



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:06 AM UTC

PDB ID : 8K6Y / pdb_00008k6y
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	:	4-5-2 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

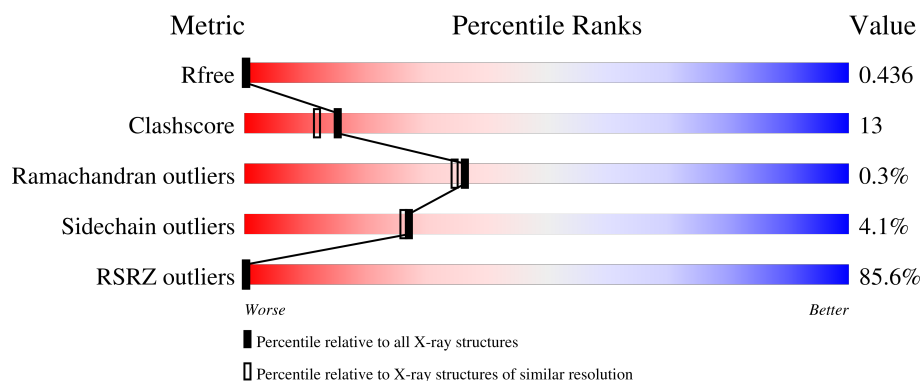
1 Overall quality at a glance

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	83% 68% 26% . .
2	B	168	84% 73% 24% . .
3	C	34	88% 76% 12% . 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	-	-	-
7	OLC	A	605	-	-	-	X
7	OLC	A	606	-	-	-	X
7	OLC	A	607	-	-	-	X
7	OLC	A	608	-	-	-	X
7	OLC	A	609	-	-	-	X
7	OLC	A	610	-	-	-	X
7	OLC	A	611	-	-	-	X
7	OLC	A	612	-	-	-	X
7	OLC	A	613	-	-	-	X
7	OLC	A	614	-	-	-	X
7	OLC	A	616	-	-	-	X
7	OLC	B	203	-	-	-	X
7	OLC	C	101	-	-	-	X

2 Entry composition

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			

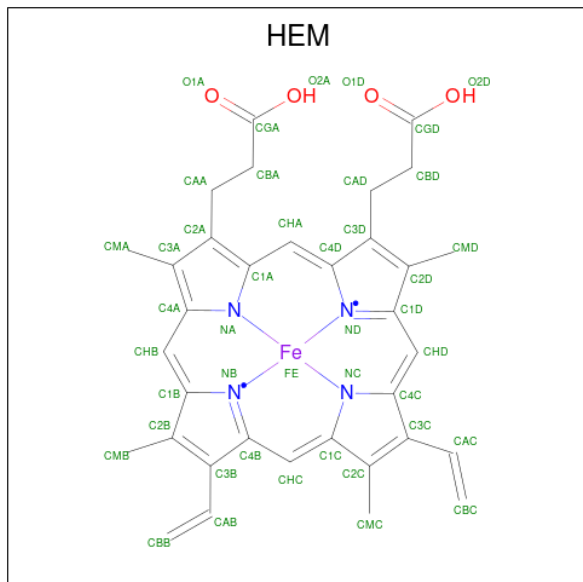
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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 (CCD ID: CU) (formula: Cu).

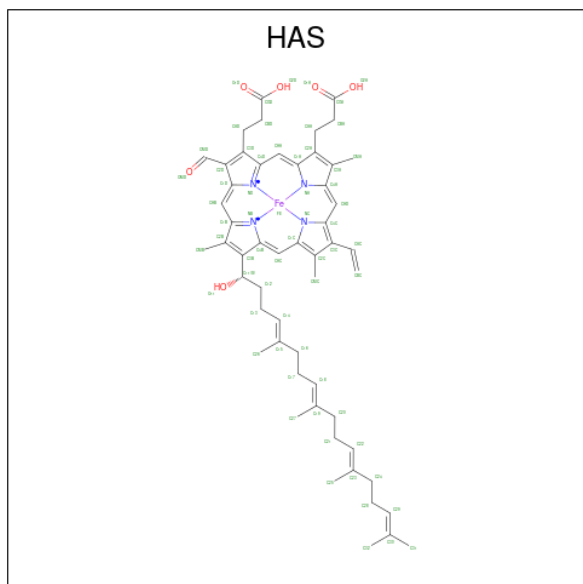
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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



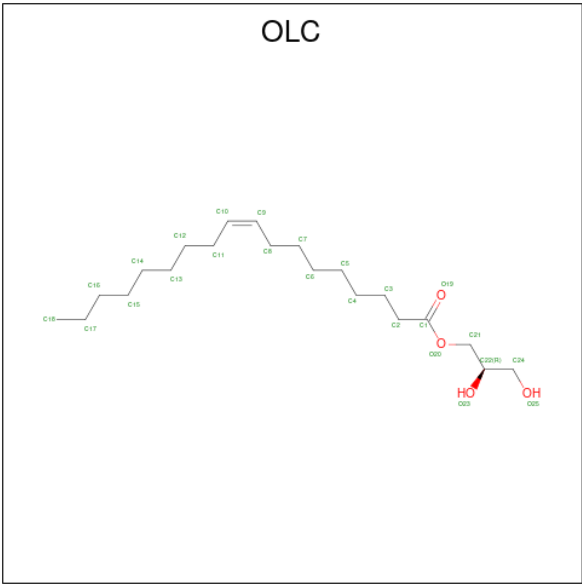
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is HEME-AS (CCD ID: 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 (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



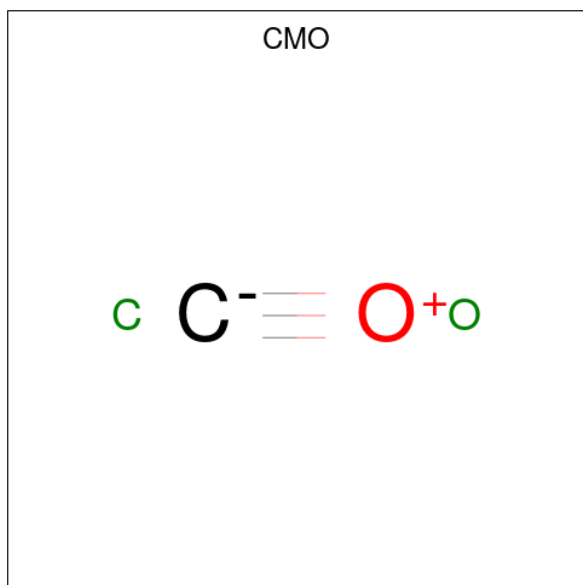
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			23	19	4		
7	A	1	Total	C	O	0	0
			18	14	4		
7	A	1	Total	C	O	0	0
			17	13	4		
7	A	1	Total	C	O	0	0
			15	11	4		
7	A	1	Total	C	O	0	0
			18	14	4		
7	A	1	Total	C	O	0	0
			15	11	4		
7	A	1	Total	C	O	0	0
			20	16	4		
7	A	1	Total	C	O	0	0
			21	17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

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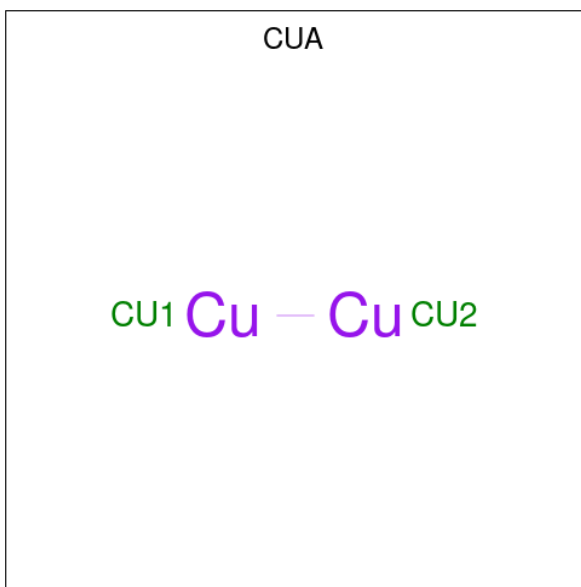
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			25	21	4		
7	B	1	Total	C	O	0	0
			24	20	4		
7	C	1	Total	C	O	0	0
			24	20	4		

- Molecule 8 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



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

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

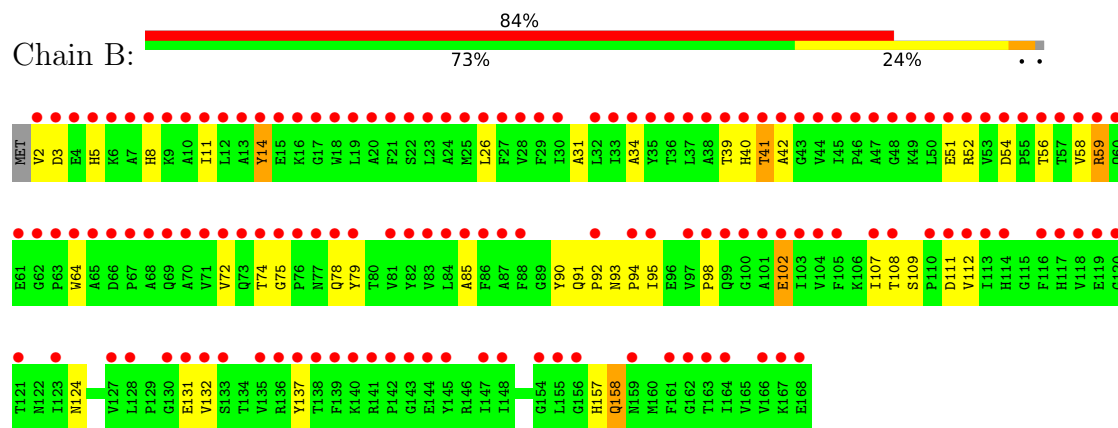


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Cu 2 2	0	0

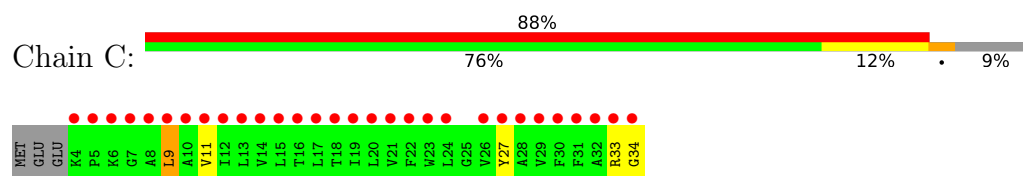
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	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

- 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	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
$\langle I/\sigma(I) \rangle$ 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)	0.39 , 79.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.58$, $\langle L^2 \rangle = 0.43$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.61	0/4525	1.28	20/6213 (0.3%)
2	B	0.63	0/1338	1.29	7/1828 (0.4%)
3	C	0.59	0/247	1.31	2/335 (0.6%)
All	All	0.61	0/6110	1.28	29/8376 (0.3%)

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 (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	HIS	CA-CB-CG	-12.09	101.71	113.80
2	B	124	ASN	CB-CA-C	-7.10	102.40	111.70
1	A	121	ALA	CA-C-N	6.36	128.78	120.26
1	A	121	ALA	C-N-CA	6.36	128.78	120.26
1	A	52	TYR	N-CA-CB	6.22	117.77	110.42
1	A	489	PHE	CB-CA-C	6.20	123.28	110.31
3	C	27	TYR	CA-C-N	6.18	128.88	120.54
3	C	27	TYR	C-N-CA	6.18	128.88	120.54
2	B	14	TYR	CB-CA-C	6.04	121.13	110.85
1	A	90	VAL	N-CA-C	-5.97	106.42	111.56
1	A	185	MET	CA-C-N	5.89	128.66	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	MET	C-N-CA	5.89	128.66	120.29
1	A	293	THR	CA-CB-OG1	-5.86	100.81	109.60
1	A	135	PHE	CA-CB-CG	5.53	119.33	113.80
2	B	124	ASN	CA-CB-CG	5.33	117.93	112.60
1	A	545	THR	CB-CA-C	5.27	119.64	110.79
1	A	137	PRO	N-CA-C	-5.25	104.30	110.70
1	A	191	LEU	CA-C-N	5.22	127.23	120.44
1	A	191	LEU	C-N-CA	5.22	127.23	120.44
1	A	335	TRP	CA-C-N	5.14	127.51	120.46
1	A	335	TRP	C-N-CA	5.14	127.51	120.46
1	A	552	HIS	CA-CB-CG	5.11	118.91	113.80
2	B	11	ILE	CA-C-N	5.08	127.08	120.28
2	B	11	ILE	C-N-CA	5.08	127.08	120.28
1	A	242	PRO	CB-CA-C	-5.07	103.81	112.64
1	A	370	THR	CA-CB-OG1	-5.05	102.02	109.60
2	B	41	THR	CB-CA-C	5.02	120.42	110.42
2	B	102	GLU	CB-CG-CD	5.02	121.13	112.60
1	A	146	TYR	CB-CA-C	5.00	119.09	110.79

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 ⓘ

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	130	0
2	B	1301	0	1278	35	0
3	C	241	0	267	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	172	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 (172) 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
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:387:LEU:HD21	1:A:433:MET:HE2	1.60	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
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
2:B:14:TYR:HE2	7:B:203:OLC:HO25	1.33	0.74
1:A:387:LEU:HD22	1:A:433:MET:HE3	1.68	0.74
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
6:A:603:HAS:HBC1	6:A:603:HAS:HMC3	1.72	0.70
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:A:616:OLC:H21A	7:C:101:OLC:O25	1.97	0.65
2:B:14:TYR:HE2	7:B:203:OLC:O25	1.78	0.64
1:A:504:ALA:O	10:A:703:HOH:O	2.14	0.64
1:A:394:THR:HG22	1:A:398:MET:HE3	1.78	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:233:HIS:CD2	1:A:233:HIS:C	2.78	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:387:LEU:CD2	1:A:433:MET:HE3	2.28	0.60
1:A:164:LEU:HD11	1:A:191:LEU:HD21	1.83	0.60
1:A:414:SER:HG	1:A:417:GLN:HG3	1.64	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:391:SER:HB2	1:A:432:MET:HG3	1.86	0.57
1:A:405:LEU:O	1:A:409:THR:OG1	2.14	0.57
1:A:270:LEU:HD22	1:A:524:MET:HG2	1.86	0.57
1:A:95:ARG:NH2	10:A:708:HOH:O	2.36	0.56
1:A:401:LEU:HG	1:A:405:LEU:HD22	1.88	0.56
1:A:433:MET:HE2	1:A:433:MET:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:230:TRP:C	1:A:230:TRP:CD1	2.87	0.53
1:A:388:GLN:HE21	6:A:603:HAS:CHC	2.22	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:492:LEU:C	1:A:493:LEU:HD12	2.37	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
2:B:137:TYR:OH	3:C:33:ARG:O	2.30	0.48
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:99:MET:HE1	1:A:169:ARG:HB3	1.96	0.47
1:A:445:LEU:HD23	7:A:616:OLC:H3A	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:ARG:NH2	10:B:306:HOH:O	2.47	0.47
6:A:603:HAS:HBC1	6:A:603:HAS:CMC	2.43	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:366:ASN:C	6:A:603:HAS:HMD	2.40	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
2:B:54:ASP:CG	2:B:56:THR:OG1	2.59	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:230:TRP:C	1:A:230:TRP:HD1	2.24	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:322:PHE:O	1:A:323:ALA:C	2.59	0.45
1:A:441:TRP:O	1:A:442:ALA:C	2.58	0.44
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
2:B:158:GLN:H	2:B:158:GLN:CD	2.25	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
2:B:91:GLN:HA	2:B:92:PRO:C	2.42	0.43
2:B:40:HIS:C	2:B:42:ALA:H	2.27	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
2:B:40:HIS:C	2:B:42:ALA:N	2.77	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:ASN:HA	2:B:94:PRO:HA	1.81	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: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:430:LEU:HD23	1:A:430:LEU:HA	1.92	0.41
1:A:416:ALA:O	1:A:417:GLN:C	2.64	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: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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	552/569 (97%)	515 (93%)	36 (6%)	1 (0%)	43	42
2	B	165/168 (98%)	155 (94%)	9 (6%)	1 (1%)	21	17
3	C	29/34 (85%)	27 (93%)	2 (7%)	0	100	100
All	All	746/771 (97%)	697 (93%)	47 (6%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	447/463 (96%)	428 (96%)	19 (4%)	26	25
2	B	136/138 (99%)	132 (97%)	4 (3%)	37	40
3	C	24/27 (89%)	22 (92%)	2 (8%)	10	7
All	All	607/628 (97%)	582 (96%)	25 (4%)	27	26

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	SER
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	270	LEU
1	A	282	HIS
1	A	326	LEU
1	A	332	LEU

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Mol	Chain	Res	Type
1	A	370	THR
1	A	401	LEU
1	A	405	LEU
1	A	424	VAL
1	A	456	VAL
1	A	498	LYS
1	A	513	SER
1	A	548	GLN
2	B	26	LEU
2	B	107	ILE
2	B	108	THR
2	B	158	GLN
3	C	9	LEU
3	C	11	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	388	GLN
1	A	455	GLN
1	A	548	GLN
1	A	552	HIS
2	B	60	GLN
2	B	91	GLN
2	B	99	GLN
2	B	158	GLN
2	B	159	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
9	CUA	B	201	2	0,1,1	-	-	-		
6	HAS	A	603	1	72,72,72	2.63	27 (37%)	87,109,109	3.01	43 (49%)
7	OLC	B	203	-	23,23,24	0.25	0	24,24,25	0.22	0
7	OLC	A	609	-	14,14,24	0.21	0	15,15,25	0.29	0
7	OLC	A	612	-	19,19,24	0.26	0	19,19,25	0.26	0
7	OLC	A	613	-	8,8,24	0.19	0	7,7,25	0.18	0
7	OLC	A	614	-	8,8,24	0.16	0	7,7,25	0.16	0
7	OLC	A	605	-	17,17,24	0.24	0	18,18,25	0.30	0
7	OLC	A	607	-	14,14,24	0.23	0	15,15,25	0.32	0
7	OLC	A	606	-	16,16,24	0.27	0	17,17,25	0.34	0
8	CMO	A	615	4	0,1,1	-	-	-		
7	OLC	C	101	-	23,23,24	0.48	1 (4%)	24,24,25	0.33	0
7	OLC	A	616	-	14,14,24	0.82	1 (7%)	15,15,25	0.67	0
5	HEM	A	602	1	50,50,50	1.59	7 (14%)	67,82,82	1.74	20 (29%)
7	OLC	A	604	-	22,22,24	0.23	0	23,23,25	0.44	0
7	OLC	A	611	-	20,20,24	0.72	1 (5%)	21,21,25	0.60	1 (4%)
7	OLC	A	610	-	19,19,24	1.23	1 (5%)	20,20,25	0.35	0
7	OLC	B	202	-	24,24,24	0.33	0	25,25,25	0.32	0
7	OLC	A	608	-	17,17,24	0.30	0	18,18,25	0.38	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	604	-	-	10/22/22/24	-
7	OLC	A	614	-	-	3/6/6/24	-
7	OLC	A	605	-	-	10/17/17/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OLC	A	607	-	-	3/14/14/24	-
6	HAS	A	603	1	1/1/8/18	9/42/82/82	-
7	OLC	A	611	-	-	8/20/20/24	-
7	OLC	B	203	-	-	9/23/23/24	-
7	OLC	A	606	-	-	7/16/16/24	-
7	OLC	A	610	-	-	10/19/19/24	-
7	OLC	A	616	-	-	2/14/14/24	-
7	OLC	B	202	-	-	10/24/24/24	-
7	OLC	A	609	-	-	7/14/14/24	-
7	OLC	A	608	-	-	9/17/17/24	-
7	OLC	A	612	-	-	9/18/18/24	-
5	HEM	A	602	1	-	2/14/54/54	-
7	OLC	A	613	-	-	5/6/6/24	-
7	OLC	C	101	-	-	16/23/23/24	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	C3B-C2B	6.22	1.48	1.34
6	A	603	HAS	FE-NA	5.92	2.14	1.95
6	A	603	HAS	CHD-C4A	5.73	1.49	1.38
6	A	603	HAS	FE-ND	5.64	2.12	1.94
5	A	602	HEM	FE-NB	5.36	2.11	1.94
6	A	603	HAS	FE-NB	5.34	2.11	1.94
7	A	610	OLC	C13-C12	5.27	1.87	1.50
6	A	603	HAS	FE-NC	5.10	2.12	1.95
6	A	603	HAS	CHA-C1A	5.08	1.48	1.38
6	A	603	HAS	CHB-C1D	4.94	1.48	1.38
6	A	603	HAS	C2A-C3A	4.70	1.46	1.36
6	A	603	HAS	C1A-C2A	4.44	1.53	1.45
6	A	603	HAS	C2D-C3D	4.32	1.47	1.37
6	A	603	HAS	C4B-C3B	4.12	1.52	1.44
6	A	603	HAS	CHC-C1C	3.94	1.48	1.39
5	A	602	HEM	FE-NC	3.90	2.08	1.95
5	A	602	HEM	C1B-NB	-3.89	1.33	1.40
6	A	603	HAS	C1B-C2B	3.83	1.52	1.44
6	A	603	HAS	C4D-C3D	3.74	1.51	1.45
6	A	603	HAS	CHC-C4B	3.74	1.46	1.38
6	A	603	HAS	C1C-C2C	3.50	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	CHA-C4D	3.33	1.46	1.39
6	A	603	HAS	CHD-C4C	3.26	1.46	1.39
5	A	602	HEM	CHB-C1B	2.98	1.44	1.38
6	A	603	HAS	O1A-CGA	2.93	1.31	1.22
6	A	603	HAS	CHB-C1B	2.84	1.45	1.39
7	A	616	OLC	C4-C5	2.69	1.65	1.51
6	A	603	HAS	CBA-CGA	2.69	1.56	1.50
6	A	603	HAS	C1D-ND	-2.56	1.35	1.40
6	A	603	HAS	C1B-NB	-2.51	1.33	1.38
6	A	603	HAS	C4B-NB	-2.35	1.36	1.40
7	A	611	OLC	C13-C12	2.27	1.65	1.51
5	A	602	HEM	C1C-C2C	-2.25	1.40	1.45
5	A	602	HEM	C4D-ND	-2.19	1.36	1.40
7	C	101	OLC	C17-C16	2.07	1.65	1.50
6	A	603	HAS	C4A-NA	-2.07	1.35	1.39
5	A	602	HEM	C1D-ND	-2.02	1.34	1.38
6	A	603	HAS	C3C-C4C	2.02	1.48	1.42

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	C2D-C3D-C4D	-11.34	98.22	106.43
6	A	603	HAS	CAD-C3D-C4D	6.73	136.42	124.70
6	A	603	HAS	C3C-C4C-NC	6.55	115.31	109.80
6	A	603	HAS	C3D-C4D-ND	6.21	116.35	110.35
6	A	603	HAS	C2B-C1B-NB	5.89	116.71	109.90
6	A	603	HAS	C3B-C4B-NB	5.86	116.58	109.84
6	A	603	HAS	C2A-C1A-NA	5.55	115.68	110.32
6	A	603	HAS	C26-C15-C16	5.18	124.22	115.23
6	A	603	HAS	CAA-CBA-CGA	-4.43	101.90	113.67
5	A	602	HEM	CHC-C4B-NB	4.38	129.13	124.42
6	A	603	HAS	C1A-C2A-C3A	-4.35	101.38	107.11
6	A	603	HAS	C3C-C2C-C1C	-4.35	102.04	107.17
6	A	603	HAS	CHA-C4D-ND	-4.20	119.90	124.42
6	A	603	HAS	OMD-CMD-C2D	-4.12	116.32	125.62
6	A	603	HAS	C1B-C2B-C3B	-4.07	102.08	106.80
5	A	602	HEM	C3B-C2B-C1B	3.97	109.39	106.41
6	A	603	HAS	C12-C13-C14	-3.77	102.25	112.16
6	A	603	HAS	C13-C12-C11	-3.72	108.44	114.39
6	A	603	HAS	C3A-C4A-NA	3.68	116.44	109.64
6	A	603	HAS	C17-C18-C19	-3.62	119.34	127.62
6	A	603	HAS	CHD-C4A-C3A	-3.59	118.01	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	CHA-C1A-C2A	-3.57	119.22	124.86
6	A	603	HAS	C4B-C3B-C2B	-3.52	101.51	107.44
5	A	602	HEM	C4B-C3B-C2B	-3.46	104.10	107.28
6	A	603	HAS	CMC-C2C-C1C	3.44	130.66	125.42
6	A	603	HAS	C2C-C1C-NC	3.33	115.48	110.14
6	A	603	HAS	CBA-CAA-C2A	3.32	121.71	112.53
5	A	602	HEM	C1A-CHA-C4D	-3.28	118.53	126.25
6	A	603	HAS	C12-C11-C3B	-3.14	107.22	112.12
6	A	603	HAS	C16-C15-C14	-3.13	114.14	121.17
5	A	602	HEM	C1B-NB-C4B	3.11	108.89	105.21
6	A	603	HAS	CBD-CAD-C3D	-3.00	104.25	112.53
6	A	603	HAS	O1A-CGA-CBA	-2.96	113.72	123.09
5	A	602	HEM	CHA-C4D-C3D	-2.83	120.01	125.23
5	A	602	HEM	CHD-C4C-NC	2.67	127.36	124.45
6	A	603	HAS	C4C-C3C-C2C	-2.63	104.03	107.30
6	A	603	HAS	C25-C23-C24	2.62	119.77	115.23
5	A	602	HEM	CHA-C1A-NA	2.54	128.47	123.86
5	A	602	HEM	O2A-CGA-CBA	2.50	121.89	114.00
5	A	602	HEM	C1C-CHC-C4B	-2.49	120.72	126.02
6	A	603	HAS	CHC-C4B-NB	-2.48	121.30	124.37
6	A	603	HAS	C32-C30-C31	2.46	120.25	114.59
6	A	603	HAS	CHB-C1B-C2B	-2.39	121.25	125.03
5	A	602	HEM	O2D-CGD-CBD	2.39	121.54	114.00
5	A	602	HEM	CHA-C4D-ND	2.36	127.28	124.37
5	A	602	HEM	C4A-C3A-C2A	2.33	109.48	106.82
5	A	602	HEM	CHC-C1C-NC	2.32	126.98	124.45
6	A	603	HAS	O2D-CGD-CBD	2.28	121.20	114.00
6	A	603	HAS	O2A-CGA-CBA	2.28	121.20	114.00
6	A	603	HAS	C32-C30-C29	-2.27	115.83	122.66
5	A	602	HEM	CHB-C1B-NB	2.27	127.17	124.37
6	A	603	HAS	CAD-CBD-CGD	-2.26	107.67	113.67
6	A	603	HAS	CHB-C1B-NB	-2.24	122.01	124.42
5	A	602	HEM	CHD-C1D-ND	2.23	126.82	124.42
5	A	602	HEM	C3D-C4D-ND	2.23	112.61	110.17
5	A	602	HEM	C4C-NC-C1C	2.20	109.41	105.82
5	A	602	HEM	CHC-C4B-C3B	-2.17	120.73	125.07
5	A	602	HEM	C2B-C1B-NB	-2.14	107.38	109.84
6	A	603	HAS	O11-C11-C3B	2.10	115.10	111.26
7	A	611	OLC	C13-C12-C11	-2.09	102.05	115.07
6	A	603	HAS	C4A-C3A-C2A	-2.08	103.89	106.97
6	A	603	HAS	CAA-C2A-C1A	2.05	129.02	124.85
6	A	603	HAS	C1A-CHA-C4D	-2.03	121.70	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	CHC-C1C-C2C	-2.00	121.61	127.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	603	HAS	NA

All (129) 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
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
6	A	603	HAS	C23-C24-C28-C29
7	A	608	OLC	O20-C21-C22-C24
7	B	202	OLC	O20-C21-C22-C24
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	612	OLC	C1-C2-C3-C4
7	A	604	OLC	O23-C22-C24-O25
7	A	611	OLC	C1-C2-C3-C4
7	B	203	OLC	C1-C2-C3-C4
7	A	616	OLC	C1-C2-C3-C4
7	A	609	OLC	O20-C21-C22-O23
7	B	202	OLC	O20-C21-C22-O23
7	A	607	OLC	C1-C2-C3-C4
7	A	609	OLC	O20-C21-C22-C24
7	A	605	OLC	C21-C22-C24-O25
7	C	101	OLC	C21-C22-C24-O25
7	A	608	OLC	C5-C6-C7-C8
7	A	611	OLC	C4-C5-C6-C7
7	A	604	OLC	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
7	A	610	OLC	C5-C6-C7-C8
7	A	608	OLC	O23-C22-C24-O25
7	B	203	OLC	O23-C22-C24-O25
7	B	202	OLC	C11-C12-C13-C14
7	B	202	OLC	C1-C2-C3-C4
7	A	612	OLC	C11-C12-C13-C14
7	C	101	OLC	C5-C6-C7-C8
7	B	202	OLC	C14-C15-C16-C17
7	B	203	OLC	C13-C14-C15-C16
7	C	101	OLC	C4-C5-C6-C7
7	A	613	OLC	C12-C13-C14-C15
7	A	604	OLC	O20-C21-C22-C24
7	A	609	OLC	C4-C5-C6-C7
7	A	616	OLC	C2-C3-C4-C5
7	A	606	OLC	C1-C2-C3-C4
7	A	608	OLC	C1-C2-C3-C4
7	A	607	OLC	C3-C4-C5-C6
7	B	202	OLC	C13-C14-C15-C16
7	A	611	OLC	C6-C7-C8-C9
7	A	612	OLC	C10-C11-C12-C13
7	B	202	OLC	C3-C4-C5-C6
7	B	202	OLC	C6-C7-C8-C9
7	A	612	OLC	C2-C3-C4-C5
7	A	605	OLC	C3-C4-C5-C6
7	A	614	OLC	C12-C13-C14-C15
7	B	203	OLC	C12-C13-C14-C15
7	A	612	OLC	C12-C13-C14-C15
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	608	OLC	C4-C5-C6-C7
7	A	610	OLC	C3-C4-C5-C6
7	A	608	OLC	C3-C4-C5-C6
7	A	606	OLC	C3-C4-C5-C6
7	A	613	OLC	C14-C15-C16-C17
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	605	OLC	C5-C6-C7-C8
7	A	613	OLC	C11-C12-C13-C14
7	A	611	OLC	C3-C4-C5-C6
7	A	605	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
7	A	606	OLC	C6-C7-C8-C9
6	A	603	HAS	C3B-C11-C12-C13
7	B	203	OLC	C2-C3-C4-C5
7	A	610	OLC	C1-C2-C3-C4
7	A	611	OLC	O23-C22-C24-O25
7	C	101	OLC	O23-C22-C24-O25
7	A	613	OLC	C10-C11-C12-C13
7	A	613	OLC	C15-C16-C17-C18
7	A	609	OLC	C5-C6-C7-C8
7	A	610	OLC	C2-C3-C4-C5
7	C	101	OLC	C12-C13-C14-C15
7	A	612	OLC	C14-C15-C16-C17
7	A	614	OLC	C15-C16-C17-C18
7	A	604	OLC	C10-C11-C12-C13
7	C	101	OLC	C11-C12-C13-C14
7	A	607	OLC	O20-C21-C22-C24
7	A	614	OLC	C10-C11-C12-C13
7	A	610	OLC	O23-C22-C24-O25
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	C9-C10-C11-C12
7	C	101	OLC	C10-C11-C12-C13
7	A	605	OLC	C1-C2-C3-C4
7	A	605	OLC	O23-C22-C24-O25
7	A	604	OLC	C7-C8-C9-C10
7	C	101	OLC	C9-C10-C11-C12
7	A	612	OLC	C13-C14-C15-C16
7	A	606	OLC	O20-C21-C22-O23
7	A	606	OLC	C5-C6-C7-C8
7	C	101	OLC	C2-C3-C4-C5
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-O1D
7	A	604	OLC	C6-C7-C8-C9
6	A	603	HAS	CAD-CBD-CGD-O2D
7	B	203	OLC	C3-C4-C5-C6
7	A	611	OLC	C7-C8-C9-C10
7	A	612	OLC	C7-C8-C9-C10
7	B	202	OLC	C5-C6-C7-C8

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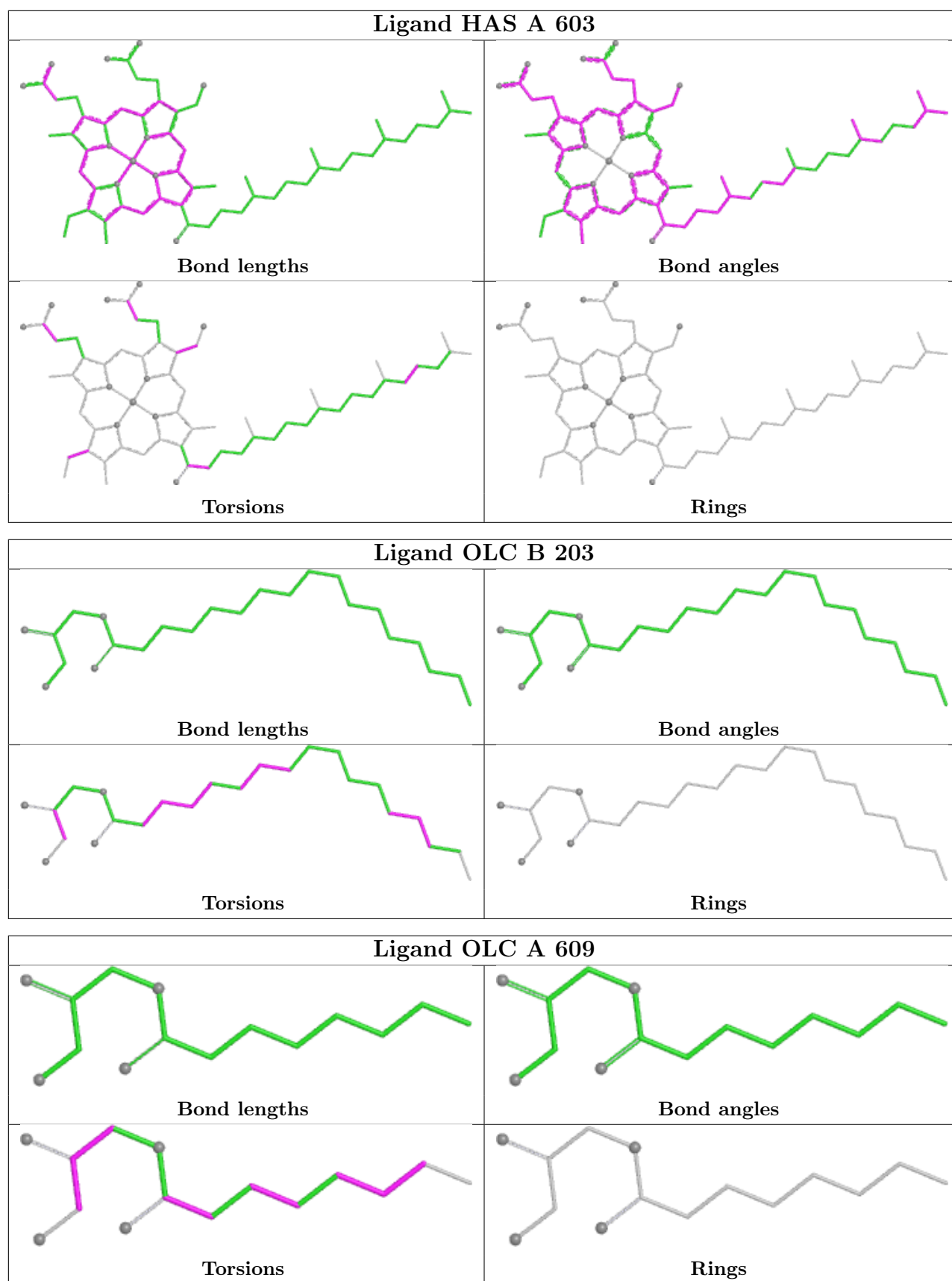
Mol	Chain	Res	Type	Atoms
6	A	603	HAS	C2C-C3C-CAC-CBC
7	A	604	OLC	C9-C10-C11-C12
7	A	605	OLC	O20-C1-C2-C3
7	A	609	OLC	C21-C22-C24-O25
7	A	606	OLC	O20-C1-C2-C3
7	A	609	OLC	C2-C3-C4-C5
7	A	606	OLC	O19-C1-C2-C3
7	B	203	OLC	C5-C6-C7-C8
5	A	602	HEM	CAA-CBA-CGA-O2A
7	A	612	OLC	O20-C1-C2-C3
5	A	602	HEM	C2B-C3B-CAB-CBB
7	A	605	OLC	O19-C1-C2-C3
7	A	609	OLC	O20-C1-C2-C3

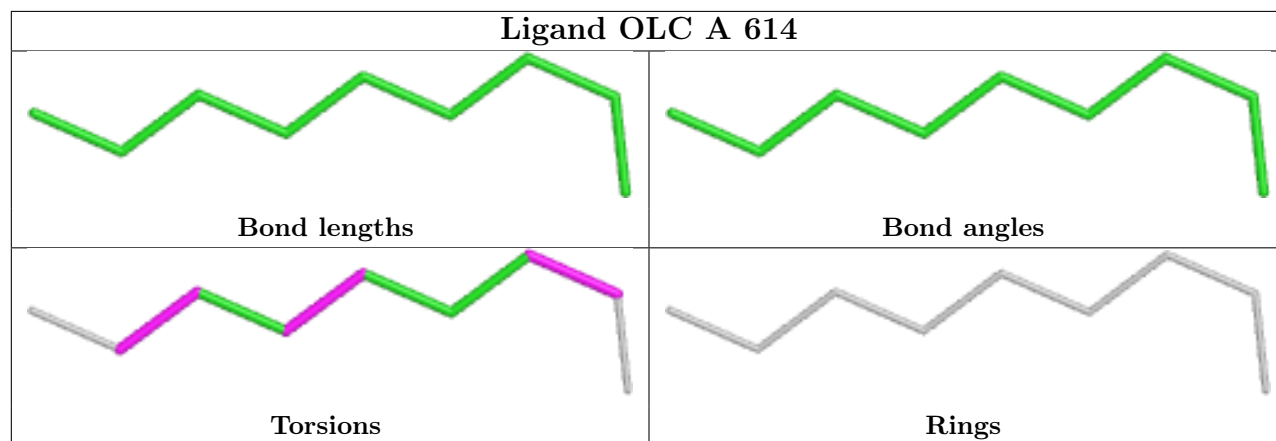
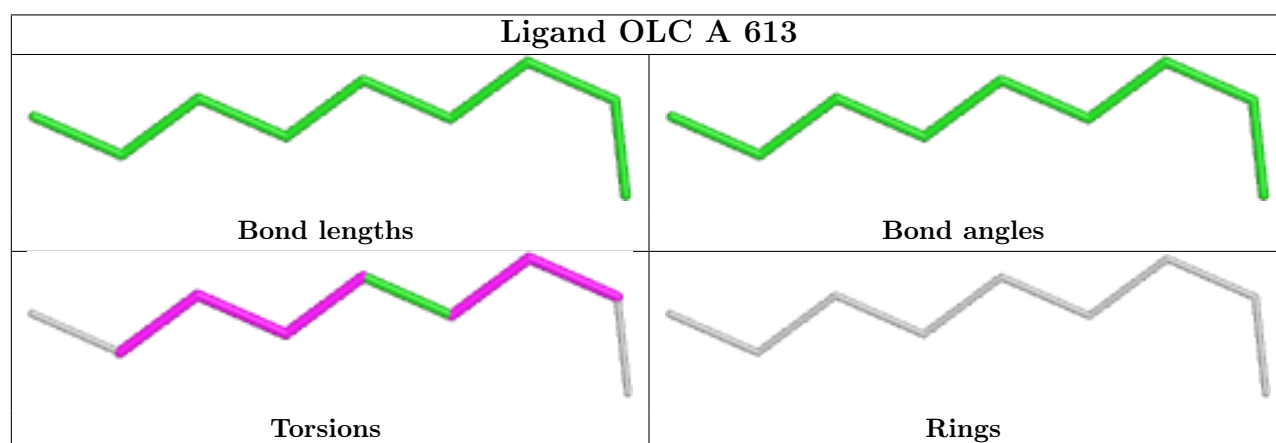
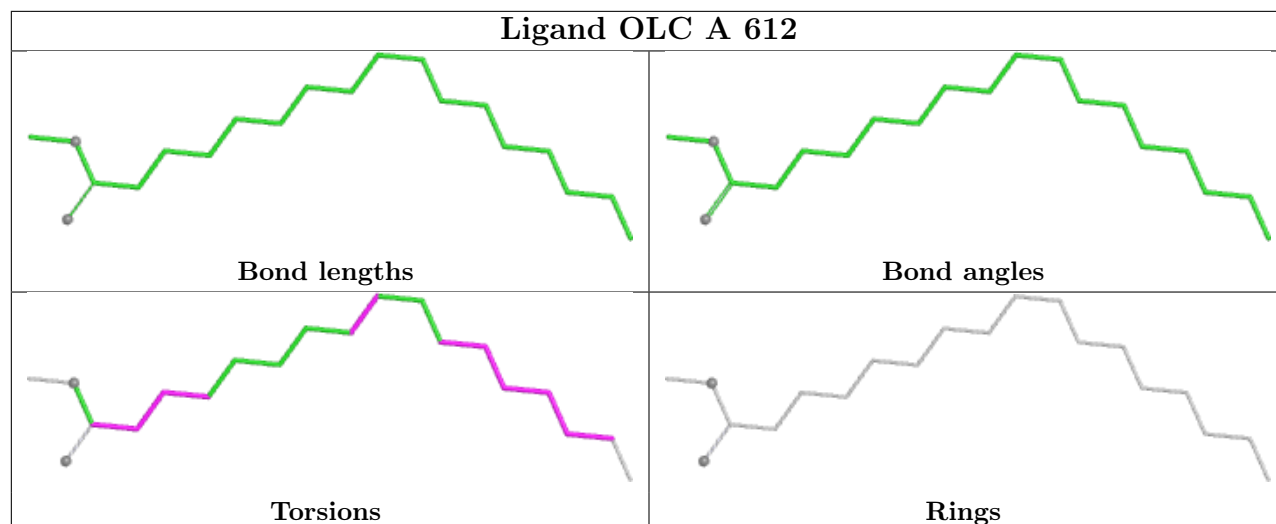
There are no ring outliers.

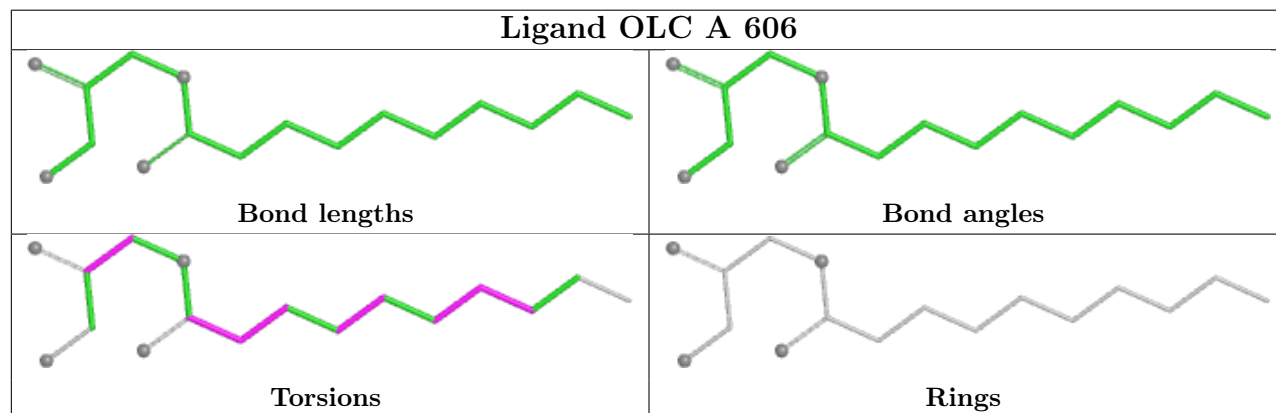
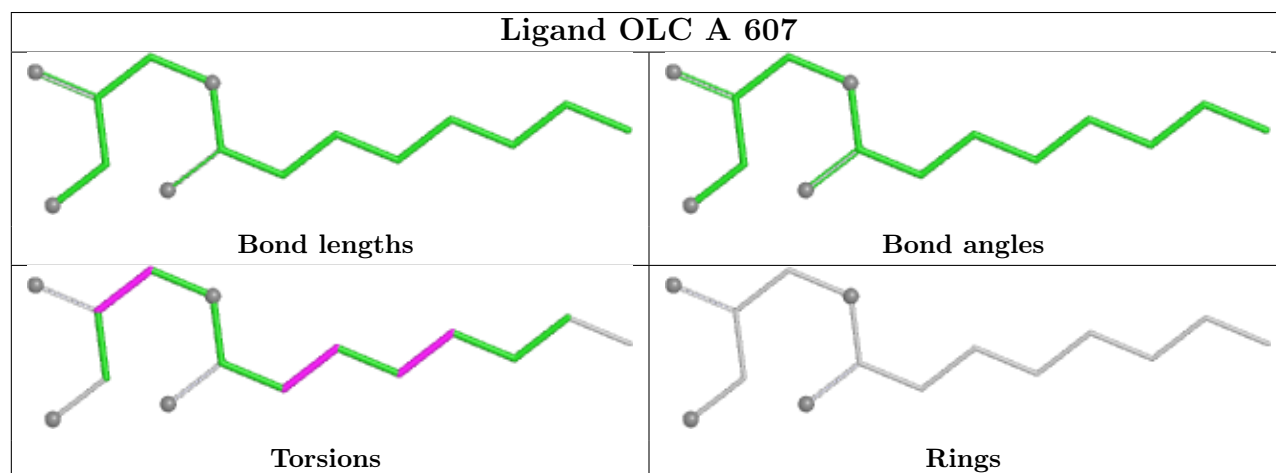
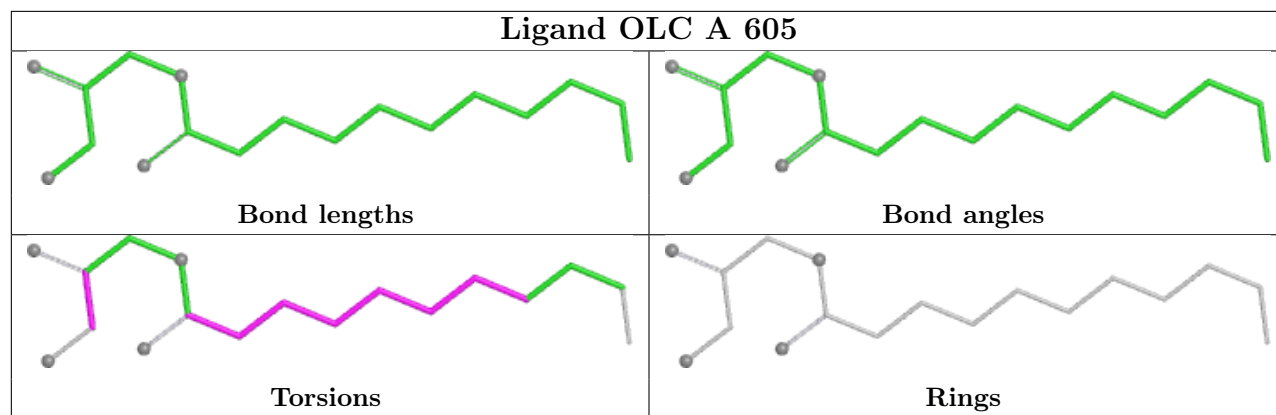
11 monomers are involved in 26 short contacts:

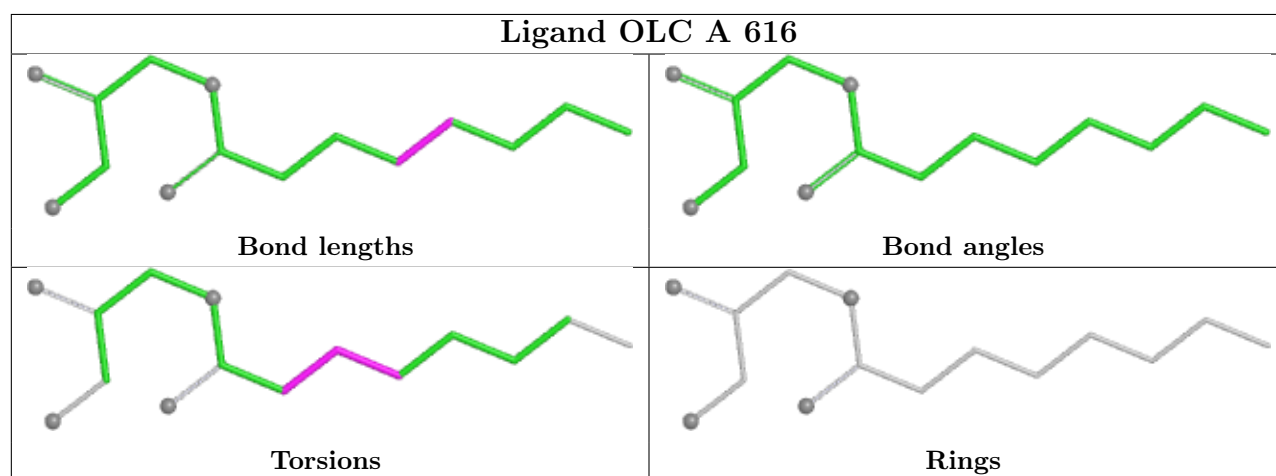
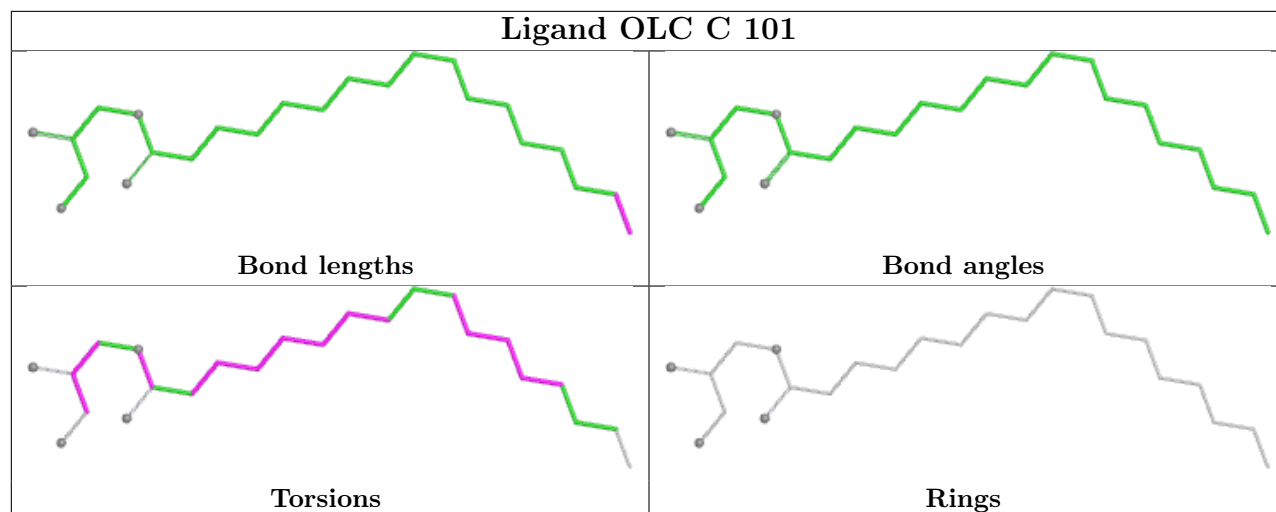
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	HAS	11	0
7	B	203	OLC	3	0
7	A	612	OLC	1	0
7	A	605	OLC	1	0
7	A	606	OLC	1	0
8	A	615	CMO	1	0
7	C	101	OLC	2	0
7	A	616	OLC	2	0
5	A	602	HEM	3	0
7	A	604	OLC	1	0
7	A	610	OLC	2	0

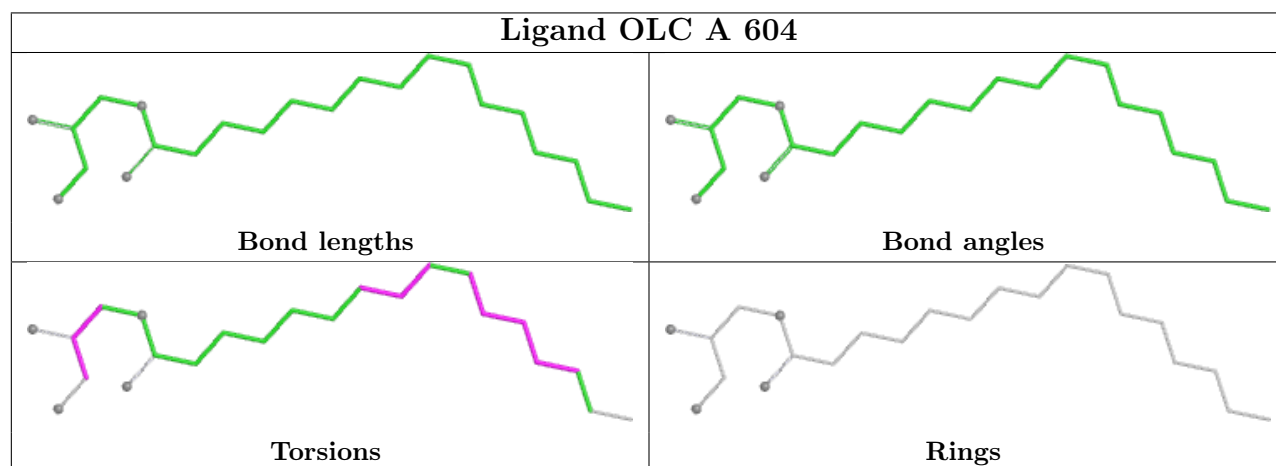
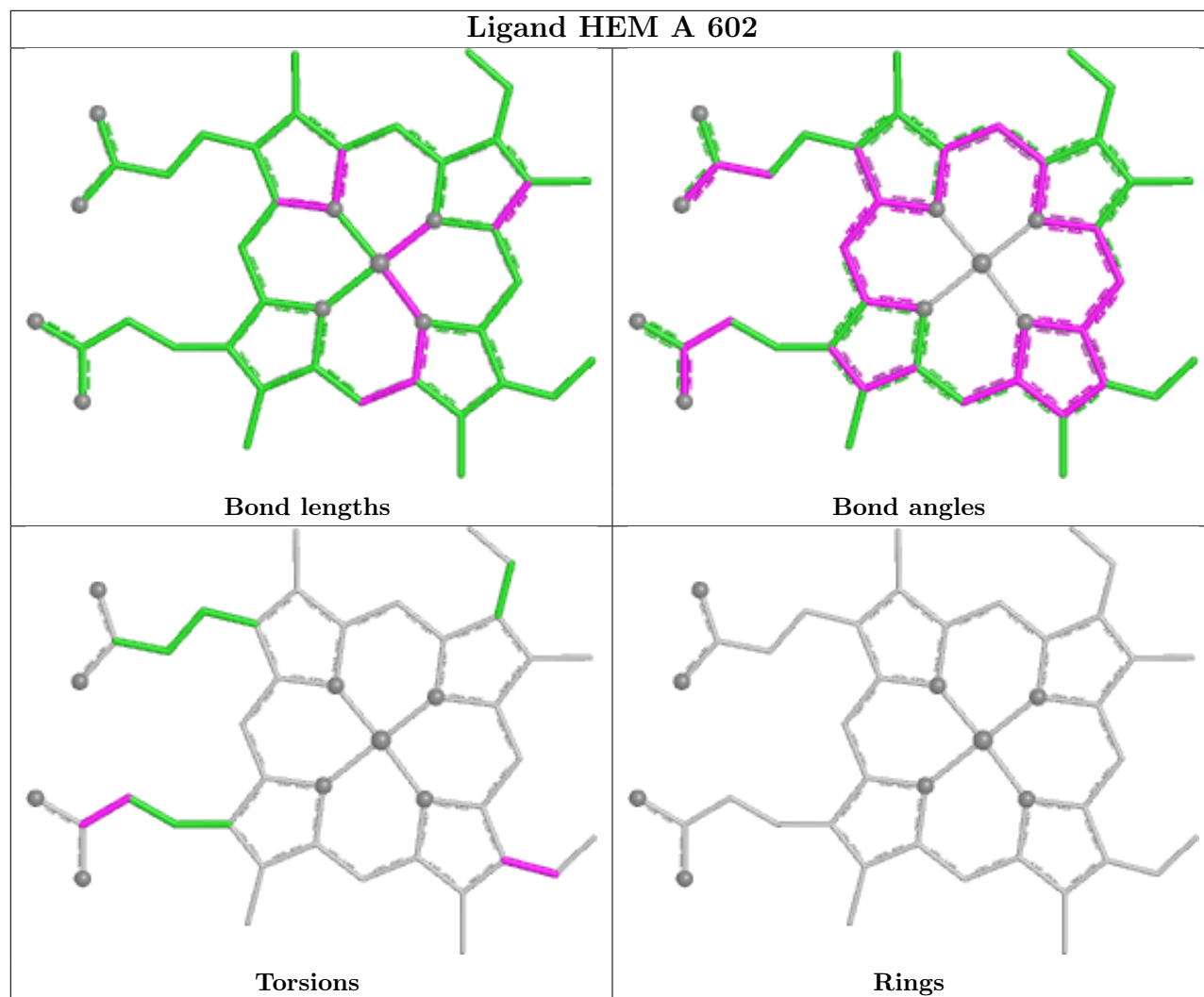
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

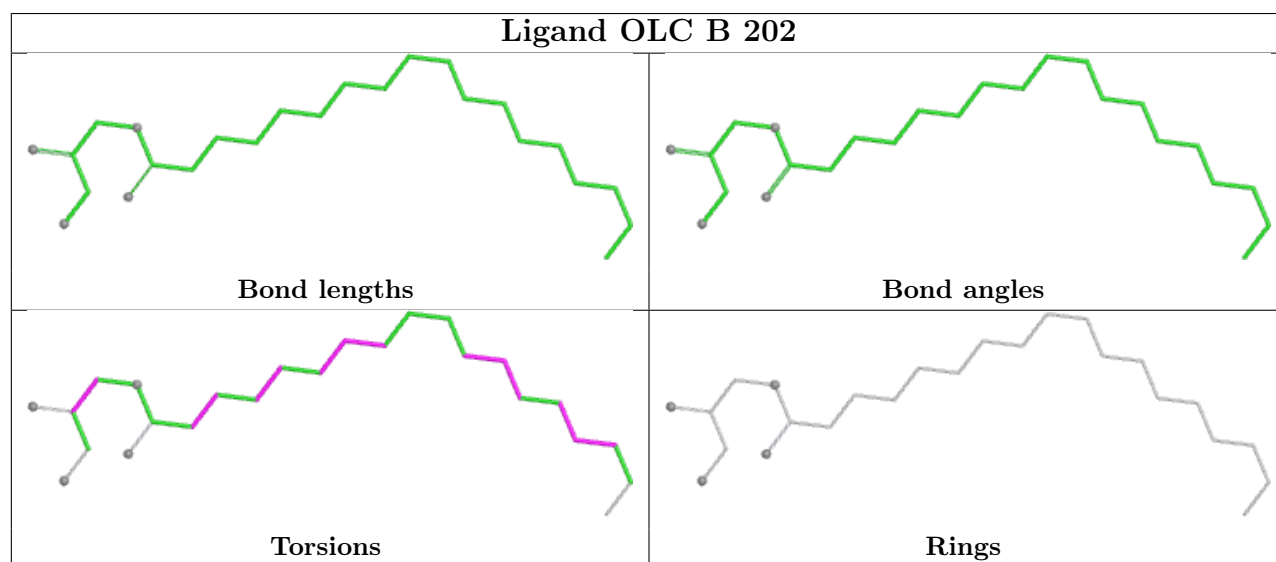
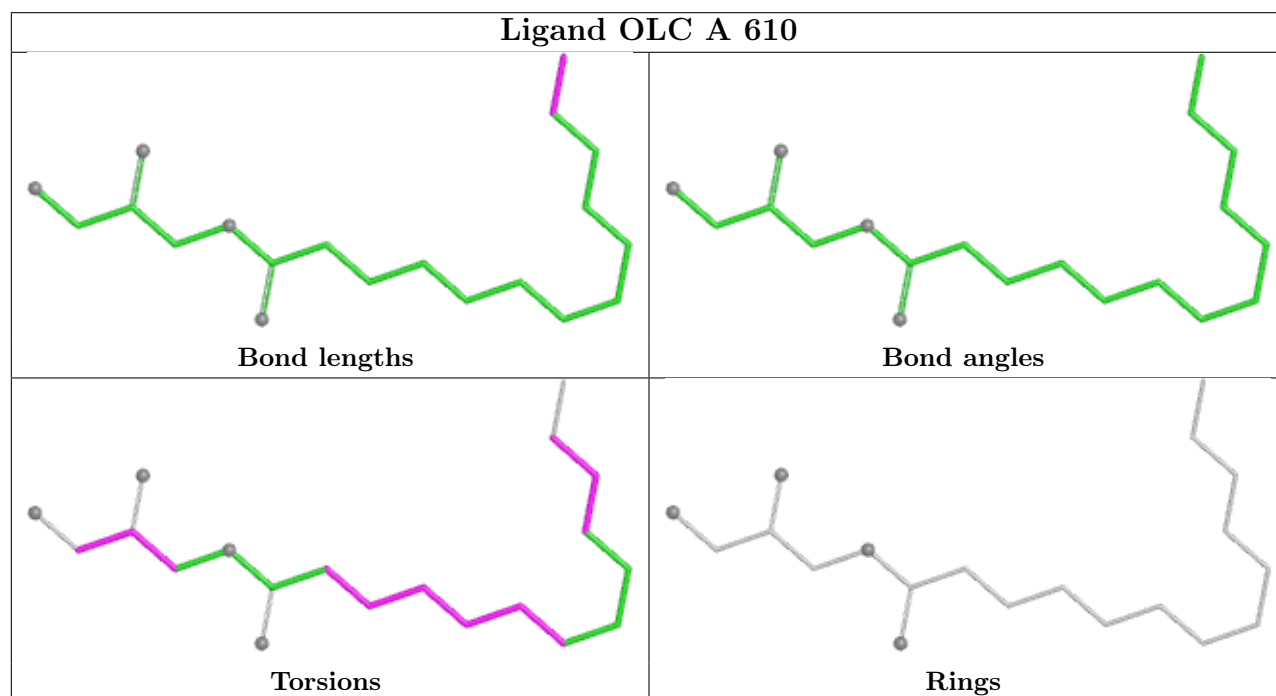
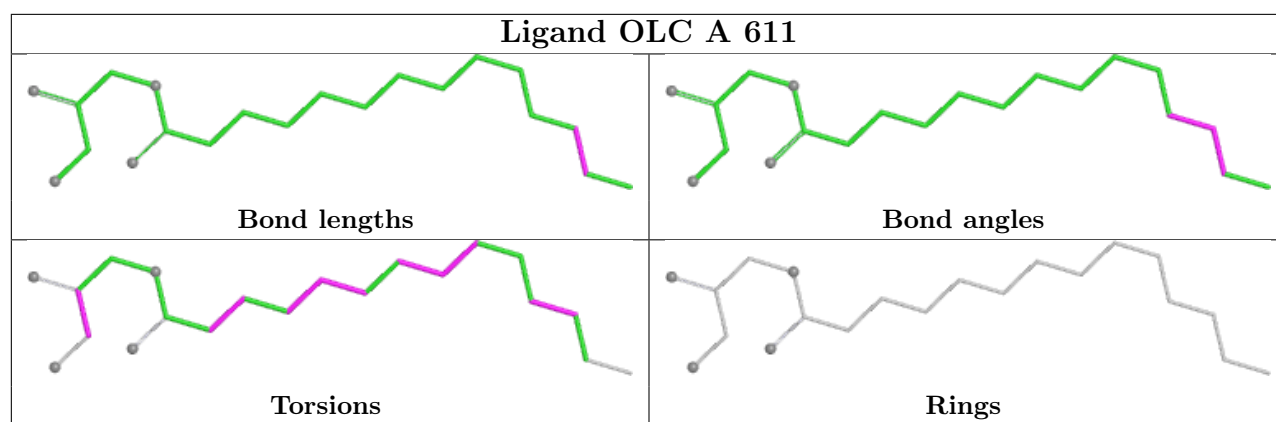


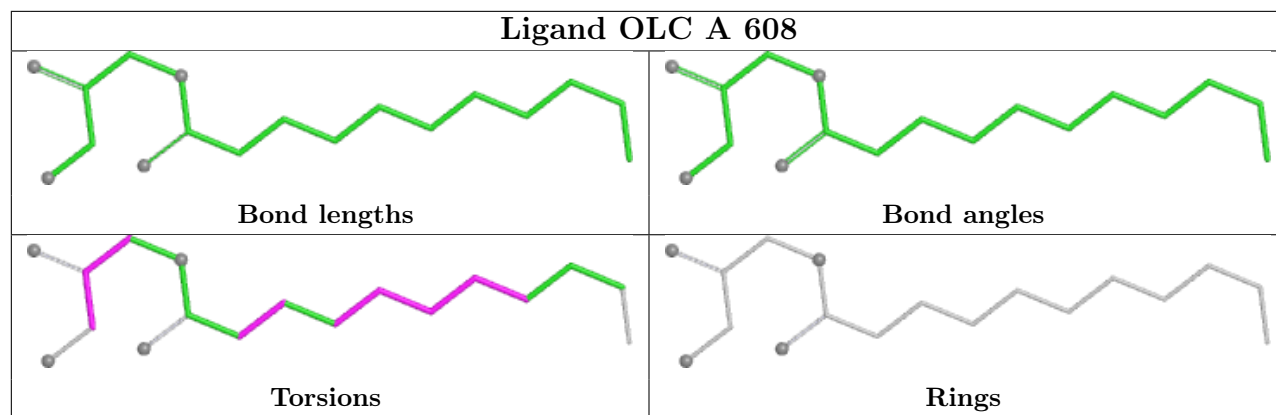












5.7 Other polymers [i](#)

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%)	3.64	473 (85%) 0 0	21, 32, 59, 91	0
2	B	167/168 (99%)	3.46	141 (84%) 0 0	22, 32, 57, 104	0
3	C	31/34 (91%)	3.52	30 (96%) 0 0	27, 34, 42, 66	0
All	All	752/771 (97%)	3.60	644 (85%) 0 0	21, 32, 59, 104	0

All (644) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	VAL	11.9
1	A	58	LEU	11.4
1	A	322	PHE	10.1
1	A	491	VAL	10.0
1	A	494	SER	9.7
1	A	11	VAL	9.3
1	A	498	LYS	8.9
1	A	520	LEU	8.6
1	A	54	LEU	8.2
2	B	3	ASP	8.2
2	B	141	ARG	8.2
1	A	326	LEU	8.2
1	A	499	PRO	8.1
1	A	504	ALA	8.1
1	A	497	ARG	8.1
1	A	332	LEU	8.0
1	A	519	ARG	7.9
1	A	176	GLY	7.9
1	A	495	ARG	7.9
2	B	140	LYS	7.9
1	A	493	LEU	7.7
1	A	527	ILE	7.7
1	A	337	ARG	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	333	PHE	7.6
1	A	107	TRP	7.6
1	A	518	ARG	7.5
1	A	175	PRO	7.5
1	A	496	GLU	7.3
1	A	219	VAL	7.3
2	B	49	LYS	7.2
1	A	513	SER	7.2
1	A	489	PHE	7.2
2	B	168	GLU	7.1
1	A	512	ILE	7.1
2	B	5	HIS	7.1
1	A	9	SER	7.1
1	A	405	LEU	7.1
1	A	515	PRO	7.0
2	B	76	PRO	7.0
1	A	536	ILE	7.0
1	A	102	ASN	6.9
1	A	12	TYR	6.8
1	A	492	LEU	6.8
1	A	174	ASN	6.8
2	B	39	THR	6.7
1	A	168	ARG	6.7
1	A	413	ILE	6.7
1	A	521	VAL	6.7
2	B	6	LYS	6.7
1	A	548	GLN	6.6
1	A	324	GLY	6.5
1	A	178	VAL	6.5
1	A	514	GLY	6.5
1	A	547	VAL	6.4
1	A	97	LEU	6.2
2	B	12	LEU	6.2
1	A	167	TRP	6.1
1	A	522	LEU	6.1
2	B	71	VAL	6.0
2	B	14	TYR	6.0
1	A	57	ARG	6.0
1	A	14	ALA	6.0
1	A	105	LEU	6.0
3	C	9	LEU	6.0
1	A	516	GLU	6.0

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Mol	Chain	Res	Type	RSRZ
2	B	48	GLY	6.0
1	A	338	ALA	5.9
1	A	455	GLN	5.9
1	A	56	LYS	5.9
1	A	230	TRP	5.9
1	A	488	LEU	5.9
1	A	336	ILE	5.9
1	A	530	TRP	5.8
1	A	553	LEU	5.8
1	A	173	ALA	5.8
1	A	172	ALA	5.8
1	A	216	VAL	5.7
1	A	169	ARG	5.7
1	A	44	LEU	5.7
1	A	412	PRO	5.7
1	A	465	VAL	5.6
1	A	538	VAL	5.6
1	A	506	LEU	5.6
1	A	60	PRO	5.6
1	A	25	LEU	5.6
1	A	182	VAL	5.6
2	B	58	VAL	5.6
1	A	331	GLY	5.5
3	C	5	PRO	5.5
1	A	320	LEU	5.5
1	A	256	GLY	5.5
1	A	486	TYR	5.5
1	A	260	VAL	5.5
1	A	490	SER	5.4
1	A	161	TYR	5.4
1	A	10	ARG	5.4
1	A	502	ALA	5.4
1	A	164	LEU	5.4
1	A	482	LEU	5.4
2	B	11	ILE	5.3
1	A	205	VAL	5.3
3	C	4	LYS	5.3
3	C	6	LYS	5.3
1	A	207	PHE	5.3
1	A	294	TRP	5.3
1	A	500	GLU	5.3
1	A	115	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
2	B	23	LEU	5.3
2	B	75	GLY	5.3
1	A	19	LYS	5.2
1	A	542	TYR	5.2
1	A	180	PRO	5.2
1	A	255	ALA	5.2
1	A	517	ASP	5.2
1	A	508	PHE	5.2
1	A	420	LEU	5.2
1	A	545	THR	5.2
1	A	402	TYR	5.1
2	B	167	LYS	5.1
1	A	13	GLU	5.1
1	A	16	PRO	5.1
1	A	330	ARG	5.1
2	B	79	TYR	5.1
1	A	198	LEU	5.1
2	B	7	ALA	5.0
1	A	206	LEU	5.0
1	A	170	TRP	5.0
1	A	55	LEU	5.0
1	A	510	GLU	5.0
1	A	15	TYR	5.0
1	A	159	SER	4.9
1	A	552	HIS	4.9
1	A	328	GLY	4.9
1	A	549	LEU	4.9
2	B	144	GLU	4.9
1	A	98	ASN	4.9
2	B	61	GLU	4.8
1	A	325	ARG	4.8
1	A	213	PHE	4.8
1	A	23	TYR	4.8
1	A	184	TYR	4.8
1	A	171	LYS	4.8
2	B	101	ALA	4.8
2	B	56	THR	4.8
1	A	501	LEU	4.7
1	A	290	ILE	4.7
1	A	263	PRO	4.7
1	A	523	ALA	4.7
1	A	417	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	20	ALA	4.7
1	A	254	GLN	4.7
1	A	289	GLY	4.7
1	A	505	PRO	4.7
2	B	63	PRO	4.7
3	C	34	GLY	4.7
1	A	503	GLU	4.7
3	C	21	VAL	4.7
2	B	77	ASN	4.7
1	A	124	LEU	4.7
1	A	543	GLY	4.7
1	A	194	PHE	4.6
2	B	50	LEU	4.6
1	A	403	TRP	4.6
3	C	13	LEU	4.6
2	B	136	ARG	4.6
1	A	529	PHE	4.6
2	B	60	GLN	4.6
1	A	111	TRP	4.6
1	A	187	VAL	4.6
1	A	201	VAL	4.6
2	B	132	VAL	4.6
1	A	301	LEU	4.6
2	B	103	ILE	4.6
2	B	29	PHE	4.6
2	B	72	VAL	4.5
1	A	335	TRP	4.5
1	A	61	PHE	4.5
2	B	105	PHE	4.5
1	A	410	GLY	4.5
1	A	27	LEU	4.5
1	A	59	LEU	4.5
1	A	122	LEU	4.5
1	A	537	LEU	4.5
1	A	401	LEU	4.5
1	A	481	LEU	4.5
1	A	540	LEU	4.5
1	A	341	TRP	4.5
1	A	428	TRP	4.4
1	A	304	PHE	4.4
1	A	531	PHE	4.4
1	A	392	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	139	PHE	4.4
2	B	8	HIS	4.4
2	B	37	LEU	4.4
2	B	73	GLN	4.4
1	A	297	ILE	4.4
1	A	551	GLY	4.4
1	A	526	ARG	4.4
1	A	200	LEU	4.4
1	A	462	HIS	4.3
2	B	59	ARG	4.3
1	A	356	PHE	4.3
1	A	177	LYS	4.3
1	A	483	LEU	4.3
1	A	49	VAL	4.3
1	A	202	LEU	4.2
2	B	40	HIS	4.2
1	A	485	ILE	4.2
1	A	509	ALA	4.2
1	A	550	PHE	4.2
2	B	104	VAL	4.2
2	B	10	ALA	4.2
2	B	20	ALA	4.2
1	A	346	PHE	4.2
2	B	135	VAL	4.2
1	A	458	ASP	4.2
2	B	35	TYR	4.2
1	A	423	ALA	4.2
1	A	314	PHE	4.2
1	A	62	VAL	4.2
2	B	100	GLY	4.1
1	A	426	TRP	4.1
1	A	475	ILE	4.1
1	A	556	VAL	4.1
2	B	30	ILE	4.1
1	A	232	GLY	4.1
2	B	22	SER	4.1
2	B	15	GLU	4.1
1	A	37	LEU	4.1
1	A	411	LYS	4.1
1	A	472	LEU	4.0
1	A	415	ASP	4.0
1	A	456	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	539	VAL	4.0
1	A	21	THR	4.0
1	A	534	ALA	4.0
2	B	68	ALA	4.0
3	C	10	ALA	4.0
2	B	69	GLN	4.0
1	A	276	SER	4.0
1	A	342	ASP	4.0
1	A	419	ARG	4.0
2	B	4	GLU	4.0
1	A	181	LEU	3.9
1	A	253	LYS	3.9
1	A	106	MET	3.9
1	A	528	GLY	3.9
2	B	70	ALA	3.9
3	C	17	LEU	3.9
1	A	190	TRP	3.9
1	A	393	VAL	3.9
1	A	257	GLY	3.9
1	A	404	LEU	3.9
1	A	408	LEU	3.9
1	A	292	PRO	3.9
1	A	358	PRO	3.9
1	A	546	LEU	3.8
2	B	118	VAL	3.8
3	C	11	VAL	3.8
1	A	24	PHE	3.8
1	A	329	GLY	3.8
1	A	125	LEU	3.8
1	A	249	THR	3.8
1	A	444	LEU	3.8
1	A	188	VAL	3.8
1	A	22	LEU	3.8
1	A	117	LEU	3.8
1	A	466	PRO	3.8
1	A	269	PHE	3.8
2	B	57	THR	3.7
2	B	127	VAL	3.7
2	B	21	PHE	3.7
1	A	110	TRP	3.7
1	A	248	TYR	3.7
1	A	532	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	42	ALA	3.7
3	C	28	ALA	3.7
1	A	293	THR	3.7
1	A	92	LEU	3.7
1	A	422	LEU	3.7
1	A	140	LYS	3.7
1	A	382	PRO	3.7
2	B	142	PRO	3.7
1	A	90	VAL	3.7
1	A	437	VAL	3.7
1	A	511	VAL	3.7
1	A	414	SER	3.7
1	A	211	TRP	3.7
1	A	108	LEU	3.7
1	A	561	LEU	3.7
2	B	99	GLN	3.7
3	C	15	LEU	3.7
1	A	101	PRO	3.7
2	B	92	PRO	3.7
1	A	334	GLY	3.7
1	A	407	ASN	3.7
1	A	307	VAL	3.7
1	A	400	SER	3.7
1	A	418	ARG	3.7
1	A	191	LEU	3.6
1	A	215	LEU	3.6
1	A	371	LEU	3.6
1	A	349	PRO	3.6
1	A	34	VAL	3.6
1	A	425	VAL	3.6
1	A	429	PHE	3.6
2	B	86	PHE	3.6
1	A	453	ILE	3.6
1	A	17	GLU	3.6
1	A	316	VAL	3.6
2	B	74	THR	3.6
1	A	274	LEU	3.6
1	A	95	ARG	3.6
2	B	28	VAL	3.6
1	A	162	ILE	3.6
2	B	27	PHE	3.6
1	A	463	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	308	PRO	3.6
2	B	84	LEU	3.6
2	B	53	VAL	3.5
1	A	41	PHE	3.5
1	A	152	PHE	3.5
1	A	484	PHE	3.5
1	A	390	ALA	3.5
1	A	535	ALA	3.5
2	B	52	ARG	3.5
1	A	241	LEU	3.5
1	A	259	LEU	3.5
1	A	339	LEU	3.5
1	A	47	GLY	3.5
1	A	212	SER	3.5
3	C	27	TYR	3.5
1	A	305	VAL	3.5
1	A	78	ILE	3.5
1	A	38	PHE	3.5
2	B	116	PHE	3.5
1	A	144	ALA	3.5
2	B	62	GLY	3.5
2	B	64	TRP	3.5
1	A	473	ALA	3.5
1	A	199	GLY	3.5
1	A	220	ASP	3.5
1	A	153	VAL	3.5
2	B	33	ILE	3.4
3	C	8	ALA	3.4
1	A	100	ARG	3.4
2	B	81	VAL	3.4
1	A	234	PRO	3.4
2	B	45	ILE	3.4
1	A	487	GLY	3.4
2	B	17	GLY	3.4
3	C	23	TRP	3.4
3	C	31	PHE	3.4
1	A	69	LEU	3.4
1	A	374	VAL	3.4
1	A	360	GLY	3.4
1	A	416	ALA	3.4
1	A	132	LEU	3.4
1	A	469	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	19	LEU	3.4
3	C	20	LEU	3.4
1	A	223	VAL	3.4
1	A	533	VAL	3.4
1	A	218	GLY	3.4
2	B	143	GLY	3.4
1	A	33	ILE	3.4
1	A	51	ALA	3.4
1	A	120	ALA	3.4
2	B	65	ALA	3.4
2	B	107	ILE	3.4
1	A	239	TRP	3.3
1	A	217	GLU	3.3
2	B	44	VAL	3.3
2	B	98	PRO	3.3
1	A	313	ALA	3.3
1	A	166	LEU	3.3
1	A	26	VAL	3.3
2	B	87	ALA	3.3
1	A	353	LEU	3.3
3	C	24	LEU	3.3
1	A	189	PHE	3.3
1	A	66	TYR	3.3
1	A	452	TYR	3.3
3	C	29	VAL	3.3
1	A	32	LEU	3.3
1	A	559	TRP	3.2
1	A	91	TYR	3.2
2	B	95	ILE	3.2
1	A	351	LEU	3.2
1	A	478	LEU	3.2
1	A	370	THR	3.2
1	A	396	THR	3.2
2	B	154	GLY	3.2
1	A	143	TRP	3.2
1	A	441	TRP	3.2
1	A	118	VAL	3.2
1	A	151	VAL	3.2
1	A	264	MET	3.2
3	C	32	ALA	3.2
1	A	99	MET	3.2
1	A	193	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	38	ALA	3.2
1	A	147	LEU	3.2
1	A	29	PHE	3.2
2	B	161	PHE	3.2
2	B	138	THR	3.2
1	A	157	TRP	3.1
1	A	85	ALA	3.1
1	A	158	VAL	3.1
1	A	154	LEU	3.1
2	B	145	TYR	3.1
1	A	252	PRO	3.1
1	A	31	ALA	3.1
1	A	94	ALA	3.1
1	A	381	VAL	3.1
1	A	376	HIS	3.1
1	A	258	LYS	3.1
3	C	30	PHE	3.1
2	B	110	PRO	3.1
1	A	142	HIS	3.1
1	A	195	LEU	3.1
2	B	155	LEU	3.1
3	C	12	ILE	3.1
1	A	179	THR	3.1
1	A	127	ASN	3.1
1	A	544	PRO	3.1
1	A	327	ARG	3.1
1	A	323	ALA	3.1
3	C	26	VAL	3.1
1	A	427	LEU	3.1
1	A	348	ALA	3.0
2	B	13	ALA	3.0
1	A	398	MET	3.0
2	B	148	ILE	3.0
2	B	9	LYS	3.0
1	A	204	ALA	3.0
1	A	541	ALA	3.0
1	A	209	LEU	3.0
1	A	375	VAL	3.0
2	B	26	LEU	3.0
3	C	14	VAL	3.0
1	A	130	THR	3.0
1	A	557	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	525	ASP	3.0
1	A	84	PHE	3.0
1	A	311	MET	3.0
1	A	113	ALA	3.0
1	A	261	SER	3.0
1	A	319	SER	3.0
1	A	367	ALA	3.0
1	A	30	LEU	3.0
1	A	445	LEU	3.0
1	A	364	ILE	3.0
2	B	156	GLY	3.0
2	B	41	THR	3.0
1	A	344	PRO	3.0
1	A	460	TYR	3.0
2	B	137	TYR	3.0
1	A	245	ALA	2.9
1	A	222	LEU	2.9
1	A	251	LEU	2.9
2	B	159	ASN	2.9
1	A	468	VAL	2.9
1	A	362	GLY	2.9
1	A	262	ASP	2.9
2	B	121	THR	2.9
1	A	192	MET	2.9
1	A	136	TYR	2.9
1	A	380	TRP	2.9
2	B	102	GLU	2.9
1	A	126	ALA	2.9
1	A	75	LEU	2.9
1	A	354	LEU	2.9
1	A	250	ILE	2.9
1	A	340	PRO	2.9
1	A	448	PRO	2.9
1	A	145	PHE	2.9
1	A	109	SER	2.9
1	A	149	ALA	2.9
1	A	397	ALA	2.9
1	A	227	LEU	2.9
1	A	303	LEU	2.9
2	B	117	HIS	2.9
1	A	163	VAL	2.9
2	B	112	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	93	PRO	2.9
1	A	278	PRO	2.9
2	B	16	LYS	2.9
1	A	345	ALA	2.9
1	A	104	GLY	2.9
1	A	88	ILE	2.8
1	A	288	PRO	2.8
1	A	48	ASN	2.8
1	A	150	SER	2.8
1	A	87	ALA	2.8
1	A	355	GLY	2.8
1	A	524	MET	2.8
2	B	24	ALA	2.8
1	A	208	LEU	2.8
1	A	409	THR	2.8
1	A	471	VAL	2.8
1	A	165	ASP	2.8
1	A	272	PHE	2.8
1	A	421	GLY	2.8
1	A	43	ALA	2.8
1	A	267	LEU	2.8
1	A	183	THR	2.8
1	A	226	THR	2.8
2	B	36	THR	2.8
1	A	406	PRO	2.8
1	A	424	VAL	2.8
2	B	164	ILE	2.8
1	A	366	ASN	2.8
1	A	114	PHE	2.8
1	A	359	GLY	2.8
1	A	121	ALA	2.8
1	A	133	TYR	2.8
2	B	123	ILE	2.8
1	A	45	ASN	2.7
1	A	442	ALA	2.7
1	A	279	VAL	2.7
1	A	350	VAL	2.7
1	A	103	MET	2.7
1	A	112	MET	2.7
1	A	432	MET	2.7
2	B	130	GLY	2.7
1	A	281	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	560	ARG	2.7
1	A	461	PRO	2.7
1	A	119	VAL	2.7
1	A	236	VAL	2.7
1	A	479	VAL	2.7
2	B	166	VAL	2.7
1	A	196	ALA	2.7
1	A	459	ALA	2.7
2	B	47	ALA	2.7
2	B	88	PHE	2.7
3	C	22	PHE	2.7
1	A	271	LEU	2.7
1	A	53	PRO	2.7
1	A	244	TYR	2.7
1	A	347	VAL	2.7
1	A	476	VAL	2.7
1	A	480	ALA	2.6
1	A	275	LEU	2.6
2	B	128	LEU	2.6
2	B	83	VAL	2.6
1	A	185	MET	2.6
1	A	139	LEU	2.6
1	A	228	PHE	2.6
2	B	55	PRO	2.6
1	A	52	TYR	2.6
2	B	82	TYR	2.6
1	A	160	ILE	2.6
1	A	357	ILE	2.6
1	A	141	GLY	2.6
2	B	120	GLY	2.6
2	B	51	GLU	2.6
2	B	131	GLU	2.6
1	A	134	THR	2.6
1	A	477	LEU	2.6
2	B	67	PRO	2.6
1	A	299	SER	2.6
2	B	97	VAL	2.6
1	A	438	GLY	2.6
1	A	70	THR	2.6
2	B	66	ASP	2.6
1	A	273	LEU	2.6
1	A	389	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	25	MET	2.5
3	C	7	GLY	2.5
1	A	50	ASP	2.5
1	A	562	TRP	2.5
1	A	116	GLY	2.5
3	C	16	THR	2.5
1	A	268	ALA	2.5
2	B	94	PRO	2.5
1	A	291	ASP	2.5
1	A	63	GLN	2.5
2	B	78	GLN	2.5
2	B	163	THR	2.5
2	B	32	LEU	2.5
3	C	33	ARG	2.5
1	A	558	GLY	2.5
1	A	229	TRP	2.5
1	A	246	ILE	2.5
1	A	312	THR	2.4
1	A	265	ALA	2.4
2	B	85	ALA	2.4
1	A	430	LEU	2.4
1	A	287	ASP	2.4
2	B	133	SER	2.4
1	A	186	ALA	2.4
2	B	108	THR	2.4
2	B	114	HIS	2.4
1	A	321	GLU	2.4
1	A	280	GLY	2.4
2	B	43	GLY	2.4
1	A	79	VAL	2.4
1	A	231	THR	2.4
1	A	555	PRO	2.4
1	A	224	ALA	2.3
1	A	379	ALA	2.3
1	A	343	ASN	2.3
1	A	387	LEU	2.3
1	A	318	ALA	2.3
2	B	113	ILE	2.3
2	B	46	PRO	2.3
1	A	80	PHE	2.3
1	A	18	LYS	2.3
1	A	214	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	238	PHE	2.2
2	B	147	ILE	2.2
1	A	399	GLY	2.2
1	A	439	LEU	2.2
1	A	65	TYR	2.2
1	A	233	HIS	2.2
1	A	266	ARG	2.2
1	A	300	VAL	2.2
1	A	457	PRO	2.2
2	B	111	ASP	2.2
1	A	277	THR	2.2
1	A	369	PHE	2.2
1	A	507	PRO	2.2
2	B	54	ASP	2.2
1	A	221	PRO	2.1
1	A	242	PRO	2.1
2	B	34	ALA	2.1
1	A	554	ASN	2.1
1	A	123	PRO	2.1
3	C	18	THR	2.1
1	A	450	ARG	2.1
1	A	373	TYR	2.1
2	B	18	TRP	2.1
1	A	454	ALA	2.1
1	A	237	TYR	2.1
1	A	434	ILE	2.1
3	C	19	ILE	2.1
2	B	162	GLY	2.0
1	A	447	VAL	2.0
2	B	119	GLU	2.0
1	A	155	SER	2.0
1	A	197	SER	2.0
1	A	76	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

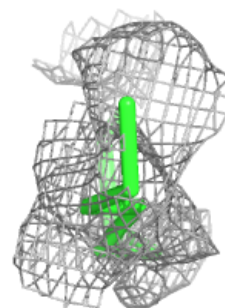
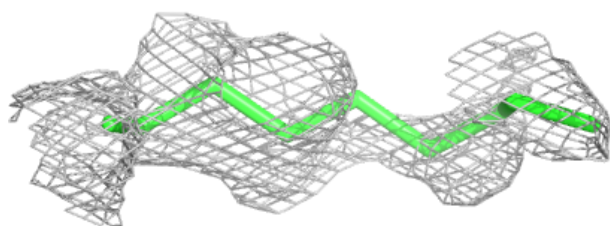
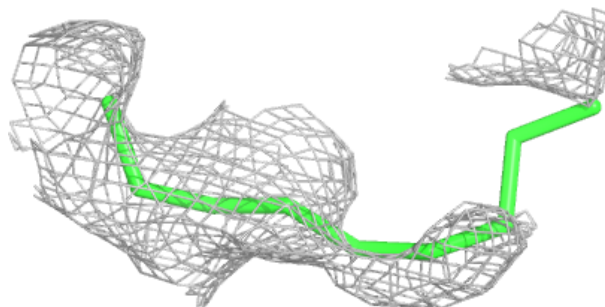
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	OLC	A	614	9/25	0.49	0.41	56,59,75,76	0
7	OLC	A	607	15/25	0.50	0.41	67,84,97,99	0
7	OLC	A	606	17/25	0.51	0.41	70,73,88,91	0
7	OLC	A	612	20/25	0.53	0.44	69,77,86,97	0
7	OLC	A	616	15/25	0.54	0.44	67,74,89,92	0
7	OLC	A	605	18/25	0.55	0.41	61,77,95,102	0
7	OLC	B	202	25/25	0.56	0.38	64,68,86,101	0
7	OLC	B	203	24/25	0.57	0.46	68,80,93,103	0
7	OLC	A	610	20/25	0.58	0.51	70,80,96,100	0
7	OLC	A	613	9/25	0.58	0.47	64,69,74,77	0
7	OLC	C	101	24/25	0.62	0.43	54,66,98,101	0
7	OLC	A	611	21/25	0.63	0.44	56,77,94,105	0
7	OLC	A	609	15/25	0.65	0.51	80,94,101,102	0
7	OLC	A	604	23/25	0.67	0.36	42,60,91,94	0
7	OLC	A	608	18/25	0.71	0.44	62,79,91,92	0
6	HAS	A	603	65/65	0.85	0.17	20,26,44,59	0
5	HEM	A	602	43/43	0.90	0.14	20,23,27,36	0
8	CMO	A	615	2/2	0.96	0.12	20,20,20,26	0
9	CUA	B	201	2/2	0.98	0.04	25,25,25,26	0
4	CU	A	601	1/1	0.99	0.05	29,29,29,29	0

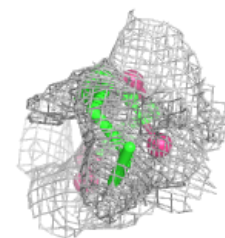
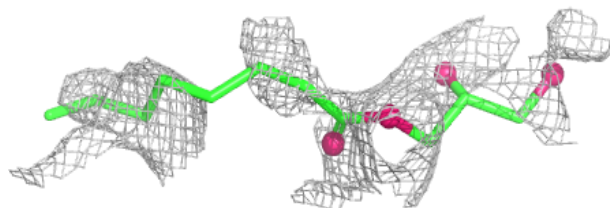
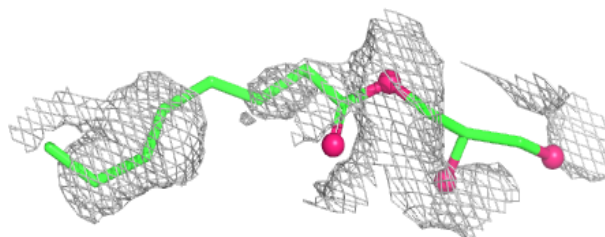
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 614:

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

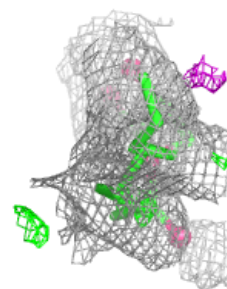
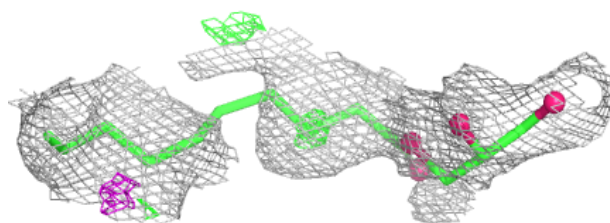
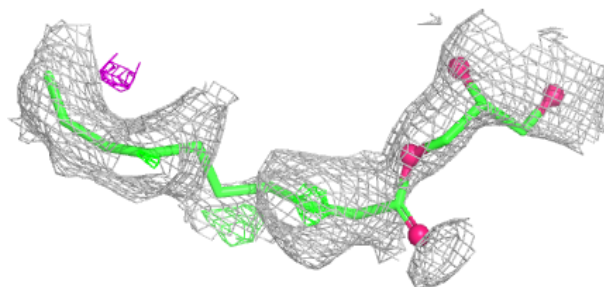
**Electron density around OLC A 607:**

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

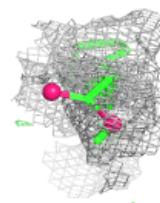
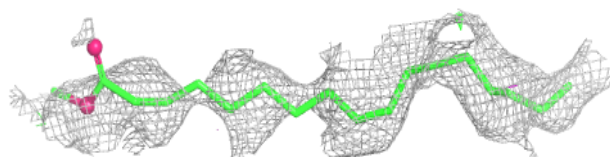
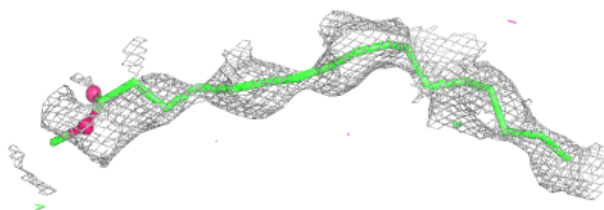


Electron density around OLC A 606:

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

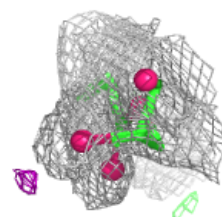
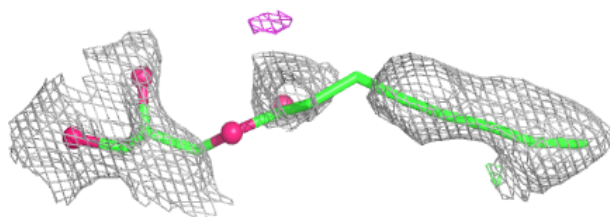
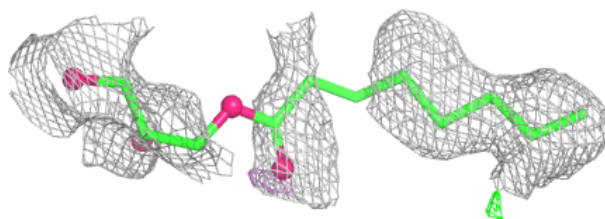
**Electron density around OLC A 612:**

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

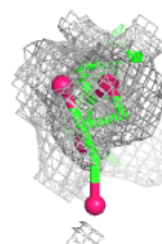
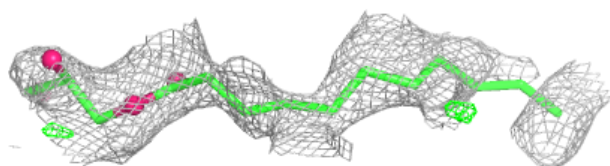
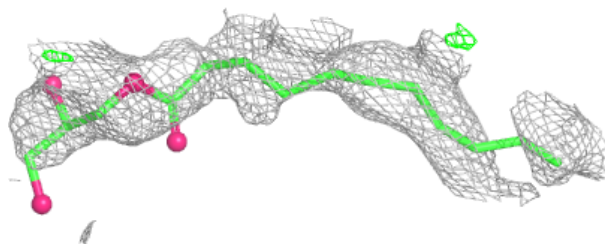


Electron density around OLC A 616:

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

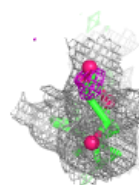
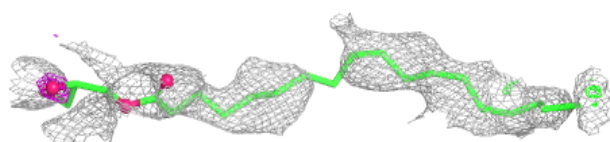
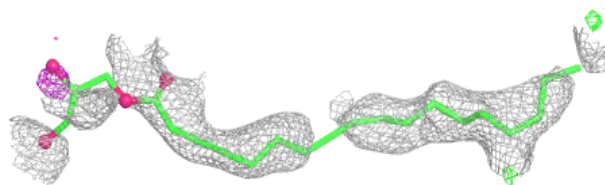
**Electron density around OLC A 605:**

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

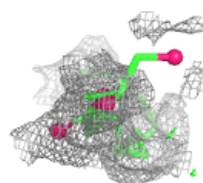
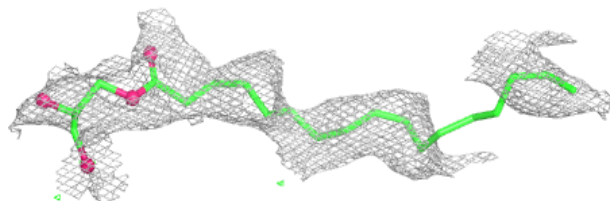
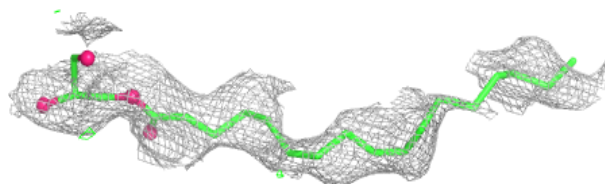


Electron density around OLC B 202:

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

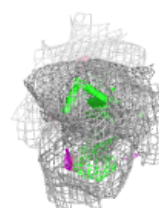
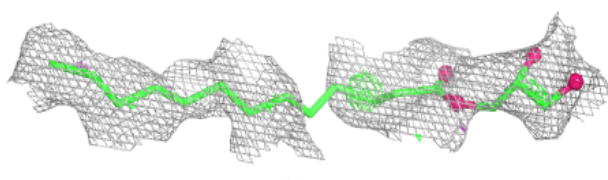
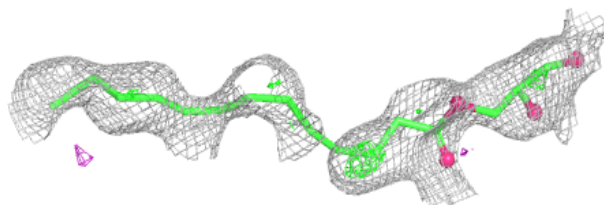
**Electron density around OLC B 203:**

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

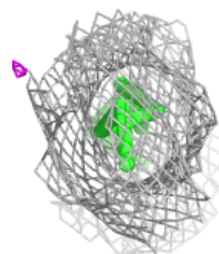
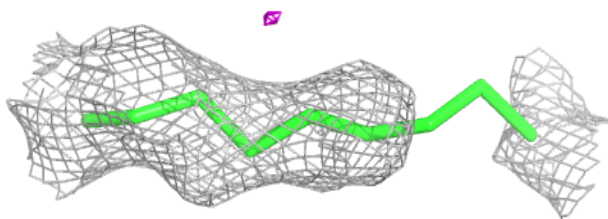
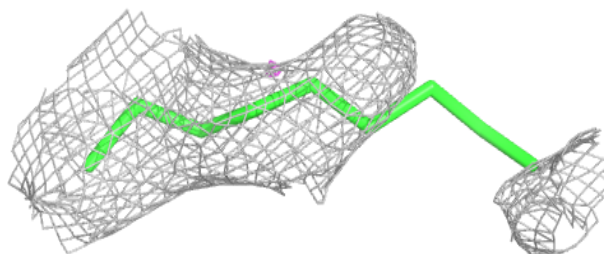


Electron density around OLC A 610:

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

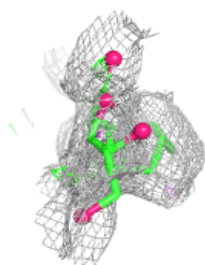
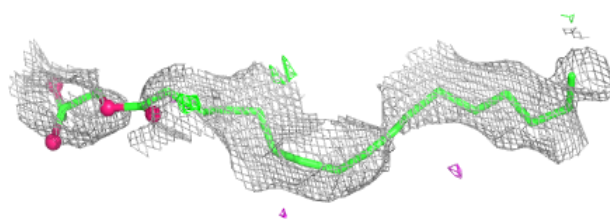
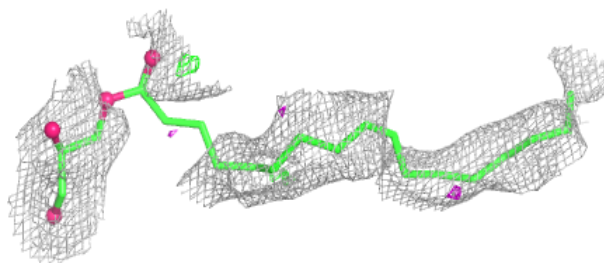
**Electron density around OLC A 613:**

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

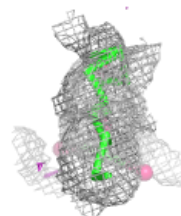
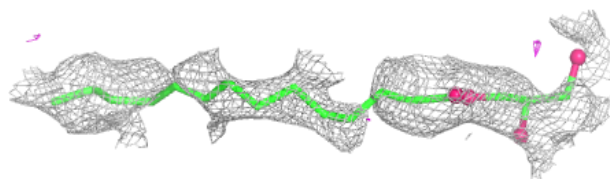
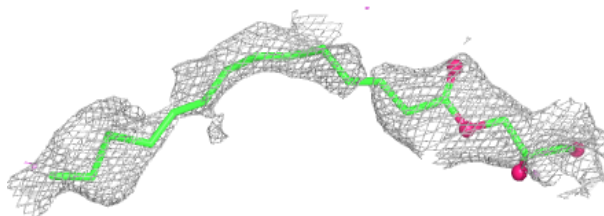


Electron density around OLC C 101:

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

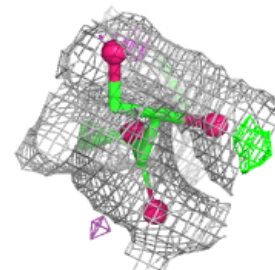
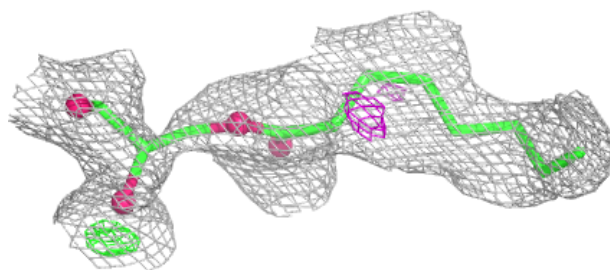
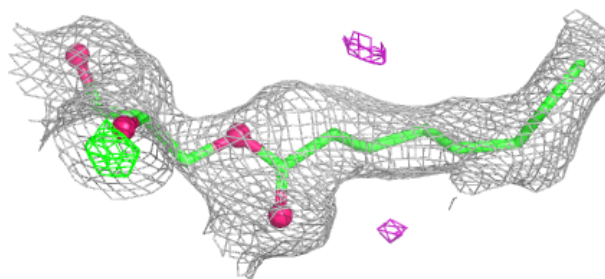
**Electron density around OLC A 611:**

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

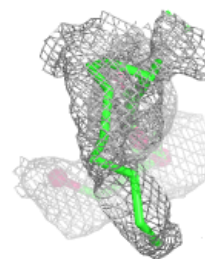
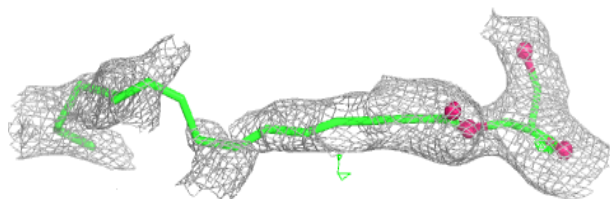
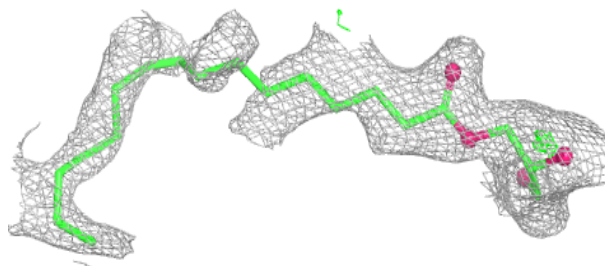


Electron density around OLC A 609:

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

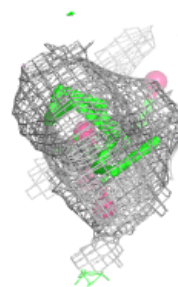
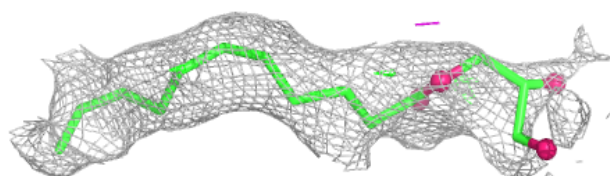
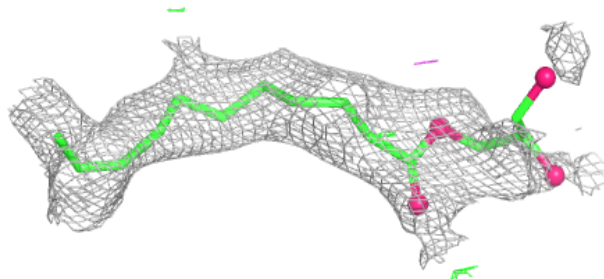
**Electron density around OLC A 604:**

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

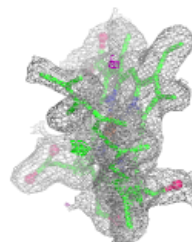
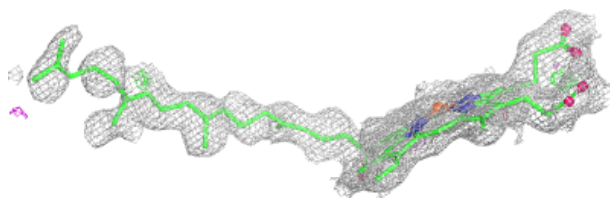
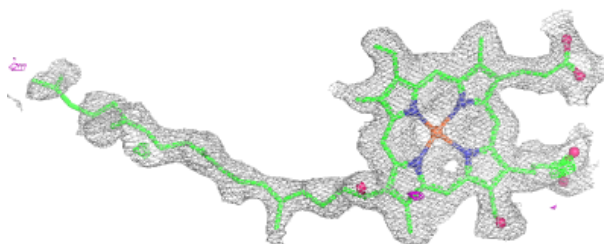


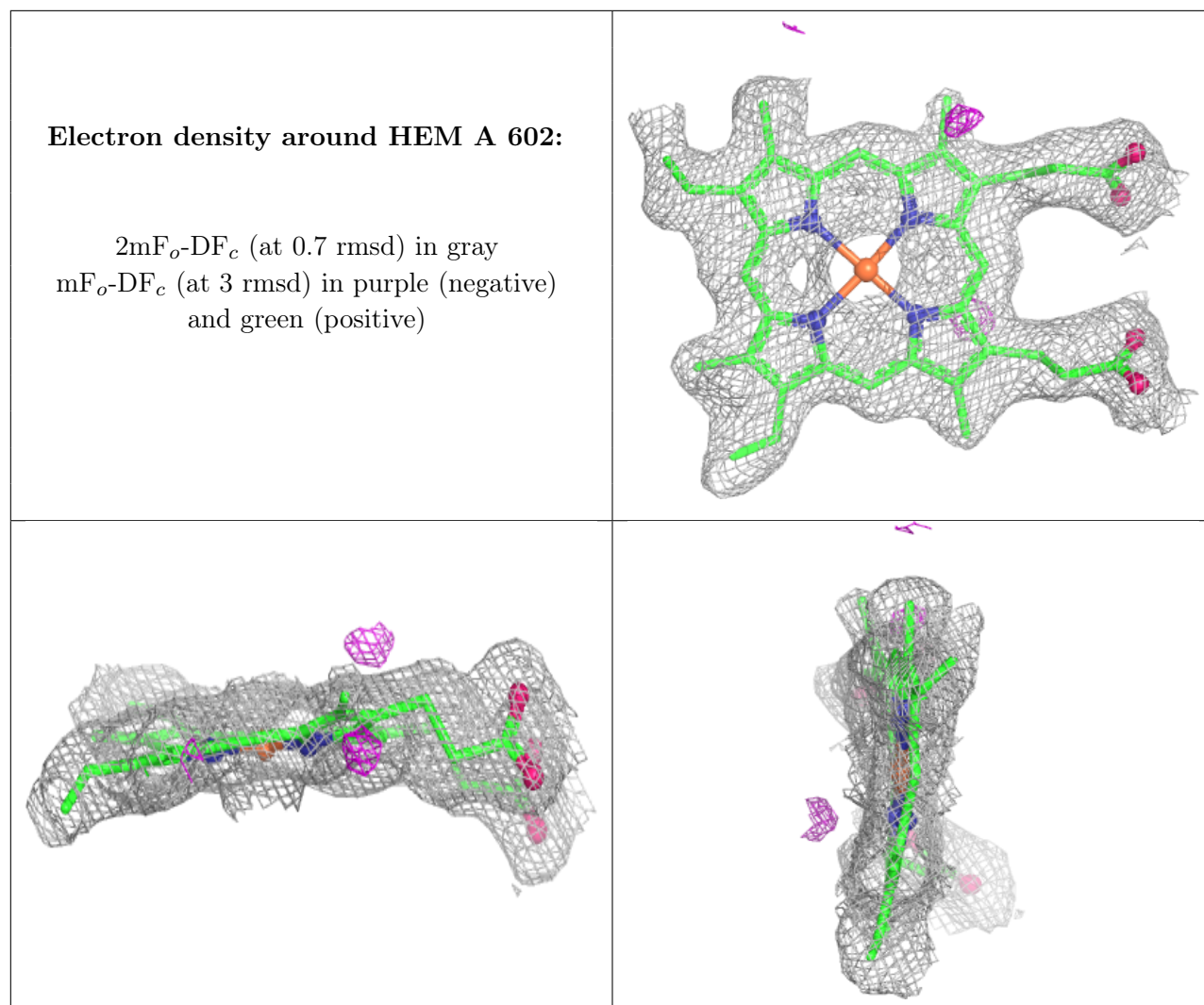
Electron density around OLC A 608:

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

**Electron density around HAS A 603:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.