



## wwPDB EM Validation Summary Report ⓘ

Apr 13, 2026 – 01:41 pm BST

PDB ID : 9QUE / pdb\_00009que  
Title : Structure of human MTH1 in complex with 8DG by continuous serial electron diffraction (SerialED)  
Authors : Hofer, G.; Wang, L.; Pacoste, L.; Hager, P.; Fonjallaz, A.; Scaletti Hutchinson, E.; Stenmark, P.; Di Palma, M.; Williams, L.; Worrall, J.; Steiner, R.; Xu, H.; Zou, X.  
Deposited on : 2025-04-10  
Resolution : 1.66 Å (reported)  
Based on initial model : 3ZR1

This is a wwPDB EM Validation Summary Report for a publicly released PDB/EMDB 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/EMValidationReportHelp>

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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.4, CSD as541be (2020)  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

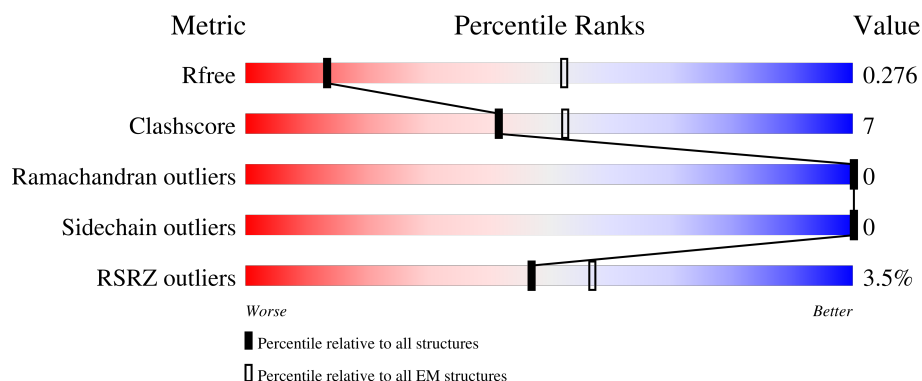
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON CRYSTALLOGRAPHY*

The reported resolution of this entry is 1.66 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
$R_{free}$	180332	208
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RSRZ outliers	180361	209

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	159	 3% 89% 10% .
1	B	159	 4% 79% 18% .

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5299 atoms, of which 2516 are hydrogens and 0 are deuteriums.

In the tables below, 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.

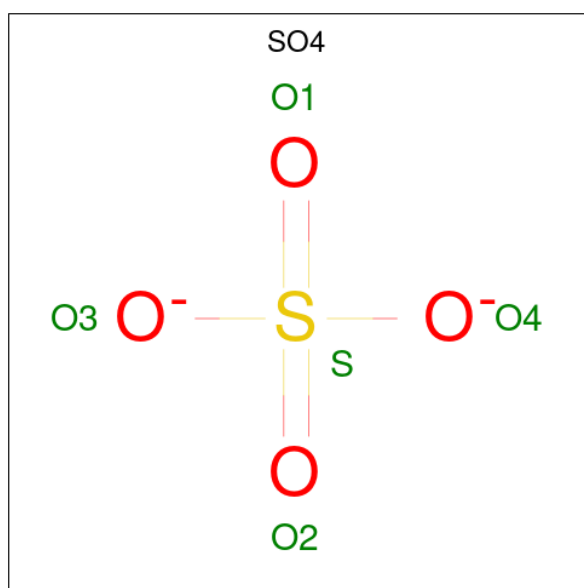
- Molecule 1 is a protein called Oxidized purine nucleoside triphosphate hydrolase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	158	Total	C	H	N	O	S	3	0
			2563	834	1264	219	238	8		
1	B	154	Total	C	H	N	O	S	1	0
			2487	811	1228	209	232	7		

There are 6 discrepancies between the modelled and reference sequences:

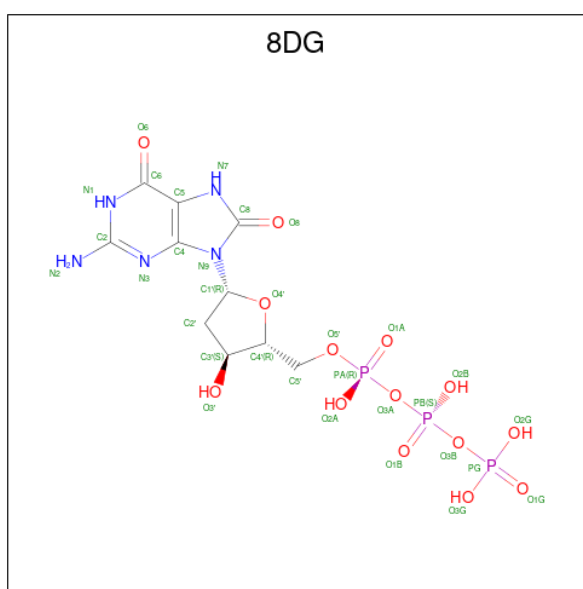
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P36639
A	-1	SER	-	expression tag	UNP P36639
A	0	HIS	-	expression tag	UNP P36639
B	-2	GLY	-	expression tag	UNP P36639
B	-1	SER	-	expression tag	UNP P36639
B	0	HIS	-	expression tag	UNP P36639

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	O	S	0
			5	4	1	
2	A	1	Total	O	S	0
			5	4	1	
2	B	1	Total	O	S	0
			5	4	1	
2	B	1	Total	O	S	0
			5	4	1	

- Molecule 3 is 8-OXO-2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: 8DG) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
3	B	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	

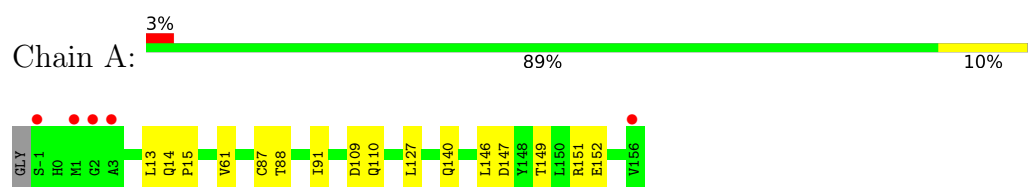
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	83	Total	O	0
			83	83	
4	B	58	Total	O	0
			58	58	

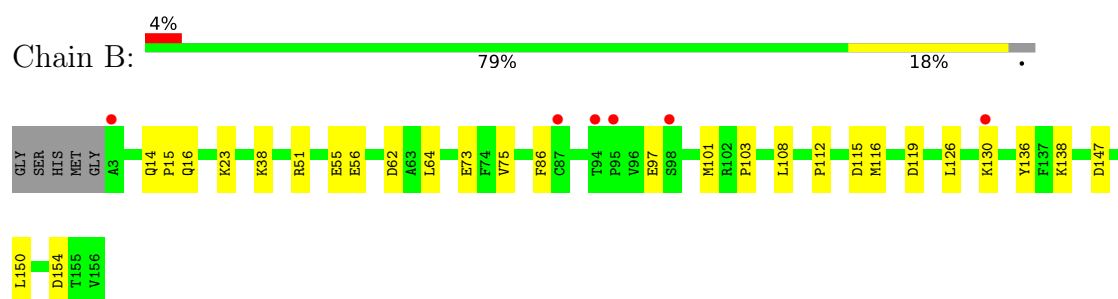
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Oxidized purine nucleoside triphosphate hydrolase



- Molecule 1: Oxidized purine nucleoside triphosphate hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.34Å 67.55Å 80.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.73 – 1.66 25.73 – 1.66	Depositor EDS
% Data completeness (in resolution range)	96.4 (25.73-1.66) 96.3 (25.73-1.66)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 1.66Å)	Xtriage
Refinement program	unknown	Depositor
R, $R_{free}$	0.205 , 0.253 0.231 , 0.276	Depositor DCC
$R_{free}$ test set	1869 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.8	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 29.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5299	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 8DG

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  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.53	0/1341	0.53	0/1808
1	B	0.48	0/1294	0.50	0/1746
All	All	0.50	0/2635	0.52	0/3554

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1299	1264	1272	12	0
1	B	1259	1228	1228	23	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
3	A	32	12	12	2	0
3	B	32	12	12	2	0
4	A	83	0	0	2	0
4	B	58	0	0	4	1
All	All	2783	2516	2524	35	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 35 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:202:8DG:C1'	3:A:202:8DG:O4'	1.64	1.20
2:A:203:SO4:O1	4:A:301:HOH:O	1.99	0.79
1:B:115:ASP:OD1	4:B:301:HOH:O	2.05	0.74
1:A:151[B]:ARG:HG3	1:B:126:LEU:HD21	1.74	0.70
1:B:108:LEU:O	4:B:302:HOH:O	2.10	0.69

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:325:HOH:O	4:B:351:HOH:O[4_455]	2.16	0.04

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	159/159 (100%)	157 (99%)	2 (1%)	0	100	100
1	B	153/159 (96%)	152 (99%)	1 (1%)	0	100	100
All	All	312/318 (98%)	309 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	141/138 (102%)	141 (100%)	0	100	100
1	B	136/138 (99%)	136 (100%)	0	100	100
All	All	277/276 (100%)	277 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	B	84	HIS
1	B	107	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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	$\# Z  > 2$
2	SO4	A	203	-	4,4,4	0.18	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	8DG	A	202	-	30,34,34	3.68	16 (53%)	43,54,54	1.88	10 (23%)
3	8DG	B	203	-	30,34,34	3.76	16 (53%)	43,54,54	1.86	12 (27%)
2	SO4	B	202	-	4,4,4	0.17	0	6,6,6	0.10	0
2	SO4	B	201	-	4,4,4	0.11	0	6,6,6	0.13	0
2	SO4	A	201	-	4,4,4	0.14	0	6,6,6	0.10	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
3	8DG	B	203	-	-	7/22/34/34	0/3/3/3
3	8DG	A	202	-	-	5/22/34/34	0/3/3/3

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	8DG	O4'-C1'	9.78	1.64	1.42
3	B	203	8DG	O4'-C1'	9.43	1.63	1.42
3	B	203	8DG	C2-N3	7.39	1.51	1.33
3	A	202	8DG	C8-N7	7.08	1.51	1.38
3	B	203	8DG	C8-N7	6.45	1.50	1.38

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	203	8DG	C5-C4-N3	-6.00	121.60	127.80
3	A	202	8DG	O4'-C1'-N9	-5.43	102.82	108.29
3	A	202	8DG	C5-C4-N3	-5.35	122.27	127.80
3	B	203	8DG	O6-C6-C5	-3.68	118.81	127.24
3	A	202	8DG	C2'-C1'-N9	3.48	120.13	116.01

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	202	8DG	C5'-O5'-PA-O1A
3	B	203	8DG	C5'-O5'-PA-O3A
3	B	203	8DG	C5'-O5'-PA-O1A
3	B	203	8DG	C5'-O5'-PA-O2A

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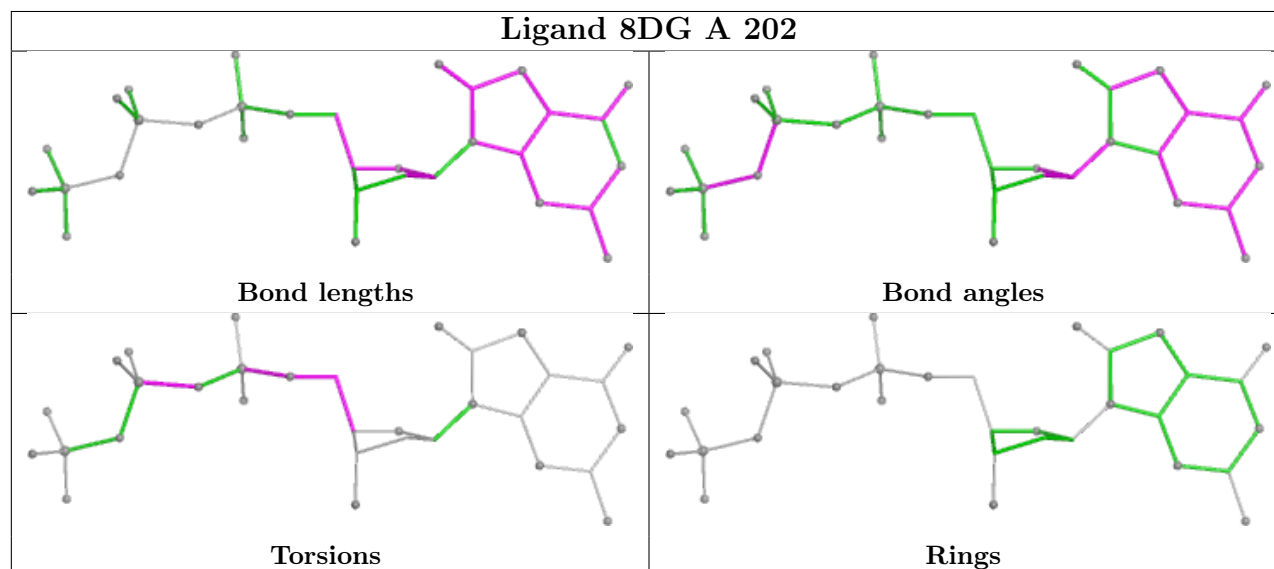
Mol	Chain	Res	Type	Atoms
3	A	202	8DG	C4'-C5'-O5'-PA

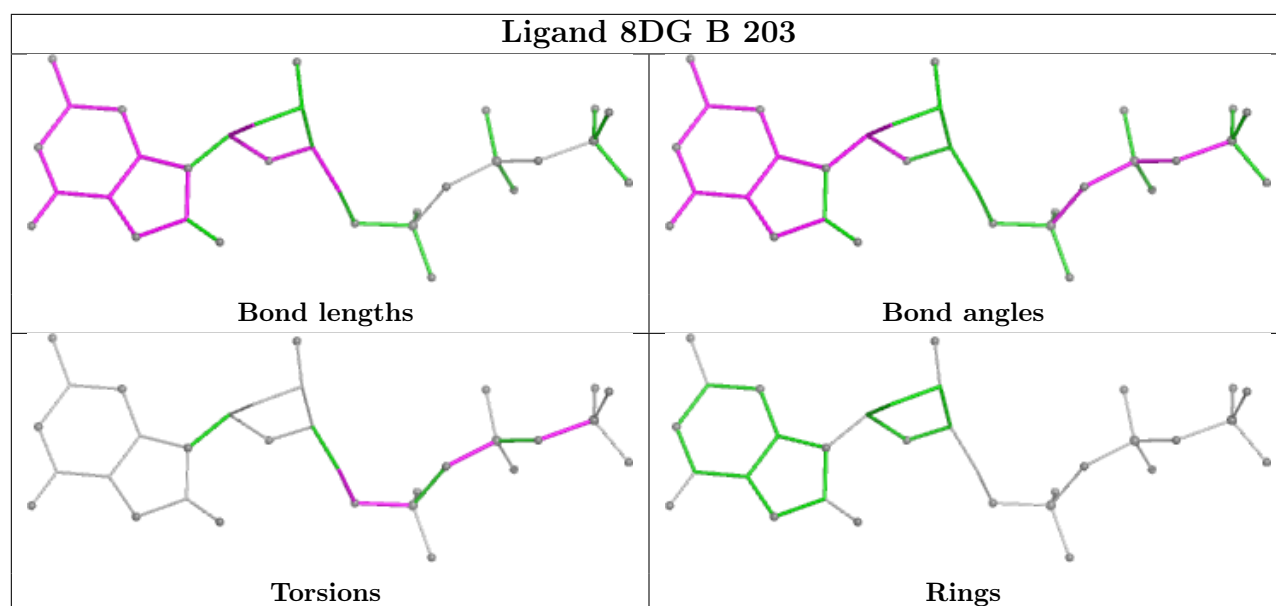
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	203	SO4	1	0
3	A	202	8DG	2	0
3	B	203	8DG	2	0

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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.