wwPDB X-ray Structure Validation Summary Report (i)

Oct 3, 2023 – 07:33 AM EDT

PDB ID	:	6Q0R
Title	:	Structure of DDB1-DDA1-DCAF15 complex bound to E7820 and RBM39
Authors	:	Faust, T.; Yoon, H.; Nowak, R.P.; Donovan, K.A.; Li, Z.; Cai, Q.; Eleuteri, N.A.; Zhang, T.; Gray, N.S.; Fischer, E.S.
Deposited on	:	2019-08-02
Resolution	:	2.90 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 2.90 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.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	OXM	B	301	-	X	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 10249 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	783	6034	3826	1008	1167	33	0	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q16531
A	-26	GLY	-	expression tag	UNP Q16531
A	-25	SER	-	expression tag	UNP Q16531
A	-24	SER	-	expression tag	UNP Q16531
A	-23	HIS	-	expression tag	UNP Q16531
A	-22	HIS	-	expression tag	UNP Q16531
A	-21	HIS	-	expression tag	UNP Q16531
A	-20	HIS	-	expression tag	UNP Q16531
A	-19	HIS	-	expression tag	UNP Q16531
A	-18	HIS	-	expression tag	UNP Q16531
A	-17	SER	-	expression tag	UNP Q16531
A	-16	ALA	-	expression tag	UNP Q16531
A	-15	ALA	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	ILE	-	expression tag	UNP Q16531
A	-12	VAL	-	expression tag	UNP Q16531
A	-11	MET	-	expression tag	UNP Q16531
A	-10	VAL	-	expression tag	UNP Q16531
A	-9	ASP	-	expression tag	UNP Q16531
A	-8	ALA	-	expression tag	UNP Q16531
A	-7	TYR	-	expression tag	UNP Q16531
A	-6	LYS	-	expression tag	UNP Q16531
A	-5	PRO	-	expression tag	UNP Q16531
A	-4	THR	-	expression tag	UNP Q16531
A	-3	LYS	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ARG	-	expression tag	UNP Q16531
A	700	GLY	-	linker	UNP Q16531
A	701	ASN	-	linker	UNP Q16531
A	702	GLY	-	linker	UNP Q16531
A	703	ASN	-	linker	UNP Q16531
A	704	SER	-	linker	UNP Q16531
A	705	GLY	-	linker	UNP Q16531

- Molecule 2 is a protein called DDB1- and CUL4-associated factor 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	0	0
			1639	1061	280	288	10			

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP Q66K64
B	-14	ASP	-	expression tag	UNP Q66K64
B	-13	TRP	-	expression tag	UNP Q66K64
B	-12	SER	-	expression tag	UNP Q66K64
B	-11	HIS	-	expression tag	UNP Q66K64
B	-10	PRO	-	expression tag	UNP Q66K64
B	-9	GLN	-	expression tag	UNP Q66K64
B	-8	PHE	-	expression tag	UNP Q66K64
B	-7	GLU	-	expression tag	UNP Q66K64
B	-6	LYS	-	expression tag	UNP Q66K64
B	-5	SER	-	expression tag	UNP Q66K64
B	-4	ALA	-	expression tag	UNP Q66K64
B	-3	VAL	-	expression tag	UNP Q66K64
B	-2	GLY	-	expression tag	UNP Q66K64
B	-1	LEU	-	expression tag	UNP Q66K64
B	0	ASN	-	expression tag	UNP Q66K64
B	1	ASP	-	expression tag	UNP Q66K64
B	2	ILE	-	expression tag	UNP Q66K64
B	3	PHE	-	expression tag	UNP Q66K64
B	4	GLU	-	expression tag	UNP Q66K64
B	5	ALA	-	expression tag	UNP Q66K64
B	6	GLN	-	expression tag	UNP Q66K64
B	7	LYS	-	expression tag	UNP Q66K64
B	8	ILE	-	expression tag	UNP Q66K64
B	9	GLU	-	expression tag	UNP Q66K64

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Chain	Residue	Modelled	Actual	Comment	Reference
B	10	TRP	-	expression tag	UNP Q66K64
B	11	HIS	-	expression tag	UNP Q66K64
B	12	GLU	-	expression tag	UNP Q66K64
B	13	GLY	-	expression tag	UNP Q66K64
B	14	GLY	-	expression tag	UNP Q66K64
B	15	GLY	-	expression tag	UNP Q66K64
B	16	GLY	-	expression tag	UNP Q66K64
B	17	SER	-	expression tag	UNP Q66K64
B	18	GLY	-	expression tag	UNP Q66K64
B	19	GLU	-	expression tag	UNP Q66K64
B	20	ASN	-	expression tag	UNP Q66K64
B	21	LEU	-	expression tag	UNP Q66K64
B	22	TYR	-	expression tag	UNP Q66K64
B	23	PHE	-	expression tag	UNP Q66K64
B	24	GLN	-	expression tag	UNP Q66K64
B	25	GLY	-	expression tag	UNP Q66K64
B	26	GLY	-	expression tag	UNP Q66K64
B	27	GLY	-	expression tag	UNP Q66K64
B	28	ARG	-	expression tag	UNP Q66K64
B	29	MET	-	expression tag	UNP Q66K64
B	30	GLY	-	expression tag	UNP Q66K64
B	31	ARG	-	expression tag	UNP Q66K64
B	32	ARG	-	expression tag	UNP Q66K64
B	33	ARG	-	expression tag	UNP Q66K64

- Molecule 3 is a protein called DDB1- and CUL4-associated factor 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	183	Total	C	N	O	S	0	0	0
			1460	941	238	274	7			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	338	MET	-	initiating methionine	UNP Q66K64
C	339	ASP	-	expression tag	UNP Q66K64
C	340	TRP	-	expression tag	UNP Q66K64
C	341	SER	-	expression tag	UNP Q66K64
C	342	HIS	-	expression tag	UNP Q66K64
C	343	PRO	-	expression tag	UNP Q66K64
C	344	GLN	-	expression tag	UNP Q66K64
C	345	PHE	-	expression tag	UNP Q66K64

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Chain	Residue	Modelled	Actual	Comment	Reference
C	346	GLU	-	expression tag	UNP Q66K64
C	347	LYS	-	expression tag	UNP Q66K64
C	348	SER	-	expression tag	UNP Q66K64
C	349	ALA	-	expression tag	UNP Q66K64
C	350	VAL	-	expression tag	UNP Q66K64
C	351	GLY	-	expression tag	UNP Q66K64
C	352	LEU	-	expression tag	UNP Q66K64
C	353	ASN	-	expression tag	UNP Q66K64
C	354	ASP	-	expression tag	UNP Q66K64
C	355	ILE	-	expression tag	UNP Q66K64
C	356	PHE	-	expression tag	UNP Q66K64
C	357	GLU	-	expression tag	UNP Q66K64
C	358	ALA	-	expression tag	UNP Q66K64
C	359	GLN	-	expression tag	UNP Q66K64
C	360	LYS	-	expression tag	UNP Q66K64
C	361	ILE	-	expression tag	UNP Q66K64
C	362	GLU	-	expression tag	UNP Q66K64
C	363	TRP	-	expression tag	UNP Q66K64
C	364	HIS	-	expression tag	UNP Q66K64
C	365	GLU	-	expression tag	UNP Q66K64
C	366	GLY	-	expression tag	UNP Q66K64
C	367	GLY	-	expression tag	UNP Q66K64
C	368	GLY	-	expression tag	UNP Q66K64
C	369	GLY	-	expression tag	UNP Q66K64
C	370	SER	-	expression tag	UNP Q66K64
C	371	GLY	-	expression tag	UNP Q66K64
C	372	GLU	-	expression tag	UNP Q66K64
C	373	ASN	-	expression tag	UNP Q66K64
C	374	LEU	-	expression tag	UNP Q66K64
C	375	TYR	-	expression tag	UNP Q66K64
C	376	PHE	-	expression tag	UNP Q66K64
C	377	GLN	-	expression tag	UNP Q66K64
C	378	GLY	-	expression tag	UNP Q66K64
C	379	GLY	-	expression tag	UNP Q66K64
C	380	GLY	-	expression tag	UNP Q66K64
C	381	ARG	-	expression tag	UNP Q66K64
C	382	MET	-	expression tag	UNP Q66K64

- Molecule 4 is a protein called RNA-binding protein 39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	82	Total	C	N	O	S	0	0	0
			612	386	103	118	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	226	MET	-	initiating methionine	UNP Q14498
D	227	GLY	-	expression tag	UNP Q14498
D	228	SER	-	expression tag	UNP Q14498
D	229	SER	-	expression tag	UNP Q14498
D	230	HIS	-	expression tag	UNP Q14498
D	231	HIS	-	expression tag	UNP Q14498
D	232	HIS	-	expression tag	UNP Q14498
D	233	HIS	-	expression tag	UNP Q14498
D	234	HIS	-	expression tag	UNP Q14498
D	235	HIS	-	expression tag	UNP Q14498
D	236	SER	-	expression tag	UNP Q14498
D	237	ALA	-	expression tag	UNP Q14498
D	238	VAL	-	expression tag	UNP Q14498
D	239	ASP	-	expression tag	UNP Q14498
D	240	GLU	-	expression tag	UNP Q14498
D	241	ASN	-	expression tag	UNP Q14498
D	242	LEU	-	expression tag	UNP Q14498
D	243	TYR	-	expression tag	UNP Q14498
D	244	PHE	-	expression tag	UNP Q14498
D	245	GLN	-	expression tag	UNP Q14498
D	246	GLY	-	expression tag	UNP Q14498
D	247	GLY	-	expression tag	UNP Q14498
D	248	GLY	-	expression tag	UNP Q14498
D	249	ARG	-	expression tag	UNP Q14498

- Molecule 5 is a protein called DET1- and DDB1-associated protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	56	Total	C	N	O	0	0	0
			457	299	76	82			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-23	MET	-	initiating methionine	UNP Q9BW61
E	-22	GLY	-	expression tag	UNP Q9BW61
E	-21	SER	-	expression tag	UNP Q9BW61
E	-20	SER	-	expression tag	UNP Q9BW61
E	-19	HIS	-	expression tag	UNP Q9BW61
E	-18	HIS	-	expression tag	UNP Q9BW61
E	-17	HIS	-	expression tag	UNP Q9BW61

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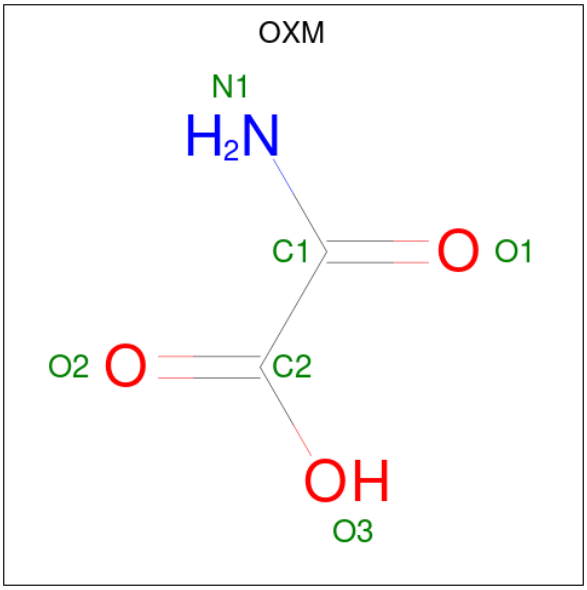
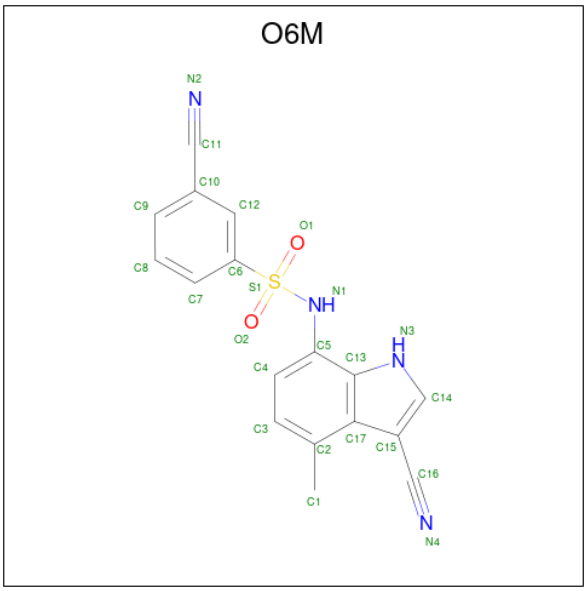
Chain	Residue	Modelled	Actual	Comment	Reference
E	-16	HIS	-	expression tag	UNP Q9BW61
E	-15	HIS	-	expression tag	UNP Q9BW61
E	-14	HIS	-	expression tag	UNP Q9BW61
E	-13	SER	-	expression tag	UNP Q9BW61
E	-12	ALA	-	expression tag	UNP Q9BW61
E	-11	VAL	-	expression tag	UNP Q9BW61
E	-10	ASP	-	expression tag	UNP Q9BW61
E	-9	GLU	-	expression tag	UNP Q9BW61
E	-8	ASN	-	expression tag	UNP Q9BW61
E	-7	LEU	-	expression tag	UNP Q9BW61
E	-6	TYR	-	expression tag	UNP Q9BW61
E	-5	PHE	-	expression tag	UNP Q9BW61
E	-4	GLN	-	expression tag	UNP Q9BW61
E	-3	GLY	-	expression tag	UNP Q9BW61
E	-2	GLY	-	expression tag	UNP Q9BW61
E	-1	GLY	-	expression tag	UNP Q9BW61
E	0	ARG	-	expression tag	UNP Q9BW61

- Molecule 6 is OXAMIC ACID (three-letter code: OXM) (formula: $C_2H_3NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	6	2	1	3	0	0

- Molecule 7 is 3-cyano-N-(3-cyano-4-methyl-1H-indol-7-yl)benzene-1-sulfonamide (three-letter code: O6M) (formula: $C_{17}H_{12}N_4O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O S 24 17 4 2 1	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Zn 1 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	8	Total O 8 8	0	0
9	B	3	Total O 3 3	0	0
9	D	3	Total O 3 3	0	0
9	E	2	Total O 2 2	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 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.11Å 93.60Å 258.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.05 – 2.90	Depositor
% Data completeness (in resolution range)	99.8 (46.05-2.90)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.205 , 0.251	Depositor
Wilson B-factor (Å^2)	97.1	Xtriage
Anisotropy	0.514	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	10249	wwPDB-VP
Average B, all atoms (Å^2)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
7	O6M	B	302	-	24,26,26	0.67	0	30,38,38	0.78	2 (6%)
6	OXM	B	301	-	5,5,5	2.10	2 (40%)	4,6,6	2.85	2 (50%)

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	O6M	B	302	-	-	0/13/15/15	0/3/3/3
6	OXM	B	301	-	-	3/3/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	301	OXM	O2-C2	3.85	1.32	1.22
6	B	301	OXM	O3-C2	-2.67	1.22	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	301	OXM	O3-C2-C1	4.24	123.64	113.84
6	B	301	OXM	O2-C2-C1	-3.78	113.64	122.06
7	B	302	O6M	C2-C17-C13	-2.16	119.14	122.67
7	B	302	O6M	C13-C5-N1	2.11	118.49	115.50

There are no chirality outliers.

All (3) torsion outliers are listed below:

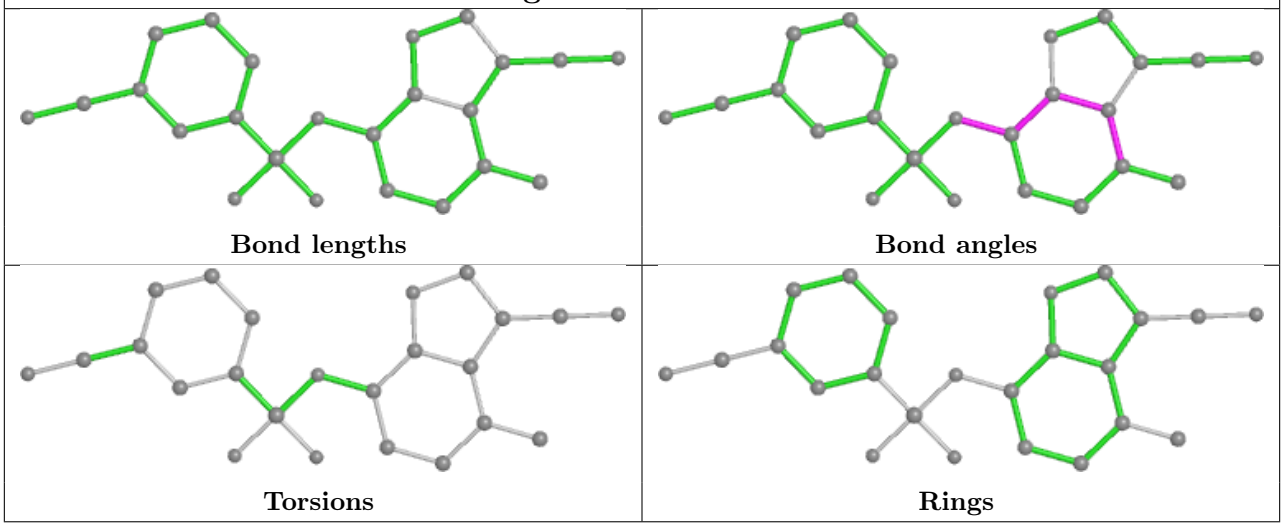
Mol	Chain	Res	Type	Atoms
6	B	301	OXM	N1-C1-C2-O2
6	B	301	OXM	N1-C1-C2-O3
6	B	301	OXM	O1-C1-C2-O2

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 O6M B 302



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.