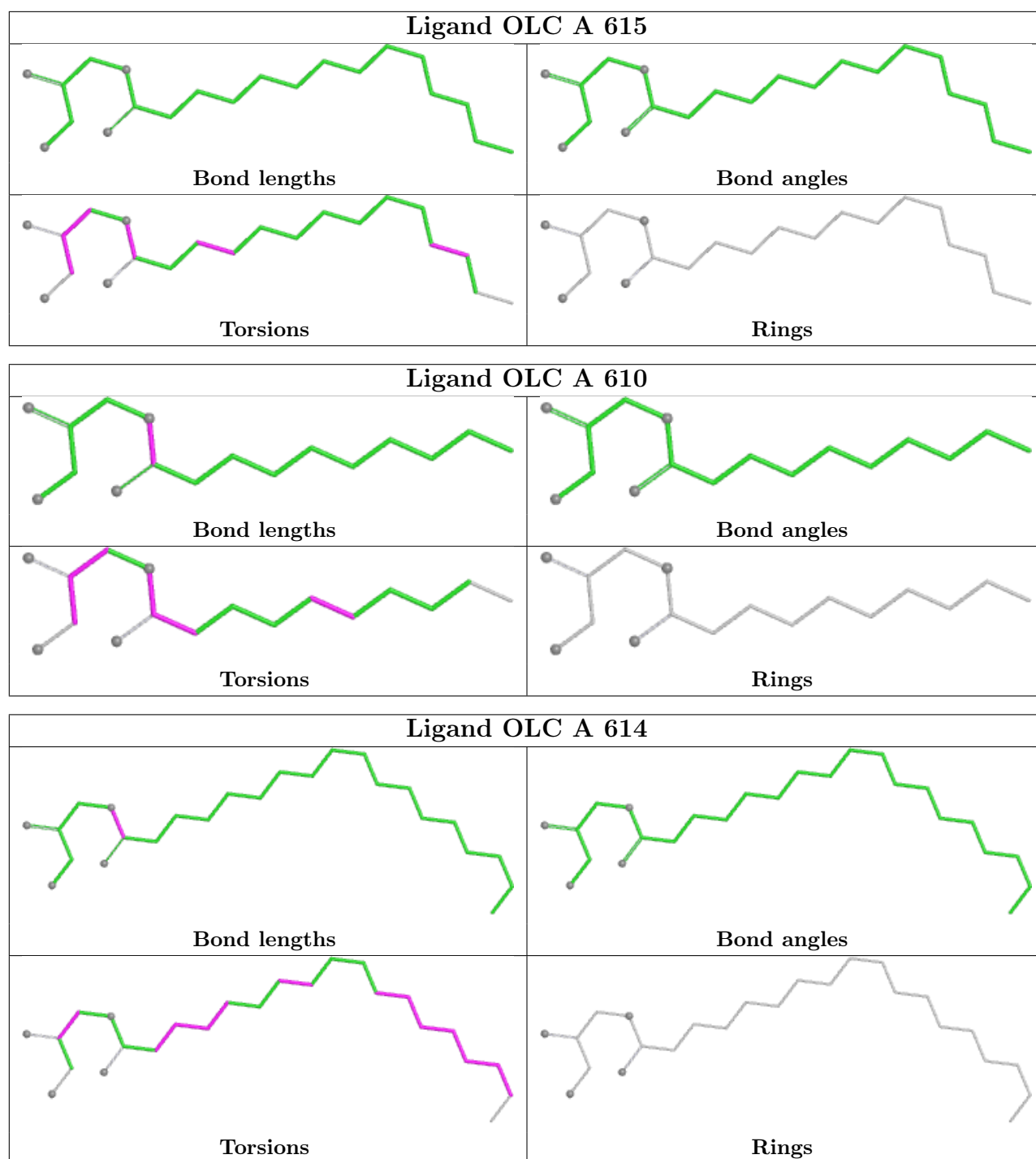












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	535/568 (94%)	-0.26	6 (1%) 78 70	21, 29, 49, 77	1 (0%)
2	B	166/168 (98%)	-0.39	0 100 100	22, 30, 46, 68	0
3	C	31/34 (91%)	-0.48	0 100 100	23, 28, 37, 49	0
All	All	732/770 (95%)	-0.30	6 (0%) 82 75	21, 29, 48, 77	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	514	GLY	5.3
1	A	368	SER	3.2
1	A	491	VAL	3.1
1	A	489	PHE	2.6
1	A	517	ASP	2.3
1	A	513	SER	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

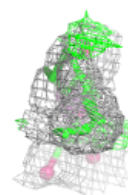
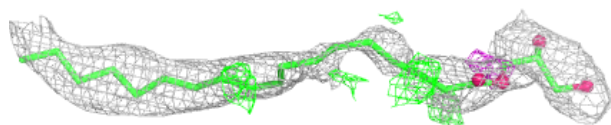
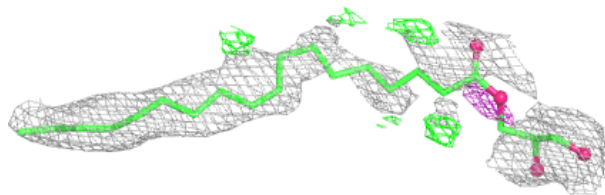
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	OLC	B	203	25/25	0.78	0.19	41,53,74,85	0
8	OLC	A	613	20/25	0.79	0.18	39,49,65,66	0
8	OLC	A	616	25/25	0.80	0.17	38,49,56,58	0
8	OLC	A	610	17/25	0.80	0.17	39,50,74,74	0
8	OLC	A	612	15/25	0.81	0.15	47,59,73,74	0
8	OLC	A	608	21/25	0.81	0.18	38,50,58,66	0
8	OLC	C	101	25/25	0.81	0.15	39,61,77,81	0
8	OLC	A	606	25/25	0.83	0.17	34,43,82,92	0
8	OLC	B	204	25/25	0.84	0.16	35,46,73,78	0
8	OLC	A	615	21/25	0.84	0.15	39,51,65,73	0
8	OLC	A	609	18/25	0.86	0.13	30,47,69,69	0
8	OLC	A	614	25/25	0.87	0.15	38,45,54,61	0
8	OLC	A	607	23/25	0.87	0.13	34,40,53,56	0
8	OLC	A	611	8/25	0.87	0.12	45,47,54,57	0
8	OLC	B	202	25/25	0.88	0.14	31,39,56,62	0
8	OLC	A	605	25/25	0.88	0.13	27,44,64,71	0
6	HAS	A	603	65/65	0.96	0.09	17,23,34,39	0
5	HEM	A	602	43/43	0.98	0.07	18,23,26,31	0
4	CU	A	601	1/1	0.98	0.03	25,25,25,25	0
7	PEO	A	604	2/2	0.99	0.15	19,19,19,25	0
9	CUA	B	201	2/2	0.99	0.03	21,21,21,24	0

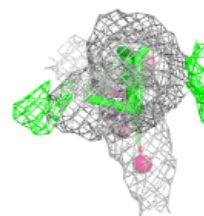
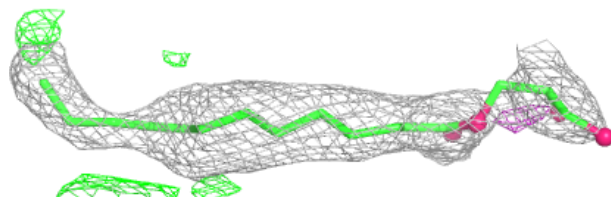
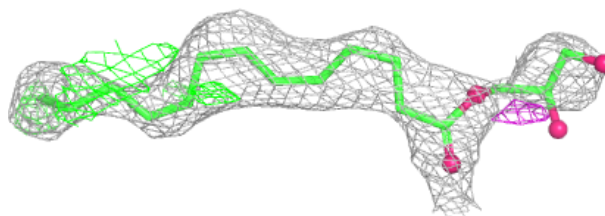
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC 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)

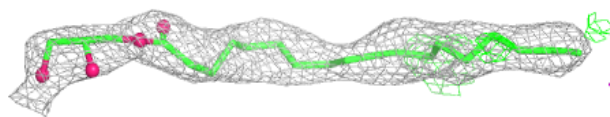
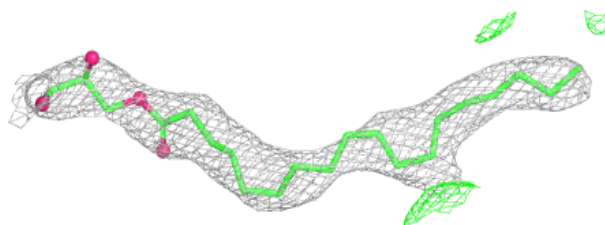
**Electron density around OLC A 613:**

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

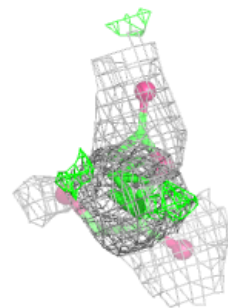
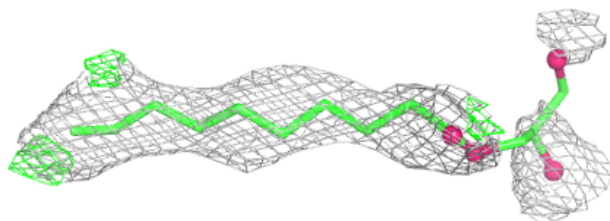
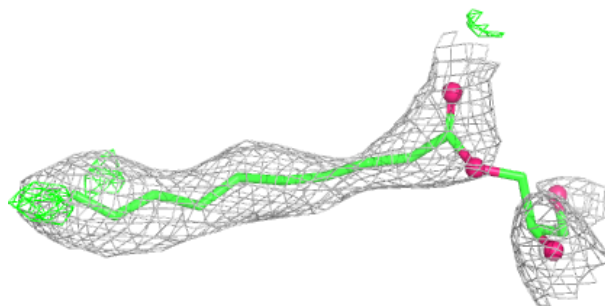


Electron density around OLC A 616:

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

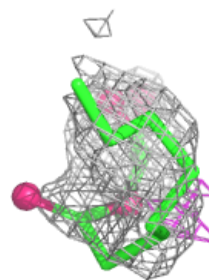
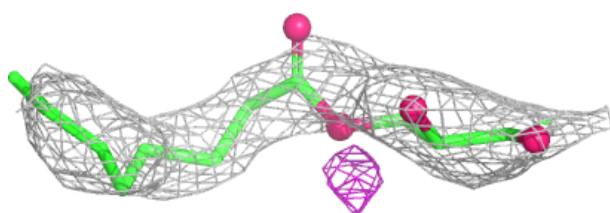
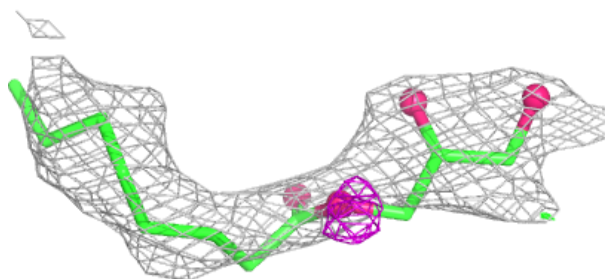
**Electron density around OLC A 610:**

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

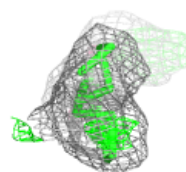
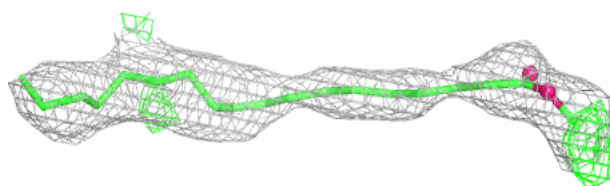
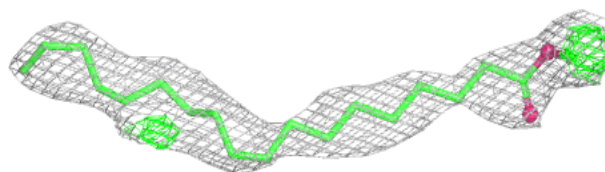


Electron density around OLC A 612:

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

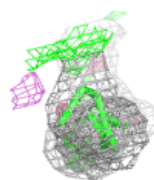
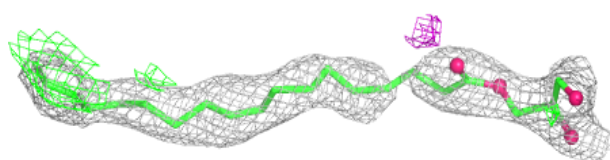
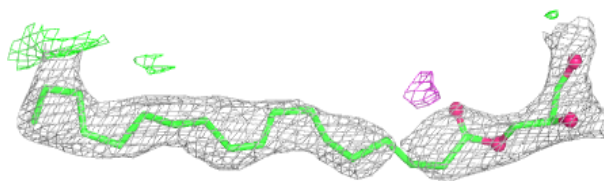
**Electron density around OLC A 608:**

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

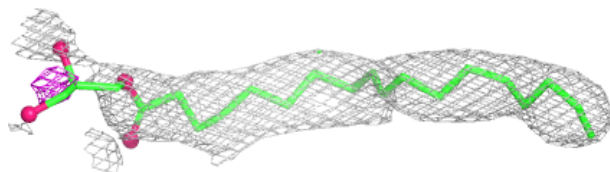
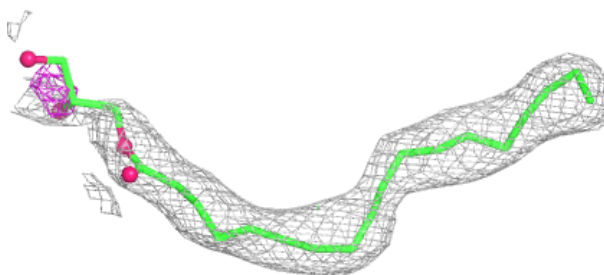


Electron density around OLC C 101:

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

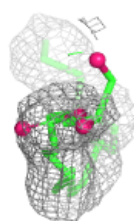
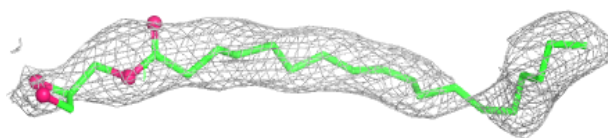
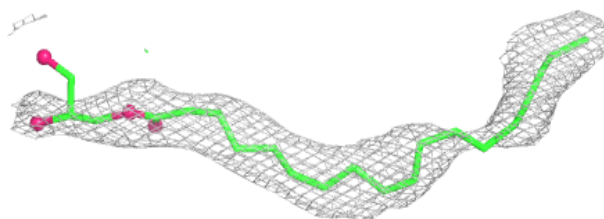
**Electron density around OLC A 606:**

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

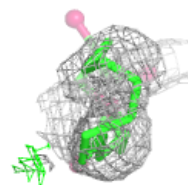
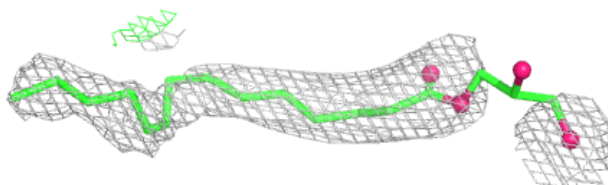
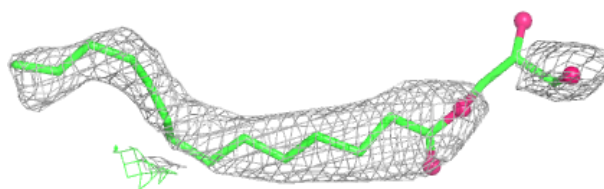


Electron density around OLC B 204:

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

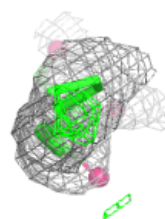
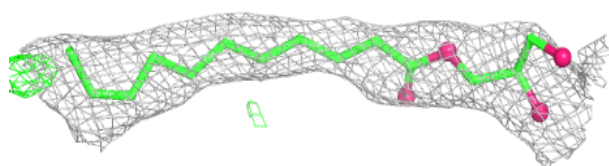
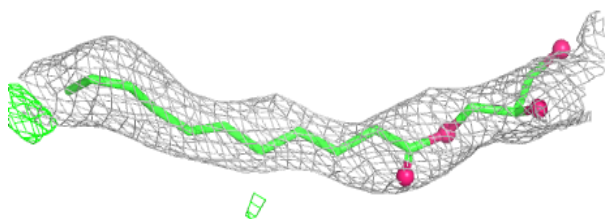
**Electron density around OLC A 615:**

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

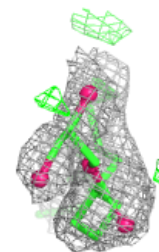
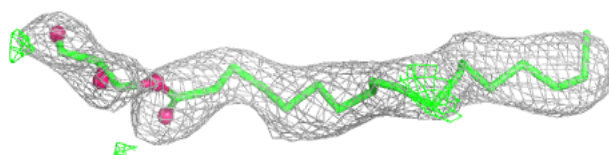
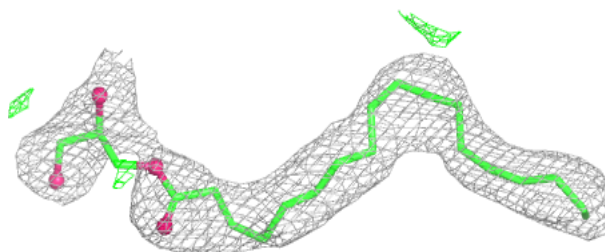


Electron density around OLC A 609:

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

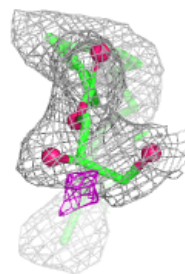
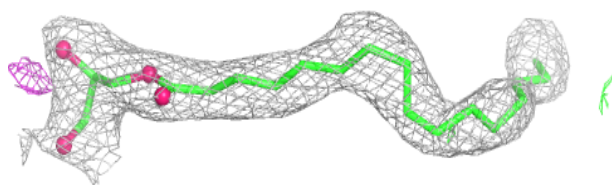
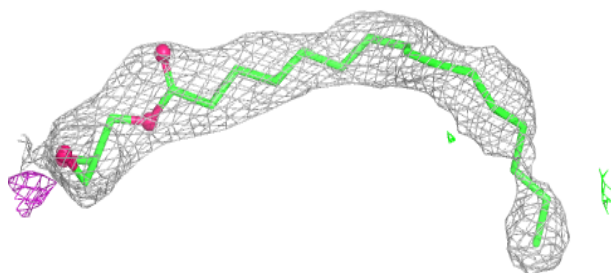
**Electron density around OLC A 614:**

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

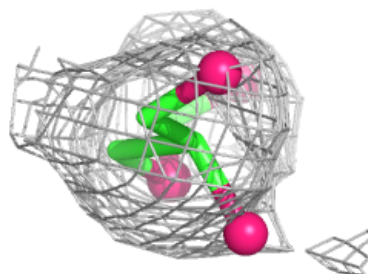
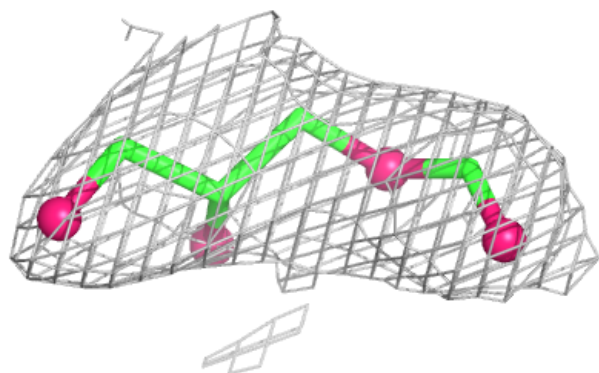
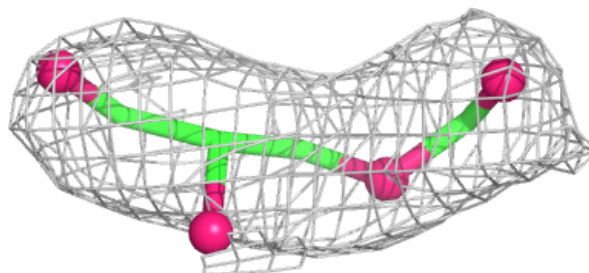


Electron density around OLC A 607:

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

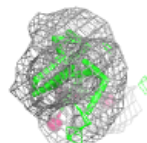
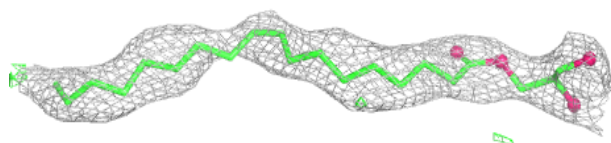
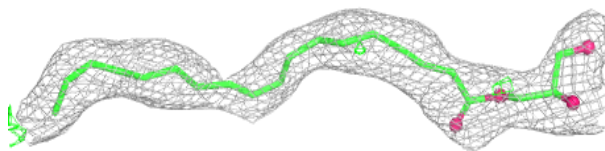
**Electron density around OLC A 611:**

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

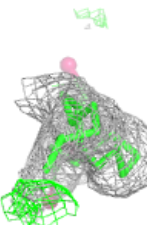
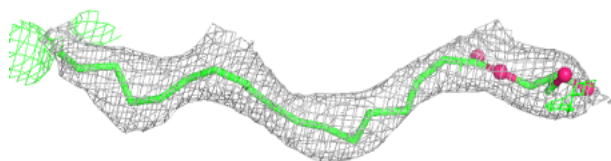
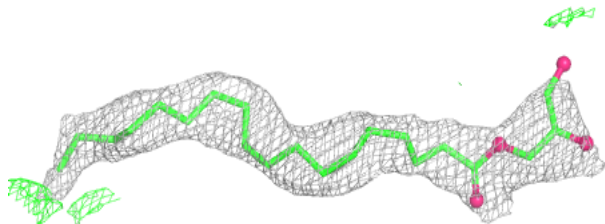


Electron density around OLC B 202:

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

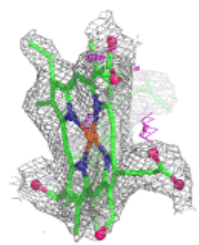
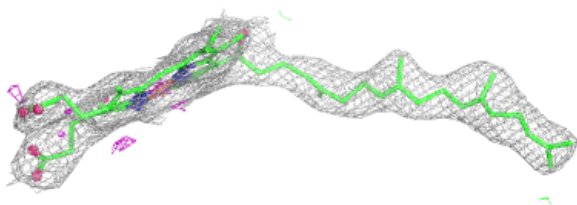
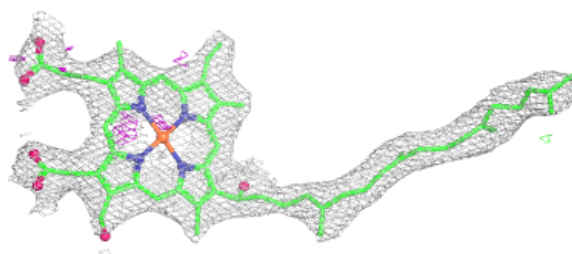
**Electron density around OLC A 605:**

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



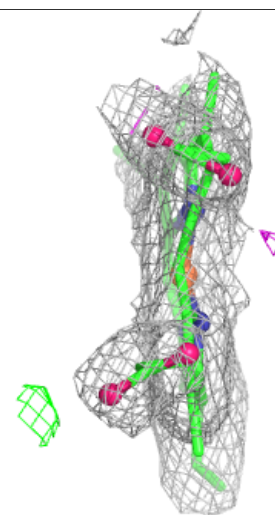
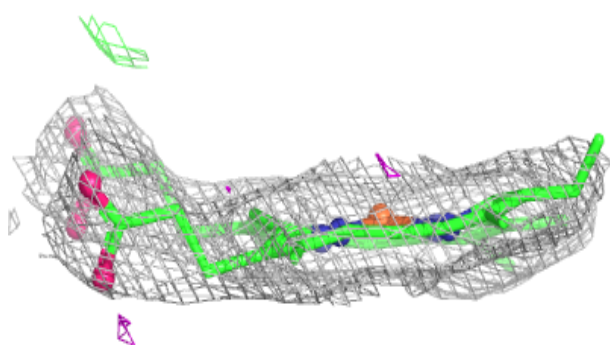
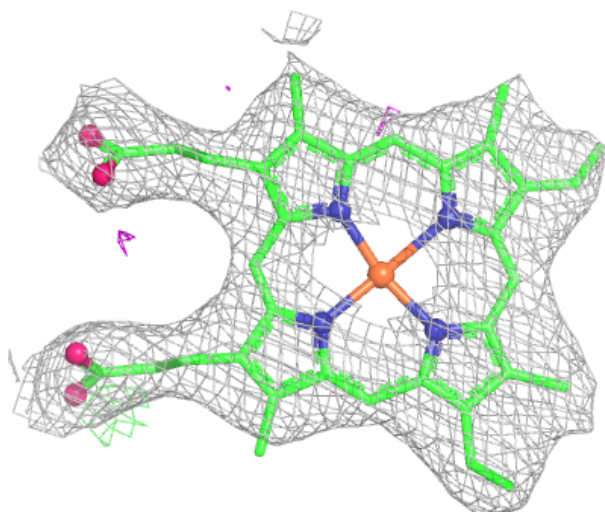
Electron density around HAS A 603:

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



Electron density around HEM A 602:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.