Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 05:36 AM EDT

PDB ID	:	6N9Q
Title	:	Structure of the Quorum Quenching lactonase from Parageobacillus caldoxylosilyticus bind to substrate C4-AHL
Authors	:	Bergonzi, C.; Schwab, M.; Elias, M.
Deposited on	:	2018-12-03
Resolution	:	2.35 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)
Xtriage (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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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 5043 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.

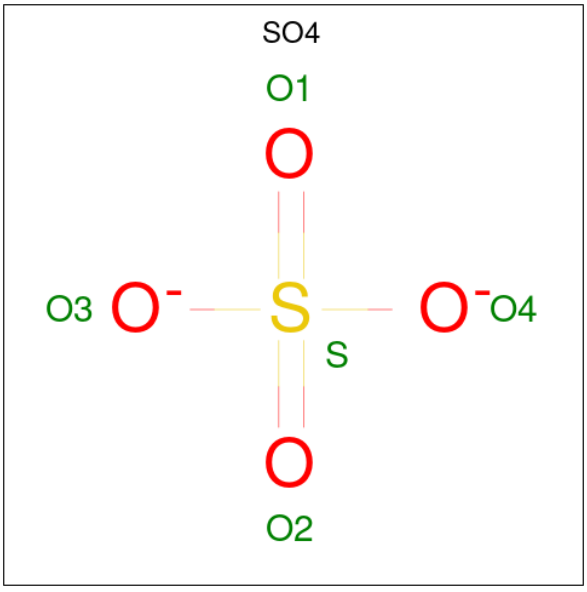
- Molecule 1 is a protein called Lactonase GcL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	277	Total	C	N	O	S	0	8	0
			2318	1469	404	431	14			
1	D	277	Total	C	N	O	S	0	7	0
			2310	1465	403	428	14			

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

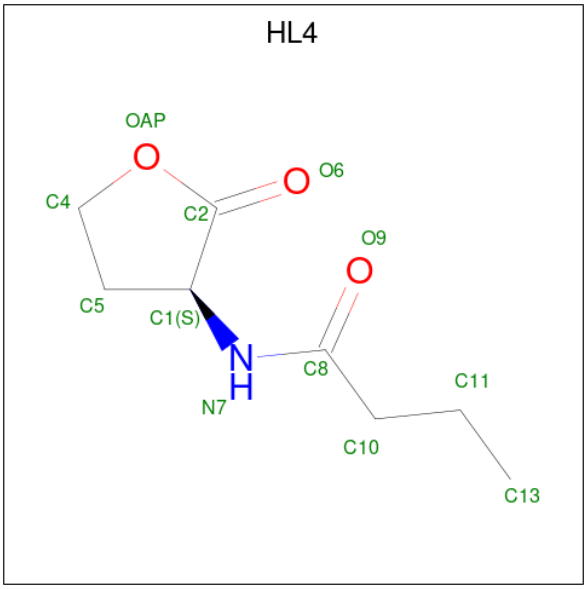
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	1	Total	Co	0	0
			1	1		
2	D	1	Total	Co	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



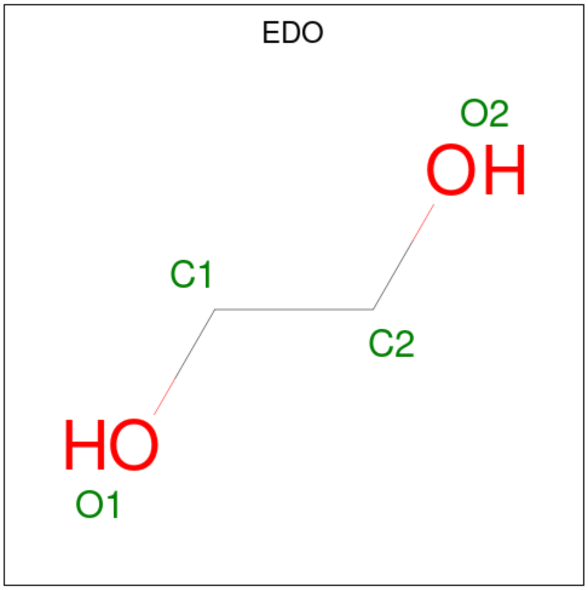
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total O S 5 4 1	0	0
3	P	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is N-[(3S)-2-oxotetrahydrofuran-3-yl]butanamide (three-letter code: HL4) (formula: $C_8H_{13}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total C N O 12 8 1 3	0	0
4	D	1	Total C N O 12 8 1 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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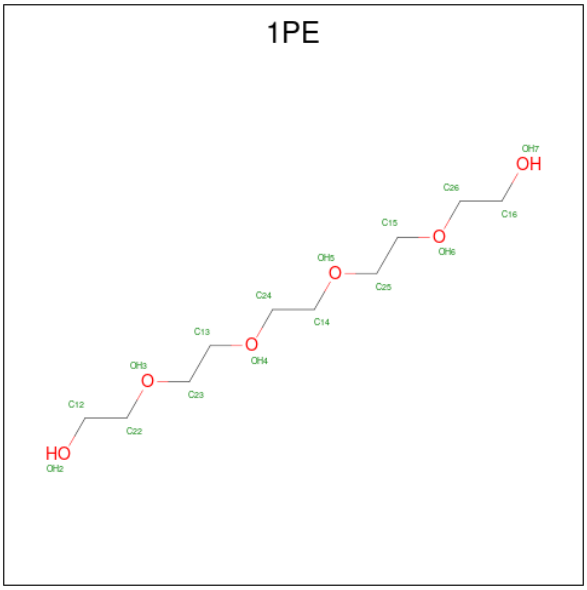
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).

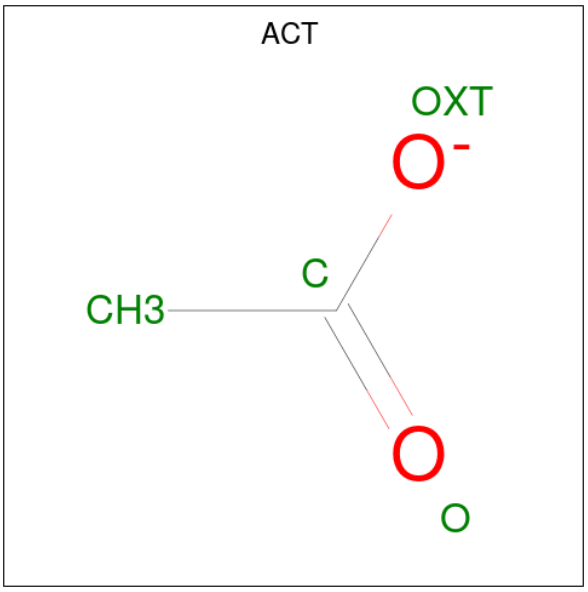


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	P	1	Total C O 16 10 6	0	0
6	P	1	Total C O 16 10 6	0	0
6	D	1	Total C O 16 10 6	0	0
6	D	1	Total C O 16 10 6	0	0

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

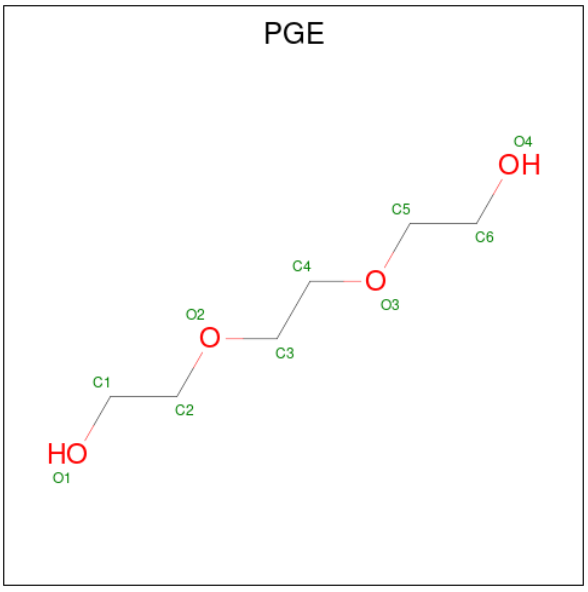
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	P	1	Total Fe 1 1	0	0
7	D	1	Total Fe 1 1	0	0

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	P	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	P	1	Total C O 10 6 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	P	1	Total C O 10 6 4	0	0
9	D	1	Total C O 10 6 4	0	0
9	D	1	Total C O 10 6 4	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	P	88	Total O 88 88	0	0
10	D	98	Total O 98 98	0	0

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

3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	108.02Å 108.02Å 222.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.74 – 2.35	Depositor
% Data completeness (in resolution range)	98.9 (19.74-2.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.55 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.166 , 0.211	Depositor
Wilson B-factor (Å^2)	40.3	Xtriage
Anisotropy	0.051	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
Total number of atoms	5043	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 37 ligands modelled in this entry, 4 are monoatomic - leaving 33 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	$\#\|Z\| > 2$
6	1PE	D	314	-	15,15,15	0.46	0	14,14,14	0.21	0
3	SO4	D	302	-	4,4,4	0.33	0	6,6,6	0.05	0
5	EDO	P	305	-	3,3,3	0.41	0	2,2,2	0.46	0
5	EDO	D	306	-	3,3,3	0.42	0	2,2,2	0.44	0
9	PGE	D	320	-	9,9,9	0.45	0	8,8,8	0.22	0
6	1PE	D	315	-	15,15,15	0.47	0	14,14,14	0.21	0
3	SO4	P	302	-	4,4,4	0.34	0	6,6,6	0.05	0
5	EDO	D	313	-	3,3,3	0.46	0	2,2,2	0.26	0
8	ACT	P	315	-	3,3,3	0.75	0	3,3,3	0.75	0
5	EDO	D	309	-	3,3,3	0.47	0	2,2,2	0.27	0
8	ACT	D	318	-	3,3,3	0.78	0	3,3,3	0.70	0
5	EDO	P	309	-	3,3,3	0.46	0	2,2,2	0.30	0
6	1PE	P	312	-	15,15,15	0.48	0	14,14,14	0.19	0
5	EDO	P	308	-	3,3,3	0.47	0	2,2,2	0.28	0
9	PGE	P	316	-	9,9,9	0.47	0	8,8,8	0.20	0
9	PGE	D	319	-	9,9,9	0.46	0	8,8,8	0.18	0
3	SO4	P	303	-	4,4,4	0.33	0	6,6,6	0.06	0
8	ACT	D	317	-	3,3,3	0.78	0	3,3,3	0.68	0
5	EDO	D	311	-	3,3,3	0.48	0	2,2,2	0.28	0
5	EDO	P	311	-	3,3,3	0.42	0	2,2,2	0.40	0
4	HL4	P	304	2,7	12,12,12	1.84	1 (8%)	11,15,15	2.40	3 (27%)
6	1PE	P	313	-	15,15,15	0.46	0	14,14,14	0.22	0
9	PGE	P	317	-	9,9,9	0.45	0	8,8,8	0.21	0
5	EDO	D	308	-	3,3,3	0.47	0	2,2,2	0.28	0
3	SO4	D	304	-	4,4,4	0.33	0	6,6,6	0.04	0
5	EDO	D	312	-	3,3,3	0.46	0	2,2,2	0.29	0
4	HL4	D	305	2,7	12,12,12	1.88	1 (8%)	11,15,15	2.02	3 (27%)
5	EDO	D	310	-	3,3,3	0.46	0	2,2,2	0.29	0
3	SO4	D	303	-	4,4,4	0.32	0	6,6,6	0.06	0
5	EDO	D	307	-	3,3,3	0.46	0	2,2,2	0.28	0
5	EDO	P	306	-	3,3,3	0.46	0	2,2,2	0.29	0
5	EDO	P	310	-	3,3,3	0.47	0	2,2,2	0.25	0
5	EDO	P	307	-	3,3,3	0.47	0	2,2,2	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	D	314	-	-	7/13/13/13	-
5	EDO	P	305	-	-	1/1/1/1	-
5	EDO	D	306	-	-	1/1/1/1	-
9	PGE	D	320	-	-	3/7/7/7	-
6	1PE	D	315	-	-	10/13/13/13	-
5	EDO	D	313	-	-	0/1/1/1	-
5	EDO	D	309	-	-	0/1/1/1	-
5	EDO	P	309	-	-	1/1/1/1	-
6	1PE	P	312	-	-	9/13/13/13	-
5	EDO	P	308	-	-	1/1/1/1	-
9	PGE	P	316	-	-	3/7/7/7	-
9	PGE	D	319	-	-	5/7/7/7	-
5	EDO	D	311	-	-	0/1/1/1	-
5	EDO	P	311	-	-	1/1/1/1	-
4	HL4	P	304	2,7	-	0/7/17/17	0/1/1/1
6	1PE	P	313	-	-	10/13/13/13	-
9	PGE	P	317	-	-	6/7/7/7	-
5	EDO	D	308	-	-	0/1/1/1	-
5	EDO	D	312	-	-	1/1/1/1	-
4	HL4	D	305	2,7	-	1/7/17/17	0/1/1/1
5	EDO	D	310	-	-	1/1/1/1	-
5	EDO	D	307	-	-	1/1/1/1	-
5	EDO	P	306	-	-	1/1/1/1	-
5	EDO	P	310	-	-	1/1/1/1	-
5	EDO	P	307	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	305	HL4	C1-C2	-6.15	1.39	1.52
4	P	304	HL4	C1-C2	-5.99	1.39	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	304	HL4	C4-OAP-C2	-6.80	104.10	110.39
4	D	305	HL4	C4-OAP-C2	-5.40	105.40	110.39
4	P	304	HL4	OAP-C2-O6	2.56	124.08	121.42
4	D	305	HL4	OAP-C2-O6	2.42	123.93	121.42
4	P	304	HL4	C5-C1-N7	-2.03	110.40	114.96
4	D	305	HL4	C5-C1-N7	-2.03	110.40	114.96

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	314	1PE	C25-C15-OH6-C26
6	D	314	1PE	OH2-C12-C22-OH3
9	P	316	PGE	O2-C3-C4-O3
6	D	315	1PE	OH4-C13-C23-OH3
9	P	317	PGE	O2-C3-C4-O3
9	D	319	PGE	O2-C3-C4-O3
9	D	319	PGE	O3-C5-C6-O4
6	D	314	1PE	OH6-C15-C25-OH5
6	D	315	1PE	OH5-C14-C24-OH4
6	P	313	1PE	OH5-C14-C24-OH4
6	P	312	1PE	OH2-C12-C22-OH3
6	D	314	1PE	OH7-C16-C26-OH6
9	P	317	PGE	O3-C5-C6-O4
9	D	320	PGE	O3-C5-C6-O4
6	D	314	1PE	OH4-C13-C23-OH3
6	D	315	1PE	C13-C23-OH3-C22
9	P	316	PGE	O3-C5-C6-O4
5	P	306	EDO	O1-C1-C2-O2
5	P	307	EDO	O1-C1-C2-O2
5	D	310	EDO	O1-C1-C2-O2
6	D	315	1PE	C23-C13-OH4-C24
6	P	313	1PE	OH2-C12-C22-OH3
6	P	313	1PE	OH7-C16-C26-OH6
6	P	312	1PE	OH6-C15-C25-OH5
9	D	319	PGE	C4-C3-O2-C2
9	D	320	PGE	O1-C1-C2-O2
5	D	307	EDO	O1-C1-C2-O2
6	D	315	1PE	C25-C15-OH6-C26
6	P	313	1PE	OH6-C15-C25-OH5
4	D	305	HL4	C8-C10-C11-C13
6	D	315	1PE	OH6-C15-C25-OH5
5	P	308	EDO	O1-C1-C2-O2
5	D	312	EDO	O1-C1-C2-O2
6	D	315	1PE	OH2-C12-C22-OH3
6	P	312	1PE	C15-C25-OH5-C14
6	P	312	1PE	C23-C13-OH4-C24
9	P	317	PGE	C4-C3-O2-C2
6	D	315	1PE	C14-C24-OH4-C13
6	P	312	1PE	C25-C15-OH6-C26
6	P	313	1PE	C24-C14-OH5-C25

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Mol	Chain	Res	Type	Atoms
6	P	312	1PE	C13-C23-OH3-C22
6	P	313	1PE	C13-C23-OH3-C22
6	P	312	1PE	C14-C24-OH4-C13
9	D	320	PGE	C4-C3-O2-C2
6	D	315	1PE	C24-C14-OH5-C25
6	P	312	1PE	OH7-C16-C26-OH6
6	D	314	1PE	C12-C22-OH3-C23
6	P	313	1PE	C12-C22-OH3-C23
6	P	313	1PE	C16-C26-OH6-C15
9	P	317	PGE	C6-C5-O3-C4
5	P	305	EDO	O1-C1-C2-O2
5	D	306	EDO	O1-C1-C2-O2
9	D	319	PGE	C1-C2-O2-C3
9	P	317	PGE	C1-C2-O2-C3
9	P	316	PGE	C3-C4-O3-C5
5	P	309	EDO	O1-C1-C2-O2
6	D	315	1PE	C15-C25-OH5-C14
6	P	313	1PE	OH4-C13-C23-OH3
6	D	314	1PE	C24-C14-OH5-C25
9	P	317	PGE	O1-C1-C2-O2
5	P	310	EDO	O1-C1-C2-O2
6	P	312	1PE	OH4-C13-C23-OH3
9	D	319	PGE	C3-C4-O3-C5
6	P	313	1PE	C23-C13-OH4-C24
5	P	311	EDO	O1-C1-C2-O2

There are no ring outliers.

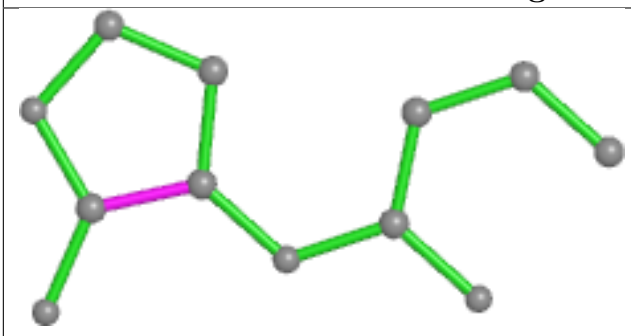
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	314	1PE	0	1
6	P	312	1PE	0	1

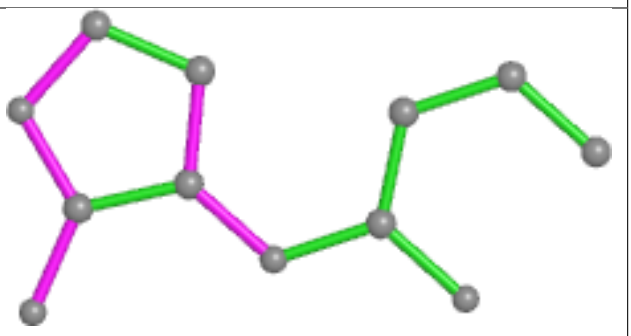
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

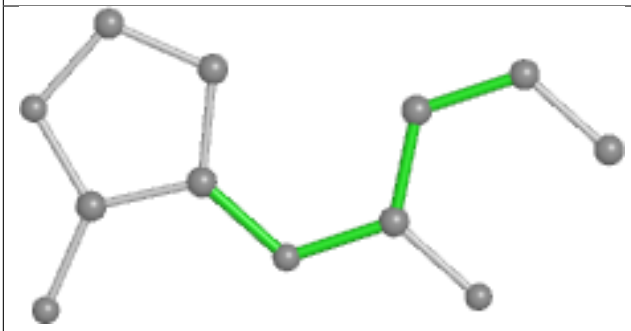
Ligand HL4 P 304



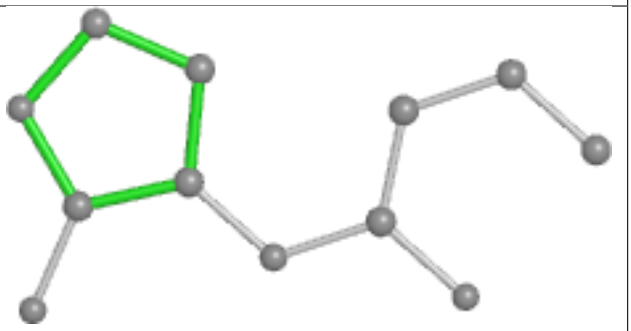
Bond lengths



Bond angles

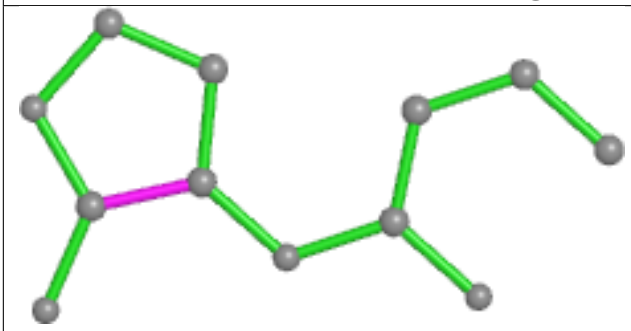


Torsions

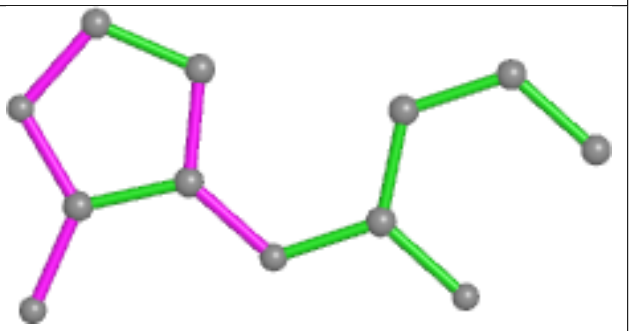


Rings

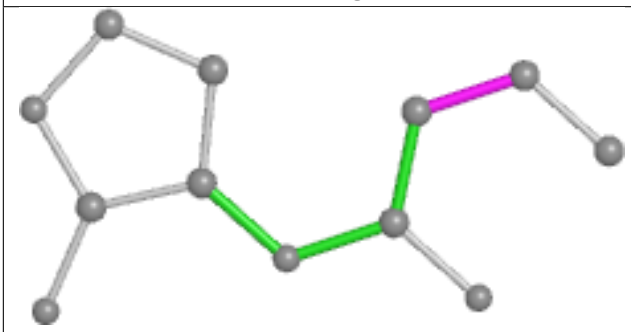
Ligand HL4 D 305



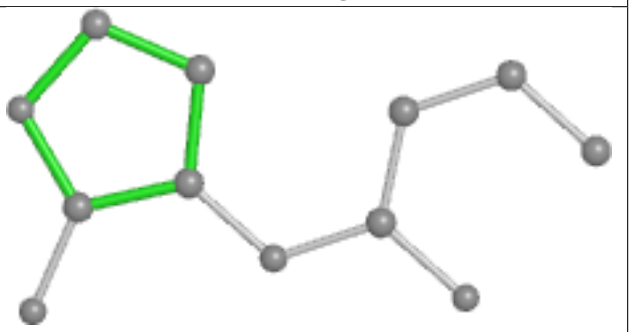
Bond lengths



Bond angles



Torsions



Rings

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

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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