wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 02:34 AM EDT

PDB ID	:	6UXE
Title	:	Structure of the human mitochondrial desulfurase complex Nfs1-ISCU2(M140I)-ISD11 with E.coli ACP1 at 1.57 A resolution showing flexibility of N terminal end of ISCU2
Authors	:	Boniecki, M.T.; Cygler, M.
Deposited on	:	2019-11-07
Resolution	:	1.57 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 1.57 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 17 unique types of molecules in this entry. The entry contains 6265 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 Cysteine desulfurase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	22	0
			3141	1993	539	587	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	MET	-	initiating methionine	UNP Q9Y697
A	53	GLY	-	expression tag	UNP Q9Y697
A	54	SER	-	expression tag	UNP Q9Y697
A	55	SER	-	expression tag	UNP Q9Y697

- Molecule 2 is a protein called LYR motif-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	85	Total	C	N	O	S	0	8	0
			728	461	142	124	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	ALA	SER	variant	UNP Q9HD34

- Molecule 3 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	75	Total	C	N	O	S	0	0	0
			535	335	84	115	1			

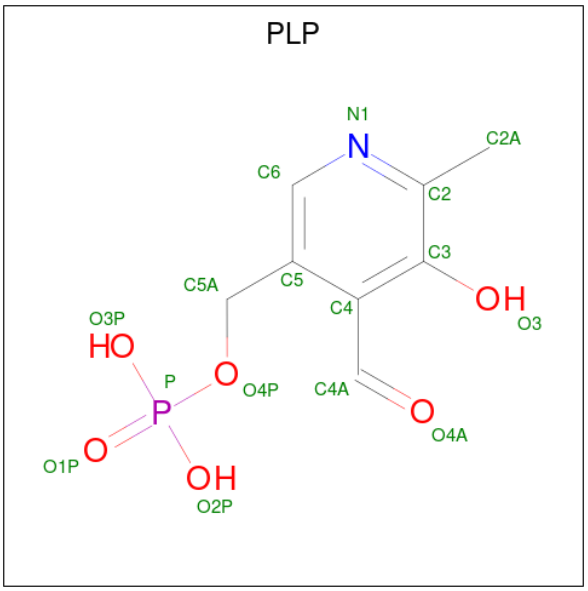
- Molecule 4 is a protein called Iron-sulfur cluster assembly enzyme ISCU, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	126	Total	C	N	O	S	0	7	0
			977	621	164	186	6			

There are 11 discrepancies between the modelled and reference sequences:

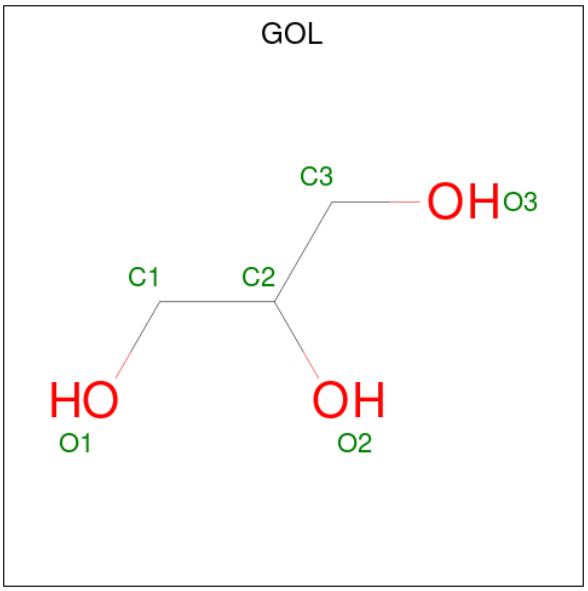
Chain	Residue	Modelled	Actual	Comment	Reference
D	33	MET	-	initiating methionine	UNP Q9H1K1
D	34	ALA	-	expression tag	UNP Q9H1K1
D	140	ILE	MET	engineered mutation	UNP Q9H1K1
D	168	LEU	-	expression tag	UNP Q9H1K1
D	169	GLU	-	expression tag	UNP Q9H1K1
D	170	HIS	-	expression tag	UNP Q9H1K1
D	171	HIS	-	expression tag	UNP Q9H1K1
D	172	HIS	-	expression tag	UNP Q9H1K1
D	173	HIS	-	expression tag	UNP Q9H1K1
D	174	HIS	-	expression tag	UNP Q9H1K1
D	175	HIS	-	expression tag	UNP Q9H1K1

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



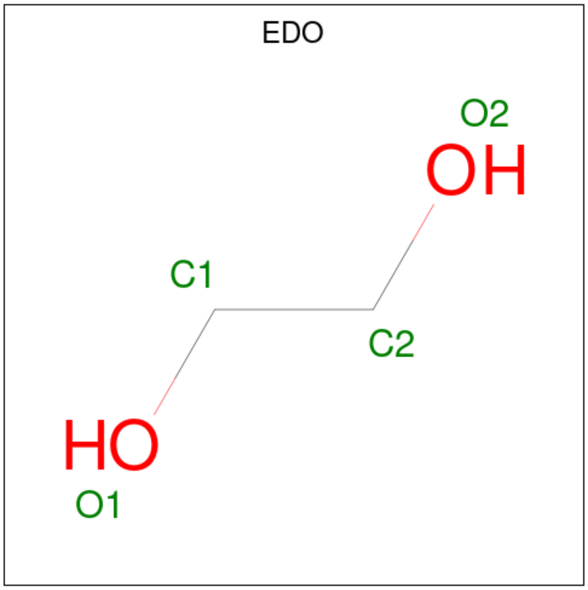
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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



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

Continued on next page...

Continued from previous page...

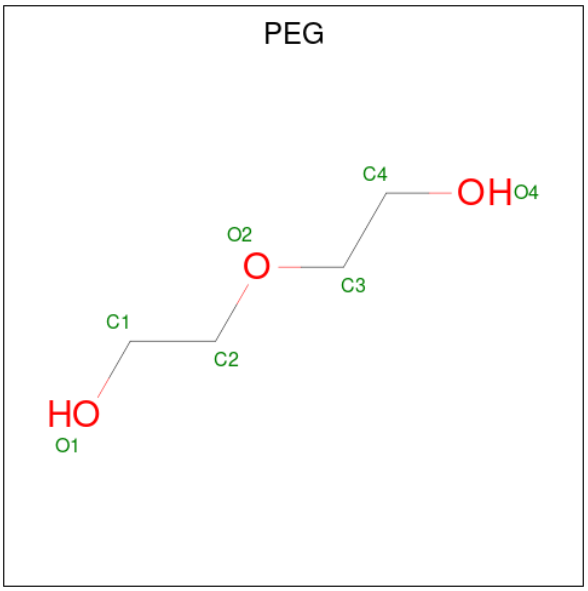
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

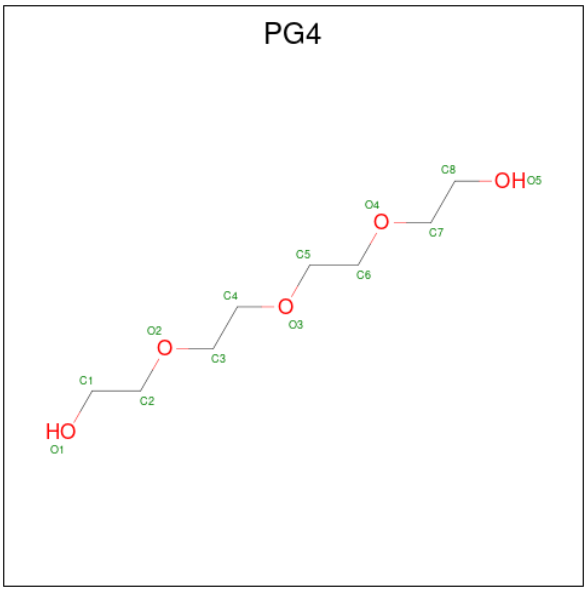
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



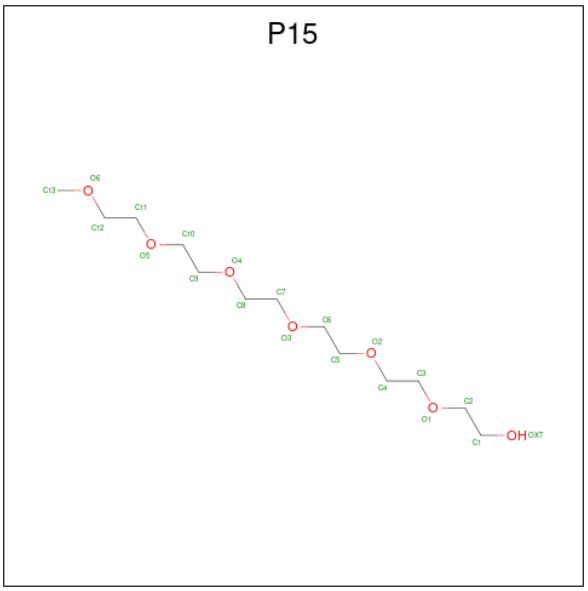
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	B	1	Total C O 7 4 3	0	0
8	B	1	Total C O 7 4 3	0	0
8	C	1	Total C O 7 4 3	0	0

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



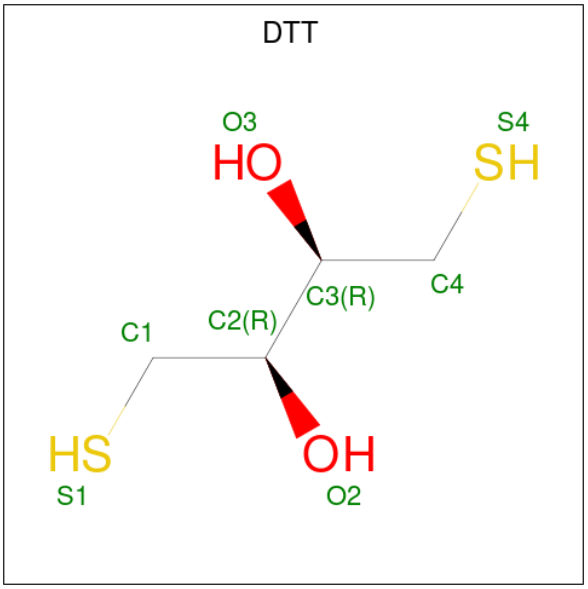
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 13 8 5	0	0
9	A	1	Total C O 13 8 5	0	0

- Molecule 10 is 2,5,8,11,14,17-HEXAOXANONADECAN-19-OL (three-letter code: P15) (formula: $C_{13}H_{28}O_7$).



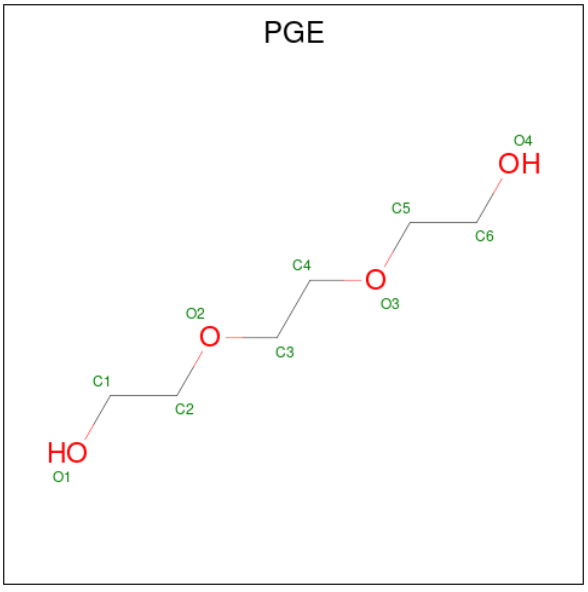
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 20 13 7	0	0

- Molecule 11 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
11	A	1	8	4	2	2	0	0

- Molecule 12 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



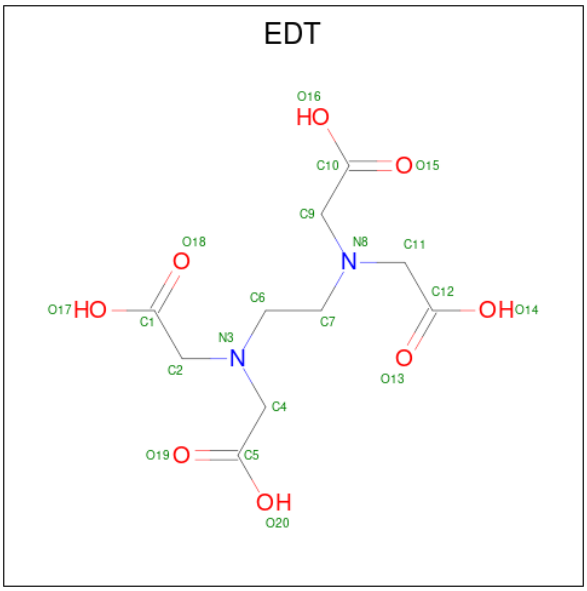
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
12	A	1	10	6	4	0	0

Continued on next page...

Continued from previous page...

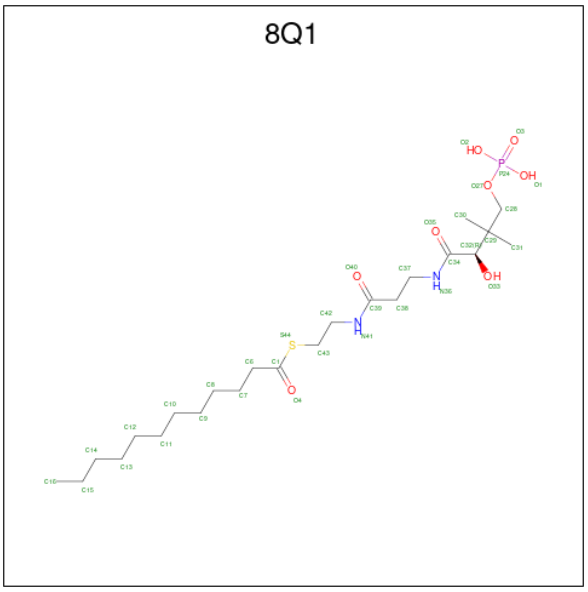
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 10 6 4	0	0
12	A	1	Total C O 10 6 4	0	0

- Molecule 13 is {[-(BIS-CARBOXYMETHYL-AMINO)-ETHYL]-CARBOXYMETHYL-AMINO}-ACETIC ACID (three-letter code: EDT) (formula: $C_{10}H_{16}N_2O_8$).



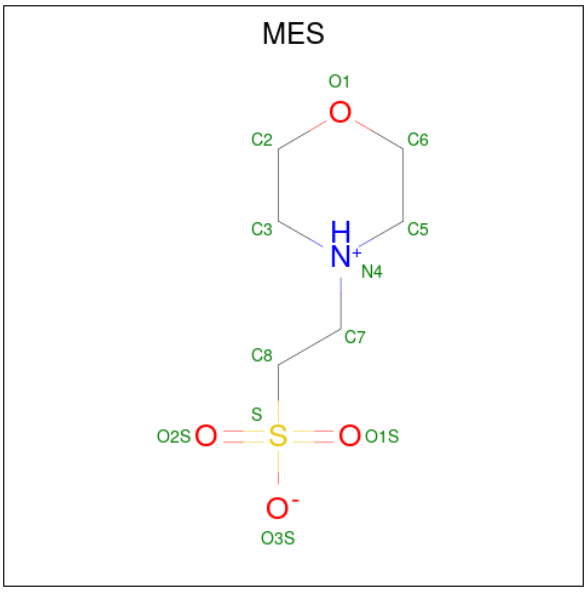
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C N O 20 10 2 8	0	0

- Molecule 14 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



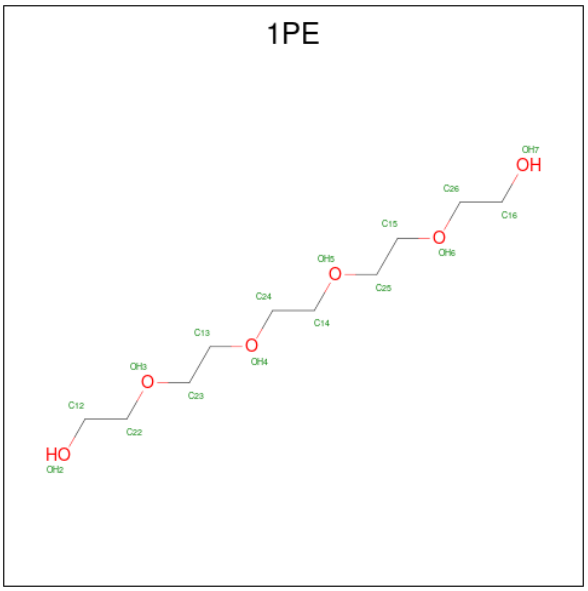
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	C	1	Total	C	N	O	P	S	0	0
			34	23	2	7	1	1		

- Molecule 15 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 16 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



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

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	260	Total O 260 260	0	0
17	B	71	Total O 71 71	0	0
17	C	18	Total O 18 18	0	0
17	D	41	Total O 41 41	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 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	86.41Å 86.41Å 245.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 1.57	Depositor
% Data completeness (in resolution range)	100.0 (48.98-1.57)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 1.57Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.156 , 0.180	Depositor
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.157	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6265	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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

79 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	$\#\|Z\| > 2$
7	EDO	C	304	-	3,3,3	0.51	0	2,2,2	0.55	0
7	EDO	B	109	-	3,3,3	0.50	0	2,2,2	0.45	0
7	EDO	A	542	-	3,3,3	0.52	0	2,2,2	0.30	0
8	PEG	A	550	-	6,6,6	0.48	0	5,5,5	0.29	0
12	PGE	A	543	-	9,9,9	0.26	0	8,8,8	0.59	0
7	EDO	C	303	-	3,3,3	0.47	0	2,2,2	0.44	0
7	EDO	A	536	-	3,3,3	0.42	0	2,2,2	0.54	0
7	EDO	D	207	-	3,3,3	0.44	0	2,2,2	0.47	0
8	PEG	B	106	-	6,6,6	0.63	0	5,5,5	0.83	0
7	EDO	A	516	-	3,3,3	0.51	0	2,2,2	0.19	0
6	GOL	D	205	-	5,5,5	0.55	0	5,5,5	0.29	0
9	PG4	A	520	-	12,12,12	0.55	0	11,11,11	0.40	0
7	EDO	A	525	-	3,3,3	0.47	0	2,2,2	0.42	0
6	GOL	A	502	-	5,5,5	0.40	0	5,5,5	1.27	1 (20%)
7	EDO	A	507	-	3,3,3	1.96	1 (33%)	2,2,2	1.64	1 (50%)
7	EDO	A	524	-	3,3,3	0.45	0	2,2,2	0.49	0
7	EDO	A	515	-	3,3,3	0.52	0	2,2,2	0.16	0
7	EDO	A	553	-	3,3,3	0.44	0	2,2,2	0.31	0
6	GOL	A	505	-	5,5,5	0.86	0	5,5,5	0.61	0
7	EDO	A	509	-	3,3,3	0.67	0	2,2,2	0.99	0
7	EDO	B	108	-	3,3,3	0.46	0	2,2,2	0.38	0
12	PGE	A	544	-	9,9,9	0.37	0	8,8,8	0.23	0
7	EDO	A	539	-	3,3,3	0.47	0	2,2,2	0.33	0
7	EDO	A	529	-	3,3,3	0.49	0	2,2,2	0.29	0
8	PEG	A	549	-	6,6,6	0.48	0	5,5,5	0.33	0
7	EDO	A	511	-	3,3,3	0.57	0	2,2,2	0.66	0
7	EDO	B	102	-	3,3,3	0.49	0	2,2,2	0.73	0
7	EDO	D	204	-	3,3,3	0.48	0	2,2,2	0.28	0
7	EDO	B	105	-	3,3,3	0.45	0	2,2,2	0.35	0
14	8Q1	C	301	3	27,33,34	2.43	9 (33%)	32,40,43	1.19	2 (6%)
8	PEG	A	531	-	6,6,6	0.54	0	5,5,5	0.86	0
7	EDO	D	201	-	3,3,3	0.47	0	2,2,2	0.24	0
7	EDO	A	545	-	3,3,3	0.47	0	2,2,2	0.25	0
10	P15	A	526	-	19,19,19	0.64	0	18,18,18	0.76	0
5	PLP	A	501	1	15,15,16	1.09	1 (6%)	20,22,23	1.06	0
7	EDO	A	506	-	3,3,3	0.40	0	2,2,2	0.21	0
7	EDO	A	522	-	3,3,3	0.74	0	2,2,2	0.76	0
7	EDO	A	530	-	3,3,3	0.52	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	EDO	A	517	-	3,3,3	0.07	0	2,2,2	0.47	0
7	EDO	B	101	-	3,3,3	0.87	0	2,2,2	1.18	0
7	EDO	A	535	-	3,3,3	0.45	0	2,2,2	0.51	0
6	GOL	A	504	-	5,5,5	0.56	0	5,5,5	0.28	0
16	1PE	D	203	-	15,15,15	0.53	0	14,14,14	0.25	0
7	EDO	A	523	-	3,3,3	0.51	0	2,2,2	0.51	0
8	PEG	B	104	-	6,6,6	0.53	0	5,5,5	0.27	0
7	EDO	A	538	-	3,3,3	0.51	0	2,2,2	0.40	0
7	EDO	A	510	-	3,3,3	0.44	0	2,2,2	0.69	0
7	EDO	B	112	-	3,3,3	0.48	0	2,2,2	0.19	0
7	EDO	D	202	-	3,3,3	0.47	0	2,2,2	0.39	0
7	EDO	A	528	-	3,3,3	0.54	0	2,2,2	0.27	0
7	EDO	A	512	-	3,3,3	0.42	0	2,2,2	0.77	0
6	GOL	A	503	-	5,5,5	0.45	0	5,5,5	0.51	0
13	EDT	B	110	-	19,19,19	1.31	2 (10%)	24,24,24	1.42	3 (12%)
7	EDO	A	547	-	3,3,3	0.45	0	2,2,2	0.48	0
7	EDO	A	546	-	3,3,3	0.78	0	2,2,2	1.40	0
7	EDO	A	514	-	3,3,3	1.28	0	2,2,2	0.83	0
15	MES	C	302	-	12,12,12	1.92	4 (33%)	14,16,16	2.24	4 (28%)
7	EDO	A	508	-	3,3,3	0.47	0	2,2,2	0.26	0
7	EDO	B	103	-	3,3,3	0.43	0	2,2,2	0.33	0
12	PGE	A	534	-	9,9,9	0.47	0	8,8,8	1.00	1 (12%)
7	EDO	A	540	-	3,3,3	0.46	0	2,2,2	0.43	0
7	EDO	B	111	-	3,3,3	0.41	0	2,2,2	0.29	0
8	PEG	A	527	-	6,6,6	0.49	0	5,5,5	0.35	0
8	PEG	A	532	-	6,6,6	0.50	0	5,5,5	0.61	0
7	EDO	A	541	-	3,3,3	0.43	0	2,2,2	0.18	0
8	PEG	C	305	-	6,6,6	0.49	0	5,5,5	0.24	0
7	EDO	A	513	-	3,3,3	0.43	0	2,2,2	0.47	0
8	PEG	A	521	-	6,6,6	0.48	0	5,5,5	0.94	0
11	DTT	A	533	-	7,7,7	0.64	0	4,8,8	0.94	0
7	EDO	A	552	-	3,3,3	0.47	0	2,2,2	0.76	0
9	PG4	A	519	-	12,12,12	0.53	0	11,11,11	0.48	0
6	GOL	A	551	-	5,5,5	0.47	0	5,5,5	0.51	0
7	EDO	D	206	-	3,3,3	0.48	0	2,2,2	0.48	0
7	EDO	A	537	-	3,3,3	0.45	0	2,2,2	0.29	0
8	PEG	A	518	-	6,6,6	0.58	0	5,5,5	0.63	0
8	PEG	A	548	-	6,6,6	0.49	0	5,5,5	0.35	0
7	EDO	B	107	-	3,3,3	0.46	0	2,2,2	0.21	0
7	EDO	A	554	-	3,3,3	0.48	0	2,2,2	0.41	0
7	EDO	C	306	-	3,3,3	0.47	0	2,2,2	0.28	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
7	EDO	C	304	-	-	1/1/1/1	-
7	EDO	B	109	-	-	0/1/1/1	-
7	EDO	A	542	-	-	0/1/1/1	-
8	PEG	A	550	-	-	2/4/4/4	-
12	PGE	A	543	-	-	3/7/7/7	-
7	EDO	C	303	-	-	1/1/1/1	-
7	EDO	A	536	-	-	1/1/1/1	-
7	EDO	D	207	-	-	0/1/1/1	-
8	PEG	B	106	-	-	3/4/4/4	-
7	EDO	A	516	-	-	1/1/1/1	-
6	GOL	D	205	-	-	1/4/4/4	-
9	PG4	A	520	-	-	5/10/10/10	-
7	EDO	A	525	-	-	1/1/1/1	-
6	GOL	A	502	-	-	0/4/4/4	-
7	EDO	A	507	-	-	0/1/1/1	-
7	EDO	A	524	-	-	1/1/1/1	-
7	EDO	A	515	-	-	1/1/1/1	-
7	EDO	A	553	-	-	1/1/1/1	-
6	GOL	A	505	-	-	2/4/4/4	-
7	EDO	A	509	-	-	0/1/1/1	-
7	EDO	B	108	-	-	1/1/1/1	-
12	PGE	A	544	-	-	3/7/7/7	-
7	EDO	A	539	-	-	0/1/1/1	-
7	EDO	A	529	-	-	1/1/1/1	-
8	PEG	A	549	-	-	2/4/4/4	-
7	EDO	A	511	-	-	0/1/1/1	-
7	EDO	B	102	-	-	1/1/1/1	-
7	EDO	D	204	-	-	0/1/1/1	-
7	EDO	B	105	-	-	1/1/1/1	-
14	8Q1	C	301	3	-	2/38/40/41	-
8	PEG	A	531	-	-	2/4/4/4	-
7	EDO	D	201	-	-	0/1/1/1	-
7	EDO	A	545	-	-	1/1/1/1	-
10	P15	A	526	-	-	10/17/17/17	-
5	PLP	A	501	1	-	0/6/6/8	0/1/1/1
7	EDO	A	506	-	-	1/1/1/1	-
7	EDO	A	522	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	530	-	-	1/1/1/1	-
7	EDO	A	517	-	-	1/1/1/1	-
7	EDO	B	101	-	-	0/1/1/1	-
7	EDO	A	535	-	-	1/1/1/1	-
6	GOL	A	504	-	-	4/4/4/4	-
16	1PE	D	203	-	-	7/13/13/13	-
7	EDO	A	523	-	-	1/1/1/1	-
8	PEG	B	104	-	-	3/4/4/4	-
7	EDO	A	538	-	-	0/1/1/1	-
7	EDO	A	510	-	-	1/1/1/1	-
7	EDO	B	112	-	-	1/1/1/1	-
7	EDO	D	202	-	-	1/1/1/1	-
7	EDO	A	528	-	-	1/1/1/1	-
7	EDO	A	512	-	-	1/1/1/1	-
6	GOL	A	503	-	-	4/4/4/4	-
13	EDT	B	110	-	-	13/21/21/21	-
7	EDO	A	547	-	-	1/1/1/1	-
7	EDO	A	546	-	-	1/1/1/1	-
7	EDO	A	514	-	-	1/1/1/1	-
15	MES	C	302	-	-	3/6/14/14	0/1/1/1
7	EDO	A	508	-	-	0/1/1/1	-
7	EDO	B	103	-	-	0/1/1/1	-
12	PGE	A	534	-	-	5/7/7/7	-
7	EDO	A	540	-	-	1/1/1/1	-
7	EDO	B	111	-	-	1/1/1/1	-
8	PEG	A	527	-	-	1/4/4/4	-
8	PEG	A	532	-	-	0/4/4/4	-
7	EDO	A	541	-	-	1/1/1/1	-
8	PEG	C	305	-	-	4/4/4/4	-
7	EDO	A	513	-	-	1/1/1/1	-
8	PEG	A	521	-	-	1/4/4/4	-
11	DTT	A	533	-	-	2/8/8/8	-
7	EDO	A	552	-	-	0/1/1/1	-
9	PG4	A	519	-	-	5/10/10/10	-
6	GOL	A	551	-	-	4/4/4/4	-
7	EDO	D	206	-	-	1/1/1/1	-
7	EDO	A	537	-	-	0/1/1/1	-
8	PEG	A	518	-	-	1/4/4/4	-
8	PEG	A	548	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	107	-	-	0/1/1/1	-
7	EDO	A	554	-	-	1/1/1/1	-
7	EDO	C	306	-	-	1/1/1/1	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	301	8Q1	O4-C1	-6.02	1.11	1.21
14	C	301	8Q1	C39-N41	4.68	1.44	1.33
14	C	301	8Q1	O40-C39	-4.67	1.13	1.23
15	C	302	MES	C8-S	4.08	1.83	1.77
14	C	301	8Q1	O35-C34	-4.08	1.15	1.23

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	302	MES	O1S-S-C8	5.52	113.56	106.92
13	B	110	EDT	C11-N8-C9	3.94	120.45	111.54
15	C	302	MES	O3S-S-O2S	-3.90	101.73	111.27
13	B	110	EDT	C11-N8-C7	2.76	118.66	111.94
14	C	301	8Q1	C42-N41-C39	-2.59	118.03	122.84

There are no chirality outliers.

5 of 129 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	503	GOL	O1-C1-C2-C3
6	A	503	GOL	C1-C2-C3-O3
6	A	504	GOL	C1-C2-C3-O3
6	A	505	GOL	O1-C1-C2-C3
6	A	551	GOL	C1-C2-C3-O3

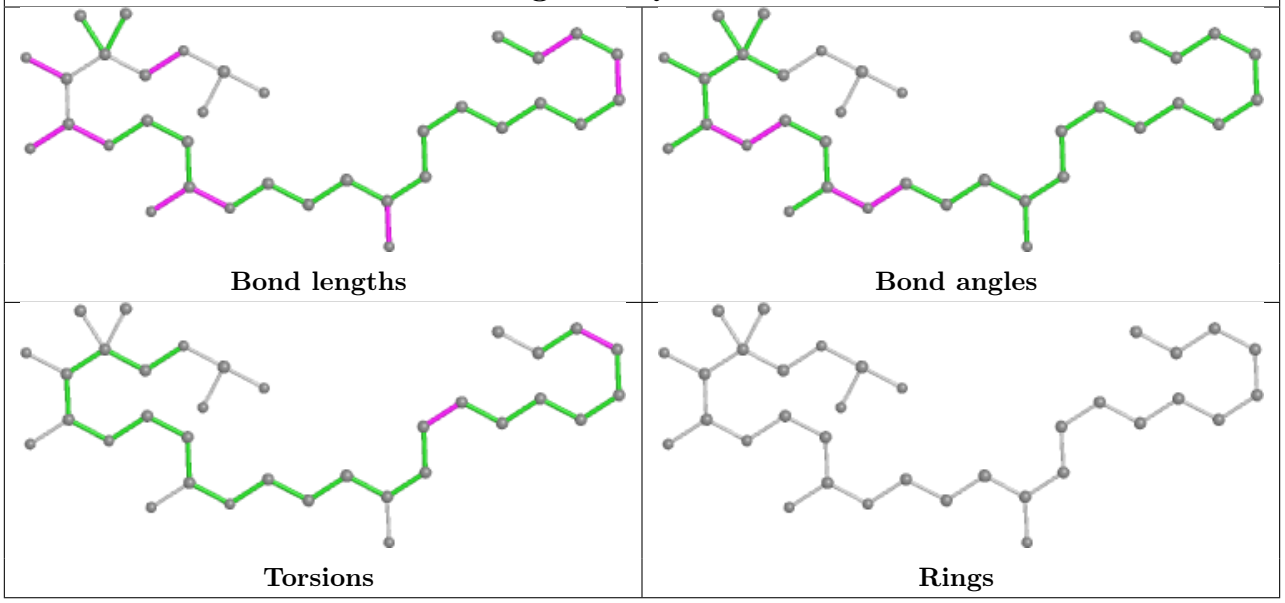
There are no ring outliers.

No monomer is involved in short contacts.

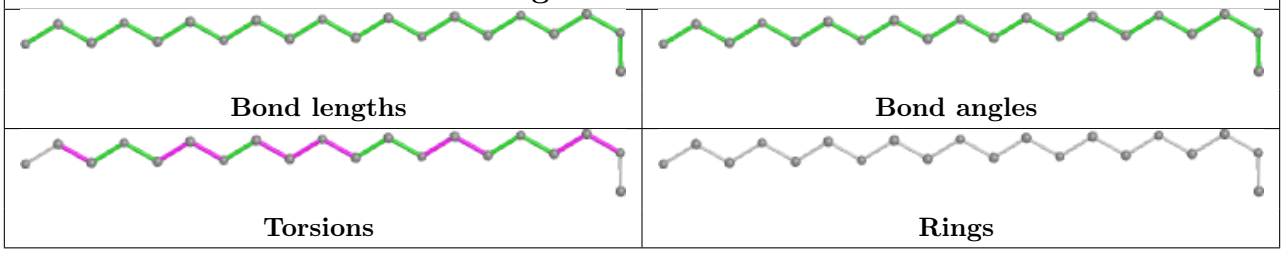
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

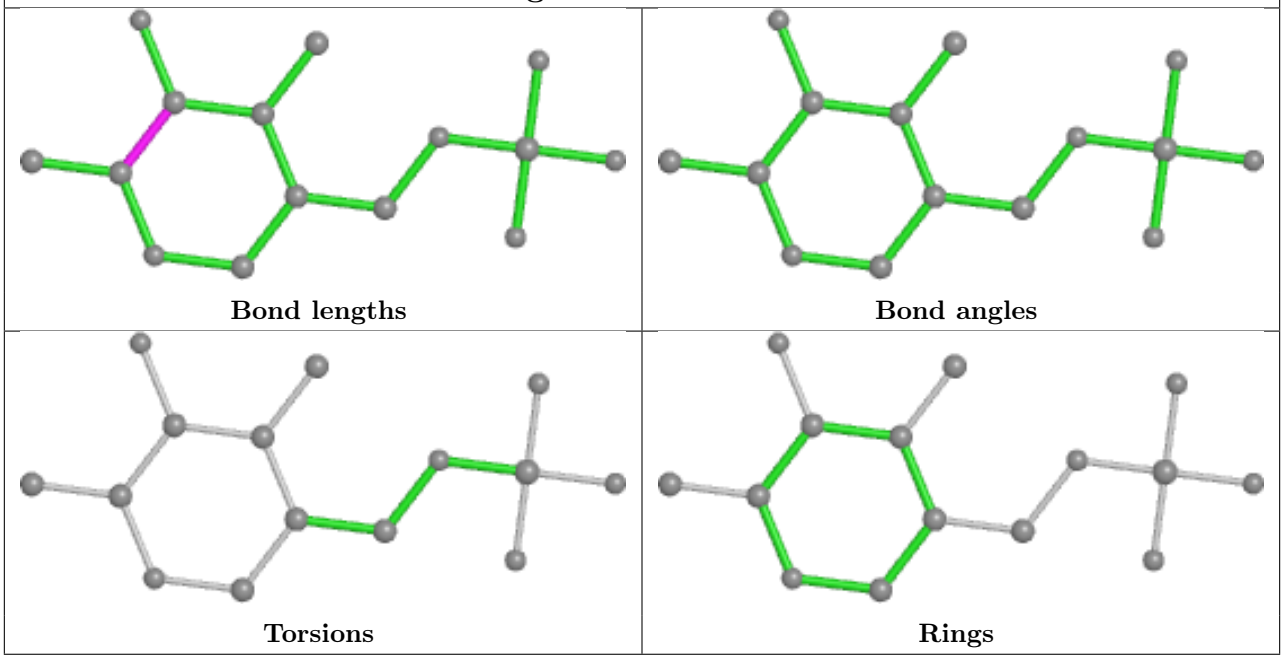
Ligand 8Q1 C 301



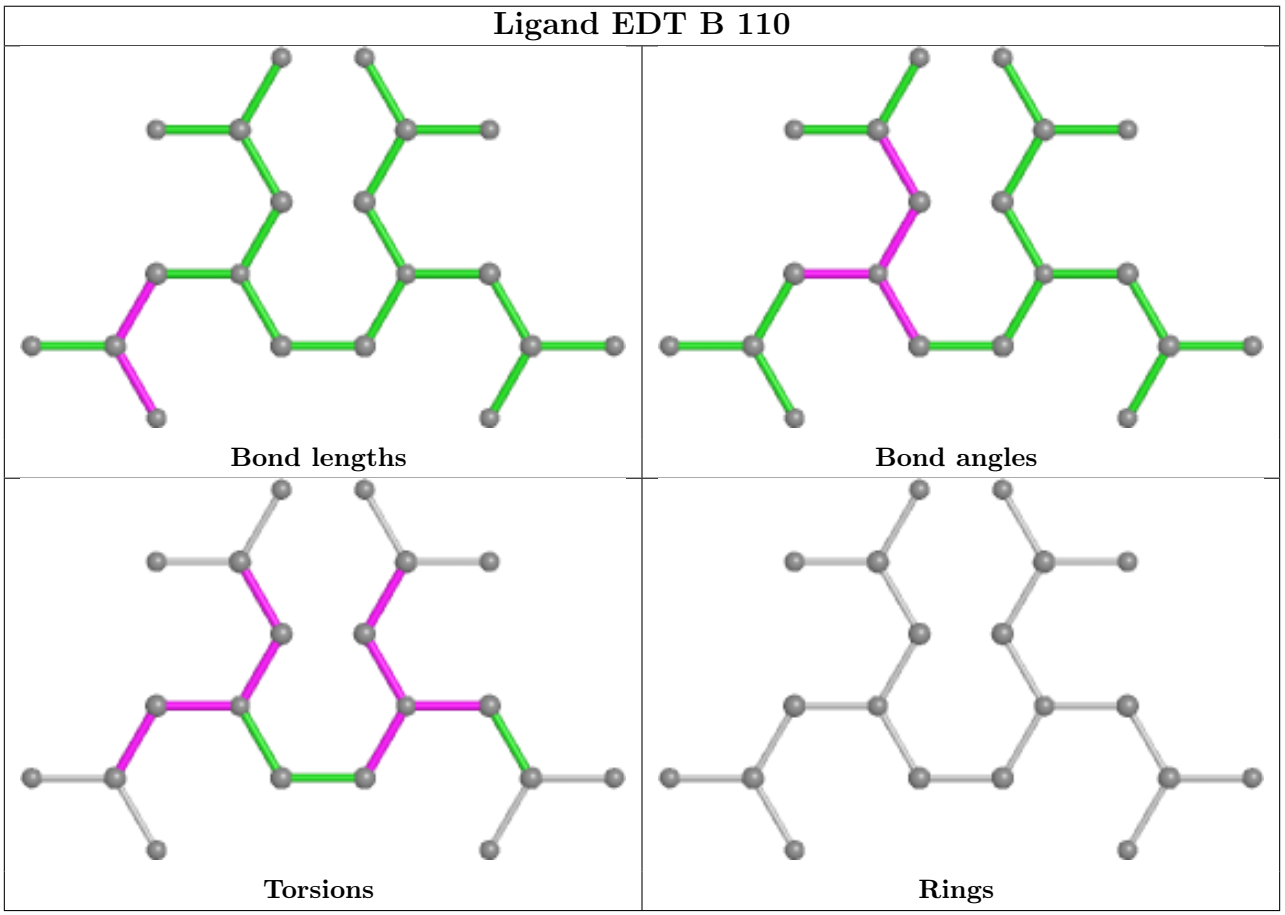
Ligand P15 A 526



Ligand PLP A 501



Ligand EDT B 110



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.