



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 03:45 PM EDT

PDB ID : 6N9R
Title : Structure of the Quorum Quenching lactonase from *Parageobacillus caldosyloticus* bound to substrate 3-oxo-C12-AHL
Authors : Bergonzi, C.; Schwab, M.; Elias, M.
Deposited on : 2018-12-03
Resolution : 1.75 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

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 1.75 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 7868 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 Putative hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2390	1515	416	443	16	0	18	0
1	P	276	2406	1521	419	451	15	0	19	0
1	X	276	2371	1501	413	442	15	0	15	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	TRP	-	expression tag	UNP A0A023DFE8
A	-12	SER	-	expression tag	UNP A0A023DFE8
A	-11	HIS	-	expression tag	UNP A0A023DFE8
A	-10	PRO	-	expression tag	UNP A0A023DFE8
A	-9	GLN	-	expression tag	UNP A0A023DFE8
A	-8	PHE	-	expression tag	UNP A0A023DFE8
A	-7	GLU	-	expression tag	UNP A0A023DFE8
A	-6	LYS	-	expression tag	UNP A0A023DFE8
A	-5	GLU	-	expression tag	UNP A0A023DFE8
A	-4	ASN	-	expression tag	UNP A0A023DFE8
A	-3	LEU	-	expression tag	UNP A0A023DFE8
A	-2	TYR	-	expression tag	UNP A0A023DFE8
A	-1	PHE	-	expression tag	UNP A0A023DFE8
A	0	GLN	-	expression tag	UNP A0A023DFE8
A	1	SER	-	expression tag	UNP A0A023DFE8
P	-13	TRP	-	expression tag	UNP A0A023DFE8
P	-12	SER	-	expression tag	UNP A0A023DFE8
P	-11	HIS	-	expression tag	UNP A0A023DFE8
P	-10	PRO	-	expression tag	UNP A0A023DFE8
P	-9	GLN	-	expression tag	UNP A0A023DFE8
P	-8	PHE	-	expression tag	UNP A0A023DFE8
P	-7	GLU	-	expression tag	UNP A0A023DFE8
P	-6	LYS	-	expression tag	UNP A0A023DFE8

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-5	GLU	-	expression tag	UNP A0A023DFE8
P	-4	ASN	-	expression tag	UNP A0A023DFE8
P	-3	LEU	-	expression tag	UNP A0A023DFE8
P	-2	TYR	-	expression tag	UNP A0A023DFE8
P	-1	PHE	-	expression tag	UNP A0A023DFE8
P	0	GLN	-	expression tag	UNP A0A023DFE8
P	1	SER	-	expression tag	UNP A0A023DFE8
X	-13	TRP	-	expression tag	UNP A0A023DFE8
X	-12	SER	-	expression tag	UNP A0A023DFE8
X	-11	HIS	-	expression tag	UNP A0A023DFE8
X	-10	PRO	-	expression tag	UNP A0A023DFE8
X	-9	GLN	-	expression tag	UNP A0A023DFE8
X	-8	PHE	-	expression tag	UNP A0A023DFE8
X	-7	GLU	-	expression tag	UNP A0A023DFE8
X	-6	LYS	-	expression tag	UNP A0A023DFE8
X	-5	GLU	-	expression tag	UNP A0A023DFE8
X	-4	ASN	-	expression tag	UNP A0A023DFE8
X	-3	LEU	-	expression tag	UNP A0A023DFE8
X	-2	TYR	-	expression tag	UNP A0A023DFE8
X	-1	PHE	-	expression tag	UNP A0A023DFE8
X	0	GLN	-	expression tag	UNP A0A023DFE8
X	1	SER	-	expression tag	UNP A0A023DFE8

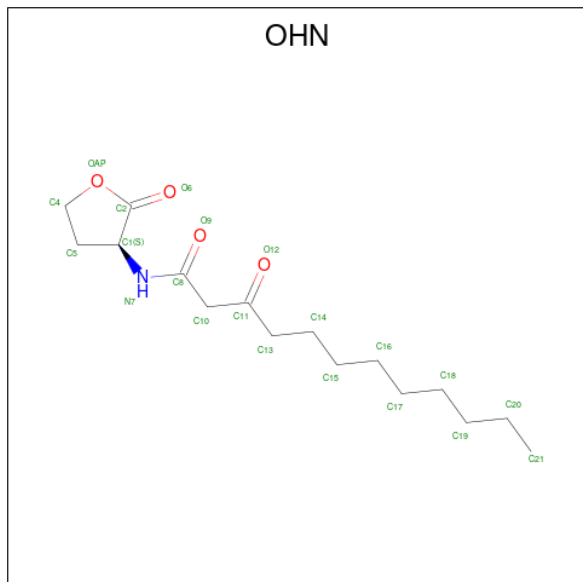
- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Co 1 1	0	0
2	P	1	Total Co 1 1	0	0
2	X	1	Total Co 1 1	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

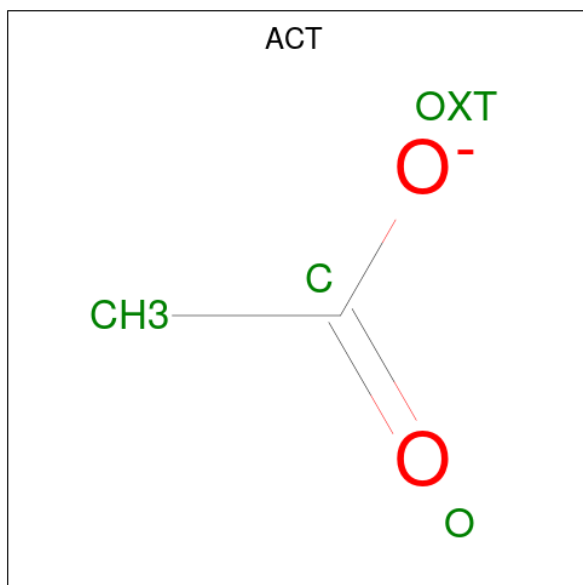
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe 1 1	0	0
3	P	1	Total Fe 1 1	0	0
3	X	1	Total Fe 1 1	0	0

- Molecule 4 is N-3-OXO-DODECANOYL-L-HOMOSERINE LACTONE (three-letter code: OHN) (formula: $C_{16}H_{27}NO_4$).



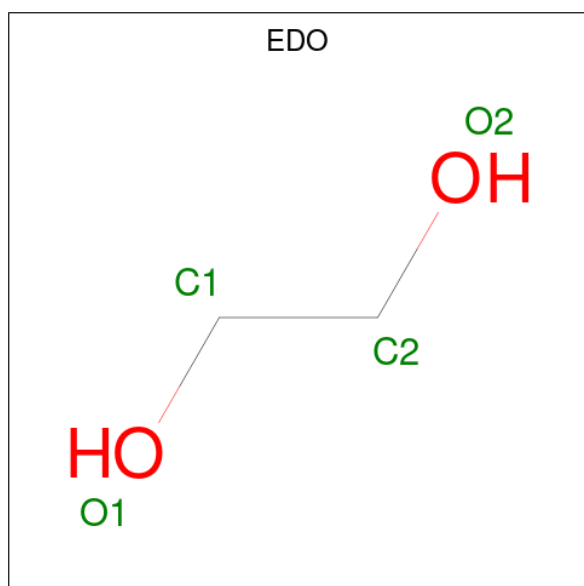
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	21	16	1	4	0	0
4	P	1	21	16	1	4	0	0
4	X	1	21	16	1	4	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	P	1	Total C O 4 2 2	0	0
5	X	1	Total C O 4 2 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



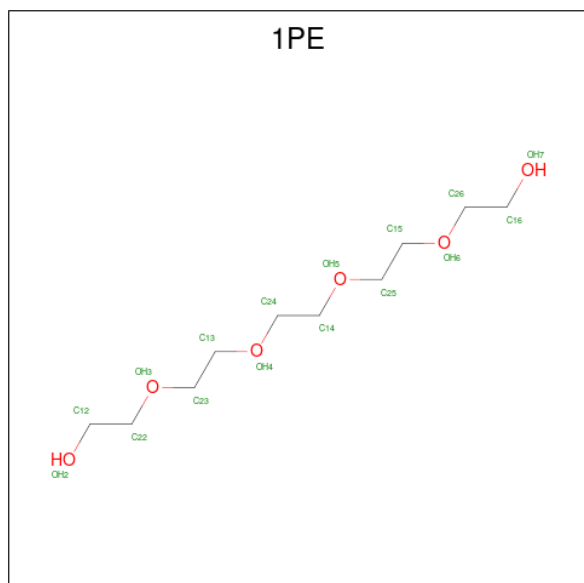
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	P	1	Total C O 4 2 2	0	0
6	P	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	P	1	Total	C	O	0	0
			4	2	2		
6	P	1	Total	C	O	0	0
			4	2	2		
6	P	1	Total	C	O	0	0
			4	2	2		
6	X	1	Total	C	O	0	0
			4	2	2		
6	X	1	Total	C	O	0	0
			4	2	2		
6	X	1	Total	C	O	0	0
			4	2	2		
6	X	1	Total	C	O	0	0
			4	2	2		
6	X	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



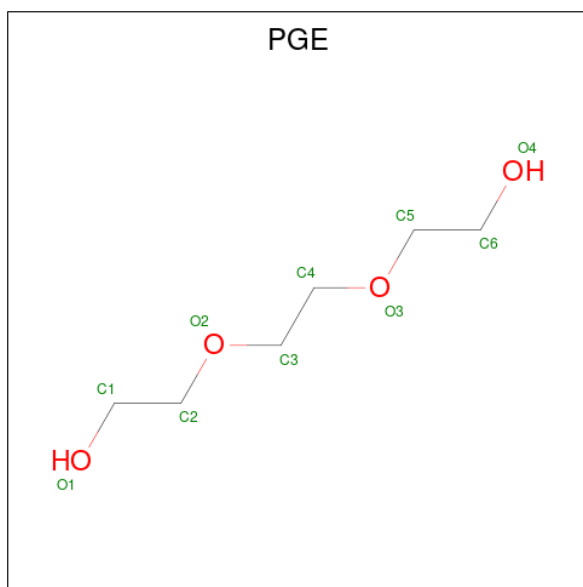
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			16	10	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	P	1	Total	C	O	0	0
			16	10	6		
7	X	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	P	1	Total	O	S	0	0
			5	4	1		
9	P	1	Total	O	S	0	0
			5	4	1		
9	P	1	Total	O	S	0	0
			5	4	1		
9	P	1	Total	O	S	0	0
			5	4	1		
9	X	1	Total	O	S	0	0
			5	4	1		
9	X	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	131	Total	O	0	0
			131	131		
10	P	175	Total	O	0	0
			175	175		
10	X	145	Total	O	0	0
			145	145		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.01Å 108.59Å 78.60Å 90.00° 115.75° 90.00°	Depositor
Resolution (Å)	70.80 – 1.75	Depositor
% Data completeness (in resolution range)	99.3 (70.80-1.75)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 1.75Å)	Xtrriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.176 , 0.235	Depositor
Wilson B-factor (Å ²)	15.8	Xtrriage
Anisotropy	0.643	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7868	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.51% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 6 are monoatomic - leaving 36 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	X	303	-	4,4,4	0.32	0	6,6,6	0.04	0
5	ACT	A	304	-	3,3,3	0.76	0	3,3,3	0.72	0
5	ACT	X	306	-	3,3,3	0.75	0	3,3,3	0.74	0
6	EDO	P	313	-	3,3,3	0.47	0	2,2,2	0.30	0
9	SO4	P	305	-	4,4,4	0.33	0	6,6,6	0.04	0
6	EDO	P	314	-	3,3,3	0.44	0	2,2,2	0.28	0
6	EDO	X	313	-	3,3,3	0.43	0	2,2,2	0.32	0
9	SO4	P	303	-	4,4,4	0.32	0	6,6,6	0.06	0
4	OHN	P	308	2,3	21,21,21	1.49	1 (4%)	20,25,25	2.03	2 (10%)
8	PGE	A	313	-	9,9,9	0.45	0	8,8,8	0.24	0
7	1PE	A	312	-	15,15,15	0.46	0	14,14,14	0.22	0
6	EDO	A	311	-	3,3,3	0.45	0	2,2,2	0.31	0
6	EDO	X	308	-	3,3,3	0.46	0	2,2,2	0.28	0
6	EDO	X	309	-	3,3,3	0.46	0	2,2,2	0.29	0
6	EDO	X	311	-	3,3,3	0.46	0	2,2,2	0.28	0
9	SO4	P	307	-	4,4,4	0.33	0	6,6,6	0.05	0
6	EDO	X	312	-	3,3,3	0.47	0	2,2,2	0.28	0
4	OHN	A	303	2,3	21,21,21	1.46	1 (4%)	20,25,25	1.92	2 (10%)
6	EDO	A	310	-	3,3,3	0.31	0	2,2,2	0.53	0
6	EDO	X	310	-	3,3,3	0.46	0	2,2,2	0.29	0
6	EDO	A	309	-	3,3,3	0.45	0	2,2,2	0.31	0
6	EDO	P	311	-	3,3,3	0.46	0	2,2,2	0.29	0
5	ACT	A	306	-	3,3,3	0.77	0	3,3,3	0.74	0
6	EDO	P	310	-	3,3,3	0.45	0	2,2,2	0.33	0
4	OHN	X	305	2,3	21,21,21	1.47	1 (4%)	20,25,25	1.95	4 (20%)
9	SO4	X	304	-	4,4,4	0.21	0	6,6,6	0.25	0
5	ACT	P	309	-	3,3,3	0.78	0	3,3,3	0.73	0
6	EDO	A	307	-	3,3,3	0.45	0	2,2,2	0.32	0
9	SO4	P	306	-	4,4,4	0.32	0	6,6,6	0.05	0
9	SO4	P	304	-	4,4,4	0.32	0	6,6,6	0.06	0
5	ACT	A	305	-	3,3,3	0.76	0	3,3,3	0.74	0
6	EDO	A	308	-	3,3,3	0.43	0	2,2,2	0.34	0
7	1PE	X	314	-	15,15,15	0.45	0	14,14,14	0.26	0
6	EDO	P	312	-	3,3,3	0.47	0	2,2,2	0.28	0
7	1PE	P	315	-	15,15,15	0.50	0	14,14,14	0.19	0
6	EDO	X	307	-	3,3,3	0.44	0	2,2,2	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	P	313	-	-	1/1/1/1	-
6	EDO	P	314	-	-	0/1/1/1	-
6	EDO	X	313	-	-	0/1/1/1	-
4	OHN	P	308	2,3	-	11/17/27/27	0/1/1/1
8	PGE	A	313	-	-	4/7/7/7	-
7	1PE	A	312	-	-	10/13/13/13	-
6	EDO	A	311	-	-	0/1/1/1	-
6	EDO	X	308	-	-	1/1/1/1	-
6	EDO	X	309	-	-	0/1/1/1	-
6	EDO	X	311	-	-	1/1/1/1	-
6	EDO	X	312	-	-	1/1/1/1	-
4	OHN	A	303	2,3	-	9/17/27/27	0/1/1/1
6	EDO	A	310	-	-	1/1/1/1	-
6	EDO	X	310	-	-	1/1/1/1	-
6	EDO	A	309	-	-	1/1/1/1	-
6	EDO	P	311	-	-	1/1/1/1	-
6	EDO	P	310	-	-	0/1/1/1	-
4	OHN	X	305	2,3	-	8/17/27/27	0/1/1/1
6	EDO	A	307	-	-	0/1/1/1	-
6	EDO	A	308	-	-	1/1/1/1	-
7	1PE	X	314	-	-	8/13/13/13	-
6	EDO	P	312	-	-	1/1/1/1	-
7	1PE	P	315	-	-	6/13/13/13	-
6	EDO	X	307	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	308	OHN	C1-C2	-6.24	1.39	1.52
4	X	305	OHN	C1-C2	-6.16	1.39	1.52
4	A	303	OHN	C1-C2	-6.08	1.39	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	308	OHN	C4-OAP-C2	-7.43	103.52	110.39
4	X	305	OHN	C4-OAP-C2	-7.01	103.91	110.39
4	A	303	OHN	C4-OAP-C2	-6.95	103.96	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	308	OHN	OAP-C2-O6	2.81	124.34	121.42
4	X	305	OHN	OAP-C2-O6	2.78	124.30	121.42
4	A	303	OHN	OAP-C2-O6	2.71	124.23	121.42
4	X	305	OHN	C14-C13-C11	-2.01	109.42	114.60
4	X	305	OHN	C5-C1-N7	-2.01	110.44	114.96

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	308	OHN	O12-C11-C13-C14
4	P	308	OHN	C10-C11-C13-C14
4	P	308	OHN	C5-C1-N7-C8
7	A	312	1PE	C16-C26-OH6-C15
7	A	312	1PE	OH4-C13-C23-OH3
7	A	312	1PE	OH6-C15-C25-OH5
8	A	313	PGE	O2-C3-C4-O3
7	P	315	1PE	OH5-C14-C24-OH4
7	P	315	1PE	OH4-C13-C23-OH3
7	P	315	1PE	OH2-C12-C22-OH3
7	X	314	1PE	OH2-C12-C22-OH3
4	X	305	OHN	C14-C15-C16-C17
4	X	305	OHN	C17-C18-C19-C20
4	A	303	OHN	C13-C14-C15-C16
4	A	303	OHN	C15-C16-C17-C18
4	P	308	OHN	C11-C13-C14-C15
4	P	308	OHN	C17-C18-C19-C20
4	X	305	OHN	C16-C17-C18-C19
6	A	308	EDO	O1-C1-C2-O2
6	P	312	EDO	O1-C1-C2-O2
6	P	313	EDO	O1-C1-C2-O2
6	X	308	EDO	O1-C1-C2-O2
6	X	312	EDO	O1-C1-C2-O2
4	P	308	OHN	C14-C15-C16-C17
7	A	312	1PE	OH7-C16-C26-OH6
4	A	303	OHN	C17-C18-C19-C20
7	X	314	1PE	C24-C14-OH5-C25
4	P	308	OHN	C15-C16-C17-C18
7	X	314	1PE	OH4-C13-C23-OH3
6	X	311	EDO	O1-C1-C2-O2
7	P	315	1PE	OH6-C15-C25-OH5
7	X	314	1PE	OH5-C14-C24-OH4

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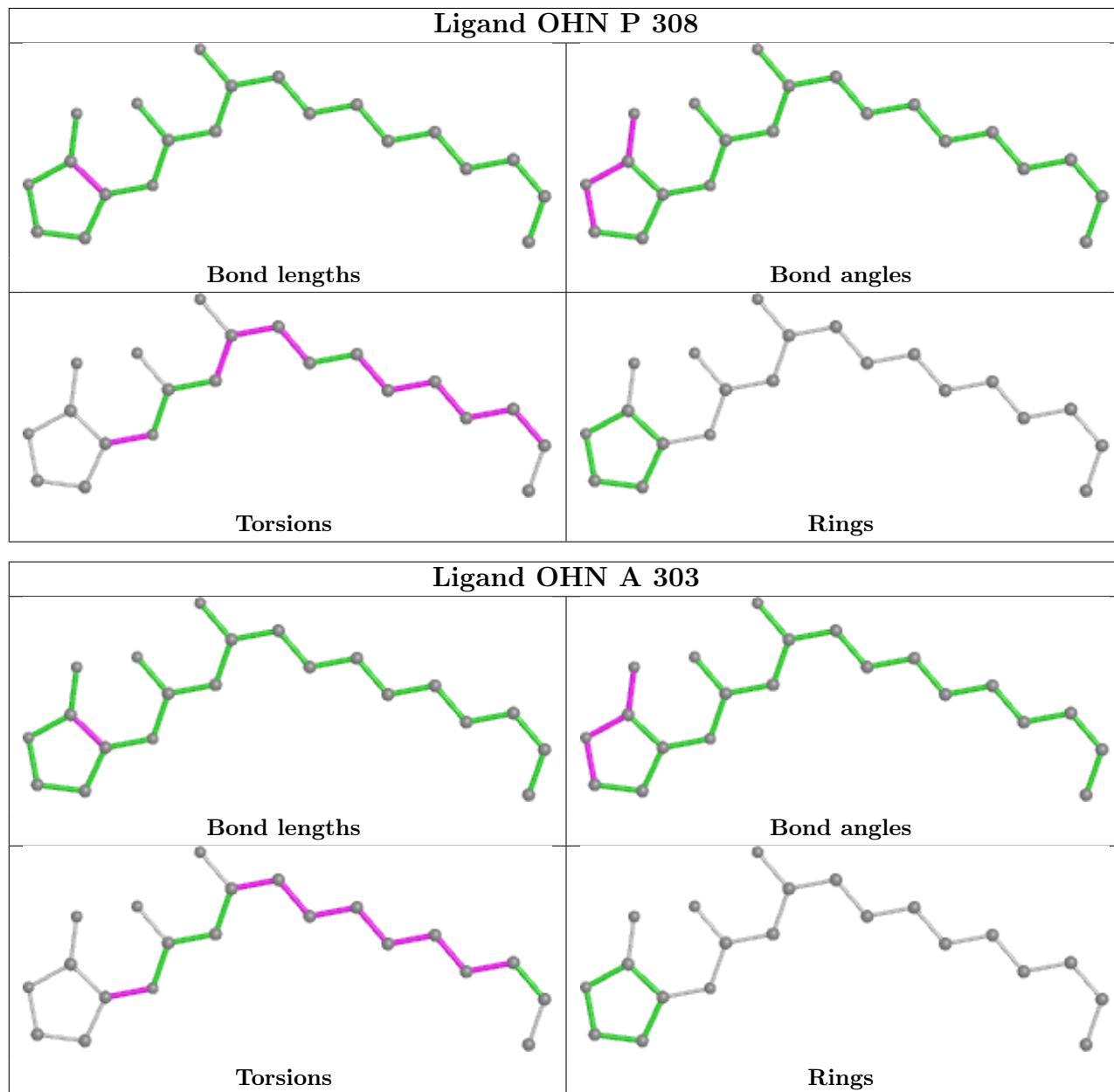
Mol	Chain	Res	Type	Atoms
4	X	305	OHN	C5-C1-N7-C8
8	A	313	PGE	O1-C1-C2-O2
6	A	310	EDO	O1-C1-C2-O2
6	P	311	EDO	O1-C1-C2-O2
6	X	310	EDO	O1-C1-C2-O2
4	X	305	OHN	C15-C16-C17-C18
4	P	308	OHN	C16-C17-C18-C19
7	A	312	1PE	C24-C14-OH5-C25
4	A	303	OHN	C14-C15-C16-C17
4	X	305	OHN	C8-C10-C11-O12
7	X	314	1PE	C13-C23-OH3-C22
7	A	312	1PE	C13-C23-OH3-C22
7	A	312	1PE	OH2-C12-C22-OH3
4	A	303	OHN	C16-C17-C18-C19
7	A	312	1PE	C25-C15-OH6-C26
4	A	303	OHN	C5-C1-N7-C8
4	P	308	OHN	C2-C1-N7-C8
4	X	305	OHN	C2-C1-N7-C8
7	A	312	1PE	C12-C22-OH3-C23
7	X	314	1PE	C25-C15-OH6-C26
7	P	315	1PE	C16-C26-OH6-C15
4	A	303	OHN	C11-C13-C14-C15
4	P	308	OHN	C18-C19-C20-C21
4	A	303	OHN	C10-C11-C13-C14
8	A	313	PGE	C4-C3-O2-C2
8	A	313	PGE	C6-C5-O3-C4
6	A	309	EDO	O1-C1-C2-O2
7	X	314	1PE	C12-C22-OH3-C23
4	A	303	OHN	O12-C11-C13-C14
7	A	312	1PE	C15-C25-OH5-C14
4	P	308	OHN	C8-C10-C11-C13
4	X	305	OHN	C8-C10-C11-C13
7	P	315	1PE	OH7-C16-C26-OH6
7	X	314	1PE	OH6-C15-C25-OH5

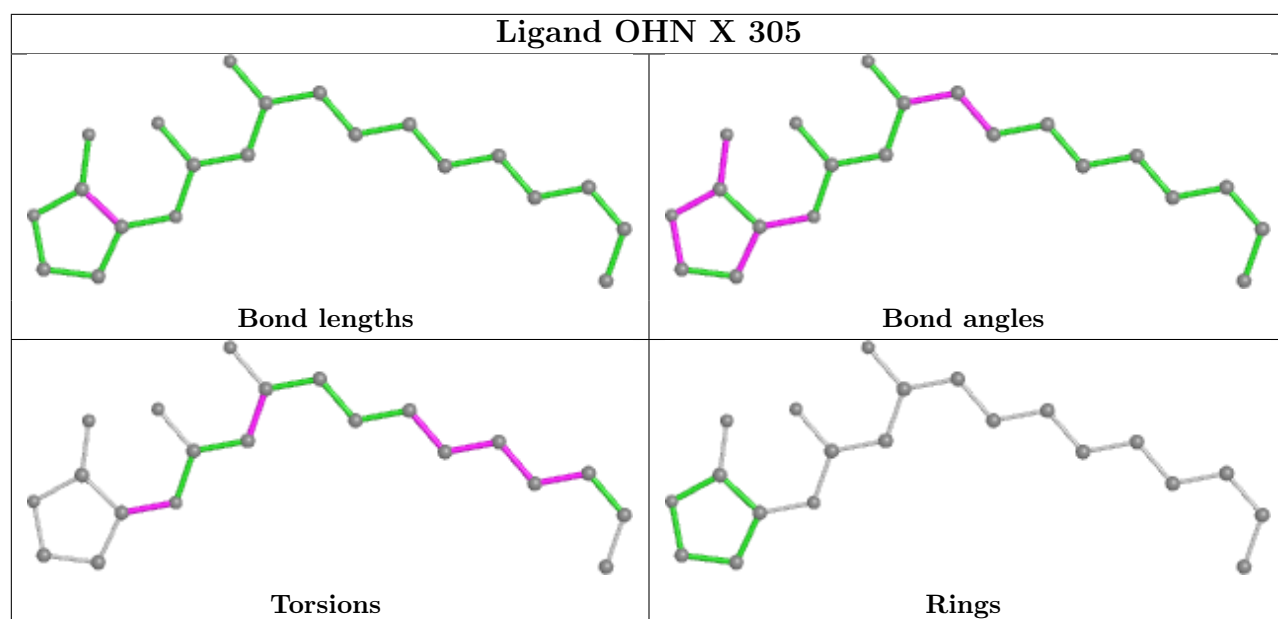
There are no ring outliers.

No monomer is involved in short contacts.

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.





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.