Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 03:56 AM EDT

PDB ID	:	6PSM
Title	:	Crystal structure of PsS1_19B C77S in complex with kappa-neocarrabiose
Authors	:	Hettle, A.G.; Boraston, A.B.
Deposited on	:	2019-07-12
Resolution	:	1.95 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 (i) 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 (1)) 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 1.95 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 8 unique types of molecules in this entry. The entry contains 22255 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.

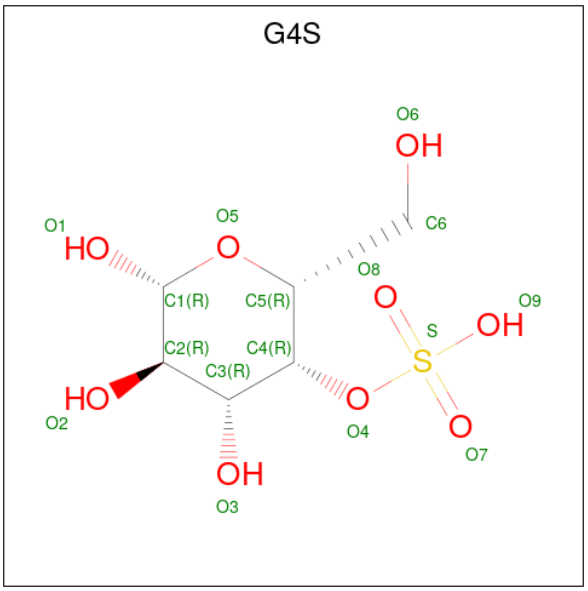
- Molecule 1 is a protein called exo-4S-kappa carrageenan S1 sulfatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	447	3537	2259	594	674	10	0	2	0
1	B	447	3526	2254	593	670	9	0	0	0
1	C	448	3540	2260	599	672	9	0	0	0
1	D	444	3505	2240	591	666	8	0	1	0
1	E	448	3545	2264	599	673	9	0	1	0
1	F	447	3522	2249	593	671	9	0	0	1

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

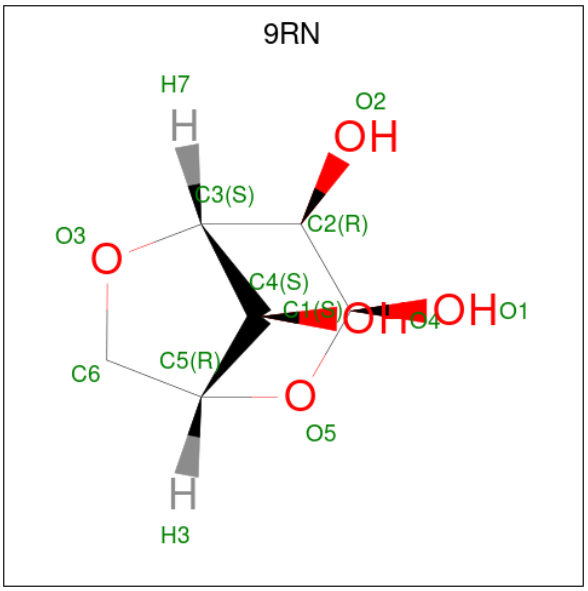
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0

- Molecule 3 is 4-O-sulfo-beta-D-galactopyranose (three-letter code: G4S) (formula: $C_6H_{12}O_9S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			16	6	9	1		
3	B	1	Total	C	O	S	0	0
			16	6	9	1		
3	C	1	Total	C	O	S	0	0
			16	6	9	1		
3	D	1	Total	C	O	S	0	0
			16	6	9	1		
3	E	1	Total	C	O	S	0	0
			16	6	9	1		
3	F	1	Total	C	O	S	0	0
			16	6	9	1		

- Molecule 4 is 3,6-anhydro-D-galactose (three-letter code: 9RN) (formula: $C_6H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	10	6	4	0	0
4	B	1	10	6	4	0	0
4	C	1	10	6	4	0	0
4	D	1	10	6	4	0	0
4	E	1	10	6	4	0	0
4	F	1	10	6	4	0	0

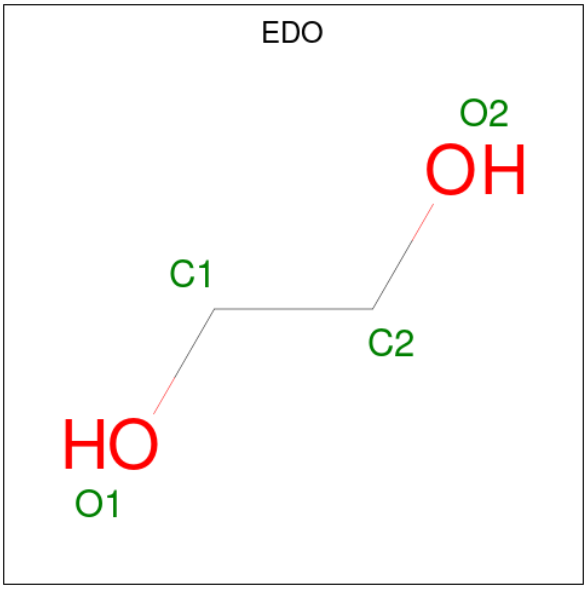
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	1	1	1	0	0
5	B	1	1	1	0	0
5	C	1	1	1	0	0
5	D	1	1	1	0	0
5	E	1	1	1	0	0
5	F	1	1	1	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	A	2	2	2	0	0
6	D	2	2	2	0	0
6	E	2	2	2	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	4	2	2	0	0
7	C	1	4	2	2	0	0
7	D	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	F	1	4	2	2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	140	140	140	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	B	121	121	121	0	0
			Total	O		
8	C	163	163	163	0	0
			Total	O		
8	D	131	131	131	0	0
			Total	O		
8	E	145	145	145	0	0
			Total	O		
8	F	186	186	186	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	P 31	Depositor
Cell constants a, b, c, α, β, γ	93.05Å 93.05Å 300.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.19 – 1.95	Depositor
% Data completeness (in resolution range)	99.7 (48.19-1.95)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.192 , 0.212	Depositor
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.703	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.110 for -h,-k,l 0.114 for h,-h-k,-l 0.178 for -k,-h,-l	Xtriage
Total number of atoms	22255	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.74% 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 (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 35 ligands modelled in this entry, 18 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
4	9RN	A	503	3	11,11,12	0.53	0	15,16,18	1.35	3 (20%)
3	G4S	B	503	4,2	16,16,16	0.85	0	19,24,24	0.77	1 (5%)
7	EDO	C	503	-	3,3,3	0.29	0	2,2,2	0.62	0
4	9RN	C	505	3	11,11,12	0.50	0	15,16,18	1.26	3 (20%)
7	EDO	A	507	-	3,3,3	0.20	0	2,2,2	0.30	0
4	9RN	D	507	3	11,11,12	0.47	0	15,16,18	1.20	2 (13%)
3	G4S	C	504	4,2	16,16,16	1.29	1 (6%)	19,24,24	0.68	0
7	EDO	D	505	-	3,3,3	0.19	0	2,2,2	0.19	0
4	9RN	E	507	3	11,11,12	0.47	0	15,16,18	1.37	2 (13%)
4	9RN	F	505	3	11,11,12	0.50	0	15,16,18	1.27	2 (13%)
7	EDO	E	505	-	3,3,3	0.30	0	2,2,2	0.13	0
4	9RN	B	504	3	11,11,12	0.50	0	15,16,18	1.25	2 (13%)
3	G4S	F	504	4,2	16,16,16	1.24	1 (6%)	19,24,24	0.64	0
7	EDO	F	503	-	3,3,3	0.13	0	2,2,2	0.43	0
3	G4S	A	502	4,2	16,16,16	1.28	1 (6%)	19,24,24	0.67	0
3	G4S	D	506	4,2	16,16,16	0.88	1 (6%)	19,24,24	0.77	0
3	G4S	E	506	4,2	16,16,16	0.88	0	19,24,24	0.79	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
4	9RN	A	503	3	-	-	0/3/2/2
3	G4S	B	503	4,2	-	0/7/27/27	0/1/1/1
7	EDO	C	503	-	-	0/1/1/1	-
7	EDO	A	507	-	-	0/1/1/1	-
4	9RN	C	505	3	-	-	0/3/2/2
4	9RN	D	507	3	-	-	0/3/2/2
3	G4S	C	504	4,2	-	0/7/27/27	0/1/1/1
7	EDO	D	505	-	-	0/1/1/1	-
4	9RN	E	507	3	-	-	0/3/2/2
4	9RN	F	505	3	-	-	0/3/2/2
7	EDO	E	505	-	-	0/1/1/1	-
4	9RN	B	504	3	-	-	0/3/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	G4S	F	504	4,2	-	0/7/27/27	0/1/1/1
7	EDO	F	503	-	-	0/1/1/1	-
3	G4S	A	502	4,2	-	0/7/27/27	0/1/1/1
3	G4S	D	506	4,2	-	0/7/27/27	0/1/1/1
3	G4S	E	506	4,2	-	0/7/27/27	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	G4S	O7-S	4.01	1.62	1.45
3	C	504	G4S	O8-S	3.99	1.62	1.45
3	F	504	G4S	O7-S	3.95	1.62	1.45
3	D	506	G4S	O9-S	2.01	1.62	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	507	9RN	O5-C5-C6	-3.27	108.47	113.33
4	D	507	9RN	C2-C3-C4	-3.12	106.12	113.85
4	F	505	9RN	C2-C3-C4	-3.09	106.21	113.85
4	A	503	9RN	O5-C5-C6	-3.01	108.87	113.33
4	B	504	9RN	O5-C5-C6	-2.98	108.91	113.33
4	E	507	9RN	C2-C3-C4	-2.86	106.78	113.85
4	B	504	9RN	C2-C3-C4	-2.70	107.16	113.85
4	F	505	9RN	O5-C5-C6	-2.65	109.39	113.33
4	C	505	9RN	O5-C5-C6	-2.57	109.51	113.33
4	D	507	9RN	O5-C5-C6	-2.55	109.54	113.33
4	C	505	9RN	C2-C3-C4	-2.54	107.56	113.85
4	A	503	9RN	C2-C3-C4	-2.51	107.65	113.85
4	A	503	9RN	C1-C2-C3	2.46	112.14	109.17
4	C	505	9RN	C1-C2-C3	2.13	111.75	109.17
3	B	503	G4S	C4-O4-S	2.11	122.95	118.88

There are no chirality outliers.

There are no torsion outliers.

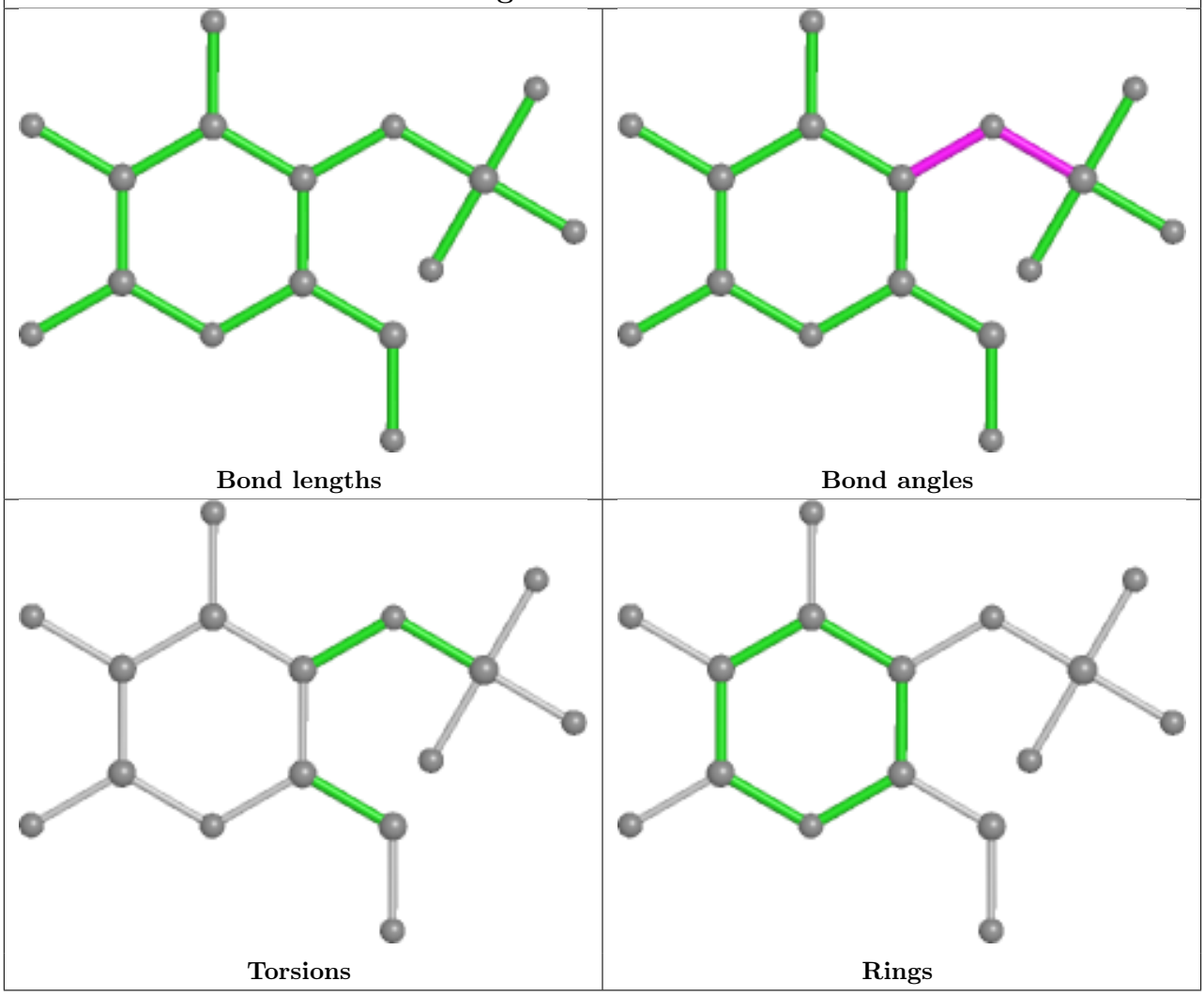
There are no ring outliers.

No monomer is involved in short contacts.

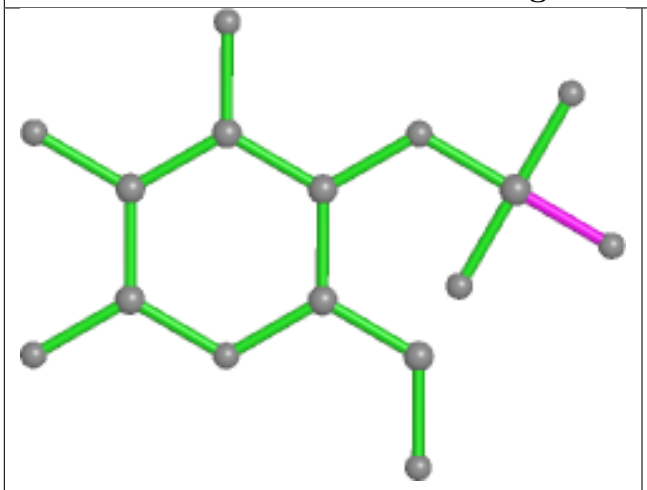
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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.

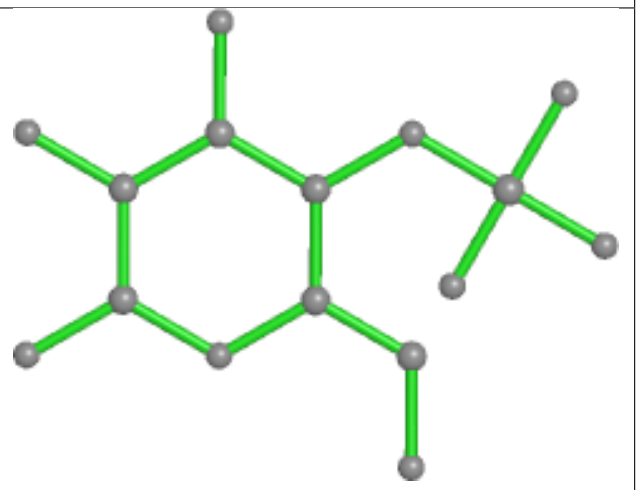
Ligand G4S B 503



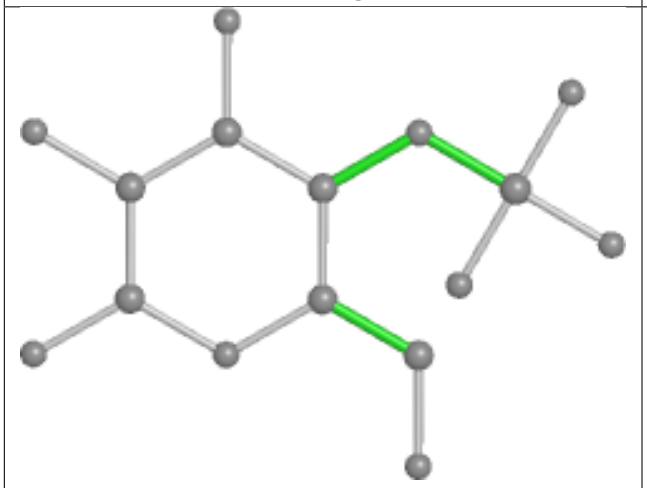
Ligand G4S C 504



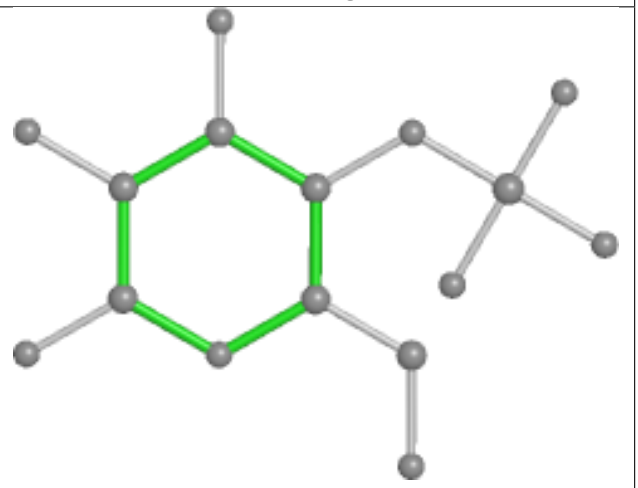
Bond lengths



Bond angles

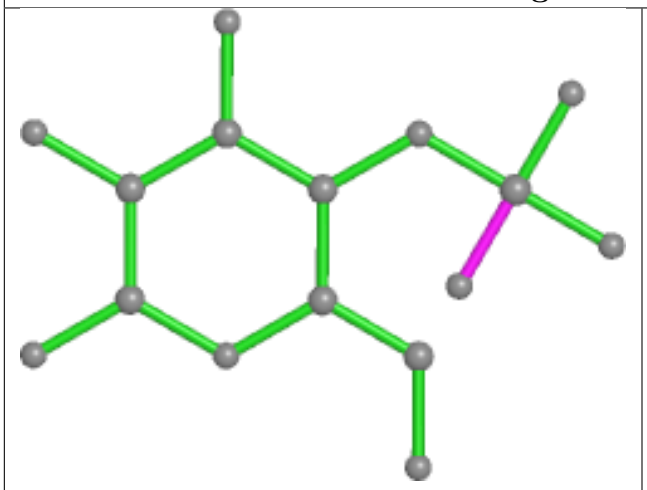


Torsions

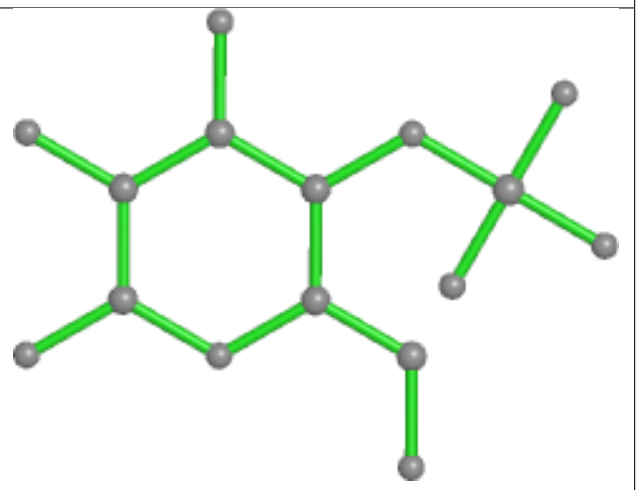


Rings

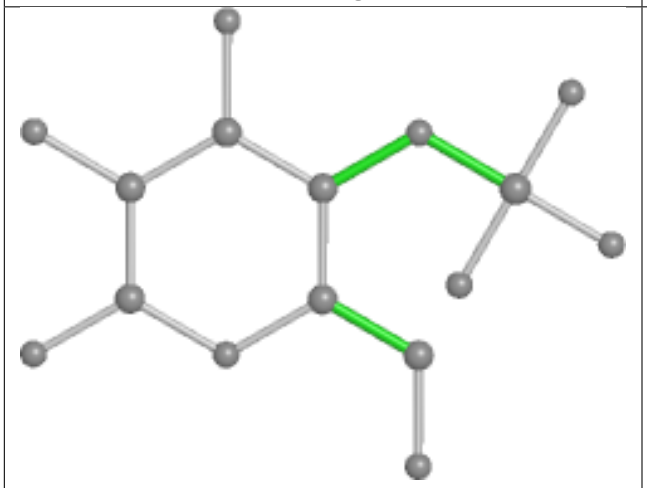
Ligand G4S F 504



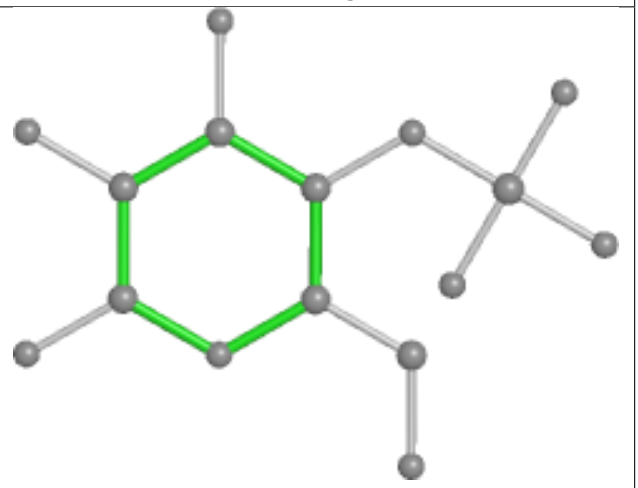
Bond lengths



Bond angles

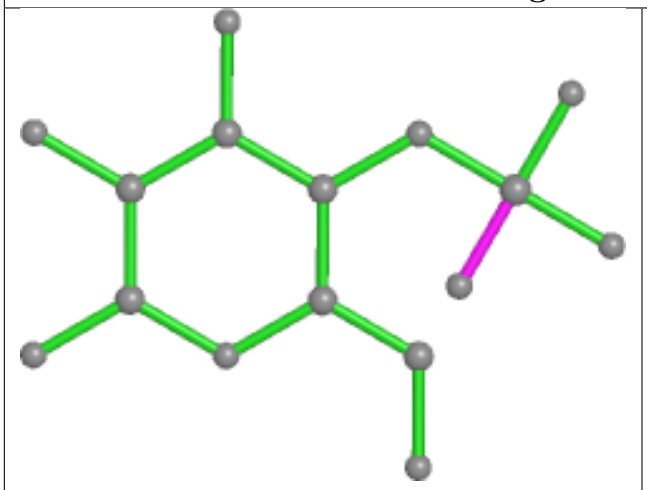


Torsions

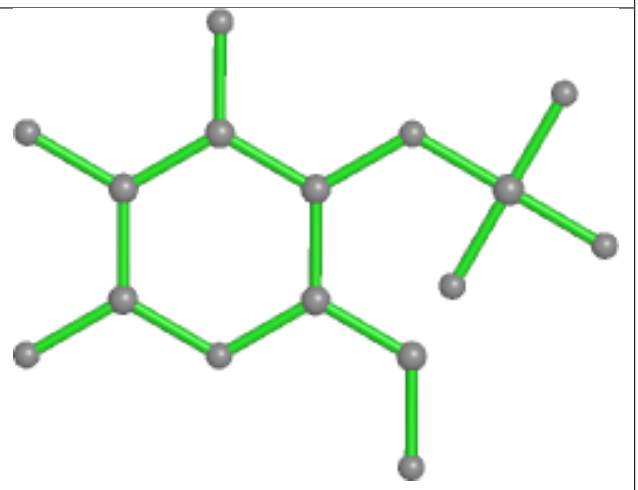


Rings

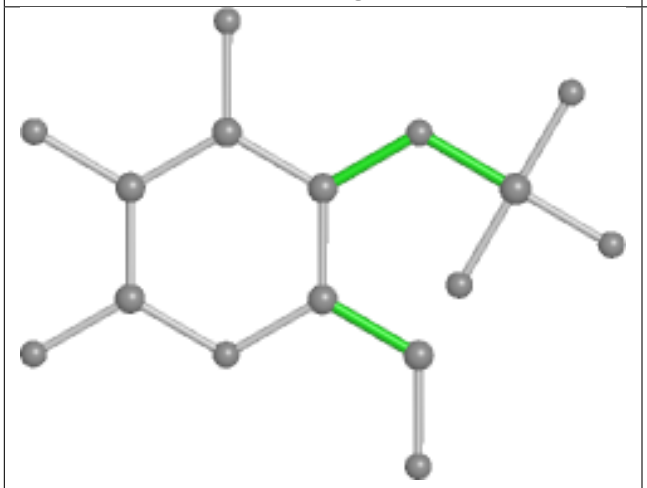
Ligand G4S A 502



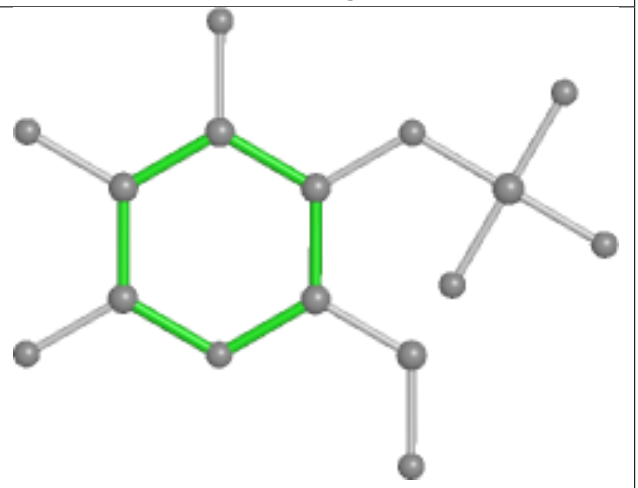
Bond lengths



Bond angles

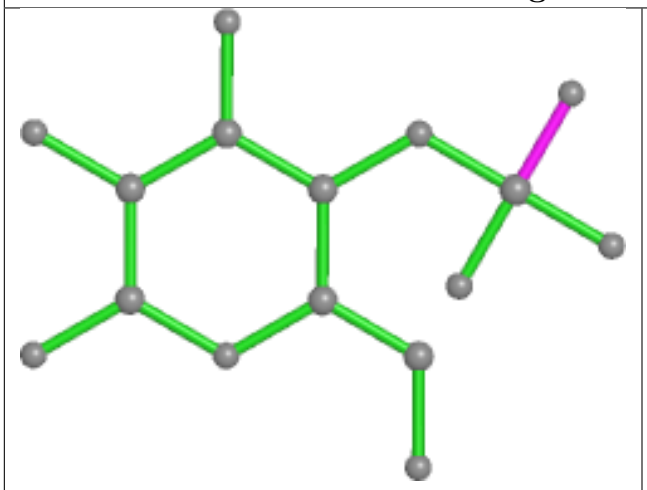


Torsions

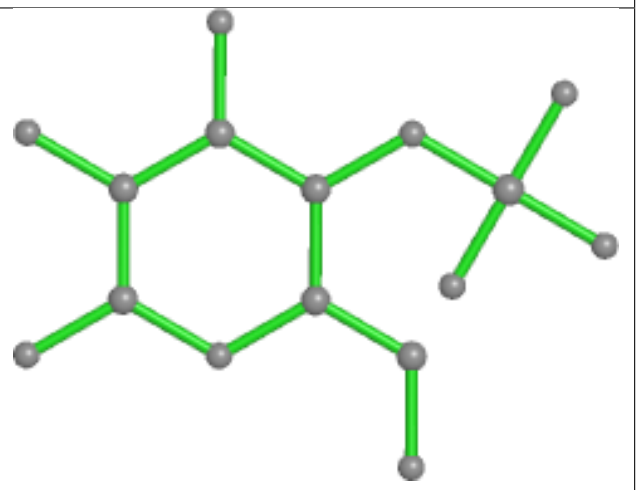


Rings

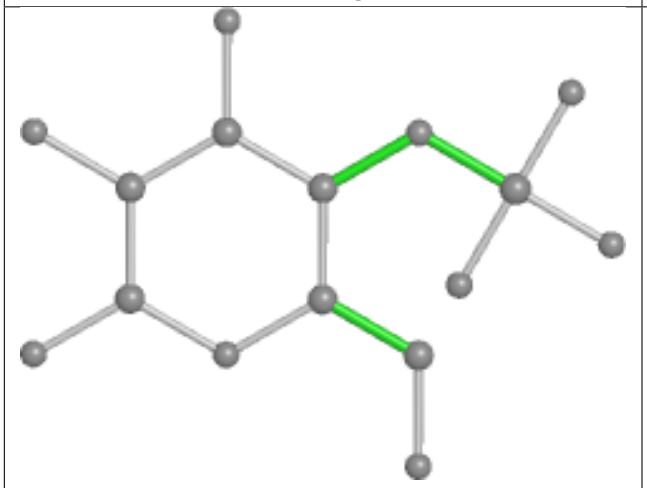
Ligand G4S D 506



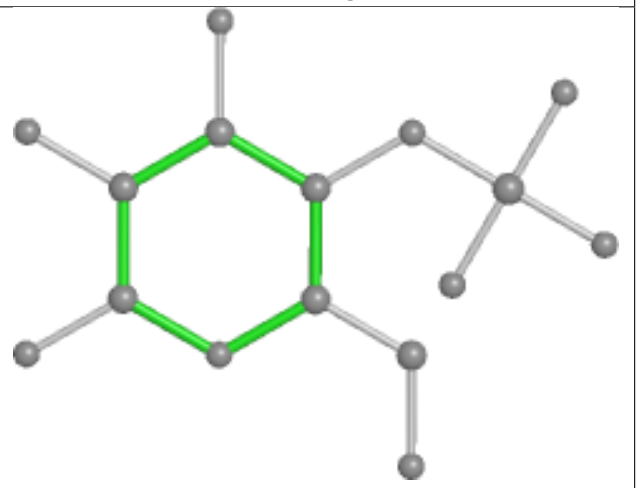
Bond lengths



Bond angles

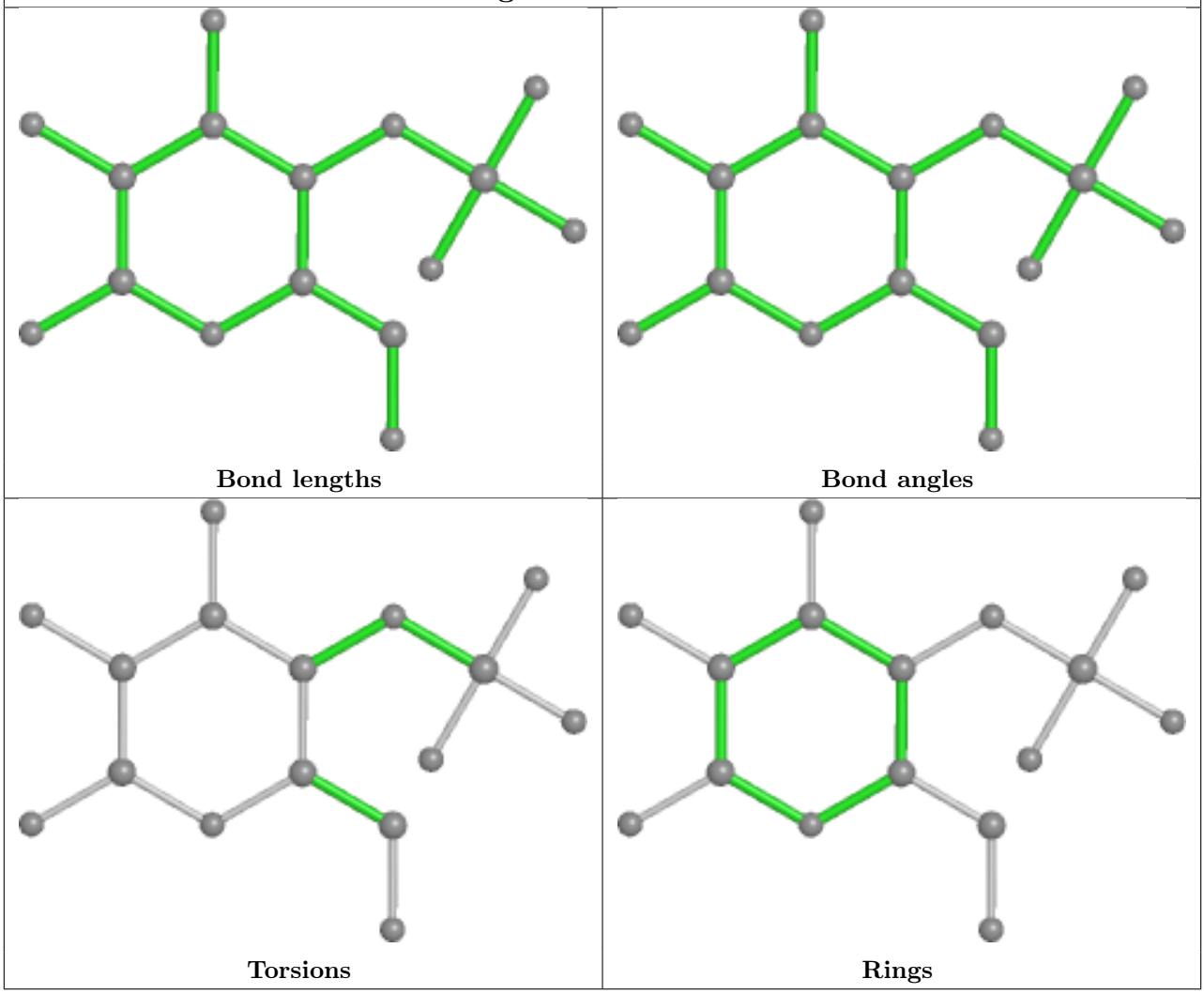


Torsions



Rings

Ligand G4S E 506



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.