Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2023 – 11:30 PM EDT

PDB ID	:	6MSO
Title	:	Crystal structure of mitochondrial fumarate hydratase from Leishmania major in a complex with inhibitor thiomalate
Authors	:	Feliciano, P.R.; Drennan, C.L.; Nonato, M.C.
Deposited on	:	2018-10-17
Resolution	:	2.05 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 2.05 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 6 unique types of molecules in this entry. The entry contains 17547 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 fumarate hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	3	0
			4169	2644	715	780	30			
1	B	540	Total	C	N	O	S	0	4	0
			4174	2649	712	780	33			
1	C	528	Total	C	N	O	S	0	3	0
			4055	2573	698	755	29			
1	D	531	Total	C	N	O	S	0	2	0
			4039	2562	693	755	29			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	initiating methionine	UNP Q4QAU9
A	-34	GLY	-	expression tag	UNP Q4QAU9
A	-33	SER	-	expression tag	UNP Q4QAU9
A	-32	SER	-	expression tag	UNP Q4QAU9
A	-31	HIS	-	expression tag	UNP Q4QAU9
A	-30	HIS	-	expression tag	UNP Q4QAU9
A	-29	HIS	-	expression tag	UNP Q4QAU9
A	-28	HIS	-	expression tag	UNP Q4QAU9
A	-27	HIS	-	expression tag	UNP Q4QAU9
A	-26	HIS	-	expression tag	UNP Q4QAU9
A	-25	SER	-	expression tag	UNP Q4QAU9
A	-24	SER	-	expression tag	UNP Q4QAU9
A	-23	GLY	-	expression tag	UNP Q4QAU9
A	-22	LEU	-	expression tag	UNP Q4QAU9
A	-21	VAL	-	expression tag	UNP Q4QAU9
A	-20	PRO	-	expression tag	UNP Q4QAU9
A	-19	ARG	-	expression tag	UNP Q4QAU9
A	-18	GLY	-	expression tag	UNP Q4QAU9
A	-17	SER	-	expression tag	UNP Q4QAU9
A	-16	HIS	-	expression tag	UNP Q4QAU9
A	-15	MET	-	expression tag	UNP Q4QAU9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	ALA	-	expression tag	UNP Q4QAU9
A	-13	SER	-	expression tag	UNP Q4QAU9
A	-12	MET	-	expression tag	UNP Q4QAU9
A	-11	THR	-	expression tag	UNP Q4QAU9
A	-10	GLY	-	expression tag	UNP Q4QAU9
A	-9	GLY	-	expression tag	UNP Q4QAU9
A	-8	GLN	-	expression tag	UNP Q4QAU9
A	-7	GLN	-	expression tag	UNP Q4QAU9
A	-6	MET	-	expression tag	UNP Q4QAU9
A	-5	GLY	-	expression tag	UNP Q4QAU9
A	-4	ARG	-	expression tag	UNP Q4QAU9
A	-3	GLY	-	expression tag	UNP Q4QAU9
A	-2	SER	-	expression tag	UNP Q4QAU9
A	-1	GLU	-	expression tag	UNP Q4QAU9
A	0	PHE	-	expression tag	UNP Q4QAU9
B	-35	MET	-	initiating methionine	UNP Q4QAU9
B	-34	GLY	-	expression tag	UNP Q4QAU9
B	-33	SER	-	expression tag	UNP Q4QAU9
B	-32	SER	-	expression tag	UNP Q4QAU9
B	-31	HIS	-	expression tag	UNP Q4QAU9
B	-30	HIS	-	expression tag	UNP Q4QAU9
B	-29	HIS	-	expression tag	UNP Q4QAU9
B	-28	HIS	-	expression tag	UNP Q4QAU9
B	-27	HIS	-	expression tag	UNP Q4QAU9
B	-26	HIS	-	expression tag	UNP Q4QAU9
B	-25	SER	-	expression tag	UNP Q4QAU9
B	-24	SER	-	expression tag	UNP Q4QAU9
B	-23	GLY	-	expression tag	UNP Q4QAU9
B	-22	LEU	-	expression tag	UNP Q4QAU9
B	-21	VAL	-	expression tag	UNP Q4QAU9
B	-20	PRO	-	expression tag	UNP Q4QAU9
B	-19	ARG	-	expression tag	UNP Q4QAU9
B	-18	GLY	-	expression tag	UNP Q4QAU9
B	-17	SER	-	expression tag	UNP Q4QAU9
B	-16	HIS	-	expression tag	UNP Q4QAU9
B	-15	MET	-	expression tag	UNP Q4QAU9
B	-14	ALA	-	expression tag	UNP Q4QAU9
B	-13	SER	-	expression tag	UNP Q4QAU9
B	-12	MET	-	expression tag	UNP Q4QAU9
B	-11	THR	-	expression tag	UNP Q4QAU9
B	-10	GLY	-	expression tag	UNP Q4QAU9
B	-9	GLY	-	expression tag	UNP Q4QAU9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLN	-	expression tag	UNP Q4QAU9
B	-7	GLN	-	expression tag	UNP Q4QAU9
B	-6	MET	-	expression tag	UNP Q4QAU9
B	-5	GLY	-	expression tag	UNP Q4QAU9
B	-4	ARG	-	expression tag	UNP Q4QAU9
B	-3	GLY	-	expression tag	UNP Q4QAU9
B	-2	SER	-	expression tag	UNP Q4QAU9
B	-1	GLU	-	expression tag	UNP Q4QAU9
B	0	PHE	-	expression tag	UNP Q4QAU9
C	-35	MET	-	initiating methionine	UNP Q4QAU9
C	-34	GLY	-	expression tag	UNP Q4QAU9
C	-33	SER	-	expression tag	UNP Q4QAU9
C	-32	SER	-	expression tag	UNP Q4QAU9
C	-31	HIS	-	expression tag	UNP Q4QAU9
C	-30	HIS	-	expression tag	UNP Q4QAU9
C	-29	HIS	-	expression tag	UNP Q4QAU9
C	-28	HIS	-	expression tag	UNP Q4QAU9
C	-27	HIS	-	expression tag	UNP Q4QAU9
C	-26	HIS	-	expression tag	UNP Q4QAU9
C	-25	SER	-	expression tag	UNP Q4QAU9
C	-24	SER	-	expression tag	UNP Q4QAU9
C	-23	GLY	-	expression tag	UNP Q4QAU9
C	-22	LEU	-	expression tag	UNP Q4QAU9
C	-21	VAL	-	expression tag	UNP Q4QAU9
C	-20	PRO	-	expression tag	UNP Q4QAU9
C	-19	ARG	-	expression tag	UNP Q4QAU9
C	-18	GLY	-	expression tag	UNP Q4QAU9
C	-17	SER	-	expression tag	UNP Q4QAU9
C	-16	HIS	-	expression tag	UNP Q4QAU9
C	-15	MET	-	expression tag	UNP Q4QAU9
C	-14	ALA	-	expression tag	UNP Q4QAU9
C	-13	SER	-	expression tag	UNP Q4QAU9
C	-12	MET	-	expression tag	UNP Q4QAU9
C	-11	THR	-	expression tag	UNP Q4QAU9
C	-10	GLY	-	expression tag	UNP Q4QAU9
C	-9	GLY	-	expression tag	UNP Q4QAU9
C	-8	GLN	-	expression tag	UNP Q4QAU9
C	-7	GLN	-	expression tag	UNP Q4QAU9
C	-6	MET	-	expression tag	UNP Q4QAU9
C	-5	GLY	-	expression tag	UNP Q4QAU9
C	-4	ARG	-	expression tag	UNP Q4QAU9
C	-3	GLY	-	expression tag	UNP Q4QAU9

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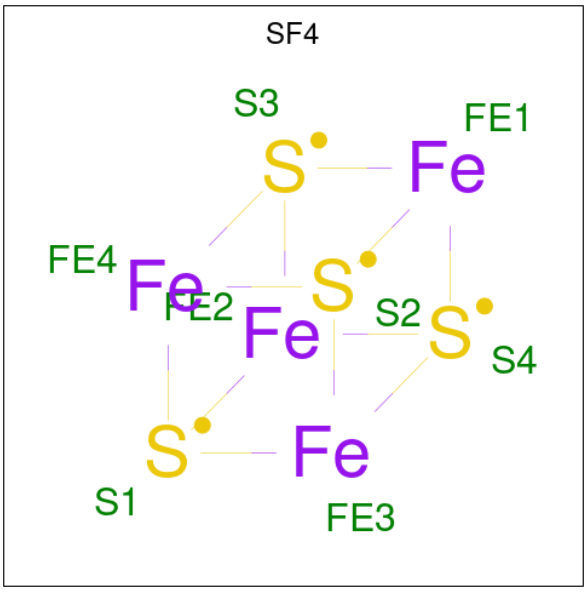
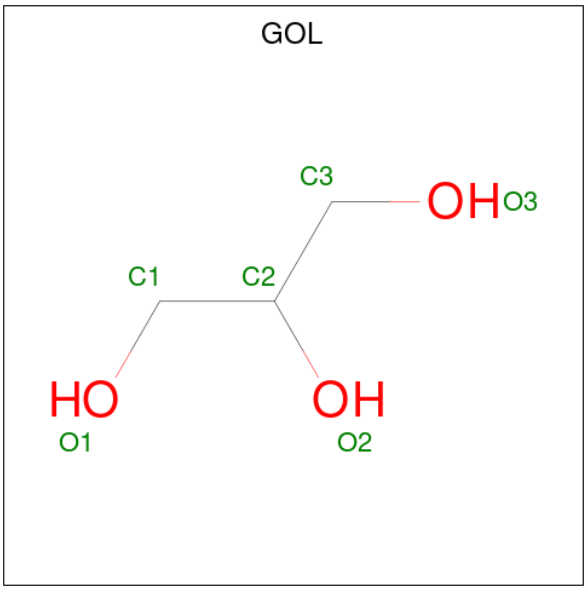
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	expression tag	UNP Q4QAU9
C	-1	GLU	-	expression tag	UNP Q4QAU9
C	0	PHE	-	expression tag	UNP Q4QAU9
D	-35	MET	-	initiating methionine	UNP Q4QAU9
D	-34	GLY	-	expression tag	UNP Q4QAU9
D	-33	SER	-	expression tag	UNP Q4QAU9
D	-32	SER	-	expression tag	UNP Q4QAU9
D	-31	HIS	-	expression tag	UNP Q4QAU9
D	-30	HIS	-	expression tag	UNP Q4QAU9
D	-29	HIS	-	expression tag	UNP Q4QAU9
D	-28	HIS	-	expression tag	UNP Q4QAU9
D	-27	HIS	-	expression tag	UNP Q4QAU9
D	-26	HIS	-	expression tag	UNP Q4QAU9
D	-25	SER	-	expression tag	UNP Q4QAU9
D	-24	SER	-	expression tag	UNP Q4QAU9
D	-23	GLY	-	expression tag	UNP Q4QAU9
D	-22	LEU	-	expression tag	UNP Q4QAU9
D	-21	VAL	-	expression tag	UNP Q4QAU9
D	-20	PRO	-	expression tag	UNP Q4QAU9
D	-19	ARG	-	expression tag	UNP Q4QAU9
D	-18	GLY	-	expression tag	UNP Q4QAU9
D	-17	SER	-	expression tag	UNP Q4QAU9
D	-16	HIS	-	expression tag	UNP Q4QAU9
D	-15	MET	-	expression tag	UNP Q4QAU9
D	-14	ALA	-	expression tag	UNP Q4QAU9
D	-13	SER	-	expression tag	UNP Q4QAU9
D	-12	MET	-	expression tag	UNP Q4QAU9
D	-11	THR	-	expression tag	UNP Q4QAU9
D	-10	GLY	-	expression tag	UNP Q4QAU9
D	-9	GLY	-	expression tag	UNP Q4QAU9
D	-8	GLN	-	expression tag	UNP Q4QAU9
D	-7	GLN	-	expression tag	UNP Q4QAU9
D	-6	MET	-	expression tag	UNP Q4QAU9
D	-5	GLY	-	expression tag	UNP Q4QAU9
D	-4	ARG	-	expression tag	UNP Q4QAU9
D	-3	GLY	-	expression tag	UNP Q4QAU9
D	-2	SER	-	expression tag	UNP Q4QAU9
D	-1	GLU	-	expression tag	UNP Q4QAU9
D	0	PHE	-	expression tag	UNP Q4QAU9

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



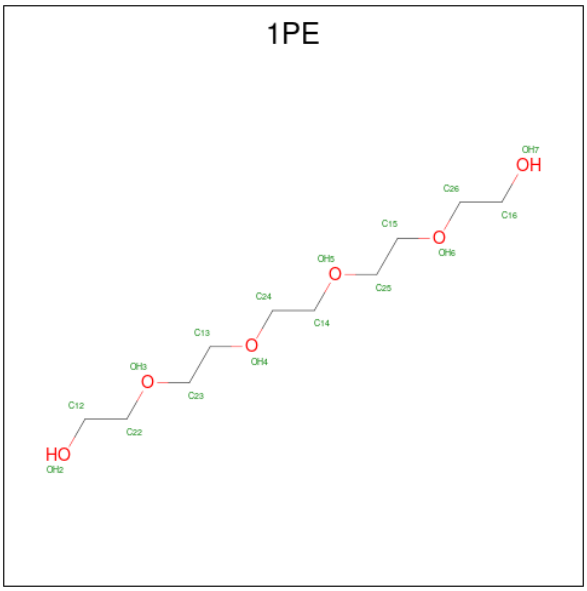
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 10 6 4	0	0
4	A	1	Total C O 10 6 4	0	0

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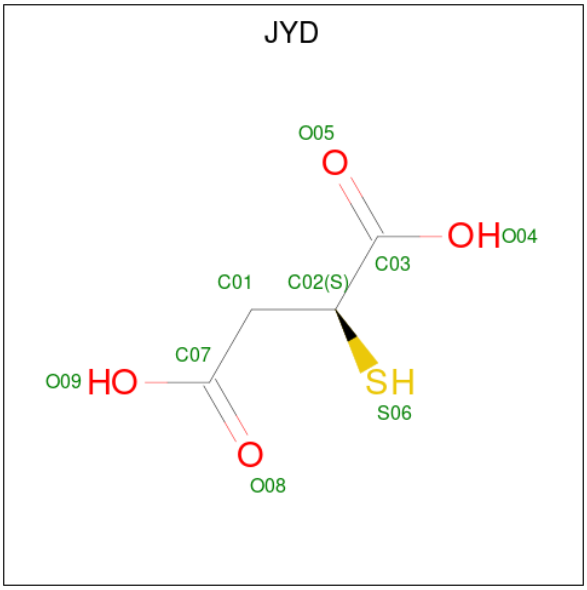
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 13 8 5	0	0
4	B	1	Total C O 10 6 4	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 10 6 4	0	0
4	C	1	Total C O 10 6 4	0	0
4	D	1	Total C O 16 10 6	0	0

- Molecule 5 is (2S)-2-sulfanylbutanedioic acid (three-letter code: JYD) (formula: $C_4H_6O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O S 18 8 8 2	0	1
5	B	1	Total C O S 18 8 8 2	0	1
5	C	1	Total C O S 9 4 4 1	0	0
5	D	1	Total C O S 9 4 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	251	Total O 252 252	0	1
6	B	282	Total O 282 282	0	0
6	C	166	Total O 167 167	0	1
6	D	168	Total O 169 169	0	1

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 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.74Å 138.44Å 138.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 2.05	Depositor
% Data completeness (in resolution range)	98.1 (48.88-2.05)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	341.80 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.159 , 0.204	Depositor
Wilson B-factor (Å^2)	24.3	Xtriage
Anisotropy	0.547	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.418 for -h,-l,-k 0.409 for -h,l,k 0.448 for h,-k,-l	Xtriage
Total number of atoms	17547	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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

28 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	$\#\|Z\| > 2$
5	JYD	A	608[A]	2	6,8,8	1.09	0	6,10,10	1.34	0
5	JYD	C	604	2	6,8,8	1.14	0	6,10,10	1.11	0
2	SF4	B	601	1,5	0,12,12	-	-	-		
3	GOL	B	602	-	5,5,5	0.84	0	5,5,5	1.56	1 (20%)
2	SF4	D	601	1,5	0,12,12	-	-	-		
3	GOL	A	605	-	5,5,5	1.30	1 (20%)	5,5,5	0.80	0
3	GOL	A	604	-	5,5,5	1.16	1 (20%)	5,5,5	1.10	0
4	1PE	A	607	-	6,6,15	0.50	0	5,5,14	0.38	0
4	1PE	D	603	-	15,15,15	0.55	0	14,14,14	0.39	0
4	1PE	B	606	-	9,9,15	0.29	0	8,8,14	0.41	0
4	1PE	A	609	-	12,12,15	0.51	0	11,11,14	0.60	0
4	1PE	B	605	-	12,12,15	0.55	0	11,11,14	0.67	0
4	1PE	C	606	-	9,9,15	0.26	0	8,8,14	0.50	0
3	GOL	A	603	-	5,5,5	1.30	1 (20%)	5,5,5	0.93	0
3	GOL	A	602	-	5,5,5	1.72	1 (20%)	5,5,5	1.08	1 (20%)
5	JYD	B	604[B]	2	6,8,8	1.13	0	6,10,10	1.18	0
5	JYD	D	602	2	6,8,8	1.02	0	6,10,10	1.92	3 (50%)
2	SF4	A	601	1,5	0,12,12	-	-	-		
4	1PE	A	611	-	9,9,15	0.28	0	8,8,14	0.39	0
5	JYD	A	608[B]	2	6,8,8	1.15	0	6,10,10	1.47	1 (16%)
4	1PE	C	605	-	9,9,15	0.27	0	8,8,14	0.50	0
4	1PE	C	603	-	6,6,15	0.50	0	5,5,14	0.37	0
5	JYD	B	604[A]	2	6,8,8	1.10	0	6,10,10	1.30	0
3	GOL	A	606	-	5,5,5	1.15	1 (20%)	5,5,5	1.00	0
2	SF4	C	601	1,5	0,12,12	-	-	-		
3	GOL	C	602	-	5,5,5	0.90	0	5,5,5	1.05	0
4	1PE	A	610	-	9,9,15	0.36	0	8,8,14	0.35	0
3	GOL	B	603	-	5,5,5	1.19	1 (20%)	5,5,5	1.09	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
5	JYD	A	608[A]	2	-	1/6/8/8	-
5	JYD	C	604	2	-	2/6/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	B	601	1,5	-	-	0/6/5/5
3	GOL	B	602	-	-	4/4/4/4	-
2	SF4	D	601	1,5	-	-	0/6/5/5
3	GOL	A	605	-	-	2/4/4/4	-
3	GOL	A	604	-	-	4/4/4/4	-
4	1PE	A	607	-	-	1/4/4/13	-
4	1PE	D	603	-	-	11/13/13/13	-
4	1PE	B	606	-	-	4/7/7/13	-
4	1PE	A	609	-	-	7/10/10/13	-
4	1PE	B	605	-	-	3/10/10/13	-
4	1PE	C	606	-	-	3/7/7/13	-
3	GOL	A	603	-	-	2/4/4/4	-
3	GOL	A	602	-	-	0/4/4/4	-
5	JYD	B	604[B]	2	-	2/6/8/8	-
5	JYD	D	602	2	-	2/6/8/8	-
2	SF4	A	601	1,5	-	-	0/6/5/5
4	1PE	A	611	-	-	5/7/7/13	-
5	JYD	A	608[B]	2	-	1/6/8/8	-
4	1PE	C	605	-	-	4/7/7/13	-
4	1PE	C	603	-	-	4/4/4/13	-
5	JYD	B	604[A]	2	-	1/6/8/8	-
3	GOL	A	606	-	-	2/4/4/4	-
2	SF4	C	601	1,5	-	-	0/6/5/5
3	GOL	C	602	-	-	2/4/4/4	-
4	1PE	A	610	-	-	5/7/7/13	-
3	GOL	B	603	-	-	0/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	GOL	O2-C2	-3.33	1.33	1.43
3	A	605	GOL	O2-C2	-2.77	1.35	1.43
3	A	603	GOL	O2-C2	-2.70	1.35	1.43
3	B	603	GOL	O2-C2	-2.32	1.36	1.43
3	A	606	GOL	O2-C2	-2.10	1.37	1.43
3	A	604	GOL	O2-C2	-2.06	1.37	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	602	JYD	O09-C07-C01	2.64	122.54	114.07
3	B	602	GOL	C3-C2-C1	-2.63	101.50	111.70
5	D	602	JYD	O08-C07-C01	-2.47	114.89	122.80
5	D	602	JYD	O04-C03-C02	2.30	120.47	114.03
3	A	602	GOL	C3-C2-C1	-2.04	103.76	111.70
5	A	608[B]	JYD	O04-C03-C02	2.02	119.71	114.03

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	GOL	O1-C1-C2-C3
3	A	604	GOL	O1-C1-C2-C3
3	A	606	GOL	C1-C2-C3-O3
3	C	602	GOL	O1-C1-C2-C3
5	A	608[A]	JYD	C07-C01-C02-S06
5	A	608[B]	JYD	C07-C01-C02-C03
5	B	604[A]	JYD	C07-C01-C02-S06
5	B	604[B]	JYD	C07-C01-C02-C03
5	B	604[B]	JYD	C07-C01-C02-S06
5	C	604	JYD	C07-C01-C02-S06
5	D	602	JYD	C07-C01-C02-S06
4	A	609	1PE	C13-C23-OH3-C22
4	A	611	1PE	C14-C24-OH4-C13
4	C	606	1PE	OH5-C14-C24-OH4
4	B	605	1PE	OH4-C13-C23-OH3
4	A	609	1PE	OH5-C14-C24-OH4
4	D	603	1PE	OH4-C13-C23-OH3
4	A	609	1PE	OH4-C13-C23-OH3
4	A	610	1PE	OH5-C14-C24-OH4
4	B	606	1PE	OH5-C14-C24-OH4
3	C	602	GOL	O1-C1-C2-O2
4	A	607	1PE	OH4-C13-C23-OH3
4	C	603	1PE	OH4-C13-C23-OH3
4	D	603	1PE	OH2-C12-C22-OH3
4	D	603	1PE	OH7-C16-C26-OH6
3	A	604	GOL	C1-C2-C3-O3
3	A	605	GOL	O1-C1-C2-C3
3	B	602	GOL	O1-C1-C2-C3
3	B	602	GOL	C1-C2-C3-O3
4	A	610	1PE	OH6-C15-C25-OH5
4	D	603	1PE	OH5-C14-C24-OH4
3	A	603	GOL	O1-C1-C2-O2

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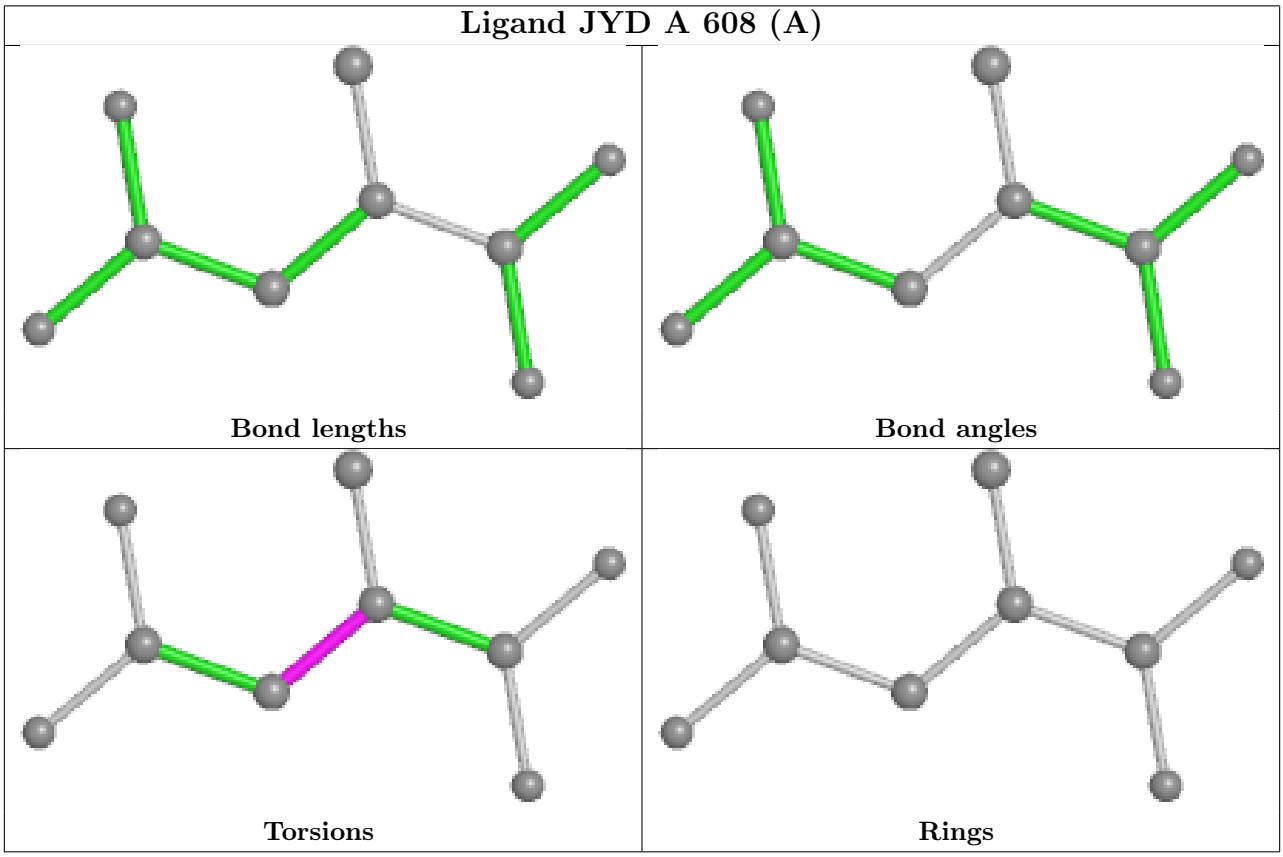
Mol	Chain	Res	Type	Atoms
3	A	604	GOL	O1-C1-C2-O2
3	A	606	GOL	O2-C2-C3-O3
3	B	602	GOL	O2-C2-C3-O3
4	A	611	1PE	OH4-C13-C23-OH3
5	D	602	JYD	C07-C01-C02-C03
4	B	606	1PE	OH4-C13-C23-OH3
4	C	606	1PE	C24-C14-OH5-C25
4	D	603	1PE	OH6-C15-C25-OH5
4	C	605	1PE	C15-C25-OH5-C14
4	C	603	1PE	OH2-C12-C22-OH3
4	C	606	1PE	OH4-C13-C23-OH3
4	A	609	1PE	OH2-C12-C22-OH3
4	B	605	1PE	OH2-C12-C22-OH3
4	A	609	1PE	C24-C14-OH5-C25
5	C	604	JYD	C07-C01-C02-C03
4	A	610	1PE	C23-C13-OH4-C24
4	A	610	1PE	C24-C14-OH5-C25
4	C	603	1PE	C13-C23-OH3-C22
4	C	605	1PE	C23-C13-OH4-C24
4	B	606	1PE	C14-C24-OH4-C13
3	A	604	GOL	O2-C2-C3-O3
4	B	606	1PE	C24-C14-OH5-C25
4	A	609	1PE	C14-C24-OH4-C13
4	A	611	1PE	OH6-C15-C25-OH5
4	A	610	1PE	C14-C24-OH4-C13
4	C	603	1PE	C12-C22-OH3-C23
4	D	603	1PE	C25-C15-OH6-C26
4	D	603	1PE	C24-C14-OH5-C25
4	D	603	1PE	C12-C22-OH3-C23
4	D	603	1PE	C23-C13-OH4-C24
4	D	603	1PE	C13-C23-OH3-C22
4	A	611	1PE	OH5-C14-C24-OH4
4	A	609	1PE	OH6-C15-C25-OH5
4	C	605	1PE	OH6-C15-C25-OH5
3	A	605	GOL	O1-C1-C2-O2
3	B	602	GOL	O1-C1-C2-O2
4	D	603	1PE	C16-C26-OH6-C15
4	A	611	1PE	C15-C25-OH5-C14
4	C	605	1PE	OH5-C14-C24-OH4
4	B	605	1PE	OH5-C14-C24-OH4

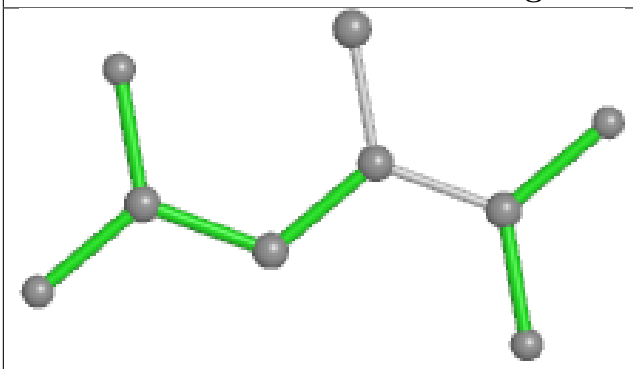
There are no ring outliers.

No monomer is involved in short contacts.

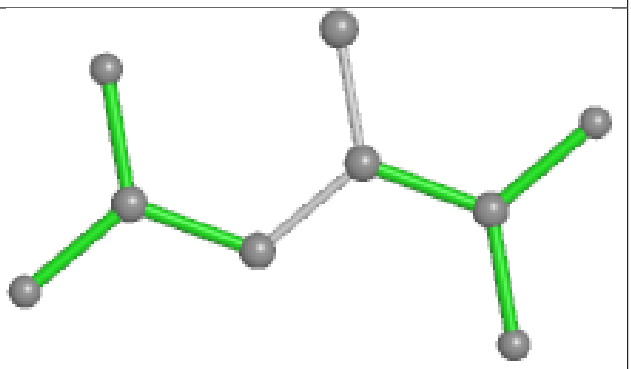
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



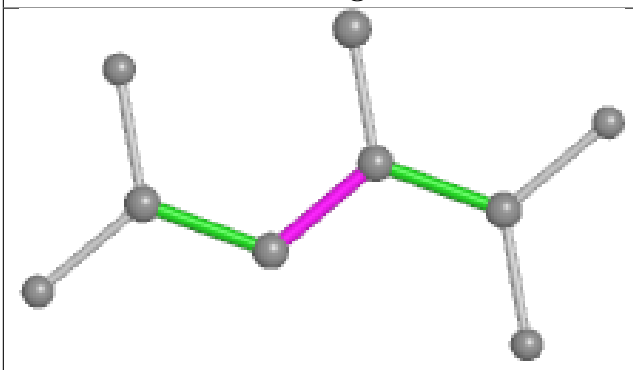
Ligand JYD C 604



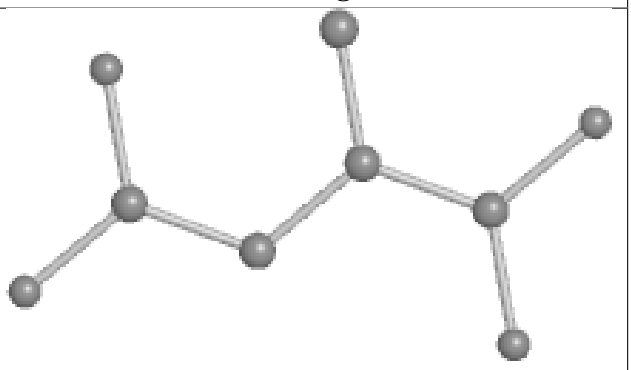
Bond lengths



Bond angles

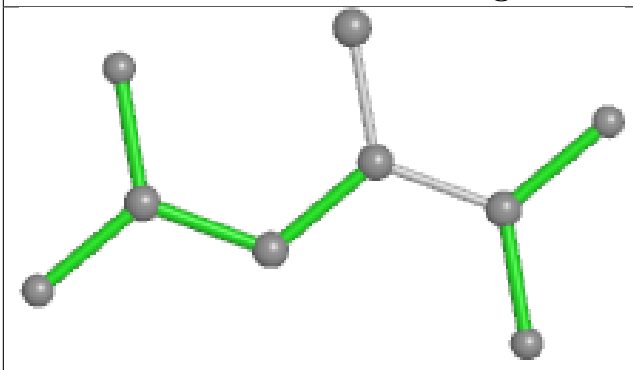


Torsions

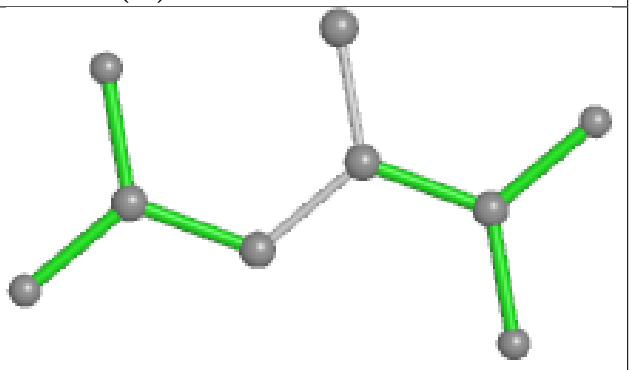


Rings

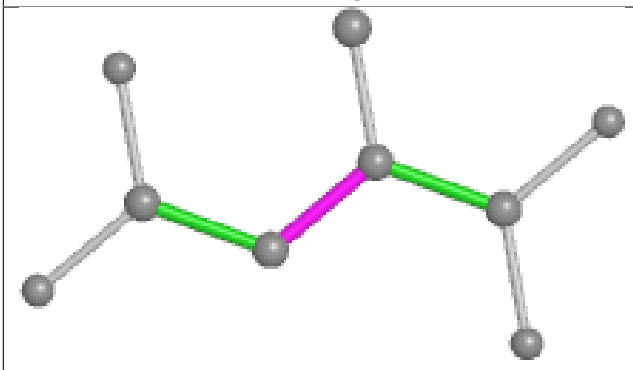
Ligand JYD B 604 (B)



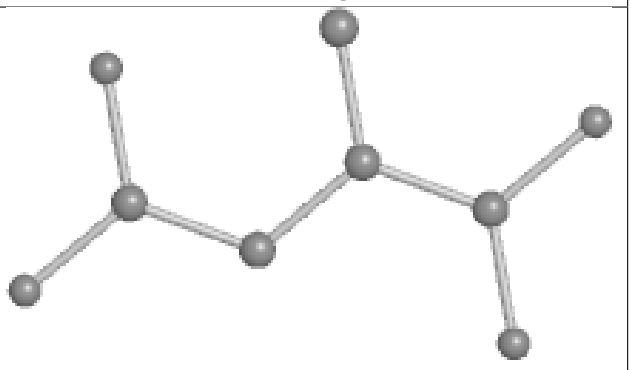
Bond lengths



Bond angles

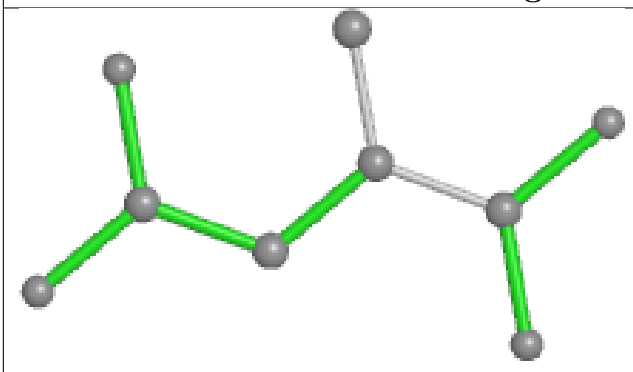


Torsions

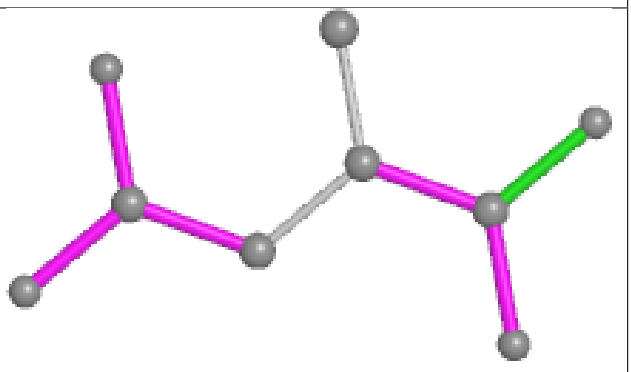


Rings

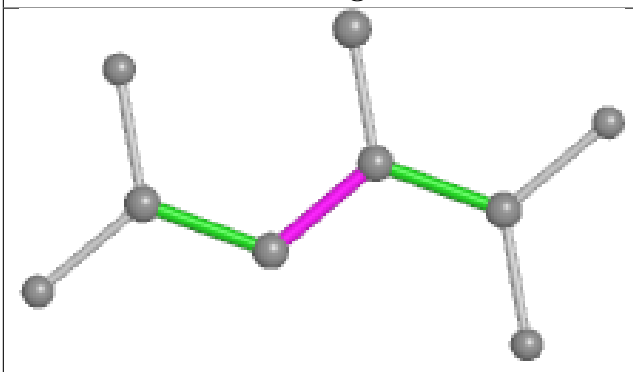
Ligand JYD D 602



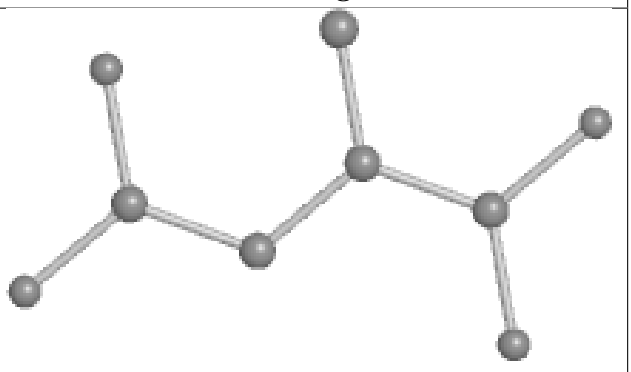
Bond lengths



Bond angles

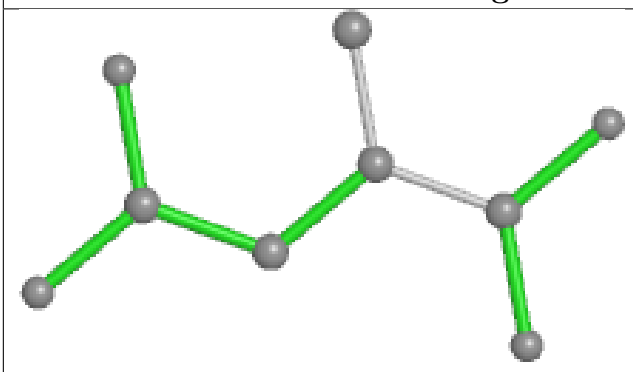


Torsions

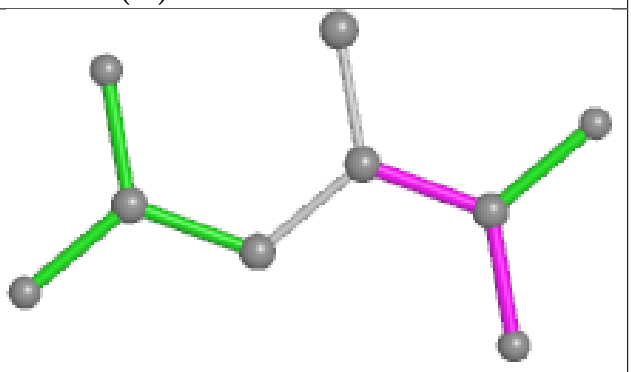


Rings

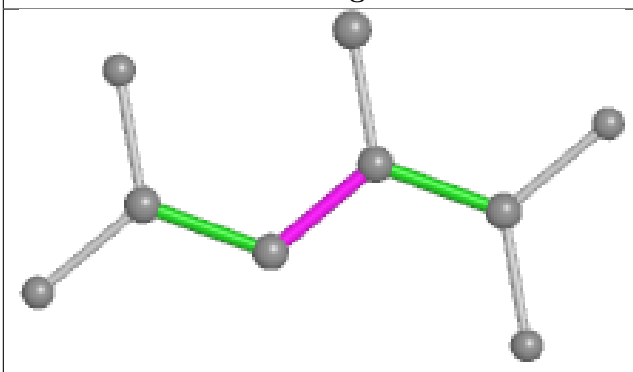
Ligand JYD A 608 (B)



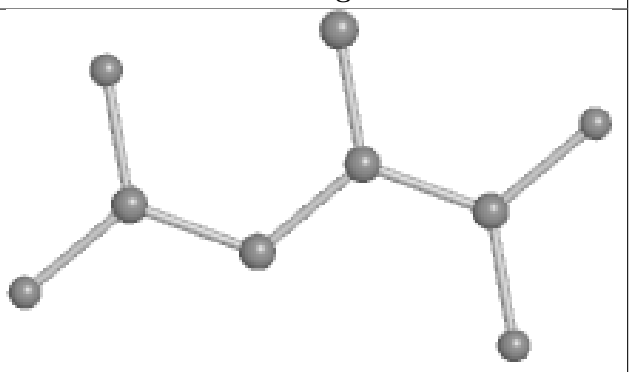
Bond lengths



Bond angles

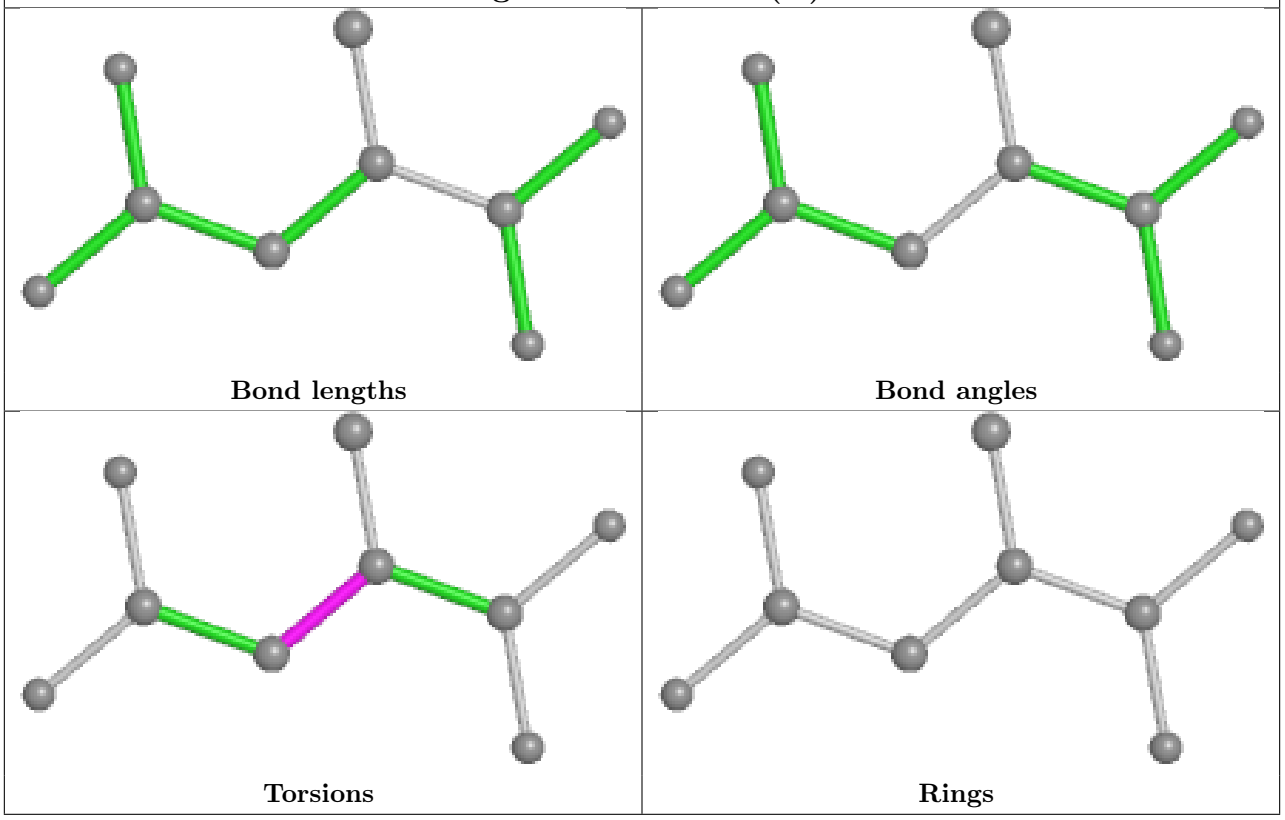


Torsions



Rings

Ligand JYD B 604 (A)



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.