



# Full wwPDB X-ray Structure Validation Report ⓘ

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 Å 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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

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
			Total	C	N	O	S			
1	A	395	3141	1993	539	587	22	0	22	0

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
			Total	C	N	O	S			
2	B	85	728	461	142	124	1	0	8	0

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
			Total	C	N	O	S			
3	C	75	535	335	84	115	1	0	0	0

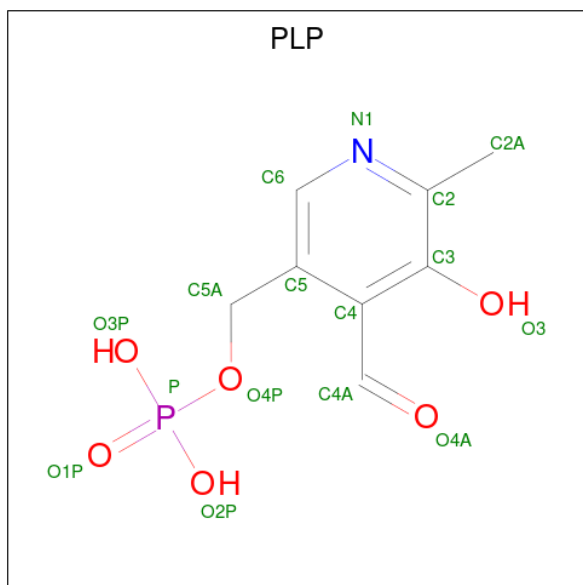
- Molecule 4 is a protein called Iron-sulfur cluster assembly enzyme ISCU, mitochondrial.

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

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
			Total	C	N	O	P		
5	A	1	15	8	1	5	1	0	0

- 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	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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	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 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0

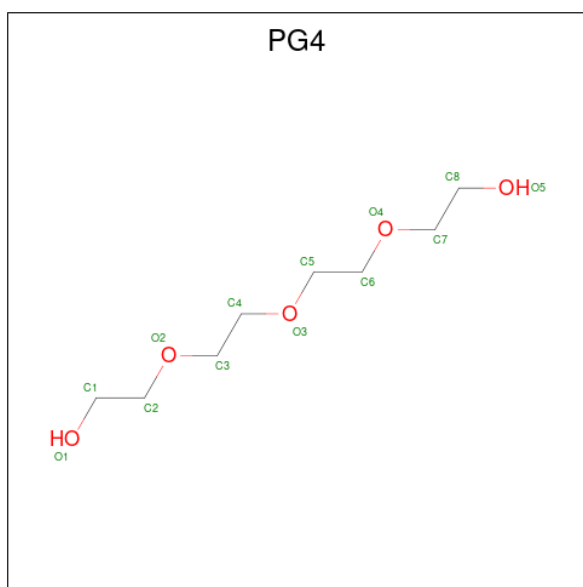
- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).





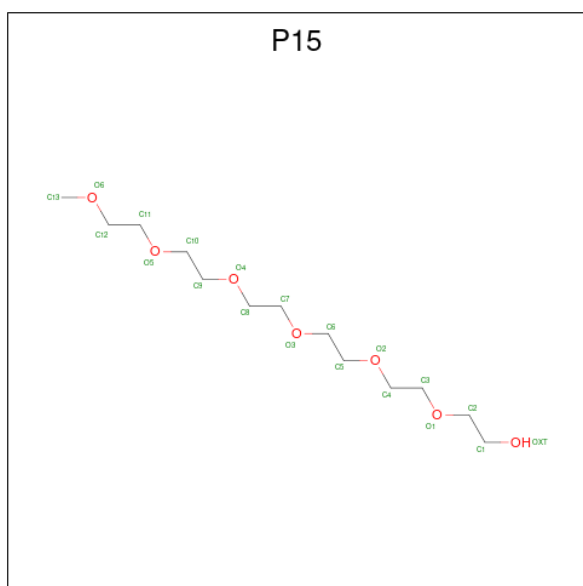
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	B	1	Total C O 7 4 3	0	0
8	B	1	Total C O 7 4 3	0	0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

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



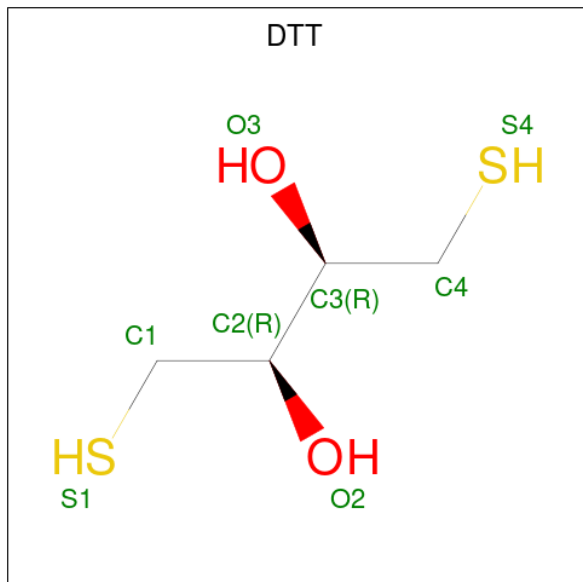
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			13	8	5		
9	A	1	Total	C	O	0	0
			13	8	5		

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



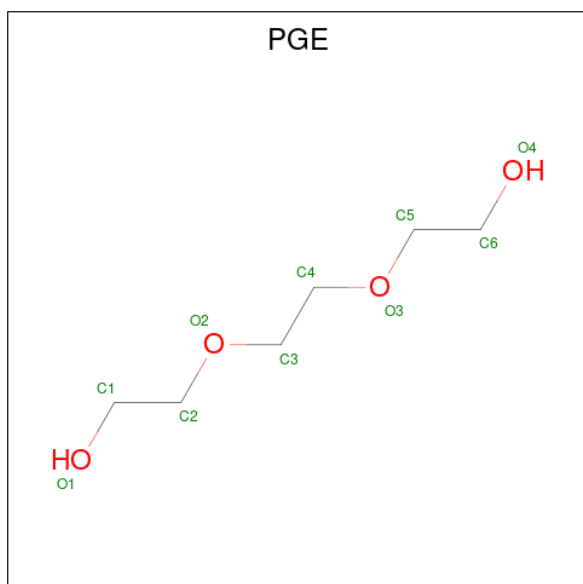
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			20	13	7		

- 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:  $C_6H_{14}O_4$ ).



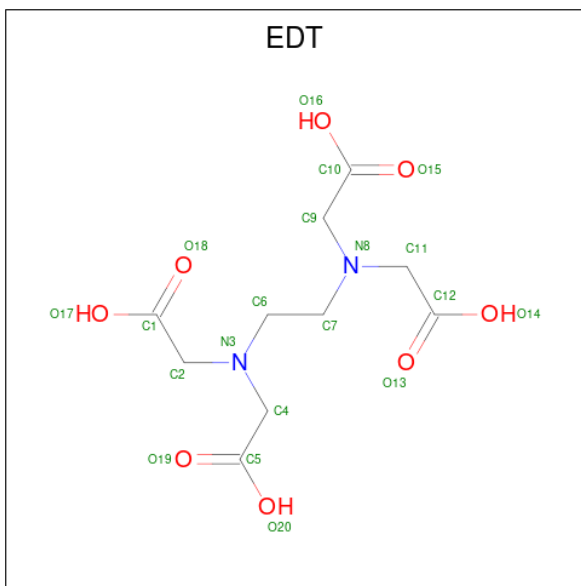
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
12	A	1	10	6	4	0	0

*Continued on next page...*

Continued from previous page...

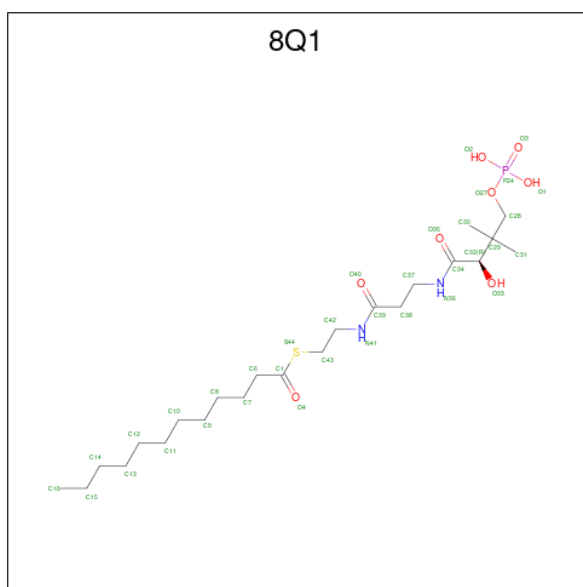
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			10	6	4		
12	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 13 is  $\{[-(\text{BIS-CARBOXYMETHYL-AMINO})\text{-ETHYL}]\text{-CARBOXYMETHYL-AMINO}\}\text{-ACETIC ACID}$  (three-letter code: EDT) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_2\text{O}_8$ ).



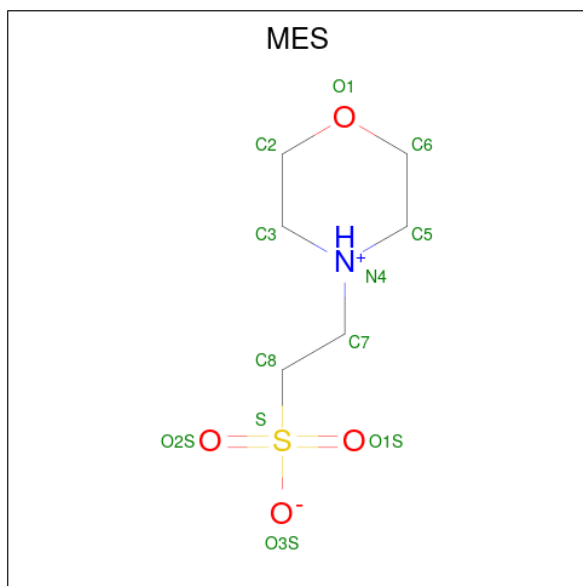
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	N	O	0	0
			20	10	2	8		

- Molecule 14 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula:  $\text{C}_{23}\text{H}_{45}\text{N}_2\text{O}_8\text{PS}$ ) (labeled as "Ligand of Interest" by depositor).



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

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



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

- 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	0	0
			16	10 6		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	260	Total	O	0	0
			260	260		
17	B	71	Total	O	0	0
			71	71		
17	C	18	Total	O	0	0
			18	18		
17	D	41	Total	O	0	0
			41	41		

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	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 1.57Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.156 , 0.180	Depositor
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtrriage
Anisotropy	0.157	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6265	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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	-

All (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
14	C	301	8Q1	O33-C32	-3.85	1.35	1.42
14	C	301	8Q1	C34-N36	3.72	1.41	1.33
14	C	301	8Q1	C12-C13	-3.14	1.34	1.51
7	A	507	EDO	O1-C1	-3.07	1.26	1.42
14	C	301	8Q1	O27-C28	-2.72	1.38	1.44
14	C	301	8Q1	C15-C14	-2.59	1.33	1.51
15	C	302	MES	O1S-S	2.53	1.52	1.45
15	C	302	MES	C7-N4	2.53	1.53	1.47
13	B	110	EDT	O13-C12	2.36	1.30	1.22
5	A	501	PLP	C3-C2	-2.13	1.38	1.40
13	B	110	EDT	C11-C12	2.05	1.55	1.51
15	C	302	MES	O2S-S	2.00	1.50	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
15	C	302	MES	O2S-S-C8	2.46	109.87	106.92
15	C	302	MES	O3S-S-C8	2.42	109.68	105.77
7	A	507	EDO	O2-C2-C1	-2.31	95.31	111.91
6	A	502	GOL	C3-C2-C1	-2.26	102.93	111.70
13	B	110	EDT	C10-C9-N8	2.20	120.82	113.63
12	A	534	PGE	O1-C1-C2	-2.10	99.63	111.81
14	C	301	8Q1	C37-N36-C34	-2.07	118.89	122.59

There are no chirality outliers.

All (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
6	A	551	GOL	O2-C2-C3-O3
11	A	533	DTT	C2-C3-C4-S4
13	B	110	EDT	C1-C2-N3-C4
15	C	302	MES	C8-C7-N4-C3
15	C	302	MES	N4-C7-C8-S
8	B	106	PEG	C1-C2-O2-C3
9	A	519	PG4	C3-C4-O3-C5
10	A	526	P15	O5-C11-C12-O6
9	A	520	PG4	O2-C3-C4-O3
16	D	203	1PE	OH6-C15-C25-OH5
10	A	526	P15	O5-C10-C9-O4
16	D	203	1PE	OH4-C13-C23-OH3
13	B	110	EDT	C10-C9-N8-C11
8	B	106	PEG	O1-C1-C2-O2
8	C	305	PEG	O1-C1-C2-O2
10	A	526	P15	O1-C3-C4-O2
13	B	110	EDT	O18-C1-C2-N3
13	B	110	EDT	O17-C1-C2-N3
6	A	503	GOL	O2-C2-C3-O3
6	A	551	GOL	O1-C1-C2-O2
8	A	518	PEG	O1-C1-C2-O2
9	A	520	PG4	O1-C1-C2-O2
10	A	526	P15	OXT-C1-C2-O1
9	A	520	PG4	C3-C4-O3-C5
8	A	548	PEG	O1-C1-C2-O2
8	A	548	PEG	O2-C3-C4-O4
8	A	549	PEG	O1-C1-C2-O2
8	A	549	PEG	O2-C3-C4-O4
12	A	534	PGE	O3-C5-C6-O4
9	A	519	PG4	O3-C5-C6-O4
16	D	203	1PE	OH5-C14-C24-OH4
6	A	504	GOL	O1-C1-C2-C3
6	A	551	GOL	O1-C1-C2-C3
8	B	104	PEG	O2-C3-C4-O4
9	A	520	PG4	O4-C7-C8-O5
12	A	534	PGE	O1-C1-C2-O2
16	D	203	1PE	OH7-C16-C26-OH6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	A	503	GOL	O1-C1-C2-O2
6	A	504	GOL	O1-C1-C2-O2
6	A	504	GOL	O2-C2-C3-O3
7	A	510	EDO	O1-C1-C2-O2
7	A	512	EDO	O1-C1-C2-O2
7	A	513	EDO	O1-C1-C2-O2
7	A	525	EDO	O1-C1-C2-O2
7	A	528	EDO	O1-C1-C2-O2
7	A	529	EDO	O1-C1-C2-O2
7	A	530	EDO	O1-C1-C2-O2
7	A	545	EDO	O1-C1-C2-O2
7	A	553	EDO	O1-C1-C2-O2
7	A	554	EDO	O1-C1-C2-O2
7	B	102	EDO	O1-C1-C2-O2
7	B	111	EDO	O1-C1-C2-O2
7	B	112	EDO	O1-C1-C2-O2
7	C	303	EDO	O1-C1-C2-O2
7	C	306	EDO	O1-C1-C2-O2
7	D	202	EDO	O1-C1-C2-O2
10	A	526	P15	O2-C5-C6-O3
14	C	301	8Q1	C6-C7-C8-C9
8	A	531	PEG	O2-C3-C4-O4
12	A	543	PGE	O1-C1-C2-O2
9	A	519	PG4	O2-C3-C4-O3
13	B	110	EDT	C7-C6-N3-C2
8	A	550	PEG	O1-C1-C2-O2
13	B	110	EDT	O16-C10-C9-N8
15	C	302	MES	C8-C7-N4-C5
6	A	505	GOL	O1-C1-C2-O2
7	A	506	EDO	O1-C1-C2-O2
7	A	514	EDO	O1-C1-C2-O2
16	D	203	1PE	C15-C25-OH5-C14
13	B	110	EDT	O15-C10-C9-N8
8	B	104	PEG	C1-C2-O2-C3
8	A	548	PEG	C1-C2-O2-C3
8	B	104	PEG	C4-C3-O2-C2
8	A	527	PEG	C1-C2-O2-C3
16	D	203	1PE	C14-C24-OH4-C13
9	A	520	PG4	C6-C5-O3-C4
10	A	526	P15	C10-C9-O4-C8
8	C	305	PEG	C4-C3-O2-C2
8	C	305	PEG	O2-C3-C4-O4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	B	110	EDT	C7-C6-N3-C4
8	A	521	PEG	O2-C3-C4-O4
7	A	546	EDO	O1-C1-C2-O2
7	B	105	EDO	O1-C1-C2-O2
10	A	526	P15	C5-C6-O3-C7
8	C	305	PEG	C1-C2-O2-C3
11	A	533	DTT	O3-C3-C4-S4
10	A	526	P15	C8-C7-O3-C6
9	A	519	PG4	O1-C1-C2-O2
13	B	110	EDT	C10-C9-N8-C7
7	A	524	EDO	O1-C1-C2-O2
7	A	540	EDO	O1-C1-C2-O2
7	A	541	EDO	O1-C1-C2-O2
7	B	108	EDO	O1-C1-C2-O2
13	B	110	EDT	N8-C11-C12-O13
12	A	543	PGE	C3-C4-O3-C5
8	A	531	PEG	C1-C2-O2-C3
8	A	548	PEG	C4-C3-O2-C2
10	A	526	P15	C3-C4-O2-C5
8	B	106	PEG	C4-C3-O2-C2
7	D	206	EDO	O1-C1-C2-O2
12	A	534	PGE	C4-C3-O2-C2
12	A	544	PGE	C1-C2-O2-C3
12	A	534	PGE	O2-C3-C4-O3
10	A	526	P15	C11-C12-O6-C13
7	A	523	EDO	O1-C1-C2-O2
7	A	536	EDO	O1-C1-C2-O2
7	A	547	EDO	O1-C1-C2-O2
12	A	534	PGE	C1-C2-O2-C3
7	A	516	EDO	O1-C1-C2-O2
7	A	517	EDO	O1-C1-C2-O2
7	A	535	EDO	O1-C1-C2-O2
7	C	304	EDO	O1-C1-C2-O2
13	B	110	EDT	N8-C11-C12-O14
12	A	544	PGE	O2-C3-C4-O3
8	A	550	PEG	C4-C3-O2-C2
14	C	301	8Q1	C12-C13-C14-C15
13	B	110	EDT	C12-C11-N8-C9
16	D	203	1PE	C24-C14-OH5-C25
6	D	205	GOL	C1-C2-C3-O3
12	A	544	PGE	O1-C1-C2-O2
13	B	110	EDT	C5-C4-N3-C2

*Continued on next page...*



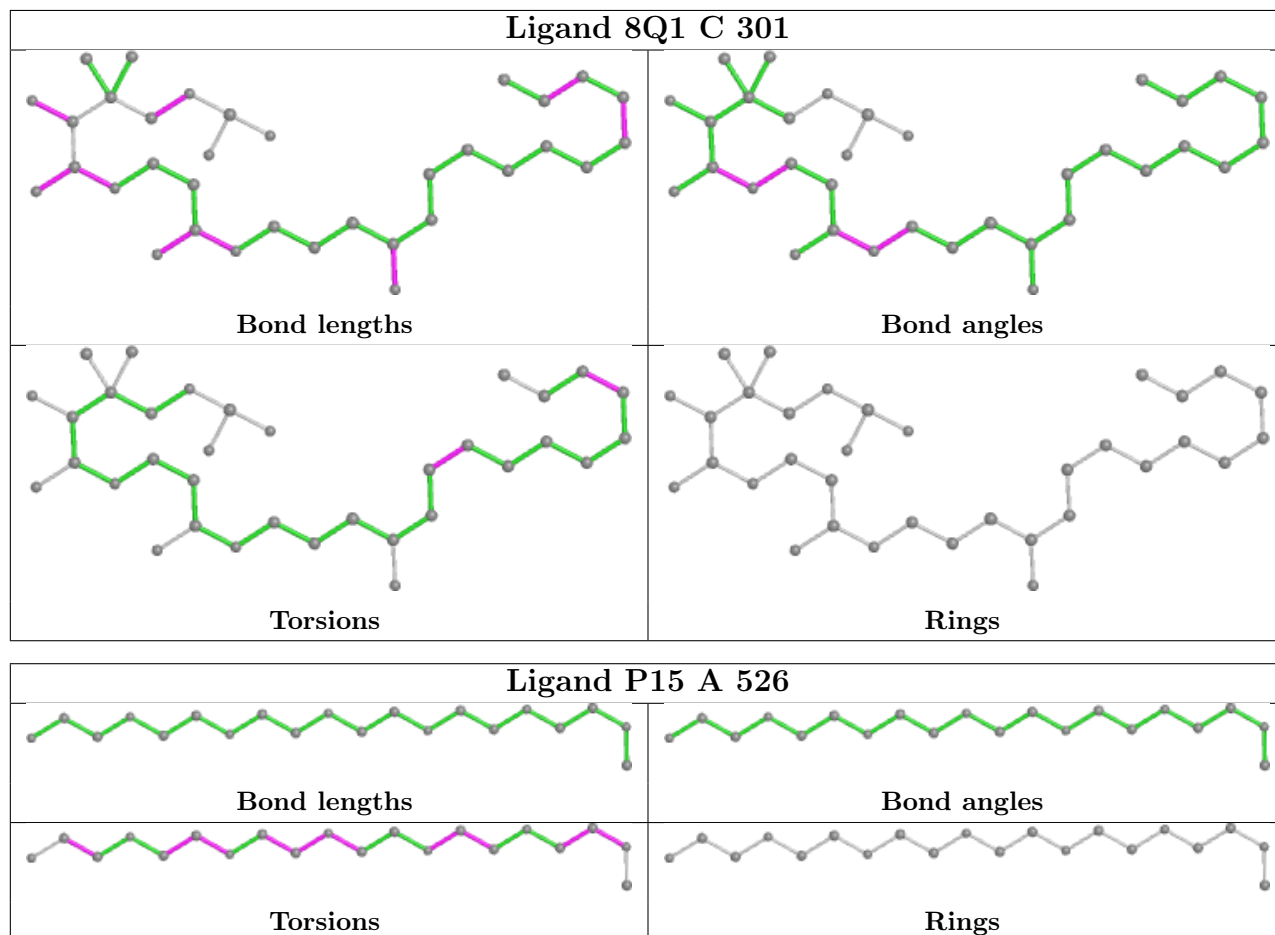
Continued from previous page...

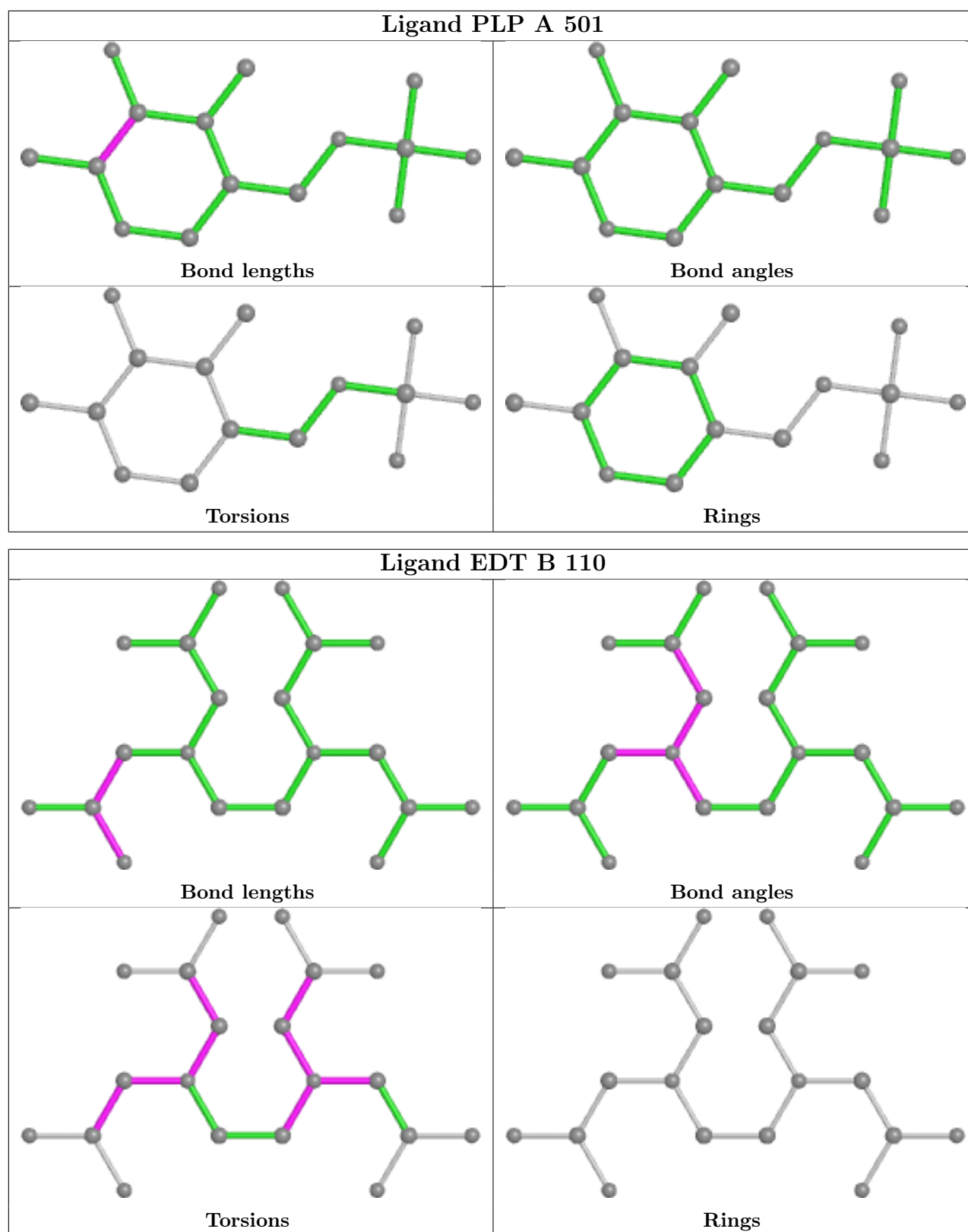
Mol	Chain	Res	Type	Atoms
12	A	543	PGE	O3-C5-C6-O4
7	A	515	EDO	O1-C1-C2-O2
9	A	519	PG4	C8-C7-O4-C6

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

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.