Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 04:20 PM JST

PDB ID	:	8K6Y
Title	:	Serial femtosecond crystallography structure of photo dissociated CO from ba3- type cytochrome c oxidase determined by extrapolation method
Authors	:	Safari, C.; Ghosh, S.; Andersson, R.; Johannesson, J.; Donoso, A.V.; Zoric, D.; Sandelin, E.; Iwata, S.; Neutze, R.; Branden, G.
Deposited on	:	2023-07-25
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:

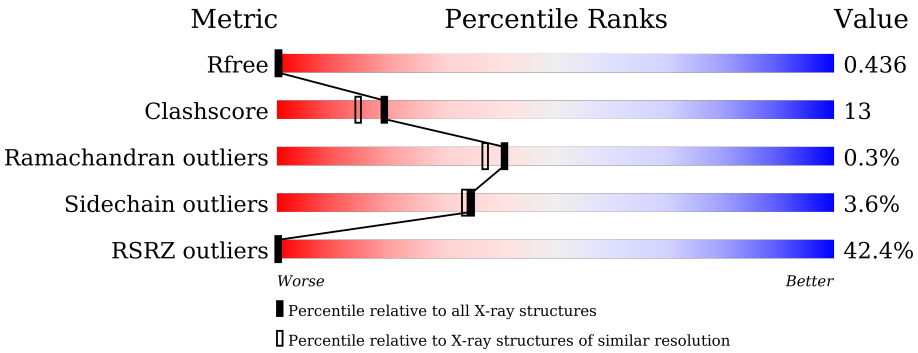
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	44% 70% 26%
2	B	168	33% 76% 22%
3	C	34	35% 85% 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	HAS	A	603	X	-	-	-
7	OLC	A	607	-	-	-	X
7	OLC	A	610	-	-	-	X
7	OLC	C	101	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 6474 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
			4368	2963	698	691	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	0	0
			1301	846	216	235	4			

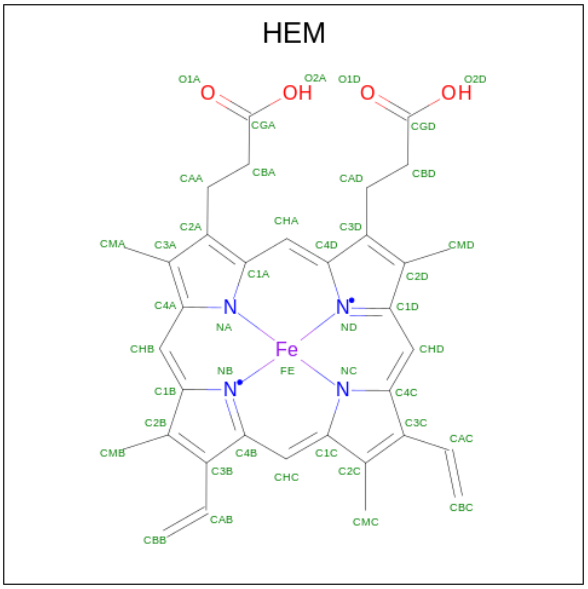
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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 (three-letter code: CU) (formula: Cu).

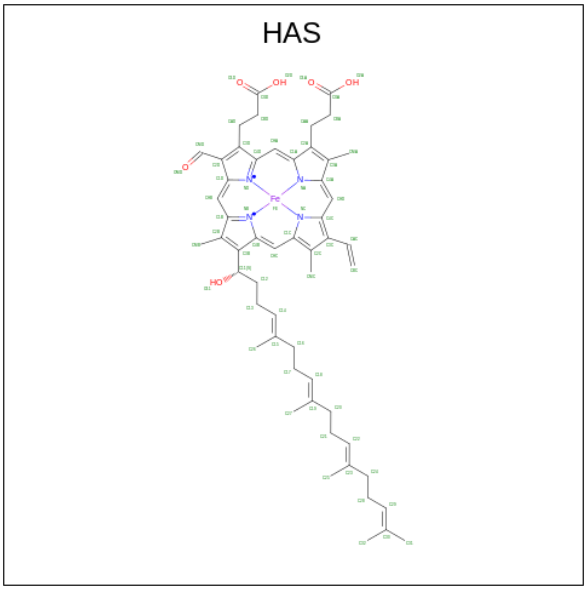
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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



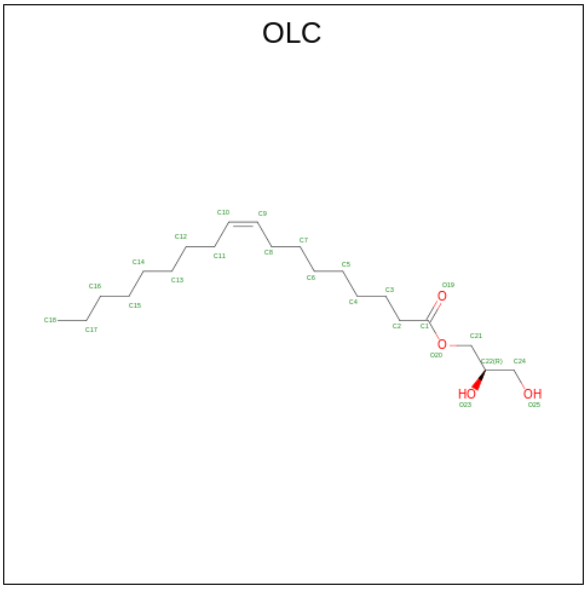
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is HEME-AS (three-letter code: HAS) (formula: $C_{54}H_{64}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 23 19 4	0	0
7	A	1	Total C O 18 14 4	0	0
7	A	1	Total C O 17 13 4	0	0
7	A	1	Total C O 15 11 4	0	0
7	A	1	Total C O 18 14 4	0	0
7	A	1	Total C O 15 11 4	0	0
7	A	1	Total C O 20 16 4	0	0
7	A	1	Total C O 21 17 4	0	0
7	A	1	Total C O 20 18 2	0	0
7	A	1	Total C 9 9	0	0
7	A	1	Total C 9 9	0	0
7	A	1	Total C O 15 11 4	0	0

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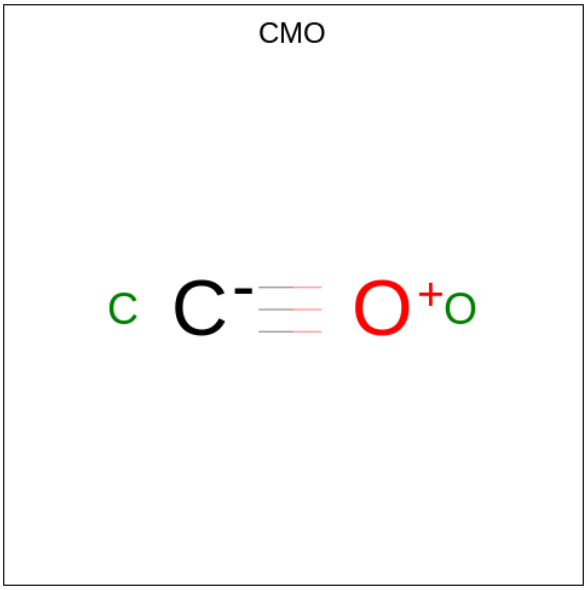
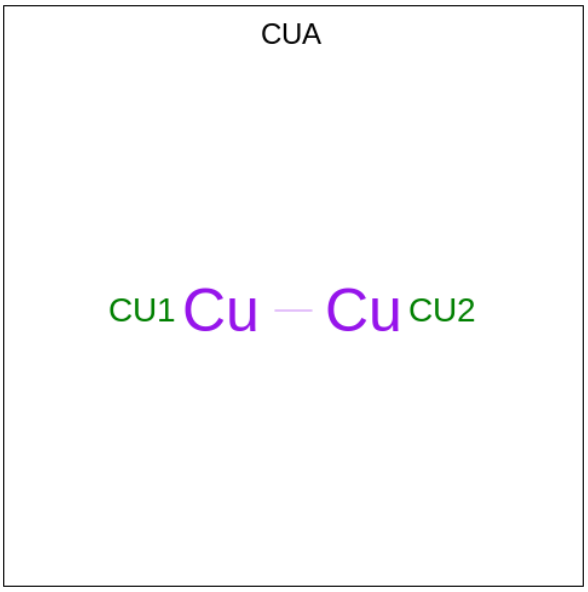
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 25 21 4	0	0
7	B	1	Total C O 24 20 4	0	0
7	C	1	Total C O 24 20 4	0	0

- Molecule 8 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



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

- Molecule 9 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	97	Total O 97 97	0	0
10	B	76	Total O 76 76	0	0
10	C	5	Total O 5 5	0	0

3 Residue-property plots (i)

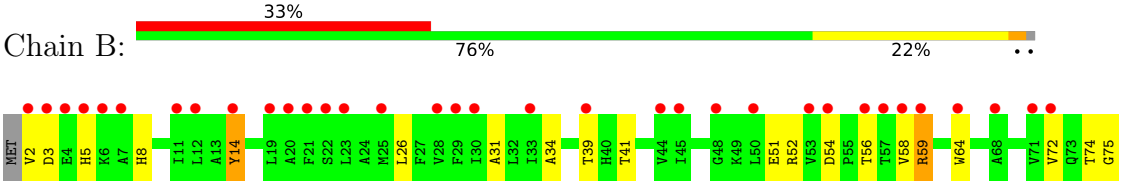
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

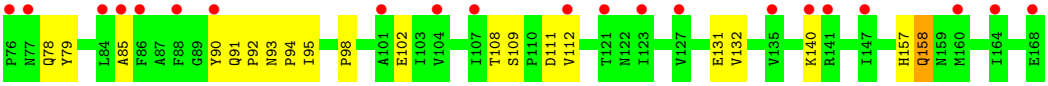
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:

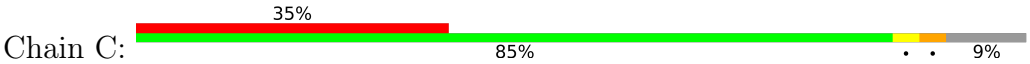
• Molecule 2: Cytochrome c oxidase subunit 2

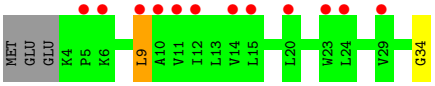
Chain B:





• Molecule 3: Cytochrome c oxidase polypeptide 2A





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	145.85Å 100.32Å 96.62Å 90.00° 126.76° 90.00°	Depositor
Resolution (Å)	37.15 – 2.00 37.15 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (37.15-2.00) 94.8 (37.15-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.48 (at 2.00Å)	Xtriage
Refinement program	REFMAC v8.0	Depositor
R, R_{free}	0.396 , 0.435 0.405 , 0.436	Depositor DCC
R_{free} test set	1877 reflections (2.63%)	wwPDB-VP
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 79.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.58$, $< L^2 > = 0.43$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	6474	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: OLC, CU, CUA, HEM, CMO, HAS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.43	0/4525	0.84	2/6213 (0.0%)
2	B	0.43	0/1338	0.88	1/1828 (0.1%)
3	C	0.43	0/247	0.79	0/335
All	All	0.43	0/6110	0.84	3/8376 (0.0%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	233	HIS	CA-CB-CG	-6.99	101.71	113.60
1	A	489	PHE	CB-CA-C	6.44	123.28	110.40
2	B	14	TYR	CB-CA-C	5.36	121.13	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ARG	Sidechain
2	B	59	ARG	Sidechain

5.2 Too-close contacts (i)

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	4467	129	0
2	B	1301	0	1278	30	0
3	C	241	0	267	2	0
4	A	1	0	0	0	0
5	A	43	0	30	3	0
6	A	65	0	62	11	0
7	A	200	0	276	8	0
7	B	49	0	75	3	0
7	C	24	0	35	2	0
8	A	2	0	0	1	0
9	B	2	0	0	0	0
10	A	97	0	0	6	0
10	B	76	0	0	7	1
10	C	5	0	0	0	0
All	All	6474	0	6490	165	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (165) 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)
7:A:610:OLC:C13	7:A:610:OLC:C12	1.87	1.51
1:A:414:SER:OG	1:A:417:GLN:HG3	1.52	1.07
5:A:602:HEM:HMC2	5:A:602:HEM:HBC2	1.49	0.95
6:A:603:HAS:HMC1	6:A:603:HAS:HBC1	1.55	0.88
1:A:387:LEU:CD2	1:A:433:MET:CE	2.53	0.85
1:A:37:LEU:HD23	1:A:481:LEU:HD21	1.58	0.84
1:A:19:LYS:NZ	7:A:606:OLC:O25	2.10	0.83
1:A:387:LEU:HD22	1:A:433:MET:CE	2.09	0.83
1:A:354:LEU:HD21	6:A:603:HAS:H313	1.61	0.82
1:A:411:LYS:HE2	1:A:494:SER:O	1.79	0.82
1:A:403:TRP:CZ3	1:A:404:LEU:HD13	2.18	0.79
5:A:602:HEM:HBC2	5:A:602:HEM:CMC	2.12	0.77
1:A:430:LEU:O	1:A:434:ILE:HG13	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:SER:HG	1:A:417:GLN:HG3	1.51	0.76
1:A:387:LEU:HD21	1:A:433:MET:CE	2.16	0.75
1:A:411:LYS:CE	1:A:494:SER:O	2.34	0.75
1:A:401:LEU:HD21	1:A:488:LEU:HD13	1.70	0.73
1:A:236:VAL:HG12	1:A:239:TRP:CZ3	2.23	0.73
1:A:387:LEU:CD2	1:A:433:MET:HE3	2.20	0.72
1:A:16:PRO:HD2	1:A:17:GLU:OE1	1.90	0.70
1:A:498:LYS:HB2	1:A:501:LEU:HD12	1.73	0.70
1:A:227:LEU:O	1:A:230:TRP:HB3	1.92	0.70
2:B:78:GLN:NE2	2:B:102:GLU:OE2	2.20	0.70
1:A:387:LEU:HD21	1:A:433:MET:HE2	1.74	0.69
1:A:398:MET:O	1:A:401:LEU:HB2	1.93	0.68
1:A:516:GLU:HA	1:A:519:ARG:HH21	1.60	0.66
1:A:411:LYS:NZ	1:A:494:SER:O	2.29	0.66
1:A:454:ALA:O	10:A:702:HOH:O	2.14	0.66
1:A:354:LEU:HD21	6:A:603:HAS:C31	2.25	0.65
1:A:53:PRO:O	1:A:57:ARG:NH2	2.29	0.65
2:B:14:TYR:HE2	7:B:203:OLC:HO25	1.45	0.65
2:B:14:TYR:HE2	7:B:203:OLC:O25	1.78	0.65
7:A:616:OLC:H21A	7:C:101:OLC:O25	1.97	0.65
1:A:504:ALA:O	10:A:703:HOH:O	2.14	0.64
1:A:282:HIS:CD2	6:A:603:HAS:OMD	2.51	0.63
2:B:31:ALA:O	2:B:34:ALA:HB3	1.97	0.63
2:B:39:THR:HG22	10:B:370:HOH:O	1.99	0.63
2:B:54:ASP:OD1	2:B:56:THR:OG1	2.14	0.62
1:A:35:GLY:HA3	1:A:76:ASN:OD1	1.99	0.62
1:A:71:LEU:O	1:A:75:LEU:HB2	1.99	0.61
2:B:52:ARG:HD3	2:B:131:GLU:OE1	2.01	0.61
1:A:391:SER:O	1:A:395:LEU:HB2	1.99	0.61
1:A:293:THR:O	1:A:297:ILE:HG13	2.00	0.61
1:A:164:LEU:HD11	1:A:191:LEU:HD21	1.83	0.60
1:A:405:LEU:O	1:A:409:THR:OG1	2.14	0.59
1:A:387:LEU:HD22	1:A:433:MET:HE3	1.80	0.59
1:A:405:LEU:HD23	1:A:491:VAL:HG11	1.83	0.59
5:A:602:HEM:HMC2	5:A:602:HEM:CBC	2.29	0.59
1:A:97:LEU:HD22	1:A:170:TRP:CD1	2.39	0.57
1:A:240:LEU:HD13	6:A:603:HAS:HMC1	1.86	0.57
1:A:391:SER:HB2	1:A:432:MET:HG3	1.86	0.57
1:A:270:LEU:HD22	1:A:524:MET:HG2	1.86	0.57
1:A:233:HIS:CD2	1:A:233:HIS:C	2.78	0.56
1:A:95:ARG:NH2	10:A:708:HOH:O	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LEU:HG	1:A:405:LEU:HD22	1.88	0.56
1:A:250:ILE:HD13	1:A:403:TRP:CH2	2.42	0.55
1:A:532:ALA:O	1:A:536:ILE:HG13	2.07	0.55
1:A:545:THR:O	1:A:549:LEU:HG	2.07	0.54
1:A:282:HIS:CG	6:A:603:HAS:OMD	2.60	0.54
1:A:220:ASP:HB3	1:A:223:VAL:HG12	1.90	0.54
1:A:193:TRP:HH2	1:A:235:ILE:HD12	1.73	0.54
1:A:260:VAL:O	2:B:8:HIS:ND1	2.41	0.54
1:A:277:THR:H	1:A:278:PRO:HD3	1.71	0.54
1:A:54:LEU:O	1:A:58:LEU:HD13	2.08	0.54
1:A:114:PHE:O	1:A:118:VAL:HG23	2.08	0.54
1:A:157:TRP:HA	1:A:160:ILE:HD12	1.89	0.54
1:A:16:PRO:CD	1:A:17:GLU:OE1	2.56	0.54
2:B:52:ARG:HG2	10:B:335:HOH:O	2.08	0.54
2:B:75:GLY:HA3	2:B:78:GLN:HB3	1.90	0.53
1:A:152:PHE:O	1:A:155:SER:HB3	2.09	0.53
1:A:277:THR:N	1:A:278:PRO:CD	2.72	0.53
1:A:388:GLN:HE21	6:A:603:HAS:CHC	2.22	0.52
1:A:387:LEU:HD22	1:A:433:MET:HE1	1.88	0.52
1:A:296:MET:HG2	7:A:612:OLC:H8	1.91	0.52
1:A:402:TYR:OH	1:A:421:GLY:HA3	2.10	0.52
1:A:277:THR:N	1:A:278:PRO:HD3	2.24	0.51
6:A:603:HAS:ND	8:A:615:CMO:C	2.73	0.51
1:A:66:TYR:OH	2:B:158:GLN:NE2	2.44	0.50
1:A:240:LEU:HD13	6:A:603:HAS:CMC	2.42	0.50
1:A:368:SER:HB2	1:A:371:LEU:HD12	1.93	0.50
1:A:489:PHE:O	1:A:493:LEU:HB2	2.10	0.50
1:A:233:HIS:O	1:A:236:VAL:HG22	2.12	0.50
1:A:193:TRP:CH2	1:A:235:ILE:HD12	2.47	0.50
1:A:51:ALA:O	1:A:54:LEU:HB3	2.12	0.49
1:A:170:TRP:CH2	1:A:180:PRO:HD3	2.48	0.49
1:A:348:ALA:HB3	1:A:349:PRO:HD3	1.94	0.49
1:A:275:LEU:O	1:A:278:PRO:HD2	2.11	0.49
1:A:414:SER:OG	1:A:417:GLN:CG	2.43	0.49
2:B:52:ARG:CD	2:B:131:GLU:OE1	2.59	0.49
1:A:400:SER:O	1:A:404:LEU:HB2	2.12	0.49
1:A:178:VAL:HG22	10:A:779:HOH:O	2.12	0.49
1:A:120:ALA:O	1:A:123:PRO:HD2	2.13	0.49
2:B:14:TYR:CD1	3:C:9:LEU:HD11	2.48	0.48
1:A:465:VAL:HB	1:A:466:PRO:CD	2.44	0.48
1:A:230:TRP:C	1:A:230:TRP:CD1	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ILE:HB	1:A:358:PRO:CD	2.44	0.48
1:A:216:VAL:HG12	7:A:610:OLC:H24A	1.95	0.48
1:A:265:ALA:O	1:A:268:ALA:HB3	2.12	0.48
1:A:270:LEU:CD2	1:A:524:MET:HG2	2.44	0.48
2:B:58:VAL:HG22	2:B:64:TRP:HB2	1.96	0.48
1:A:291:ASP:HA	1:A:292:PRO:HD2	1.70	0.47
2:B:94:PRO:HD2	10:B:357:HOH:O	2.13	0.47
7:C:101:OLC:H21A	7:C:101:OLC:H2	1.39	0.47
1:A:52:TYR:N	1:A:53:PRO:HD2	2.30	0.47
1:A:445:LEU:HD23	7:A:616:OLC:H3A	1.96	0.47
2:B:59:ARG:NH2	10:B:306:HOH:O	2.47	0.47
1:A:403:TRP:CZ3	1:A:404:LEU:CD1	2.95	0.46
1:A:542:TYR:O	1:A:546:LEU:HG	2.16	0.46
1:A:143:TRP:CE2	7:A:605:OLC:H4	2.51	0.46
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.80	0.46
2:B:59:ARG:NH1	10:B:307:HOH:O	2.48	0.46
1:A:41:PHE:CE2	1:A:55:LEU:HD13	2.51	0.46
2:B:51:GLU:O	2:B:132:VAL:HG23	2.17	0.45
1:A:411:LYS:HD3	1:A:494:SER:HB3	1.99	0.45
1:A:206:LEU:O	1:A:207:PHE:CD1	2.69	0.45
2:B:41:THR:HA	10:B:356:HOH:O	2.16	0.45
1:A:111:TRP:O	1:A:115:ILE:HG12	2.16	0.45
1:A:189:PHE:CE1	1:A:242:PRO:HD3	2.51	0.45
1:A:192:MET:HE2	1:A:193:TRP:HA	1.99	0.45
1:A:492:LEU:C	1:A:493:LEU:HD12	2.37	0.45
1:A:536:ILE:HG22	1:A:540:LEU:HD12	1.99	0.44
2:B:72:VAL:O	2:B:74:THR:HG23	2.17	0.44
1:A:97:LEU:HD11	1:A:183:THR:HG21	2.00	0.44
1:A:146:TYR:OH	10:A:704:HOH:O	2.21	0.43
1:A:343:ASN:HA	1:A:344:PRO:HD2	1.86	0.43
2:B:2:VAL:HG22	2:B:5:HIS:HB2	2.00	0.43
1:A:391:SER:O	1:A:395:LEU:CB	2.64	0.43
1:A:366:ASN:CB	6:A:603:HAS:HMD	2.49	0.43
1:A:302:THR:O	1:A:305:VAL:HG12	2.18	0.43
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.84	0.43
1:A:33:ILE:O	1:A:37:LEU:HG	2.19	0.42
1:A:252:PRO:HB2	1:A:509:ALA:HB2	2.01	0.42
1:A:401:LEU:CD2	1:A:488:LEU:HD13	2.44	0.42
1:A:95:ARG:NH2	1:A:95:ARG:HA	2.34	0.42
1:A:25:LEU:HD11	1:A:404:LEU:HD23	2.01	0.42
1:A:57:ARG:HG2	1:A:57:ARG:HH21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:TYR:HE1	10:A:733:HOH:O	2.02	0.42
2:B:14:TYR:CE2	7:B:203:OLC:O25	2.57	0.42
2:B:93:ASN:HA	2:B:94:PRO:HA	1.81	0.42
1:A:441:TRP:O	1:A:442:ALA:C	2.58	0.42
10:B:315:HOH:O	3:C:34:GLY:HA2	2.20	0.42
1:A:146:TYR:CD1	1:A:208:LEU:HD13	2.54	0.42
1:A:400:SER:O	1:A:404:LEU:CB	2.68	0.41
1:A:220:ASP:HB3	1:A:223:VAL:CG1	2.50	0.41
2:B:90:TYR:O	2:B:91:GLN:HG2	2.21	0.41
1:A:366:ASN:C	6:A:603:HAS:HMD	2.40	0.41
1:A:498:LYS:HB2	1:A:501:LEU:CD1	2.48	0.41
2:B:85:ALA:O	2:B:109:SER:HA	2.21	0.41
1:A:467:MET:O	1:A:471:VAL:HG23	2.20	0.41
1:A:511:VAL:HG12	1:A:512:ILE:O	2.21	0.41
1:A:539:VAL:O	1:A:543:GLY:HA3	2.21	0.41
2:B:92:PRO:HG2	2:B:95:ILE:HG12	2.01	0.41
1:A:230:TRP:C	1:A:230:TRP:HD1	2.24	0.41
1:A:430:LEU:HD23	1:A:430:LEU:HA	1.92	0.41
2:B:54:ASP:CG	2:B:56:THR:OG1	2.59	0.41
1:A:450:ARG:O	2:B:157:HIS:CD2	2.74	0.41
1:A:196:ALA:O	1:A:231:THR:HA	2.21	0.40
1:A:241:LEU:HD12	1:A:241:LEU:HA	1.91	0.40
1:A:322:PHE:O	1:A:323:ALA:C	2.59	0.40
1:A:348:ALA:HB3	1:A:349:PRO:CD	2.51	0.40
1:A:95:ARG:HH22	1:A:98:ASN:HA	1.86	0.40
1:A:105:LEU:HB3	1:A:162:ILE:HD11	2.04	0.40
2:B:111:ASP:OD1	2:B:112:VAL:N	2.48	0.40
1:A:426:TRP:CD1	7:A:604:OLC:O19	2.74	0.40
2:B:79:TYR:CE1	2:B:98:PRO:HG3	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:359:HOH:O	10:B:365:HOH:O[2_556]	1.95	0.25

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	552/569 (97%)	515 (93%)	36 (6%)	1 (0%)	47 44
2	B	165/168 (98%)	155 (94%)	9 (6%)	1 (1%)	25 19
3	C	29/34 (85%)	27 (93%)	2 (7%)	0	100 100
All	All	746/771 (97%)	697 (93%)	47 (6%)	2 (0%)	41 37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3	ASP
1	A	322	PHE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	447/463 (96%)	430 (96%)	17 (4%)	33 31
2	B	136/138 (99%)	132 (97%)	4 (3%)	42 43
3	C	24/27 (89%)	23 (96%)	1 (4%)	30 27
All	All	607/628 (97%)	585 (96%)	22 (4%)	35 34

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	SER

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Mol	Chain	Res	Type
1	A	133	TYR
1	A	192	MET
1	A	215	LEU
1	A	230	TRP
1	A	241	LEU
1	A	252	PRO
1	A	262	ASP
1	A	282	HIS
1	A	332	LEU
1	A	369	PHE
1	A	401	LEU
1	A	405	LEU
1	A	456	VAL
1	A	513	SER
1	A	525	ASP
1	A	548	GLN
2	B	26	LEU
2	B	108	THR
2	B	140	LYS
2	B	158	GLN
3	C	9	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	388	GLN
1	A	446	ASN
1	A	455	GLN
1	A	548	GLN
2	B	60	GLN
2	B	99	GLN
2	B	158	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 monosaccharides 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	$\#\|Z\| > 2$
7	OLC	A	616	-	14,14,24	0.75	1 (7%)	15,15,25	0.67	0
7	OLC	A	610	-	19,19,24	1.09	1 (5%)	20,20,25	0.34	0
7	OLC	A	604	-	22,22,24	0.24	0	23,23,25	0.43	0
7	OLC	C	101	-	23,23,24	0.44	0	24,24,25	0.33	0
7	OLC	B	202	-	24,24,24	0.32	0	25,25,25	0.32	0
6	HAS	A	603	1	69,72,72	2.67	25 (36%)	73,109,109	3.13	39 (53%)
7	OLC	A	608	-	17,17,24	0.31	0	18,18,25	0.38	0
8	CMO	A	615	4	0,1,1	-	-	-		
7	OLC	A	614	-	8,8,24	0.17	0	7,7,25	0.14	0
7	OLC	A	605	-	17,17,24	0.24	0	18,18,25	0.31	0
7	OLC	A	606	-	16,16,24	0.27	0	17,17,25	0.35	0
7	OLC	A	609	-	14,14,24	0.21	0	15,15,25	0.29	0
7	OLC	A	613	-	8,8,24	0.18	0	7,7,25	0.16	0
5	HEM	A	602	1	41,50,50	1.49	6 (14%)	45,82,82	1.96	16 (35%)
7	OLC	A	611	-	20,20,24	0.69	0	21,21,25	0.56	0
7	OLC	A	612	-	19,19,24	0.27	0	19,19,25	0.26	0
7	OLC	B	203	-	23,23,24	0.26	0	24,24,25	0.22	0
9	CUA	B	201	2	0,1,1	-	-	-		
7	OLC	A	607	-	14,14,24	0.23	0	15,15,25	0.33	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
7	OLC	A	605	-	-	10/17/17/24	-
7	OLC	A	606	-	-	8/16/16/24	-
7	OLC	A	609	-	-	8/14/14/24	-
7	OLC	A	616	-	-	2/14/14/24	-
7	OLC	A	610	-	-	11/19/19/24	-
7	OLC	A	604	-	-	10/22/22/24	-
7	OLC	C	101	-	-	16/23/23/24	-
7	OLC	A	613	-	-	5/6/6/24	-
7	OLC	A	612	-	-	9/18/18/24	-
7	OLC	B	202	-	-	11/24/24/24	-
6	HAS	A	603	1	1/1/8/18	8/40/82/82	-
7	OLC	A	608	-	-	10/17/17/24	-
7	OLC	B	203	-	-	9/23/23/24	-
7	OLC	A	611	-	-	8/20/20/24	-
7	OLC	A	614	-	-	3/6/6/24	-
5	HEM	A	602	1	-	1/12/54/54	-
7	OLC	A	607	-	-	3/14/14/24	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	CHD-C4A	10.31	1.49	1.35
6	A	603	HAS	C3B-C2B	6.29	1.48	1.34
6	A	603	HAS	CHA-C1A	5.13	1.48	1.38
6	A	603	HAS	C3C-C2C	4.99	1.47	1.40
6	A	603	HAS	FE-NA	4.88	2.14	1.95
6	A	603	HAS	CHB-C1D	4.86	1.48	1.38
6	A	603	HAS	C2D-C3D	4.81	1.47	1.36
6	A	603	HAS	C2A-C3A	4.79	1.46	1.36
7	A	610	OLC	C13-C12	4.61	1.87	1.49
6	A	603	HAS	C4B-C3B	4.38	1.52	1.44
6	A	603	HAS	C1A-C2A	4.38	1.53	1.45
6	A	603	HAS	CHC-C4B	4.29	1.46	1.35
6	A	603	HAS	C1B-C2B	3.99	1.52	1.44
5	A	602	HEM	C1B-NB	-3.94	1.33	1.40
5	A	602	HEM	CHB-C1B	3.70	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	C4D-C3D	3.68	1.51	1.45
6	A	603	HAS	CHA-C4D	3.30	1.46	1.39
5	A	602	HEM	FE-NB	2.94	2.11	1.96
6	A	603	HAS	O1A-CGA	2.87	1.31	1.22
6	A	603	HAS	CHB-C1B	2.82	1.45	1.39
6	A	603	HAS	FE-ND	2.75	2.12	1.97
6	A	603	HAS	CBA-CGA	2.68	1.56	1.50
6	A	603	HAS	C1C-CHC	2.61	1.48	1.41
6	A	603	HAS	C1D-ND	-2.61	1.35	1.40
6	A	603	HAS	FE-NB	2.59	2.11	1.97
5	A	602	HEM	C1A-NA	2.53	1.41	1.36
7	A	616	OLC	C4-C5	2.42	1.65	1.51
6	A	603	HAS	C4B-NB	-2.40	1.36	1.40
6	A	603	HAS	C1B-NB	-2.37	1.33	1.38
5	A	602	HEM	C4D-ND	-2.24	1.36	1.40
6	A	603	HAS	C4A-NA	-2.08	1.35	1.39
6	A	603	HAS	C4C-CHD	2.06	1.46	1.41
5	A	602	HEM	C1D-C2D	2.04	1.48	1.44

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	603	HAS	C2D-C3D-C4D	-11.60	98.22	106.49
6	A	603	HAS	CAD-C3D-C4D	6.73	136.42	124.66
6	A	603	HAS	C3D-C4D-ND	6.19	116.35	110.36
6	A	603	HAS	C2B-C1B-NB	5.70	116.71	109.88
6	A	603	HAS	C3B-C4B-NB	5.69	116.58	109.84
6	A	603	HAS	C2A-C1A-NA	5.50	115.68	110.32
6	A	603	HAS	CAA-CBA-CGA	-5.44	101.90	113.60
6	A	603	HAS	C26-C15-C16	5.32	124.22	115.27
6	A	603	HAS	C3C-C4C-NC	4.72	115.31	109.21
6	A	603	HAS	C1A-C2A-C3A	-4.41	101.38	107.13
5	A	602	HEM	CHC-C4B-NB	4.33	129.13	124.43
6	A	603	HAS	CHA-C4D-ND	-4.16	119.90	124.42
6	A	603	HAS	OMD-CMD-C2D	-4.14	116.32	125.69
6	A	603	HAS	C1B-C2B-C3B	-3.95	102.08	106.80
6	A	603	HAS	C13-C12-C11	-3.93	108.44	114.35
5	A	602	HEM	C3B-C2B-C1B	3.92	109.39	106.49
5	A	602	HEM	C4B-C3B-C2B	-3.80	104.10	107.11
6	A	603	HAS	C12-C13-C14	-3.78	102.25	112.23
5	A	602	HEM	C1B-NB-C4B	3.69	108.89	105.07
6	A	603	HAS	C3A-C4A-NA	3.66	116.44	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	602	HEM	C4A-C3A-C2A	3.57	109.48	107.00
6	A	603	HAS	CHA-C1A-C2A	-3.53	119.22	124.94
6	A	603	HAS	C17-C18-C19	-3.45	119.34	127.66
6	A	603	HAS	C4B-C3B-C2B	-3.45	101.51	107.41
6	A	603	HAS	C16-C15-C14	-3.45	114.14	121.12
6	A	603	HAS	CBA-CAA-C2A	3.27	121.71	112.63
6	A	603	HAS	CBD-CAD-C3D	-3.02	104.25	112.63
6	A	603	HAS	O1A-CGA-CBA	-2.91	113.72	123.08
5	A	602	HEM	CHA-C4D-C3D	-2.83	120.01	125.33
6	A	603	HAS	C4A-NA-C1A	-2.80	102.61	105.35
6	A	603	HAS	CAD-CBD-CGD	-2.76	107.67	113.60
6	A	603	HAS	C25-C23-C24	2.68	119.77	115.27
6	A	603	HAS	C32-C30-C31	2.56	120.25	114.60
5	A	602	HEM	CHC-C4B-C3B	-2.51	120.73	124.57
6	A	603	HAS	C20-C21-C22	-2.50	103.66	111.88
6	A	603	HAS	CHC-C4B-NB	-2.50	121.30	124.38
5	A	602	HEM	O2A-CGA-CBA	2.45	121.89	114.03
6	A	603	HAS	CHB-C1B-C2B	-2.39	121.25	124.98
6	A	603	HAS	C32-C30-C29	-2.36	115.83	122.65
5	A	602	HEM	CHA-C4D-ND	2.35	127.28	124.38
5	A	602	HEM	O2D-CGD-CBD	2.34	121.54	114.03
5	A	602	HEM	C3C-C4C-NC	-2.26	106.67	110.94
5	A	602	HEM	CHB-C1B-NB	2.26	127.17	124.38
6	A	603	HAS	O2D-CGD-CBD	2.23	121.20	114.03
6	A	603	HAS	O2A-CGA-CBA	2.23	121.20	114.03
6	A	603	HAS	CHB-C1B-NB	-2.22	122.01	124.42
5	A	602	HEM	CHD-C1D-ND	2.20	126.82	124.43
5	A	602	HEM	C3D-C4D-ND	2.20	112.61	110.17
6	A	603	HAS	CAA-C2A-C1A	2.19	129.02	124.89
6	A	603	HAS	C4B-NB-C1B	-2.13	102.87	105.07
5	A	602	HEM	CMA-C3A-C4A	-2.11	125.22	128.46
6	A	603	HAS	C4A-C3A-C2A	-2.09	103.89	106.94
5	A	602	HEM	C2B-C1B-NB	-2.08	107.38	109.84
6	A	603	HAS	C1D-C2D-C3D	2.06	108.75	107.11
6	A	603	HAS	C1A-CHA-C4D	-2.02	121.70	126.06

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	603	HAS	NA

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	603	HAS	C1D-C2D-CMD-OMD
6	A	603	HAS	C3D-C2D-CMD-OMD
6	A	603	HAS	C23-C24-C28-C29
7	A	604	OLC	C21-C22-C24-O25
7	A	608	OLC	C21-C22-C24-O25
7	A	610	OLC	C10-C11-C12-C13
7	A	610	OLC	O20-C21-C22-C24
7	A	611	OLC	C21-C22-C24-O25
7	B	203	OLC	C21-C22-C24-O25
7	C	101	OLC	O20-C21-C22-C24
7	C	101	OLC	O20-C21-C22-O23
7	C	101	OLC	C2-C1-O20-C21
7	C	101	OLC	O19-C1-O20-C21
7	A	608	OLC	O20-C21-C22-C24
7	B	202	OLC	O20-C21-C22-C24
7	A	612	OLC	C1-C2-C3-C4
7	A	604	OLC	O20-C21-C22-O23
7	A	608	OLC	O20-C21-C22-O23
7	A	610	OLC	O20-C21-C22-O23
7	A	611	OLC	C1-C2-C3-C4
7	A	604	OLC	O23-C22-C24-O25
7	B	203	OLC	C1-C2-C3-C4
7	A	616	OLC	C1-C2-C3-C4
7	A	607	OLC	C1-C2-C3-C4
7	A	609	OLC	O20-C21-C22-O23
7	B	202	OLC	O20-C21-C22-O23
7	A	608	OLC	C5-C6-C7-C8
7	A	611	OLC	C4-C5-C6-C7
7	A	609	OLC	O20-C21-C22-C24
7	A	604	OLC	C12-C13-C14-C15
7	B	202	OLC	C11-C12-C13-C14
7	A	610	OLC	C5-C6-C7-C8
7	B	202	OLC	C14-C15-C16-C17
7	B	202	OLC	C1-C2-C3-C4
7	C	101	OLC	C5-C6-C7-C8
7	A	613	OLC	C12-C13-C14-C15
7	C	101	OLC	C4-C5-C6-C7
7	A	605	OLC	C21-C22-C24-O25
7	C	101	OLC	C21-C22-C24-O25
7	A	609	OLC	C4-C5-C6-C7
7	A	612	OLC	C11-C12-C13-C14
7	A	616	OLC	C2-C3-C4-C5
7	B	203	OLC	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
7	A	614	OLC	C12-C13-C14-C15
7	A	605	OLC	C3-C4-C5-C6
7	A	612	OLC	C2-C3-C4-C5
7	A	608	OLC	O23-C22-C24-O25
7	B	203	OLC	O23-C22-C24-O25
7	B	203	OLC	C12-C13-C14-C15
7	A	611	OLC	C6-C7-C8-C9
7	A	612	OLC	C10-C11-C12-C13
7	A	607	OLC	C3-C4-C5-C6
7	B	202	OLC	C13-C14-C15-C16
7	B	202	OLC	C3-C4-C5-C6
7	A	606	OLC	C1-C2-C3-C4
7	A	608	OLC	C1-C2-C3-C4
7	B	202	OLC	C6-C7-C8-C9
7	A	604	OLC	O20-C21-C22-C24
7	A	608	OLC	C3-C4-C5-C6
7	A	610	OLC	C3-C4-C5-C6
7	A	612	OLC	C12-C13-C14-C15
7	A	613	OLC	C14-C15-C16-C17
7	A	608	OLC	C6-C7-C8-C9
7	A	611	OLC	C10-C11-C12-C13
7	B	203	OLC	C6-C7-C8-C9
7	A	605	OLC	C5-C6-C7-C8
7	A	608	OLC	C4-C5-C6-C7
7	A	613	OLC	C11-C12-C13-C14
7	A	605	OLC	C2-C3-C4-C5
7	A	606	OLC	C3-C4-C5-C6
7	A	604	OLC	C11-C12-C13-C14
7	B	202	OLC	C10-C11-C12-C13
7	C	101	OLC	C6-C7-C8-C9
7	A	611	OLC	C3-C4-C5-C6
7	A	610	OLC	C1-C2-C3-C4
7	A	613	OLC	C10-C11-C12-C13
7	A	606	OLC	C6-C7-C8-C9
7	B	203	OLC	C2-C3-C4-C5
7	A	609	OLC	C5-C6-C7-C8
7	A	613	OLC	C15-C16-C17-C18
7	C	101	OLC	C12-C13-C14-C15
7	A	612	OLC	C14-C15-C16-C17
7	A	610	OLC	C2-C3-C4-C5
7	A	614	OLC	C15-C16-C17-C18
7	C	101	OLC	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
7	A	607	OLC	O20-C21-C22-C24
7	A	611	OLC	O23-C22-C24-O25
7	C	101	OLC	O23-C22-C24-O25
7	A	604	OLC	C10-C11-C12-C13
7	A	614	OLC	C10-C11-C12-C13
7	A	605	OLC	C4-C5-C6-C7
7	C	101	OLC	C3-C4-C5-C6
7	A	610	OLC	C4-C5-C6-C7
7	C	101	OLC	C1-C2-C3-C4
7	A	610	OLC	O23-C22-C24-O25
7	A	606	OLC	O20-C21-C22-O23
7	A	605	OLC	C1-C2-C3-C4
7	C	101	OLC	C10-C11-C12-C13
7	A	612	OLC	C13-C14-C15-C16
7	A	606	OLC	C5-C6-C7-C8
7	A	610	OLC	C9-C10-C11-C12
7	A	604	OLC	C7-C8-C9-C10
7	C	101	OLC	C2-C3-C4-C5
7	A	609	OLC	C21-C22-C24-O25
7	C	101	OLC	C9-C10-C11-C12
7	A	605	OLC	O23-C22-C24-O25
6	A	603	HAS	CAD-CBD-CGD-O1D
7	A	604	OLC	C6-C7-C8-C9
7	A	605	OLC	C6-C7-C8-C9
6	A	603	HAS	CAA-CBA-CGA-O1A
6	A	603	HAS	CAA-CBA-CGA-O2A
6	A	603	HAS	CAD-CBD-CGD-O2D
7	B	203	OLC	C3-C4-C5-C6
7	A	610	OLC	C21-C22-C24-O25
7	A	611	OLC	C7-C8-C9-C10
7	B	202	OLC	C5-C6-C7-C8
7	A	605	OLC	O20-C1-C2-C3
7	A	604	OLC	C9-C10-C11-C12
7	A	612	OLC	C7-C8-C9-C10
7	A	606	OLC	O20-C1-C2-C3
7	A	606	OLC	O19-C1-C2-C3
5	A	602	HEM	CAA-CBA-CGA-O2A
7	A	605	OLC	O19-C1-C2-C3
7	A	606	OLC	O20-C21-C22-C24
6	A	603	HAS	C3B-C11-C12-C13
7	A	609	OLC	C2-C3-C4-C5
7	A	609	OLC	O20-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	A	612	OLC	O20-C1-C2-C3
7	B	203	OLC	C5-C6-C7-C8
7	B	202	OLC	C9-C10-C11-C12
7	A	609	OLC	O19-C1-C2-C3
7	A	608	OLC	C2-C3-C4-C5

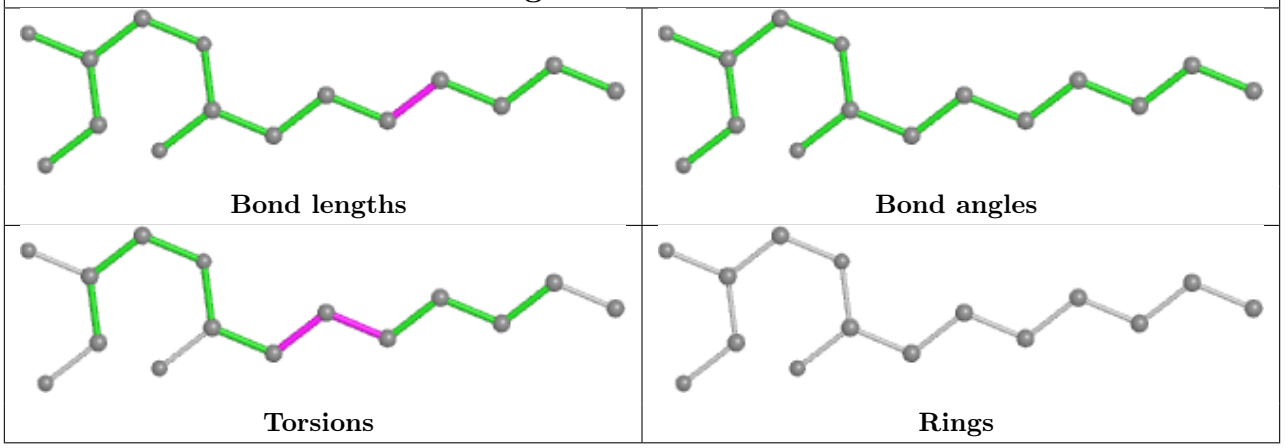
There are no ring outliers.

11 monomers are involved in 26 short contacts:

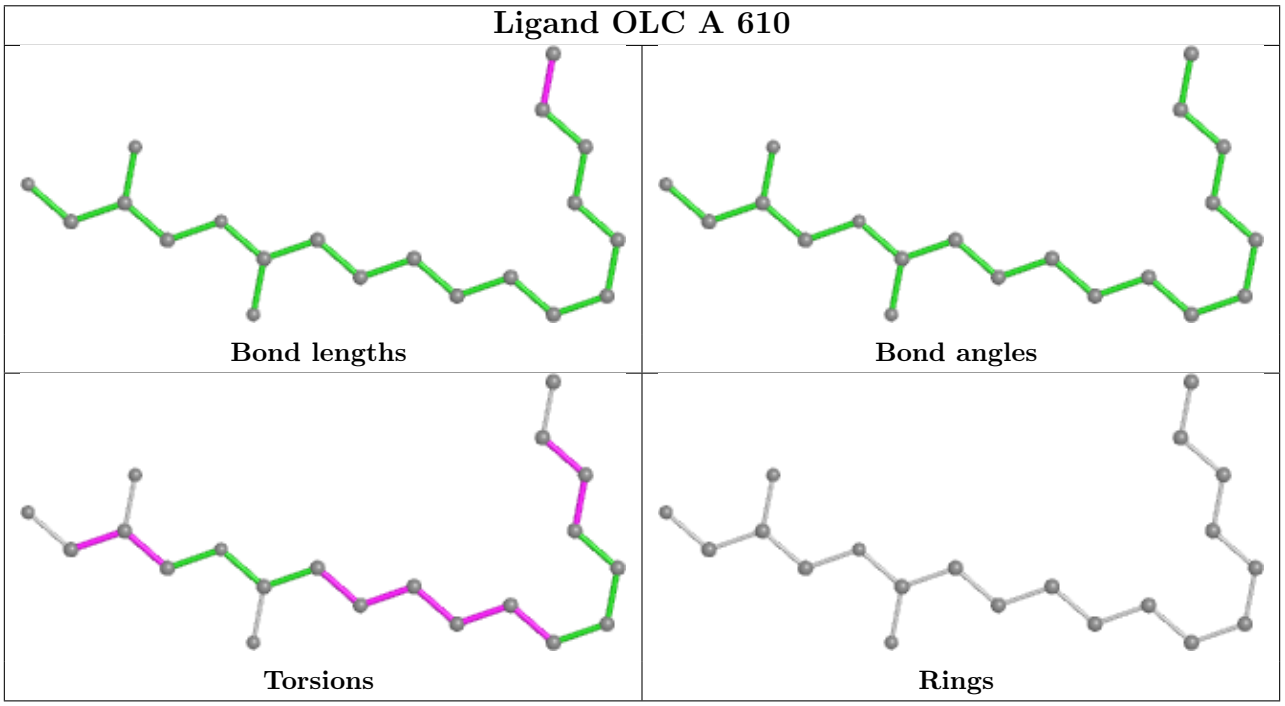
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	616	OLC	2	0
7	A	610	OLC	2	0
7	A	604	OLC	1	0
7	C	101	OLC	2	0
6	A	603	HAS	11	0
8	A	615	CMO	1	0
7	A	605	OLC	1	0
7	A	606	OLC	1	0
5	A	602	HEM	3	0
7	A	612	OLC	1	0
7	B	203	OLC	3	0

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

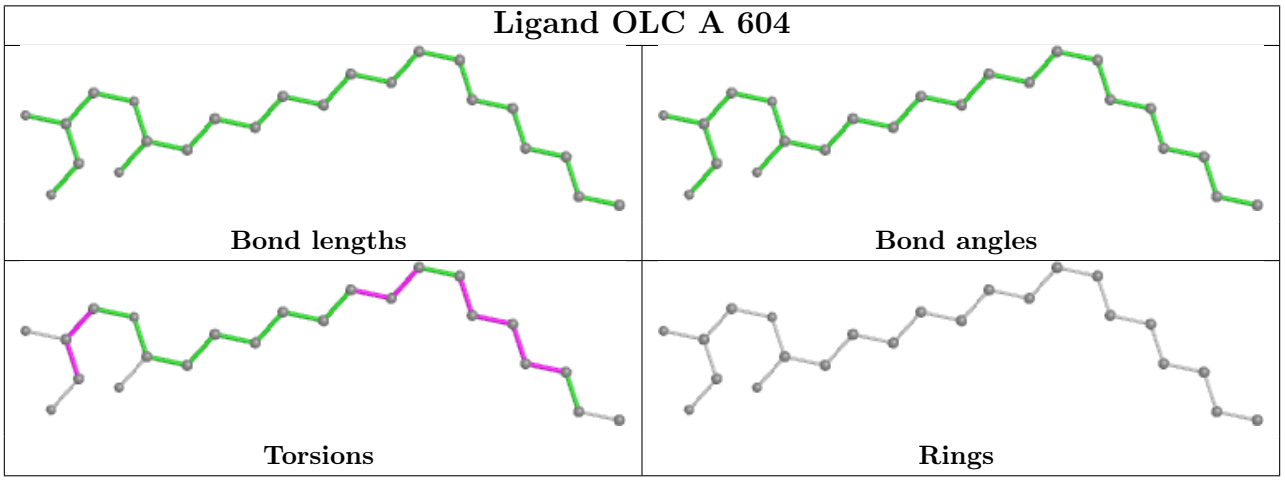
Ligand OLC A 616



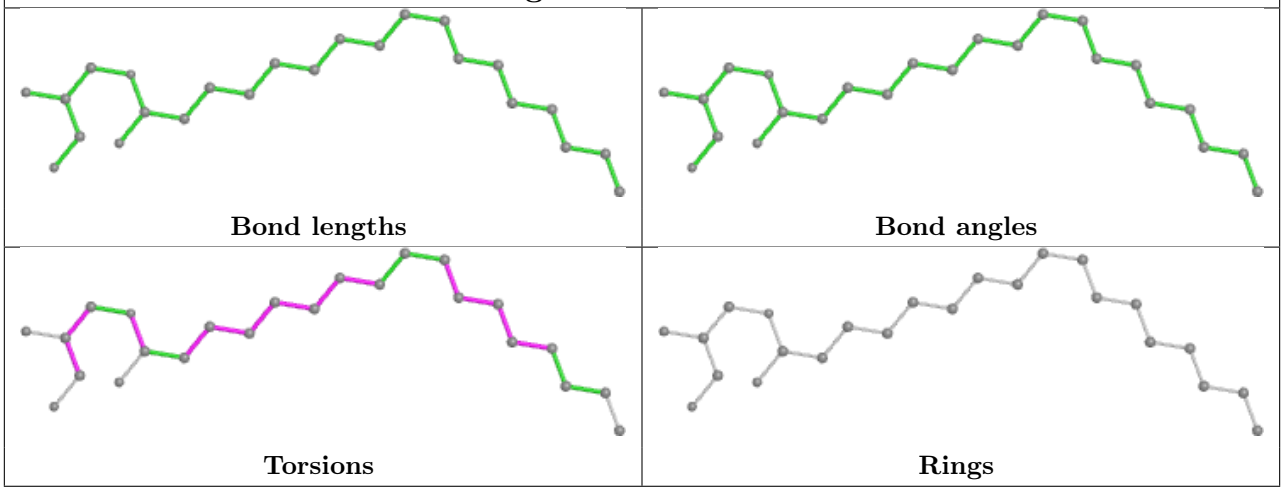
Ligand OLC A 610



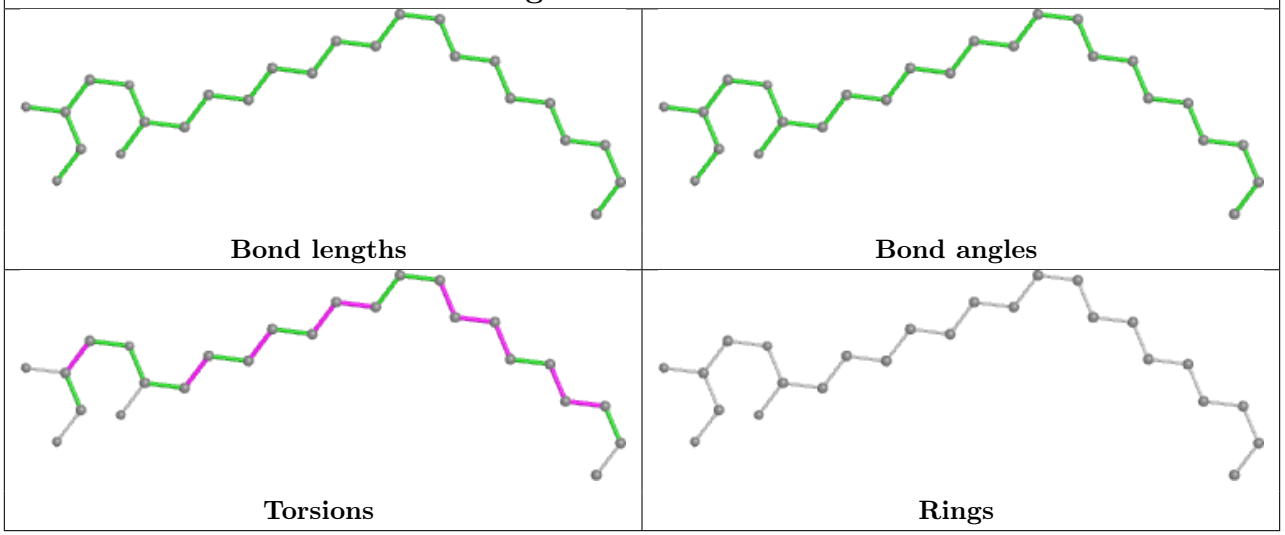
Ligand OLC A 604



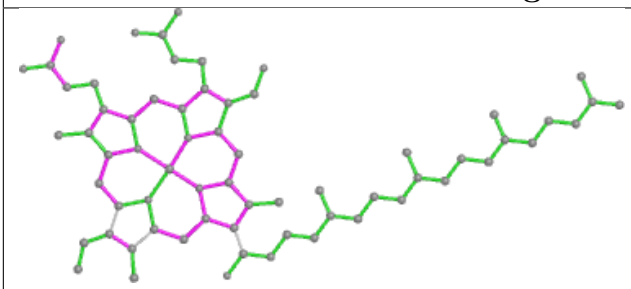
Ligand OLC C 101



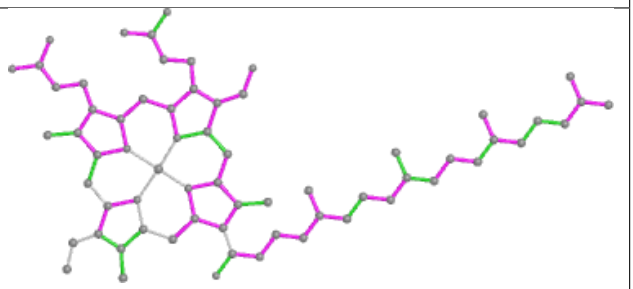
Ligand OLC B 202



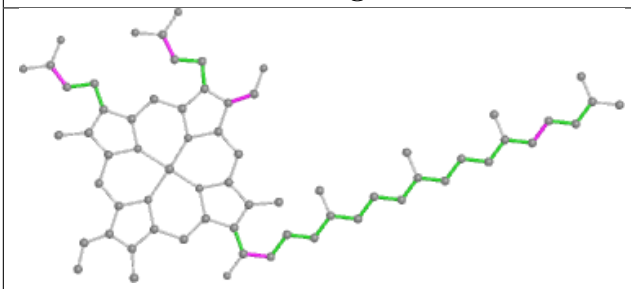
Ligand HAS A 603



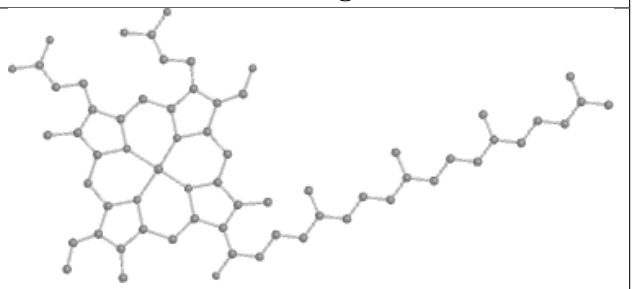
Bond lengths



Bond angles

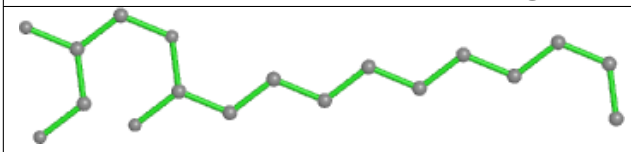


Torsions

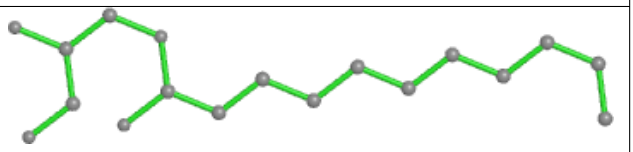


Rings

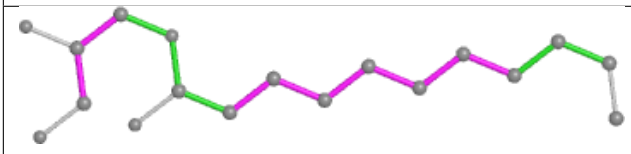
Ligand OLC A 608



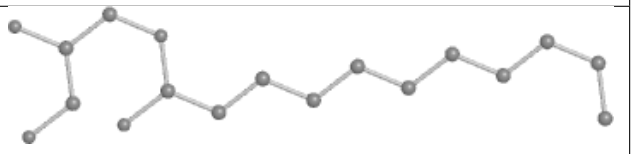
Bond lengths



Bond angles

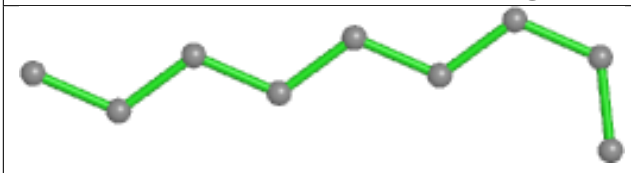


Torsions

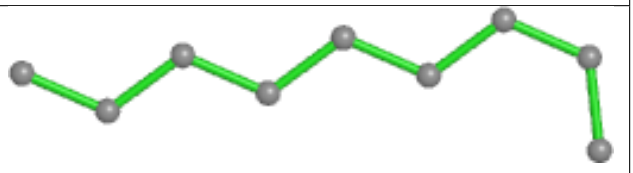


Rings

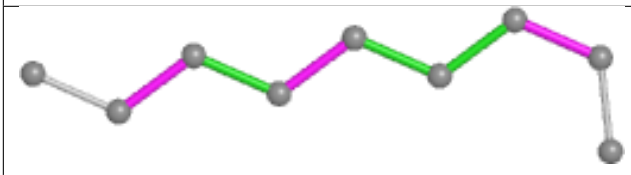
Ligand OLC A 614



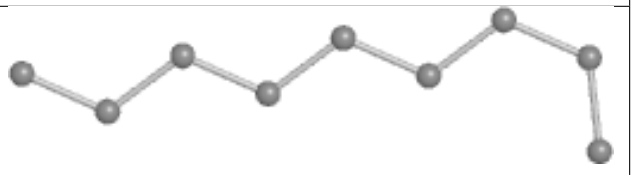
Bond lengths



Bond angles

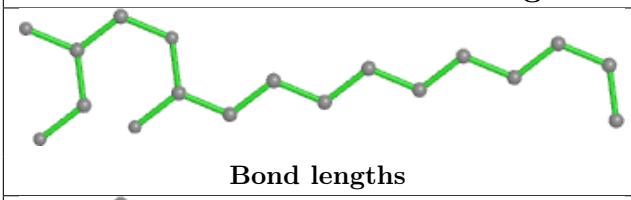


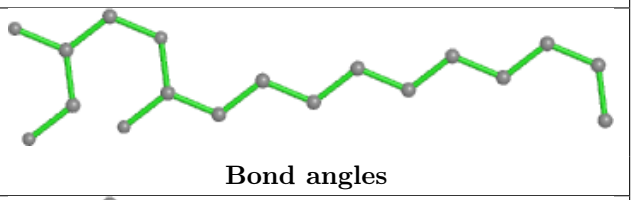
Torsions

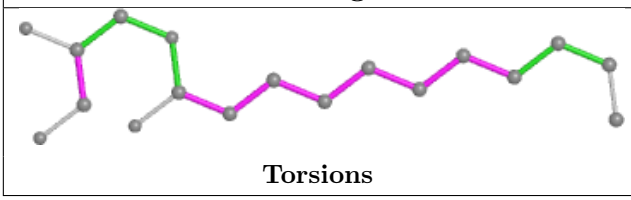


Rings

Ligand OLC A 605


Bond lengths


Bond angles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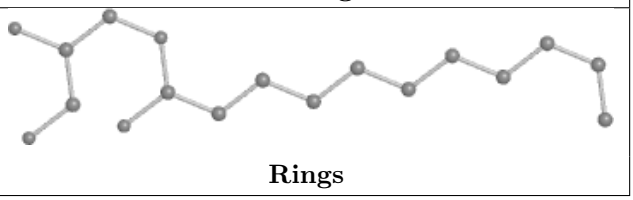
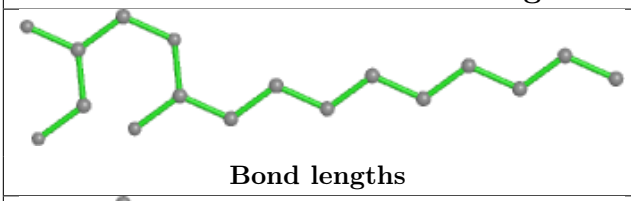
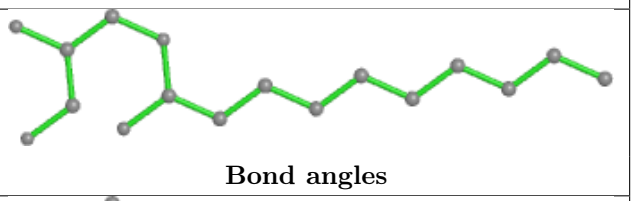
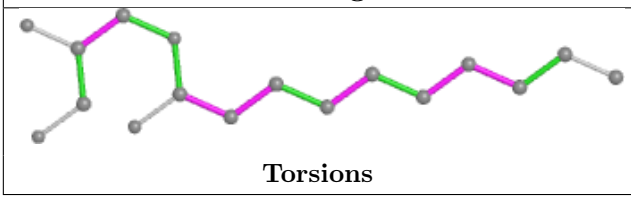

Rings

Ligand OLC A 606


Bond lengths


Bond angles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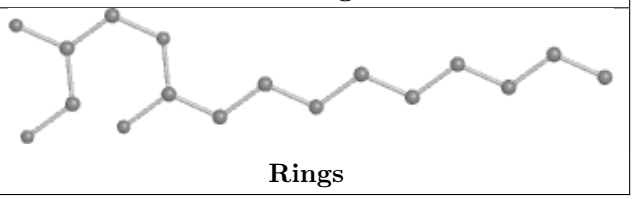
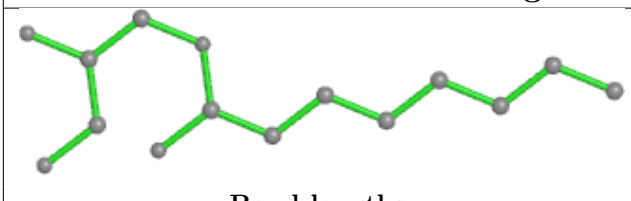
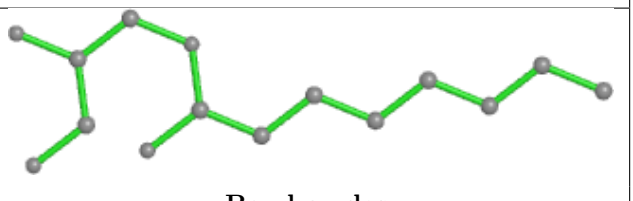
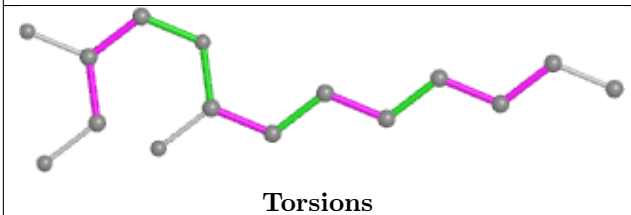
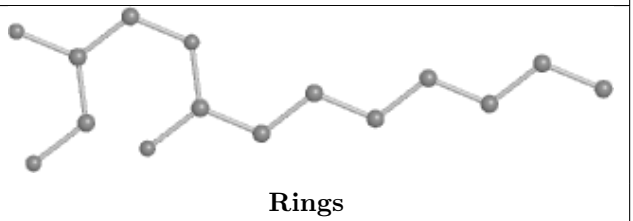

Rings

Ligand OLC A 609

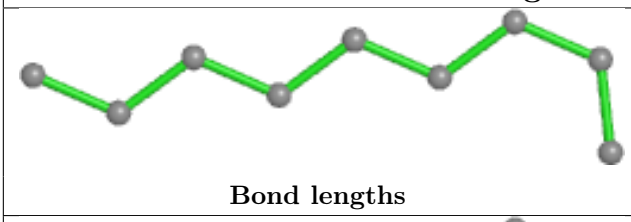

Bond lengths


Bond angles

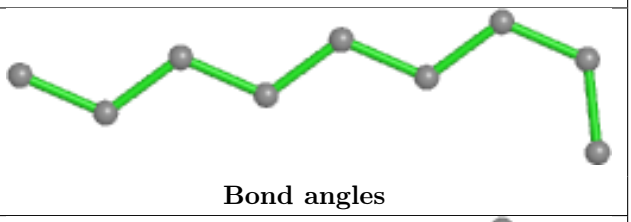

Torsions


Rings

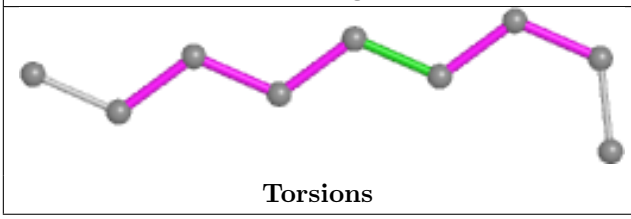
Ligand OLC A 613



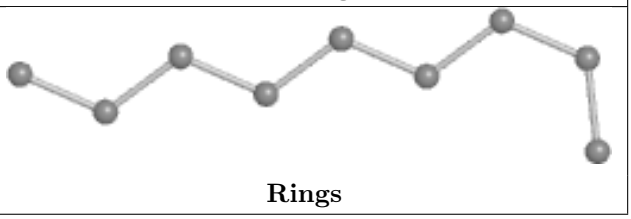
Bond lengths



Bond angles

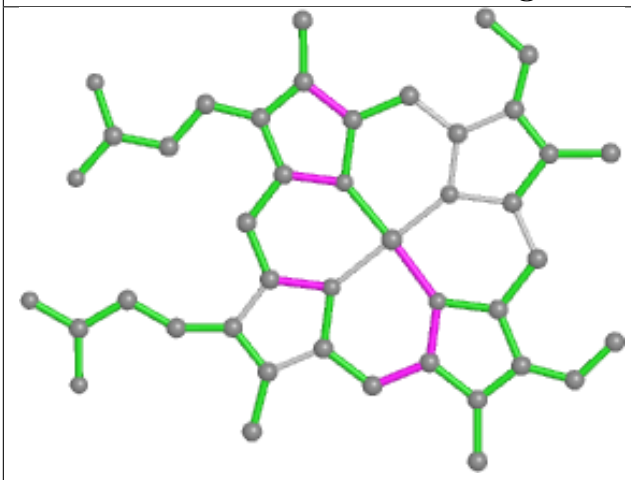


Torsions

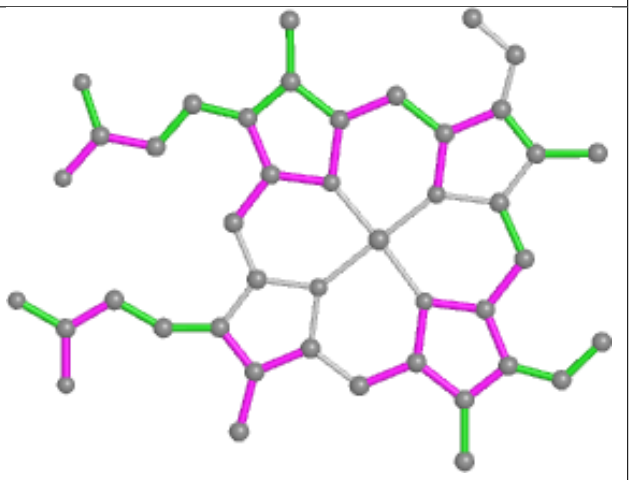


Rings

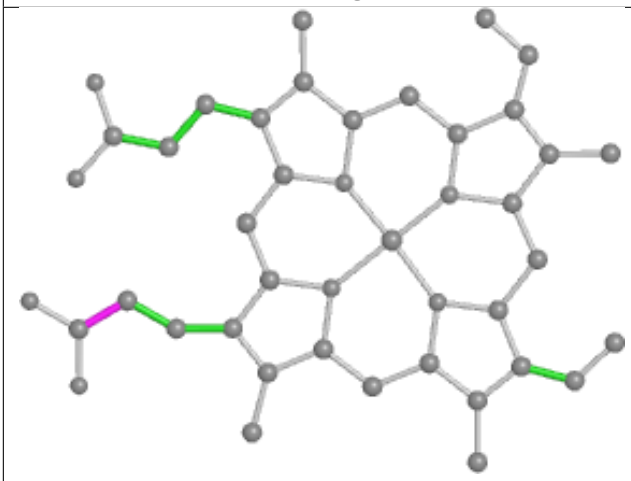
Ligand HEM A 602



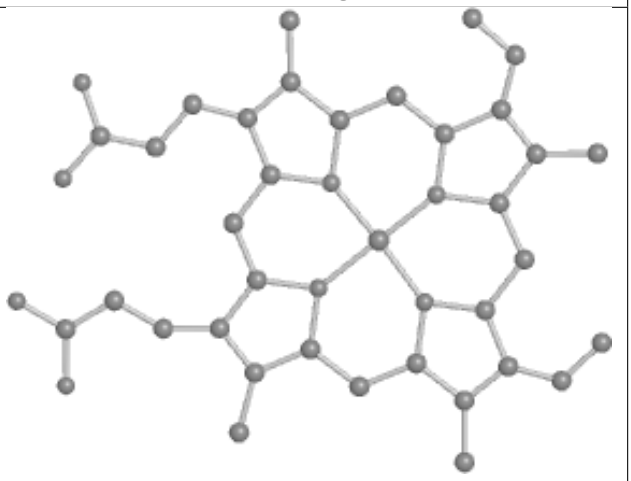
Bond lengths



Bond angles

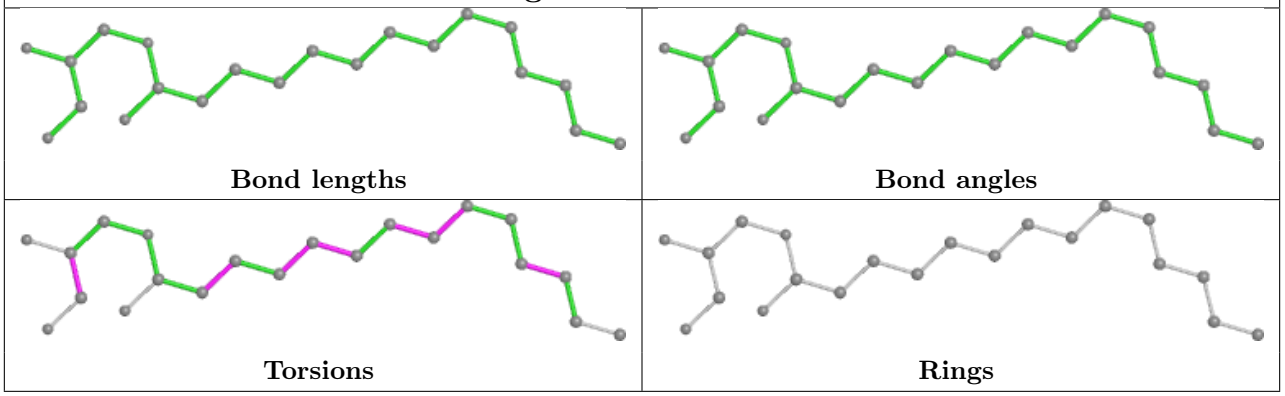


Torsions

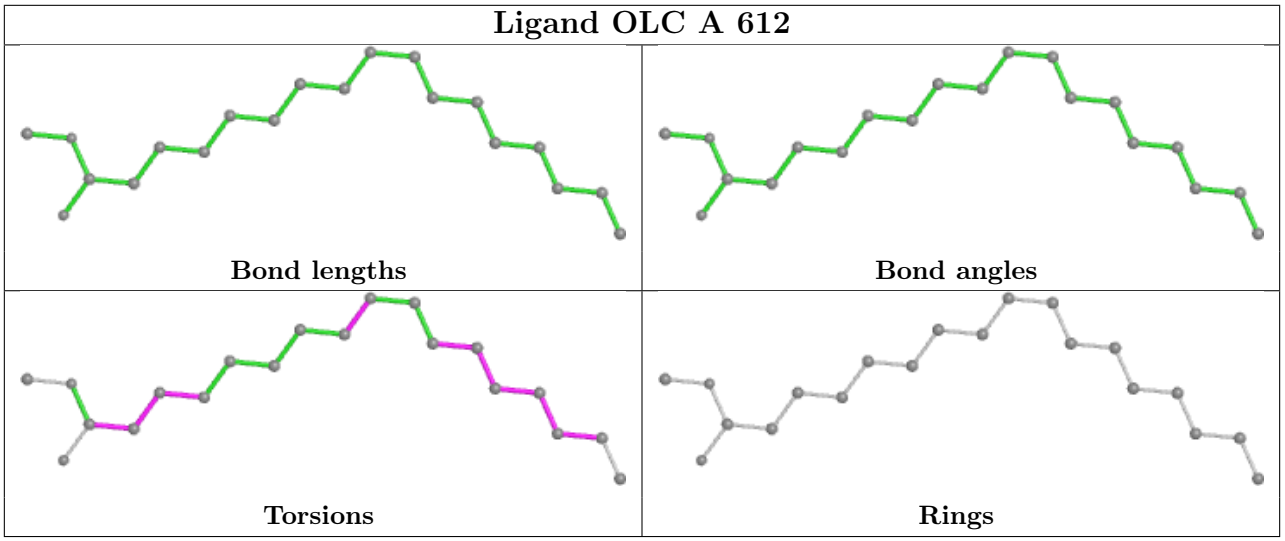


Rings

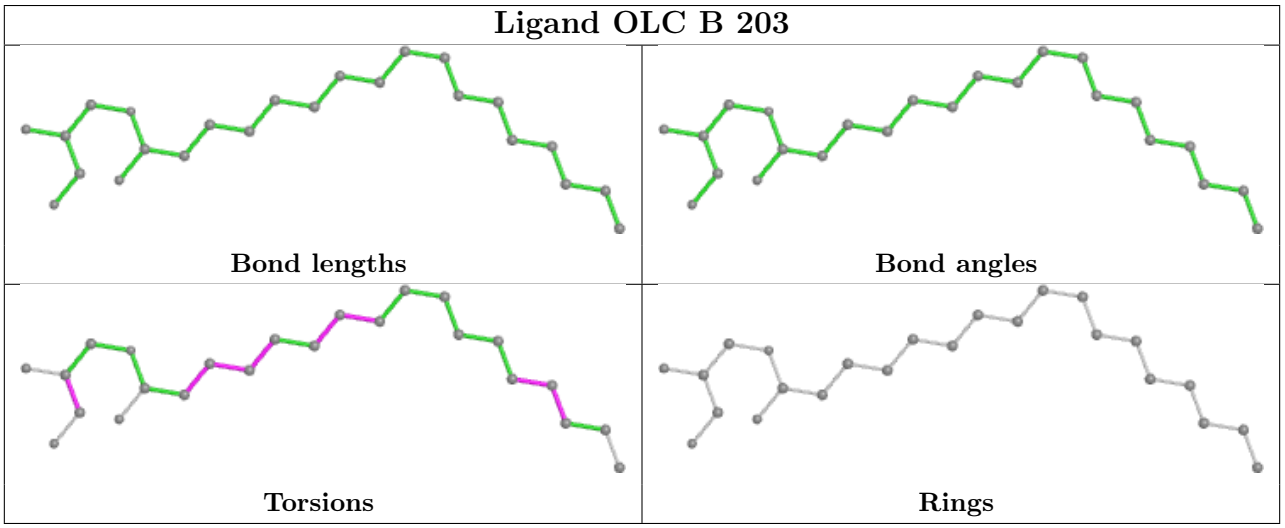
Ligand OLC A 611

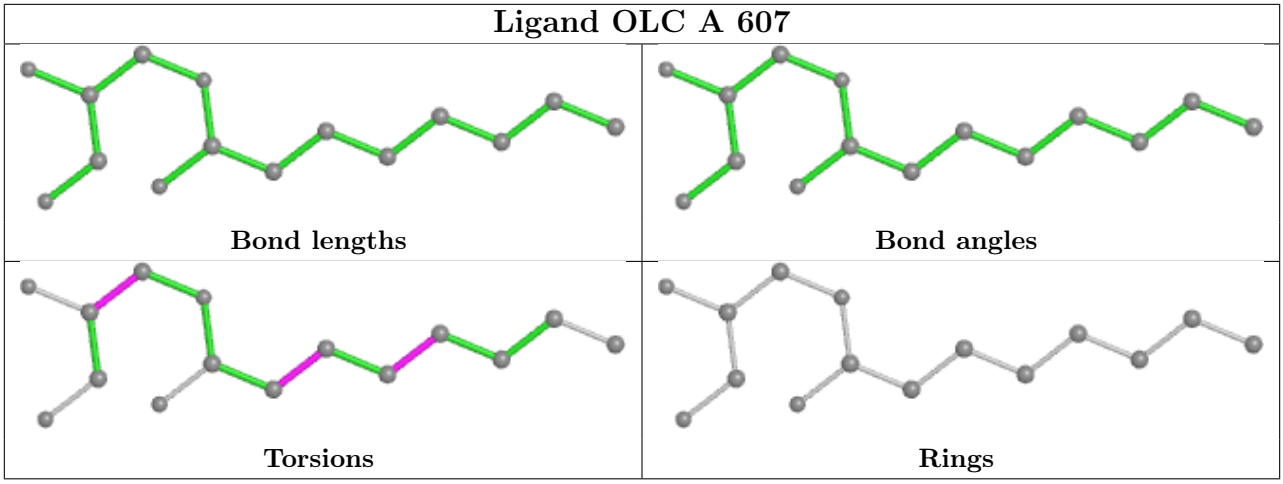


Ligand OLC A 612



Ligand OLC B 203





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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%)	2.07	252 (45%)	0	0	21, 32, 59, 91	0
2	B	167/168 (99%)	1.70	55 (32%)	0	0	22, 32, 57, 104	0
3	C	31/34 (91%)	1.86	12 (38%)	0	0	27, 34, 42, 66	0
All	All	752/771 (97%)	1.98	319 (42%)	0	0	21, 32, 59, 104	0

All (319) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	VAL	11.8
1	A	331	GLY	7.7
1	A	496	GLU	7.2
1	A	495	ARG	7.1
1	A	494	SER	6.6
1	A	536	ILE	6.6
1	A	527	ILE	5.8
1	A	54	LEU	5.6
1	A	326	LEU	5.6
1	A	413	ILE	5.4
1	A	404	LEU	5.4
2	B	141	ARG	5.4
1	A	393	VAL	5.3
1	A	520	LEU	5.2
1	A	489	PHE	5.2
1	A	515	PRO	5.1
1	A	205	VAL	5.1
1	A	58	LEU	5.1
1	A	504	ALA	5.0
1	A	514	GLY	4.9
1	A	176	GLY	4.8
2	B	76	PRO	4.8
1	A	545	THR	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	39	THR	4.7
2	B	5	HIS	4.6
1	A	20	ALA	4.5
1	A	174	ASN	4.4
3	C	5	PRO	4.4
1	A	392	LEU	4.4
1	A	16	PRO	4.3
1	A	170	TRP	4.3
1	A	307	VAL	4.2
2	B	72	VAL	4.2
1	A	25	LEU	4.2
1	A	516	GLU	4.2
1	A	482	LEU	4.2
1	A	553	LEU	4.2
1	A	532	ALA	4.2
1	A	328	GLY	4.2
1	A	92	LEU	4.1
1	A	519	ARG	4.1
1	A	506	LEU	4.1
1	A	178	VAL	4.1
1	A	201	VAL	4.1
1	A	9	SER	4.0
1	A	159	SER	4.0
1	A	11	VAL	4.0
1	A	164	LEU	4.0
2	B	56	THR	4.0
1	A	105	LEU	4.0
2	B	3	ASP	4.0
3	C	11	VAL	3.9
1	A	59	LEU	3.9
2	B	84	LEU	3.9
1	A	396	THR	3.9
2	B	29	PHE	3.9
1	A	246	ILE	3.9
1	A	26	VAL	3.8
1	A	308	PRO	3.8
1	A	401	LEU	3.8
1	A	219	VAL	3.8
1	A	548	GLN	3.8
1	A	498	LYS	3.7
1	A	522	LEU	3.7
1	A	492	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	389	VAL	3.7
1	A	552	HIS	3.7
1	A	102	ASN	3.7
2	B	140	LYS	3.6
1	A	324	GLY	3.6
1	A	410	GLY	3.6
1	A	330	ARG	3.6
1	A	256	GLY	3.6
1	A	437	VAL	3.6
1	A	322	PHE	3.6
1	A	172	ALA	3.6
1	A	78	ILE	3.6
1	A	187	VAL	3.6
1	A	403	TRP	3.5
1	A	198	LEU	3.5
1	A	488	LEU	3.5
2	B	58	VAL	3.5
1	A	512	ILE	3.5
1	A	487	GLY	3.5
1	A	561	LEU	3.5
1	A	465	VAL	3.5
2	B	168	GLU	3.4
1	A	60	PRO	3.4
1	A	181	LEU	3.4
1	A	353	LEU	3.4
3	C	9	LEU	3.4
1	A	207	PHE	3.4
1	A	462	HIS	3.4
1	A	55	LEU	3.4
1	A	301	LEU	3.4
1	A	517	ASP	3.4
2	B	6	LYS	3.4
3	C	15	LEU	3.4
1	A	304	PHE	3.4
1	A	425	VAL	3.4
1	A	21	THR	3.3
1	A	182	VAL	3.3
1	A	69	LEU	3.3
1	A	538	VAL	3.3
1	A	417	GLN	3.3
1	A	33	ILE	3.3
1	A	485	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	549	LEU	3.3
1	A	381	VAL	3.3
1	A	350	VAL	3.3
2	B	85	ALA	3.3
1	A	333	PHE	3.2
1	A	108	LEU	3.2
1	A	236	VAL	3.2
1	A	546	LEU	3.2
1	A	168	ARG	3.2
1	A	426	TRP	3.2
1	A	513	SER	3.2
1	A	518	ARG	3.1
1	A	32	LEU	3.1
1	A	249	THR	3.1
3	C	20	LEU	3.1
1	A	98	ASN	3.1
1	A	491	VAL	3.1
1	A	171	LYS	3.1
2	B	57	THR	3.1
1	A	132	LEU	3.1
1	A	405	LEU	3.1
1	A	150	SER	3.1
1	A	265	ALA	3.1
1	A	356	PHE	3.1
1	A	169	ARG	3.1
1	A	502	ALA	3.1
1	A	143	TRP	3.1
1	A	497	ARG	3.0
2	B	19	LEU	3.0
2	B	20	ALA	3.0
1	A	400	SER	3.0
3	C	24	LEU	3.0
1	A	31	ALA	3.0
1	A	336	ILE	3.0
1	A	523	ALA	3.0
1	A	107	TRP	3.0
1	A	191	LEU	3.0
1	A	230	TRP	3.0
1	A	533	VAL	3.0
2	B	104	VAL	3.0
1	A	402	TYR	3.0
1	A	243	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	420	LEU	3.0
2	B	71	VAL	2.9
1	A	97	LEU	2.9
2	B	107	ILE	2.9
2	B	22	SER	2.9
2	B	12	LEU	2.9
3	C	23	TRP	2.9
1	A	218	GLY	2.9
1	A	251	LEU	2.9
2	B	30	ILE	2.9
1	A	412	PRO	2.9
1	A	184	TYR	2.9
2	B	101	ALA	2.9
2	B	23	LEU	2.9
1	A	349	PRO	2.9
3	C	12	ILE	2.8
1	A	29	PHE	2.8
1	A	61	PHE	2.8
1	A	238	PHE	2.8
1	A	274	LEU	2.8
2	B	11	ILE	2.8
1	A	269	PHE	2.8
1	A	134	THR	2.8
1	A	44	LEU	2.8
1	A	305	VAL	2.8
1	A	271	LEU	2.8
1	A	320	LEU	2.8
1	A	124	LEU	2.8
1	A	121	ALA	2.7
1	A	115	ILE	2.7
1	A	335	TRP	2.7
2	B	135	VAL	2.7
1	A	432	MET	2.7
1	A	530	TRP	2.7
1	A	423	ALA	2.7
1	A	200	LEU	2.7
1	A	408	LEU	2.7
2	B	48	GLY	2.7
1	A	27	LEU	2.7
1	A	499	PRO	2.7
1	A	415	ASP	2.7
1	A	263	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	422	LEU	2.6
1	A	481	LEU	2.6
1	A	429	PHE	2.6
1	A	23	TYR	2.6
1	A	341	TRP	2.6
1	A	366	ASN	2.6
1	A	317	ALA	2.6
1	A	83	LEU	2.6
1	A	241	LEU	2.6
1	A	133	TYR	2.6
1	A	87	ALA	2.6
1	A	180	PRO	2.6
1	A	222	LEU	2.6
1	A	53	PRO	2.5
1	A	111	TRP	2.5
1	A	254	GLN	2.5
1	A	213	PHE	2.5
2	B	50	LEU	2.5
1	A	255	ALA	2.5
1	A	455	GLN	2.5
1	A	68	GLY	2.5
1	A	90	VAL	2.5
1	A	163	VAL	2.5
1	A	555	PRO	2.5
1	A	235	ILE	2.5
1	A	94	ALA	2.5
1	A	240	LEU	2.5
1	A	501	LEU	2.5
2	B	64	TRP	2.5
1	A	547	VAL	2.5
1	A	56	LYS	2.5
1	A	346	PHE	2.5
2	B	21	PHE	2.5
1	A	22	LEU	2.4
1	A	186	ALA	2.4
1	A	185	MET	2.4
1	A	49	VAL	2.4
2	B	14	TYR	2.4
1	A	473	ALA	2.4
1	A	311	MET	2.4
3	C	6	LYS	2.4
1	A	199	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	259	LEU	2.4
1	A	535	ALA	2.4
1	A	37	LEU	2.4
2	B	88	PHE	2.4
1	A	79	VAL	2.4
1	A	542	TYR	2.4
1	A	477	LEU	2.3
1	A	118	VAL	2.3
1	A	57	ARG	2.3
1	A	323	ALA	2.3
2	B	4	GLU	2.3
2	B	33	ILE	2.3
1	A	15	TYR	2.3
1	A	229	TRP	2.3
1	A	279	VAL	2.3
1	A	103	MET	2.3
2	B	25	MET	2.3
1	A	47	GLY	2.3
1	A	113	ALA	2.3
1	A	220	ASP	2.3
1	A	490	SER	2.3
1	A	248	TYR	2.3
1	A	445	LEU	2.3
3	C	10	ALA	2.3
3	C	29	VAL	2.3
1	A	193	TRP	2.3
2	B	77	ASN	2.3
1	A	162	ILE	2.3
1	A	71	LEU	2.2
1	A	313	ALA	2.2
1	A	226	THR	2.2
1	A	149	ALA	2.2
1	A	444	LEU	2.2
2	B	7	ALA	2.2
2	B	68	ALA	2.2
1	A	216	VAL	2.2
1	A	316	VAL	2.2
1	A	239	TRP	2.2
1	A	189	PHE	2.2
1	A	365	VAL	2.2
2	B	44	VAL	2.2
2	B	53	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	112	VAL	2.2
1	A	179	THR	2.2
1	A	117	LEU	2.2
1	A	427	LEU	2.2
1	A	212	SER	2.2
1	A	74	VAL	2.2
1	A	120	ALA	2.2
2	B	121	THR	2.2
1	A	453	ILE	2.1
1	A	294	TRP	2.1
1	A	354	LEU	2.1
1	A	272	PHE	2.1
1	A	397	ALA	2.1
1	A	88	ILE	2.1
3	C	14	VAL	2.1
1	A	192	MET	2.1
1	A	277	THR	2.1
1	A	160	ILE	2.1
1	A	273	LEU	2.1
1	A	493	LEU	2.1
2	B	160	MET	2.1
1	A	139	LEU	2.1
1	A	188	VAL	2.1
2	B	54	ASP	2.1
2	B	59	ARG	2.1
1	A	247	ILE	2.1
2	B	123	ILE	2.1
1	A	260	VAL	2.1
1	A	526	ARG	2.1
1	A	472	LEU	2.0
1	A	152	PHE	2.0
1	A	161	TYR	2.0
1	A	510	GLU	2.0
2	B	90	TYR	2.0
1	A	303	LEU	2.0
1	A	395	LEU	2.0
2	B	45	ILE	2.0
2	B	164	ILE	2.0
1	A	500	GLU	2.0
2	B	127	VAL	2.0
2	B	86	PHE	2.0
1	A	376	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	147	ILE	2.0
2	B	28	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

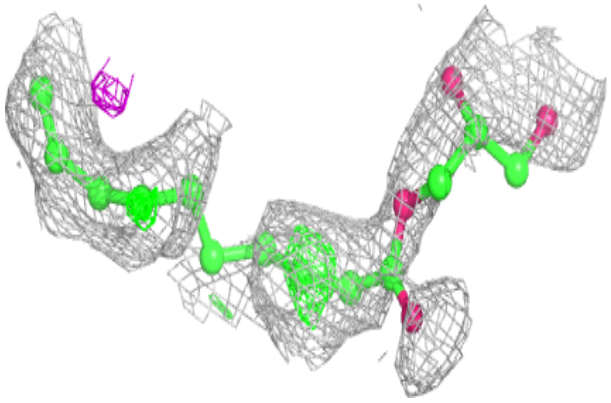
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

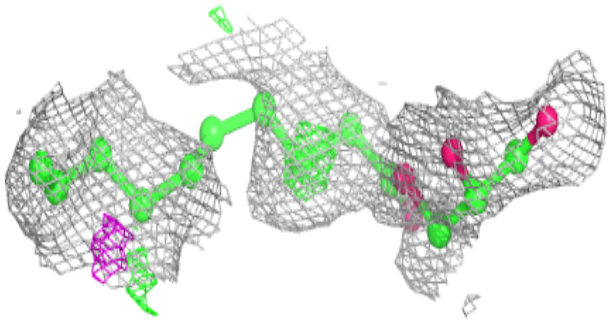
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	OLC	A	606	17/25	0.18	0.38	70,73,88,91	0
7	OLC	A	616	15/25	0.21	0.36	67,74,89,92	0
7	OLC	B	202	25/25	0.26	0.38	64,68,86,101	0
7	OLC	A	609	15/25	0.27	0.39	80,94,101,102	0
7	OLC	A	610	20/25	0.28	0.42	70,80,96,100	0
7	OLC	A	607	15/25	0.32	0.49	67,84,97,99	0
7	OLC	C	101	24/25	0.38	0.41	54,66,98,101	0
7	OLC	A	614	9/25	0.44	0.31	56,59,75,76	0
7	OLC	B	203	24/25	0.47	0.33	68,80,93,103	0
7	OLC	A	612	20/25	0.47	0.34	69,77,86,97	0
7	OLC	A	608	18/25	0.48	0.36	62,79,91,92	0
7	OLC	A	611	21/25	0.49	0.34	56,77,94,105	0
7	OLC	A	613	9/25	0.56	0.31	64,69,74,77	0
7	OLC	A	605	18/25	0.57	0.35	61,77,95,102	0
7	OLC	A	604	23/25	0.63	0.28	42,60,91,94	0
6	HAS	A	603	65/65	0.75	0.25	20,26,44,59	0
5	HEM	A	602	43/43	0.79	0.23	20,23,27,36	0
8	CMO	A	615	2/2	0.97	0.14	20,20,20,26	0
9	CUA	B	201	2/2	0.98	0.05	25,25,25,26	0
4	CU	A	601	1/1	0.99	0.08	29,29,29,29	0

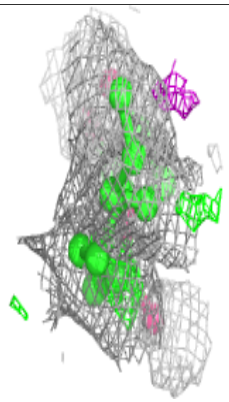
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC 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)

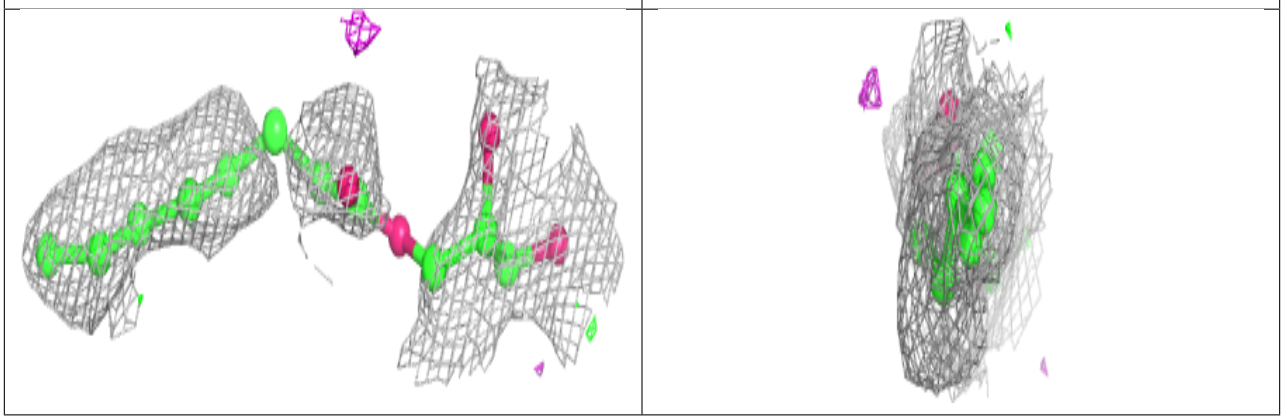






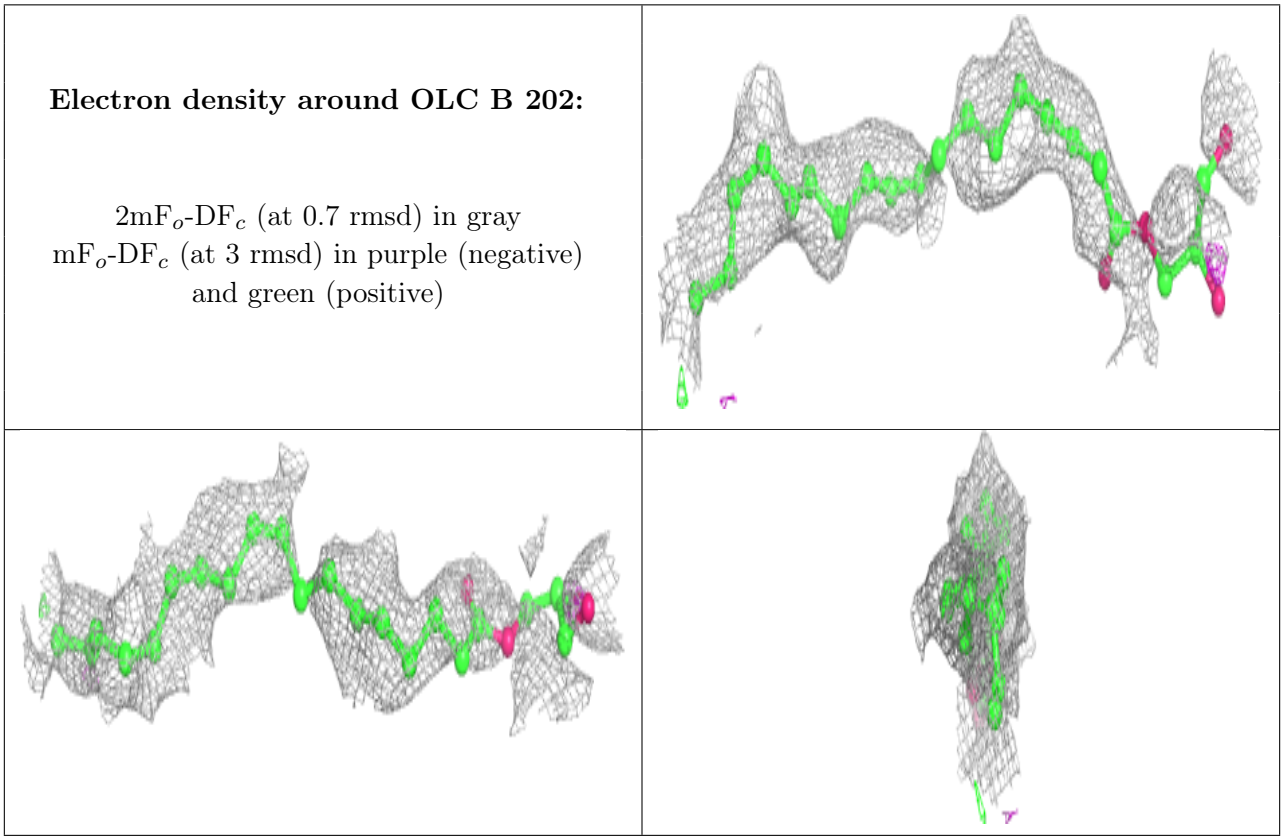
Electron density around OLC A 616:

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



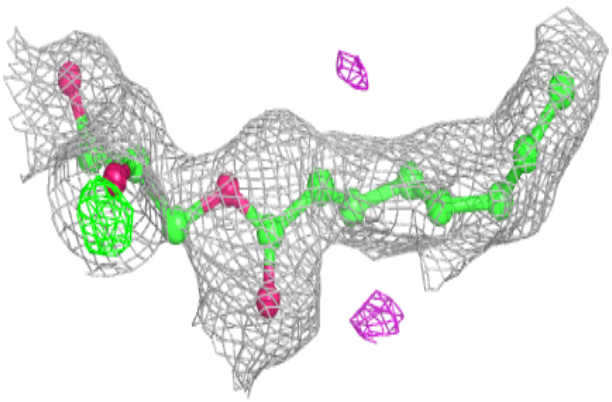
Electron density around OLC B 202:

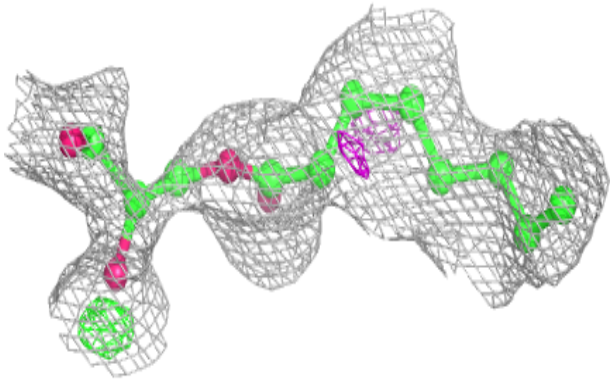
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

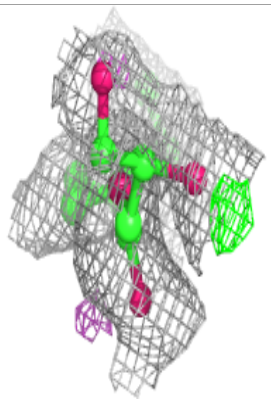


Electron density around OLC A 609:

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

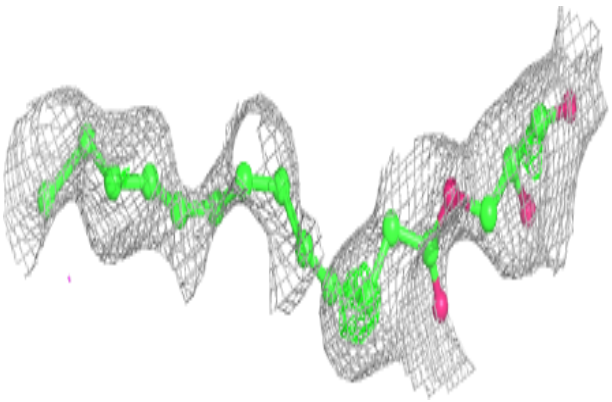


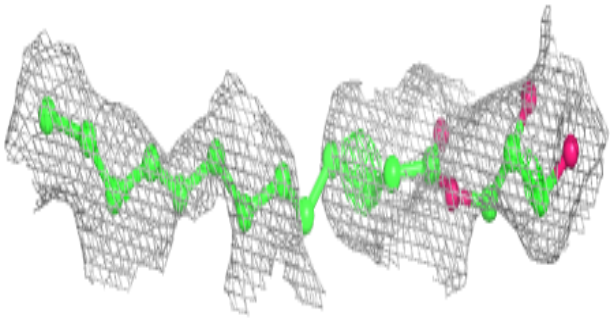


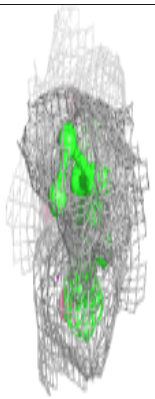


Electron density around OLC A 610:

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

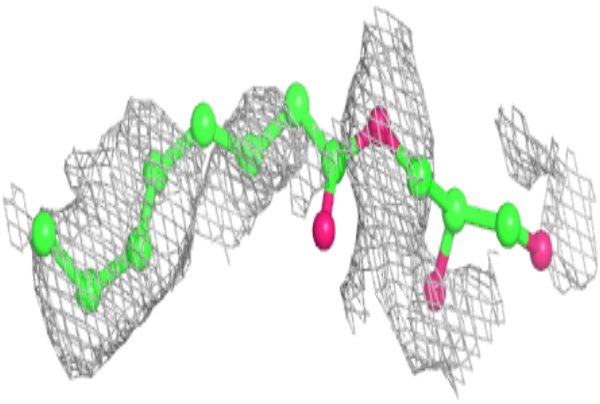


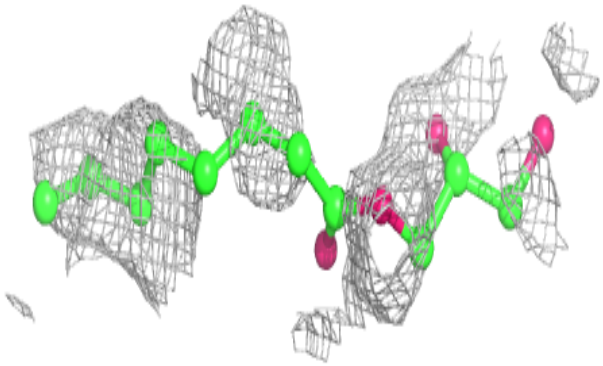


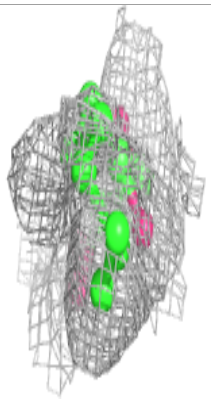


Electron density around OLC A 607:

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

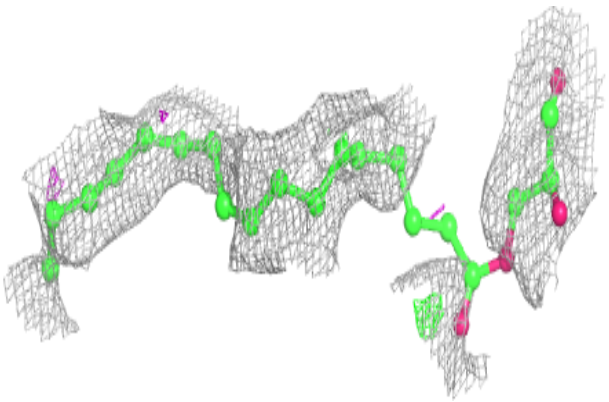


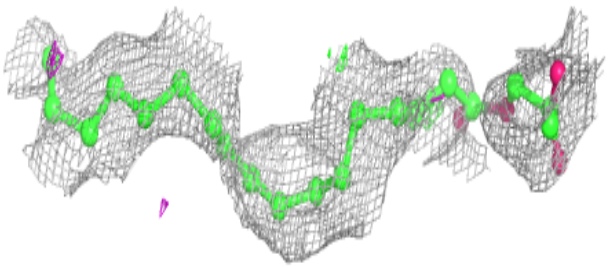


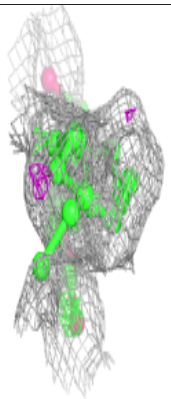


Electron density around OLC C 101:

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

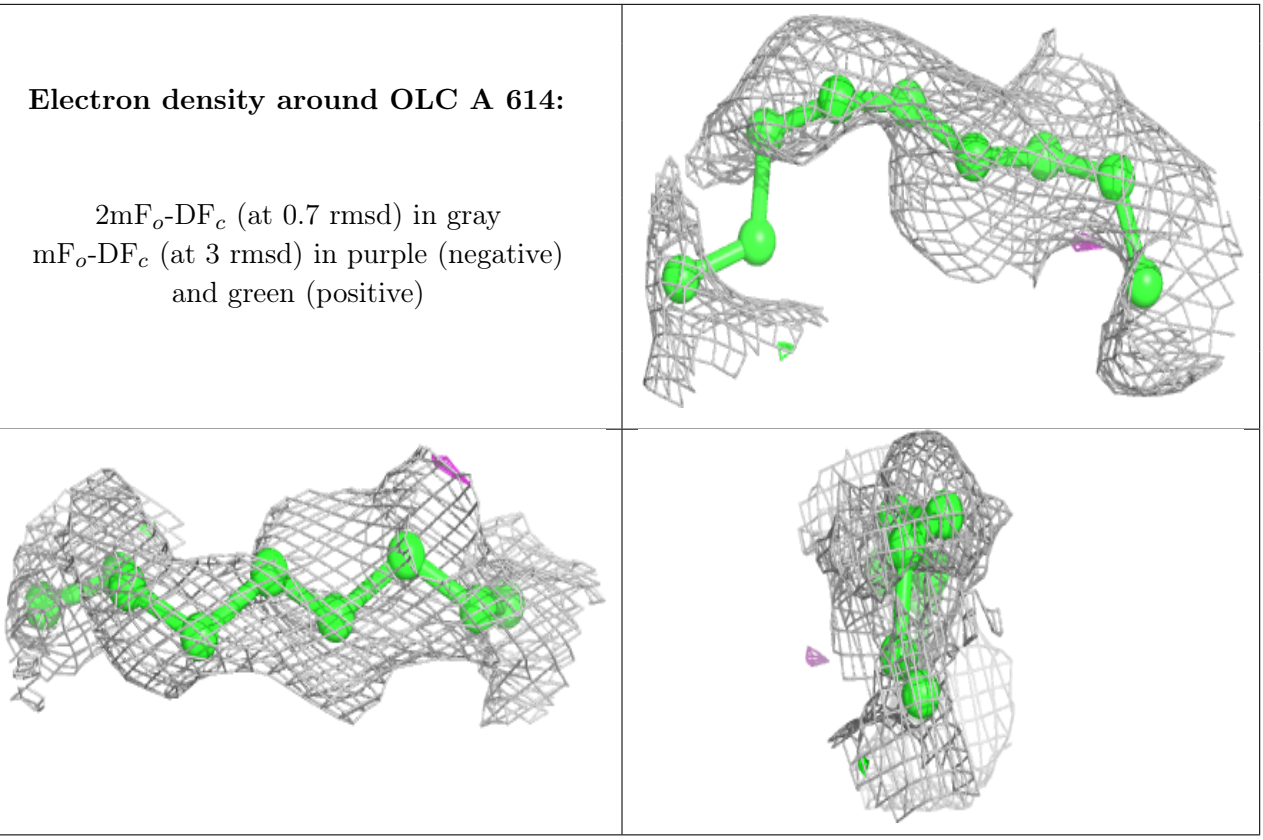






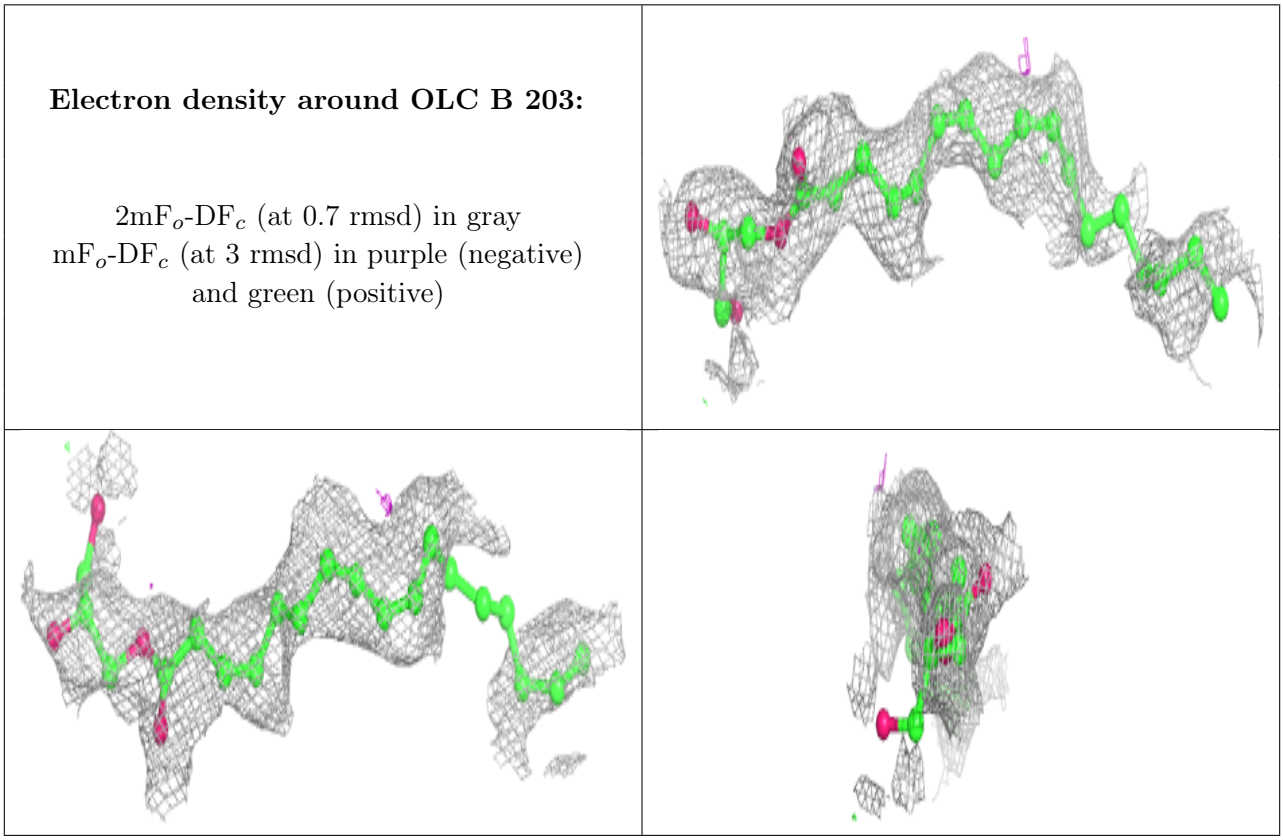
Electron density around OLC A 614:

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



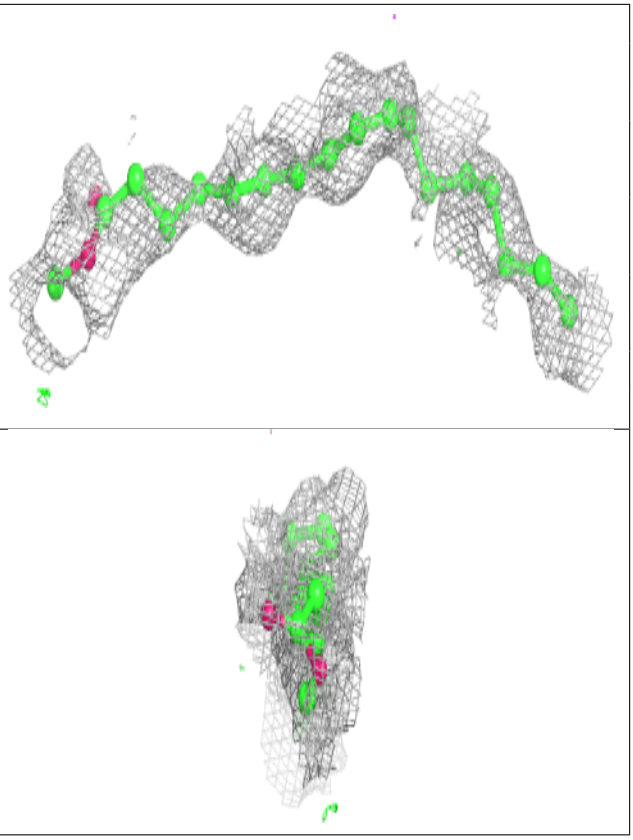
Electron density around OLC B 203:

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



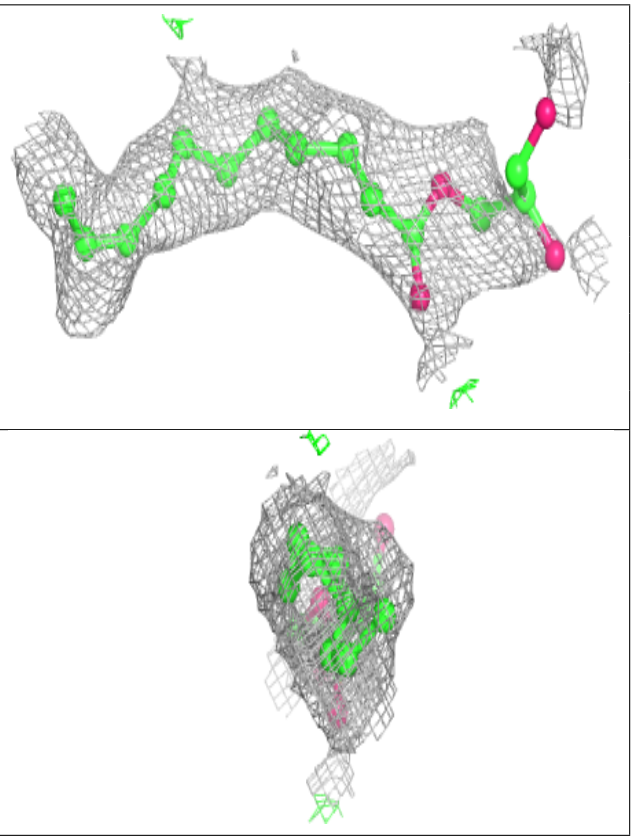
Electron density around OLC A 612:

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



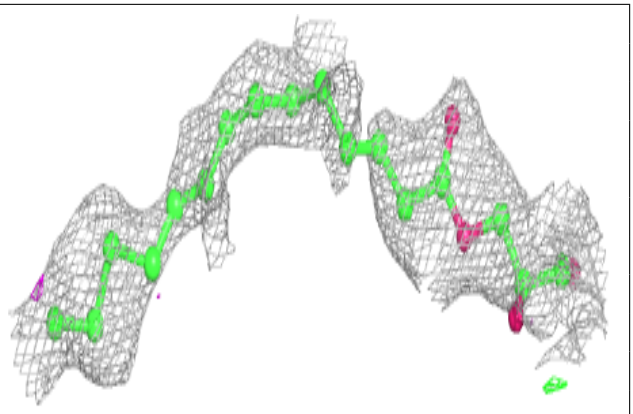
Electron density around OLC A 608:

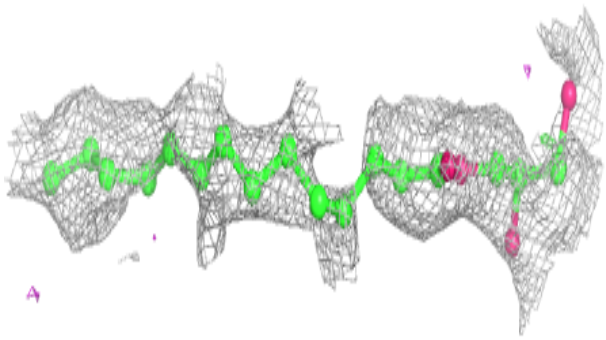
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

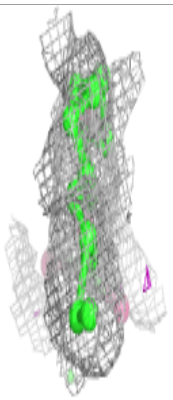


Electron density around OLC A 611:

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

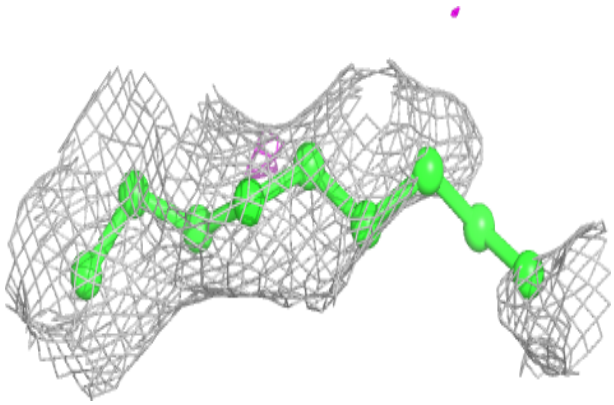


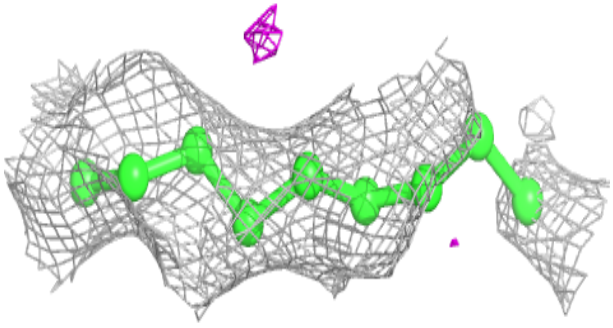


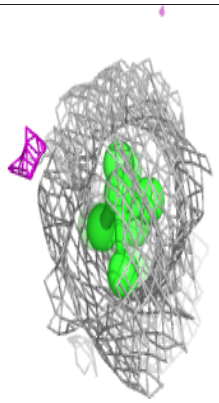


Electron density around OLC A 613:

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

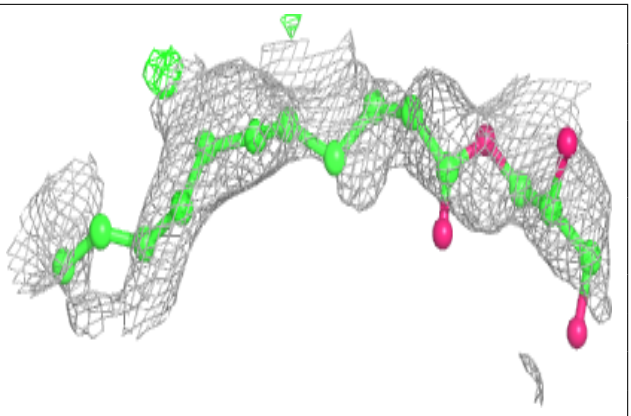


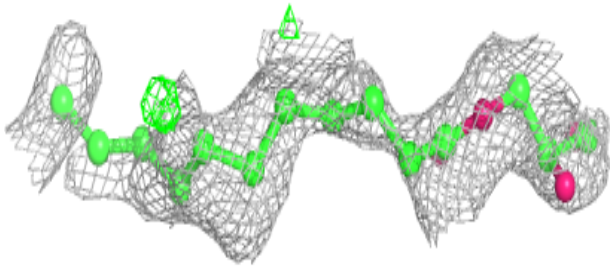


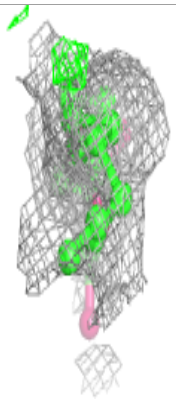


Electron density around OLC A 605:

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

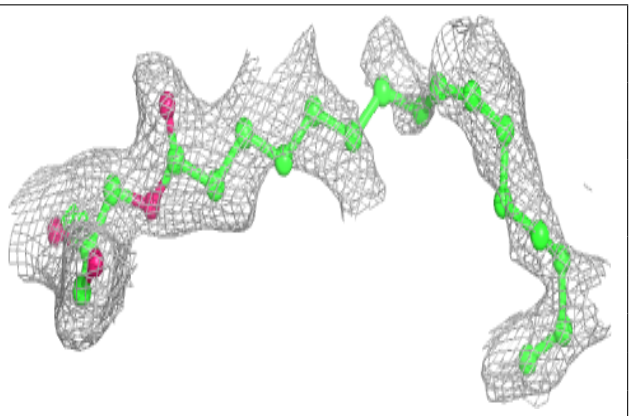


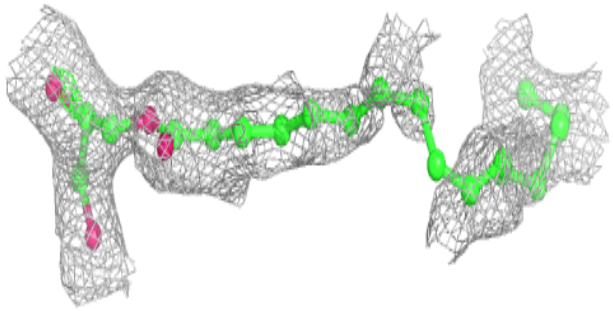


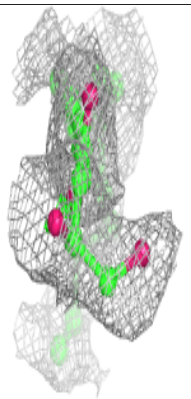


Electron density around OLC A 604:

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

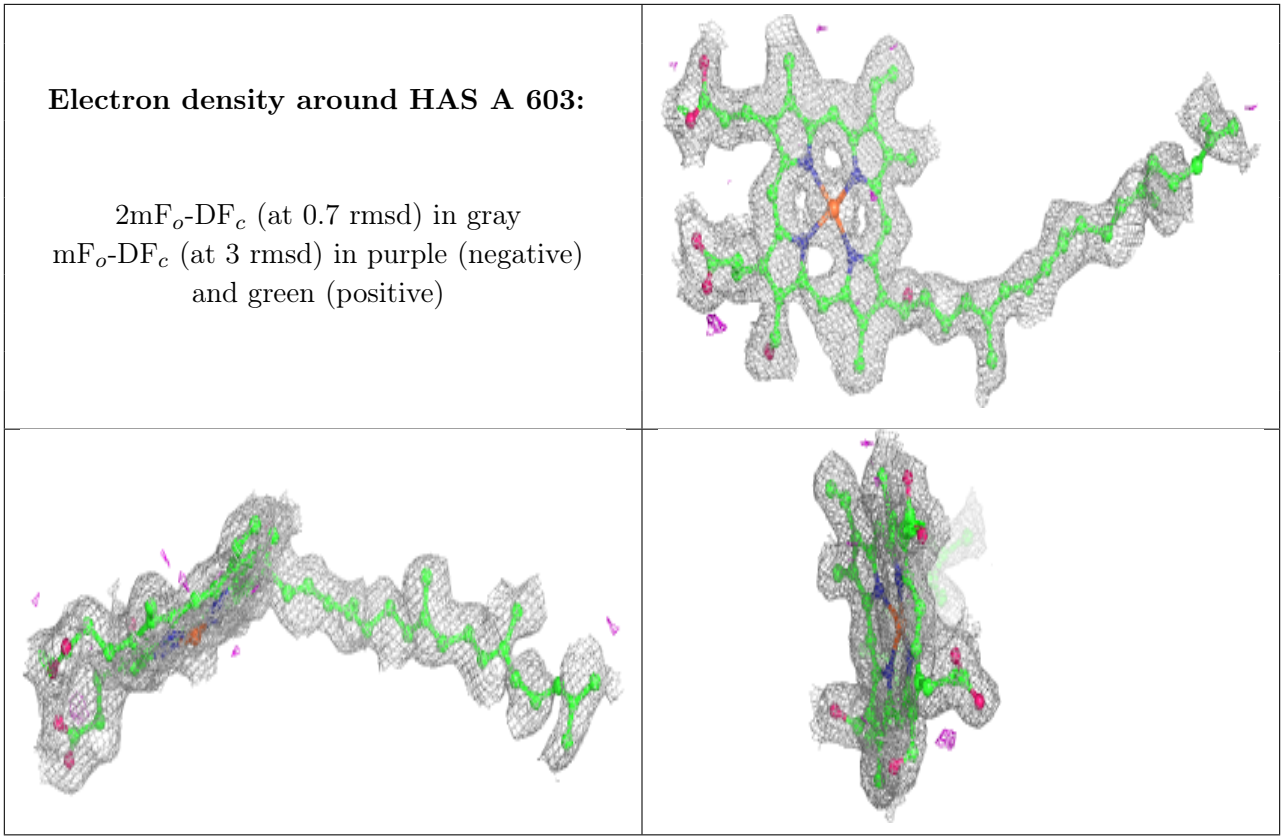






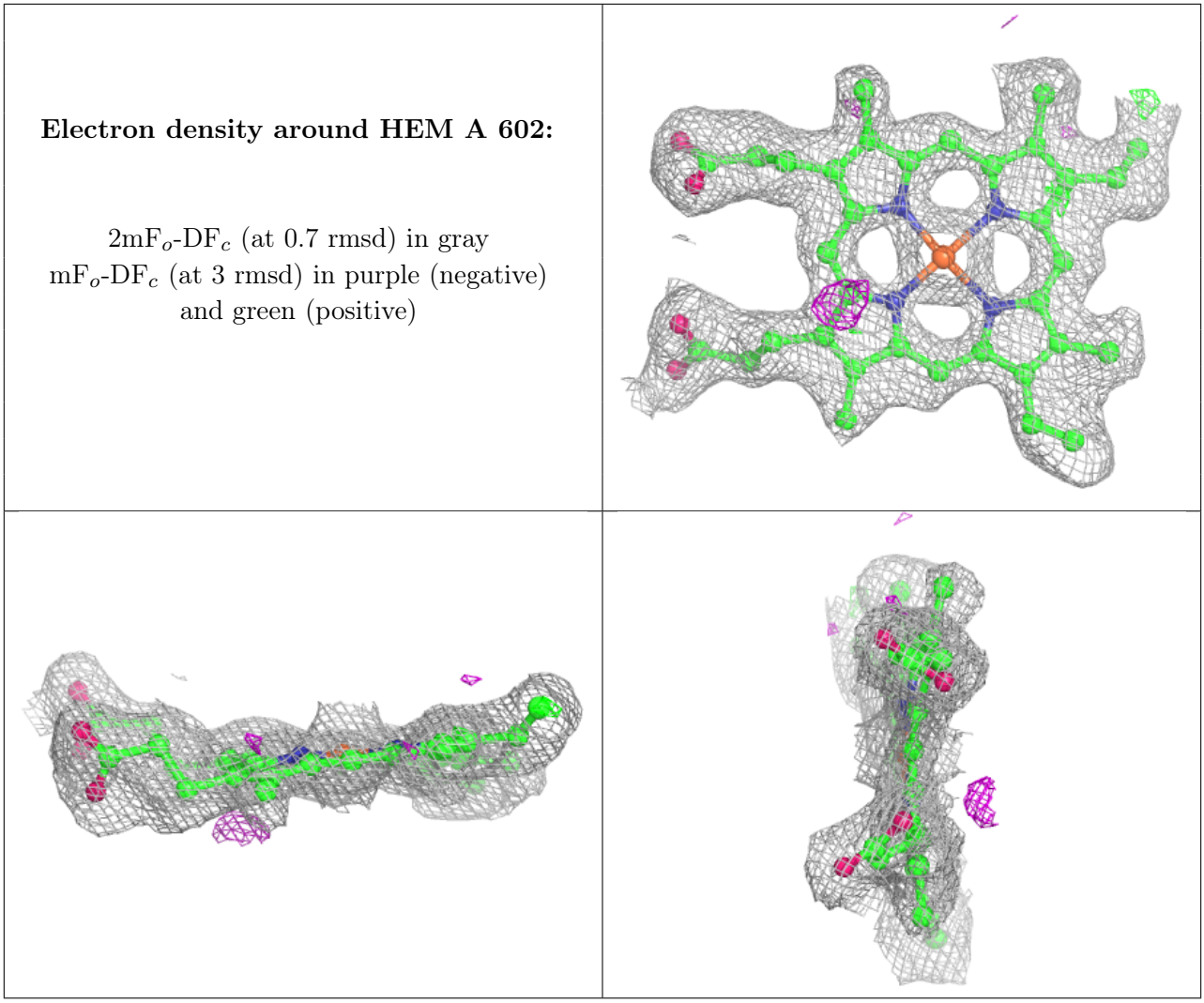
Electron density around HAS A 603:

$2mF_o$-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

There are no such residues in this entry.