



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:46 AM UTC

PDB ID : 5ITE / pdb\_00005ite  
Title : 2.2-Angstrom in meso crystal structure of Haloquadratum Walsbyi Bacteriorhodopsin (HwBR) from Octylglucoside (OG) Detergent Micelles  
Authors : Broecker, J.; Eger, B.T.; Ernst, O.P.  
Deposited on : 2016-03-16  
Resolution : 2.18 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](mailto: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>.

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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

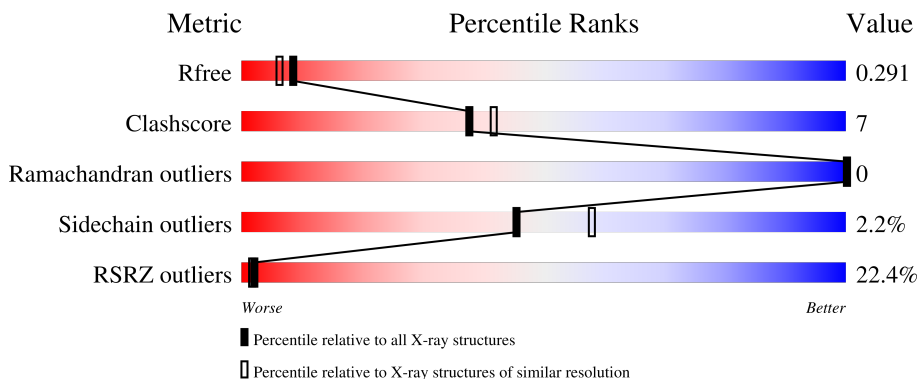
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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  $\geq 3$ , 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	268	19% (Poor fit) 74% (0 outliers) 12% (1 outlier) 15% (2+ outliers)
1	B	268	15% (Poor fit) 73% (0 outliers) 12% (1 outlier) 15% (2+ outliers)
1	C	268	23% (Poor fit) 72% (0 outliers) 12% (1 outlier) 15% (2+ outliers)

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5686 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 Bacteriorhodopsin-I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	228	Total 1777	C 1184	N 274	O 312	S 7	0	3	0
1	B	228	Total 1772	C 1181	N 271	O 313	S 7	0	3	0
1	C	228	Total 1783	C 1187	N 275	O 314	S 7	0	4	0

There are 48 discrepancies between the modelled and reference sequences:

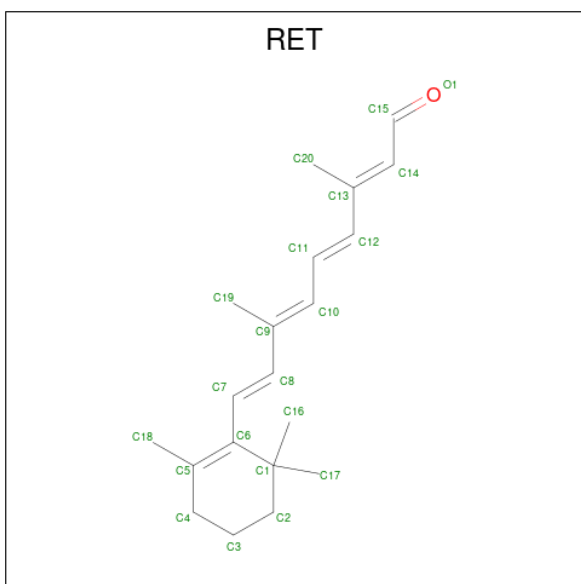
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q18DH8
A	2	ALA	-	expression tag	UNP Q18DH8
A	255	LEU	-	expression tag	UNP Q18DH8
A	256	VAL	-	expression tag	UNP Q18DH8
A	257	PRO	-	expression tag	UNP Q18DH8
A	258	ARG	-	expression tag	UNP Q18DH8
A	259	GLY	-	expression tag	UNP Q18DH8
A	260	SER	-	expression tag	UNP Q18DH8
A	261	LEU	-	expression tag	UNP Q18DH8
A	262	GLU	-	expression tag	UNP Q18DH8
A	263	HIS	-	expression tag	UNP Q18DH8
A	264	HIS	-	expression tag	UNP Q18DH8
A	265	HIS	-	expression tag	UNP Q18DH8
A	266	HIS	-	expression tag	UNP Q18DH8
A	267	HIS	-	expression tag	UNP Q18DH8
A	268	HIS	-	expression tag	UNP Q18DH8
B	1	MET	-	initiating methionine	UNP Q18DH8
B	2	ALA	-	expression tag	UNP Q18DH8
B	255	LEU	-	expression tag	UNP Q18DH8
B	256	VAL	-	expression tag	UNP Q18DH8
B	257	PRO	-	expression tag	UNP Q18DH8
B	258	ARG	-	expression tag	UNP Q18DH8
B	259	GLY	-	expression tag	UNP Q18DH8

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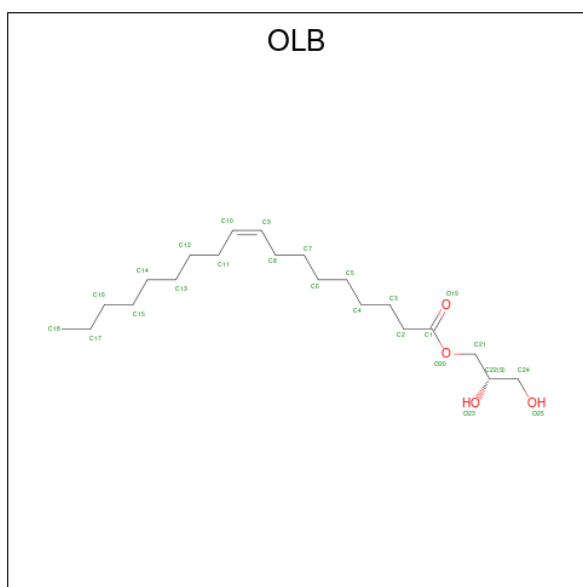
Chain	Residue	Modelled	Actual	Comment	Reference
B	260	SER	-	expression tag	UNP Q18DH8
B	261	LEU	-	expression tag	UNP Q18DH8
B	262	GLU	-	expression tag	UNP Q18DH8
B	263	HIS	-	expression tag	UNP Q18DH8
B	264	HIS	-	expression tag	UNP Q18DH8
B	265	HIS	-	expression tag	UNP Q18DH8
B	266	HIS	-	expression tag	UNP Q18DH8
B	267	HIS	-	expression tag	UNP Q18DH8
B	268	HIS	-	expression tag	UNP Q18DH8
C	1	MET	-	initiating methionine	UNP Q18DH8
C	2	ALA	-	expression tag	UNP Q18DH8
C	255	LEU	-	expression tag	UNP Q18DH8
C	256	VAL	-	expression tag	UNP Q18DH8
C	257	PRO	-	expression tag	UNP Q18DH8
C	258	ARG	-	expression tag	UNP Q18DH8
C	259	GLY	-	expression tag	UNP Q18DH8
C	260	SER	-	expression tag	UNP Q18DH8
C	261	LEU	-	expression tag	UNP Q18DH8
C	262	GLU	-	expression tag	UNP Q18DH8
C	263	HIS	-	expression tag	UNP Q18DH8
C	264	HIS	-	expression tag	UNP Q18DH8
C	265	HIS	-	expression tag	UNP Q18DH8
C	266	HIS	-	expression tag	UNP Q18DH8
C	267	HIS	-	expression tag	UNP Q18DH8
C	268	HIS	-	expression tag	UNP Q18DH8

- Molecule 2 is RETINAL (CCD ID: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



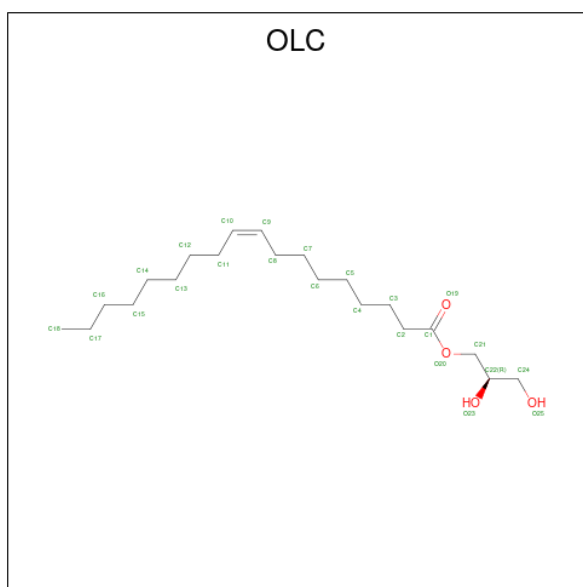
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 20 20	0	0
2	B	1	Total C 20 20	0	0
2	C	1	Total C 20 20	0	0

- Molecule 3 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLB) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 25 21 4	0	0
3	B	1	Total C O 25 21 4	0	0
3	C	1	Total C O 25 21 4	0	0

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 25 21 4	0	0
4	B	1	Total C O 25 21 4	0	0
4	B	1	Total C O 25 21 4	0	0
4	B	1	Total C O 25 21 4	0	0
4	C	1	Total C O 25 21 4	0	0
4	C	1	Total C O 25 21 4	0	0

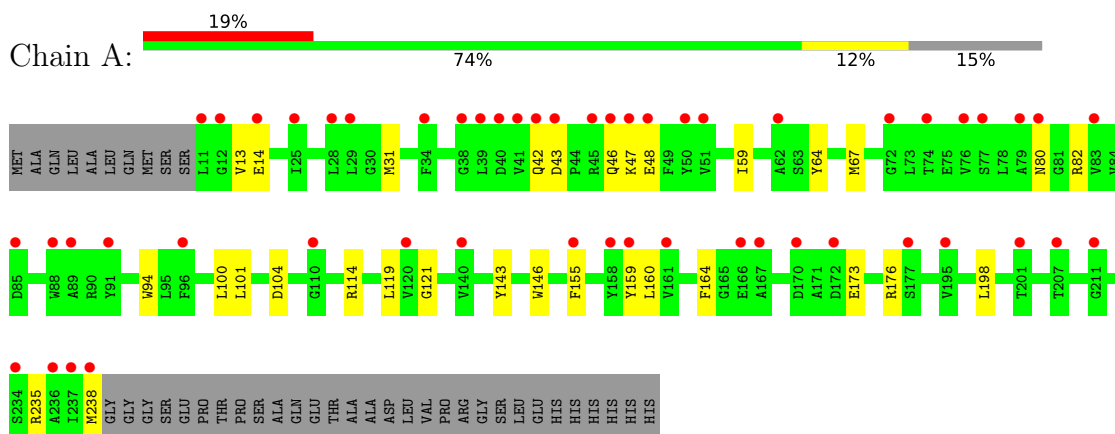
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	25	Total O 25 25	0	0
5	B	21	Total O 21 21	0	0
5	C	23	Total O 23 23	0	0

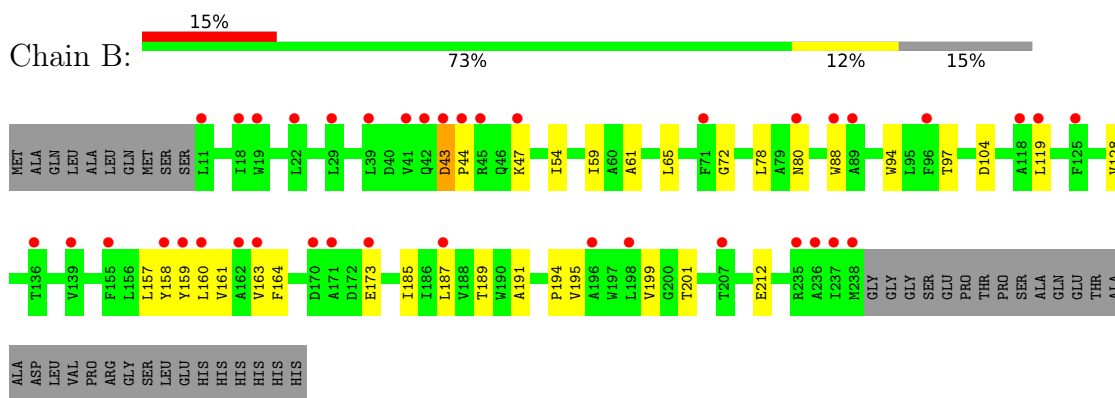
### 3 Residue-property plots

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.

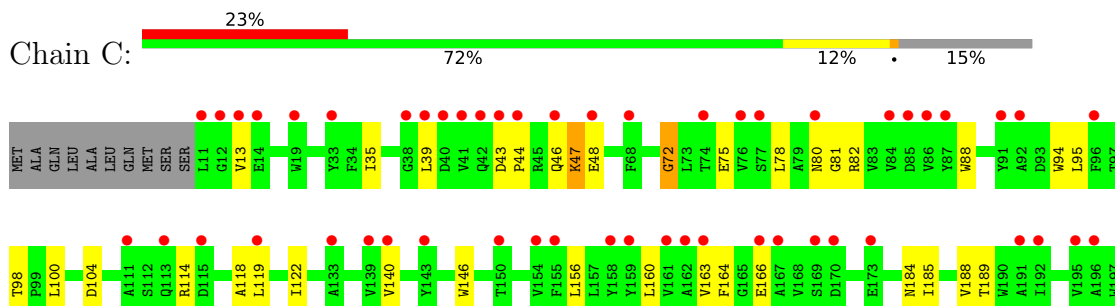
- Molecule 1: Bacteriorhodopsin-I



- Molecule 1: Bacteriorhodopsin-I



- Molecule 1: Bacteriorhodopsin-I



L198	E202	L206	T207	F216	S234	R235	A236	L237	N238	GLY	GLY	GLY	SER	GLU	PRO	THR	PRO	SER	ALA	GLN	GLU	THR	ALA	ALA	ALA	ASP	LEU	VAL	PRO	ARG	GLY	SER	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.44Å 61.56Å 119.69Å 90.00° 116.80° 90.00°	Depositor
Resolution (Å)	47.51 – 2.18 47.51 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.51-2.18) 99.1 (47.51-2.18)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.18Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.259 , 0.289 0.262 , 0.291	Depositor DCC
$R_{free}$ test set	1738 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtrriage
Anisotropy	0.147	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	5686	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5752e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OLC, RET, OLB

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	0.60	0/1822	0.99	4/2486 (0.2%)
1	B	0.58	0/1817	0.98	4/2480 (0.2%)
1	C	0.58	0/1828	0.98	7/2494 (0.3%)
All	All	0.59	0/5467	0.98	15/7460 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	VAL	N-CA-C	-9.76	101.35	110.53
1	B	43	ASP	CA-C-N	6.47	126.23	119.05
1	B	43	ASP	C-N-CA	6.47	126.23	119.05
1	C	198	LEU	N-CA-C	6.43	118.29	111.28
1	C	39	LEU	N-CA-C	5.99	118.58	111.33
1	B	97	THR	N-CA-C	5.89	117.78	111.36
1	C	72	GLY	N-CA-C	-5.33	107.43	115.32
1	A	143	TYR	N-CA-C	5.30	117.14	111.36
1	C	81	GLY	N-CA-C	5.26	122.11	115.42
1	A	101	LEU	N-CA-C	-5.24	105.57	111.28
1	A	43	ASP	CA-C-N	5.23	124.86	119.05
1	A	43	ASP	C-N-CA	5.23	124.86	119.05
1	B	161	VAL	N-CA-C	5.18	115.39	110.42
1	C	98	THR	CA-C-N	-5.04	113.46	119.05
1	C	98	THR	C-N-CA	-5.04	113.46	119.05

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1777	0	1831	21	0
1	B	1772	0	1822	23	0
1	C	1783	0	1834	27	0
2	A	20	0	27	2	0
2	B	20	0	27	3	0
2	C	20	0	27	4	0
3	A	25	0	40	2	0
3	B	25	0	40	4	0
3	C	25	0	40	5	0
4	A	25	0	40	2	0
4	B	75	0	120	12	0
4	C	50	0	80	5	0
5	A	25	0	0	0	0
5	B	21	0	0	0	0
5	C	23	0	0	1	0
All	All	5686	0	5928	81	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (81) 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:173:GLU:OE1	1:A:176:ARG:NH2	2.13	0.80
1:B:191:ALA:HB1	4:B:304:OLC:H16	1.66	0.77
1:B:94:TRP:CD1	2:B:301:RET:H14	2.20	0.77
4:C:302:OLC:H9	3:C:304:OLB:H4A	1.67	0.77
1:B:128:VAL:HG11	4:B:302:OLC:H12A	1.68	0.74
1:A:59:ILE:HG23	4:B:302:OLC:H13A	1.72	0.72
1:A:94:TRP:CD1	2:A:301:RET:H14	2.25	0.71
1:B:61:ALA:HB1	3:B:305:OLB:H32	1.76	0.67
1:C:146:TRP:CE2	1:C:198:LEU:HD13	2.30	0.66
1:A:114:ARG:HA	3:C:304:OLB:H24A	1.78	0.66
1:A:48:GLU:HG3	4:B:302:OLC:H24A	1.81	0.63
1:A:146:TRP:CE2	1:A:198:LEU:HD13	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LEU:HD21	3:C:304:OLB:H4	1.81	0.61
1:C:47:LYS:NZ	5:C:401:HOH:O	2.11	0.60
1:C:80:ASN:HD21	1:C:82:ARG:HB2	1.66	0.60
1:B:72:GLY:HA2	1:B:88:TRP:CE2	2.36	0.60
1:B:78:LEU:HB2	1:B:80:ASN:OD1	2.05	0.57
1:C:43:ASP:HB3	1:C:46:GLN:HE21	1.69	0.57
1:C:78:LEU:HB2	1:C:80:ASN:OD1	2.04	0.57
1:A:46:GLN:NE2	1:A:238:MET:SD	2.76	0.56
1:C:163:VAL:O	1:C:166:GLU:HG2	2.06	0.56
2:B:301:RET:H8	2:B:301:RET:H161	1.86	0.56
1:C:94:TRP:CD1	2:C:301:RET:H14	2.41	0.56
1:B:72:GLY:HA2	1:B:88:TRP:CZ2	2.41	0.54
1:A:114:ARG:NE	1:C:48:GLU:OE2	2.33	0.54
1:A:80:ASN:HB3	1:A:82[A]:ARG:H	1.74	0.52
1:C:160:LEU:O	1:C:164:PHE:HB2	2.09	0.52
1:C:119:LEU:HD12	1:C:164:PHE:CZ	2.45	0.52
1:A:80:ASN:HB3	1:A:82[B]:ARG:HB2	1.92	0.51
1:A:13:VAL:HG12	1:A:14:GLU:HG3	1.92	0.51
2:A:301:RET:H8	2:A:301:RET:H161	1.91	0.51
1:A:80:ASN:HB3	1:A:82[B]:ARG:H	1.74	0.51
1:C:80:ASN:ND2	1:C:82:ARG:HB2	2.25	0.50
1:A:114:ARG:HD3	1:C:48:GLU:HG2	1.94	0.50
1:A:59:ILE:HD11	4:B:302:OLC:H7	1.92	0.50
4:A:303:OLC:H13A	4:B:302:OLC:H4A	1.94	0.50
1:A:160:LEU:O	1:A:164:PHE:HB2	2.12	0.49
1:C:44:PRO:O	1:C:48:GLU:HG3	2.12	0.49
1:B:160:LEU:O	1:B:164:PHE:HB2	2.13	0.48
1:B:65:LEU:HD22	3:B:305:OLB:H36	1.95	0.48
1:A:119:LEU:HD12	1:A:164:PHE:CZ	2.49	0.48
1:C:72:GLY:HA2	1:C:88:TRP:CZ2	2.49	0.47
1:B:44:PRO:O	1:B:47:LYS:HG2	2.15	0.47
1:C:95:LEU:HD11	4:C:302:OLC:H18A	1.97	0.47
1:B:59:ILE:HG12	4:C:303:OLC:H17	1.96	0.46
1:B:185:ILE:O	1:B:189:THR:HG23	2.16	0.46
3:B:305:OLB:C3	1:C:122:ILE:HG12	2.46	0.45
1:C:185:ILE:O	1:C:189:THR:HG23	2.17	0.45
1:C:43:ASP:HB3	1:C:46:GLN:NE2	2.32	0.44
1:B:43:ASP:HA	1:B:44:PRO:HD3	1.84	0.44
1:B:44:PRO:HA	1:B:47:LYS:HD3	2.00	0.44
1:B:158:TYR:CD1	4:B:304:OLC:H4	2.52	0.44
1:B:201[A]:THR:HG22	1:B:212:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:302:OLB:H25	3:A:302:OLB:H20	1.64	0.43
1:B:54:ILE:HD13	3:B:305:OLB:H24A	2.00	0.43
3:A:302:OLB:O23	1:C:35:ILE:HG12	2.18	0.43
1:B:195:VAL:O	1:B:199:VAL:HG13	2.19	0.43
1:C:72:GLY:HA2	1:C:88:TRP:CE2	2.53	0.43
1:C:118:ALA:HB2	4:C:303:OLC:O20	2.19	0.42
1:B:159:TYR:O	1:B:163:VAL:HB	2.19	0.42
1:C:119:LEU:HD23	1:C:119:LEU:HA	1.83	0.42
4:A:303:OLC:H12A	4:A:303:OLC:H15A	1.86	0.42
4:B:304:OLC:H8	4:B:304:OLC:H11A	1.65	0.42
2:C:301:RET:H171	2:C:301:RET:H8	2.00	0.42
4:B:303:OLC:H11	4:B:303:OLC:H8	1.64	0.42
1:B:158:TYR:CE1	4:B:304:OLC:H2A	2.55	0.42
1:C:114:ARG:O	4:C:303:OLC:H3	2.20	0.42
1:A:155:PHE:HD2	1:A:159:TYR:CE2	2.38	0.42
1:C:95:LEU:HD12	1:C:95:LEU:HA	1.92	0.42
1:A:31:MET:HE2	1:A:31:MET:HB3	1.96	0.41
2:C:301:RET:H181	2:C:301:RET:H7	1.57	0.41
1:B:158:TYR:HD1	4:B:304:OLC:H4	1.85	0.41
1:A:100:LEU:HD21	4:B:302:OLC:H3A	2.02	0.41
2:C:301:RET:H11	2:C:301:RET:H191	1.94	0.41
1:B:194:PRO:HD3	2:B:301:RET:H7	2.03	0.40
1:A:121:GLY:HA2	3:C:304:OLB:H5A	2.02	0.40
1:B:157:LEU:HD22	1:B:187:LEU:HD23	2.04	0.40
1:A:64:TYR:HA	1:A:67:MET:HE3	2.04	0.40
1:C:80:ASN:OD1	1:C:82:ARG:N	2.48	0.40
1:C:184:ASN:O	1:C:188:VAL:HG12	2.21	0.40
3:C:304:OLB:H241	3:C:304:OLB:H211	1.70	0.40

There are no symmetry-related clashes.

## 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	229/268 (85%)	227 (99%)	2 (1%)	0	100	100
1	B	229/268 (85%)	228 (100%)	1 (0%)	0	100	100
1	C	230/268 (86%)	229 (100%)	1 (0%)	0	100	100
All	All	688/804 (86%)	684 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	184/212 (87%)	180 (98%)	4 (2%)	45	58
1	B	184/212 (87%)	181 (98%)	3 (2%)	55	68
1	C	185/212 (87%)	180 (97%)	5 (3%)	39	50
All	All	553/636 (87%)	541 (98%)	12 (2%)	45	58

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	47	LYS
1	A	104	ASP
1	A	235	ARG
1	B	104	ASP
1	B	119	LEU
1	B	173	GLU
1	C	47	LYS
1	C	75	GLU
1	C	104	ASP
1	C	140	VAL
1	C	156	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	46	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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$
4	OLC	A	303	-	24,24,24	0.95	1 (4%)	25,25,25	0.89	1 (4%)
3	OLB	A	302	-	24,24,24	0.94	1 (4%)	25,25,25	0.99	1 (4%)
4	OLC	B	302	-	24,24,24	0.93	1 (4%)	25,25,25	1.04	1 (4%)
4	OLC	B	303	-	24,24,24	0.93	1 (4%)	25,25,25	0.96	1 (4%)
4	OLC	B	304	-	24,24,24	0.94	1 (4%)	25,25,25	0.91	1 (4%)
2	RET	B	301	1	20,20,21	0.87	2 (10%)	27,27,28	1.74	6 (22%)
3	OLB	C	304	-	24,24,24	0.94	1 (4%)	25,25,25	0.92	1 (4%)
3	OLB	B	305	-	24,24,24	0.95	1 (4%)	25,25,25	1.05	2 (8%)
4	OLC	C	302	-	24,24,24	0.95	1 (4%)	25,25,25	0.92	1 (4%)
2	RET	C	301	1	20,20,21	0.90	2 (10%)	27,27,28	1.92	9 (33%)
2	RET	A	301	1	20,20,21	0.88	2 (10%)	27,27,28	1.71	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	OLC	C	303	-	24,24,24	0.96	1 (4%)	25,25,25	1.03	1 (4%)

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
4	OLC	A	303	-	-	4/24/24/24	-
3	OLB	A	302	-	-	6/24/24/24	-
4	OLC	B	302	-	-	2/24/24/24	-
4	OLC	B	303	-	-	1/24/24/24	-
4	OLC	B	304	-	-	2/24/24/24	-
2	RET	B	301	1	-	4/13/30/31	0/1/1/1
3	OLB	C	304	-	-	0/24/24/24	-
3	OLB	B	305	-	-	2/24/24/24	-
4	OLC	C	302	-	-	2/24/24/24	-
2	RET	C	301	1	-	0/13/30/31	0/1/1/1
2	RET	A	301	1	-	4/13/30/31	0/1/1/1
4	OLC	C	303	-	-	5/24/24/24	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	303	OLC	O20-C1	3.56	1.43	1.33
4	C	302	OLC	O20-C1	3.51	1.43	1.33
4	B	304	OLC	O20-C1	3.51	1.43	1.33
3	B	305	OLB	O20-C1	3.50	1.43	1.33
3	A	302	OLB	O20-C1	3.50	1.43	1.33
4	A	303	OLC	O20-C1	3.50	1.43	1.33
3	C	304	OLB	O20-C1	3.49	1.43	1.33
4	B	302	OLC	O20-C1	3.48	1.43	1.33
4	B	303	OLC	O20-C1	3.42	1.43	1.33
2	C	301	RET	C14-C13	2.54	1.35	1.33
2	A	301	RET	C11-C10	-2.52	1.35	1.43
2	C	301	RET	C11-C10	-2.46	1.35	1.43
2	B	301	RET	C14-C13	2.42	1.35	1.33
2	B	301	RET	C11-C10	-2.41	1.35	1.43
2	A	301	RET	C14-C13	2.40	1.35	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	RET	C18-C5-C6	-4.19	119.91	124.48
2	C	301	RET	C18-C5-C6	-4.11	120.00	124.48
2	B	301	RET	C18-C5-C6	-4.07	120.04	124.48
2	B	301	RET	C3-C4-C5	-3.56	107.71	114.06
2	C	301	RET	C10-C11-C12	-3.45	113.22	123.20
2	B	301	RET	C7-C8-C9	-3.26	121.42	126.23
2	C	301	RET	C3-C4-C5	-3.23	108.30	114.06
4	C	303	OLC	O20-C1-C2	2.94	120.81	111.83
3	B	305	OLB	O20-C1-C2	2.93	120.77	111.83
2	C	301	RET	C1-C6-C7	2.89	123.50	115.65
2	A	301	RET	C3-C4-C5	-2.87	108.95	114.06
2	C	301	RET	C19-C9-C8	2.84	122.43	118.09
3	A	302	OLB	O20-C1-C2	2.80	120.37	111.83
2	C	301	RET	C7-C6-C5	-2.77	115.18	121.56
4	B	302	OLC	O20-C1-C2	2.76	120.25	111.83
4	B	303	OLC	O20-C1-C2	2.72	120.14	111.83
2	A	301	RET	C7-C8-C9	-2.60	122.39	126.23
2	C	301	RET	C2-C3-C4	-2.50	105.79	111.28
2	B	301	RET	C11-C10-C9	-2.46	123.82	127.28
3	C	304	OLB	O20-C1-C2	2.44	119.28	111.83
2	A	301	RET	C10-C11-C12	-2.43	116.15	123.20
2	B	301	RET	C10-C11-C12	-2.36	116.35	123.20
2	A	301	RET	C11-C10-C9	-2.36	123.97	127.28
4	C	302	OLC	O20-C1-C2	2.34	118.96	111.83
4	B	304	OLC	O20-C1-C2	2.23	118.62	111.83
2	C	301	RET	C20-C13-C12	2.22	121.48	118.09
3	B	305	OLB	O20-C1-O19	-2.21	118.10	123.63
4	A	303	OLC	O20-C1-C2	2.09	118.19	111.83
2	A	301	RET	C18-C5-C4	2.07	118.01	113.60
2	B	301	RET	C18-C5-C4	2.05	117.97	113.60
2	C	301	RET	C11-C10-C9	-2.01	124.45	127.28

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	RET	C1-C6-C7-C8
2	A	301	RET	C7-C8-C9-C10
2	B	301	RET	C1-C6-C7-C8
2	B	301	RET	C5-C6-C7-C8
2	B	301	RET	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	B	301	RET	C7-C8-C9-C19
2	A	301	RET	C7-C8-C9-C19
3	B	305	OLB	C2-C3-C4-C5
4	B	303	OLC	C2-C3-C4-C5
2	A	301	RET	C5-C6-C7-C8
3	A	302	OLB	C5-C6-C7-C8
4	C	303	OLC	C4-C5-C6-C7
4	A	303	OLC	C6-C7-C8-C9
4	A	303	OLC	C11-C12-C13-C14
3	A	302	OLB	O20-C1-C2-C3
3	A	302	OLB	C1-C2-C3-C4
4	C	303	OLC	C5-C6-C7-C8
3	A	302	OLB	C12-C13-C14-C15
4	B	304	OLC	C22-C21-O20-C1
3	B	305	OLB	C6-C7-C8-C9
4	C	302	OLC	C9-C10-C11-C12
4	C	302	OLC	C15-C16-C17-C18
4	A	303	OLC	C9-C10-C11-C12
4	B	302	OLC	C9-C10-C11-C12
4	B	304	OLC	C11-C12-C13-C14
4	A	303	OLC	C22-C21-O20-C1
3	A	302	OLB	O19-C1-C2-C3
4	C	303	OLC	C21-C22-C24-O25
3	A	302	OLB	C11-C12-C13-C14
4	B	302	OLC	C22-C21-O20-C1
4	C	303	OLC	C9-C10-C11-C12
4	C	303	OLC	C2-C3-C4-C5

There are no ring outliers.

12 monomers are involved in 37 short contacts:

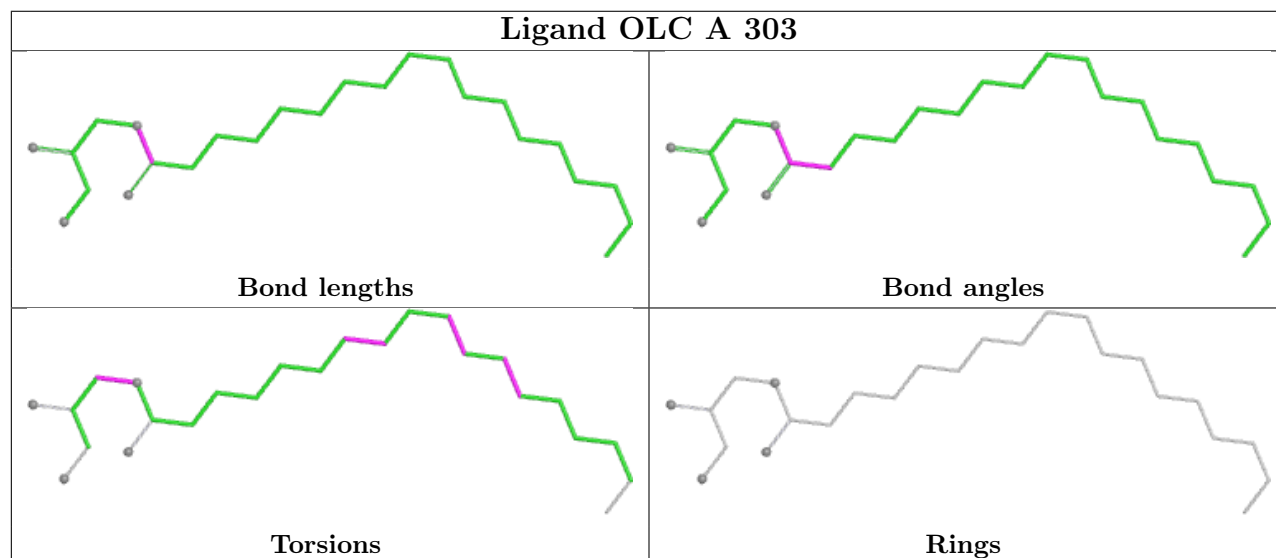
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	OLC	2	0
3	A	302	OLB	2	0
4	B	302	OLC	6	0
4	B	303	OLC	1	0
4	B	304	OLC	5	0
2	B	301	RET	3	0
3	C	304	OLB	5	0
3	B	305	OLB	4	0
4	C	302	OLC	2	0
2	C	301	RET	4	0

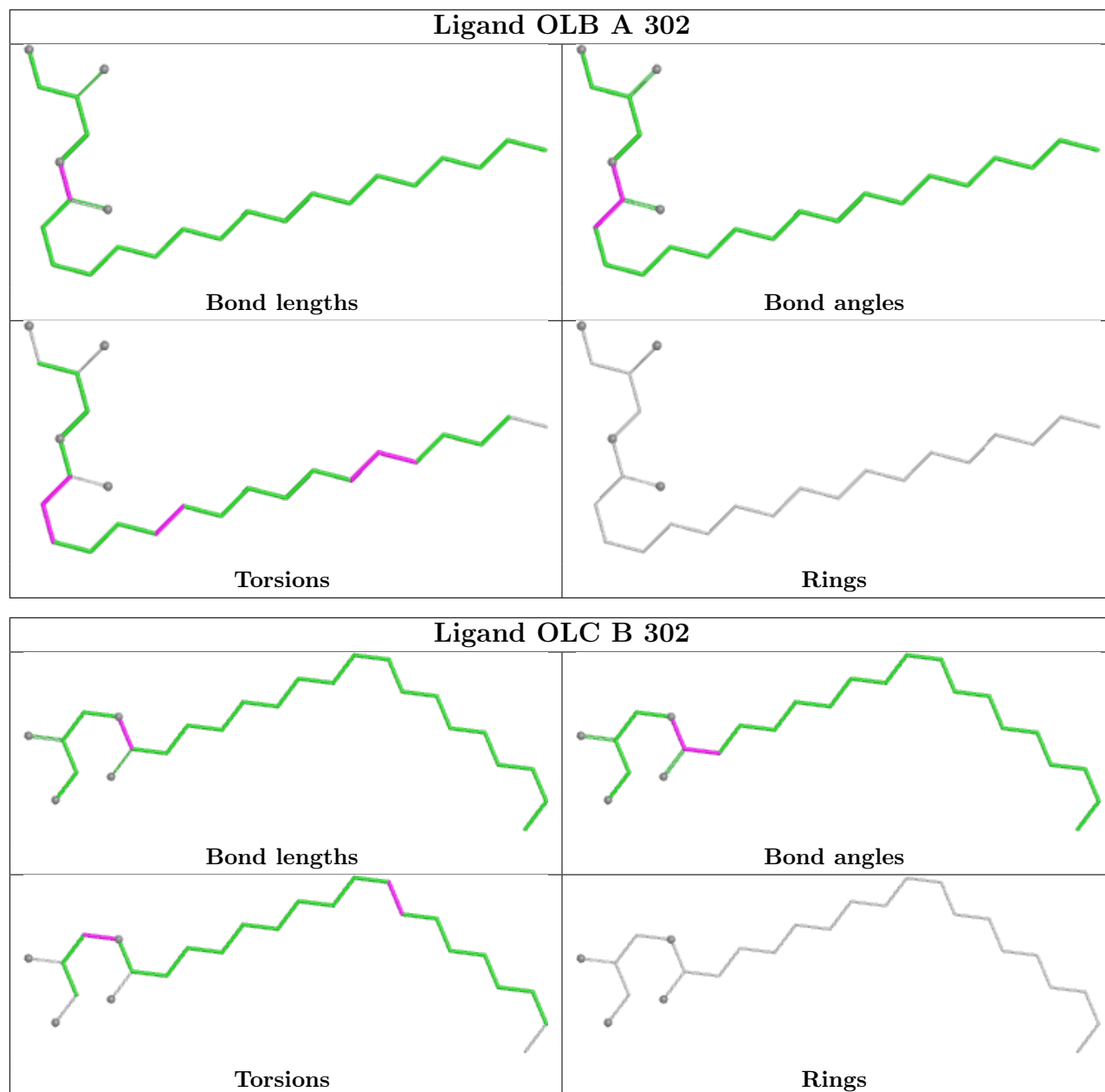
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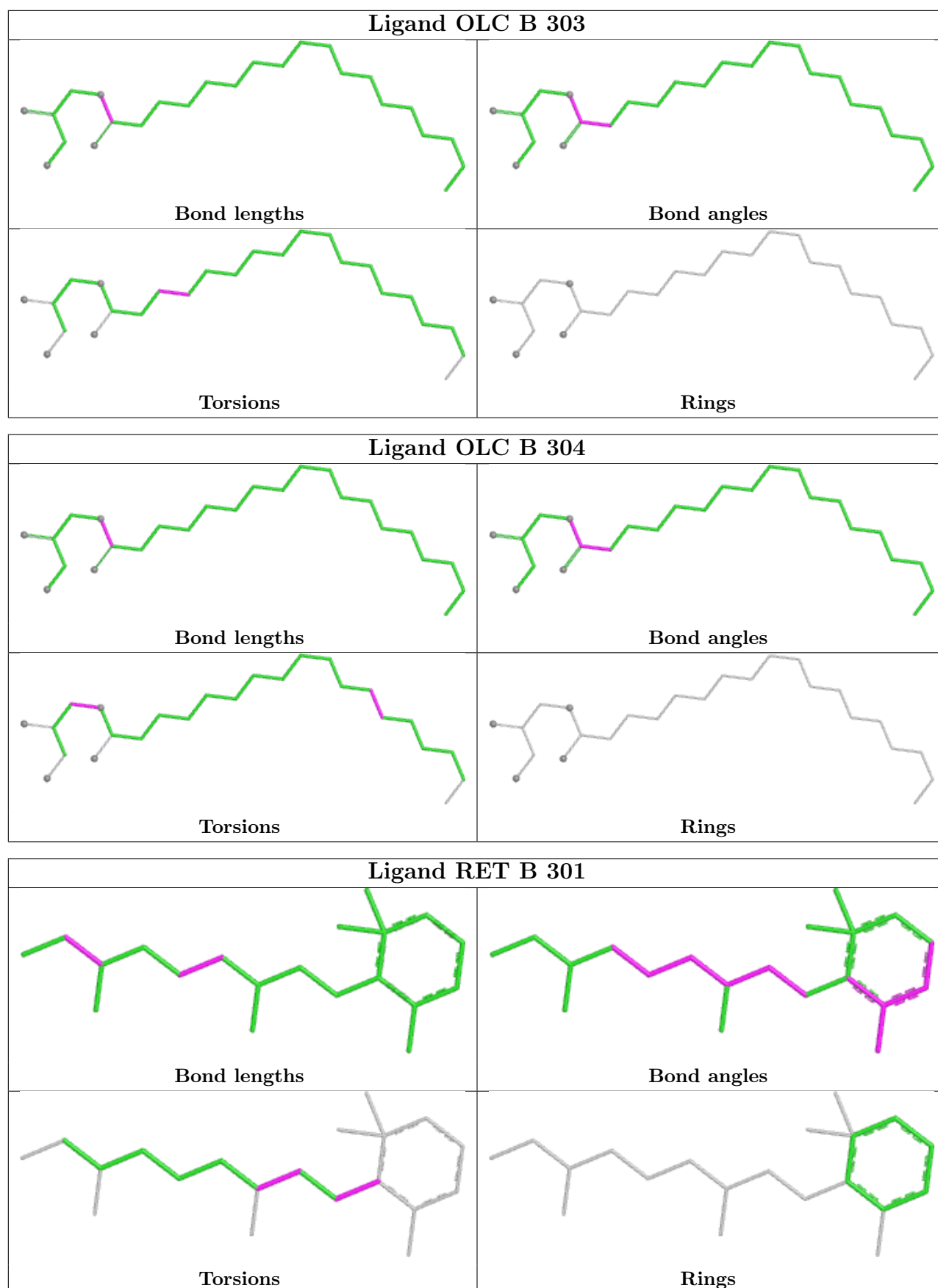
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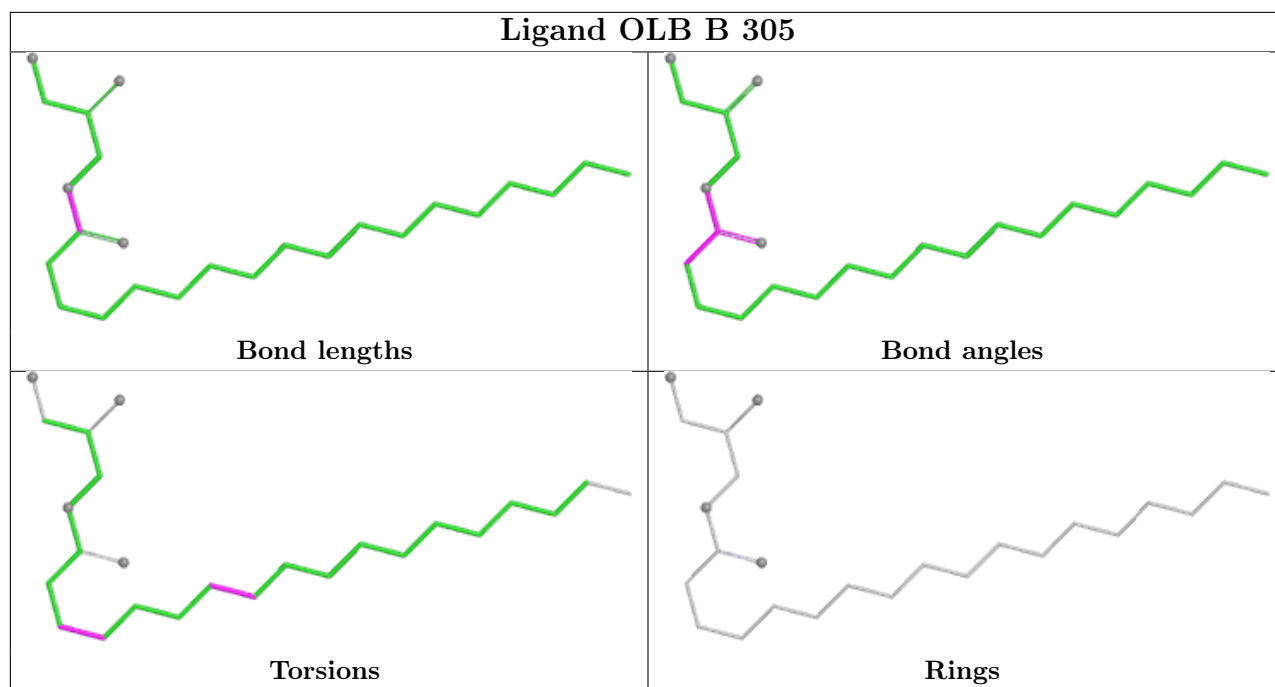
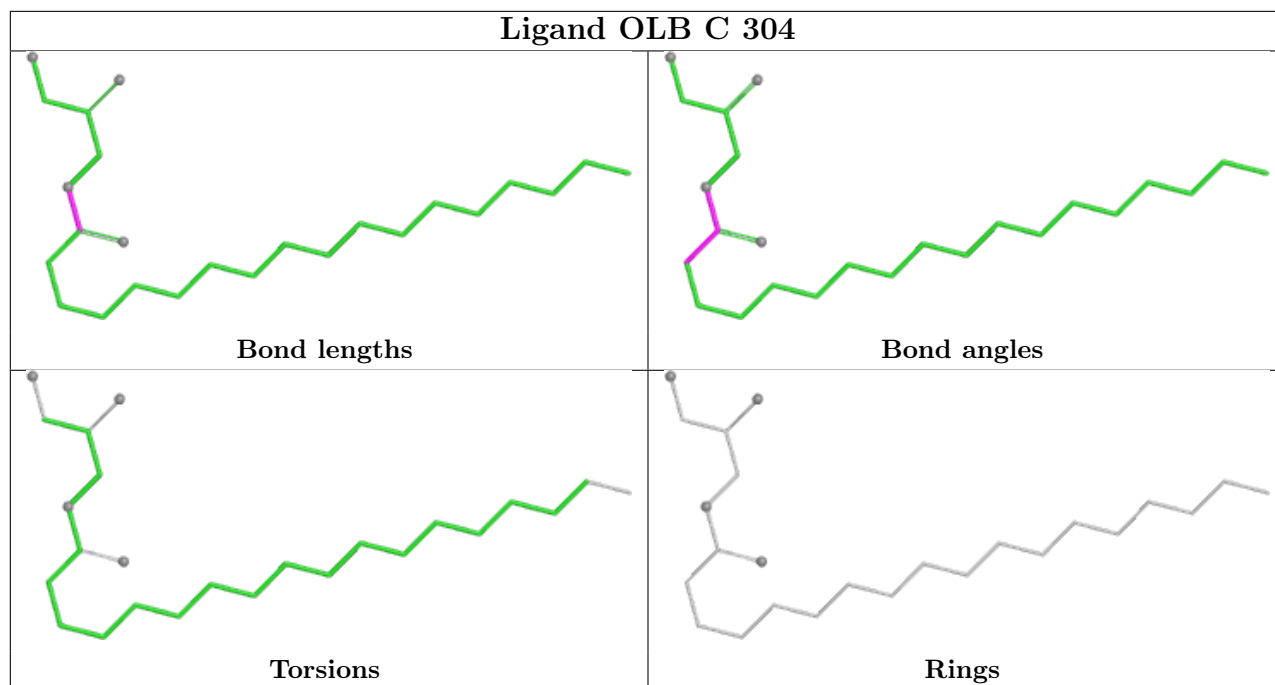
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	RET	2	0
4	C	303	OLC	3	0

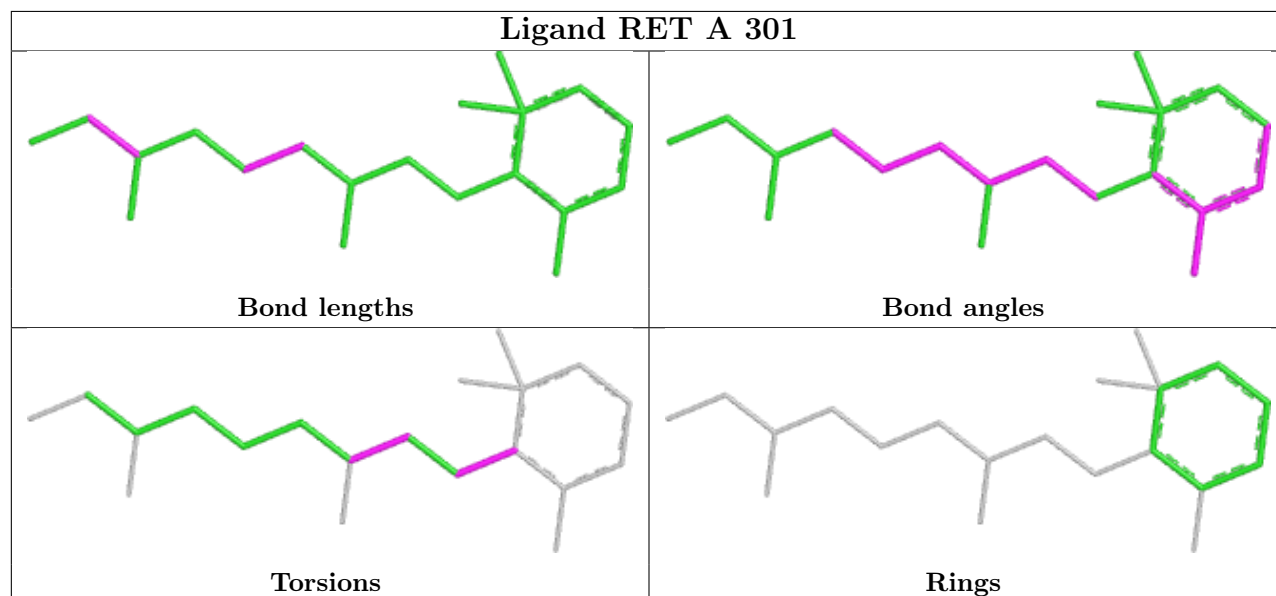
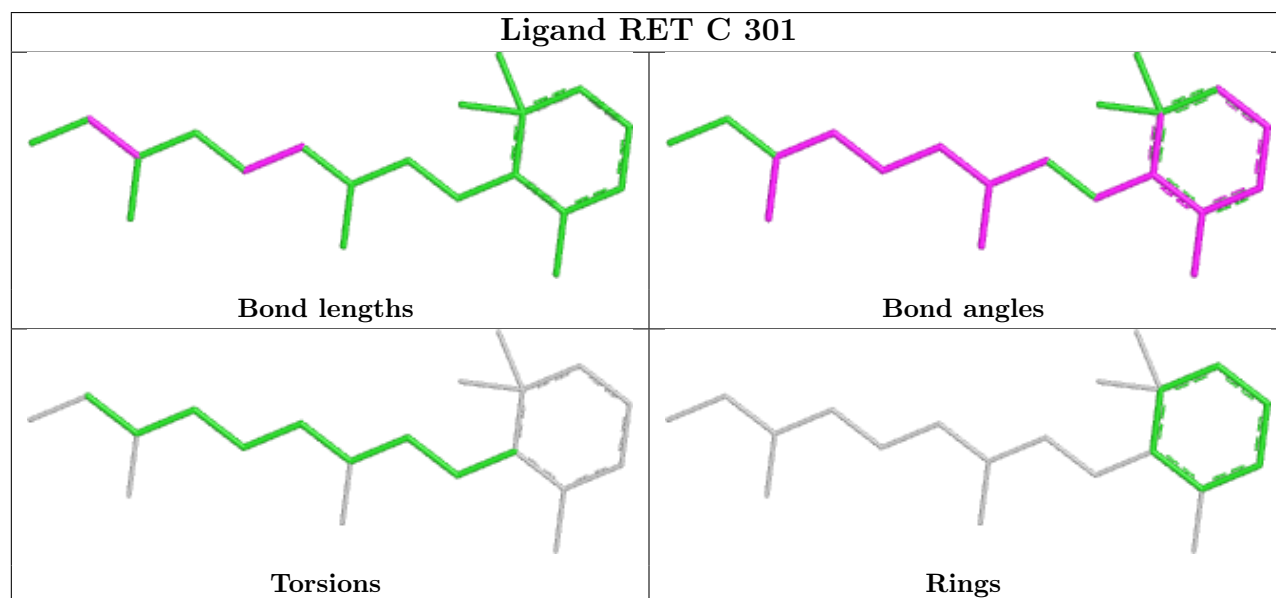
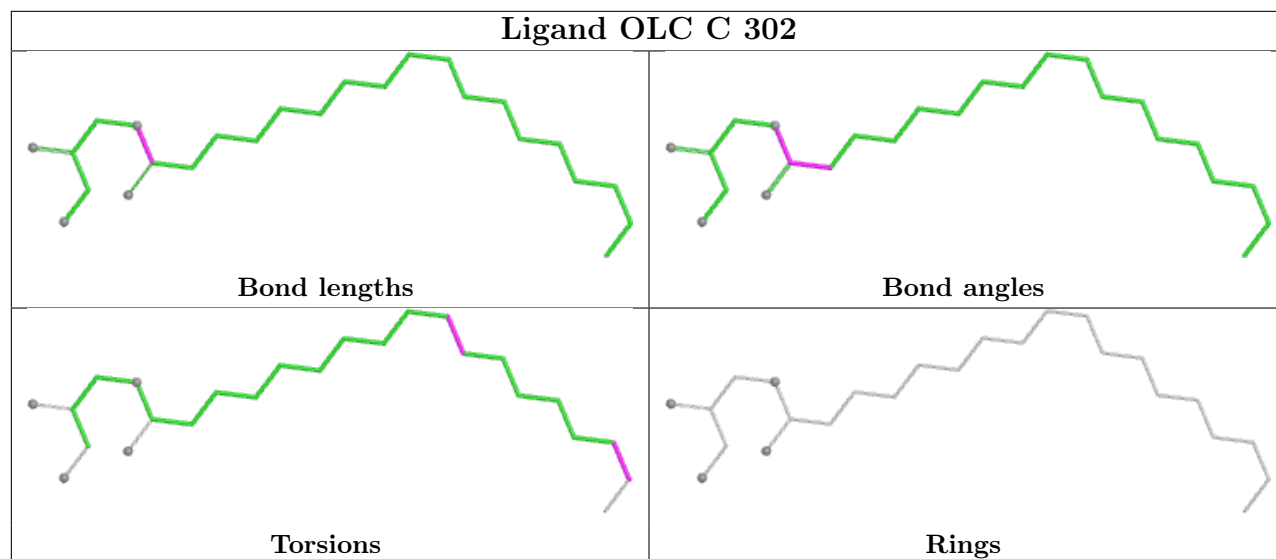
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

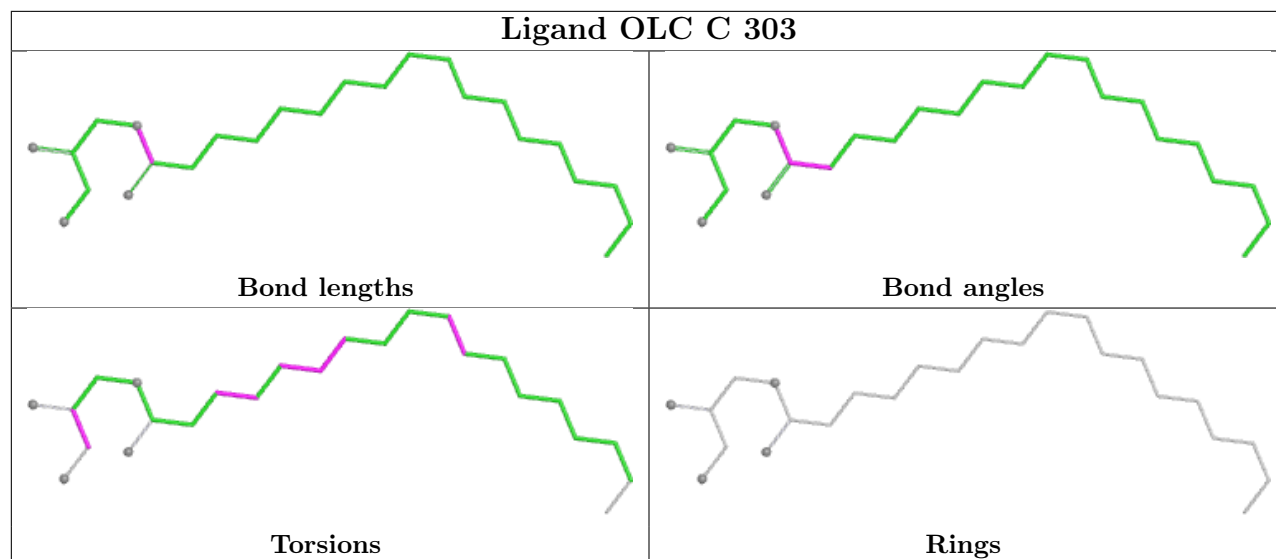












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	228/268 (85%)	1.36	52 (22%) <b>2</b> <b>2</b>	8, 20, 43, 73	3 (1%)
1	B	228/268 (85%)	1.17	39 (17%) <b>4</b> <b>4</b>	10, 20, 39, 74	3 (1%)
1	C	228/268 (85%)	1.44	62 (27%) <b>1</b> <b>1</b>	6, 21, 43, 84	4 (1%)
All	All	684/804 (85%)	1.32	153 (22%) <b>2</b> <b>2</b>	6, 20, 42, 84	10 (1%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	11	LEU	9.0
1	A	11	LEU	6.5
1	C	39	LEU	6.2
1	C	12	GLY	6.0
1	C	238	MET	6.0
1	A	40	ASP	5.5
1	A	41	VAL	5.0
1	A	42	GLN	4.6
1	B	11	LEU	4.6
1	A	39	LEU	4.5
1	C	42	GLN	4.4
1	C	155	PHE	4.3
1	A	155	PHE	4.2
1	B	42	GLN	4.2
1	C	40	ASP	4.2
1	A	238	MET	4.1
1	A	83	VAL	4.1
1	C	41	VAL	4.1
1	C	235	ARG	4.0
1	B	80	ASN	3.8
1	A	38	GLY	3.7
1	B	155	PHE	3.7
1	C	170	ASP	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	236	ALA	3.6
1	C	159	TYR	3.5
1	A	43	ASP	3.5
1	B	159	TYR	3.5
1	B	238	MET	3.5
1	A	237	ILE	3.5
1	A	170	ASP	3.5
1	C	158	TYR	3.4
1	B	187	LEU	3.4
1	C	154	VAL	3.4
1	B	171	ALA	3.4
1	C	167	ALA	3.3
1	A	72	GLY	3.3
1	B	158	TYR	3.3
1	A	236	ALA	3.2
1	B	39	LEU	3.2
1	B	18	ILE	3.2
1	C	161	VAL	3.1
1	B	45	ARG	3.1
1	C	77	SER	3.1
1	A	158	TYR	3.1
1	A	159	TYR	3.1
1	C	87	TYR	3.1
1	C	115	ASP	3.0
1	B	118	ALA	3.0
1	A	207	THR	3.0
1	C	43	ASP	3.0
1	C	46	GLN	3.0
1	B	41	VAL	3.0
1	C	80	ASN	3.0
1	C	198	LEU	2.9
1	C	86	VAL	2.9
1	B	236	ALA	2.9
1	C	237	ILE	2.8
1	C	74	THR	2.8
1	B	44	PRO	2.8
1	B	163	VAL	2.8
1	C	13	VAL	2.8
1	B	235	ARG	2.7
1	B	170	ASP	2.7
1	A	12	GLY	2.7
1	A	110	GLY	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	47	LYS	2.7
1	C	38	GLY	2.7
1	B	196	ALA	2.7
1	A	76	VAL	2.7
1	A	14	GLU	2.6
1	B	88	TRP	2.6
1	C	140	VAL	2.6
1	A	195	VAL	2.6
1	A	48	GLU	2.6
1	A	80	ASN	2.6
1	B	47	LYS	2.6
1	C	111	ALA	2.6
1	B	237	ILE	2.5
1	C	162	ALA	2.5
1	A	201[A]	THR	2.5
1	B	96	PHE	2.5
1	C	96	PHE	2.5
1	C	216	PHE	2.5
1	A	91	TYR	2.5
1	C	33	TYR	2.5
1	B	162	ALA	2.5
1	B	43	ASP	2.4
1	B	119	LEU	2.4
1	C	195	VAL	2.4
1	A	50	TYR	2.4
1	C	191	ALA	2.4
1	B	125	PHE	2.4
1	C	166	GLU	2.4
1	A	25	ILE	2.4
1	B	207	THR	2.4
1	C	91	TYR	2.4
1	A	140	VAL	2.4
1	C	196	ALA	2.3
1	B	22	LEU	2.3
1	B	160	LEU	2.3
1	A	166	GLU	2.3
1	C	48	GLU	2.3
1	C	206	LEU	2.3
1	C	14	GLU	2.3
1	C	44	PRO	2.3
1	C	92	ALA	2.3
1	A	34	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	46	GLN	2.3
1	B	139	VAL	2.3
1	A	29	LEU	2.3
1	C	119	LEU	2.3
1	A	167	ALA	2.2
1	B	136	THR	2.2
1	C	76	VAL	2.2
1	A	79	ALA	2.2
1	A	89	ALA	2.2
1	B	89	ALA	2.2
1	B	173	GLU	2.2
1	A	77	SER	2.2
1	A	96	PHE	2.2
1	C	68	PHE	2.2
1	A	85	ASP	2.2
1	C	202	GLU	2.2
1	C	133	ALA	2.2
1	B	198	LEU	2.2
1	A	74	THR	2.2
1	C	192	ILE	2.1
1	C	163	VAL	2.1
1	A	211	GLY	2.1
1	C	113	GLN	2.1
1	A	28	LEU	2.1
1	A	234	SER	2.1
1	C	169	SER	2.1
1	C	150	THR	2.1
1	A	88	TRP	2.1
1	C	19	TRP	2.1
1	A	120	VAL	2.1
1	A	62	ALA	2.1
1	A	177	SER	2.1
1	B	29	LEU	2.1
1	C	173	GLU	2.1
1	A	45	ARG	2.1
1	B	19	TRP	2.1
1	C	139	VAL	2.1
1	A	161	VAL	2.1
1	B	71	PHE	2.1
1	C	234	SER	2.1
1	C	207	THR	2.0
1	A	51	VAL	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	84	VAL	2.0
1	A	172	ASP	2.0
1	C	85	ASP	2.0
1	C	143	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

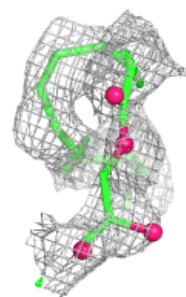
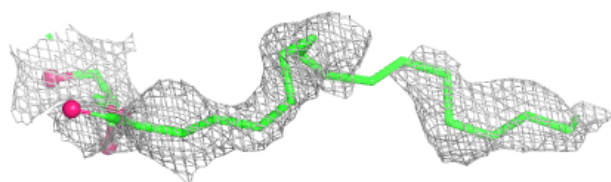
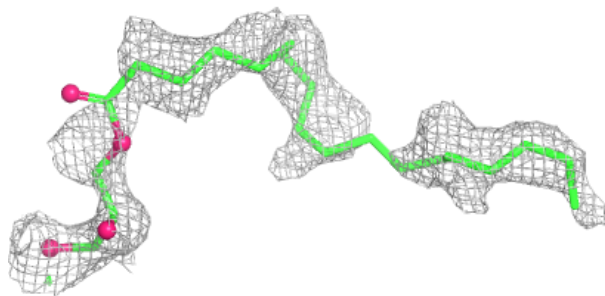
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	OLB	A	302	25/25	0.62	0.27	45,52,58,59	0
3	OLB	B	305	25/25	0.62	0.31	55,57,69,70	0
4	OLC	C	303	25/25	0.63	0.25	33,39,51,52	0
4	OLC	A	303	25/25	0.64	0.25	46,57,65,65	0
4	OLC	B	304	25/25	0.67	0.23	26,41,51,51	0
3	OLB	C	304	25/25	0.67	0.24	39,46,55,55	0
4	OLC	C	302	25/25	0.68	0.23	38,43,60,60	0
4	OLC	B	302	25/25	0.69	0.23	36,42,46,46	0
4	OLC	B	303	25/25	0.71	0.20	35,42,51,52	0
2	RET	C	301	20/21	0.84	0.13	3,8,13,13	0
2	RET	B	301	20/21	0.84	0.12	13,16,19,19	0
2	RET	A	301	20/21	0.89	0.11	12,15,17,17	0

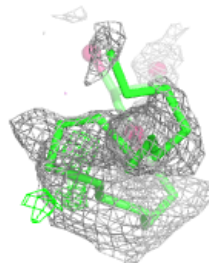
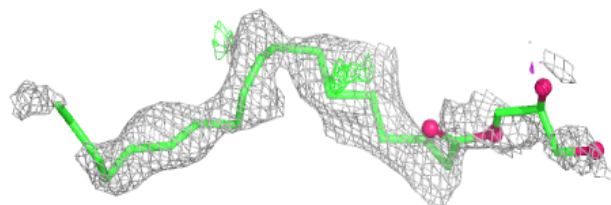
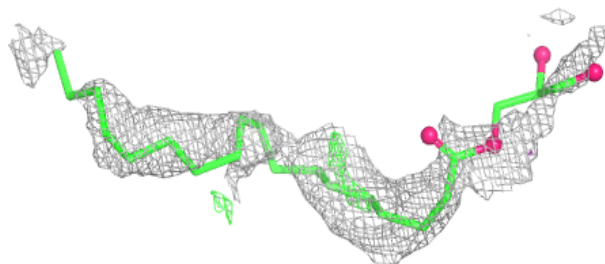
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OLB A 302:**

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

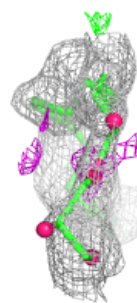
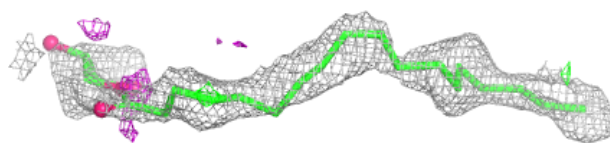
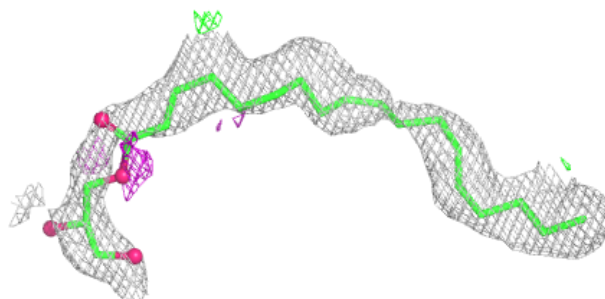
**Electron density around OLB B 305:**

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

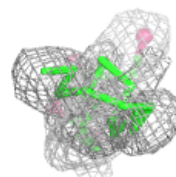
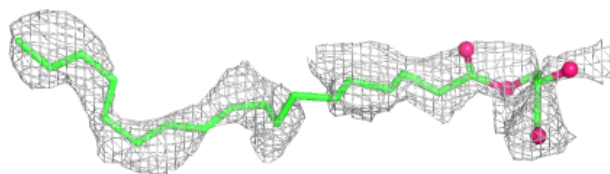
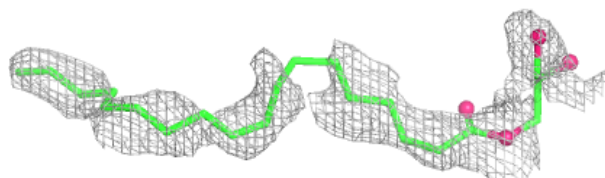


**Electron density around OLC C 303:**

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

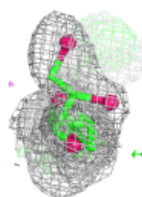
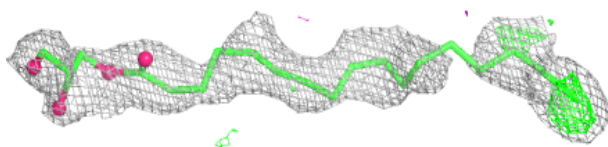
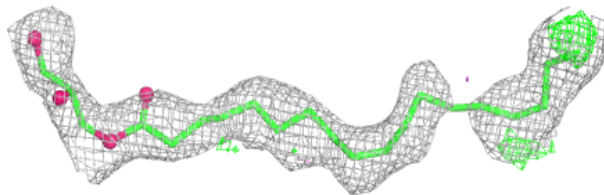
**Electron density around OLC A 303:**

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

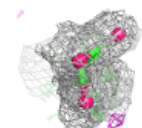
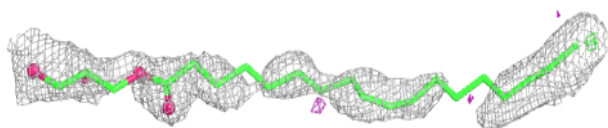
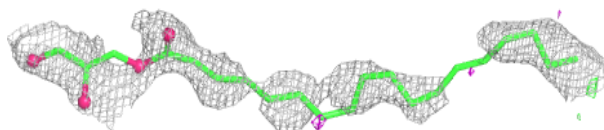


**Electron density around OLC B 304:**

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

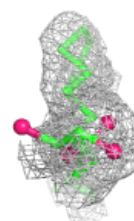
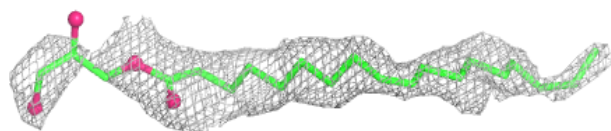
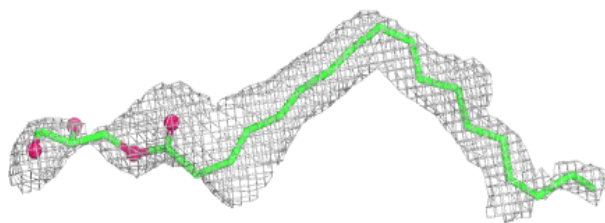
**Electron density around OLB C 304:**

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

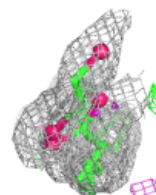
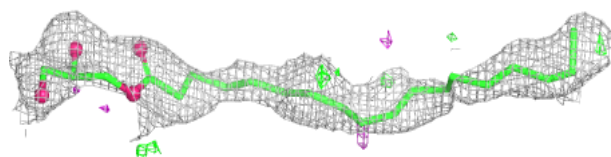
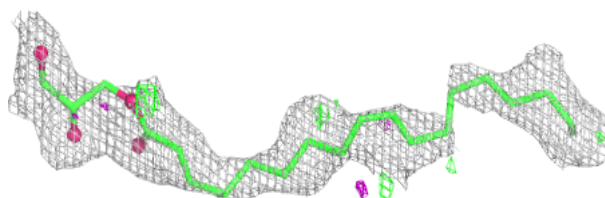


**Electron density around OLC C 302:**

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

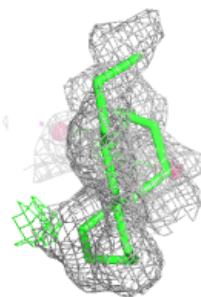
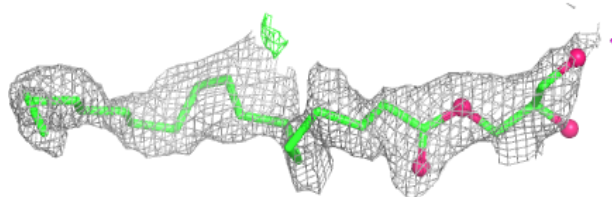
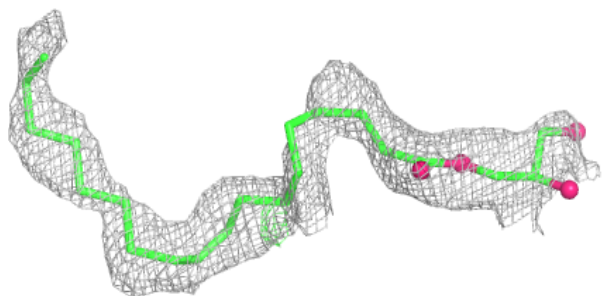
**Electron density around OLC B 302:**

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

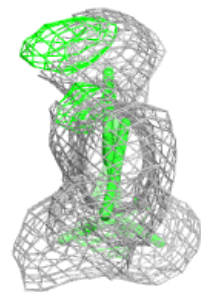
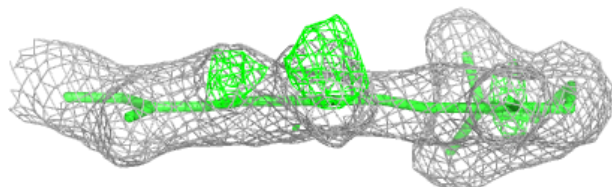
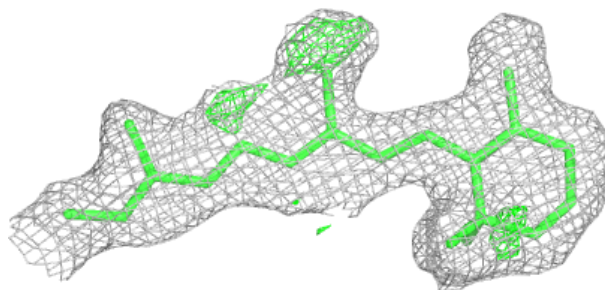


**Electron density around OLC B 303:**

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

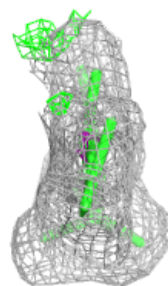
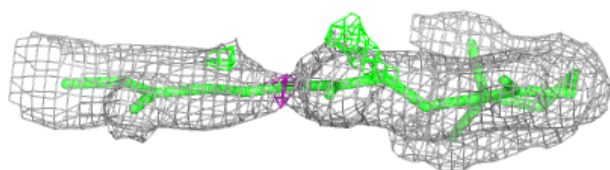
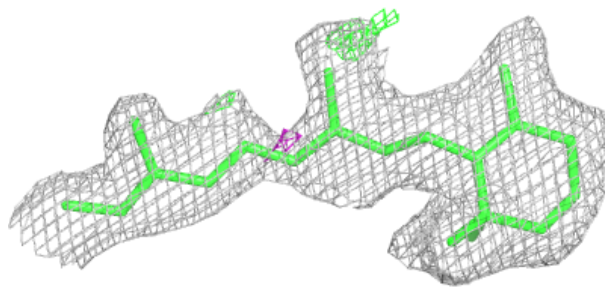
**Electron density around RET C 301:**

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

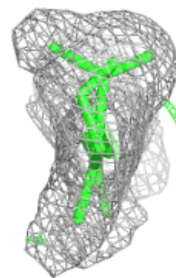
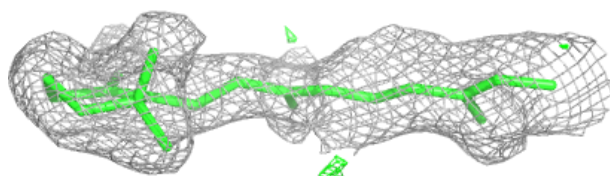
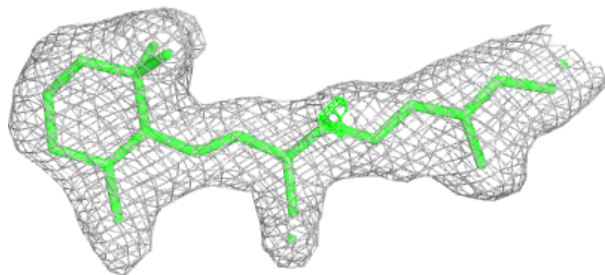


**Electron density around RET B 301:**

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

**Electron density around RET A 301:**

$2mF_o-DF_c$  (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.