



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 02:58 PM EDT

PDB ID : 4G71 / pdb_00004g71
Title : Structure of Recombinant Cytochrome ba3 Oxidase mutant V236N from *Thermus thermophilus*
Authors : Li, Y.; Chen, Y.; Stout, C.D.
Deposited on : 2012-07-19
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

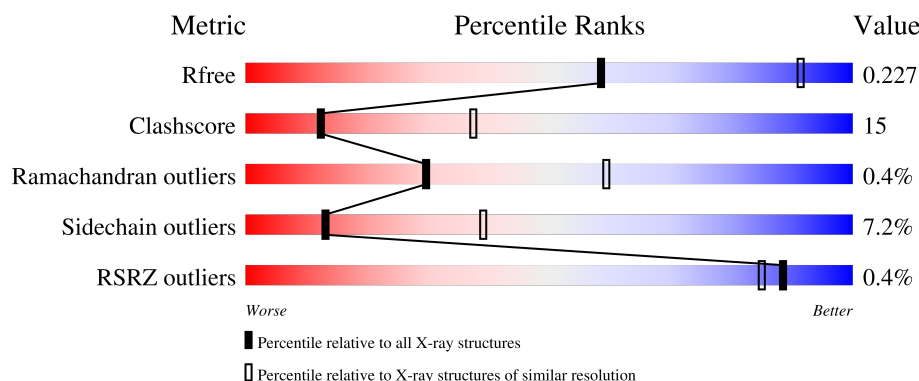
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

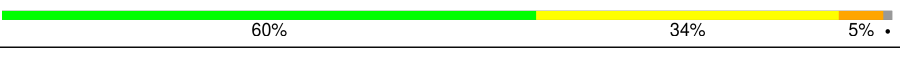
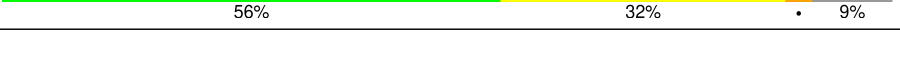
The reported resolution of this entry is 2.90 Å.

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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	 65% 29% 5% 1%
2	B	168	 60% 34% 5% 1%
3	C	34	 56% 32% 9% 3%

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
7	PER	A	604	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6389 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	3	0
			4358	2962	688	692	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP Q5SJ79
A	-5	HIS	-	expression tag	UNP Q5SJ79
A	-4	HIS	-	expression tag	UNP Q5SJ79
A	-3	HIS	-	expression tag	UNP Q5SJ79
A	-2	HIS	-	expression tag	UNP Q5SJ79
A	-1	HIS	-	expression tag	UNP Q5SJ79
A	0	HIS	-	expression tag	UNP Q5SJ79
A	1	HIS	-	expression tag	UNP Q5SJ79
A	120	PHE	ALA	engineered mutation	UNP Q5SJ79
A	236	ASN	VAL	engineered mutation	UNP Q5SJ79

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	1	0
			1283	833	213	233	4			

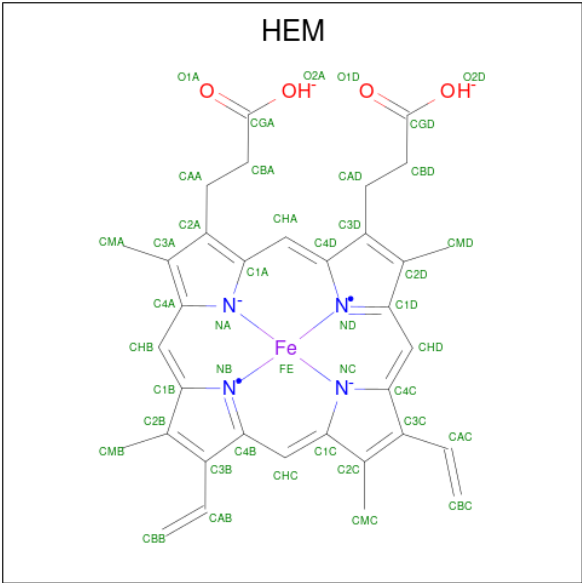
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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

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

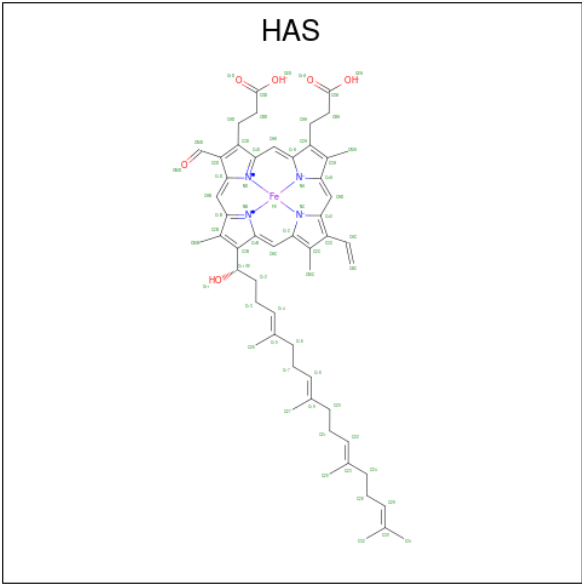
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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



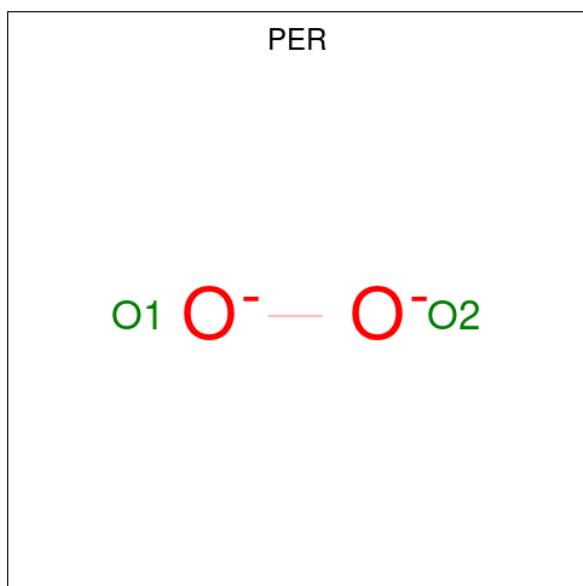
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



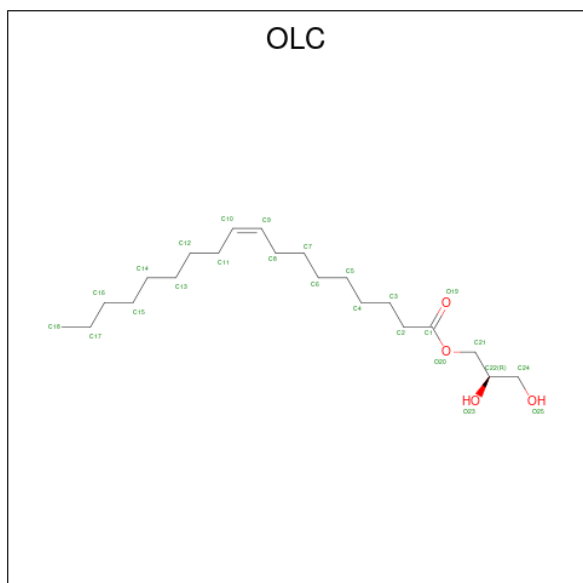
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	
			65	54	1	4	6	
							0	0

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



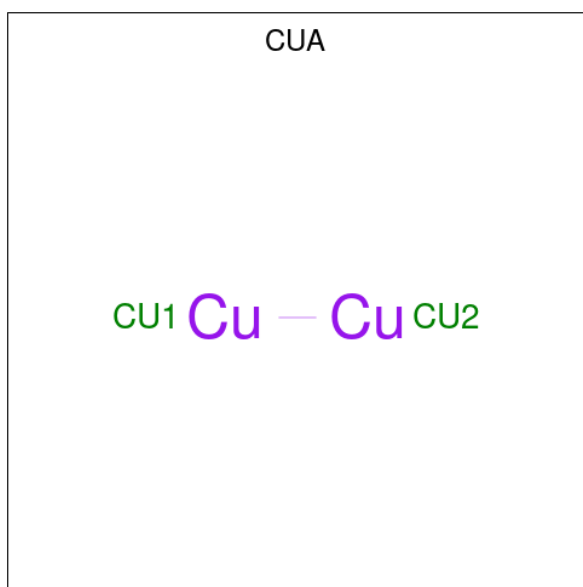
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O		
			2	2	0	0

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



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

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



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

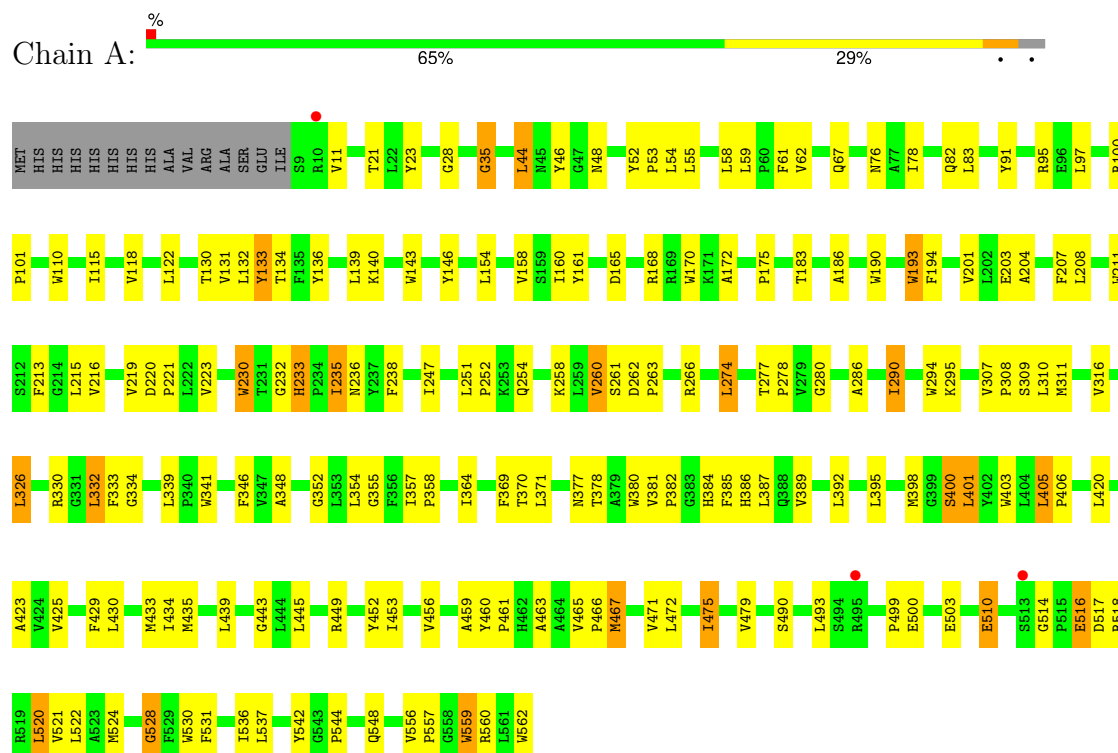
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	39	Total O 39 39	0	0
10	B	23	Total O 23 23	0	0
10	C	2	Total O 2 2	0	0

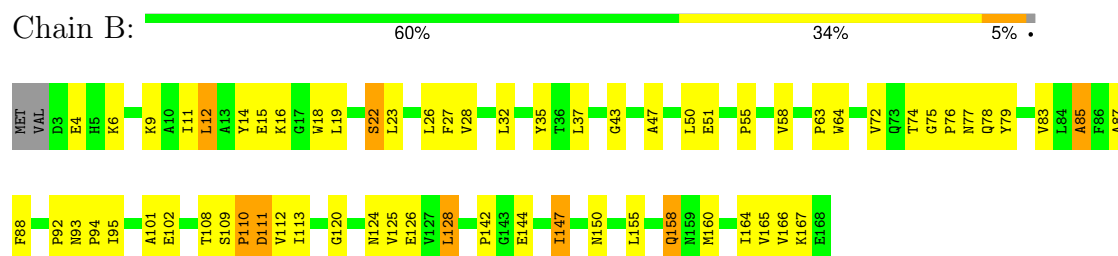
3 Residue-property plots

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

• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 3: Cytochrome c oxidase polypeptide 2A



MET	GLU	GLU	K4	P5	K6	L9	I12	L15	I19	L20	V21	L24	Y27	A28	R33	G34
-----	-----	-----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.44Å 98.36Å 94.84Å 90.00° 127.81° 90.00°	Depositor
Resolution (Å)	74.93 – 2.90 74.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (74.93-2.90) 99.1 (74.93-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.180 , 0.224 0.183 , 0.227	Depositor DCC
R_{free} test set	1183 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6389	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.15	9/4520 (0.2%)	1.14	15/6210 (0.2%)
2	B	1.08	2/1323 (0.2%)	1.12	4/1807 (0.2%)
3	C	1.09	0/247	1.09	1/335 (0.3%)
All	All	1.13	11/6090 (0.2%)	1.14	20/8352 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	HIS	ND1-CE1	6.54	1.39	1.32
2	B	112	VAL	C-O	-6.35	1.16	1.24
1	A	115	ILE	CA-CB	6.20	1.60	1.54
1	A	233	HIS	CG-CD2	6.12	1.42	1.35
1	A	384	HIS	CG-CD2	5.80	1.42	1.35
1	A	559	TRP	CA-C	-5.57	1.45	1.52
1	A	370	THR	C-O	-5.50	1.17	1.24
1	A	193	TRP	CD2-CE2	5.39	1.50	1.41
2	B	110	PRO	C-O	-5.38	1.17	1.24
1	A	233	HIS	CE1-NE2	5.24	1.37	1.32
1	A	531	PHE	C-O	-5.20	1.18	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	VAL	N-CA-C	7.86	118.66	110.72
1	A	465	VAL	CB-CA-C	-6.83	107.21	113.70
1	A	516	GLU	N-CA-C	6.44	116.56	108.45
1	A	514	GLY	N-CA-C	-5.83	100.45	112.34
1	A	35	GLY	N-CA-C	-5.82	105.33	112.77
1	A	479	VAL	N-CA-CB	5.76	116.90	110.62
3	C	28	ALA	N-CA-C	-5.63	104.84	110.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	83	VAL	N-CA-C	5.61	116.38	108.36
1	A	183	THR	N-CA-C	5.50	117.28	111.28
1	A	62	VAL	CB-CA-C	-5.48	103.48	110.98
1	A	467	MET	N-CA-C	5.46	118.75	111.75
1	A	528	GLY	N-CA-C	-5.45	106.04	112.64
1	A	459	ALA	N-CA-C	5.37	118.99	112.23
2	B	85	ALA	N-CA-C	-5.35	100.68	109.40
2	B	43	GLY	N-CA-C	-5.27	107.78	114.16
1	A	536	ILE	N-CA-C	-5.19	105.54	110.42
1	A	260	VAL	N-CA-C	5.14	117.52	111.09
1	A	266	ARG	N-CA-C	-5.07	105.66	111.14
2	B	74	THR	N-CA-C	-5.03	106.56	113.30
1	A	136	TYR	N-CA-C	5.01	116.82	109.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4358	0	4422	143	0
2	B	1283	0	1245	47	0
3	C	241	0	267	14	0
4	A	1	0	0	0	0
5	A	43	0	30	3	0
6	A	65	0	62	4	0
7	A	2	0	0	3	0
8	A	210	0	289	16	0
8	B	75	0	120	10	0
8	C	45	0	64	6	0
9	B	2	0	0	0	0
10	A	39	0	0	4	0
10	B	23	0	0	6	1
10	C	2	0	0	1	0
All	All	6389	0	6499	198	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 15.

All (198) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ILE:HD11	8:A:605:OLC:H11	1.27	1.11
1:A:263:PRO:HG2	1:A:516:GLU:HG2	1.37	1.05
2:B:14:TYR:CD2	2:B:14:TYR:CD1	2.40	1.01
1:A:516:GLU:HG3	1:A:517:ASP:H	1.27	0.97
2:B:14:TYR:CD2	2:B:14:TYR:CB	2.49	0.95
2:B:14:TYR:CD1	2:B:14:TYR:CB	2.53	0.91
1:A:233:HIS:O	1:A:236:ASN:HB2	1.76	0.85
1:A:236:ASN:OD1	6:A:603:HAS:C4C	2.26	0.84
1:A:290:ILE:HG22	1:A:295:LYS:HE3	1.60	0.83
1:A:168:ARG:NH2	8:A:611:OLC:H3A	1.94	0.83
1:A:236:ASN:OD1	6:A:603:HAS:CHD	2.28	0.82
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.16	0.80
1:A:475:ILE:CD1	8:A:605:OLC:H11	2.08	0.79
2:B:47:ALA:O	10:B:322:HOH:O	2.03	0.76
1:A:82:GLN:HB2	10:A:739:HOH:O	1.86	0.74
2:B:144:GLU:HG2	2:B:165:VAL:HG22	1.69	0.74
1:A:377:ASN:OD1	10:A:725:HOH:O	2.06	0.73
1:A:475:ILE:HD11	8:A:605:OLC:C11	2.15	0.71
1:A:516:GLU:HG3	1:A:517:ASP:N	2.06	0.70
1:A:381:VAL:HB	1:A:382:PRO:HD3	1.73	0.70
2:B:51:GLU:OE2	10:B:305:HOH:O	2.11	0.69
1:A:168:ARG:HH11	8:A:610:OLC:H22	1.58	0.69
8:B:203:OLC:H5A	3:C:33:ARG:HE	1.60	0.67
2:B:18:TRP:CE3	3:C:12:ILE:HD13	2.30	0.67
2:B:14:TYR:CD2	3:C:9:LEU:HD11	2.30	0.66
3:C:4:LYS:HG3	3:C:6:LYS:HG2	1.78	0.66
1:A:46:TYR:HA	1:A:453:ILE:HD11	1.78	0.66
1:A:236:ASN:ND2	7:A:604:PER:O2	2.29	0.65
1:A:280:GLY:HA3	1:A:542:TYR:OH	1.97	0.64
1:A:168:ARG:HH21	8:A:611:OLC:H3A	1.64	0.63
1:A:294:TRP:CH2	1:A:544:PRO:HG2	2.33	0.63
8:A:605:OLC:H2A	8:A:613:OLC:H3A	1.81	0.62
1:A:560:ARG:O	1:A:560:ARG:HG2	1.96	0.62
1:A:398:MET:O	1:A:401:LEU:HB2	2.00	0.62
1:A:216:VAL:HG12	8:A:614:OLC:H21A	1.82	0.61
1:A:332:LEU:HD13	1:A:333:PHE:CE1	2.35	0.61
1:A:400:SER:HA	1:A:403:TRP:NE1	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HD22	1:A:61:PHE:HE1	1.65	0.61
1:A:165:ASP:OD1	10:A:721:HOH:O	2.17	0.61
1:A:520:LEU:O	1:A:521:VAL:C	2.43	0.60
8:B:203:OLC:H18A	8:C:102:OLC:H6	1.83	0.60
1:A:260:VAL:HG11	2:B:11:ILE:HD13	1.84	0.60
1:A:456:VAL:HG23	1:A:456:VAL:O	2.01	0.60
1:A:528:GLY:HA2	8:A:611:OLC:H2	1.84	0.60
1:A:341:TRP:CZ2	8:A:615:OLC:H3	2.36	0.60
1:A:445:LEU:HD12	1:A:463:ALA:HB2	1.84	0.59
1:A:286:ALA:HB1	2:B:125:VAL:HA	1.84	0.58
3:C:4:LYS:N	10:C:202:HOH:O	2.36	0.57
1:A:348:ALA:HA	1:A:425:VAL:HG11	1.87	0.57
1:A:341:TRP:CE2	8:A:615:OLC:H3	2.40	0.56
1:A:355:GLY:O	1:A:358:PRO:HG2	2.05	0.56
1:A:435:MET:HE3	1:A:439:LEU:HD12	1.85	0.56
1:A:357:ILE:HG23	3:C:15:LEU:HD13	1.88	0.55
8:B:203:OLC:H17	8:C:101:OLC:H11	1.89	0.55
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.42	0.55
2:B:78:GLN:NE2	2:B:102:GLU:OE2	2.38	0.55
2:B:120:GLY:HA2	8:B:203:OLC:H4	1.88	0.55
1:A:434:ILE:HG21	1:A:472:LEU:HD23	1.89	0.55
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.87	0.55
1:A:78:ILE:HD11	1:A:133:TYR:HB2	1.89	0.55
1:A:168:ARG:HH22	8:A:611:OLC:C6	2.20	0.55
2:B:93:ASN:ND2	10:B:316:HOH:O	2.39	0.55
1:A:435:MET:HE3	1:A:439:LEU:CD1	2.37	0.54
1:A:348:ALA:HB1	1:A:395:LEU:O	2.08	0.54
2:B:76:PRO:HG2	10:B:318:HOH:O	2.07	0.54
1:A:35:GLY:HA3	1:A:76:ASN:OD1	2.08	0.54
1:A:405:LEU:HB3	1:A:406:PRO:HD3	1.91	0.53
1:A:562:TRP:HA	2:B:155:LEU:HG	1.91	0.52
1:A:52:TYR:N	1:A:53:PRO:CD	2.72	0.52
1:A:429:PHE:CE2	1:A:433:MET:HE3	2.45	0.52
1:A:263:PRO:HG2	1:A:516:GLU:CG	2.25	0.52
1:A:521:VAL:HA	1:A:524:MET:HE2	1.92	0.52
1:A:357:ILE:HG23	3:C:15:LEU:CD1	2.41	0.51
1:A:161:TYR:CE2	8:A:610:OLC:H21	2.45	0.51
1:A:204:ALA:HA	1:A:208:LEU:HB2	1.93	0.51
1:A:430:LEU:O	1:A:434:ILE:HG13	2.10	0.51
3:C:21:VAL:HG11	8:C:102:OLC:H9	1.93	0.50
8:B:203:OLC:H12	8:C:102:OLC:H21A	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LEU:HD13	2:B:22:SER:HB2	1.93	0.50
1:A:499:PRO:O	1:A:503:GLU:HG3	2.12	0.50
2:B:108:THR:OG1	2:B:109:SER:N	2.45	0.50
1:A:97:LEU:HD22	1:A:170:TRP:CD1	2.46	0.50
1:A:168:ARG:NH1	8:A:610:OLC:H22	2.25	0.50
1:A:193:TRP:CH2	1:A:235:ILE:HG13	2.46	0.50
1:A:140:LYS:HE3	1:A:211:TRP:NE1	2.27	0.50
1:A:332:LEU:HD13	1:A:333:PHE:HE1	1.74	0.50
2:B:125:VAL:HG22	2:B:126:GLU:O	2.12	0.49
1:A:23:TYR:HB3	1:A:110:TRP:NE1	2.28	0.49
1:A:52:TYR:N	1:A:53:PRO:HD2	2.26	0.49
1:A:220:ASP:HB3	1:A:223:VAL:HG12	1.94	0.49
1:A:332:LEU:CD1	1:A:333:PHE:HE1	2.26	0.49
1:A:517:ASP:OD2	1:A:520:LEU:HB2	2.12	0.49
2:B:92:PRO:HG3	10:B:323:HOH:O	2.11	0.48
1:A:377:ASN:O	1:A:449:ARG:HG2	2.12	0.48
1:A:307:VAL:N	1:A:308:PRO:HD2	2.28	0.48
1:A:556:VAL:HG12	2:B:55:PRO:HG3	1.96	0.48
1:A:230:TRP:C	1:A:230:TRP:CD1	2.92	0.48
2:B:142:PRO:HA	2:B:166:VAL:HG12	1.96	0.48
1:A:233:HIS:CD2	1:A:233:HIS:C	2.92	0.48
1:A:445:LEU:HD12	1:A:463:ALA:CB	2.44	0.48
1:A:236:ASN:CG	7:A:604:PER:O2	2.57	0.47
2:B:12:LEU:O	2:B:16:LYS:HG3	2.13	0.47
1:A:377:ASN:HB2	2:B:150:ASN:ND2	2.30	0.47
2:B:95:ILE:HD12	2:B:164:ILE:HG12	1.95	0.47
8:B:203:OLC:H17	8:C:101:OLC:H12	1.95	0.47
2:B:93:ASN:HA	2:B:94:PRO:HA	1.75	0.47
1:A:258:LYS:HG2	1:A:510:GLU:HB3	1.95	0.47
2:B:113:ILE:HG23	2:B:128:LEU:HD12	1.96	0.47
1:A:277:THR:N	1:A:278:PRO:HD2	2.29	0.47
2:B:23:LEU:HD12	2:B:23:LEU:HA	1.59	0.46
2:B:35:TYR:OH	8:B:202:OLC:H24A	2.14	0.46
1:A:371:LEU:HD21	3:C:27:TYR:HD1	1.81	0.46
2:B:77:ASN:OD1	2:B:101:ALA:HA	2.15	0.46
1:A:67:GLN:HA	1:A:130:THR:HG23	1.97	0.46
1:A:341:TRP:HB3	8:A:606:OLC:H24A	1.96	0.46
1:A:401:LEU:O	1:A:405:LEU:HB2	2.15	0.46
2:B:63:PRO:HD2	2:B:64:TRP:CE3	2.50	0.46
2:B:85:ALA:O	2:B:110:PRO:HD2	2.16	0.46
3:C:20:LEU:HD12	3:C:20:LEU:HA	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ALA:HA	1:A:425:VAL:CG1	2.45	0.46
1:A:140:LYS:HE3	1:A:211:TRP:CD1	2.51	0.46
1:A:277:THR:N	1:A:278:PRO:CD	2.79	0.46
1:A:172:ALA:O	1:A:175:PRO:HD3	2.16	0.45
1:A:236:ASN:OD1	6:A:603:HAS:C3C	2.64	0.45
1:A:247:ILE:HG21	1:A:316:VAL:HG21	1.97	0.45
1:A:354:LEU:HD13	8:A:615:OLC:H8	1.97	0.45
2:B:88:PHE:HB3	2:B:160:MET:HB2	1.98	0.45
1:A:76:ASN:HB3	5:A:602:HEM:CAC	2.46	0.45
1:A:186:ALA:O	1:A:190:TRP:CD1	2.70	0.45
1:A:203:GLU:O	1:A:207:PHE:HB2	2.17	0.45
1:A:232:GLY:O	1:A:235:ILE:HG22	2.17	0.45
1:A:247:ILE:CG2	1:A:316:VAL:HG21	2.47	0.45
1:A:290:ILE:CG2	1:A:295:LYS:HE3	2.41	0.45
1:A:254:GLN:H	1:A:254:GLN:HG2	1.63	0.45
1:A:386:HIS:CE1	5:A:602:HEM:C1A	3.05	0.44
2:B:87:ALA:HB1	2:B:88:PHE:CE1	2.52	0.44
1:A:59:LEU:HD22	1:A:61:PHE:CE1	2.48	0.44
6:A:603:HAS:C4A	7:A:604:PER:O2	2.65	0.44
1:A:100:ARG:HG2	1:A:101:PRO:O	2.17	0.44
1:A:211:TRP:CG	1:A:219:VAL:HG23	2.52	0.44
3:C:6:LYS:HB2	3:C:6:LYS:HZ3	1.83	0.44
1:A:251:LEU:N	1:A:252:PRO:CD	2.81	0.44
2:B:144:GLU:CG	2:B:165:VAL:HG22	2.43	0.44
1:A:44:LEU:HD12	1:A:471:VAL:HA	1.99	0.43
1:A:326:LEU:HA	1:A:326:LEU:HD12	1.43	0.43
1:A:357:ILE:HB	1:A:358:PRO:CD	2.48	0.43
1:A:452:TYR:HB3	2:B:158[A]:GLN:OE1	2.17	0.43
8:B:203:OLC:H17	8:C:101:OLC:C12	2.49	0.43
1:A:463:ALA:C	1:A:466:PRO:HD2	2.43	0.43
1:A:548:GLN:NE2	2:B:50:LEU:HD12	2.33	0.43
1:A:146:TYR:CD2	1:A:208:LEU:HD13	2.53	0.43
1:A:146:TYR:CE2	1:A:208:LEU:HD13	2.53	0.43
1:A:274:LEU:HD21	1:A:530:TRP:CE3	2.54	0.43
2:B:124:ASN:OD1	2:B:150:ASN:ND2	2.44	0.43
1:A:131:VAL:O	1:A:132:LEU:HB2	2.19	0.43
1:A:143:TRP:HB2	1:A:213:PHE:CE2	2.54	0.43
1:A:139:LEU:HA	1:A:559:TRP:O	2.19	0.43
1:A:154:LEU:HD23	1:A:154:LEU:HA	1.64	0.43
1:A:516:GLU:HA	1:A:516:GLU:OE1	2.19	0.42
2:B:109:SER:OG	2:B:111:ASP:OD2	2.38	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:THR:HG22	10:B:315:HOH:O	2.19	0.42
1:A:380:TRP:H	1:A:443:GLY:HA3	1.85	0.42
1:A:516:GLU:CG	1:A:517:ASP:N	2.76	0.42
2:B:32:LEU:HD21	8:B:202:OLC:H7A	2.01	0.42
1:A:339:LEU:HB3	1:A:346:PHE:CZ	2.54	0.42
1:A:364:ILE:HD12	3:C:19:ILE:HG12	2.02	0.42
2:B:19:LEU:HD23	2:B:19:LEU:HA	1.95	0.42
2:B:32:LEU:HA	2:B:32:LEU:HD23	1.82	0.42
2:B:77:ASN:O	2:B:77:ASN:CG	2.62	0.42
3:C:6:LYS:HB2	3:C:6:LYS:NZ	2.35	0.42
1:A:460:TYR:N	1:A:461:PRO:CD	2.83	0.41
1:A:28:GLY:HA2	1:A:83:LEU:HD12	2.01	0.41
1:A:387:LEU:HD22	1:A:433:MET:HE1	2.03	0.41
2:B:72:VAL:O	2:B:79:TYR:HA	2.19	0.41
1:A:21:THR:OG1	1:A:91:TYR:HB2	2.21	0.41
1:A:48:ASN:HB2	1:A:467:MET:SD	2.61	0.41
1:A:220:ASP:HA	1:A:221:PRO:HD3	1.79	0.41
5:A:602:HEM:HMC2	5:A:602:HEM:HBC2	2.02	0.41
1:A:235:ILE:CG2	1:A:236:ASN:N	2.84	0.41
1:A:308:PRO:O	1:A:311:MET:HB3	2.21	0.41
1:A:330:ARG:O	1:A:334:GLY:HA3	2.20	0.41
2:B:6:LYS:O	2:B:9:LYS:N	2.54	0.41
1:A:522:LEU:HD23	1:A:522:LEU:HA	1.91	0.41
1:A:55:LEU:HD11	1:A:59:LEU:HD12	2.03	0.40
1:A:95:ARG:HD2	1:A:95:ARG:HA	1.92	0.40
1:A:377:ASN:N	10:A:716:HOH:O	2.41	0.40
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.78	0.40
1:A:420:LEU:O	1:A:423:ALA:HB3	2.20	0.40
1:A:258:LYS:HE2	1:A:510:GLU:HB3	2.02	0.40
2:B:147:ILE:HD11	2:B:164:ILE:HG13	2.02	0.40
1:A:235:ILE:HA	1:A:238:PHE:HB3	2.04	0.40
2:B:75:GLY:HA3	2:B:78:GLN:HB3	2.03	0.40
1:A:332:LEU:HD13	1:A:333:PHE:CD1	2.57	0.40
1:A:517:ASP:O	1:A:518:ARG:C	2.64	0.40
2:B:27:PHE:O	2:B:28:VAL:C	2.64	0.40
8:B:204:OLC:H9	3:C:12:ILE:CD1	2.52	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:308:HOH:O	10:B:319:HOH:O[2_556]	2.15	0.05

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	554/569 (97%)	497 (90%)	54 (10%)	3 (0%)	24	54
2	B	165/168 (98%)	154 (93%)	11 (7%)	0	100	100
3	C	29/34 (85%)	27 (93%)	2 (7%)	0	100	100
All	All	748/771 (97%)	678 (91%)	67 (9%)	3 (0%)	30	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	537	LEU
1	A	369	PHE
1	A	557	PRO

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	442/464 (95%)	413 (93%)	29 (7%)	15	43
2	B	132/138 (96%)	119 (90%)	13 (10%)	7	25
3	C	24/27 (89%)	22 (92%)	2 (8%)	10	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	598/629 (95%)	554 (93%)	44 (7%)	13	38

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	44	LEU
1	A	54	LEU
1	A	58	LEU
1	A	118	VAL
1	A	122	LEU
1	A	133	TYR
1	A	134	THR
1	A	158	VAL
1	A	201	VAL
1	A	215	LEU
1	A	230	TRP
1	A	235	ILE
1	A	261	SER
1	A	262	ASP
1	A	274	LEU
1	A	290	ILE
1	A	309	SER
1	A	326	LEU
1	A	332	LEU
1	A	400	SER
1	A	401	LEU
1	A	405	LEU
1	A	475	ILE
1	A	490	SER
1	A	493	LEU
1	A	500	GLU
1	A	510	GLU
1	A	520	LEU
2	B	4	GLU
2	B	12	LEU
2	B	15	GLU
2	B	22	SER
2	B	26	LEU
2	B	37	LEU
2	B	58	VAL
2	B	111	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	128	LEU
2	B	147	ILE
2	B	158[A]	GLN
2	B	158[B]	GLN
2	B	167	LYS
3	C	6	LYS
3	C	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	343	ASN
1	A	377	ASN
1	A	548	GLN
2	B	93	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 [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	OLC	B	203	-	24,24,24	0.76	1 (4%)	25,25,25	1.01	2 (8%)
8	OLC	A	613	-	23,23,24	0.55	1 (4%)	24,24,25	0.81	2 (8%)
8	OLC	A	607	-	20,20,24	0.56	0	20,20,25	0.70	1 (5%)
8	OLC	A	609	-	15,15,24	0.71	1 (6%)	16,16,25	0.68	0
8	OLC	A	608	-	17,17,24	0.53	0	18,18,25	0.67	0
8	OLC	B	204	-	24,24,24	0.57	0	25,25,25	0.59	0
8	OLC	A	612	-	19,19,24	0.59	0	20,20,25	0.71	0
8	OLC	A	610	-	7,7,24	0.49	0	6,7,25	0.49	0
8	OLC	A	606	-	21,21,24	0.63	0	22,22,25	0.79	1 (4%)
7	PER	A	604	6	1,1,1	0.32	0	-		
8	OLC	A	611	-	12,12,24	0.68	0	13,13,25	0.82	1 (7%)
6	HAS	A	603	7,1	72,72,72	2.32	30 (41%)	87,109,109	1.67	18 (20%)
8	OLC	C	102	-	22,22,24	0.56	1 (4%)	23,23,25	0.64	0
5	HEM	A	602	1	50,50,50	3.44	31 (62%)	67,82,82	2.19	16 (23%)
8	OLC	A	614	-	19,19,24	0.68	1 (5%)	20,20,25	0.84	1 (5%)
8	OLC	A	615	-	23,23,24	0.62	1 (4%)	24,24,25	1.14	2 (8%)
8	OLC	B	202	-	24,24,24	0.60	0	25,25,25	0.56	0
8	OLC	C	101	-	21,21,24	0.67	1 (4%)	22,22,25	0.70	0
8	OLC	A	605	-	23,23,24	0.63	1 (4%)	24,24,25	1.03	1 (4%)
9	CUA	B	201	2	0,1,1	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OLC	C	102	-	-	11/22/22/24	-
5	HEM	A	602	1	-	5/14/54/54	-
8	OLC	B	204	-	-	8/24/24/24	-
8	OLC	A	612	-	-	7/19/19/24	-
8	OLC	B	203	-	-	12/24/24/24	-
8	OLC	A	605	-	-	9/23/23/24	-
8	OLC	A	614	-	-	9/19/19/24	-
8	OLC	A	613	-	-	11/23/23/24	-
8	OLC	A	615	-	-	10/23/23/24	-
8	OLC	A	607	-	-	8/19/19/24	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OLC	A	606	-	-	8/21/21/24	-
8	OLC	A	609	-	-	10/15/15/24	-
8	OLC	A	608	-	-	9/17/17/24	-
8	OLC	A	610	-	-	3/6/6/24	-
8	OLC	A	611	-	-	6/12/12/24	-
8	OLC	B	202	-	-	8/24/24/24	-
8	OLC	C	101	-	-	6/21/21/24	-
6	HAS	A	603	7,1	-	11/42/82/82	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEM	FE-NB	7.15	2.16	1.94
5	A	602	HEM	C1B-C2B	-6.79	1.30	1.44
5	A	602	HEM	CHD-C4C	6.68	1.51	1.38
5	A	602	HEM	C3C-C4C	-6.67	1.34	1.46
5	A	602	HEM	C3C-C2C	6.04	1.49	1.37
5	A	602	HEM	C3B-C2B	5.97	1.49	1.37
6	A	603	HAS	CHD-C4C	5.83	1.52	1.39
6	A	603	HAS	CAC-C3C	-5.73	1.32	1.47
6	A	603	HAS	CHB-C1D	5.46	1.49	1.38
5	A	602	HEM	CAB-C3B	-5.31	1.33	1.47
5	A	602	HEM	CHB-C1B	5.20	1.48	1.38
5	A	602	HEM	C1C-C2C	-5.18	1.35	1.45
5	A	602	HEM	CHC-C1C	5.14	1.48	1.38
5	A	602	HEM	CHA-C1A	4.69	1.49	1.39
6	A	603	HAS	CHC-C1C	4.55	1.49	1.39
5	A	602	HEM	CBB-CAB	4.33	1.51	1.30
6	A	603	HAS	CBC-CAC	4.32	1.51	1.30
5	A	602	HEM	CHA-C4D	-4.28	1.29	1.38
5	A	602	HEM	C4D-ND	-4.00	1.33	1.40
6	A	603	HAS	C4D-ND	3.99	1.46	1.38
6	A	603	HAS	CHA-C4D	3.93	1.48	1.39
6	A	603	HAS	C4B-C3B	3.70	1.51	1.44
6	A	603	HAS	O1D-CGD	3.64	1.34	1.22
6	A	603	HAS	CHB-C1B	-3.60	1.31	1.39
6	A	603	HAS	C2D-C1D	3.54	1.51	1.44
5	A	602	HEM	CHB-C4A	-3.51	1.31	1.39
6	A	603	HAS	C1D-ND	3.46	1.46	1.40
5	A	602	HEM	FE-NC	3.45	2.06	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	CHA-C1A	-3.45	1.31	1.38
6	A	603	HAS	C4B-NB	-3.43	1.34	1.40
5	A	602	HEM	C4A-NA	-3.34	1.33	1.39
6	A	603	HAS	C1C-C2C	-3.27	1.35	1.43
6	A	603	HAS	C1C-NC	-3.16	1.33	1.39
5	A	602	HEM	C1B-NB	-3.14	1.34	1.40
6	A	603	HAS	FE-NA	3.14	2.05	1.95
6	A	603	HAS	CHC-C4B	-3.13	1.32	1.38
5	A	602	HEM	C4A-C3A	2.99	1.50	1.43
5	A	602	HEM	FE-ND	2.91	2.03	1.94
5	A	602	HEM	CHC-C4B	-2.91	1.32	1.39
6	A	603	HAS	C2A-C3A	-2.77	1.30	1.36
6	A	603	HAS	C1B-NB	-2.58	1.33	1.38
5	A	602	HEM	C1C-NC	-2.57	1.34	1.39
8	B	203	OLC	O20-C1	2.54	1.40	1.33
5	A	602	HEM	C1D-C2D	2.46	1.49	1.44
6	A	603	HAS	C4A-C3A	2.44	1.50	1.45
6	A	603	HAS	C3C-C2C	2.42	1.49	1.41
5	A	602	HEM	C4B-NB	-2.40	1.34	1.38
6	A	603	HAS	C4D-C3D	2.39	1.49	1.45
5	A	602	HEM	CMC-C2C	2.37	1.55	1.50
8	A	614	OLC	O20-C1	2.36	1.40	1.33
5	A	602	HEM	C1D-ND	-2.34	1.34	1.38
5	A	602	HEM	C1A-C2A	2.31	1.49	1.44
8	A	605	OLC	O20-C1	2.30	1.40	1.33
5	A	602	HEM	C4C-NC	-2.30	1.35	1.39
6	A	603	HAS	O2D-CGD	-2.28	1.23	1.30
8	A	615	OLC	O20-C1	2.22	1.39	1.33
5	A	602	HEM	C4D-C3D	2.21	1.48	1.45
5	A	602	HEM	CHD-C1D	-2.15	1.34	1.39
8	C	101	OLC	O20-C1	2.14	1.39	1.33
6	A	603	HAS	C4C-NC	2.13	1.43	1.39
6	A	603	HAS	C1B-C2B	2.13	1.48	1.44
5	A	602	HEM	FE-NA	2.08	2.02	1.95
8	A	609	OLC	O20-C1	2.08	1.39	1.33
8	C	102	OLC	O20-C1	2.02	1.39	1.33
6	A	603	HAS	C1A-NA	-2.01	1.35	1.39
8	A	613	OLC	O20-C1	2.01	1.39	1.33
6	A	603	HAS	C3C-C4C	2.01	1.48	1.42
6	A	603	HAS	CMD-C2D	2.01	1.49	1.45
6	A	603	HAS	FE-NC	2.00	2.01	1.95

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	HEM	CHC-C4B-NB	7.35	132.33	124.42
5	A	602	HEM	C3B-C4B-NB	-7.14	104.34	109.47
5	A	602	HEM	C1B-NB-C4B	6.29	112.65	105.21
6	A	603	HAS	C1D-ND-C4D	-5.01	99.28	105.21
5	A	602	HEM	C3C-C2C-C1C	-4.30	102.98	107.05
6	A	603	HAS	CHA-C1A-C2A	-4.24	118.18	124.86
6	A	603	HAS	CHB-C1D-ND	-4.21	119.16	124.37
6	A	603	HAS	C4C-C3C-C2C	-4.12	102.18	107.30
6	A	603	HAS	C25-C23-C24	3.85	121.92	115.23
5	A	602	HEM	C4B-C3B-C2B	-3.66	103.91	107.28
5	A	602	HEM	CHB-C1B-NB	3.41	128.59	124.37
8	B	203	OLC	O20-C21-C22	3.24	121.08	105.85
5	A	602	HEM	O2D-CGD-O1D	-3.24	115.00	123.33
8	A	615	OLC	C3-C2-C1	-3.17	102.08	113.69
5	A	602	HEM	C4C-C3C-C2C	-3.13	104.10	106.81
6	A	603	HAS	C2C-C1C-NC	3.09	115.10	110.14
6	A	603	HAS	CHC-C1C-NC	-3.08	118.28	123.86
5	A	602	HEM	C4A-CHB-C1B	-3.05	119.07	126.25
6	A	603	HAS	CAA-CBA-CGA	-2.94	105.86	113.67
6	A	603	HAS	CHA-C4D-ND	-2.81	121.40	124.42
6	A	603	HAS	CHD-C4A-NA	-2.79	121.42	124.45
5	A	602	HEM	O2D-CGD-CBD	2.79	122.81	114.00
5	A	602	HEM	CMD-C2D-C1D	-2.77	120.71	125.03
6	A	603	HAS	CMB-C2B-C3B	-2.68	125.08	130.28
5	A	602	HEM	CHA-C1A-NA	2.68	128.72	123.86
5	A	602	HEM	CBA-CAA-C2A	-2.59	105.36	112.53
6	A	603	HAS	O11-C11-C3B	-2.54	106.60	111.26
5	A	602	HEM	CHB-C1B-C2B	-2.49	119.88	126.95
5	A	602	HEM	C4D-C3D-C2D	-2.37	103.44	106.89
8	A	606	OLC	C21-O20-C1	2.30	125.52	117.12
6	A	603	HAS	C12-C11-C3B	2.28	115.69	112.12
8	A	614	OLC	C21-O20-C1	2.23	125.26	117.12
5	A	602	HEM	CBB-CAB-C3B	-2.20	116.55	127.53
8	A	615	OLC	C21-O20-C1	2.11	124.84	117.12
8	A	613	OLC	C21-O20-C1	2.10	124.81	117.12
8	A	607	OLC	C21-O20-C1	2.10	122.81	116.07
6	A	603	HAS	C12-C13-C14	2.09	117.65	112.16
6	A	603	HAS	C3D-C4D-ND	2.08	112.36	110.35
8	B	203	OLC	C21-O20-C1	2.08	124.72	117.12
6	A	603	HAS	CHA-C1A-NA	2.07	126.71	124.45
8	A	613	OLC	O20-C1-O19	2.05	128.76	123.63
8	A	611	OLC	C21-O20-C1	2.04	124.56	117.12
6	A	603	HAS	C21-C22-C23	-2.03	122.98	127.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	O1A-CGA-CBA	-2.03	116.67	123.09
8	A	605	OLC	C21-O20-C1	2.01	124.46	117.12

There are no chirality outliers.

All (151) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	HEM	C2B-C3B-CAB-CBB
5	A	602	HEM	C4B-C3B-CAB-CBB
8	A	605	OLC	C21-C22-C24-O25
8	A	606	OLC	C21-C22-C24-O25
8	A	610	OLC	O20-C21-C22-C24
8	A	610	OLC	O19-C1-O20-C21
8	A	611	OLC	C21-C22-C24-O25
8	A	611	OLC	O20-C21-C22-C24
8	A	613	OLC	C21-C22-C24-O25
8	A	613	OLC	O23-C22-C24-O25
8	A	613	OLC	O20-C21-C22-C24
8	A	614	OLC	C10-C11-C12-C13
8	A	614	OLC	C21-C22-C24-O25
8	C	102	OLC	C21-C22-C24-O25
8	A	605	OLC	O19-C1-O20-C21
8	A	609	OLC	O19-C1-O20-C21
8	A	614	OLC	O19-C1-O20-C21
8	B	204	OLC	O19-C1-O20-C21
8	A	614	OLC	C2-C1-O20-C21
8	A	605	OLC	C2-C1-O20-C21
8	A	609	OLC	C2-C1-O20-C21
8	B	204	OLC	C2-C1-O20-C21
8	B	203	OLC	O19-C1-O20-C21
8	B	202	OLC	C2-C1-O20-C21
8	B	202	OLC	O19-C1-O20-C21
8	A	610	OLC	O20-C21-C22-O23
8	A	613	OLC	O20-C21-C22-O23
8	A	607	OLC	C2-C1-O20-C21
8	B	203	OLC	C2-C1-O20-C21
6	A	603	HAS	C25-C23-C24-C28
8	A	612	OLC	C2-C1-O20-C21
8	A	615	OLC	C2-C1-O20-C21
8	C	101	OLC	C2-C1-O20-C21
6	A	603	HAS	C22-C23-C24-C28
8	A	609	OLC	O20-C21-C22-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	609	OLC	O20-C21-C22-O23
8	A	611	OLC	O20-C21-C22-O23
8	A	607	OLC	O19-C1-O20-C21
8	C	101	OLC	O19-C1-O20-C21
8	A	615	OLC	C1-C2-C3-C4
8	A	612	OLC	O19-C1-O20-C21
8	A	615	OLC	O19-C1-O20-C21
8	B	203	OLC	C6-C7-C8-C9
8	A	608	OLC	C2-C1-O20-C21
8	C	102	OLC	C2-C1-O20-C21
8	A	613	OLC	C11-C12-C13-C14
8	A	605	OLC	O23-C22-C24-O25
8	A	606	OLC	O23-C22-C24-O25
8	A	611	OLC	O23-C22-C24-O25
8	A	614	OLC	O23-C22-C24-O25
8	C	102	OLC	O23-C22-C24-O25
8	A	614	OLC	C1-C2-C3-C4
8	C	102	OLC	C2-C3-C4-C5
8	C	102	OLC	C11-C12-C13-C14
8	A	608	OLC	O19-C1-O20-C21
8	C	102	OLC	O19-C1-O20-C21
8	A	607	OLC	C10-C11-C12-C13
8	B	202	OLC	C3-C4-C5-C6
8	A	614	OLC	C3-C4-C5-C6
8	B	202	OLC	C14-C15-C16-C17
8	A	606	OLC	C11-C12-C13-C14
8	C	101	OLC	C5-C6-C7-C8
8	A	615	OLC	C6-C7-C8-C9
8	B	204	OLC	C10-C11-C12-C13
8	A	613	OLC	C2-C1-O20-C21
8	A	611	OLC	C3-C4-C5-C6
8	C	102	OLC	C4-C5-C6-C7
8	A	615	OLC	C12-C13-C14-C15
8	B	202	OLC	C12-C13-C14-C15
8	A	608	OLC	C6-C7-C8-C9
8	A	612	OLC	C6-C7-C8-C9
8	A	612	OLC	C3-C4-C5-C6
8	B	203	OLC	C3-C4-C5-C6
8	A	613	OLC	O19-C1-O20-C21
8	A	613	OLC	C12-C13-C14-C15
8	A	605	OLC	C4-C5-C6-C7
6	A	603	HAS	C3D-C2D-CMD-OMD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	608	OLC	C4-C5-C6-C7
8	A	611	OLC	C1-C2-C3-C4
8	A	609	OLC	C2-C3-C4-C5
8	A	607	OLC	C2-C3-C4-C5
8	B	204	OLC	C12-C13-C14-C15
8	A	613	OLC	C13-C14-C15-C16
8	C	102	OLC	C3-C4-C5-C6
8	A	607	OLC	C6-C7-C8-C9
8	A	608	OLC	C2-C3-C4-C5
8	B	204	OLC	C15-C16-C17-C18
8	C	102	OLC	C13-C14-C15-C16
8	C	102	OLC	C1-C2-C3-C4
6	A	603	HAS	C3D-CAD-CBD-CGD
8	A	609	OLC	C3-C4-C5-C6
8	B	202	OLC	O20-C21-C22-C24
8	B	204	OLC	O20-C21-C22-C24
8	A	605	OLC	C14-C15-C16-C17
8	C	101	OLC	C3-C4-C5-C6
8	A	613	OLC	C4-C5-C6-C7
8	B	204	OLC	C6-C7-C8-C9
8	B	203	OLC	C4-C5-C6-C7
8	B	204	OLC	O20-C21-C22-O23
8	A	605	OLC	C13-C14-C15-C16
8	A	606	OLC	O19-C1-O20-C21
8	A	606	OLC	O20-C21-C22-O23
8	A	615	OLC	C10-C11-C12-C13
8	A	607	OLC	C3-C4-C5-C6
6	A	603	HAS	C1D-C2D-CMD-OMD
8	A	606	OLC	C2-C1-O20-C21
8	A	612	OLC	C2-C3-C4-C5
8	A	605	OLC	C5-C6-C7-C8
8	B	203	OLC	C10-C11-C12-C13
8	A	615	OLC	C9-C10-C11-C12
8	C	101	OLC	C9-C10-C11-C12
8	A	614	OLC	O20-C21-C22-O23
8	B	203	OLC	C11-C12-C13-C14
8	A	615	OLC	C11-C12-C13-C14
8	A	609	OLC	C1-C2-C3-C4
8	A	614	OLC	C6-C7-C8-C9
8	B	202	OLC	O20-C21-C22-O23
8	A	609	OLC	C21-C22-C24-O25
6	A	603	HAS	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	605	OLC	C1-C2-C3-C4
8	C	101	OLC	C10-C11-C12-C13
8	A	606	OLC	C2-C3-C4-C5
6	A	603	HAS	CAA-CBA-CGA-O2A
8	A	613	OLC	C7-C8-C9-C10
8	A	615	OLC	C7-C8-C9-C10
8	B	202	OLC	C7-C8-C9-C10
8	A	607	OLC	C13-C14-C15-C16
8	A	608	OLC	O20-C21-C22-C24
8	A	608	OLC	O20-C21-C22-O23
8	B	203	OLC	O20-C21-C22-O23
8	A	606	OLC	C7-C8-C9-C10
8	A	612	OLC	C9-C10-C11-C12
6	A	603	HAS	C11-C12-C13-C14
8	A	612	OLC	O20-C1-C2-C3
8	B	203	OLC	C9-C10-C11-C12
8	B	203	OLC	C5-C6-C7-C8
8	A	607	OLC	C7-C8-C9-C10
8	A	608	OLC	C7-C8-C9-C10
6	A	603	HAS	CAD-CBD-CGD-O1D
8	B	203	OLC	C7-C8-C9-C10
8	C	102	OLC	C7-C8-C9-C10
6	A	603	HAS	C3A-C2A-CAA-CBA
8	A	609	OLC	O20-C1-C2-C3
8	A	608	OLC	C1-C2-C3-C4
8	B	203	OLC	O20-C21-C22-C24
6	A	603	HAS	CAD-CBD-CGD-O2D
5	A	602	HEM	CAA-CBA-CGA-O2A
8	A	615	OLC	C4-C5-C6-C7
5	A	602	HEM	CAA-CBA-CGA-O1A
8	A	609	OLC	O19-C1-C2-C3
5	A	602	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

15 monomers are involved in 36 short contacts:

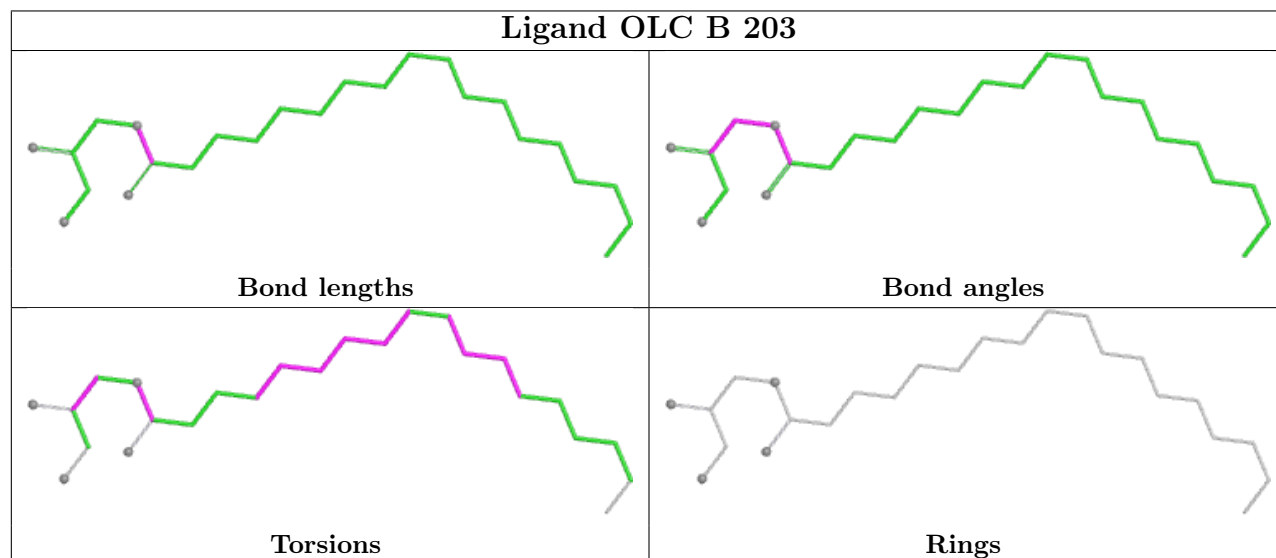
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	203	OLC	7	0
8	A	613	OLC	1	0
8	B	204	OLC	1	0
8	A	610	OLC	3	0
8	A	606	OLC	1	0

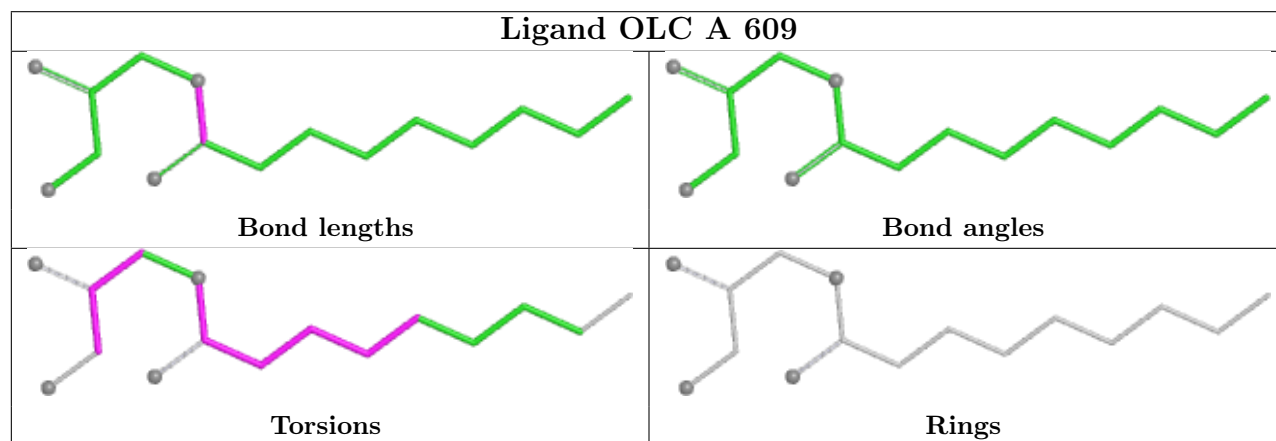
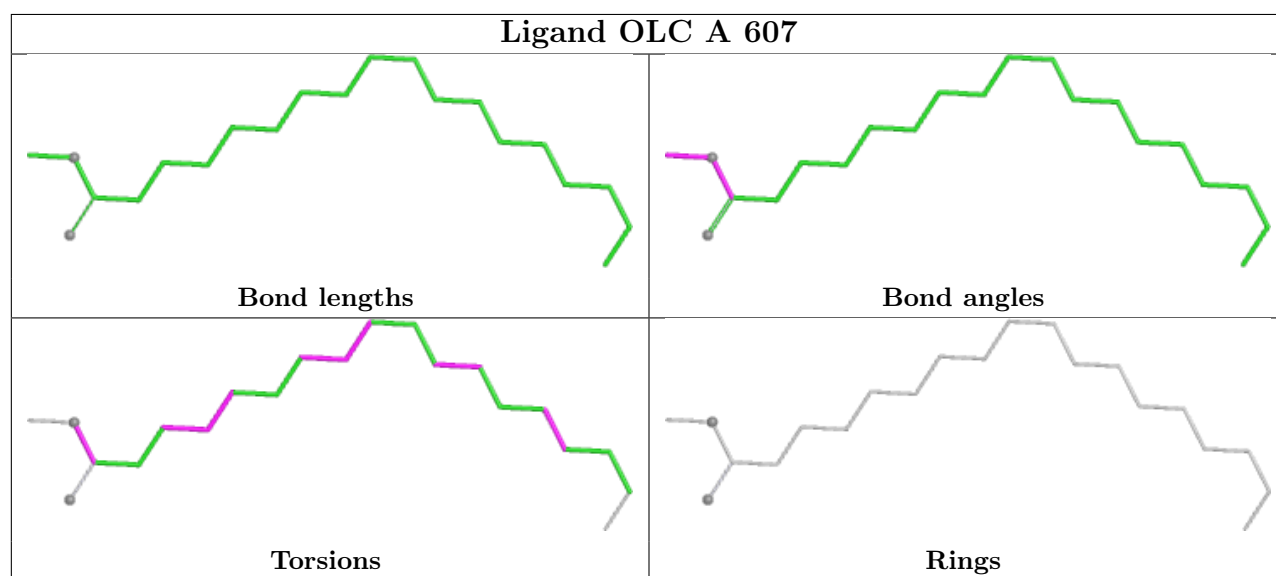
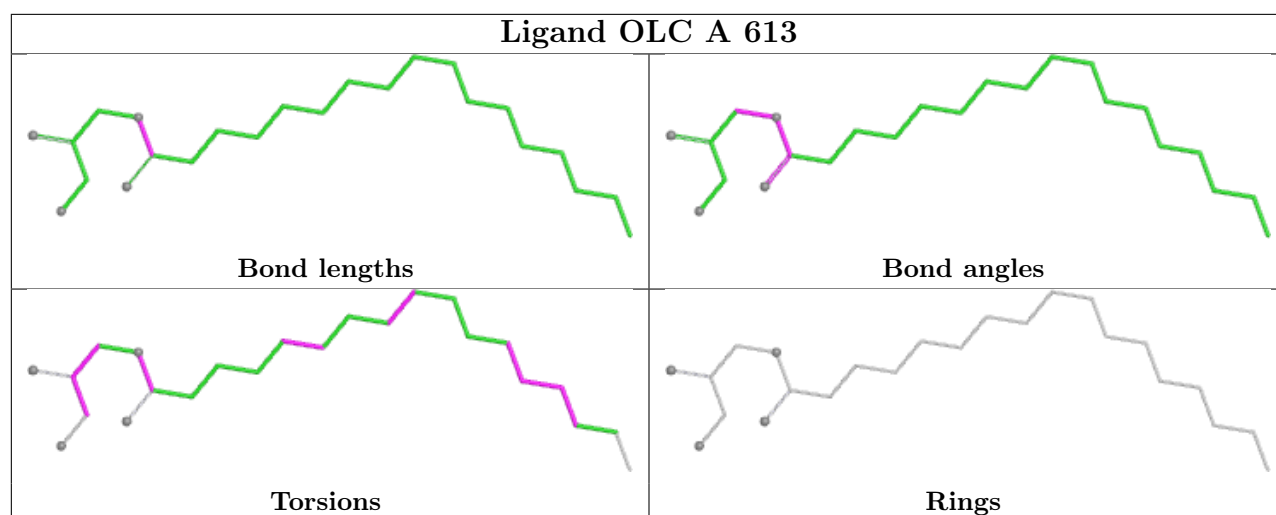
Continued on next page...

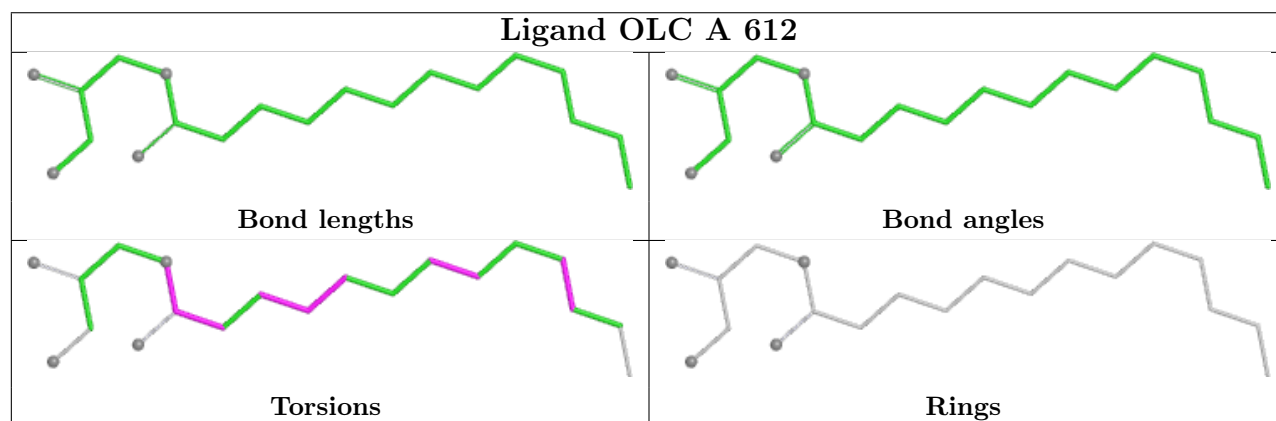
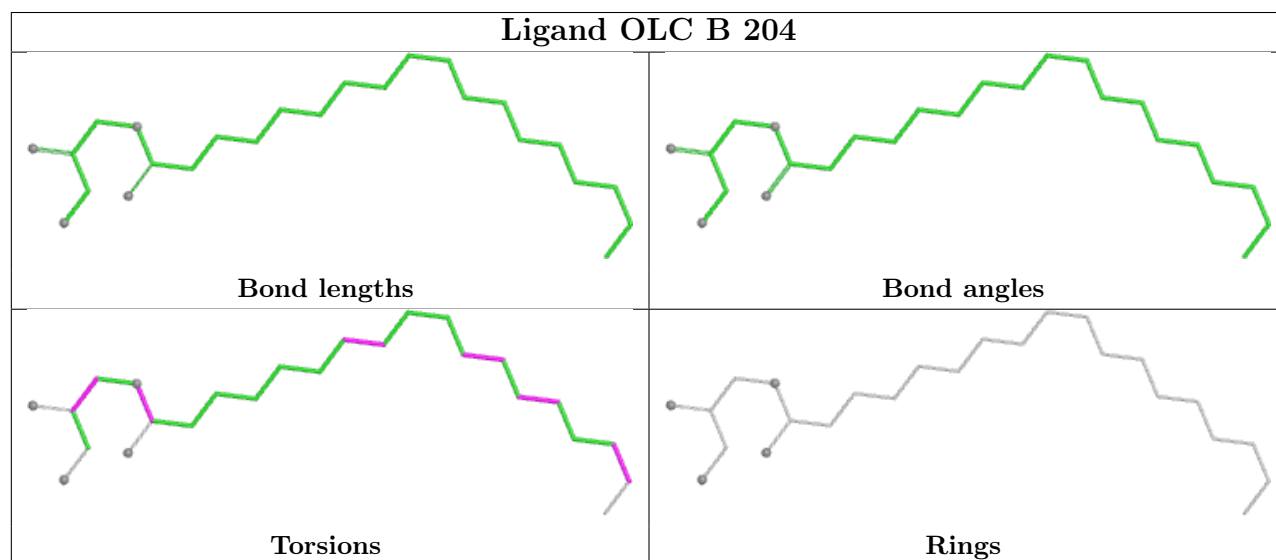
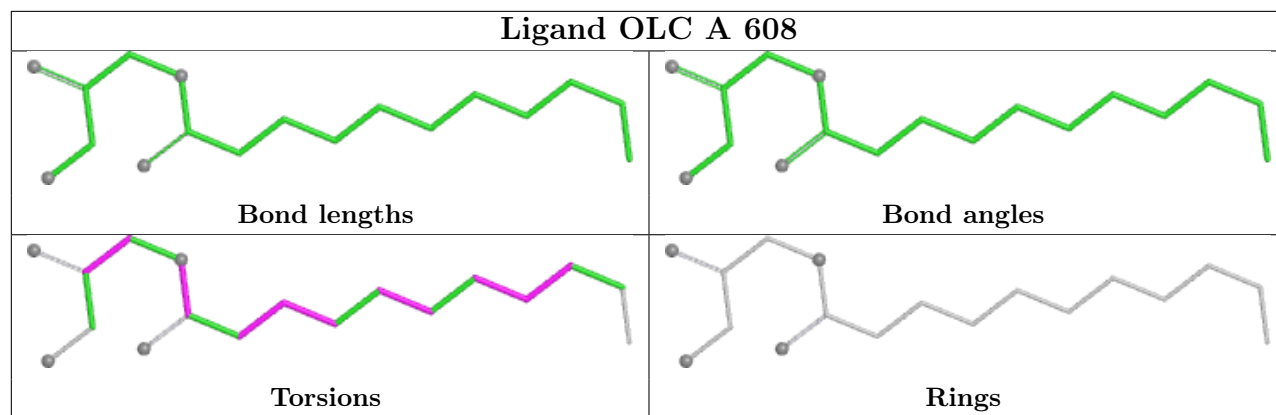
Continued from previous page...

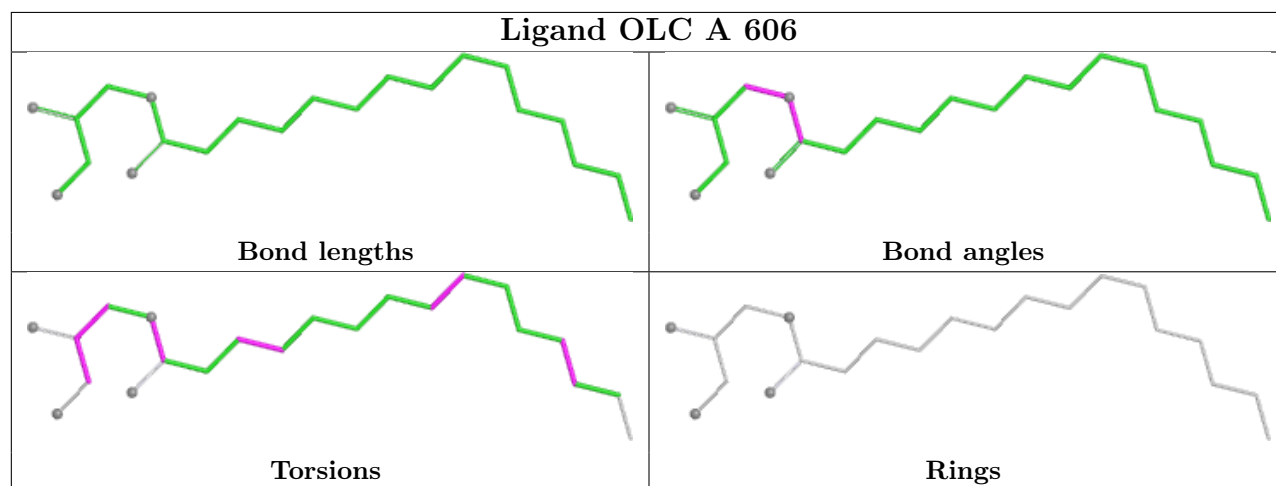
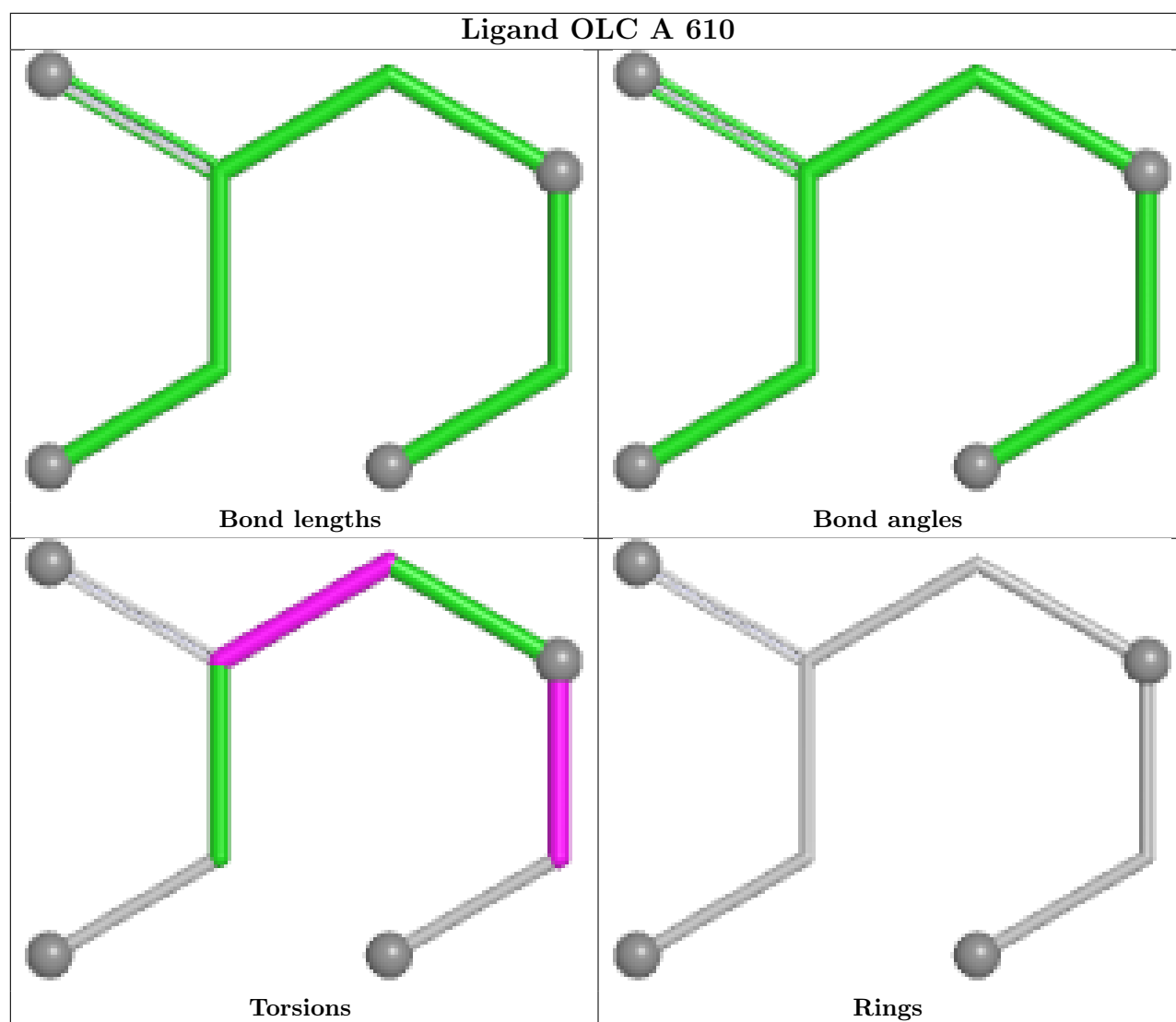
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	604	PER	3	0
8	A	611	OLC	4	0
6	A	603	HAS	4	0
8	C	102	OLC	3	0
5	A	602	HEM	3	0
8	A	614	OLC	1	0
8	A	615	OLC	3	0
8	B	202	OLC	2	0
8	C	101	OLC	3	0
8	A	605	OLC	4	0

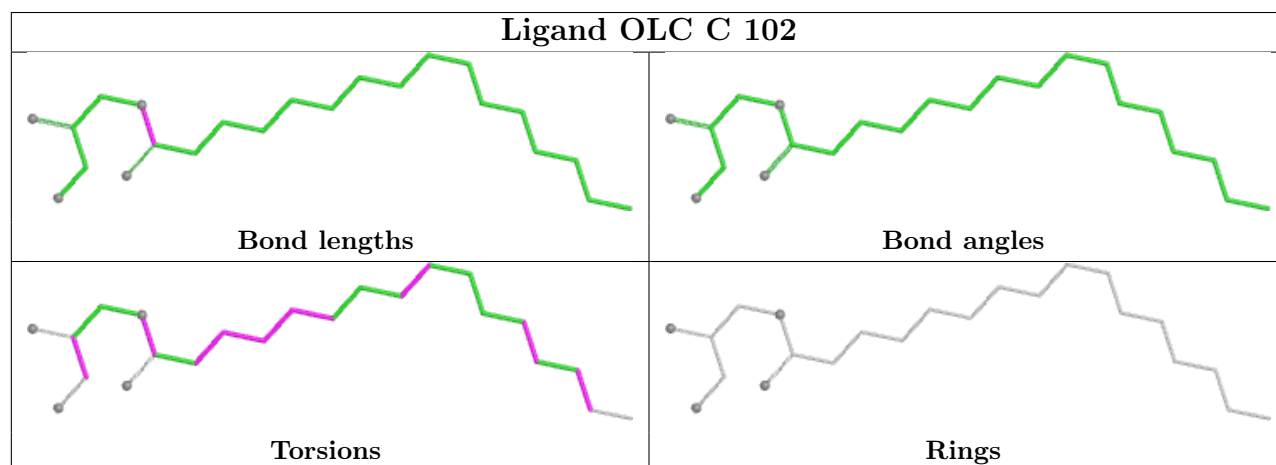
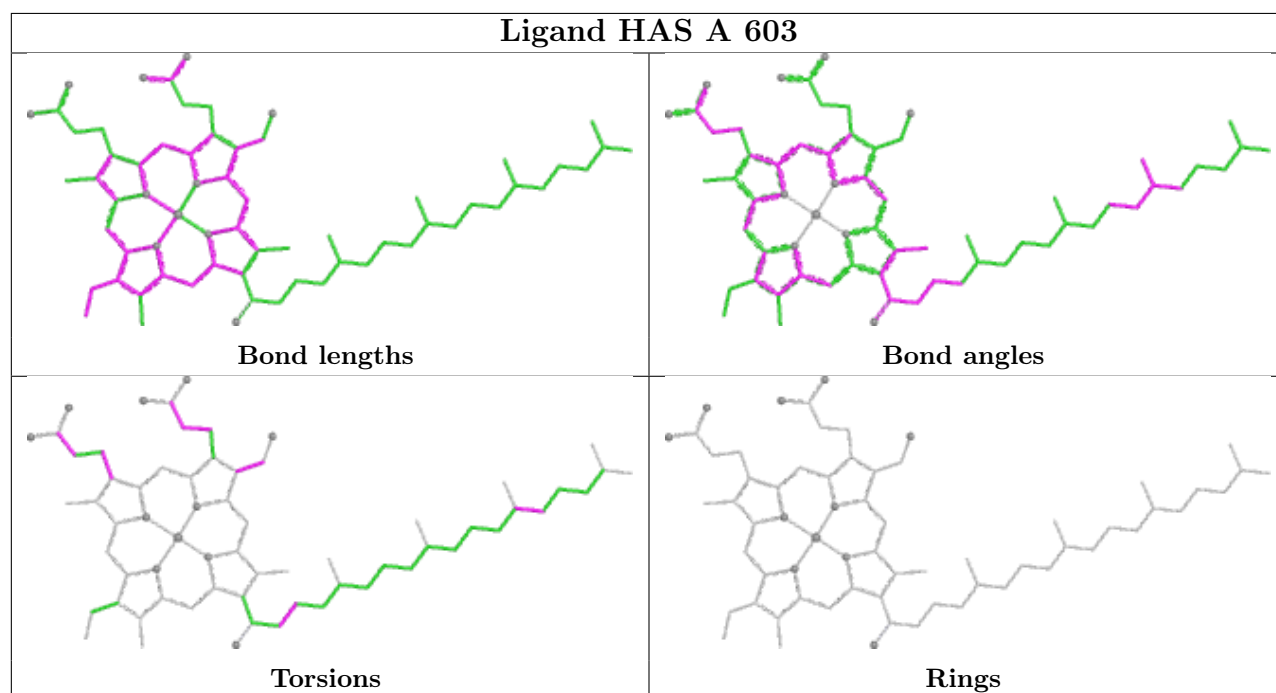
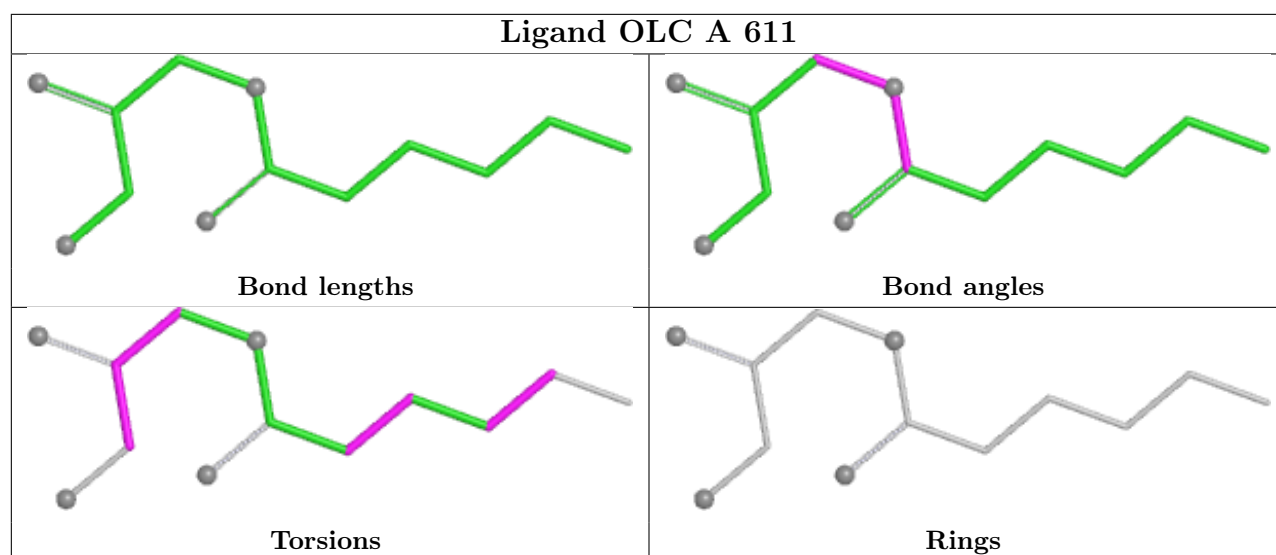
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

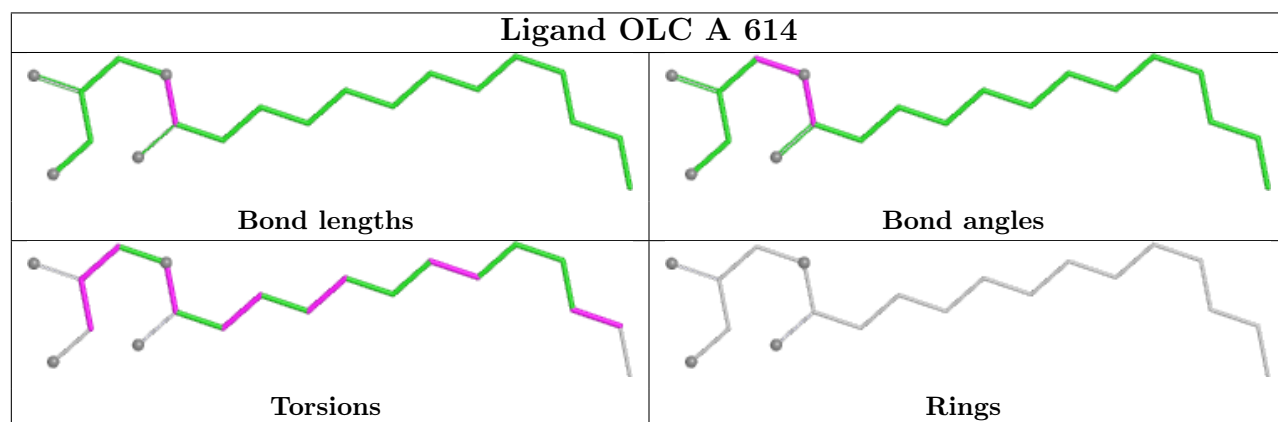
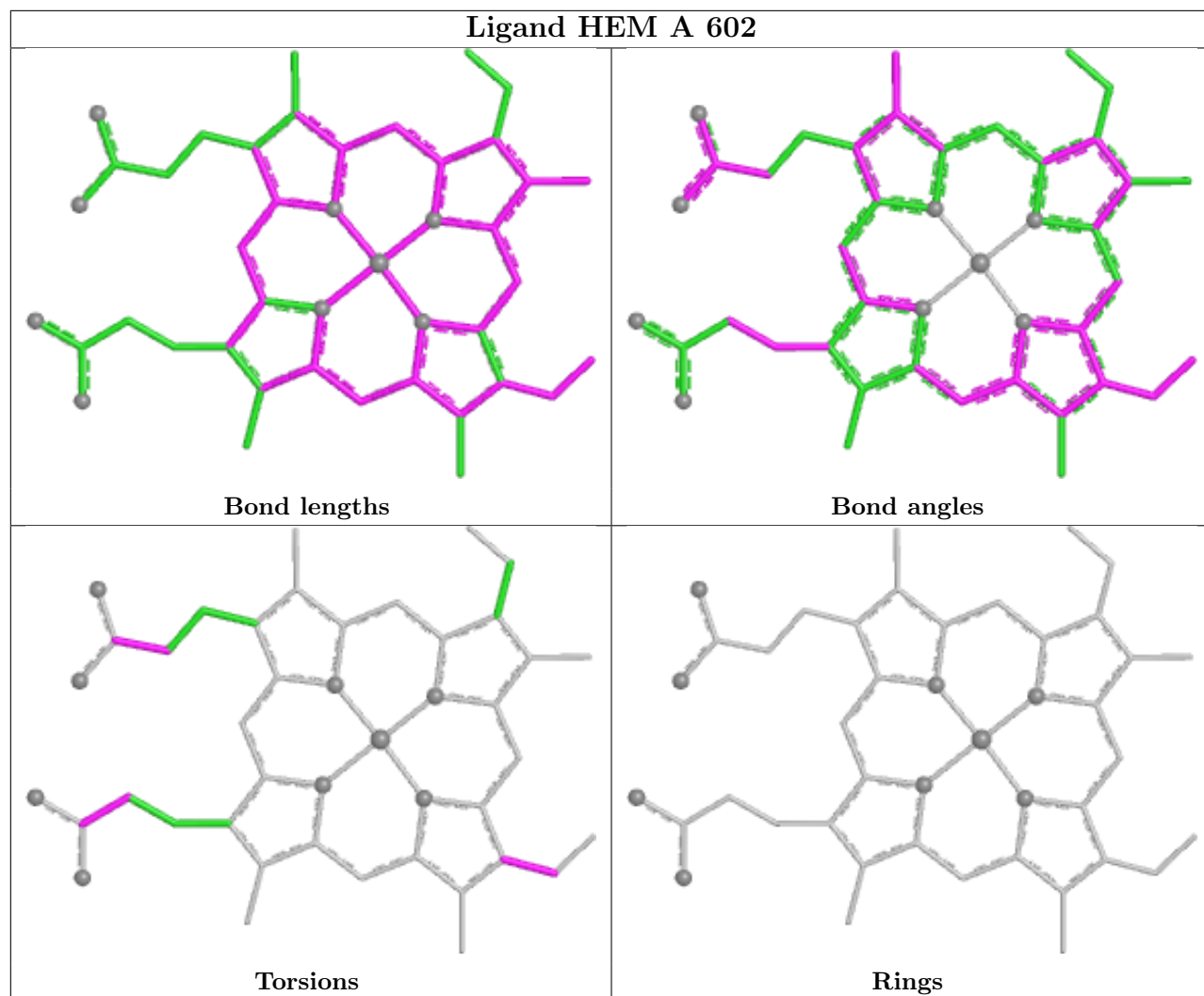


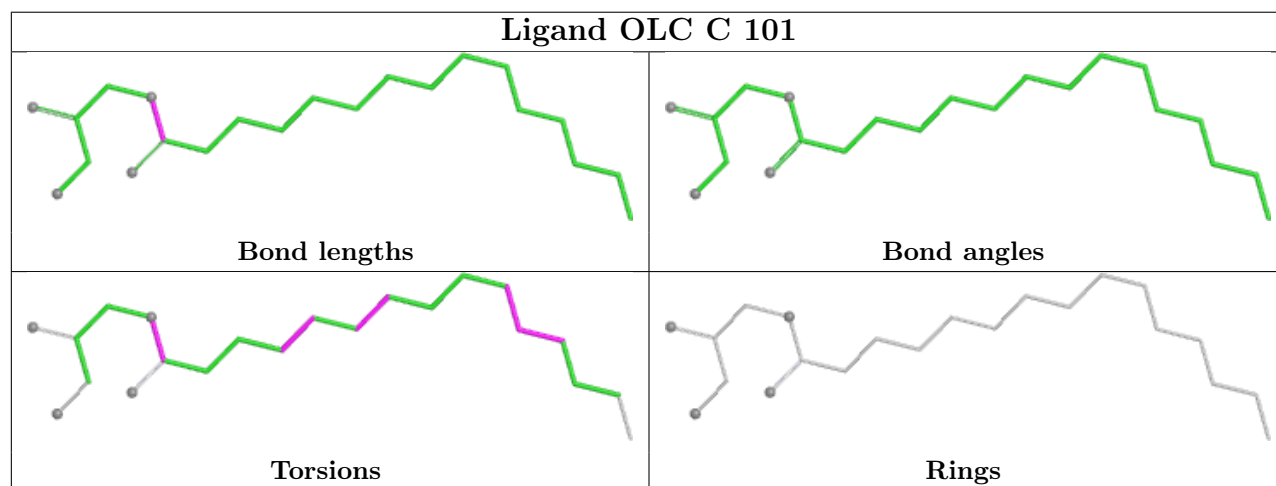
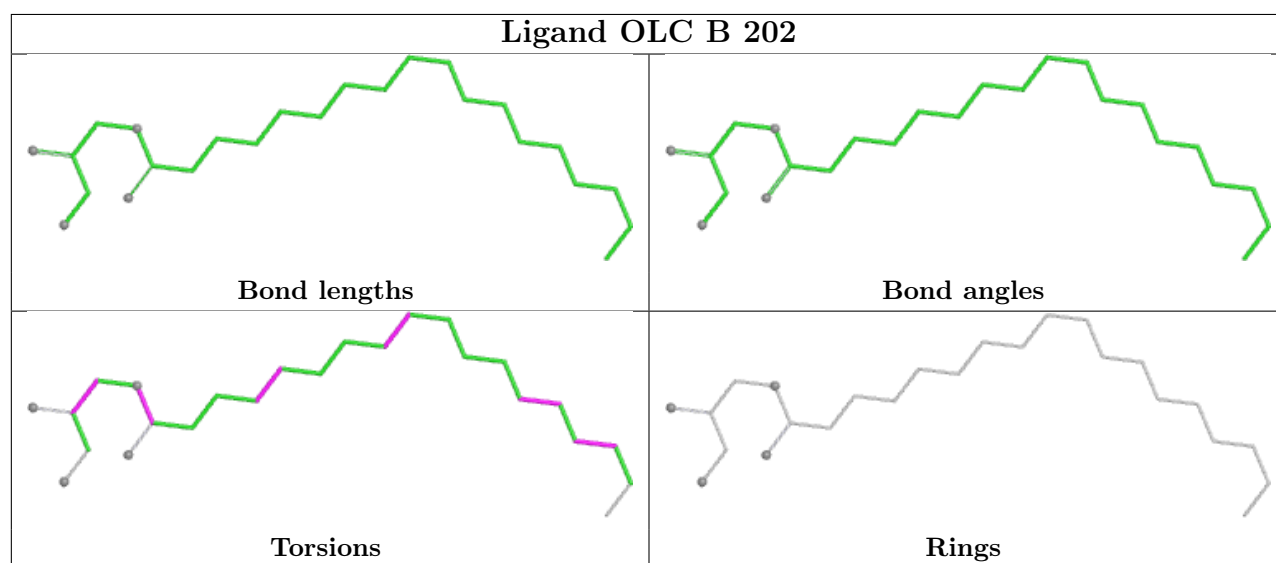
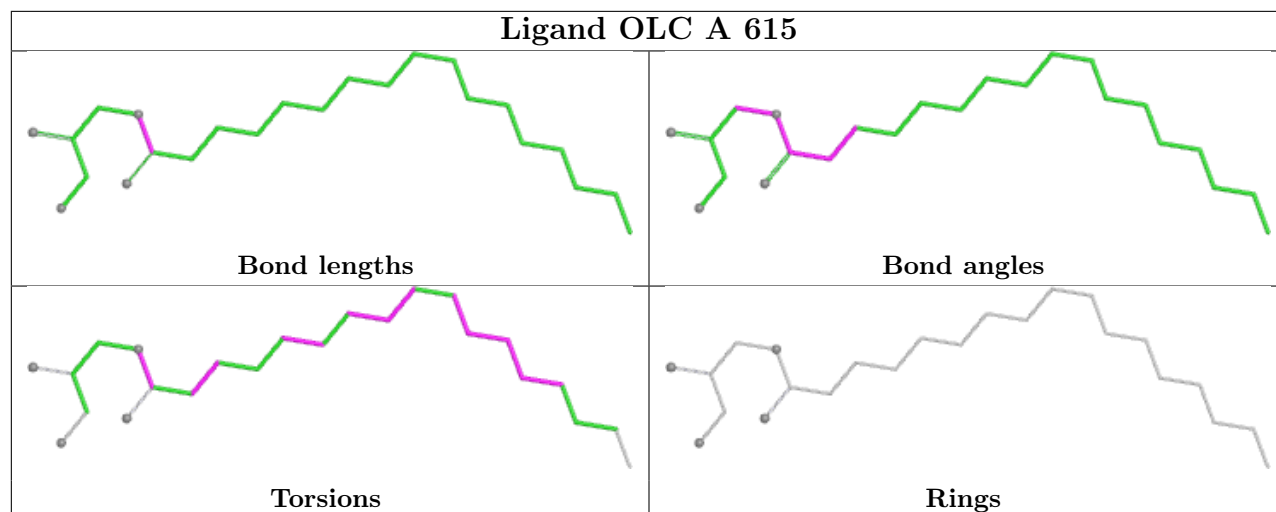


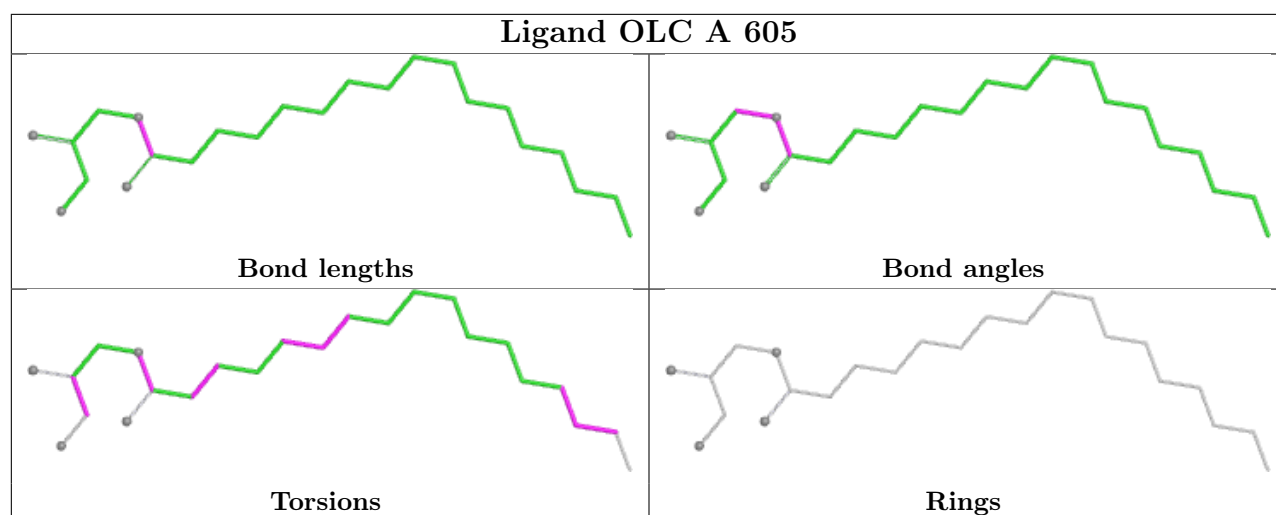












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	554/569 (97%)	-0.59	3 (0%) 87 83	16, 32, 57, 86	2 (0%)
2	B	166/168 (98%)	-0.67	0 100 100	21, 32, 49, 73	1 (0%)
3	C	31/34 (91%)	-0.62	0 100 100	25, 30, 43, 50	0
All	All	751/771 (97%)	-0.61	3 (0%) 88 85	16, 32, 54, 86	3 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	SER	2.4
1	A	10	ARG	2.3
1	A	495	ARG	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	OLC	A	611	13/25	0.71	0.17	50,67,74,83	0

Continued on next page...

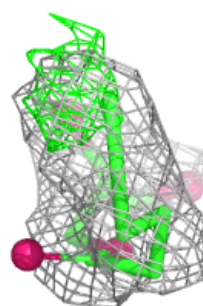
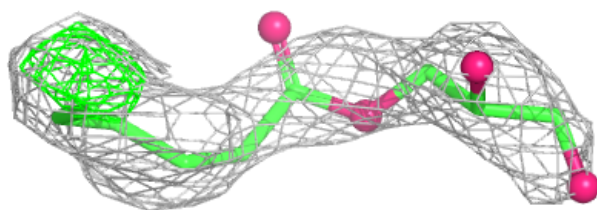
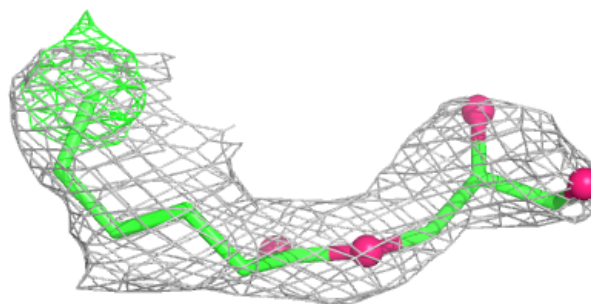
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	OLC	C	102	23/25	0.75	0.14	50,65,91,92	0
8	OLC	C	101	22/25	0.79	0.14	39,52,84,101	0
8	OLC	A	609	16/25	0.80	0.15	36,64,100,105	0
8	OLC	A	605	24/25	0.82	0.13	45,59,71,71	0
8	OLC	A	606	22/25	0.84	0.11	38,51,60,66	0
8	OLC	A	614	20/25	0.85	0.13	41,46,81,82	0
8	OLC	A	615	24/25	0.85	0.13	43,59,75,81	0
8	OLC	B	202	25/25	0.86	0.13	37,56,68,82	0
8	OLC	B	204	25/25	0.86	0.13	40,58,74,75	0
8	OLC	A	607	21/25	0.88	0.09	41,51,53,54	0
8	OLC	A	612	20/25	0.88	0.12	45,60,68,69	0
8	OLC	A	613	24/25	0.88	0.11	43,58,68,70	0
8	OLC	B	203	25/25	0.89	0.12	37,53,84,91	0
8	OLC	A	610	8/25	0.91	0.10	57,60,64,66	0
7	PER	A	604	2/2	0.92	0.15	36,36,36,38	0
8	OLC	A	608	18/25	0.94	0.09	31,55,68,76	0
6	HAS	A	603	65/65	0.98	0.06	25,28,35,40	0
5	HEM	A	602	43/43	0.98	0.07	19,22,27,31	0
4	CU	A	601	1/1	0.99	0.03	29,29,29,29	0
9	CUA	B	201	2/2	0.99	0.02	22,22,22,25	0

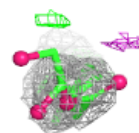
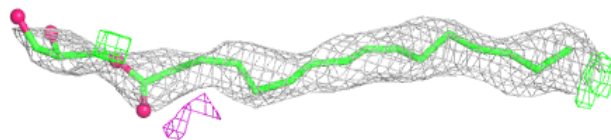
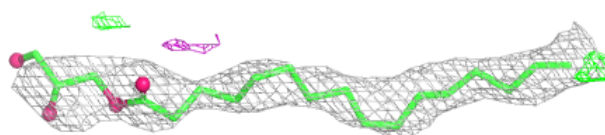
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 611:

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

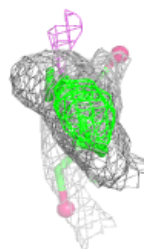
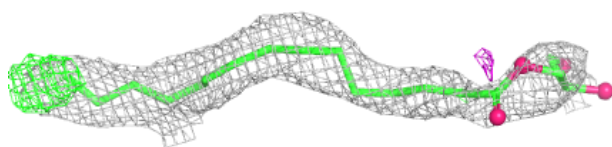
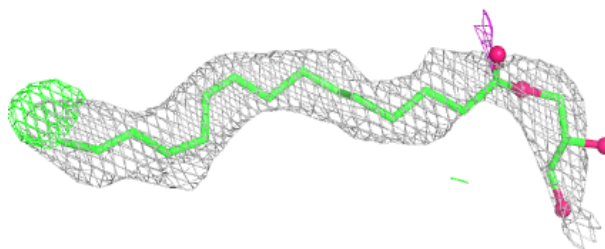
**Electron density around OLC C 102:**

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

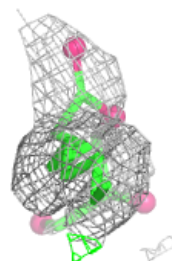
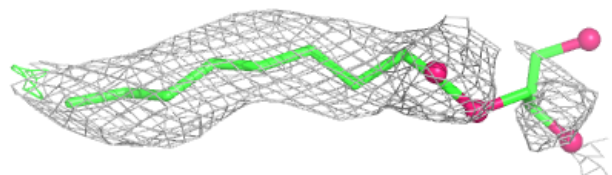
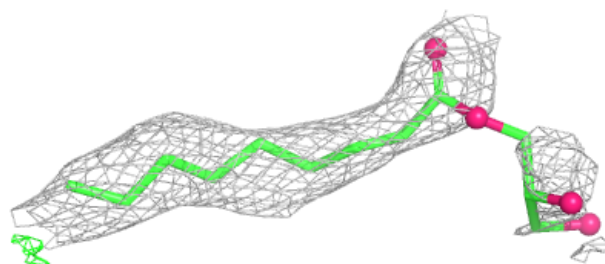


Electron density around OLC C 101:

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

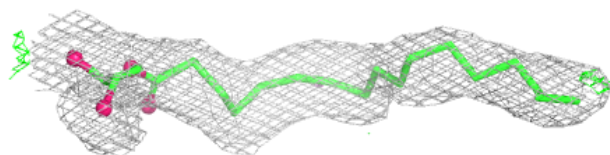
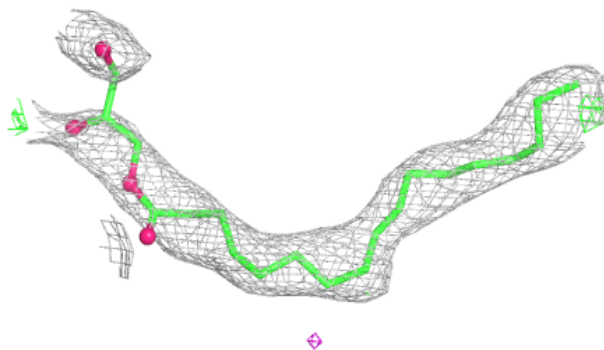
**Electron density around OLC A 609:**

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

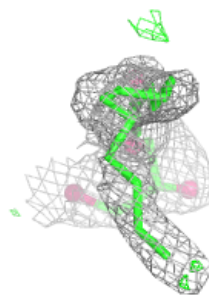
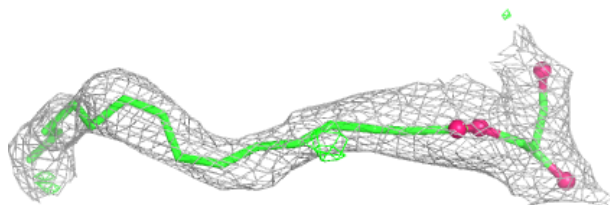
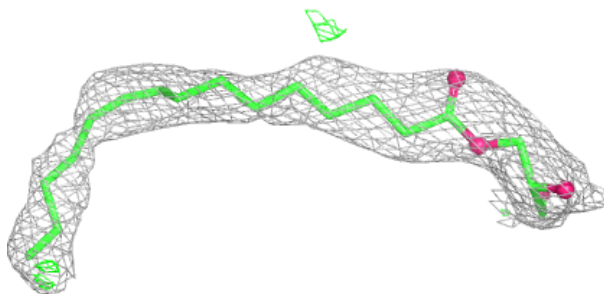


Electron density around OLC A 605:

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

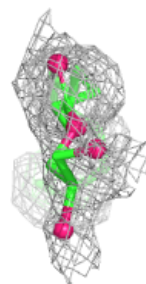
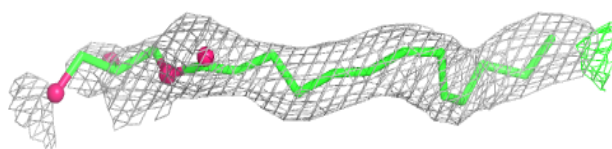
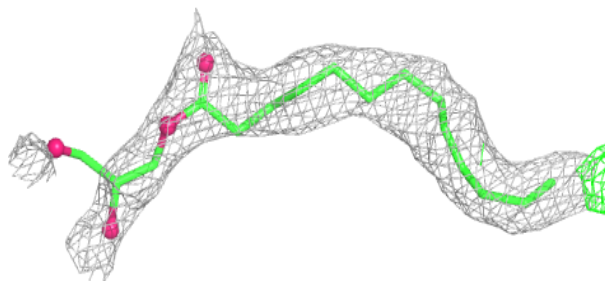
**Electron density around OLC A 606:**

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

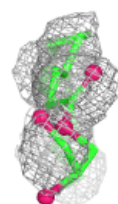
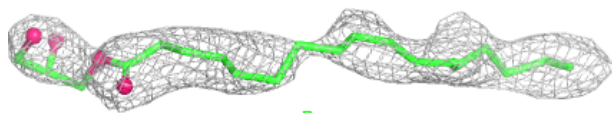
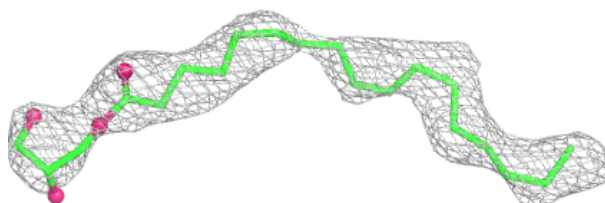


Electron density around OLC A 614:

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

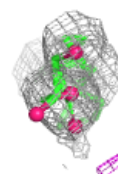
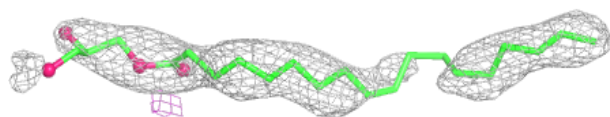
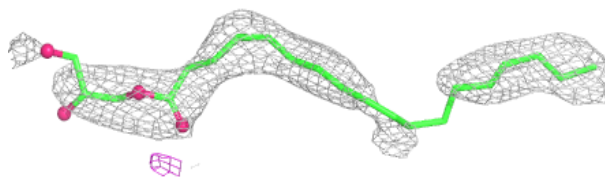
**Electron density around OLC A 615:**

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

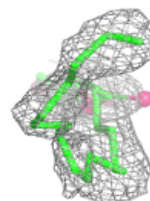
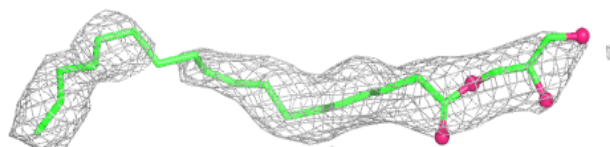
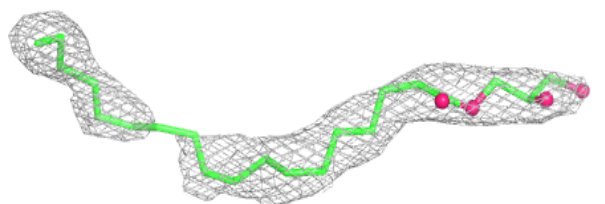


Electron density around OLC B 202:

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

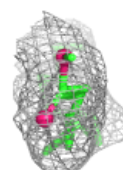
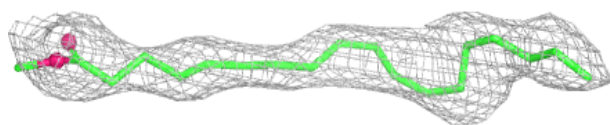
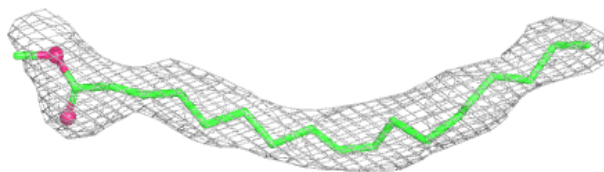
**Electron density around OLC B 204:**

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

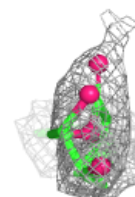
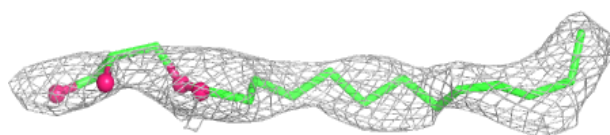
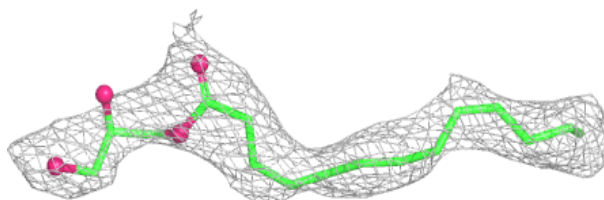


Electron density around OLC A 607:

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

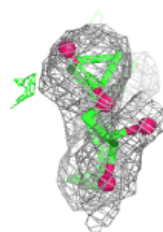
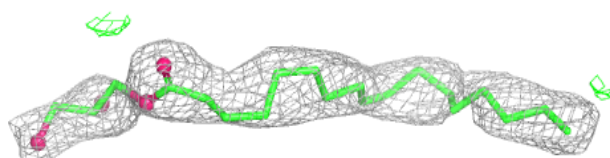
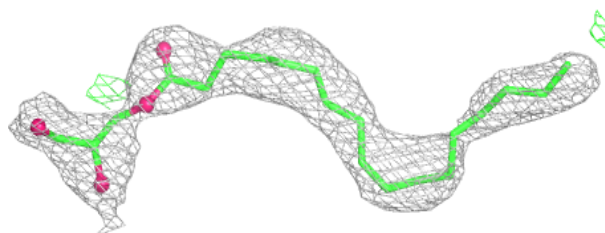
**Electron density around OLC A 612:**

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

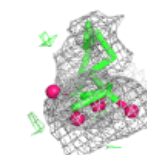
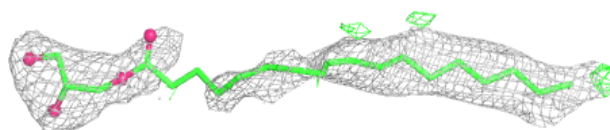
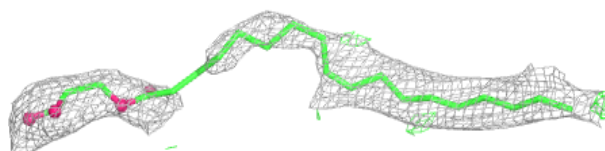


Electron density around OLC A 613:

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

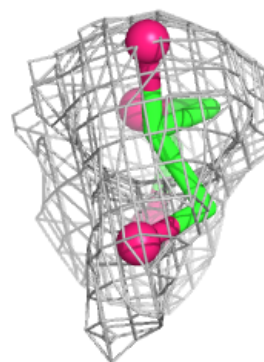
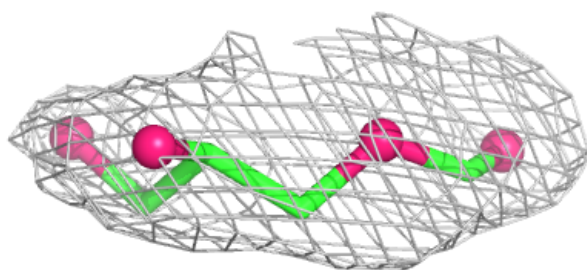
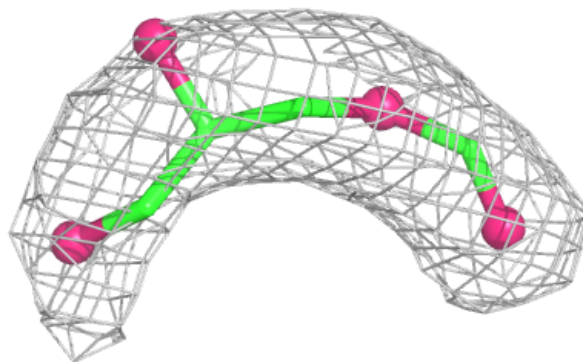
**Electron density around OLC B 203:**

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

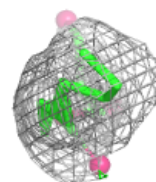
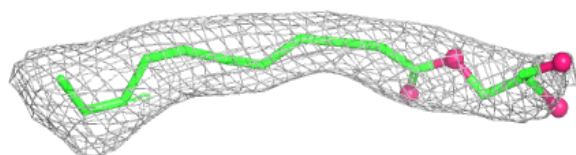
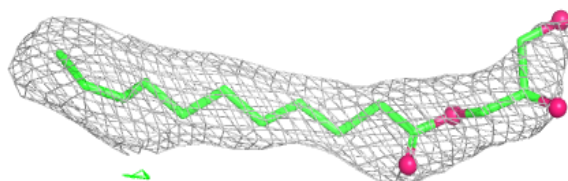


Electron density around OLC A 610:

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

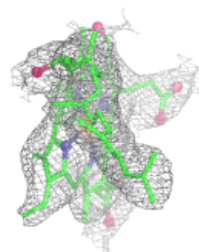
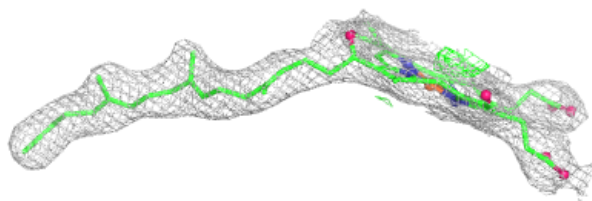
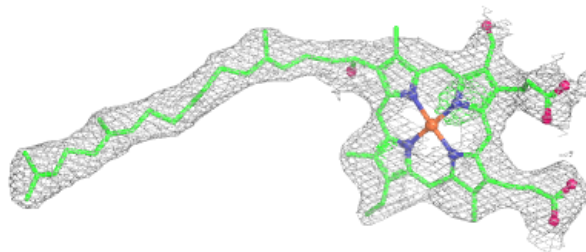
**Electron density around OLC A 608:**

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



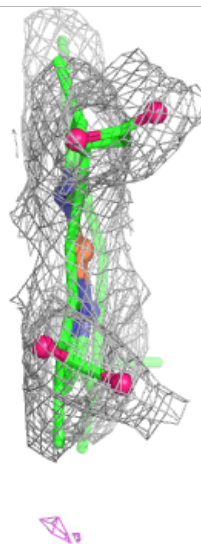
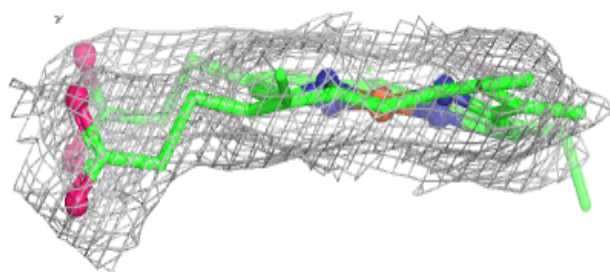
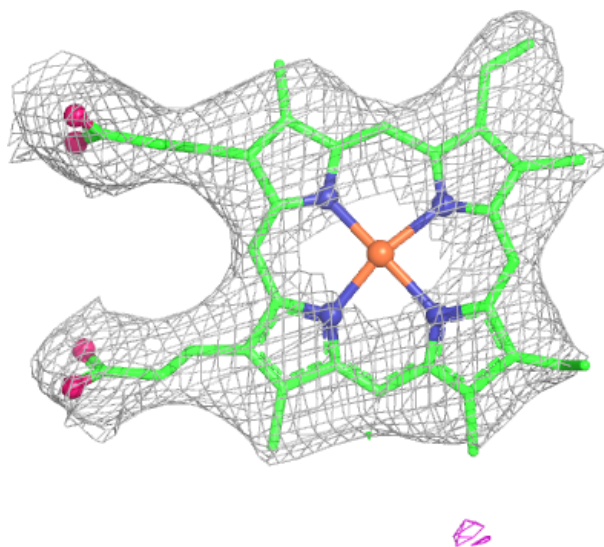
Electron density around HAS A 603:

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



Electron density around HEM A 602:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.