



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:52 AM UTC

PDB ID : 4G70 / pdb_00004g70
Title : Structure of Recombinant Cytochrome ba3 Oxidase mutant V236T from *Thermus thermophilus*
Authors : Li, Y.; Chen, Y.; Stout, C.D.
Deposited on : 2012-07-19
Resolution : 2.60 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

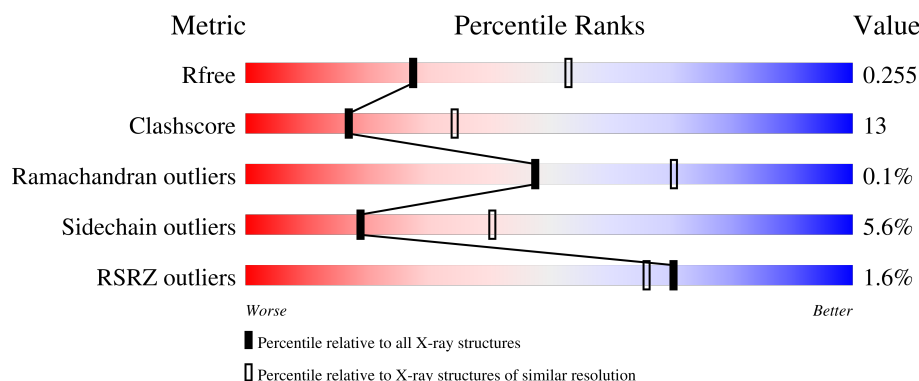
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	569	
2	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
5	HAS	A	602	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6374 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4346	2950	692	688	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	THR	VAL	engineered mutation	UNP Q5SJ79

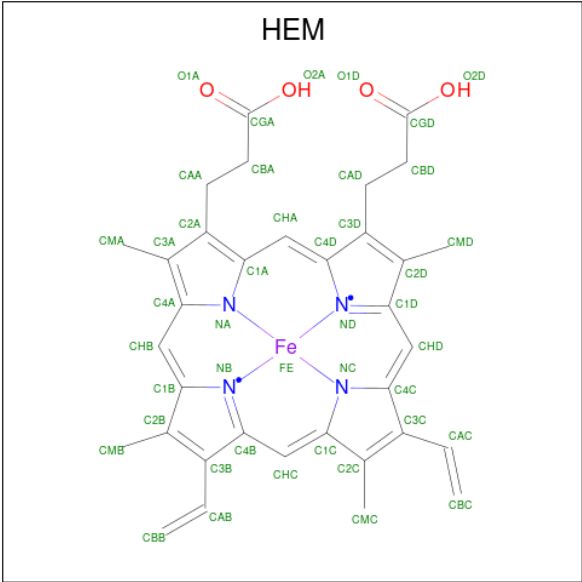
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1275	829	211	231	4			

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

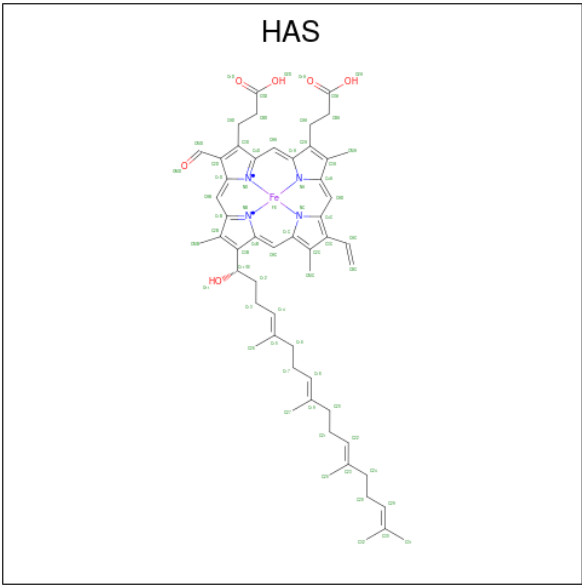
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	31	Total	C	N	O	0	0	0
			237	166	36	35			

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 5 is HEME-AS (CCD ID: HAS) (formula: $C_{54}H_{64}FeN_4O_6$).

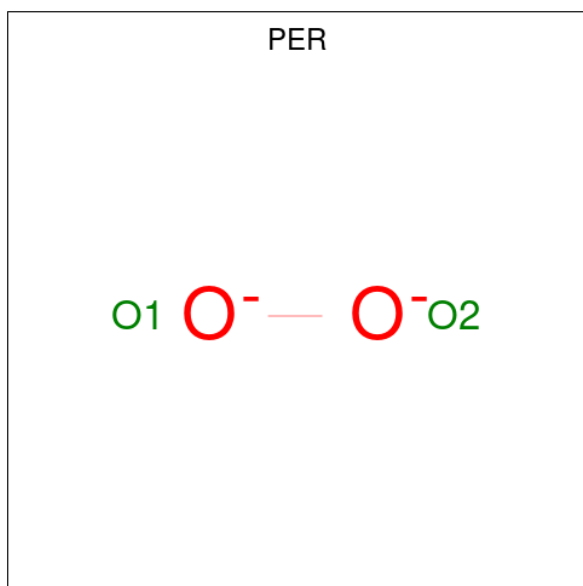


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

- Molecule 6 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

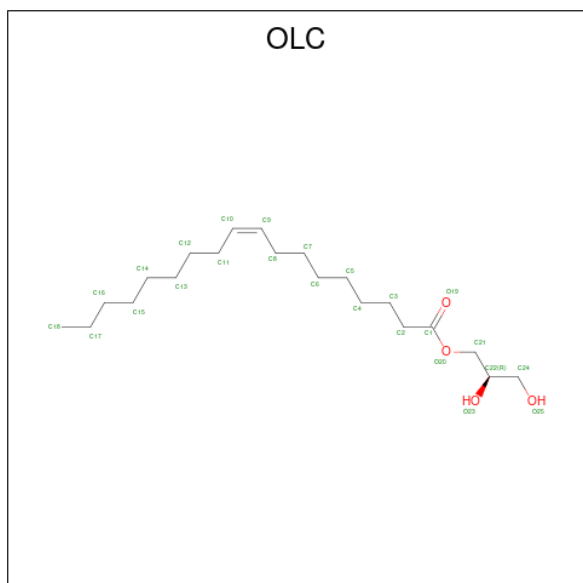
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cu	0	0
			1	1		

- Molecule 7 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



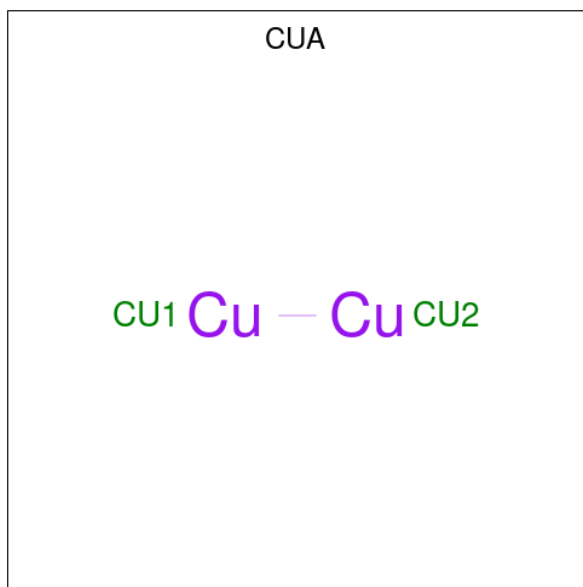
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			2	2		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 20 18 2	0	0
8	A	1	Total C O 22 18 4	0	0
8	A	1	Total C O 20 18 2	0	0
8	A	1	Total C O 18 14 4	0	0
8	A	1	Total C O 13 9 4	0	0
8	A	1	Total C O 8 4 4	0	0
8	A	1	Total C O 12 8 4	0	0
8	A	1	Total C O 9 7 2	0	0
8	A	1	Total C O 25 21 4	0	0
8	A	1	Total C O 13 9 4	0	0
8	A	1	Total C O 24 20 4	0	0
8	B	1	Total C O 24 20 4	0	0
8	B	1	Total C O 23 19 4	0	0
8	B	1	Total C O 16 12 4	0	0
8	C	1	Total C O 23 19 4	0	0
8	C	1	Total C 13 13	0	0

- Molecule 9 is DINUCLEAR COPPER ION (CCD ID: 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	71	Total	O	0	0
			71	71		
10	B	44	Total	O	0	0
			44	44		
10	C	5	Total	O	0	0
			5	5		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.48Å 98.36Å 94.78Å 90.00° 127.39° 90.00°	Depositor
Resolution (Å)	75.30 – 2.60 75.30 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (75.30-2.60) 97.9 (75.30-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.194 , 0.252 0.208 , 0.255	Depositor DCC
R_{free} test set	1603 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6374	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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: CUA, CU, PER, OLC, 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	1.46	6/4503 (0.1%)	1.23	27/6186 (0.4%)
2	B	1.13	1/1311 (0.1%)	1.09	1/1795 (0.1%)
3	C	1.07	0/243	1.24	2/331 (0.6%)
All	All	1.38	7/6057 (0.1%)	1.20	30/8312 (0.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	354	LEU	CA-CB	52.67	2.36	1.53
1	A	354	LEU	CG-CD2	30.01	2.51	1.52
1	A	137	PRO	CA-C	7.02	1.55	1.51
1	A	453	ILE	C-O	-5.89	1.17	1.24
1	A	386	HIS	CG-CD2	5.69	1.42	1.35
2	B	148	ILE	CA-C	5.64	1.59	1.52
1	A	282	HIS	CG-CD2	5.23	1.41	1.35

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	LEU	CB-CG-CD2	-25.23	35.00	110.70
1	A	354	LEU	CB-CA-C	21.86	144.62	110.96
1	A	514	GLY	N-CA-C	-10.11	91.72	112.34
1	A	515	PRO	N-CA-C	-7.87	98.71	111.15
3	C	23	TRP	N-CA-C	7.75	119.42	110.97
1	A	516	GLU	N-CA-C	-7.61	98.57	110.36
2	B	47	ALA	N-CA-C	-7.30	99.22	110.10
1	A	208	LEU	N-CA-C	6.75	118.30	111.07
1	A	527	ILE	N-CA-C	6.75	117.50	110.62
1	A	514	GLY	CA-C-N	-6.45	113.32	119.90
1	A	514	GLY	C-N-CA	-6.45	113.32	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	GLY	N-CA-C	-6.36	104.79	112.49
1	A	516	GLU	CA-C-N	-6.26	113.85	122.30
1	A	516	GLU	C-N-CA	-6.26	113.85	122.30
1	A	233	HIS	N-CA-CB	6.08	116.17	110.39
1	A	316	VAL	N-CA-C	-5.90	104.99	110.53
1	A	91	TYR	N-CA-C	5.71	117.51	111.28
1	A	496	GLU	N-CA-C	5.69	117.64	110.24
1	A	354	LEU	CA-CB-CG	-5.61	96.66	116.30
1	A	70	THR	N-CA-C	-5.54	104.94	110.97
1	A	181	LEU	N-CA-C	5.52	120.42	111.37
1	A	310	LEU	N-CA-C	-5.46	105.33	111.28
1	A	29	PHE	N-CA-C	5.36	117.13	111.28
1	A	354	LEU	N-CA-CB	-5.34	102.11	109.91
1	A	385	PHE	N-CA-C	5.10	119.21	112.89
1	A	451	ALA	N-CA-C	5.09	117.70	109.40
3	C	28	ALA	N-CA-C	-5.08	105.63	111.07
1	A	261	SER	N-CA-C	5.06	116.30	107.49
1	A	30	LEU	N-CA-C	-5.04	105.68	111.07
1	A	151	VAL	N-CA-C	-5.00	104.74	111.44

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	4346	0	4417	116	0
2	B	1275	0	1234	28	0
3	C	237	0	256	7	0
4	A	43	0	30	5	0
5	A	65	0	62	3	0
6	A	1	0	0	0	0
7	A	2	0	0	1	0
8	A	184	0	245	26	0
8	B	63	0	89	10	0
8	C	36	0	53	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	2	0	0	0	0
10	A	71	0	0	6	0
10	B	44	0	0	6	2
10	C	5	0	0	0	0
All	All	6374	0	6386	160	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 (160) 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:CE1	1.70	1.56
1:A:233:HIS:NE2	1:A:237:TYR:HE1	0.78	1.26
7:A:604:PER:O1	7:A:604:PER:O2	1.52	1.23
1:A:233:HIS:CD2	1:A:237:TYR:HE1	1.74	1.05
1:A:354:LEU:CA	1:A:354:LEU:CB	2.36	1.04
8:B:203:OLC:H6	3:C:33:ARG:HE	1.39	0.87
2:B:120:GLY:HA2	8:B:203:OLC:H2	1.59	0.85
1:A:233:HIS:CD2	1:A:237:TYR:CE1	2.55	0.84
10:A:705:HOH:O	8:B:203:OLC:H4A	1.79	0.83
1:A:517:ASP:HA	1:A:519:ARG:HH21	1.43	0.82
1:A:514:GLY:O	1:A:515:PRO:C	2.20	0.80
8:A:605:OLC:H12	8:A:613:OLC:H14A	1.65	0.78
1:A:411:LYS:HE3	1:A:497:ARG:HH21	1.49	0.76
1:A:517:ASP:HB2	1:A:519:ARG:HE	1.50	0.76
8:A:613:OLC:H21A	10:A:706:HOH:O	1.84	0.76
1:A:220:ASP:HB3	1:A:223:VAL:HG12	1.68	0.75
2:B:101:ALA:O	10:B:314:HOH:O	2.05	0.74
2:B:47:ALA:O	10:B:341:HOH:O	2.07	0.73
5:A:602:HAS:HMC1	5:A:602:HAS:HBC1	1.72	0.71
1:A:465:VAL:HG13	8:A:612:OLC:H5A	1.73	0.71
2:B:35:TYR:OH	8:B:202:OLC:H24A	1.91	0.70
2:B:141:ARG:HH12	8:B:203:OLC:H24A	1.57	0.69
1:A:168:ARG:HH11	8:A:610:OLC:C22	2.08	0.67
4:A:601:HEM:O2A	10:A:717:HOH:O	2.13	0.67
1:A:167:TRP:CZ3	8:A:611:OLC:H22	2.29	0.67
4:A:601:HEM:HBC2	4:A:601:HEM:HMC1	1.76	0.66
1:A:167:TRP:CH2	8:A:611:OLC:H22	2.31	0.65
8:C:101:OLC:H10	8:C:102:OLC:H8	1.79	0.65
1:A:161:TYR:CE2	8:A:610:OLC:H21	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:PRO:HG3	1:A:144:ALA:HB3	1.80	0.64
1:A:443:GLY:O	10:A:737:HOH:O	2.15	0.63
1:A:233:HIS:CE1	1:A:237:TYR:CE1	2.75	0.63
1:A:293:THR:HG23	8:A:607:OLC:H8	1.82	0.61
1:A:463:ALA:O	1:A:467:MET:HG3	1.99	0.61
2:B:17:GLY:HA3	8:B:204:OLC:H3	1.84	0.60
1:A:156:THR:O	1:A:160:ILE:HG13	2.01	0.59
1:A:174:ASN:HB3	1:A:177:LYS:HD2	1.85	0.59
1:A:111:TRP:HE3	1:A:115:ILE:CD1	2.16	0.58
8:A:606:OLC:H13A	8:A:613:OLC:H12	1.84	0.58
1:A:69:LEU:HD11	4:A:601:HEM:HBD2	1.86	0.58
1:A:232:GLY:O	1:A:235:ILE:HG22	2.04	0.58
1:A:233:HIS:NE2	1:A:237:TYR:CZ	2.62	0.58
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.39	0.58
1:A:401:LEU:O	1:A:405:LEU:HB2	2.04	0.58
8:B:203:OLC:H7A	8:C:101:OLC:O25	2.04	0.57
1:A:168:ARG:NH1	8:A:610:OLC:C22	2.68	0.57
1:A:403:TRP:CZ3	1:A:404:LEU:HD13	2.40	0.57
8:A:613:OLC:C8	8:A:613:OLC:H13A	2.34	0.56
3:C:18:THR:HG23	8:C:102:OLC:H12A	1.86	0.56
1:A:277:THR:N	1:A:278:PRO:CD	2.69	0.55
1:A:229:TRP:CE3	1:A:232:GLY:HA3	2.43	0.54
3:C:18:THR:HG23	8:C:102:OLC:C12	2.38	0.54
1:A:339:LEU:HD13	1:A:346:PHE:HZ	1.73	0.54
1:A:398:MET:O	1:A:401:LEU:HB2	2.08	0.53
2:B:58:VAL:O	10:B:344:HOH:O	2.17	0.53
1:A:341:TRP:CZ2	8:A:615:OLC:H3	2.44	0.53
1:A:429:PHE:CE2	1:A:433:MET:HE3	2.44	0.53
1:A:341:TRP:CE2	8:A:615:OLC:H3	2.43	0.53
2:B:91:GLN:OE1	10:B:319:HOH:O	2.19	0.53
4:A:601:HEM:HBC2	4:A:601:HEM:CMC	2.38	0.52
1:A:517:ASP:CA	1:A:519:ARG:HH21	2.20	0.52
2:B:93:ASN:O	10:B:309:HOH:O	2.19	0.52
10:A:705:HOH:O	8:B:203:OLC:H6A	2.09	0.52
8:B:203:OLC:H6	3:C:33:ARG:NE	2.19	0.52
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.45	0.52
1:A:562:TRP:HA	2:B:155:LEU:HG	1.92	0.52
1:A:55:LEU:HD11	1:A:59:LEU:HD12	1.92	0.52
1:A:382:PRO:HA	1:A:385:PHE:CZ	2.46	0.51
1:A:465:VAL:HG22	8:A:612:OLC:H3A	1.91	0.51
1:A:400:SER:HB2	1:A:403:TRP:CZ2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ASN:HB3	2:B:150:ASN:HB2	1.93	0.50
2:B:11:ILE:HA	3:C:5:PRO:HG3	1.92	0.50
1:A:292:PRO:CB	8:A:607:OLC:H3A	2.41	0.50
1:A:518:ARG:NH2	10:A:760:HOH:O	2.44	0.50
1:A:111:TRP:HE3	1:A:115:ILE:HD11	1.75	0.50
1:A:290:ILE:HB	1:A:295:LYS:HE3	1.93	0.50
1:A:280:GLY:HA3	1:A:542:TYR:OH	2.13	0.49
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.48	0.49
1:A:371:LEU:HD21	3:C:27:TYR:HD1	1.77	0.49
8:A:613:OLC:H13A	8:A:613:OLC:H8A	1.93	0.49
1:A:341:TRP:HB3	8:A:606:OLC:H24A	1.95	0.49
2:B:18:TRP:CE3	3:C:12:ILE:HD13	2.47	0.49
1:A:90:VAL:HG11	1:A:106:MET:HE3	1.94	0.49
2:B:158:GLN:H	2:B:158:GLN:NE2	2.11	0.49
1:A:254:GLN:HG2	1:A:343:ASN:HD21	1.78	0.48
1:A:263:PRO:HG2	1:A:516:GLU:HB3	1.94	0.48
1:A:514:GLY:C	1:A:515:PRO:O	2.50	0.48
1:A:247:ILE:HA	1:A:251:LEU:HB2	1.96	0.48
1:A:213:PHE:CD2	8:A:608:OLC:H4	2.48	0.48
1:A:472:LEU:HD22	8:A:613:OLC:H11	1.95	0.48
1:A:300:VAL:HG11	8:A:607:OLC:H16	1.94	0.47
1:A:140:LYS:HE3	1:A:211:TRP:NE1	2.29	0.47
1:A:233:HIS:CD2	1:A:233:HIS:C	2.93	0.47
1:A:517:ASP:OD1	1:A:517:ASP:N	2.37	0.47
8:A:607:OLC:H4A	2:B:37:LEU:HG	1.96	0.47
8:C:101:OLC:C10	8:C:102:OLC:H7A	2.44	0.47
1:A:369:PHE:C	1:A:369:PHE:CD2	2.92	0.47
1:A:262:ASP:C	1:A:262:ASP:OD2	2.57	0.47
1:A:330:ARG:O	1:A:334:GLY:HA3	2.14	0.47
1:A:277:THR:N	1:A:278:PRO:HD2	2.30	0.47
1:A:292:PRO:HB2	8:A:607:OLC:H3A	1.96	0.47
1:A:435:MET:HB2	1:A:473:ALA:HB1	1.96	0.47
1:A:233:HIS:CD2	1:A:237:TYR:CD1	3.01	0.47
2:B:120:GLY:CA	8:B:203:OLC:H2	2.37	0.47
1:A:28:GLY:HA2	1:A:83:LEU:HD12	1.97	0.46
1:A:91:TYR:OH	1:A:407:ASN:ND2	2.48	0.46
1:A:556:VAL:CG1	2:B:55:PRO:HG3	2.45	0.46
1:A:263:PRO:HG2	1:A:516:GLU:CB	2.44	0.46
1:A:511:VAL:HG12	1:A:512:ILE:N	2.31	0.46
2:B:45:ILE:O	10:B:302:HOH:O	2.20	0.46
1:A:277:THR:H	1:A:278:PRO:CD	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:VAL:O	1:A:308:PRO:HD2	2.16	0.45
1:A:310:LEU:HD13	2:B:22:SER:HB3	1.97	0.45
2:B:67:PRO:O	2:B:92:PRO:HG3	2.17	0.45
1:A:381:VAL:HB	1:A:382:PRO:HD3	1.97	0.45
1:A:241:LEU:N	1:A:242:PRO:CD	2.80	0.45
1:A:300:VAL:HG11	8:A:607:OLC:C16	2.47	0.45
1:A:286:ALA:HB1	2:B:125:VAL:HA	1.98	0.45
1:A:16:PRO:HB2	1:A:103:MET:HE2	1.98	0.44
1:A:111:TRP:CE3	1:A:115:ILE:HD11	2.53	0.44
1:A:254:GLN:CG	1:A:343:ASN:HD21	2.30	0.44
1:A:302:THR:O	1:A:305:VAL:HG12	2.18	0.44
1:A:548:GLN:O	1:A:548:GLN:HG2	2.16	0.44
1:A:236:THR:HB	5:A:602:HAS:CAC	2.48	0.44
1:A:264:MET:HE1	2:B:19:LEU:HD11	1.99	0.44
1:A:354:LEU:CA	1:A:354:LEU:CG	2.96	0.44
1:A:339:LEU:HD13	1:A:346:PHE:CZ	2.51	0.44
1:A:195:LEU:HD23	1:A:195:LEU:HA	1.82	0.43
1:A:258:LYS:HB3	1:A:510:GLU:O	2.18	0.43
8:A:607:OLC:H11A	8:A:607:OLC:H14A	1.79	0.43
2:B:64:TRP:HB3	2:B:84:LEU:HD13	2.00	0.43
1:A:114:PHE:O	1:A:118:VAL:HG23	2.18	0.43
2:B:113:ILE:HA	2:B:127:VAL:O	2.19	0.43
1:A:311:MET:HG3	2:B:19:LEU:HD21	2.01	0.43
1:A:96:GLU:OE2	1:A:180:PRO:HB2	2.19	0.43
1:A:438:GLY:HA3	1:A:470:ASN:OD1	2.19	0.43
1:A:477:LEU:HD13	4:A:601:HEM:HMB3	2.01	0.43
1:A:387:LEU:HD22	1:A:433:MET:HE1	2.00	0.43
1:A:81:THR:HB	1:A:239:TRP:CD1	2.54	0.42
1:A:105:LEU:HA	1:A:105:LEU:HD23	1.76	0.42
1:A:184:TYR:CE2	1:A:266:ARG:HB3	2.55	0.42
1:A:230:TRP:C	1:A:230:TRP:CD1	2.98	0.42
1:A:285:PHE:CZ	1:A:369:PHE:HA	2.54	0.42
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.96	0.42
1:A:46:TYR:HA	1:A:453:ILE:HD11	2.01	0.42
1:A:233:HIS:N	1:A:234:PRO:HD2	2.35	0.42
8:A:615:OLC:H13	8:A:615:OLC:H10	1.58	0.42
1:A:307:VAL:N	1:A:308:PRO:HD2	2.35	0.41
2:B:46:PRO:HA	2:B:134:THR:O	2.20	0.41
1:A:369:PHE:C	1:A:369:PHE:HD2	2.28	0.41
1:A:483:LEU:HD23	1:A:483:LEU:HA	1.85	0.41
2:B:78:GLN:HG3	2:B:102:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:101:OLC:H10	8:C:102:OLC:C8	2.48	0.41
1:A:235:ILE:O	1:A:238:PHE:HB3	2.21	0.41
5:A:602:HAS:HMC1	5:A:602:HAS:CBC	2.44	0.41
1:A:134:THR:O	1:A:135:PHE:C	2.64	0.41
1:A:191:LEU:HD11	8:A:611:OLC:H3	2.04	0.40
1:A:56:LYS:O	1:A:60:PRO:HA	2.22	0.40
1:A:204:ALA:HA	1:A:208:LEU:HB2	2.04	0.40
2:B:71:VAL:HG22	2:B:81:VAL:HG22	2.04	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:306:HOH:O	10:B:320:HOH:O[2_556]	1.32	0.88
10:B:323:HOH:O	10:B:323:HOH:O[2_556]	1.41	0.79

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	552/569 (97%)	522 (95%)	29 (5%)	1 (0%)	43	66
2	B	164/168 (98%)	158 (96%)	6 (4%)	0	100	100
3	C	29/34 (85%)	28 (97%)	1 (3%)	0	100	100
All	All	745/771 (97%)	708 (95%)	36 (5%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/464 (95%)	419 (95%)	21 (5%)	23	47
2	B	131/138 (95%)	124 (95%)	7 (5%)	20	43
3	C	23/27 (85%)	18 (78%)	5 (22%)	1	2
All	All	594/629 (94%)	561 (94%)	33 (6%)	19	40

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	54	LEU
1	A	58	LEU
1	A	133	TYR
1	A	215	LEU
1	A	230	TRP
1	A	254	GLN
1	A	262	ASP
1	A	274	LEU
1	A	290	ILE
1	A	332	LEU
1	A	392	LEU
1	A	405	LEU
1	A	413	ILE
1	A	425	VAL
1	A	456	VAL
1	A	516	GLU
1	A	517	ASP
1	A	518	ARG
1	A	519	ARG
1	A	520	LEU
2	B	12	LEU
2	B	26	LEU
2	B	37	LEU
2	B	58	VAL
2	B	61	GLU

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Mol	Chain	Res	Type
2	B	158	GLN
2	B	167	LYS
3	C	13	LEU
3	C	17	LEU
3	C	20	LEU
3	C	23	TRP
3	C	24	LEU

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

Mol	Chain	Res	Type
1	A	254	GLN
1	A	407	ASN
1	A	455	GLN
2	B	91	GLN
2	B	158	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HAS	A	602	1,7	72,72,72	2.21	29 (40%)	87,109,109	1.76	20 (22%)
8	OLC	A	609	-	12,12,24	0.75	0	13,13,25	0.61	0
8	OLC	A	606	-	21,21,24	0.56	0	22,22,25	1.25	3 (13%)
8	OLC	A	607	-	19,19,24	0.66	1 (5%)	19,19,25	0.69	1 (5%)
8	OLC	B	203	-	22,22,24	0.85	1 (4%)	23,23,25	1.57	3 (13%)
8	OLC	A	610	-	7,7,24	0.41	0	6,7,25	0.89	0
8	OLC	C	102	-	12,12,24	0.12	0	11,11,25	0.67	0
8	OLC	A	614	-	12,12,24	0.62	0	13,13,25	0.87	0
8	OLC	A	605	-	19,19,24	0.49	0	19,19,25	0.85	0
9	CUA	B	201	2	0,1,1	-	-	-	-	-
8	OLC	A	608	-	17,17,24	0.56	0	18,18,25	0.54	0
8	OLC	A	612	-	8,8,24	0.64	0	8,8,25	1.45	1 (12%)
8	OLC	A	613	-	24,24,24	0.67	1 (4%)	25,25,25	0.95	1 (4%)
4	HEM	A	601	1	50,50,50	3.27	30 (60%)	67,82,82	2.29	23 (34%)
8	OLC	A	615	-	23,23,24	0.49	0	24,24,25	0.96	2 (8%)
8	OLC	B	202	-	23,23,24	0.51	0	24,24,25	0.74	1 (4%)
7	PER	A	604	5,6	1,1,1	0.71	0	-	-	-
8	OLC	C	101	-	22,22,24	0.54	0	23,23,25	0.75	0
8	OLC	A	611	-	11,11,24	0.74	0	12,12,25	0.57	0
8	OLC	B	204	-	15,15,24	0.51	0	16,16,25	0.64	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
5	HAS	A	602	1,7	1/1/8/18	10/42/82/82	-
8	OLC	A	609	-	-	6/12/12/24	-
8	OLC	C	102	-	-	8/10/10/24	-
8	OLC	A	614	-	-	8/12/12/24	-
8	OLC	A	606	-	-	9/21/21/24	-
8	OLC	A	605	-	-	8/18/18/24	-
8	OLC	A	615	-	-	9/23/23/24	-
8	OLC	B	202	-	-	11/23/23/24	-
4	HEM	A	601	1	-	5/14/54/54	-
8	OLC	A	607	-	-	9/18/18/24	-
8	OLC	A	608	-	-	6/17/17/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OLC	A	612	-	-	5/6/6/24	-
8	OLC	A	613	-	-	16/24/24/24	-
8	OLC	B	203	-	-	9/22/22/24	-
8	OLC	A	611	-	-	5/11/11/24	-
8	OLC	C	101	-	-	11/22/22/24	-
8	OLC	B	204	-	-	5/15/15/24	-
8	OLC	A	610	-	-	4/6/6/24	-

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	HEM	C3C-C4C	-8.69	1.30	1.46
4	A	601	HEM	C3B-C2B	6.30	1.50	1.37
5	A	602	HAS	CHB-C1D	6.06	1.50	1.38
4	A	601	HEM	CAB-C3B	-5.85	1.31	1.47
4	A	601	HEM	CHC-C1C	5.61	1.49	1.38
4	A	601	HEM	C1C-C2C	-5.50	1.34	1.45
4	A	601	HEM	C3C-C2C	5.49	1.48	1.37
4	A	601	HEM	C1B-C2B	-5.27	1.33	1.44
4	A	601	HEM	CHB-C1B	5.26	1.49	1.38
5	A	602	HAS	CAC-C3C	-5.18	1.33	1.47
5	A	602	HAS	CHA-C4D	5.08	1.50	1.39
4	A	601	HEM	CHD-C4C	4.99	1.48	1.38
4	A	601	HEM	CHA-C1A	4.84	1.50	1.39
4	A	601	HEM	CBB-CAB	4.52	1.52	1.30
5	A	602	HAS	CBC-CAC	4.32	1.51	1.30
5	A	602	HAS	CHC-C1C	4.15	1.48	1.39
4	A	601	HEM	FE-NB	4.13	2.07	1.94
5	A	602	HAS	C4D-ND	3.91	1.46	1.38
5	A	602	HAS	CHD-C4A	-3.86	1.30	1.38
5	A	602	HAS	O1D-CGD	3.76	1.34	1.22
4	A	601	HEM	FE-NC	3.54	2.06	1.95
4	A	601	HEM	FE-ND	3.43	2.05	1.94
5	A	602	HAS	CHD-C4C	3.34	1.46	1.39
5	A	602	HAS	FE-NA	3.32	2.06	1.95
5	A	602	HAS	C3C-C2C	3.19	1.51	1.41
5	A	602	HAS	C1D-ND	3.18	1.45	1.40
5	A	602	HAS	CHA-C1A	-3.09	1.32	1.38
5	A	602	HAS	C1C-C2C	-3.05	1.36	1.43
5	A	602	HAS	CMD-C2D	2.95	1.52	1.45
4	A	601	HEM	CHA-C4D	-2.94	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	HEM	C1A-NA	2.94	1.45	1.39
4	A	601	HEM	CHD-C1D	-2.92	1.32	1.39
4	A	601	HEM	C4A-NA	-2.88	1.34	1.39
4	A	601	HEM	C4A-C3A	2.88	1.49	1.43
5	A	602	HAS	C4B-C3B	2.87	1.49	1.44
5	A	602	HAS	CHB-C1B	-2.85	1.32	1.39
4	A	601	HEM	C4D-ND	-2.82	1.35	1.40
4	A	601	HEM	C1A-C2A	2.79	1.50	1.44
4	A	601	HEM	C1B-NB	-2.76	1.35	1.40
4	A	601	HEM	C1D-C2D	2.74	1.50	1.44
5	A	602	HAS	O2D-CGD	-2.61	1.22	1.30
5	A	602	HAS	C4C-NC	2.59	1.44	1.39
5	A	602	HAS	C1A-C2A	2.58	1.49	1.45
5	A	602	HAS	FE-ND	2.54	2.02	1.94
8	B	203	OLC	O20-C1	2.53	1.40	1.33
4	A	601	HEM	C3B-C4B	2.47	1.49	1.44
4	A	601	HEM	C1C-NC	-2.47	1.35	1.39
5	A	602	HAS	C2A-C3A	-2.36	1.31	1.36
4	A	601	HEM	CHB-C4A	-2.35	1.34	1.39
4	A	601	HEM	FE-NA	2.33	2.02	1.95
8	A	607	OLC	O20-C1	2.23	1.39	1.33
5	A	602	HAS	C2D-C1D	2.22	1.49	1.44
4	A	601	HEM	C1D-ND	-2.21	1.34	1.38
4	A	601	HEM	C4D-C3D	2.18	1.48	1.45
5	A	602	HAS	C1B-C2B	2.17	1.48	1.44
5	A	602	HAS	C1B-NB	-2.11	1.34	1.38
8	A	613	OLC	O20-C1	2.08	1.39	1.33
5	A	602	HAS	C4A-C3A	2.05	1.49	1.45
4	A	601	HEM	CHC-C4B	-2.05	1.34	1.39
5	A	602	HAS	FE-NB	2.04	2.01	1.94
5	A	602	HAS	C4A-NA	-2.03	1.35	1.39
5	A	602	HAS	C4B-NB	-2.03	1.36	1.40

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	HEM	CHC-C4B-NB	7.08	132.05	124.42
4	A	601	HEM	C4B-C3B-C2B	-6.78	101.05	107.28
4	A	601	HEM	C3B-C4B-NB	-6.18	105.03	109.47
5	A	602	HAS	C4C-C3C-C2C	-4.95	101.14	107.30
5	A	602	HAS	C1D-ND-C4D	-4.79	99.54	105.21
5	A	602	HAS	CHB-C1B-C2B	-4.77	117.50	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	203	OLC	O20-C21-C22	4.09	125.10	105.85
4	A	601	HEM	C1B-NB-C4B	3.92	109.84	105.21
5	A	602	HAS	C12-C11-C3B	3.86	118.16	112.12
5	A	602	HAS	C27-C19-C20	3.78	121.80	115.23
8	B	203	OLC	C21-C22-C24	3.75	124.40	111.77
4	A	601	HEM	CHA-C4D-ND	3.74	128.99	124.37
8	B	203	OLC	C21-O20-C1	3.73	130.74	117.12
5	A	602	HAS	CAA-CBA-CGA	-3.55	104.25	113.67
5	A	602	HAS	CAD-CBD-CGD	-3.51	104.36	113.67
4	A	601	HEM	C3C-C2C-C1C	-3.30	103.93	107.05
4	A	601	HEM	CHD-C1D-ND	3.29	127.96	124.42
8	A	612	OLC	C4-C3-C2	-3.23	101.25	113.13
4	A	601	HEM	C3B-C2B-C1B	3.17	108.79	106.41
4	A	601	HEM	CHD-C4C-C3C	-3.16	119.89	125.21
8	A	606	OLC	O20-C21-C22	-3.04	91.56	105.85
4	A	601	HEM	CMA-C3A-C4A	-3.01	120.83	125.42
4	A	601	HEM	C4D-ND-C1D	3.01	108.77	105.21
4	A	601	HEM	CHD-C4C-NC	3.00	127.72	124.45
5	A	602	HAS	C21-C22-C23	-2.95	120.86	127.62
5	A	602	HAS	C12-C13-C14	2.91	119.82	112.16
5	A	602	HAS	CMB-C2B-C3B	-2.91	124.64	130.28
5	A	602	HAS	CHB-C1D-ND	-2.76	120.95	124.37
4	A	601	HEM	CHA-C4D-C3D	-2.74	120.17	125.23
5	A	602	HAS	CHC-C4B-NB	2.69	127.70	124.37
4	A	601	HEM	CHA-C1A-NA	2.64	128.65	123.86
5	A	602	HAS	C2C-C1C-NC	2.62	114.34	110.14
4	A	601	HEM	CAD-CBD-CGD	-2.61	106.74	113.67
5	A	602	HAS	C20-C19-C18	-2.59	115.35	121.17
4	A	601	HEM	CHB-C1B-C2B	-2.59	119.59	126.95
4	A	601	HEM	CMC-C2C-C1C	2.57	129.25	124.73
4	A	601	HEM	CHC-C1C-NC	-2.56	121.67	124.45
5	A	602	HAS	O11-C11-C3B	-2.53	106.62	111.26
4	A	601	HEM	O2A-CGA-CBA	2.51	121.92	114.00
8	A	615	OLC	C3-C2-C1	-2.41	104.85	113.69
5	A	602	HAS	CHD-C4A-C3A	-2.41	120.47	125.49
8	A	606	OLC	C21-C22-C24	2.39	119.84	111.77
8	A	606	OLC	C21-O20-C1	2.37	125.79	117.12
8	A	607	OLC	C21-O20-C1	2.36	123.63	116.07
4	A	601	HEM	C2A-C1A-NA	-2.27	107.64	110.15
8	A	613	OLC	O20-C21-C22	2.26	116.50	105.85
4	A	601	HEM	CMB-C2B-C3B	-2.24	123.01	128.43
5	A	602	HAS	CHC-C1C-NC	-2.22	119.84	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	HAS	CHA-C1A-C2A	-2.20	121.38	124.86
5	A	602	HAS	C25-C23-C24	2.16	118.98	115.23
4	A	601	HEM	O1A-CGA-CBA	-2.13	116.33	123.09
8	B	202	OLC	O20-C21-C22	2.06	115.55	105.85
5	A	602	HAS	C4A-C3A-C2A	-2.04	103.94	106.97
8	A	615	OLC	C21-C22-C24	-2.02	104.98	111.77
4	A	601	HEM	CMC-C2C-C3C	-2.00	123.58	128.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	602	HAS	NA

All (144) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	HEM	C2B-C3B-CAB-CBB
5	A	602	HAS	C1D-C2D-CMD-OMD
8	A	606	OLC	C21-C22-C24-O25
8	A	609	OLC	O20-C21-C22-C24
8	A	610	OLC	O20-C21-C22-C24
8	A	610	OLC	O19-C1-O20-C21
8	A	611	OLC	O20-C21-C22-C24
8	A	613	OLC	C21-C22-C24-O25
8	A	613	OLC	O20-C21-C22-C24
8	A	614	OLC	C21-C22-C24-O25
8	A	614	OLC	O20-C21-C22-C24
8	A	615	OLC	O20-C21-C22-C24
8	A	615	OLC	O20-C21-C22-O23
8	B	202	OLC	C21-C22-C24-O25
8	B	204	OLC	C21-C22-C24-O25
8	A	609	OLC	O19-C1-O20-C21
8	A	609	OLC	C2-C1-O20-C21
8	A	610	OLC	O20-C21-C22-O23
8	A	611	OLC	O20-C21-C22-O23
8	A	613	OLC	O20-C21-C22-O23
8	A	614	OLC	O20-C21-C22-O23
8	A	613	OLC	C2-C3-C4-C5
5	A	602	HAS	C17-C18-C19-C27
8	B	203	OLC	C2-C1-O20-C21
8	C	101	OLC	C2-C1-O20-C21
8	A	606	OLC	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
8	A	608	OLC	O20-C21-C22-C24
8	B	203	OLC	O20-C21-C22-C24
8	A	605	OLC	C2-C1-O20-C21
8	A	607	OLC	C2-C1-O20-C21
8	B	203	OLC	O19-C1-O20-C21
8	A	608	OLC	O20-C21-C22-O23
8	A	609	OLC	O20-C21-C22-O23
8	B	203	OLC	O20-C21-C22-O23
8	C	101	OLC	O19-C1-O20-C21
8	B	204	OLC	C1-C2-C3-C4
8	A	606	OLC	O23-C22-C24-O25
8	A	614	OLC	C1-C2-C3-C4
8	A	615	OLC	C10-C11-C12-C13
8	A	606	OLC	O20-C21-C22-O23
8	A	613	OLC	C2-C1-O20-C21
8	A	613	OLC	O19-C1-O20-C21
8	A	607	OLC	C13-C14-C15-C16
8	C	101	OLC	C5-C6-C7-C8
8	A	613	OLC	C12-C13-C14-C15
8	A	613	OLC	O23-C22-C24-O25
8	A	614	OLC	O23-C22-C24-O25
8	B	202	OLC	O23-C22-C24-O25
8	B	204	OLC	O23-C22-C24-O25
8	A	613	OLC	C13-C14-C15-C16
8	C	102	OLC	C12-C13-C14-C15
8	B	202	OLC	C3-C4-C5-C6
8	A	605	OLC	O19-C1-O20-C21
8	A	607	OLC	O19-C1-O20-C21
8	A	615	OLC	C6-C7-C8-C9
8	A	605	OLC	C4-C5-C6-C7
8	A	612	OLC	C2-C3-C4-C5
8	B	203	OLC	C22-C21-O20-C1
8	A	608	OLC	C6-C7-C8-C9
8	B	203	OLC	C6-C7-C8-C9
8	C	102	OLC	C6-C7-C8-C9
8	A	607	OLC	C11-C12-C13-C14
8	B	202	OLC	C6-C7-C8-C9
8	C	102	OLC	C10-C11-C12-C13
8	B	203	OLC	C2-C3-C4-C5
8	A	615	OLC	C12-C13-C14-C15
8	B	204	OLC	C5-C6-C7-C8
8	C	101	OLC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
8	A	614	OLC	C2-C1-O20-C21
8	C	101	OLC	C11-C12-C13-C14
8	B	203	OLC	C3-C4-C5-C6
8	A	612	OLC	C3-C4-C5-C6
8	A	605	OLC	C10-C11-C12-C13
8	A	613	OLC	C4-C5-C6-C7
8	B	202	OLC	C14-C15-C16-C17
8	A	605	OLC	C3-C4-C5-C6
8	C	101	OLC	C4-C5-C6-C7
8	C	102	OLC	C14-C15-C16-C17
8	C	102	OLC	C11-C12-C13-C14
8	A	614	OLC	C3-C4-C5-C6
8	A	606	OLC	C12-C13-C14-C15
8	A	613	OLC	C14-C15-C16-C17
8	A	615	OLC	C4-C5-C6-C7
8	A	614	OLC	O19-C1-O20-C21
8	A	607	OLC	C4-C5-C6-C7
8	A	613	OLC	C11-C12-C13-C14
8	A	608	OLC	C1-C2-C3-C4
8	A	606	OLC	C11-C12-C13-C14
8	A	611	OLC	C21-C22-C24-O25
8	A	606	OLC	C6-C7-C8-C9
8	B	202	OLC	C11-C12-C13-C14
8	C	102	OLC	C13-C14-C15-C16
8	A	613	OLC	C15-C16-C17-C18
8	B	202	OLC	C2-C1-O20-C21
8	A	605	OLC	C2-C3-C4-C5
8	A	607	OLC	C10-C11-C12-C13
8	C	101	OLC	C6-C7-C8-C9
8	A	608	OLC	C4-C5-C6-C7
8	B	202	OLC	O19-C1-O20-C21
8	A	615	OLC	C14-C15-C16-C17
8	A	606	OLC	C7-C8-C9-C10
8	C	101	OLC	C9-C10-C11-C12
5	A	602	HAS	O11-C11-C3B-C2B
8	B	202	OLC	C7-C8-C9-C10
8	C	101	OLC	C1-C2-C3-C4
5	A	602	HAS	C17-C18-C19-C20
5	A	602	HAS	C23-C24-C28-C29
8	B	203	OLC	C9-C10-C11-C12
8	A	605	OLC	C6-C7-C8-C9
8	C	101	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	A	601	HEM	C4B-C3B-CAB-CBB
8	C	101	OLC	C12-C13-C14-C15
8	A	605	OLC	C9-C10-C11-C12
5	A	602	HAS	C25-C23-C24-C28
8	A	613	OLC	C9-C10-C11-C12
8	A	608	OLC	C3-C4-C5-C6
5	A	602	HAS	CAA-CBA-CGA-O1A
8	A	613	OLC	C10-C11-C12-C13
8	A	612	OLC	C4-C5-C6-C7
5	A	602	HAS	CAA-CBA-CGA-O2A
8	A	606	OLC	C3-C4-C5-C6
8	B	202	OLC	C10-C11-C12-C13
8	A	607	OLC	C5-C6-C7-C8
8	C	102	OLC	C9-C10-C11-C12
5	A	602	HAS	C11-C12-C13-C14
8	B	202	OLC	C13-C14-C15-C16
4	A	601	HEM	CAD-CBD-CGD-O1D
8	A	611	OLC	O23-C22-C24-O25
8	A	613	OLC	C3-C4-C5-C6
5	A	602	HAS	C22-C23-C24-C28
8	A	610	OLC	C22-C21-O20-C1
8	C	102	OLC	C7-C8-C9-C10
8	A	607	OLC	C7-C8-C9-C10
8	A	615	OLC	C7-C8-C9-C10
8	B	204	OLC	C6-C7-C8-C9
8	A	615	OLC	C1-C2-C3-C4
8	A	609	OLC	O20-C1-C2-C3
8	A	612	OLC	O19-C1-C2-C3
8	A	612	OLC	O20-C1-C2-C3
4	A	601	HEM	CAD-CBD-CGD-O2D
8	A	607	OLC	C14-C15-C16-C17
4	A	601	HEM	CAA-CBA-CGA-O2A
8	A	611	OLC	C1-C2-C3-C4
8	A	609	OLC	O19-C1-C2-C3

There are no ring outliers.

17 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	HAS	3	0
8	A	606	OLC	2	0
8	A	607	OLC	7	0

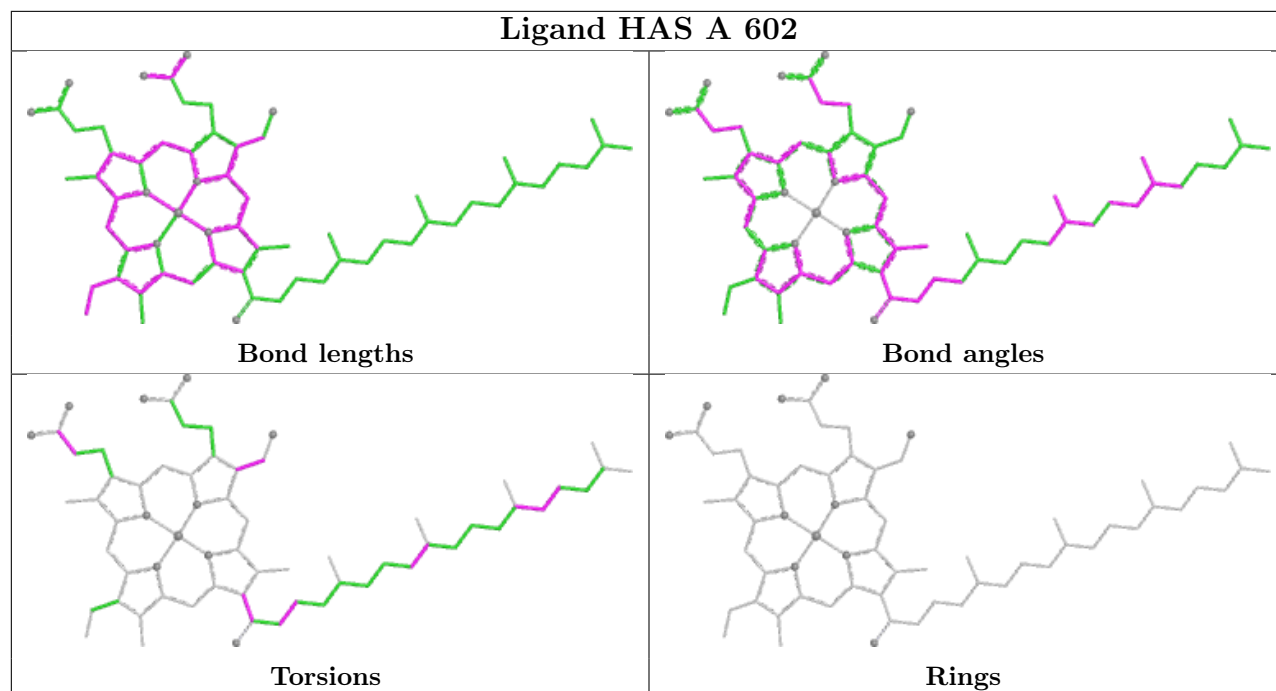
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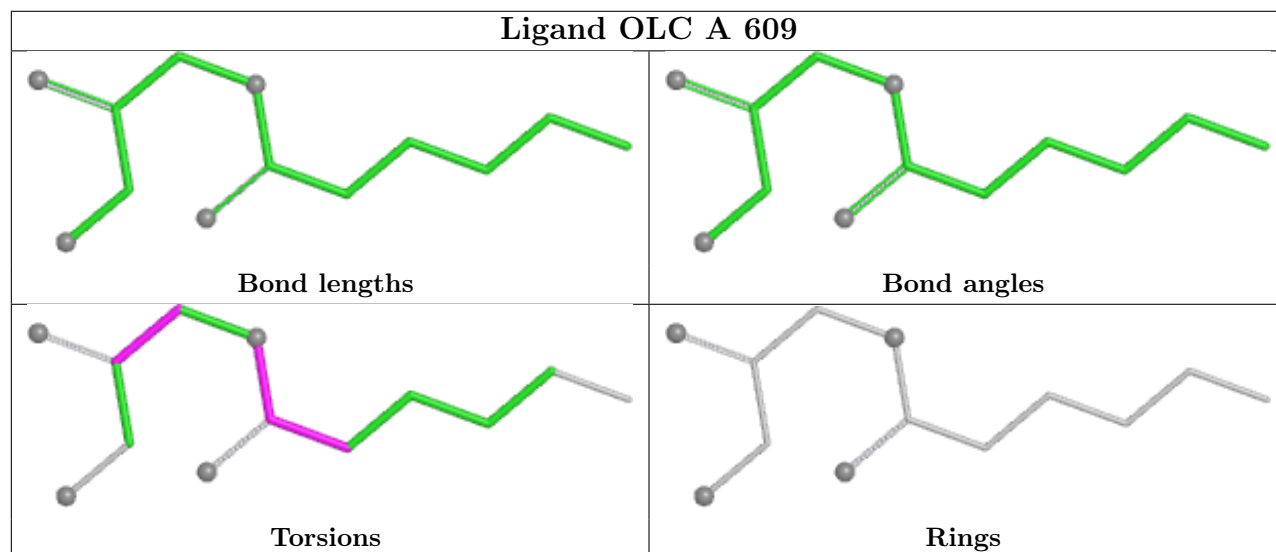
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	203	OLC	8	0
8	A	610	OLC	3	0
8	C	102	OLC	5	0
8	A	605	OLC	1	0
8	A	608	OLC	1	0
8	A	612	OLC	2	0
8	A	613	OLC	6	0
4	A	601	HEM	5	0
8	A	615	OLC	3	0
8	B	202	OLC	1	0
7	A	604	PER	1	0
8	C	101	OLC	4	0
8	A	611	OLC	3	0
8	B	204	OLC	1	0

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

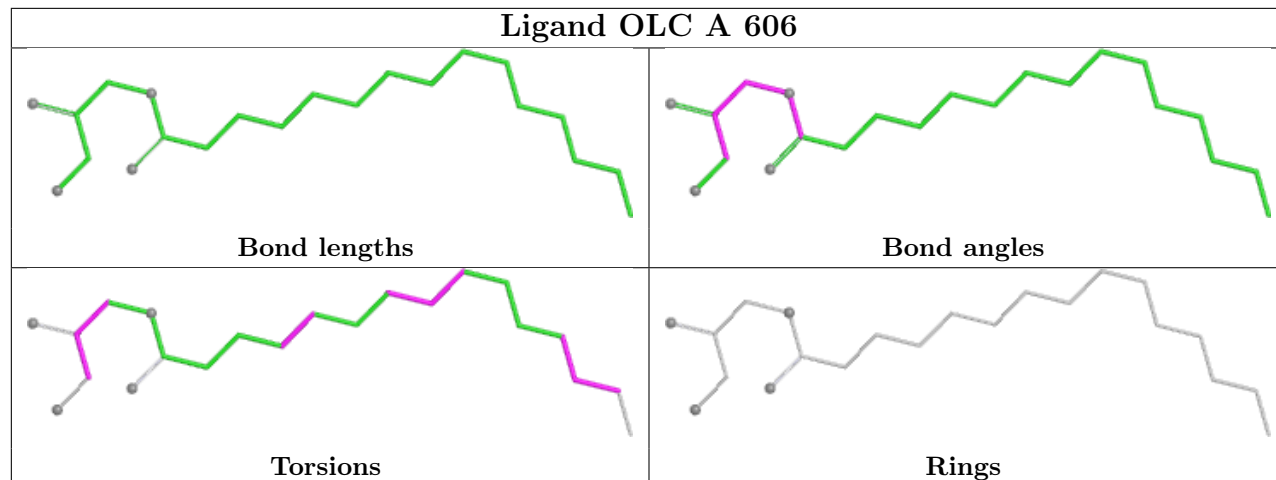
Ligand HAS A 602

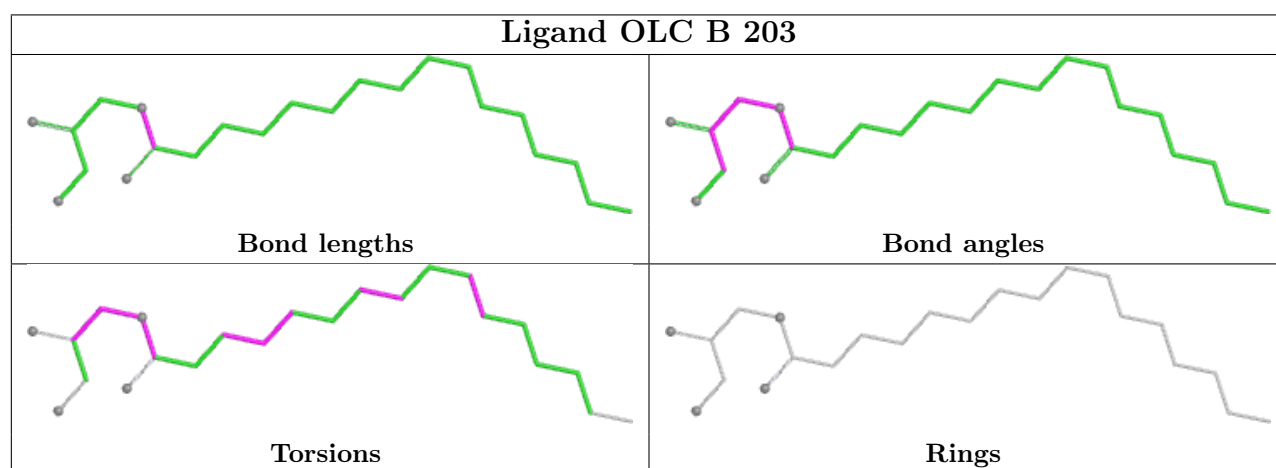
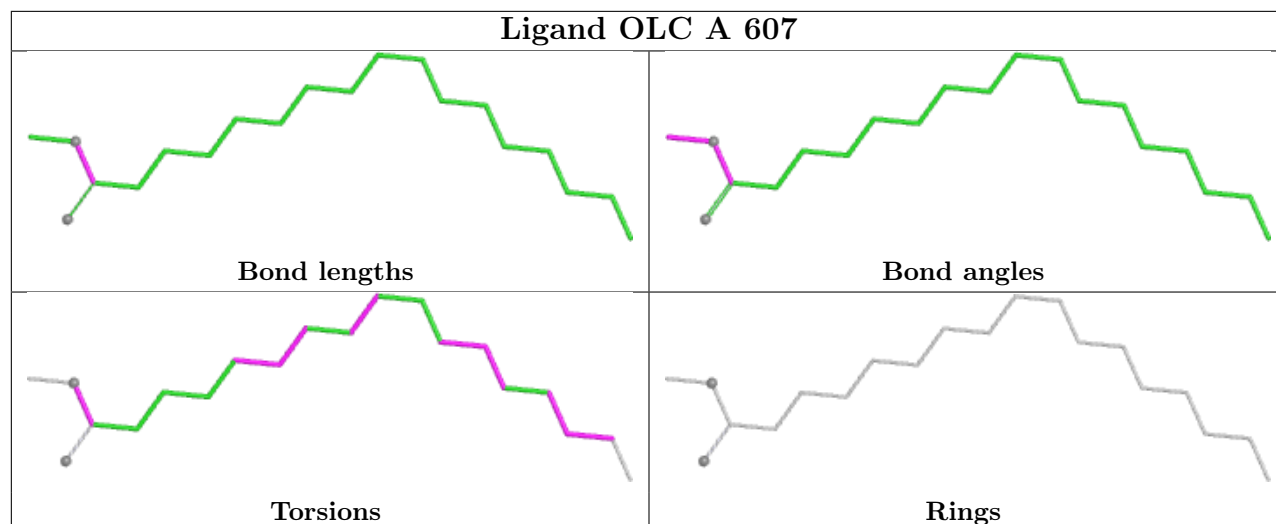


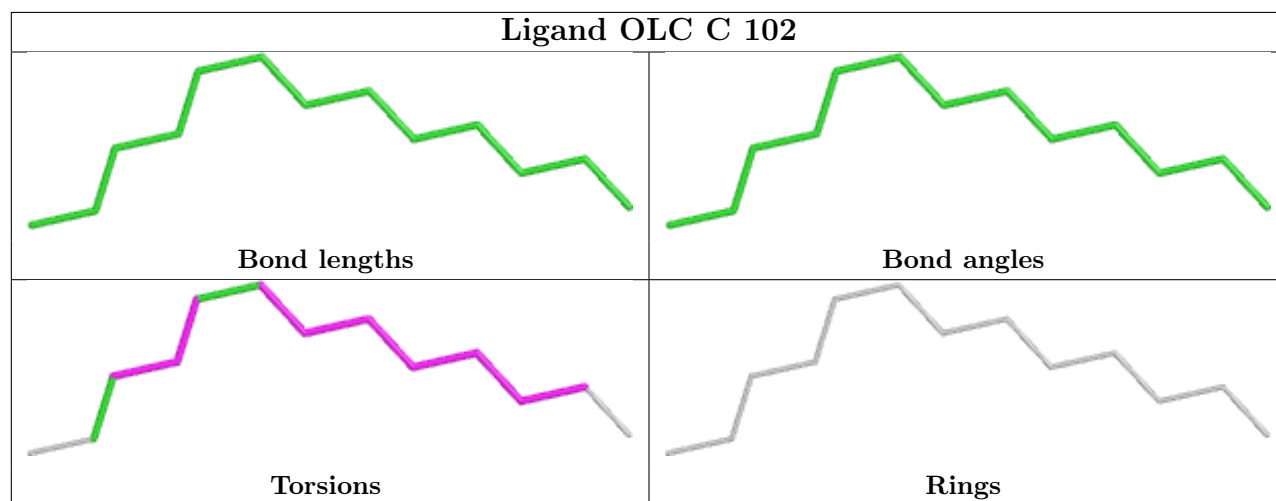
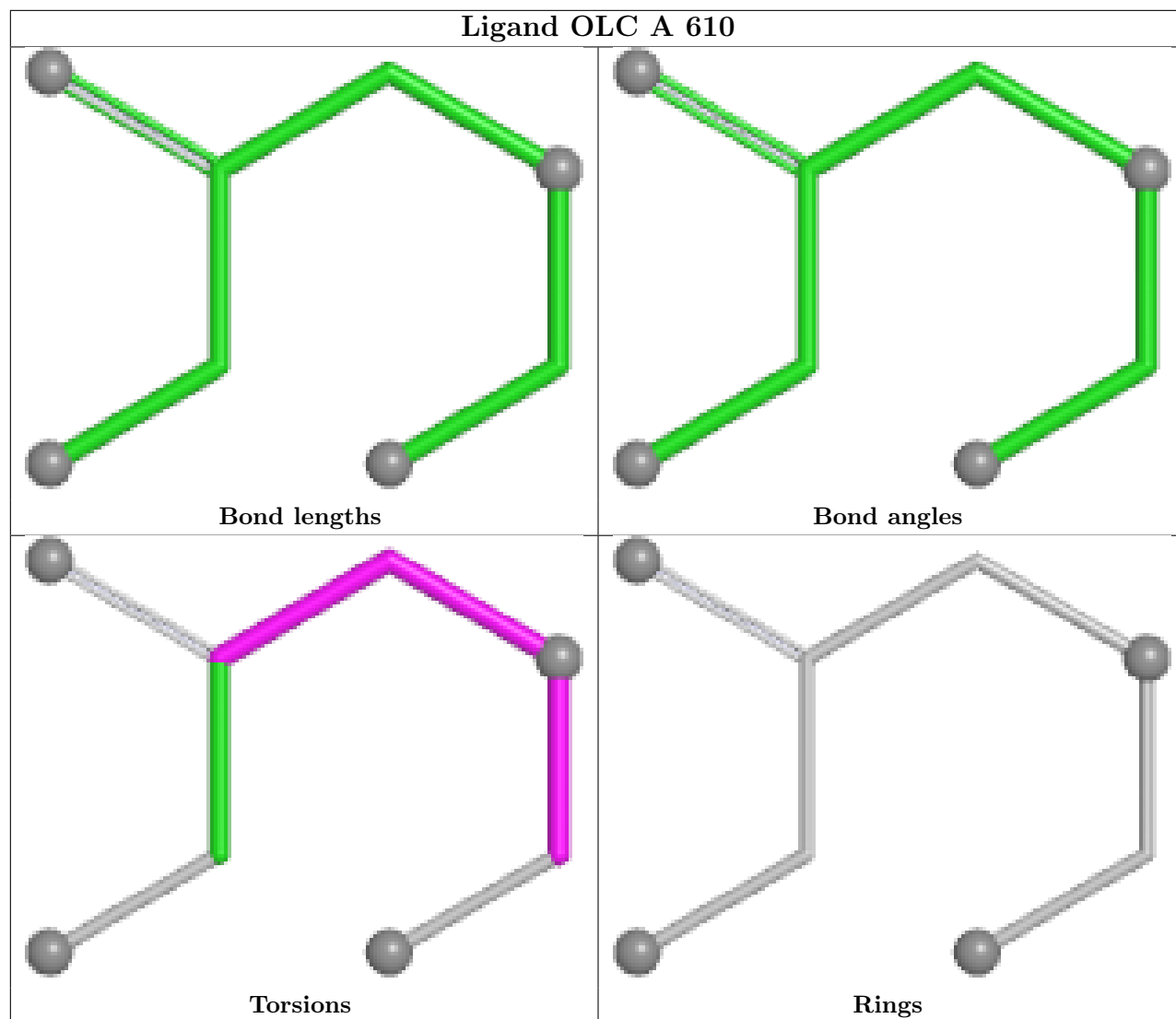
Ligand OLC A 609

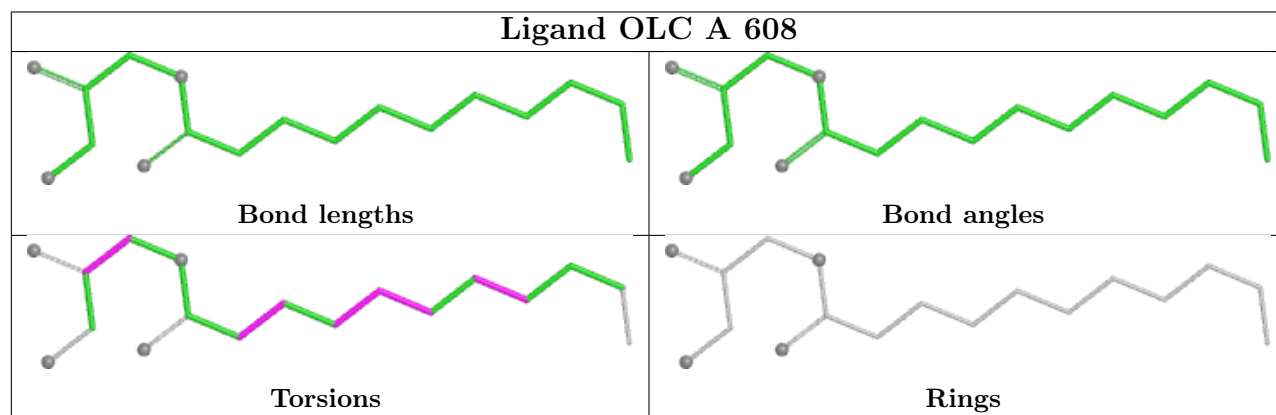
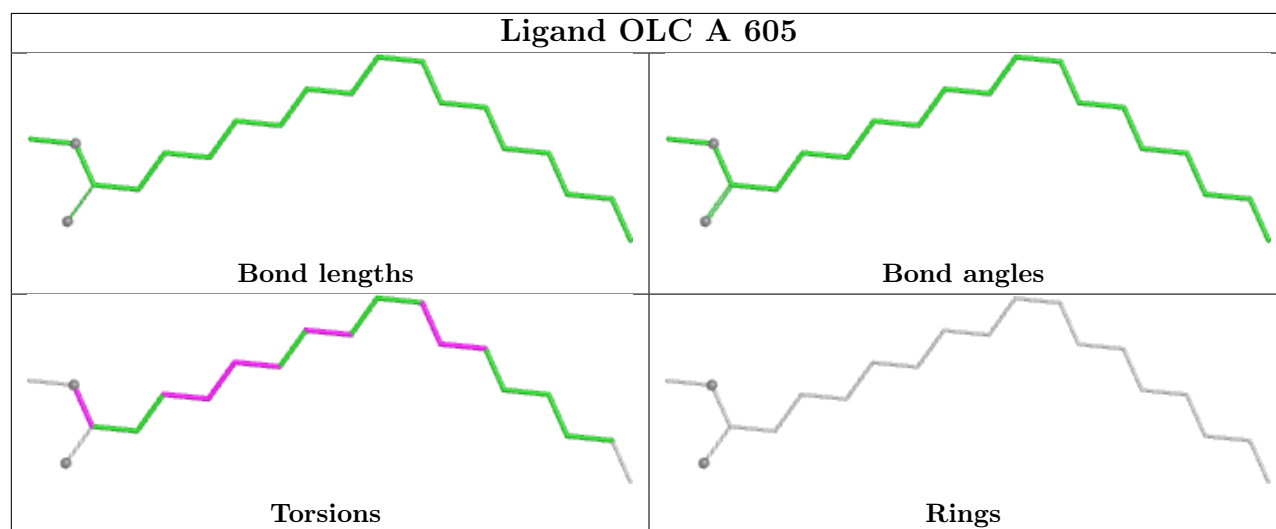
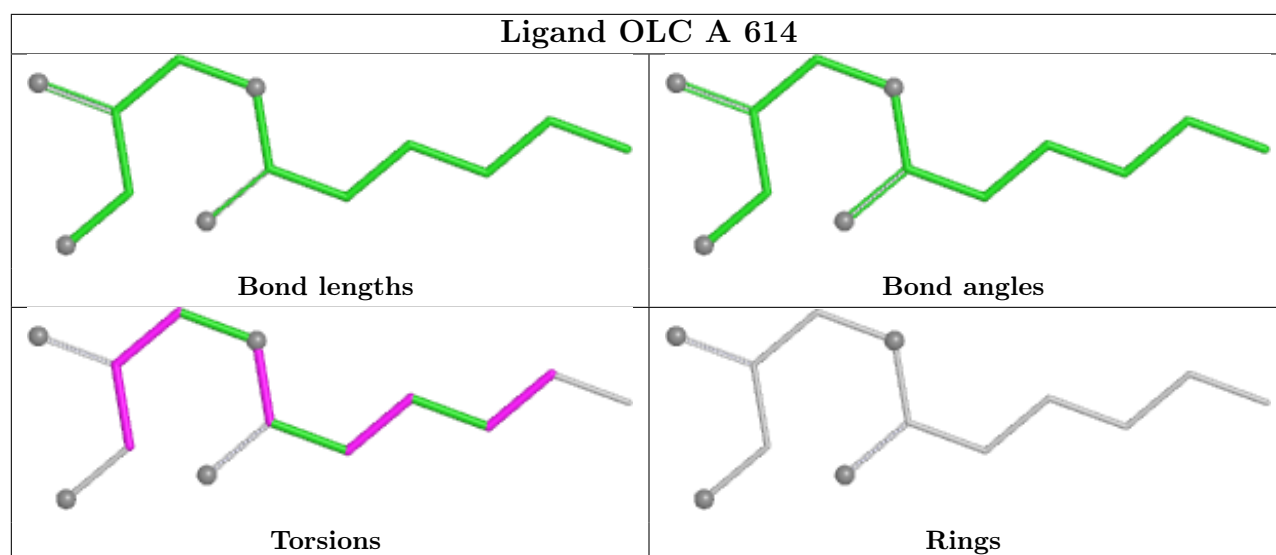


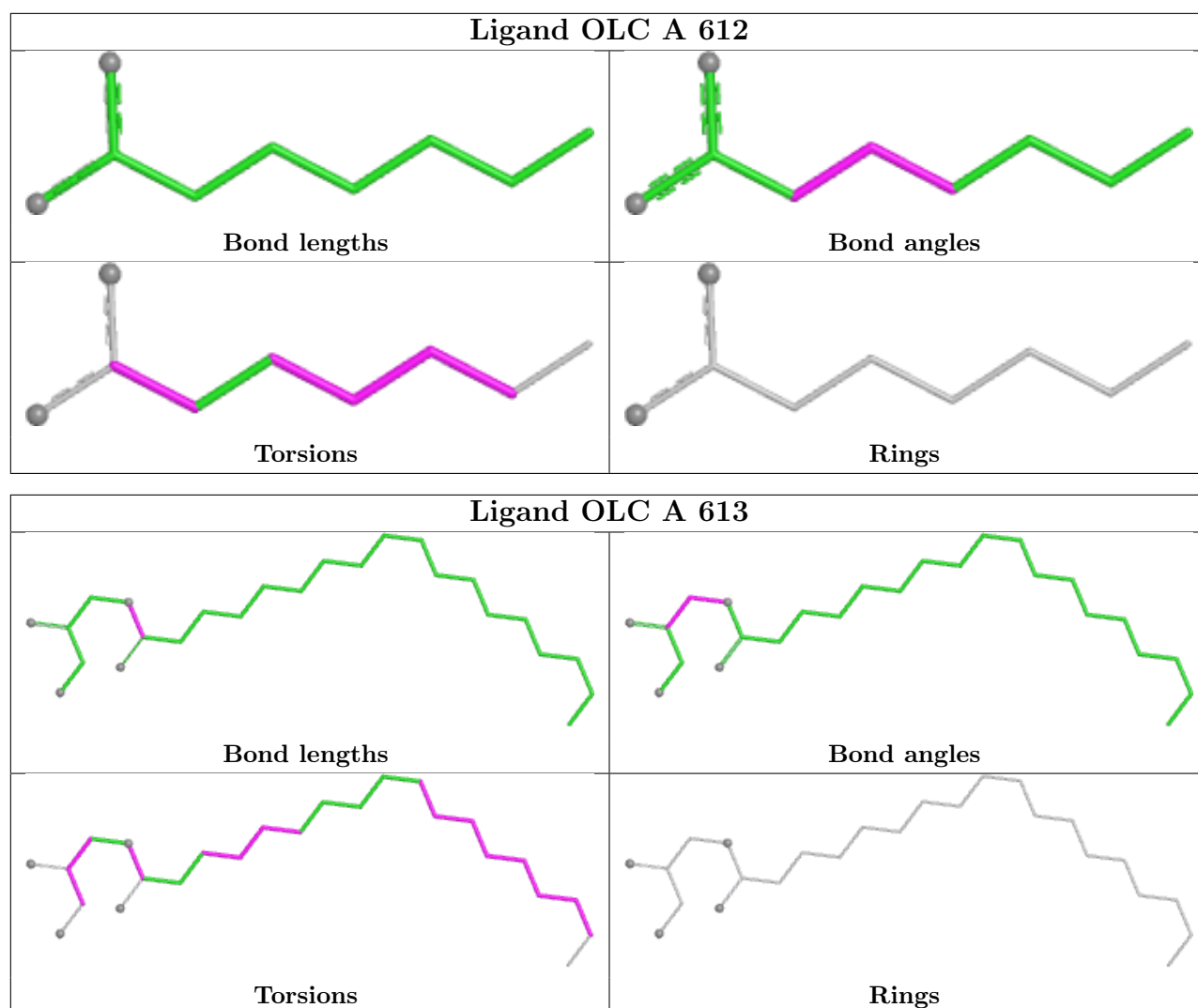
Ligand OLC A 606

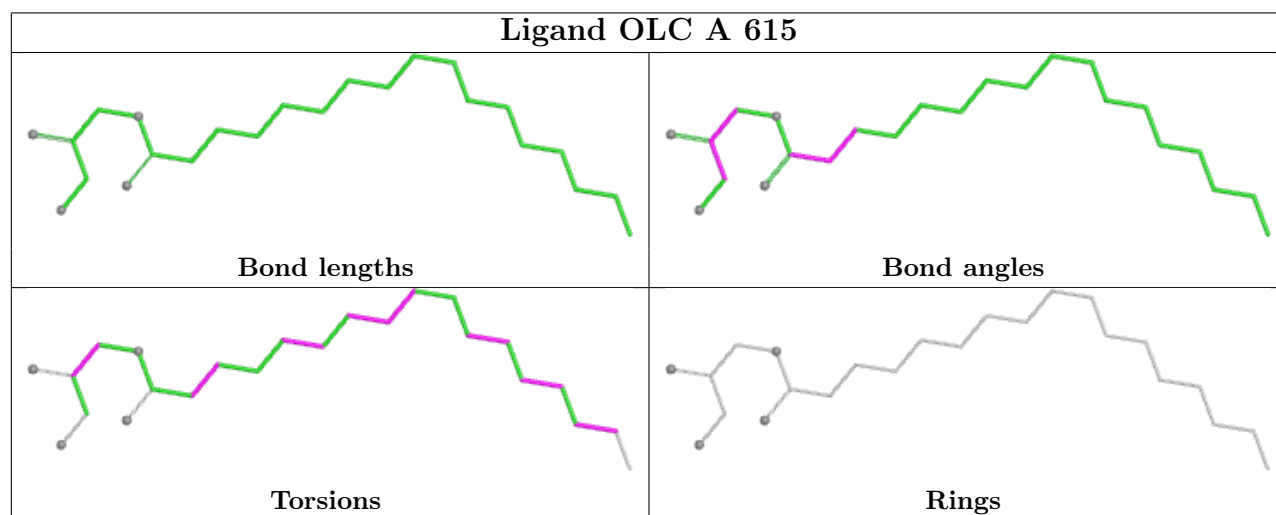
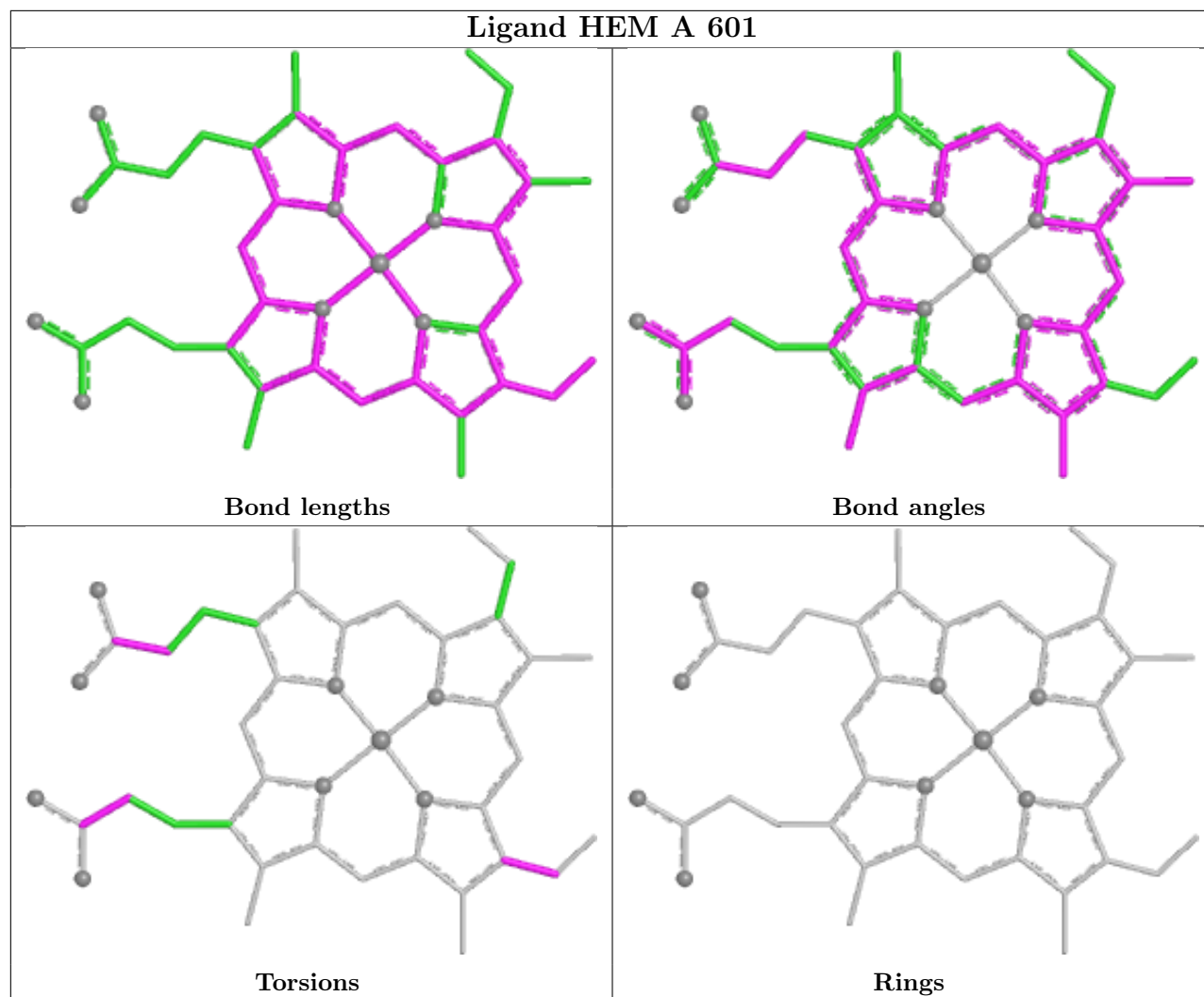


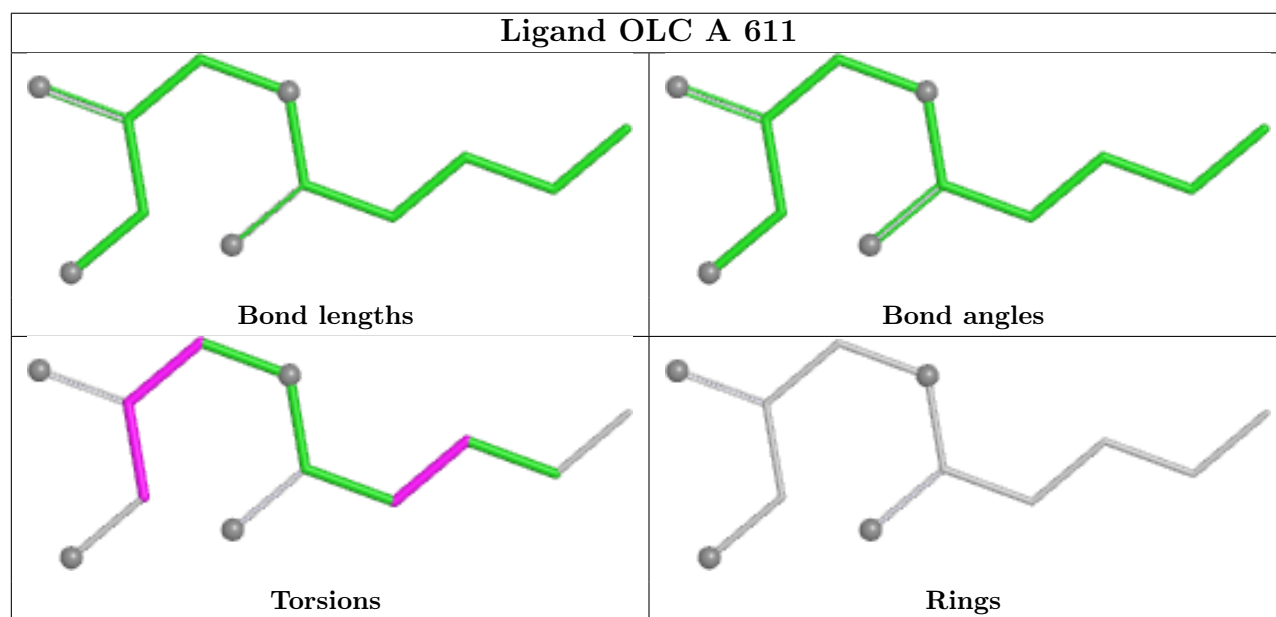
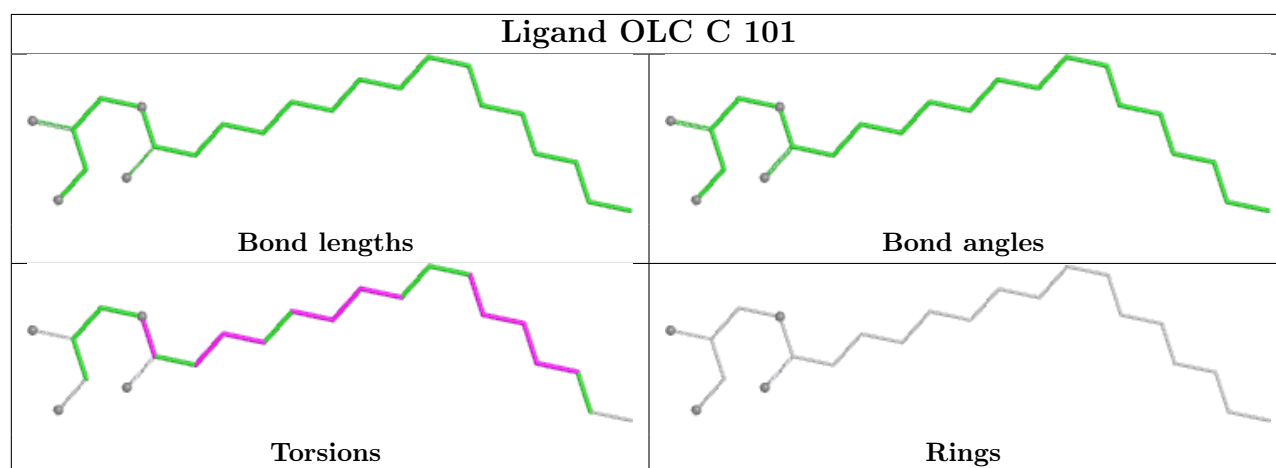
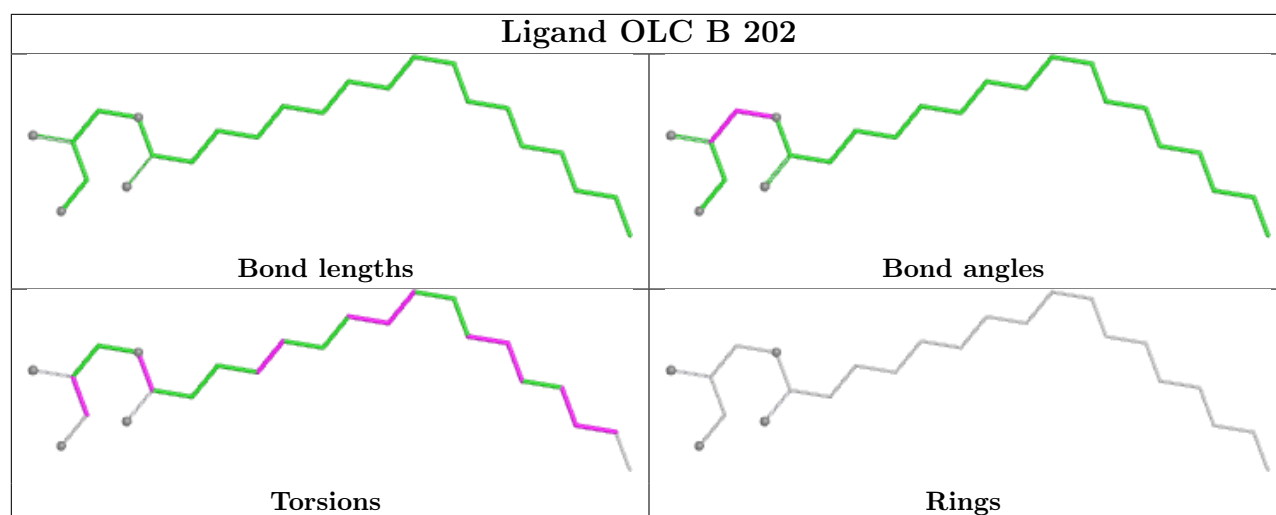


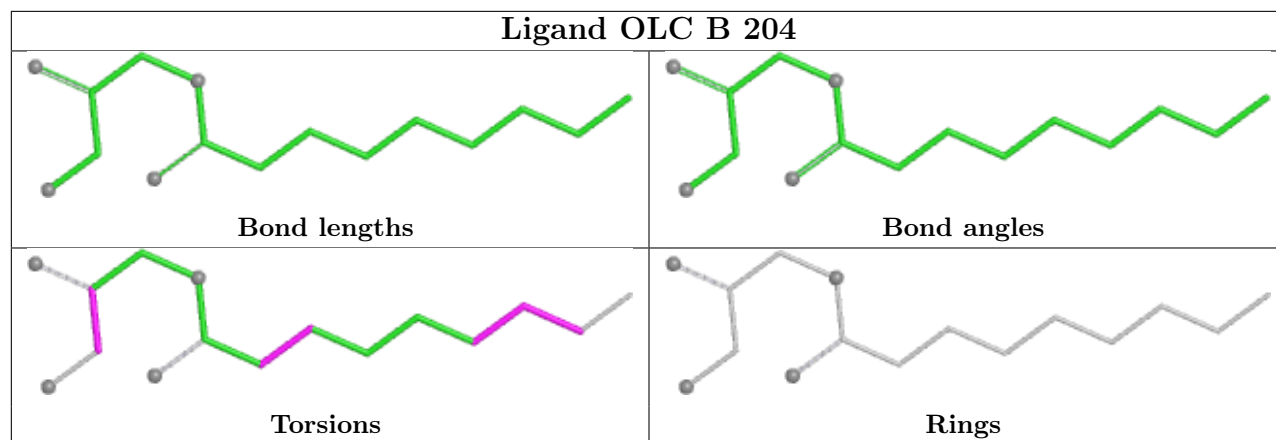












5.7 Other polymers [i](#)

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%)	-0.27	12 (2%) 62 57	19, 30, 61, 95	1 (0%)
2	B	166/168 (98%)	-0.40	0 100 100	21, 31, 50, 70	0
3	C	31/34 (91%)	-0.34	0 100 100	24, 30, 42, 55	0
All	All	751/771 (97%)	-0.30	12 (1%) 70 66	19, 30, 57, 95	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	SER	4.4
1	A	489	PHE	4.0
1	A	495	ARG	3.5
1	A	515	PRO	3.4
1	A	494	SER	3.3
1	A	10	ARG	3.3
1	A	492	LEU	2.7
1	A	333	PHE	2.6
1	A	516	GLU	2.3
1	A	201	VAL	2.2
1	A	217	GLU	2.1
1	A	501	LEU	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

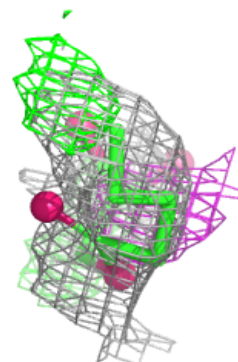
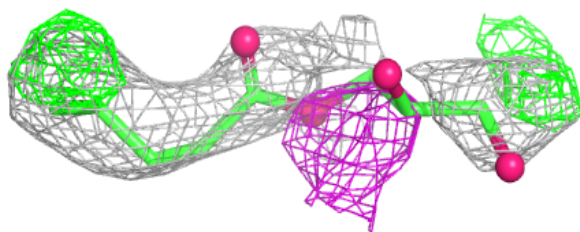
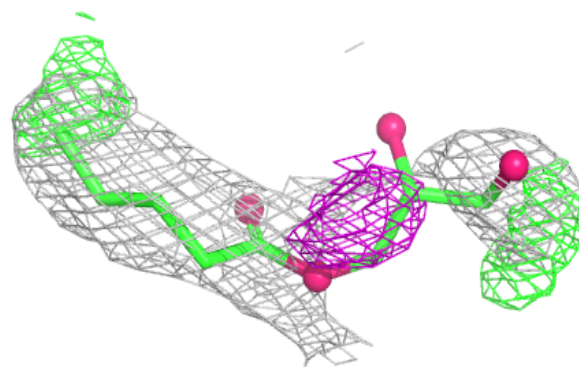
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	OLC	A	611	12/25	0.57	0.26	48,73,75,75	0
8	OLC	A	609	13/25	0.61	0.25	59,65,77,78	0
8	OLC	A	615	24/25	0.64	0.26	52,59,67,69	0
8	OLC	A	612	9/25	0.70	0.24	53,55,62,64	0
8	OLC	A	607	20/25	0.71	0.27	57,62,75,77	0
8	OLC	A	605	20/25	0.72	0.26	45,65,84,87	0
8	OLC	A	608	18/25	0.72	0.22	47,60,72,72	0
8	OLC	B	203	23/25	0.72	0.24	57,63,72,76	0
8	OLC	A	614	13/25	0.74	0.29	62,75,81,81	0
8	OLC	B	204	16/25	0.78	0.23	65,66,70,72	0
8	OLC	C	101	23/25	0.78	0.20	46,56,71,74	0
8	OLC	A	613	25/25	0.79	0.21	48,59,64,67	0
8	OLC	C	102	13/25	0.81	0.26	63,70,79,81	0
8	OLC	A	610	8/25	0.82	0.14	67,68,70,70	0
8	OLC	A	606	22/25	0.83	0.18	30,45,62,64	0
8	OLC	B	202	24/25	0.83	0.21	53,66,71,73	0
5	HAS	A	602	65/65	0.96	0.09	19,25,42,47	0
4	HEM	A	601	43/43	0.98	0.05	18,21,23,26	0
7	PER	A	604	2/2	0.99	0.11	27,27,27,29	0
6	CU	A	603	1/1	1.00	0.02	27,27,27,27	0
9	CUA	B	201	2/2	1.00	0.01	24,24,24,26	0

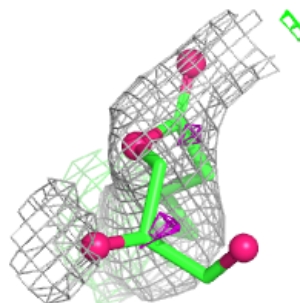
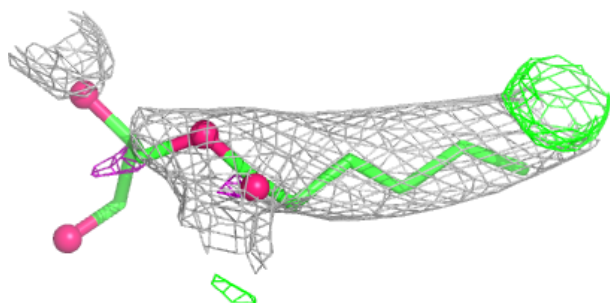
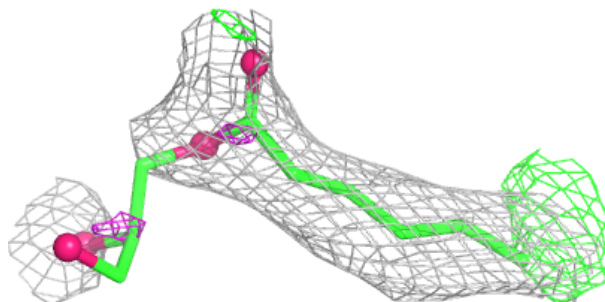
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 611:

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

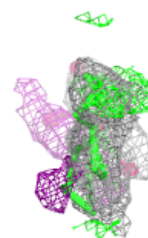
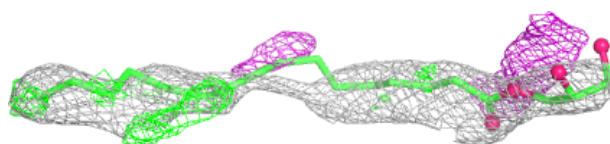
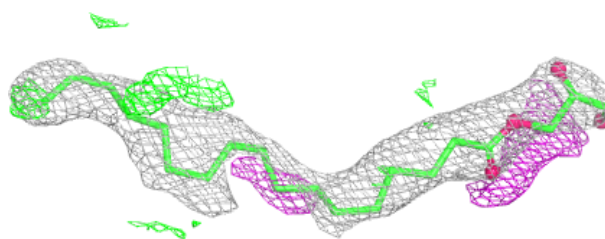
**Electron density around OLC A 609:**

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

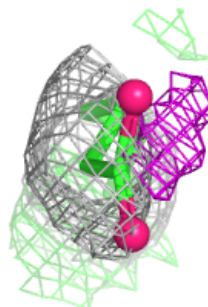
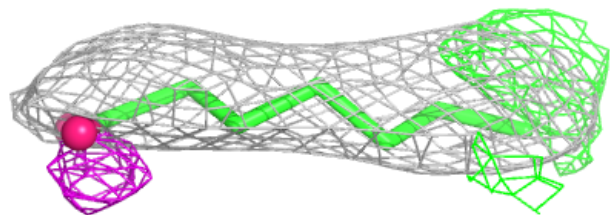
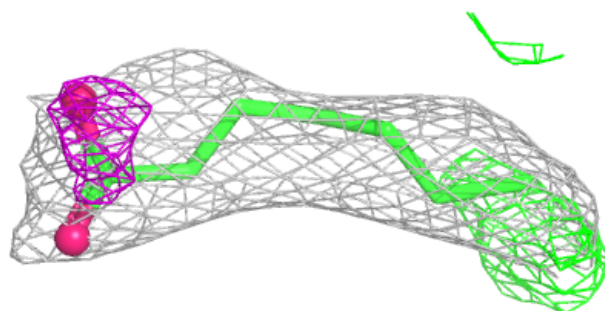


Electron density around OLC A 615:

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

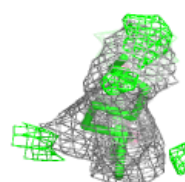
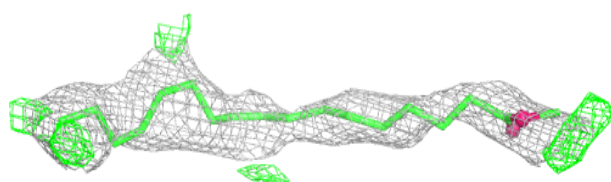
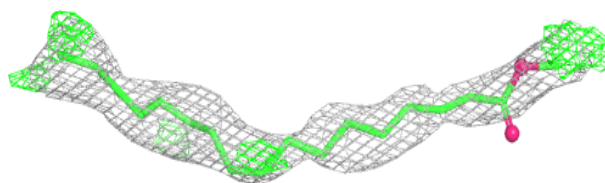
**Electron density around OLC A 612:**

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

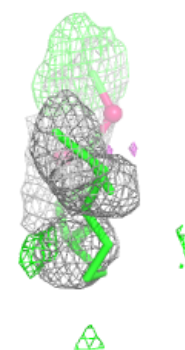
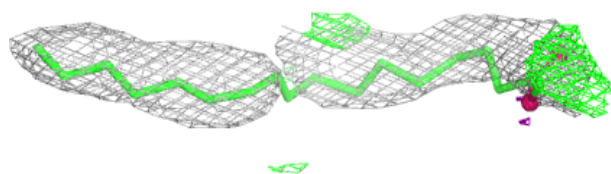
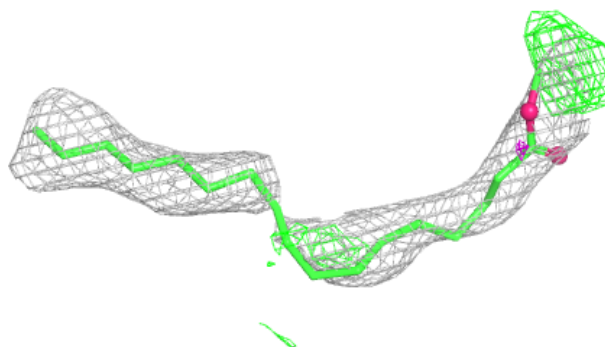


Electron density around OLC A 607:

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

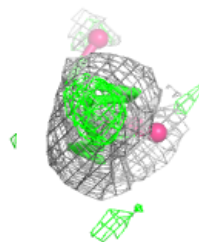
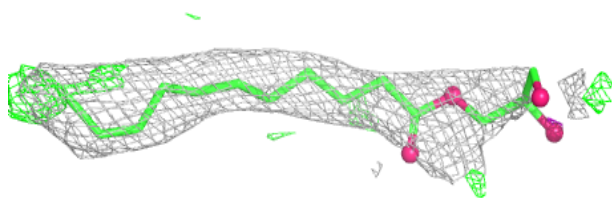
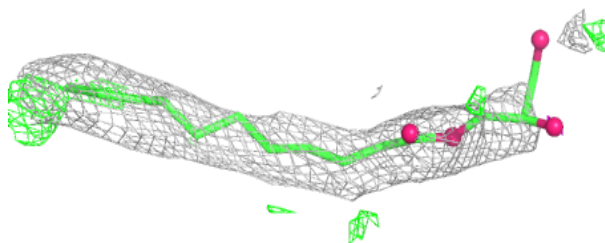
**Electron density around OLC A 605:**

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

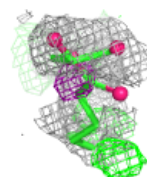
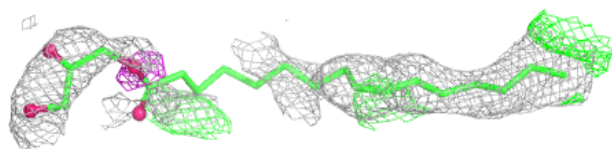
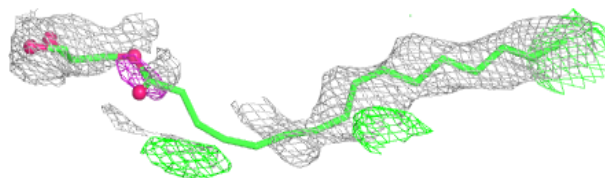


Electron density around OLC A 608:

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

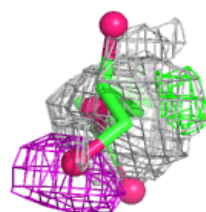
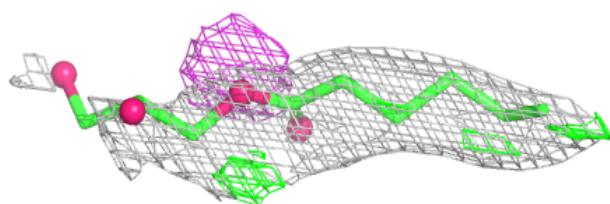
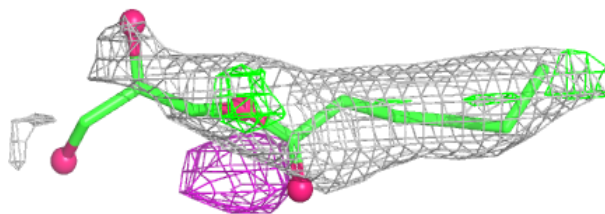
**Electron density around OLC B 203:**

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

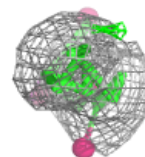
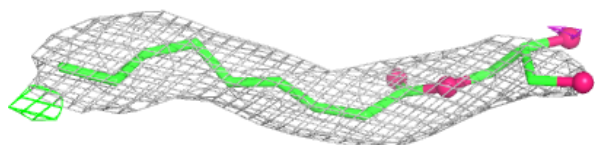
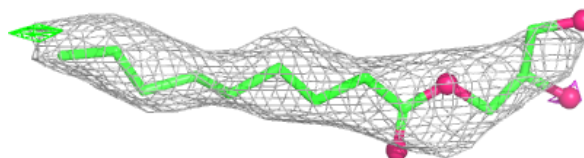


Electron density around OLC A 614:

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

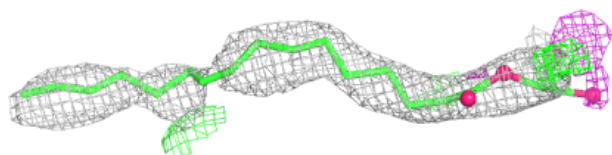
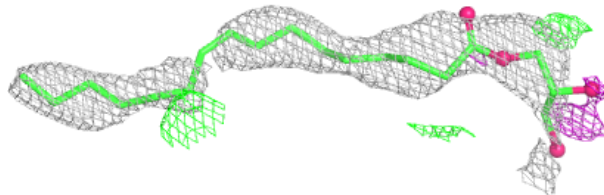
**Electron density around OLC B 204:**

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

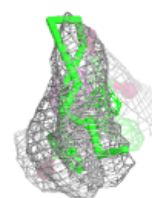
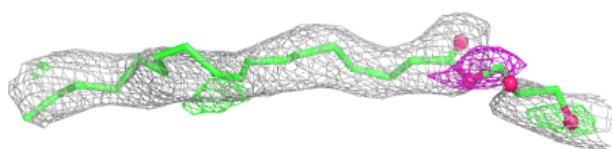
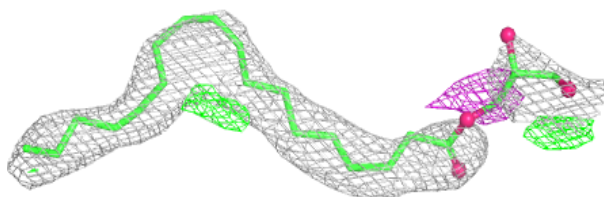


Electron density around OLC C 101:

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

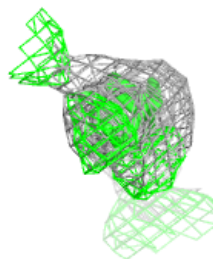
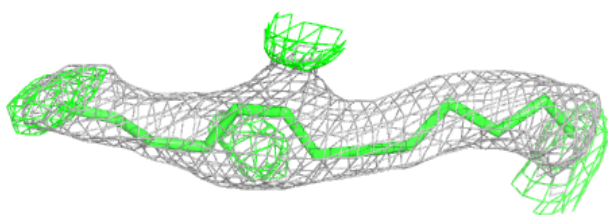
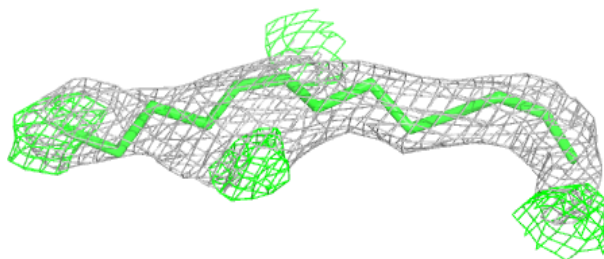
**Electron density around OLC A 613:**

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

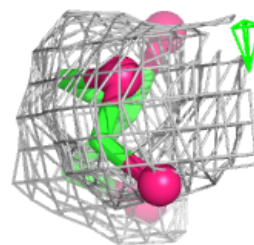
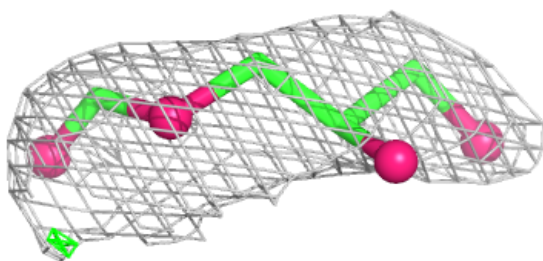
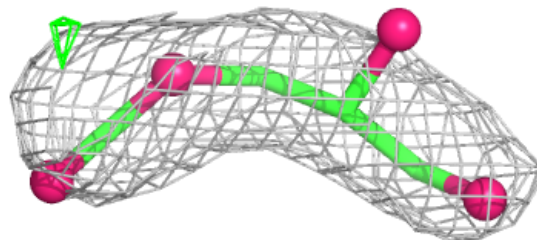


Electron density around OLC C 102:

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

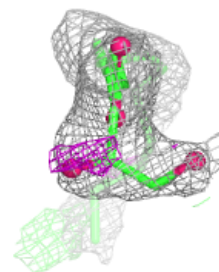
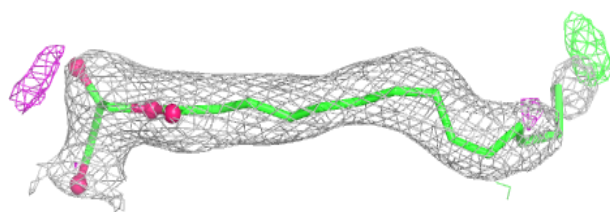
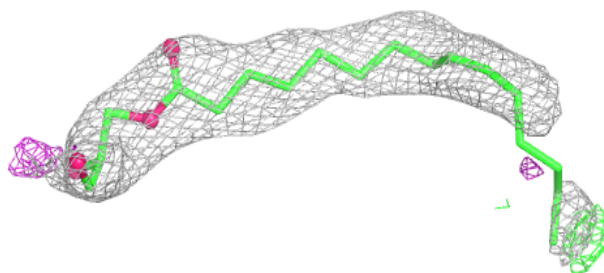
**Electron density around OLC A 610:**

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

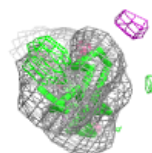
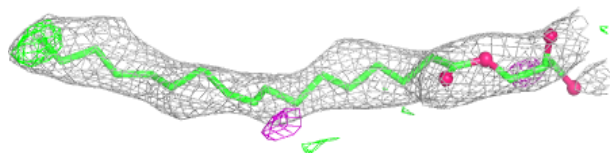
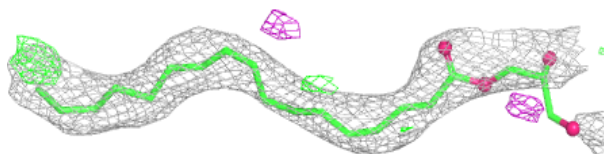


Electron density around OLC A 606:

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

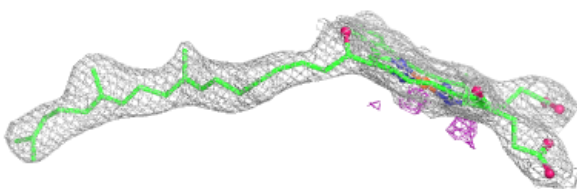
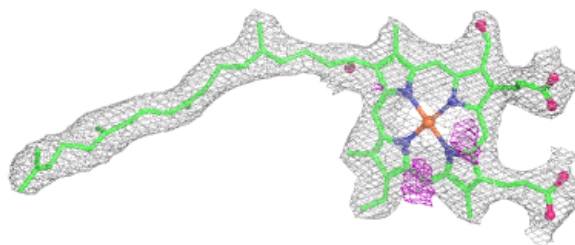
**Electron density around OLC B 202:**

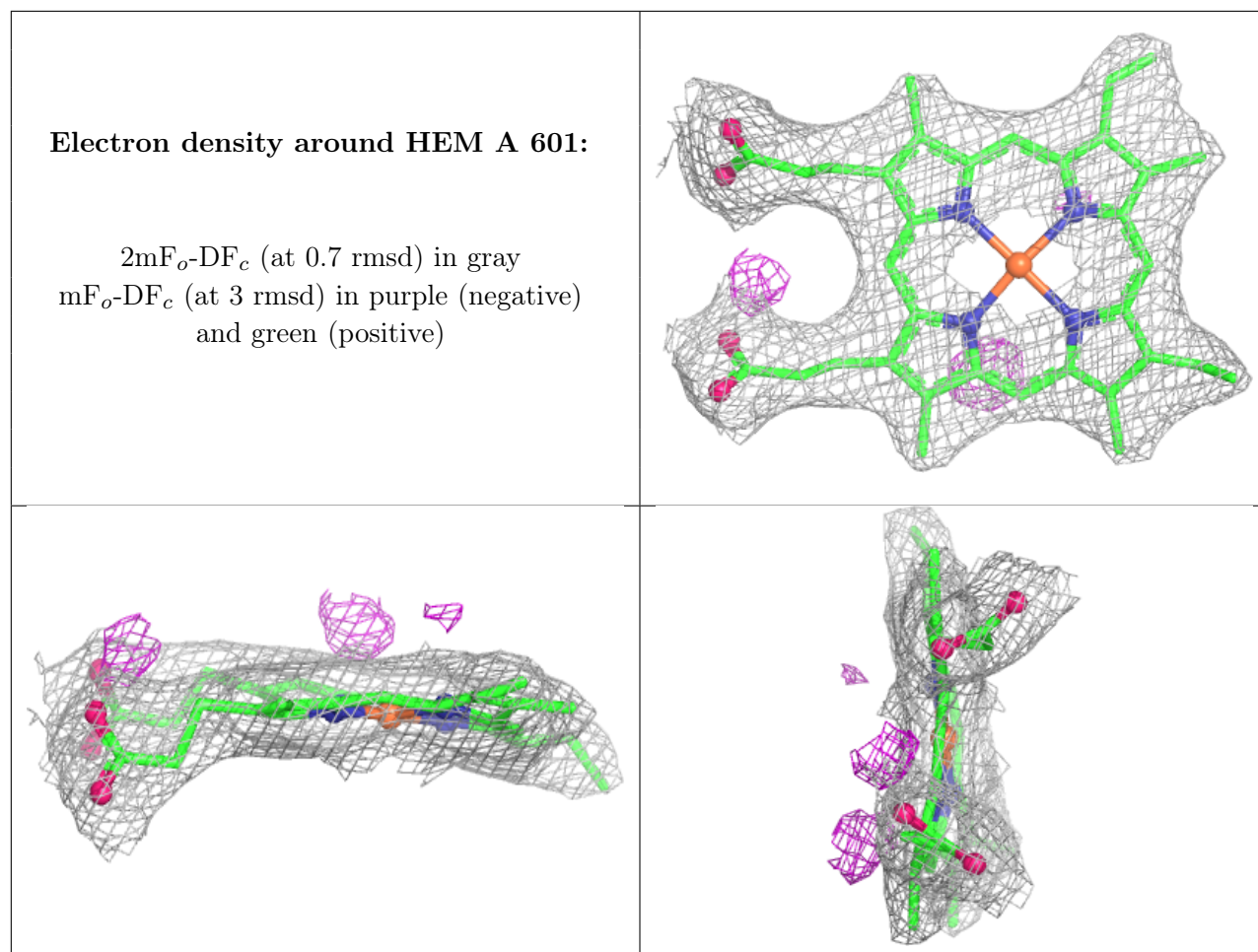
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HAS 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.