



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:08 PM UTC

PDB ID : 4G7S / pdb_00004g7s
Title : Structure of Recombinant Cytochrome ba3 Oxidase mutant V236I from *Thermus thermophilus*
Authors : Li, Y.; Chen, Y.; Stout, C.D.
Deposited on : 2012-07-20
Resolution : 2.00 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

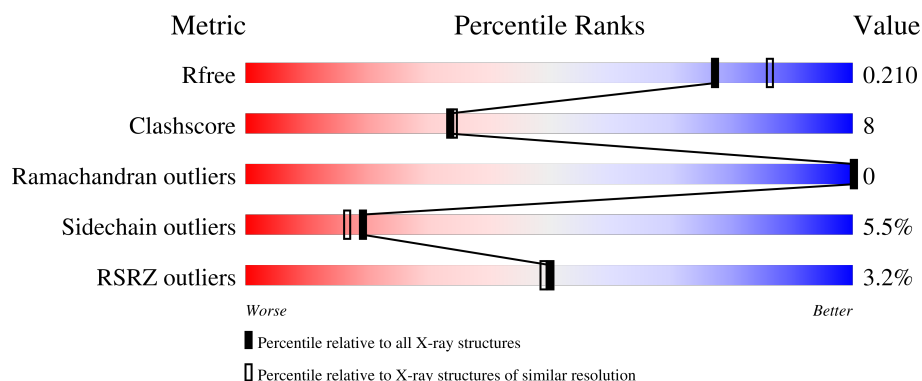
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	3% 77% 17% • •
2	B	168	4% 81% 18% •
3	C	34	65% 24% • 9%

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

There are 10 unique types of molecules in this entry. The entry contains 6475 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	3	0
			4368	2966	695	691	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	ILE	VAL	engineered mutation	UNP Q5SJ79

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	1	0
			1288	837	214	233	4			

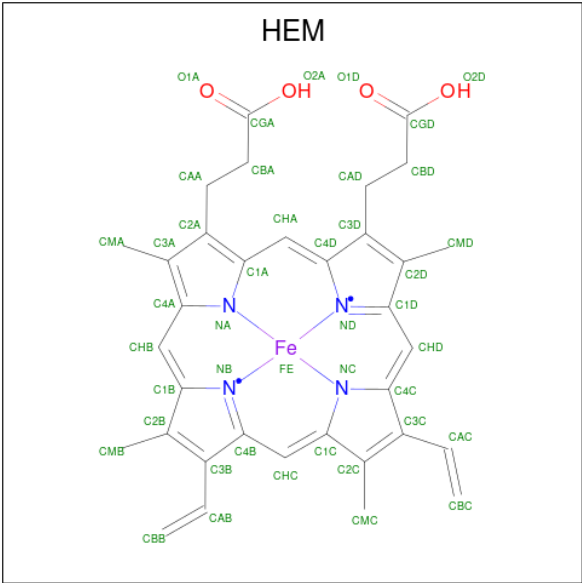
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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

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

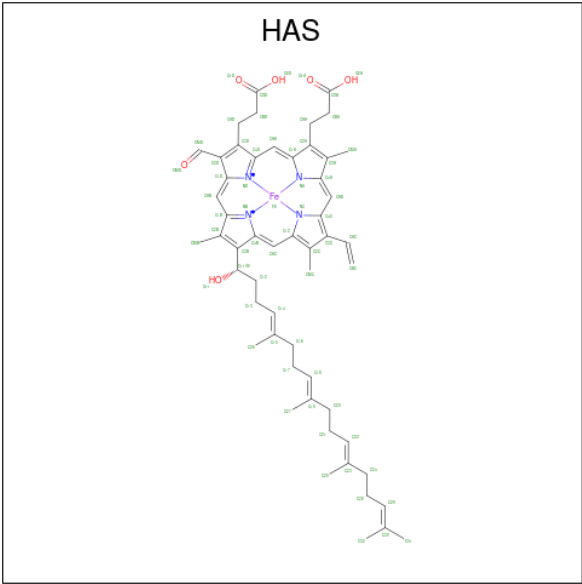
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Cu			0	0
			1	1				

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



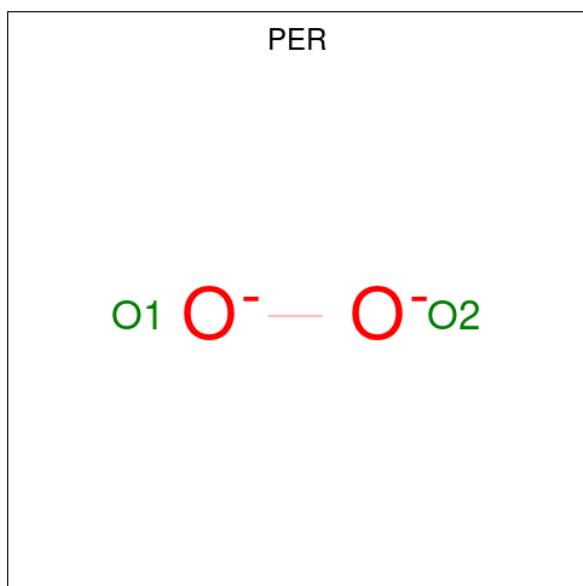
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

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



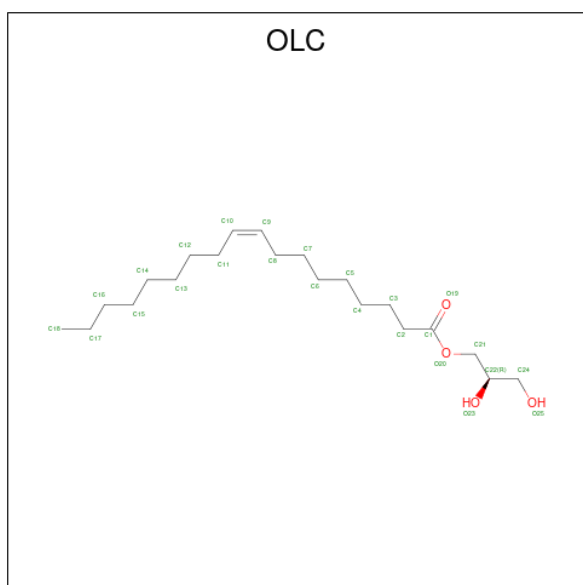
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	
			65	54	1	4	6	
							0	0

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



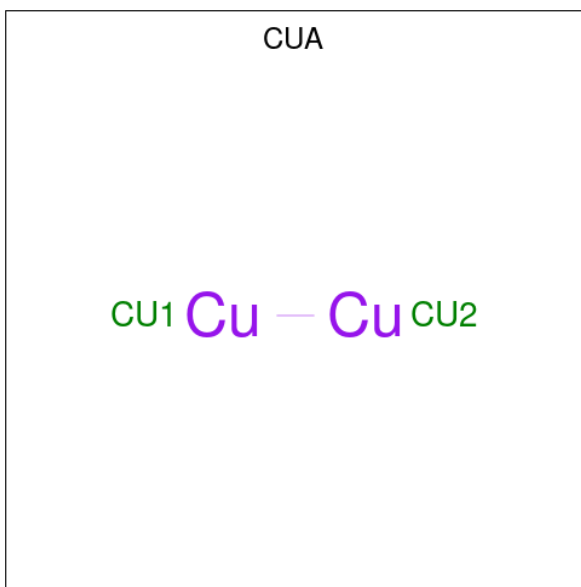
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O		
			2	2	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 19 17 2	0	0
8	A	1	Total C O 23 19 4	0	0
8	A	1	Total C O 14 12 2	0	0
8	A	1	Total C O 12 10 2	0	0
8	A	1	Total C O 15 11 4	0	0
8	A	1	Total C O 20 16 4	0	0
8	A	1	Total C O 25 21 4	0	0
8	A	1	Total C O 21 17 4	0	0
8	A	1	Total C O 25 21 4	0	0
8	B	1	Total C O 20 18 2	0	0
8	B	1	Total C O 24 20 4	0	0
8	B	1	Total C O 16 12 4	0	0
8	B	1	Total C O 20 18 2	0	0
8	C	1	Total C O 23 19 4	0	0
8	C	1	Total C 9 9	0	0

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



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

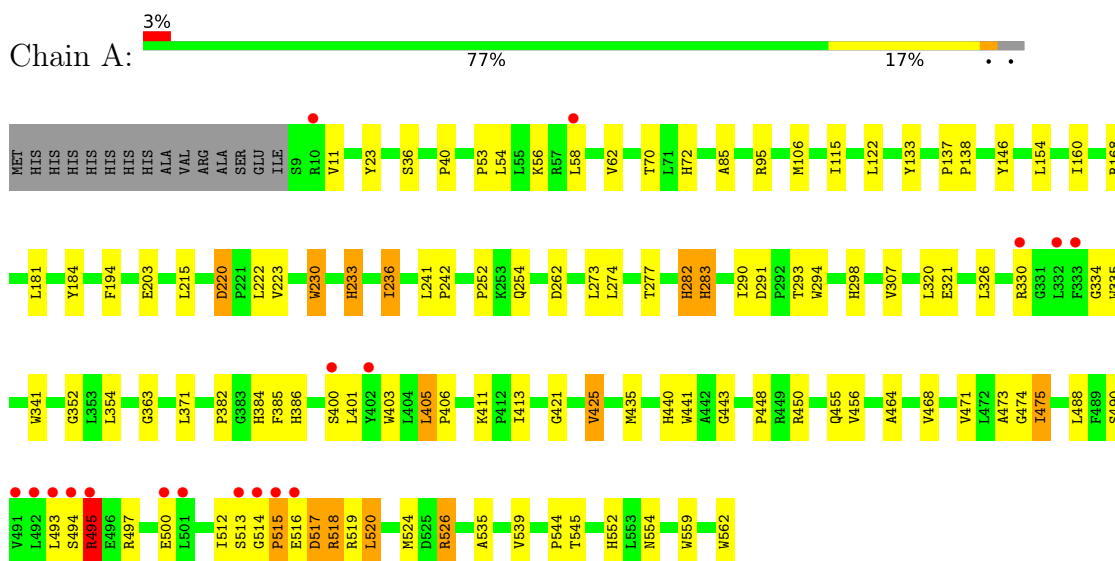
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	106	Total 106	O 106	0	0
10	B	67	Total 67	O 67	0	0
10	C	6	Total 6	O 6	0	0

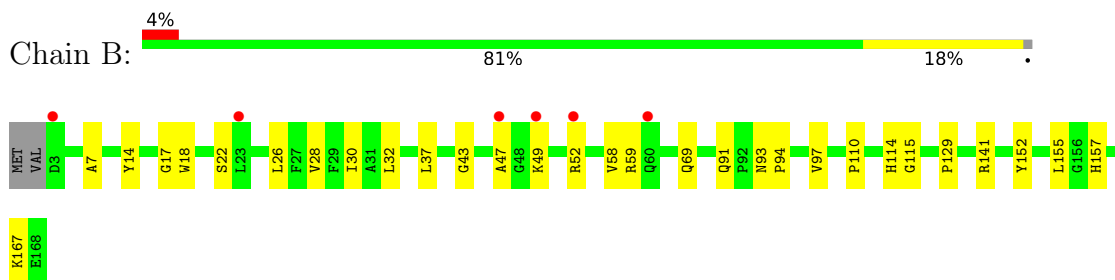
3 Residue-property plots [i](#)

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.

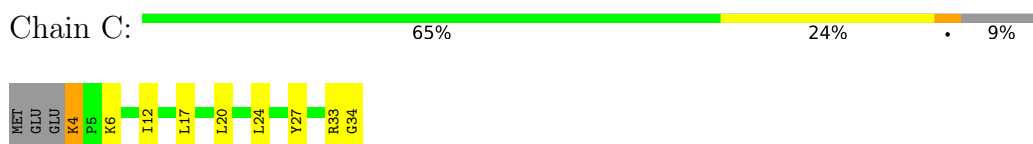
• Molecule 1: Cytochrome c oxidase subunit 1



• 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	143.57Å 98.39Å 94.58Å 90.00° 127.64° 90.00°	Depositor
Resolution (Å)	74.89 – 2.00 74.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (74.89-2.00) 93.5 (74.89-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.182 , 0.207 0.183 , 0.210	Depositor DCC
R_{free} test set	3316 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.2	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	0.95	EDS
Total number of atoms	6475	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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: CU, CUA, OLC, HAS, PER, HEM

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	1.70	43/4535 (0.9%)	1.27	26/6227 (0.4%)
2	B	1.63	8/1330 (0.6%)	1.25	8/1817 (0.4%)
3	C	1.51	0/247	1.21	0/335
All	All	1.68	51/6112 (0.8%)	1.26	34/8379 (0.4%)

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	PRO	C-O	-10.10	1.16	1.25
1	A	298	HIS	CG-CD2	9.60	1.46	1.35
1	A	137	PRO	CA-C	9.19	1.56	1.51
1	A	72	HIS	CG-CD2	8.51	1.45	1.35
1	A	443	GLY	N-CA	7.63	1.55	1.45
1	A	220	ASP	CA-C	7.49	1.62	1.52
1	A	282	HIS	CE1-NE2	7.07	1.39	1.32
2	B	97	VAL	C-O	-7.02	1.19	1.24
1	A	282	HIS	CG-CD2	6.86	1.43	1.35
2	B	152	TYR	C-O	6.77	1.32	1.23
1	A	471	VAL	N-CA	6.65	1.54	1.46
1	A	386	HIS	ND1-CE1	6.50	1.39	1.32
1	A	222	LEU	CA-C	6.47	1.60	1.52
1	A	440	HIS	N-CA	6.38	1.53	1.46
1	A	448	PRO	C-O	6.36	1.31	1.23
2	B	115	GLY	N-CA	6.35	1.51	1.44
1	A	273	LEU	CA-C	6.31	1.60	1.52
1	A	53	PRO	N-CA	6.24	1.56	1.47
2	B	91	GLN	CA-C	6.13	1.58	1.52
1	A	283	HIS	CD2-NE2	-6.12	1.31	1.37
2	B	28	VAL	CA-C	5.91	1.60	1.52
1	A	539	VAL	C-O	-5.90	1.17	1.24
1	A	23	TYR	C-O	-5.87	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	110	PRO	C-O	-5.87	1.17	1.24
1	A	146	TYR	CA-C	5.77	1.60	1.52
1	A	283	HIS	CG-ND1	-5.76	1.31	1.38
1	A	106	MET	C-O	5.69	1.30	1.24
2	B	157	HIS	CE1-NE2	5.65	1.38	1.32
1	A	298	HIS	CG-ND1	-5.64	1.32	1.38
2	B	43	GLY	N-CA	5.61	1.53	1.45
1	A	384	HIS	CE1-NE2	5.61	1.38	1.32
1	A	122	LEU	CA-C	5.58	1.58	1.52
1	A	72	HIS	CE1-NE2	5.57	1.38	1.32
1	A	252	PRO	CA-C	5.49	1.60	1.52
1	A	474	GLY	C-O	5.45	1.30	1.23
1	A	421	GLY	N-CA	5.43	1.52	1.45
1	A	468	VAL	N-CA	5.43	1.52	1.46
1	A	456	VAL	C-O	5.42	1.31	1.24
1	A	85	ALA	CA-C	5.41	1.59	1.52
1	A	545	THR	CA-C	-5.33	1.45	1.52
1	A	11	VAL	N-CA	5.32	1.52	1.46
1	A	184	TYR	CA-C	5.32	1.59	1.52
1	A	277	THR	CA-C	5.30	1.59	1.52
1	A	518	ARG	C-O	-5.24	1.17	1.24
1	A	441	TRP	CD2-CE2	5.23	1.50	1.41
1	A	282	HIS	ND1-CE1	5.22	1.37	1.32
1	A	384	HIS	CA-CB	5.18	1.61	1.53
1	A	559	TRP	CA-C	-5.18	1.46	1.52
1	A	320	LEU	N-CA	-5.12	1.40	1.46
1	A	298	HIS	CE1-NE2	5.09	1.37	1.32
1	A	464	ALA	N-CA	5.08	1.52	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	PRO	CA-C-N	7.51	135.21	121.70
1	A	515	PRO	C-N-CA	7.51	135.21	121.70
1	A	475	ILE	CB-CG1-CD1	-7.35	98.36	113.80
1	A	95	ARG	NE-CZ-NH1	-7.28	114.22	121.50
1	A	519	ARG	CA-C-N	6.92	129.85	120.44
1	A	519	ARG	C-N-CA	6.92	129.85	120.44
1	A	233	HIS	N-CA-CB	6.92	120.07	110.11
1	A	490	SER	N-CA-C	6.91	119.69	111.33
1	A	515	PRO	CA-C-O	-6.87	112.93	120.97
1	A	233	HIS	CA-CB-CG	-6.62	107.18	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	59	ARG	NE-CZ-NH2	6.45	125.01	119.20
1	A	203	GLU	N-CA-C	-6.23	104.49	111.28
1	A	488	LEU	N-CA-C	-6.04	104.70	111.28
1	A	70	THR	N-CA-C	-5.89	104.78	111.14
1	A	535	ALA	N-CA-C	5.70	117.50	111.28
1	A	352	GLY	N-CA-C	-5.67	105.93	112.73
2	B	22	SER	CB-CA-C	5.56	120.02	110.79
2	B	69	GLN	CA-CB-CG	-5.55	103.01	114.10
1	A	363	GLY	N-CA-C	-5.54	105.68	112.77
1	A	95	ARG	NE-CZ-NH2	5.53	124.17	119.20
1	A	181	LEU	N-CA-C	5.50	117.72	111.11
1	A	475	ILE	CA-CB-CG2	5.49	119.83	110.50
2	B	30	ILE	N-CA-C	5.46	116.09	110.36
1	A	425	VAL	N-CA-CB	-5.40	102.49	110.58
2	B	114	HIS	CA-C-N	-5.37	116.03	122.16
2	B	114	HIS	C-N-CA	-5.37	116.03	122.16
2	B	7	ALA	N-CA-C	-5.32	105.56	111.36
1	A	517	ASP	N-CA-C	5.29	118.63	111.17
1	A	307	VAL	O-C-N	5.26	123.79	120.42
2	B	157	HIS	N-CA-C	5.22	117.38	111.11
1	A	495	ARG	N-CA-C	5.14	116.57	110.97
1	A	450	ARG	NE-CZ-NH1	-5.09	116.41	121.50
1	A	514	GLY	N-CA-C	-5.08	101.97	112.34
1	A	115	ILE	N-CA-C	5.01	115.23	110.42

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	4368	0	4462	67	0
2	B	1288	0	1260	15	0
3	C	241	0	267	5	0
4	A	1	0	0	0	0
5	A	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	65	0	62	5	0
7	A	2	0	0	0	0
8	A	174	0	247	31	0
8	B	80	0	112	12	0
8	C	32	0	50	2	0
9	B	2	0	0	0	0
10	A	106	0	0	3	0
10	B	67	0	0	1	0
10	C	6	0	0	1	0
All	All	6475	0	6490	99	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (99) 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:168:ARG:HH22	8:A:609:OLC:C2	1.62	1.11
1:A:330[B]:ARG:HH11	1:A:330[B]:ARG:CG	1.67	1.07
1:A:168:ARG:NH1	8:A:609:OLC:H7A	1.77	0.99
1:A:168:ARG:HH12	8:A:609:OLC:H5	1.26	0.99
1:A:330[B]:ARG:HG2	1:A:330[B]:ARG:NH1	1.54	0.94
1:A:168:ARG:HH12	8:A:609:OLC:C5	1.80	0.93
3:C:34:GLY:OXT	10:C:204:HOH:O	1.89	0.90
1:A:168:ARG:HH22	8:A:609:OLC:H2A	1.43	0.83
1:A:495:ARG:HH21	1:A:495:ARG:HA	1.42	0.83
8:A:606:OLC:H13A	8:A:611:OLC:H12	1.61	0.82
1:A:168:ARG:NH2	8:A:609:OLC:O23	2.12	0.81
1:A:330[B]:ARG:HH11	1:A:330[B]:ARG:HG2	0.74	0.81
1:A:516:GLU:O	1:A:516:GLU:CG	2.30	0.79
2:B:141:ARG:HH12	8:B:203:OLC:H24A	1.49	0.77
1:A:168:ARG:HH22	8:A:609:OLC:H2	1.45	0.77
2:B:141:ARG:NH1	8:B:203:OLC:H24A	2.00	0.76
1:A:168:ARG:NH2	8:A:609:OLC:C2	2.46	0.75
8:B:203:OLC:H7A	8:C:101:OLC:O25	1.88	0.74
1:A:330[B]:ARG:CG	1:A:330[B]:ARG:NH1	2.35	0.74
8:A:605:OLC:H12	8:A:611:OLC:H14A	1.70	0.73
1:A:168:ARG:HH12	8:A:609:OLC:H7A	1.53	0.72
1:A:236:ILE:HD13	6:A:603:HAS:C3C	2.21	0.70
8:A:605:OLC:C12	8:A:611:OLC:H14A	2.23	0.69
1:A:516:GLU:O	1:A:516:GLU:HG3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ILE:HD13	6:A:603:HAS:C2C	2.25	0.67
1:A:168:ARG:NH1	8:A:609:OLC:C7	2.60	0.62
1:A:168:ARG:NH1	8:A:609:OLC:C5	2.59	0.62
1:A:168:ARG:NH2	8:A:609:OLC:H2A	2.11	0.61
1:A:168:ARG:HH11	8:A:609:OLC:H7A	1.65	0.60
8:A:606:OLC:H13A	8:A:611:OLC:C12	2.30	0.59
1:A:282:HIS:CD2	1:A:283:HIS:CD2	2.91	0.58
1:A:236:ILE:HD12	1:A:236:ILE:C	2.28	0.57
2:B:18:TRP:CE3	3:C:12:ILE:HD13	2.40	0.56
2:B:14:TYR:OH	8:B:204:OLC:H24A	2.06	0.55
1:A:168:ARG:HH22	8:A:609:OLC:C1	2.19	0.55
8:B:203:OLC:H6	3:C:33:ARG:HE	1.72	0.54
8:A:611:OLC:C8	8:A:611:OLC:H13A	2.37	0.54
1:A:220:ASP:HB3	1:A:223:VAL:HG12	1.90	0.54
1:A:354:LEU:HD21	6:A:603:HAS:H323	1.88	0.54
8:A:610:OLC:O19	8:A:611:OLC:O23	2.25	0.53
1:A:526:ARG:NH2	10:A:781:HOH:O	2.29	0.53
1:A:168:ARG:NH2	8:A:609:OLC:H2	2.19	0.52
2:B:141:ARG:NH1	8:B:203:OLC:O19	2.41	0.52
1:A:526:ARG:HB3	1:A:526:ARG:CZ	2.40	0.52
2:B:14:TYR:CZ	8:B:204:OLC:H24A	2.45	0.51
1:A:241:LEU:N	1:A:242:PRO:CD	2.74	0.51
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.46	0.51
5:A:602:HEM:CMC	5:A:602:HEM:HBC2	2.41	0.51
1:A:405:LEU:HB3	1:A:406:PRO:HD3	1.94	0.50
1:A:516:GLU:O	1:A:516:GLU:HG2	2.10	0.50
2:B:32:LEU:HD21	8:B:202:OLC:H7A	1.92	0.50
1:A:401:LEU:O	1:A:405:LEU:HB2	2.11	0.50
6:A:603:HAS:HMC1	6:A:603:HAS:HBC1	1.93	0.49
1:A:435:MET:HB2	1:A:473:ALA:HB1	1.94	0.49
8:A:611:OLC:H21A	10:A:711:HOH:O	2.12	0.49
1:A:400:SER:HA	1:A:403:TRP:NE1	2.28	0.49
1:A:56:LYS:HG2	1:A:62:VAL:O	2.13	0.49
3:C:4:LYS:HG3	3:C:6:LYS:HG2	1.95	0.49
1:A:254:GLN:HE22	1:A:403:TRP:CD1	2.31	0.48
1:A:138:PRO:HG2	2:B:129:PRO:HG2	1.95	0.48
1:A:168:ARG:HH12	8:A:609:OLC:H5A	1.74	0.47
1:A:168:ARG:HH12	8:A:609:OLC:H2	1.80	0.47
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.50	0.47
8:B:203:OLC:H7A	8:C:101:OLC:C24	2.44	0.47
1:A:168:ARG:NH1	8:A:609:OLC:H5A	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ARG:HA	1:A:495:ARG:NH2	2.23	0.46
8:A:605:OLC:H12A	8:A:611:OLC:H14A	1.97	0.46
1:A:411:LYS:HE3	1:A:497:ARG:NH2	2.30	0.46
1:A:405:LEU:CB	1:A:406:PRO:HD3	2.47	0.45
8:A:609:OLC:H5	8:A:609:OLC:H2	1.29	0.45
1:A:341:TRP:HB3	8:A:606:OLC:H24A	1.99	0.45
1:A:233:HIS:CD2	1:A:233:HIS:C	2.96	0.44
8:A:612:OLC:H8	8:A:612:OLC:H11	1.81	0.44
1:A:154:LEU:HD23	1:A:154:LEU:HA	1.82	0.44
1:A:562:TRP:HA	2:B:155:LEU:HG	1.99	0.44
1:A:291:ASP:OD2	1:A:293:THR:HB	2.18	0.44
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.99	0.43
1:A:293:THR:HG23	8:B:205:OLC:H8	1.99	0.43
5:A:602:HEM:HBC2	5:A:602:HEM:HMC2	2.00	0.43
1:A:371:LEU:HD21	3:C:27:TYR:HD1	1.83	0.43
2:B:47:ALA:HA	10:B:351:HOH:O	2.17	0.43
1:A:552:HIS:HB3	2:B:52:ARG:NH1	2.33	0.43
1:A:230:TRP:C	1:A:230:TRP:CD1	2.97	0.43
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.90	0.43
8:A:613:OLC:H13	8:A:613:OLC:H10	1.04	0.42
1:A:515:PRO:HA	1:A:516:GLU:HB3	2.01	0.42
2:B:17:GLY:HA3	8:B:204:OLC:H3	2.01	0.42
1:A:520:LEU:HD22	1:A:524:MET:HG3	2.02	0.42
6:A:603:HAS:HHA	6:A:603:HAS:HAA2	1.83	0.42
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.55	0.41
1:A:554:ASN:HB2	2:B:52:ARG:HD2	2.02	0.41
1:A:233:HIS:O	1:A:236:ILE:HG13	2.21	0.41
1:A:36:SER:O	1:A:40:PRO:HD3	2.20	0.41
8:A:611:OLC:H13A	8:A:611:OLC:H8A	2.02	0.41
1:A:517:ASP:OD2	1:A:520:LEU:HB2	2.22	0.40
2:B:93:ASN:HA	2:B:94:PRO:HA	1.90	0.40
2:B:141:ARG:NH2	8:B:203:OLC:O19	2.54	0.40
1:A:382:PRO:HG2	10:A:742:HOH:O	2.22	0.40

There are no symmetry-related clashes.

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	554/569 (97%)	539 (97%)	15 (3%)	0	100	100
2	B	165/168 (98%)	163 (99%)	2 (1%)	0	100	100
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	748/771 (97%)	731 (98%)	17 (2%)	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	447/464 (96%)	423 (95%)	24 (5%)	20	17
2	B	134/138 (97%)	129 (96%)	5 (4%)	30	30
3	C	24/27 (89%)	20 (83%)	4 (17%)	2	1
All	All	605/629 (96%)	572 (94%)	33 (6%)	19	17

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

Mol	Chain	Res	Type
1	A	54	LEU
1	A	58	LEU
1	A	133	TYR
1	A	215	LEU
1	A	230	TRP

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Mol	Chain	Res	Type
1	A	236	ILE
1	A	262	ASP
1	A	274	LEU
1	A	290	ILE
1	A	326	LEU
1	A	405	LEU
1	A	413	ILE
1	A	425	VAL
1	A	455	GLN
1	A	475	ILE
1	A	493	LEU
1	A	494	SER
1	A	495	ARG
1	A	500	GLU
1	A	512	ILE
1	A	513	SER
1	A	518	ARG
1	A	520	LEU
1	A	526	ARG
2	B	26	LEU
2	B	37	LEU
2	B	49	LYS
2	B	58	VAL
2	B	167	LYS
3	C	4	LYS
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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	455	GLN
2	B	8	HIS
2	B	40	HIS
2	B	69	GLN
2	B	91	GLN

5.3.3 RNA ⓘ

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 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	OLC	A	612	-	20,20,24	0.51	0	21,21,25	0.86	0
8	OLC	A	605	-	18,18,24	0.50	0	18,18,25	1.14	2 (11%)
8	OLC	A	610	-	19,19,24	0.41	0	20,20,25	0.84	0
8	OLC	A	606	-	22,22,24	0.71	0	23,23,25	1.20	2 (8%)
5	HEM	A	602	1	50,50,50	2.73	21 (42%)	67,82,82	2.83	30 (44%)
8	OLC	B	203	-	23,23,24	1.01	1 (4%)	24,24,25	1.72	4 (16%)
8	OLC	A	607	-	13,13,24	0.66	0	13,13,25	0.82	0
8	OLC	A	608	-	11,11,24	0.76	0	11,11,25	0.99	1 (9%)
9	CUA	B	201	2	0,1,1	-	-	-	-	-
7	PER	A	604	6,4	1,1,1	0.31	0	-	-	-
8	OLC	A	613	-	24,24,24	0.36	0	25,25,25	1.16	3 (12%)
8	OLC	A	609	-	14,14,24	1.20	1 (7%)	15,15,25	1.63	2 (13%)
8	OLC	B	202	-	19,19,24	0.66	1 (5%)	19,19,25	0.77	0
8	OLC	A	611	-	24,24,24	0.68	1 (4%)	25,25,25	1.10	2 (8%)
8	OLC	B	204	-	15,15,24	0.50	0	16,16,25	0.74	0
8	OLC	C	101	-	22,22,24	0.59	0	23,23,25	1.08	1 (4%)
8	OLC	C	102	-	8,8,24	0.10	0	7,7,25	0.43	0
6	HAS	A	603	1,7	72,72,72	2.11	22 (30%)	87,109,109	1.81	21 (24%)
8	OLC	B	205	-	19,19,24	0.54	0	19,19,25	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OLC	A	611	-	-	15/24/24/24	-
8	OLC	A	612	-	-	4/20/20/24	-
8	OLC	B	202	-	-	9/18/18/24	-
8	OLC	A	609	-	-	9/14/14/24	-
8	OLC	B	204	-	-	6/15/15/24	-
8	OLC	A	610	-	-	9/19/19/24	-
8	OLC	A	606	-	-	8/22/22/24	-
8	OLC	C	101	-	-	9/22/22/24	-
5	HEM	A	602	1	-	1/14/54/54	-
8	OLC	B	203	-	-	10/23/23/24	-
8	OLC	A	613	-	-	10/24/24/24	-
8	OLC	C	102	-	-	3/6/6/24	-
8	OLC	A	607	-	-	3/12/12/24	-
6	HAS	A	603	1,7	1/1/8/18	5/42/82/82	-
8	OLC	A	608	-	-	3/9/9/24	-
8	OLC	B	205	-	-	7/18/18/24	-
8	OLC	A	605	-	-	5/16/16/24	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEM	C3C-C4C	-7.34	1.33	1.46
5	A	602	HEM	C1C-C2C	-6.80	1.31	1.45
5	A	602	HEM	CHB-C1B	5.33	1.49	1.38
6	A	603	HAS	CHC-C1C	5.27	1.51	1.39
6	A	603	HAS	C1D-ND	5.22	1.49	1.40
5	A	602	HEM	CHC-C1C	5.02	1.48	1.38
6	A	603	HAS	CAC-C3C	-4.97	1.34	1.47
5	A	602	HEM	CHD-C4C	4.92	1.48	1.38
5	A	602	HEM	CAB-C3B	-4.36	1.35	1.47
6	A	603	HAS	CHB-C1D	4.23	1.47	1.38
6	A	603	HAS	CHA-C4D	4.17	1.48	1.39
5	A	602	HEM	C1A-NA	4.17	1.47	1.39
5	A	602	HEM	C3C-C2C	4.10	1.45	1.37
5	A	602	HEM	CBB-CAB	4.09	1.50	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEM	C1B-C2B	-3.88	1.36	1.44
6	A	603	HAS	CHD-C4C	3.79	1.47	1.39
8	A	609	OLC	O20-C1	3.74	1.44	1.33
6	A	603	HAS	FE-NA	3.66	2.07	1.95
6	A	603	HAS	C4D-ND	3.63	1.46	1.38
8	B	203	OLC	O20-C1	3.50	1.43	1.33
6	A	603	HAS	CBC-CAC	3.47	1.47	1.30
5	A	602	HEM	CHA-C1A	3.40	1.47	1.39
5	A	602	HEM	FE-ND	3.29	2.05	1.94
6	A	603	HAS	CHA-C1A	-3.20	1.32	1.38
6	A	603	HAS	C3C-C2C	2.98	1.51	1.41
6	A	603	HAS	FE-NC	2.77	2.04	1.95
5	A	602	HEM	CMB-C2B	2.75	1.56	1.50
5	A	602	HEM	CMA-C3A	2.70	1.56	1.50
6	A	603	HAS	O1D-CGD	2.67	1.30	1.22
6	A	603	HAS	C4D-C3D	2.62	1.49	1.45
5	A	602	HEM	FE-NB	2.55	2.02	1.94
8	A	611	OLC	O20-C1	2.53	1.40	1.33
5	A	602	HEM	C1D-C2D	2.51	1.49	1.44
6	A	603	HAS	C1C-C2C	-2.51	1.37	1.43
6	A	603	HAS	C4C-NC	2.48	1.44	1.39
6	A	603	HAS	CHB-C1B	-2.46	1.33	1.39
6	A	603	HAS	FE-NB	2.43	2.02	1.94
6	A	603	HAS	C3C-C4C	2.39	1.49	1.42
8	B	202	OLC	O20-C1	2.36	1.40	1.33
5	A	602	HEM	CHD-C1D	-2.34	1.33	1.39
6	A	603	HAS	C4A-C3A	2.28	1.49	1.45
5	A	602	HEM	C3B-C2B	2.26	1.41	1.37
6	A	603	HAS	CHC-C4B	-2.22	1.34	1.38
5	A	602	HEM	FE-NA	2.15	2.02	1.95
5	A	602	HEM	C4D-C3D	2.13	1.48	1.45
6	A	603	HAS	C1C-NC	-2.12	1.35	1.39
5	A	602	HEM	FE-NC	2.08	2.02	1.95

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	HEM	CHC-C4B-NB	9.90	135.07	124.42
5	A	602	HEM	CHD-C1D-ND	7.41	132.40	124.42
6	A	603	HAS	C4C-C3C-C2C	-6.63	99.05	107.30
5	A	602	HEM	CHA-C4D-ND	6.44	132.34	124.37
5	A	602	HEM	C4D-ND-C1D	6.20	112.55	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	CHA-C1A-NA	4.79	129.67	124.45
5	A	602	HEM	C1A-CHA-C4D	-4.58	115.48	126.25
6	A	603	HAS	CHA-C1A-C2A	-4.52	117.72	124.86
5	A	602	HEM	C4C-C3C-C2C	-4.34	103.05	106.81
5	A	602	HEM	CMD-C2D-C1D	-4.29	118.33	125.03
8	A	609	OLC	O20-C1-C2	4.26	124.82	111.83
8	B	203	OLC	C21-O20-C1	4.15	132.29	117.12
5	A	602	HEM	C1C-CHC-C4B	-4.10	117.30	126.02
8	B	203	OLC	O20-C21-C22	4.06	124.94	105.85
5	A	602	HEM	C2D-C1D-ND	-4.00	105.28	109.90
5	A	602	HEM	CHC-C4B-C3B	-3.73	117.62	125.07
5	A	602	HEM	C4B-C3B-C2B	-3.73	103.85	107.28
5	A	602	HEM	CHA-C1A-NA	3.67	130.51	123.86
5	A	602	HEM	C4A-CHB-C1B	-3.63	117.72	126.25
5	A	602	HEM	C2A-C1A-NA	-3.48	106.29	110.15
6	A	603	HAS	C2D-C3D-C4D	3.47	108.94	106.43
6	A	603	HAS	CAA-CBA-CGA	-3.29	104.94	113.67
5	A	602	HEM	C3D-C4D-ND	-3.27	106.58	110.17
8	B	203	OLC	C21-C22-C24	3.23	122.65	111.77
8	A	606	OLC	O20-C21-C22	-3.21	90.77	105.85
5	A	602	HEM	C3B-C4B-NB	-3.12	107.23	109.47
6	A	603	HAS	CMB-C2B-C3B	-3.11	124.26	130.28
8	A	613	OLC	C3-C2-C1	-3.09	102.39	113.69
5	A	602	HEM	CHB-C1B-NB	3.03	128.12	124.37
6	A	603	HAS	CHD-C4A-NA	2.95	127.66	124.45
6	A	603	HAS	CHB-C1D-ND	-2.86	120.83	124.37
6	A	603	HAS	C1D-C2D-C3D	2.73	109.79	107.28
6	A	603	HAS	C2C-C1C-NC	2.70	114.47	110.14
8	B	203	OLC	O23-C22-C24	-2.66	98.15	109.18
5	A	602	HEM	CHA-C4D-C3D	-2.63	120.38	125.23
8	A	606	OLC	C21-C22-C24	2.63	120.62	111.77
8	A	611	OLC	O20-C21-C22	2.57	117.93	105.85
8	A	605	OLC	C3-C2-C1	-2.55	107.85	114.51
6	A	603	HAS	CHD-C4A-C3A	-2.55	120.19	125.49
5	A	602	HEM	CAD-CBD-CGD	-2.51	107.00	113.67
6	A	603	HAS	C20-C19-C18	-2.47	115.61	121.17
5	A	602	HEM	CMC-C2C-C3C	-2.44	122.52	128.43
5	A	602	HEM	O2A-CGA-CBA	2.41	121.60	114.00
6	A	603	HAS	CMB-C2B-C1B	2.37	128.74	125.03
8	A	613	OLC	C13-C12-C11	-2.34	102.59	113.86
5	A	602	HEM	CBD-CAD-C3D	-2.34	106.08	112.53
8	A	605	OLC	C13-C14-C15	-2.32	102.63	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	C27-C19-C20	2.29	119.21	115.23
6	A	603	HAS	O2D-CGD-CBD	2.29	121.24	114.00
8	C	101	OLC	C21-O20-C1	2.28	125.44	117.12
6	A	603	HAS	CHA-C4D-ND	-2.28	121.97	124.42
5	A	602	HEM	O2A-CGA-O1A	-2.23	117.61	123.33
5	A	602	HEM	O2D-CGD-O1D	-2.22	117.62	123.33
6	A	603	HAS	C2A-C1A-NA	2.22	112.46	110.32
8	A	611	OLC	C21-O20-C1	2.21	125.19	117.12
8	A	613	OLC	C3-C4-C5	-2.19	103.30	114.37
5	A	602	HEM	C4A-C3A-C2A	2.16	109.29	106.82
5	A	602	HEM	CHB-C1B-C2B	-2.15	120.83	126.95
6	A	603	HAS	C12-C11-C3B	2.13	115.45	112.12
8	A	608	OLC	C3-C4-C5	-2.12	103.65	114.37
6	A	603	HAS	C1A-CHA-C4D	-2.11	121.54	126.02
5	A	602	HEM	C1B-NB-C4B	2.09	107.68	105.21
6	A	603	HAS	C17-C18-C19	-2.06	122.90	127.62
5	A	602	HEM	O2D-CGD-CBD	2.04	120.46	114.00
5	A	602	HEM	C3B-C2B-C1B	2.04	107.94	106.41
8	A	609	OLC	C21-O20-C1	2.03	124.55	117.12
6	A	603	HAS	CHA-C4D-C3D	2.03	127.74	124.77
5	A	602	HEM	CHC-C1C-NC	-2.00	122.27	124.45

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	603	HAS	NA

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	HEM	C2B-C3B-CAB-CBB
8	A	606	OLC	C21-C22-C24-O25
8	A	609	OLC	C21-C22-C24-O25
8	A	610	OLC	O20-C21-C22-O23
8	A	612	OLC	C21-C22-C24-O25
8	A	613	OLC	O20-C21-C22-C24
8	A	613	OLC	O20-C21-C22-O23
8	B	203	OLC	C21-C22-C24-O25
8	B	204	OLC	C21-C22-C24-O25
8	B	203	OLC	C22-C21-O20-C1
8	A	611	OLC	O20-C21-C22-O23
8	B	202	OLC	C2-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
8	A	609	OLC	C2-C1-O20-C21
8	A	610	OLC	C2-C1-O20-C21
8	A	605	OLC	C2-C3-C4-C5
8	A	609	OLC	C2-C3-C4-C5
8	A	611	OLC	C2-C3-C4-C5
8	A	610	OLC	O20-C21-C22-C24
8	A	610	OLC	O19-C1-O20-C21
8	A	613	OLC	C4-C5-C6-C7
8	B	205	OLC	C2-C1-O20-C21
8	A	612	OLC	O23-C22-C24-O25
8	A	609	OLC	O19-C1-O20-C21
8	A	607	OLC	C1-C2-C3-C4
8	B	203	OLC	C1-C2-C3-C4
6	A	603	HAS	C23-C24-C28-C29
8	A	606	OLC	O20-C21-C22-O23
8	C	101	OLC	C2-C1-O20-C21
8	B	202	OLC	O19-C1-O20-C21
8	A	606	OLC	O20-C21-C22-C24
8	B	204	OLC	C1-C2-C3-C4
8	C	101	OLC	O19-C1-O20-C21
8	A	611	OLC	C12-C13-C14-C15
8	C	101	OLC	C5-C6-C7-C8
8	A	606	OLC	O23-C22-C24-O25
8	B	204	OLC	O23-C22-C24-O25
8	A	613	OLC	C10-C11-C12-C13
8	B	202	OLC	C3-C4-C5-C6
8	A	606	OLC	C12-C13-C14-C15
8	A	611	OLC	C2-C1-O20-C21
8	C	101	OLC	C1-C2-C3-C4
8	B	203	OLC	C2-C3-C4-C5
8	A	606	OLC	C11-C12-C13-C14
8	A	611	OLC	C13-C14-C15-C16
8	A	605	OLC	C10-C11-C12-C13
8	B	203	OLC	C6-C7-C8-C9
8	C	102	OLC	C14-C15-C16-C17
8	A	611	OLC	O19-C1-O20-C21
8	A	613	OLC	C12-C13-C14-C15
8	A	611	OLC	C1-C2-C3-C4
8	B	202	OLC	C6-C7-C8-C9
8	C	101	OLC	C10-C11-C12-C13
8	A	610	OLC	C2-C3-C4-C5
8	A	610	OLC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
8	B	205	OLC	O19-C1-O20-C21
8	A	611	OLC	C14-C15-C16-C17
8	A	611	OLC	C4-C5-C6-C7
8	A	609	OLC	O23-C22-C24-O25
8	A	605	OLC	C4-C5-C6-C7
8	A	613	OLC	C14-C15-C16-C17
8	B	203	OLC	C3-C4-C5-C6
8	A	610	OLC	C6-C7-C8-C9
8	A	611	OLC	C10-C11-C12-C13
8	A	609	OLC	C3-C4-C5-C6
8	B	203	OLC	C2-C1-O20-C21
8	A	612	OLC	C10-C11-C12-C13
8	B	203	OLC	O19-C1-O20-C21
8	A	611	OLC	C15-C16-C17-C18
8	A	610	OLC	C4-C5-C6-C7
8	B	202	OLC	C14-C15-C16-C17
8	A	609	OLC	O20-C21-C22-O23
8	A	611	OLC	O20-C21-C22-C24
8	A	611	OLC	C11-C12-C13-C14
8	A	609	OLC	C5-C6-C7-C8
8	B	202	OLC	C11-C12-C13-C14
8	C	102	OLC	C11-C12-C13-C14
8	C	101	OLC	C11-C12-C13-C14
8	A	613	OLC	C1-C2-C3-C4
8	A	609	OLC	O20-C21-C22-C24
8	C	101	OLC	C4-C5-C6-C7
8	A	612	OLC	C3-C4-C5-C6
8	B	203	OLC	O23-C22-C24-O25
8	B	205	OLC	C13-C14-C15-C16
8	B	205	OLC	C10-C11-C12-C13
8	A	605	OLC	C6-C7-C8-C9
8	A	606	OLC	C13-C14-C15-C16
8	C	102	OLC	C10-C11-C12-C13
8	A	607	OLC	C6-C7-C8-C9
8	A	606	OLC	C7-C8-C9-C10
8	B	202	OLC	C7-C8-C9-C10
8	B	202	OLC	C1-C2-C3-C4
8	A	611	OLC	C3-C4-C5-C6
8	C	101	OLC	C9-C10-C11-C12
8	A	611	OLC	C9-C10-C11-C12
6	A	603	HAS	CAD-CBD-CGD-O1D
8	B	204	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
6	A	603	HAS	CAA-CBA-CGA-O2A
6	A	603	HAS	CAA-CBA-CGA-O1A
8	A	610	OLC	C9-C10-C11-C12
8	B	204	OLC	C2-C1-O20-C21
8	A	608	OLC	O20-C1-C2-C3
8	A	608	OLC	C7-C8-C9-C10
8	A	608	OLC	O19-C1-C2-C3
8	B	204	OLC	C6-C7-C8-C9
8	B	203	OLC	C9-C10-C11-C12
8	B	205	OLC	C7-C8-C9-C10
8	C	101	OLC	C3-C4-C5-C6
8	A	613	OLC	C7-C8-C9-C10
6	A	603	HAS	CAD-CBD-CGD-O2D
8	B	205	OLC	C2-C3-C4-C5
8	B	205	OLC	C5-C6-C7-C8
8	A	613	OLC	C15-C16-C17-C18
8	B	202	OLC	C10-C11-C12-C13
8	A	607	OLC	C7-C8-C9-C10
8	A	605	OLC	C3-C4-C5-C6
8	A	613	OLC	C9-C10-C11-C12

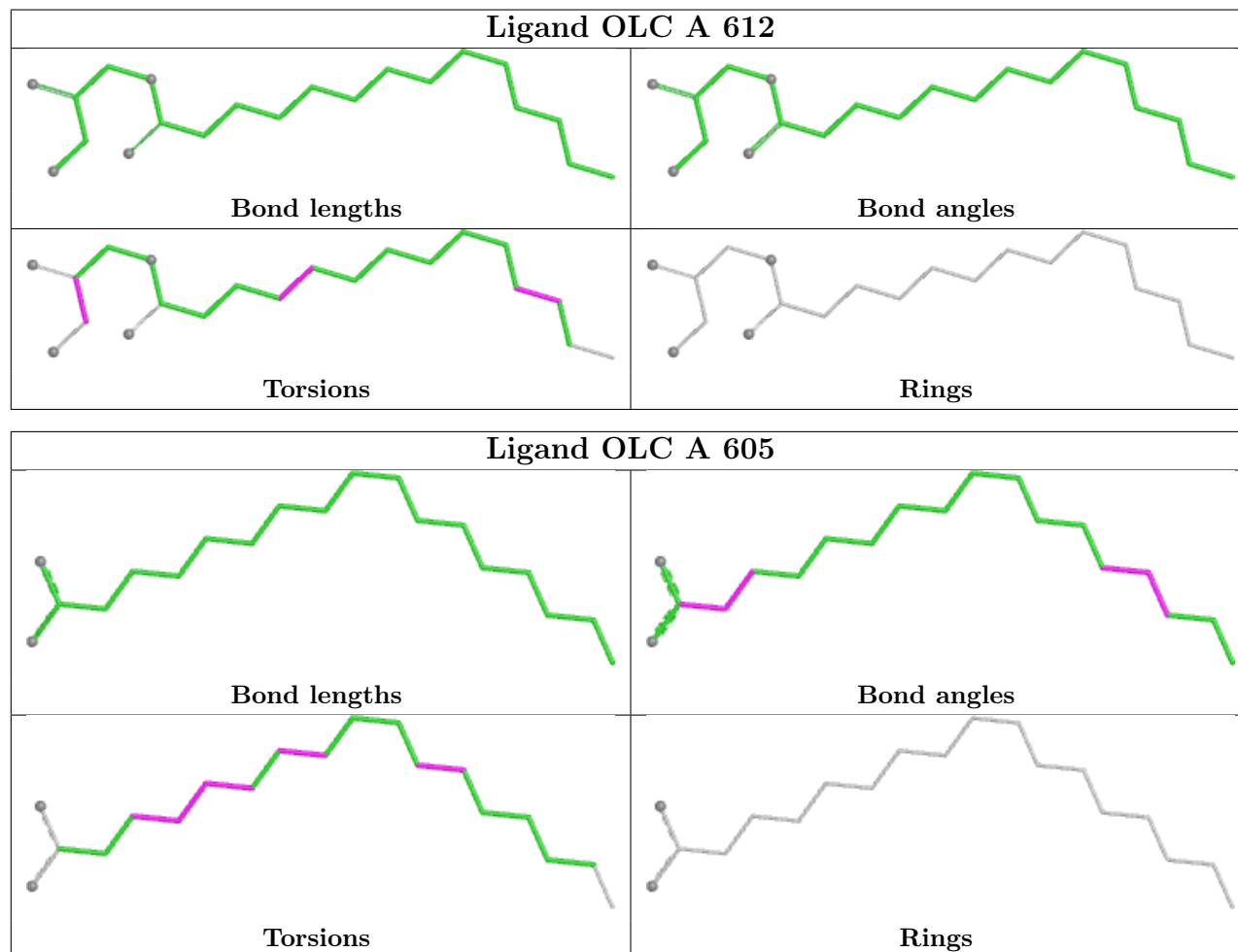
There are no ring outliers.

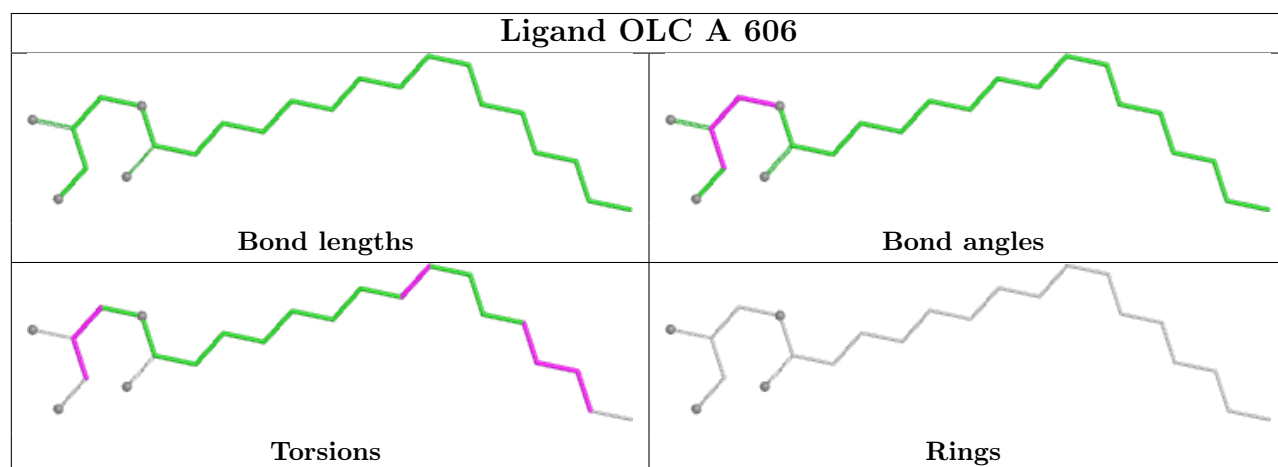
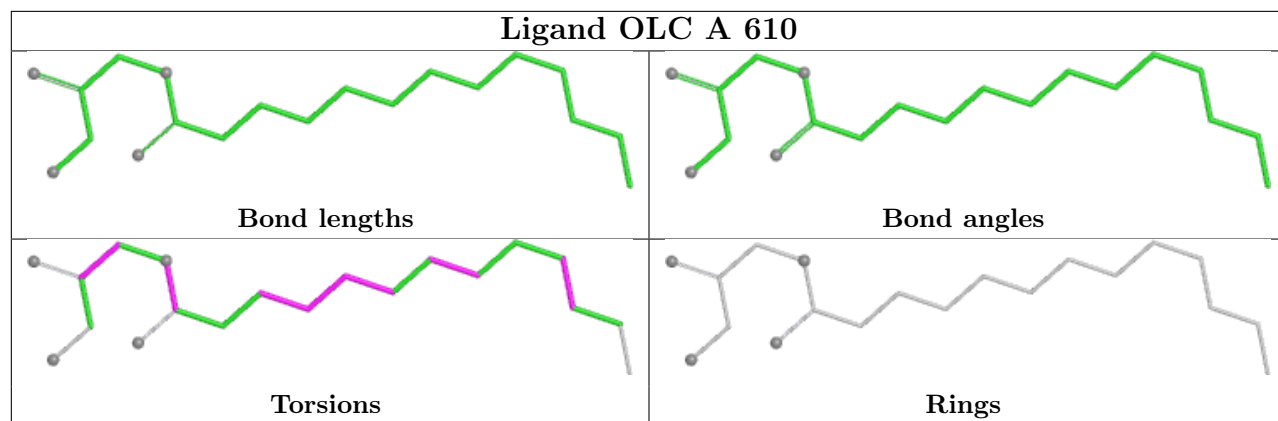
14 monomers are involved in 50 short contacts:

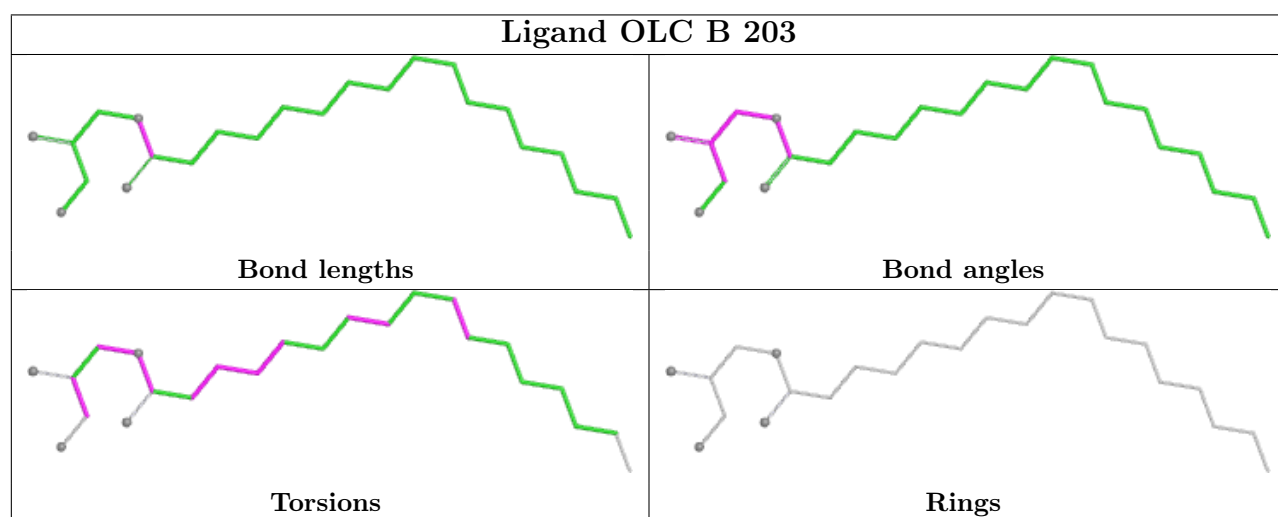
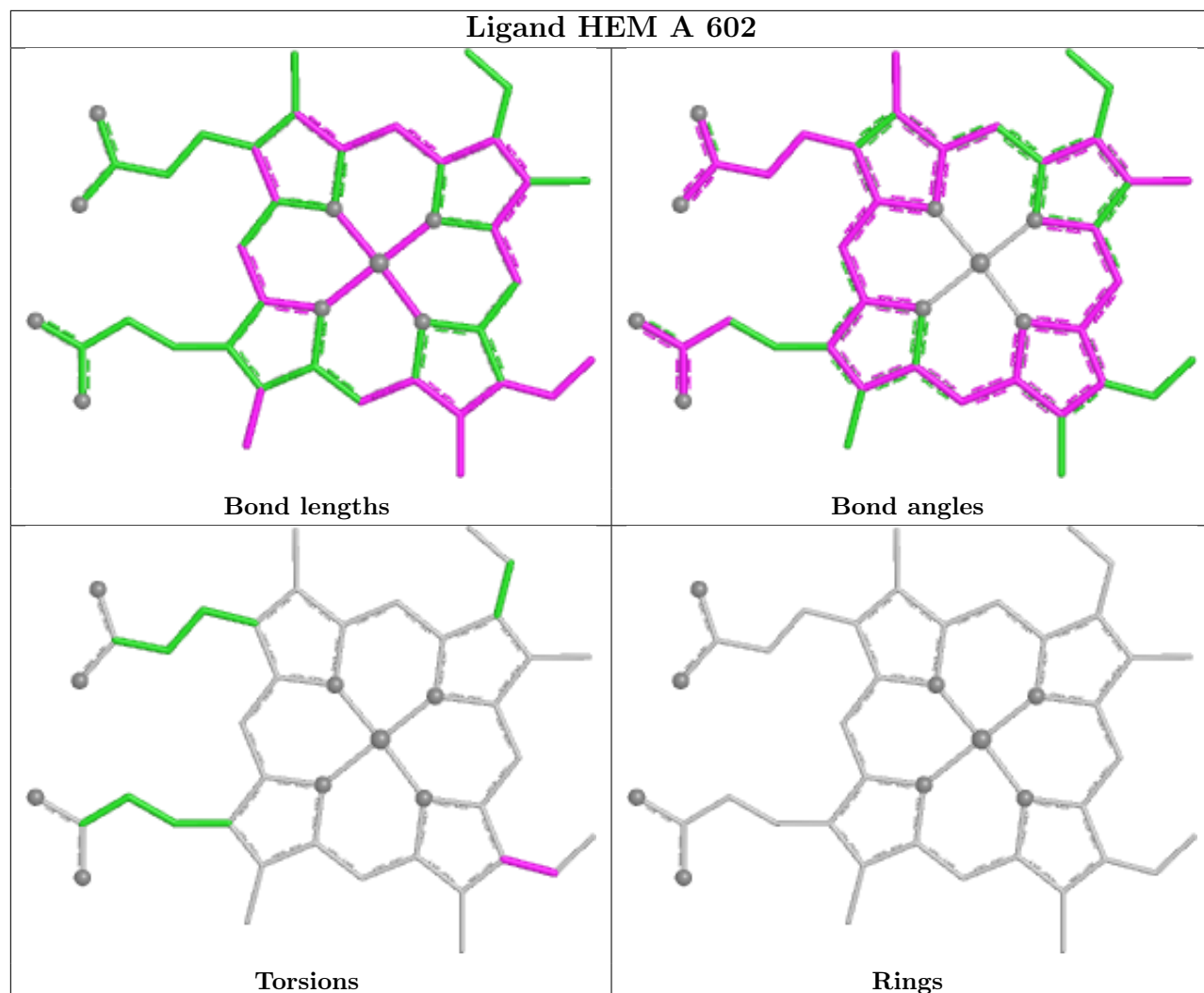
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	612	OLC	1	0
8	A	605	OLC	3	0
8	A	610	OLC	1	0
8	A	606	OLC	3	0
5	A	602	HEM	2	0
8	B	203	OLC	7	0
8	A	613	OLC	1	0
8	A	609	OLC	19	0
8	B	202	OLC	1	0
8	A	611	OLC	9	0
8	B	204	OLC	3	0
8	C	101	OLC	2	0
6	A	603	HAS	5	0
8	B	205	OLC	1	0

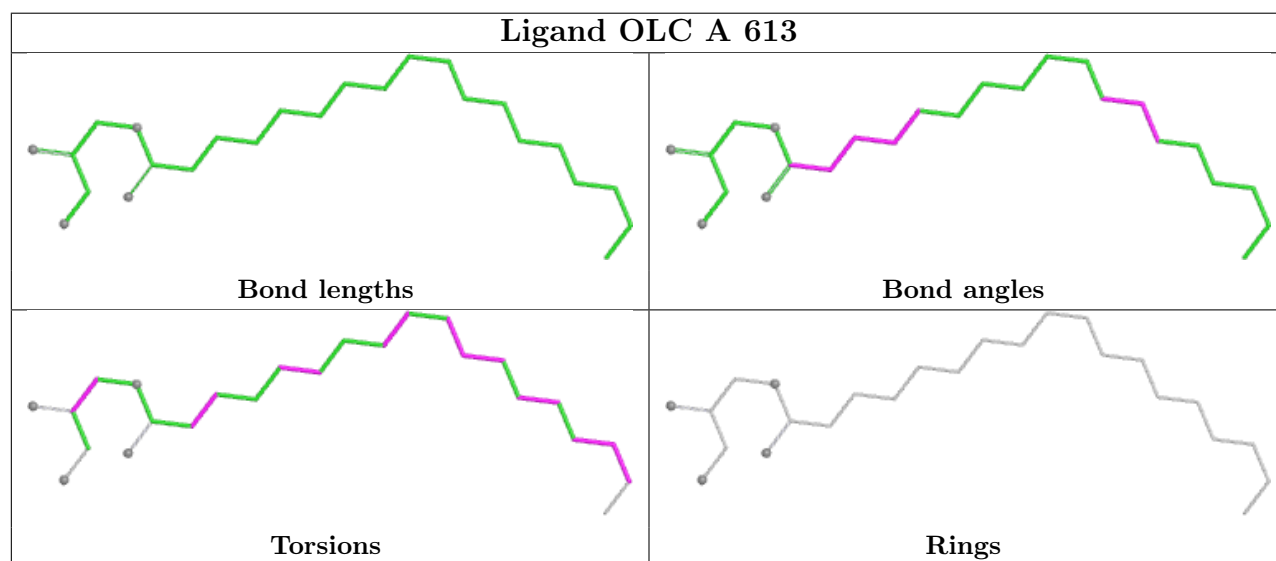
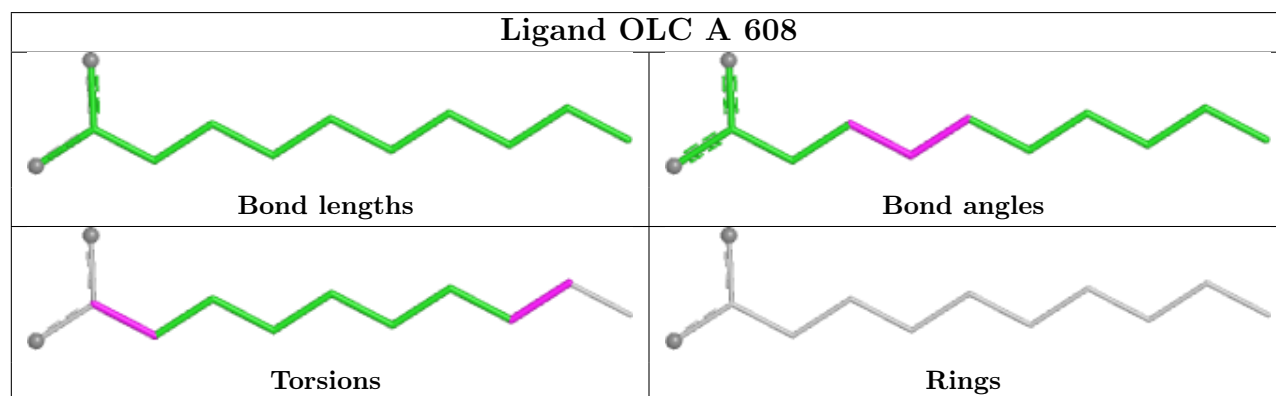
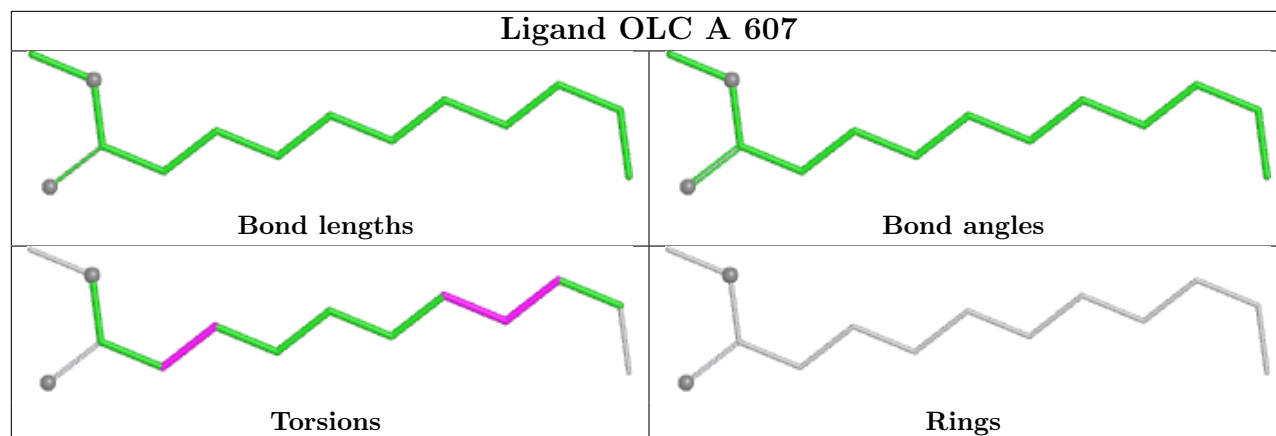
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

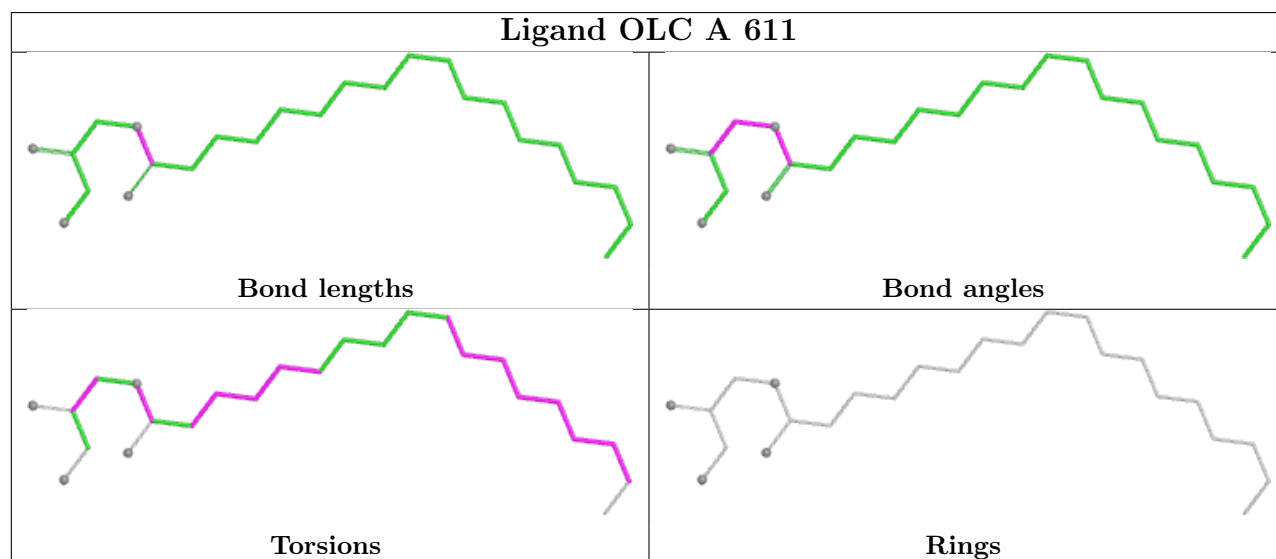
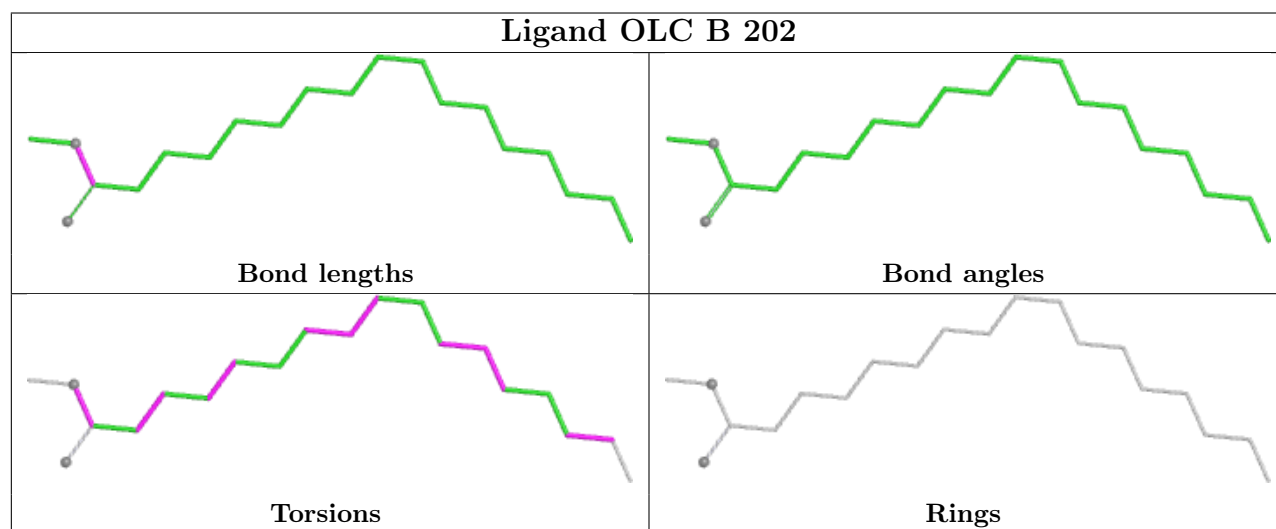
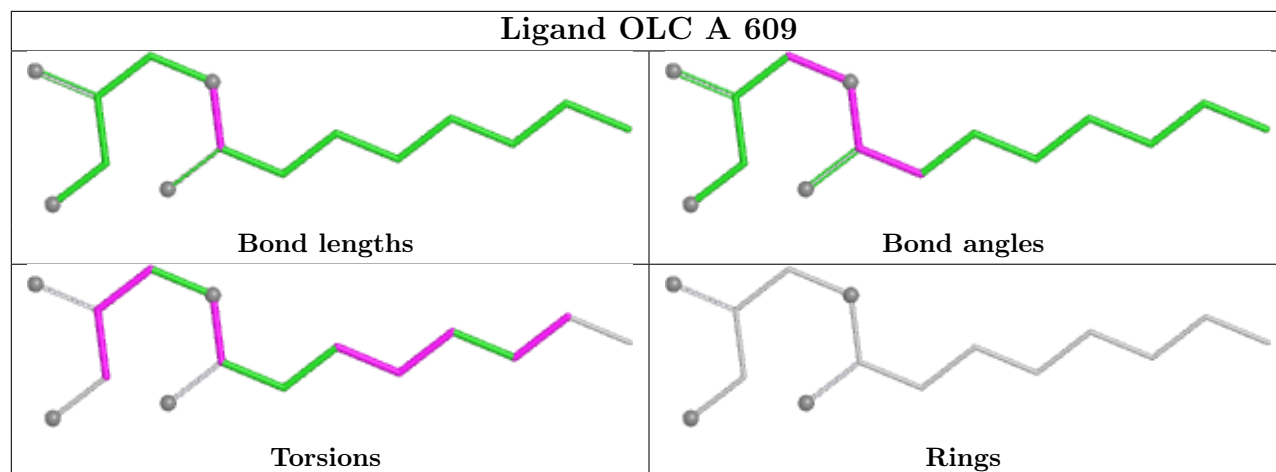
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

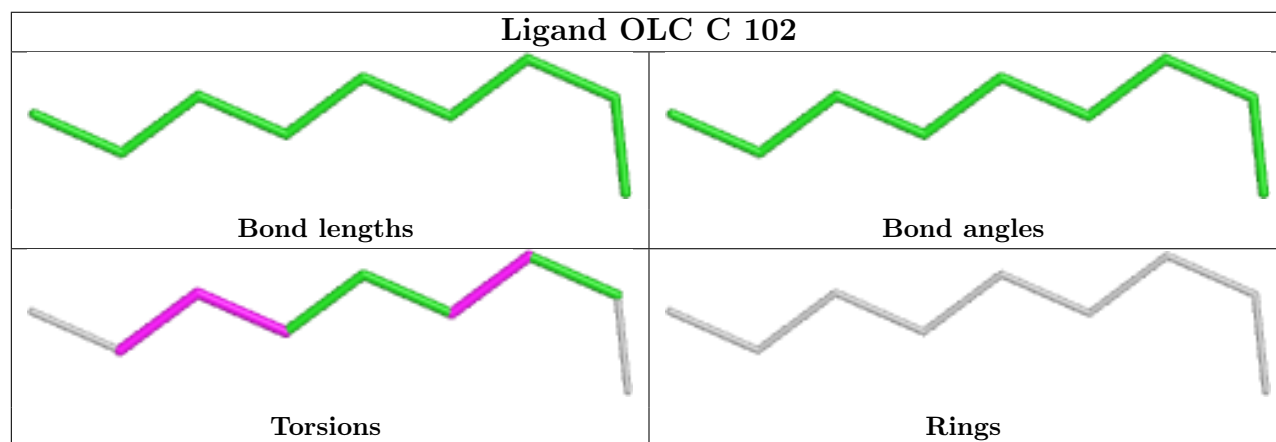
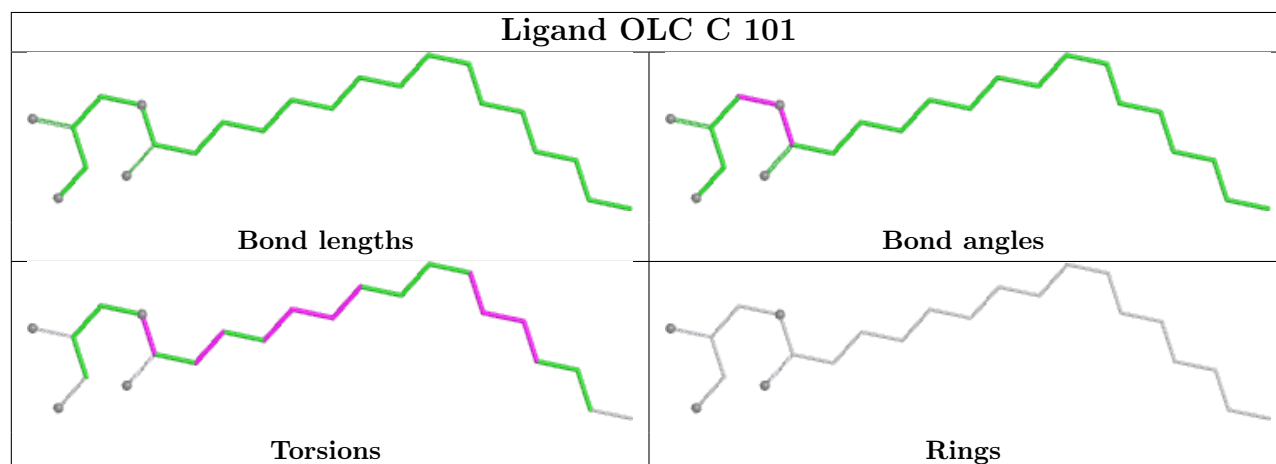
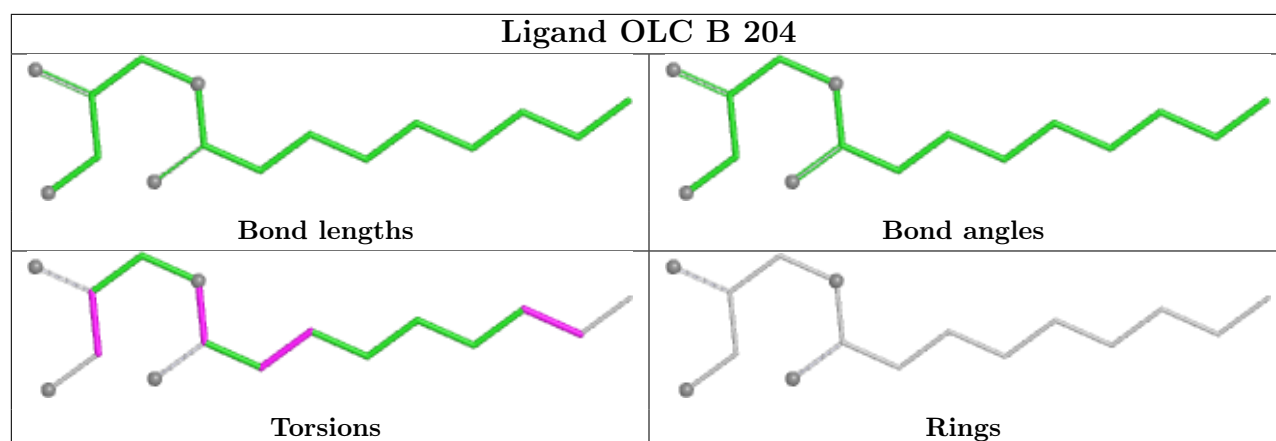


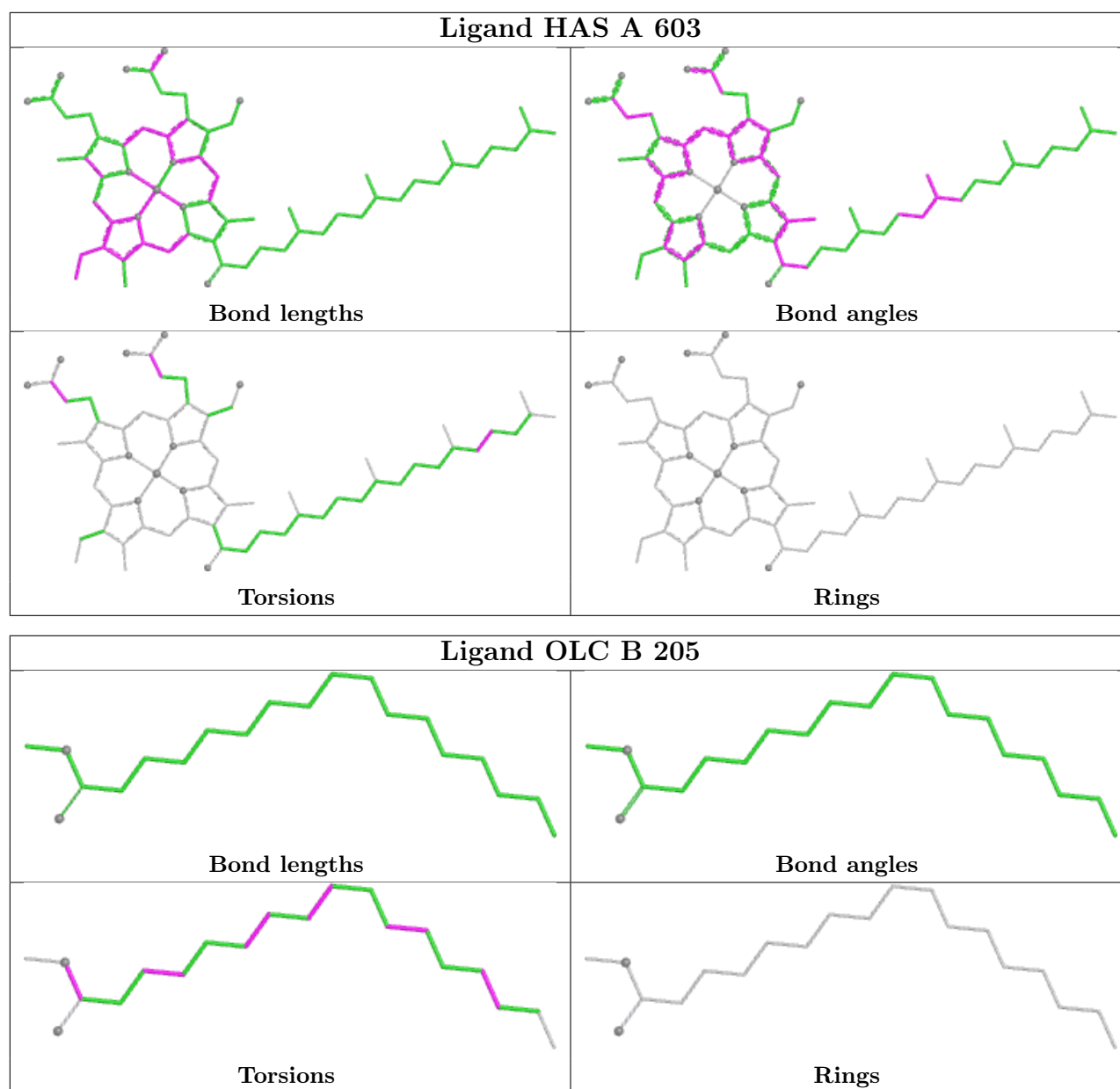












5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

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%)	-0.07	18 (3%) 50 49	15, 25, 49, 100	2 (0%)
2	B	166/168 (98%)	-0.18	6 (3%) 46 45	14, 26, 45, 64	1 (0%)
3	C	31/34 (91%)	-0.21	0 100 100	20, 26, 37, 59	0
All	All	751/771 (97%)	-0.10	24 (3%) 50 49	14, 26, 49, 100	3 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	516	GLU	5.3
1	A	515	PRO	4.3
1	A	513	SER	3.9
1	A	492	LEU	3.7
1	A	491	VAL	3.1
1	A	493	LEU	3.1
1	A	494	SER	2.9
1	A	10	ARG	2.9
2	B	52	ARG	2.8
1	A	400	SER	2.7
1	A	402	TYR	2.6
1	A	500	GLU	2.4
1	A	333	PHE	2.4
1	A	501	LEU	2.3
2	B	3	ASP	2.3
2	B	47	ALA	2.3
1	A	514	GLY	2.3
2	B	49	LYS	2.2
1	A	58	LEU	2.2
1	A	330[A]	ARG	2.1
1	A	495	ARG	2.1
2	B	23	LEU	2.1
1	A	332	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	60	GLN	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.

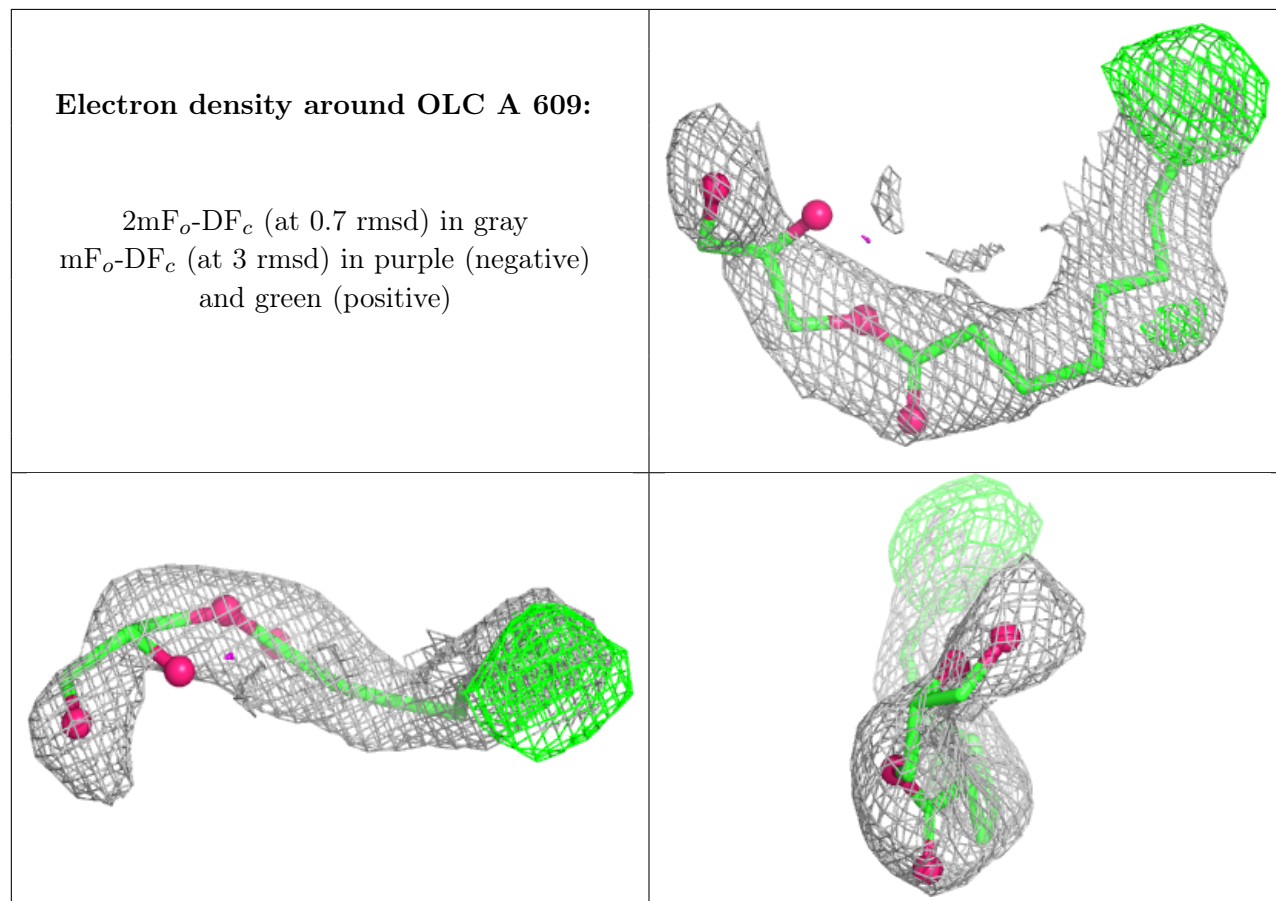
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	OLC	A	609	15/25	0.72	0.22	50,62,84,92	0
8	OLC	A	607	14/25	0.80	0.21	46,55,74,79	0
8	OLC	A	613	25/25	0.80	0.20	47,57,69,87	0
8	OLC	B	203	24/25	0.81	0.20	46,62,86,100	0
8	OLC	C	102	9/25	0.82	0.28	56,60,62,66	0
8	OLC	C	101	23/25	0.83	0.18	37,53,73,79	0
8	OLC	A	608	12/25	0.83	0.20	48,54,71,86	0
8	OLC	B	204	16/25	0.84	0.18	49,60,80,93	0
8	OLC	B	205	20/25	0.84	0.20	47,55,80,82	0
8	OLC	A	610	20/25	0.85	0.18	46,66,86,87	0
8	OLC	B	202	20/25	0.86	0.18	46,57,65,67	0
8	OLC	A	612	21/25	0.86	0.14	46,57,86,96	0
8	OLC	A	611	25/25	0.86	0.18	42,59,71,76	0
8	OLC	A	606	23/25	0.87	0.14	29,40,58,68	0
8	OLC	A	605	19/25	0.89	0.17	43,57,83,84	0
7	PER	A	604	2/2	0.93	0.17	21,21,21,23	0
6	HAS	A	603	65/65	0.98	0.06	14,18,33,36	0
5	HEM	A	602	43/43	0.99	0.04	12,15,18,19	0
4	CU	A	601	1/1	1.00	0.01	21,21,21,21	0
9	CUA	B	201	2/2	1.00	0.01	19,19,19,19	0

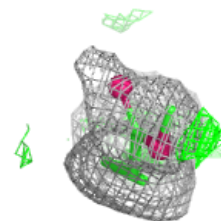
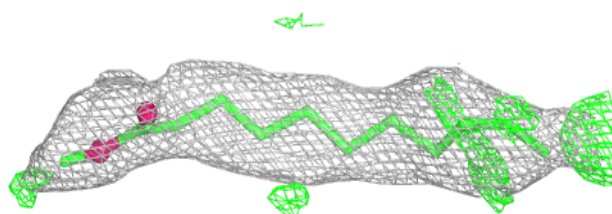
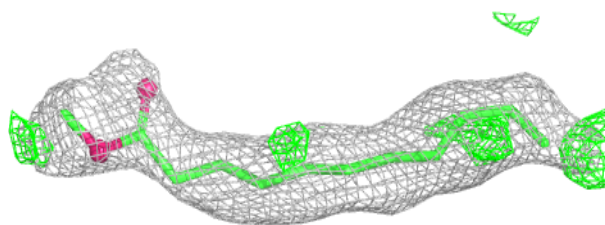
The following is a graphical depiction of the model fit to experimental electron density of all

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.

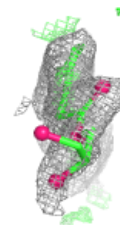
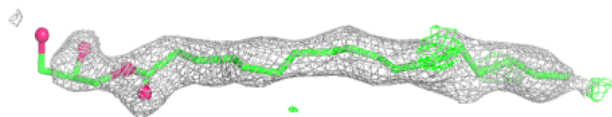
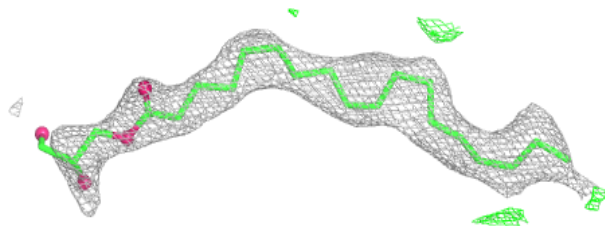


Electron density around OLC A 607:

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

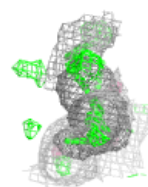
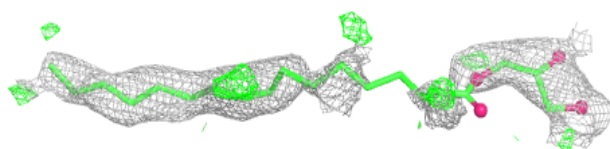
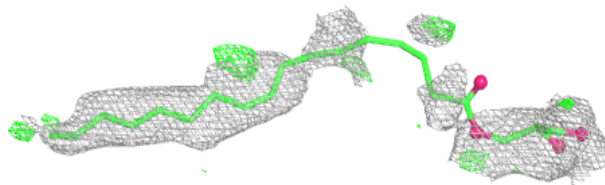
**Electron density around OLC A 613:**

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

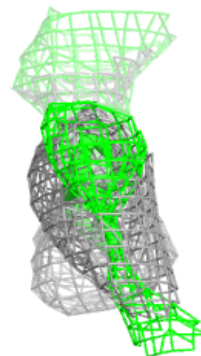
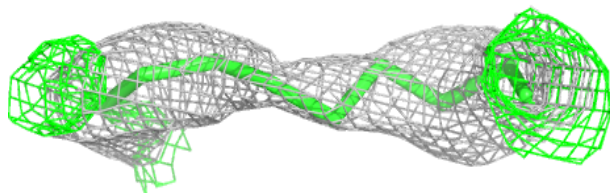
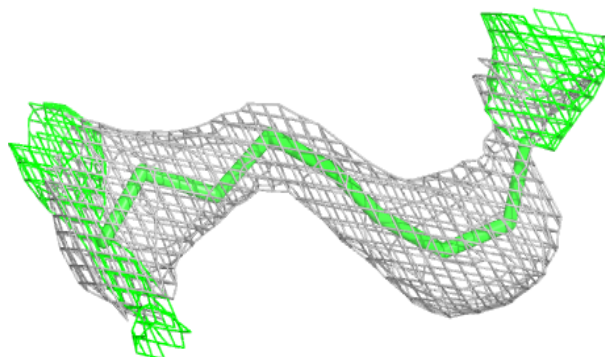


Electron density around OLC B 203:

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

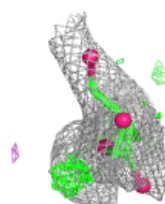
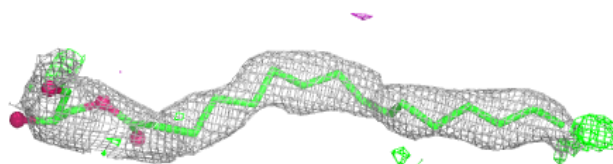
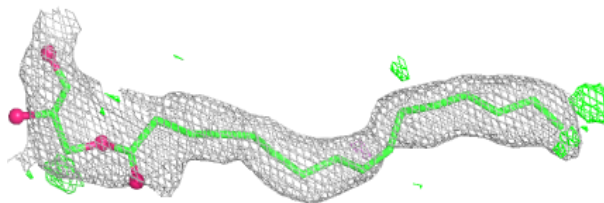
**Electron density around OLC C 102:**

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

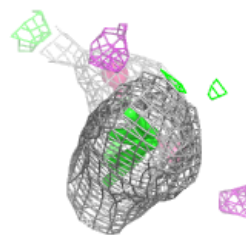
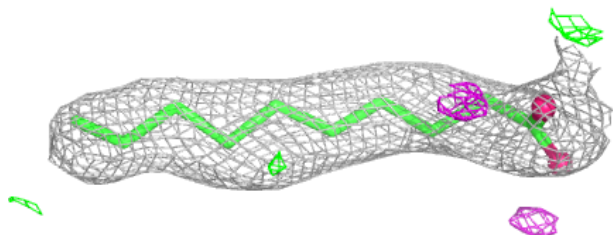
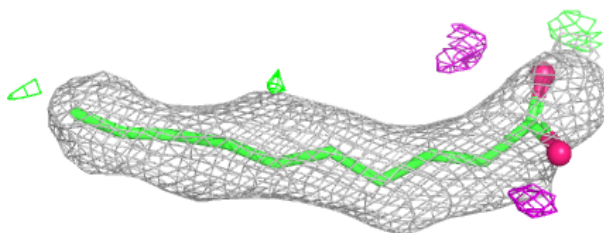


Electron density around OLC C 101:

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

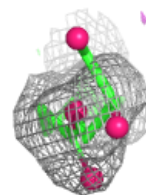
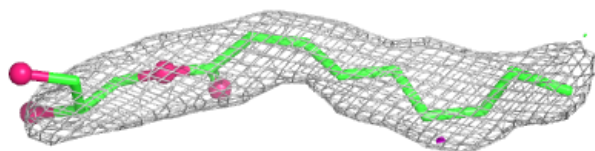
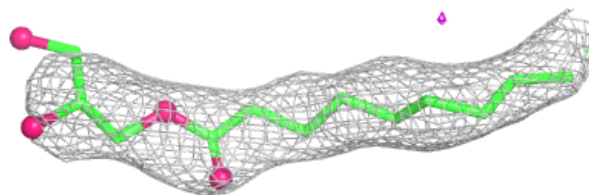
**Electron density around OLC A 608:**

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

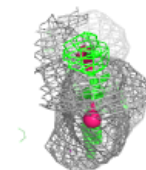
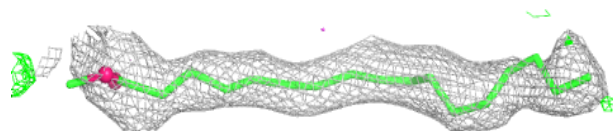
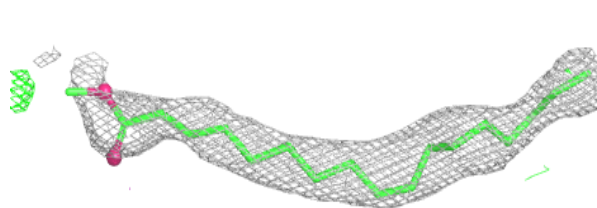


Electron density around OLC B 204:

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

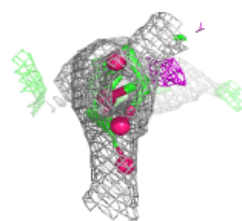
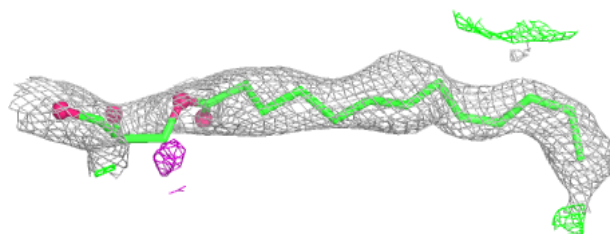
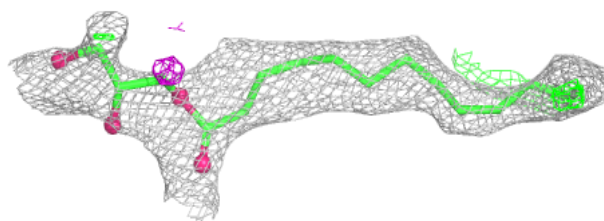
**Electron density around OLC B 205:**

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

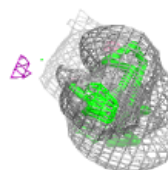
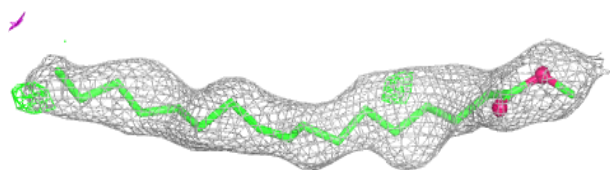
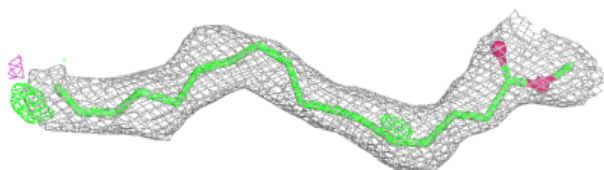


Electron density around OLC A 610:

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

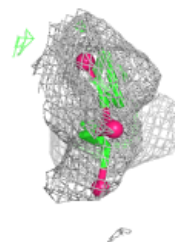
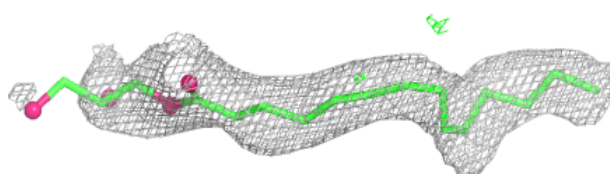
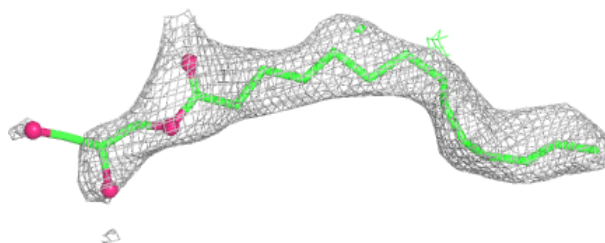
**Electron density around OLC B 202:**

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

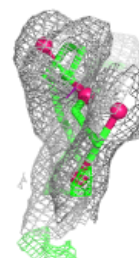
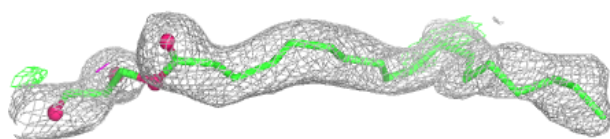
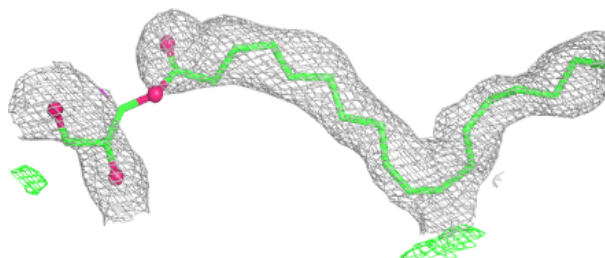


Electron density around OLC A 612:

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

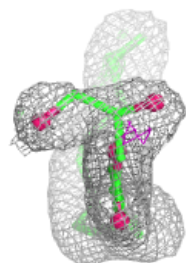
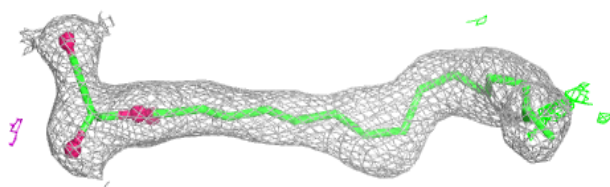
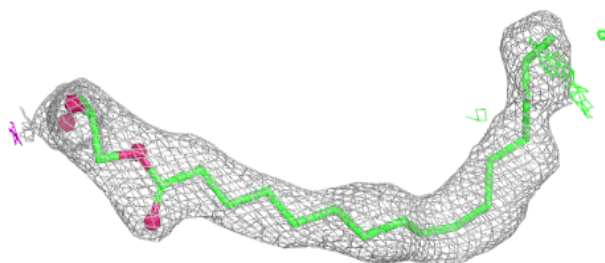
**Electron density around OLC A 611:**

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

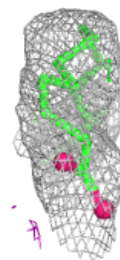
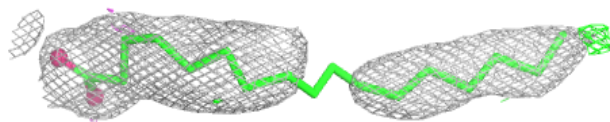
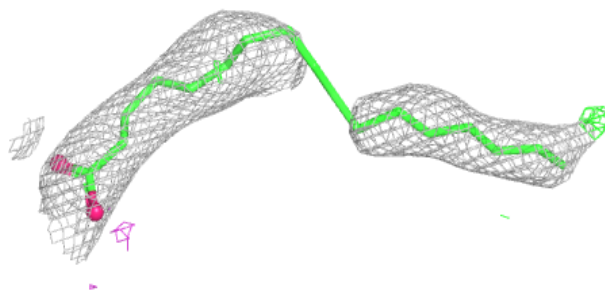


Electron density around OLC A 606:

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

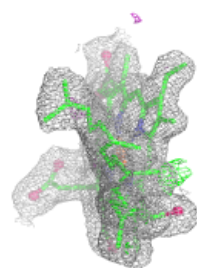
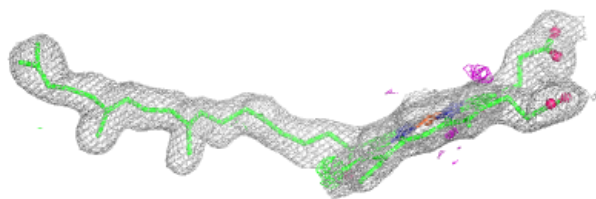
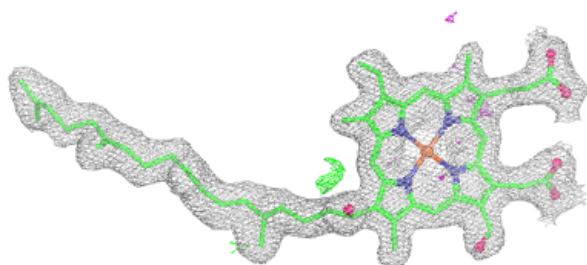
**Electron density around OLC A 605:**

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



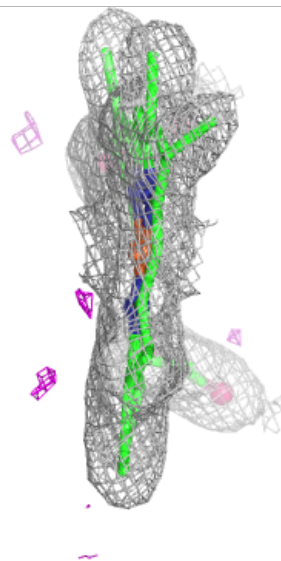
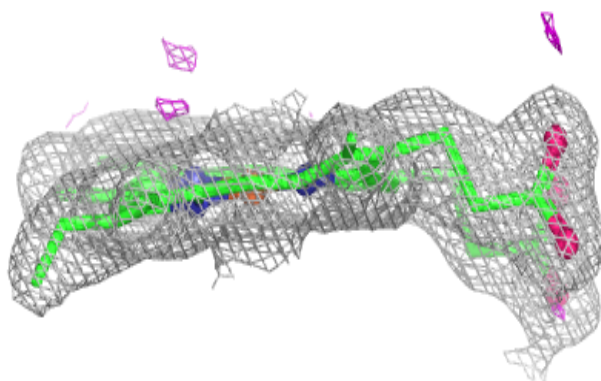
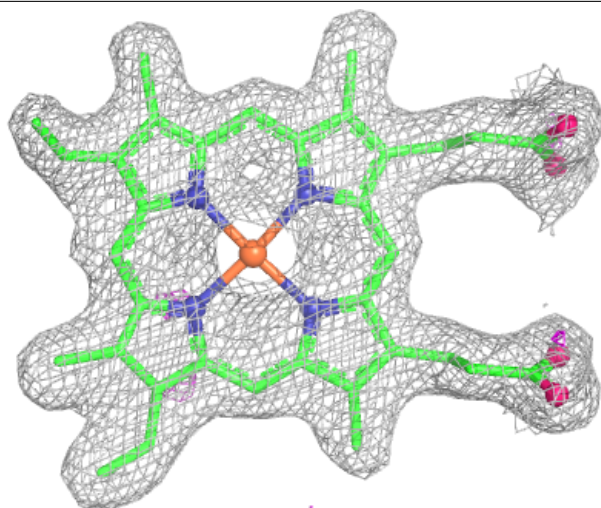
Electron density around HAS A 603:

$2mF_o-DF_c$ (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.