



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2022 – 02:10 PM EDT

PDB ID : 7N3S
Title : Human bisphosphoglycerate mutase complex with 2-phosphoglycolate
Authors : Aljahdali, A.S.; Musayev, F.N.; Safo, M.K.
Deposited on : 2021-06-01
Resolution : 2.48 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
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) : 2.27

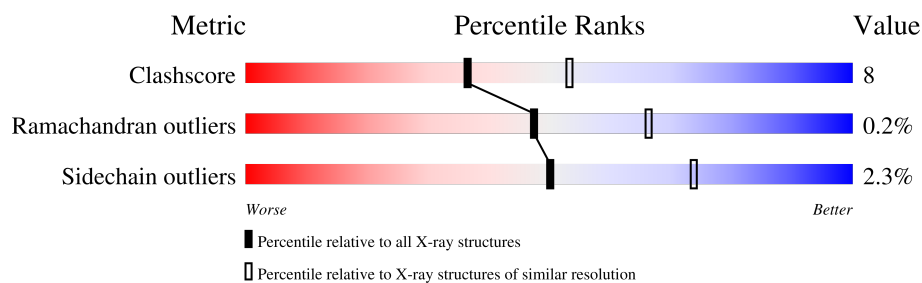
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4201 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.

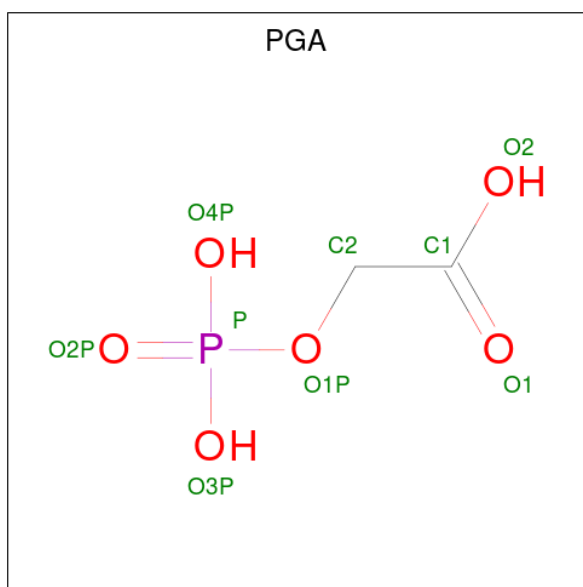
- Molecule 1 is a protein called Bisphosphoglycerate mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			2067	1308	369	384	6			
1	B	243	Total	C	N	O	S	0	0	0
			1989	1260	355	368	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	260	LEU	-	expression tag	UNP P07738
A	261	GLU	-	expression tag	UNP P07738
A	262	HIS	-	expression tag	UNP P07738
A	263	HIS	-	expression tag	UNP P07738
A	264	HIS	-	expression tag	UNP P07738
A	265	HIS	-	expression tag	UNP P07738
A	266	HIS	-	expression tag	UNP P07738
A	267	HIS	-	expression tag	UNP P07738
B	260	LEU	-	expression tag	UNP P07738
B	261	GLU	-	expression tag	UNP P07738
B	262	HIS	-	expression tag	UNP P07738
B	263	HIS	-	expression tag	UNP P07738
B	264	HIS	-	expression tag	UNP P07738
B	265	HIS	-	expression tag	UNP P07738
B	266	HIS	-	expression tag	UNP P07738
B	267	HIS	-	expression tag	UNP P07738

- Molecule 2 is 2-PHOSPHOGLYCOLIC ACID (three-letter code: PGA) (formula: C₂H₅O₆P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			9	2	6	1		
2	A	1	Total	C	O	P	0	0
			9	2	6	1		
2	B	1	Total	C	O	P	0	0
			9	2	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	37	Total	O	0	0
			37	37		

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

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	52.64Å 70.81Å 158.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 2.48	Depositor
% Data completeness (in resolution range)	99.7 (29.00-2.48)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.210 , 0.284	Depositor
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.563	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4201	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGA

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	0.44	0/2113	0.62	1/2863 (0.0%)
1	B	0.37	0/2035	0.57	1/2760 (0.0%)
All	All	0.41	0/4148	0.60	2/5623 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	117	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	117	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	238	GLN	Peptide

4.2 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	2067	0	2041	25	0
1	B	1989	0	1962	40	0
2	A	18	0	4	0	0
2	B	9	0	2	1	0
3	A	81	0	0	3	0
3	B	37	0	0	0	0
All	All	4201	0	4009	64	0

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 8.

All (64) 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)
1:B:119:TYR:CZ	1:B:159:LYS:HD3	1.82	1.14
1:B:119:TYR:CE2	1:B:159:LYS:HD3	2.02	0.92
1:B:119:TYR:OH	1:B:159:LYS:HD3	1.72	0.88
1:B:114:LEU:HD11	1:B:121:VAL:HG21	1.59	0.84
1:B:158:LEU:HD22	1:B:193:ARG:HH21	1.42	0.82
1:A:196:LEU:CD2	1:A:220:LEU:HD21	2.18	0.73
1:B:119:TYR:OH	1:B:159:LYS:CD	2.37	0.72
1:B:102:GLN:HG3	1:B:105:LEU:HD12	1.74	0.69
1:B:152:LEU:O	1:B:154:ARG:NH1	2.27	0.67
1:A:48:LEU:O	3:A:401:HOH:O	2.15	0.64
1:A:95:LEU:HA	1:A:98:LEU:HD12	1.81	0.62
1:B:116:ARG:NH2	2:B:301:PGA:O2P	2.32	0.61
1:B:37:GLU:HG2	1:B:215:GLY:HA3	1.83	0.60
1:A:114:LEU:O	1:A:118:SER:HB3	2.02	0.59
1:A:199:LEU:HD13	1:A:222:LEU:HD21	1.84	0.59
1:B:44:GLN:O	1:B:48:LEU:HD12	2.03	0.59
1:B:116:ARG:HG3	1:B:117:ARG:HD2	1.85	0.59
1:B:119:TYR:CE2	1:B:159:LYS:CD	2.84	0.59
1:B:116:ARG:HD3	1:B:117:ARG:HE	1.68	0.58
1:A:117:ARG:HE	1:A:211:THR:HG22	1.70	0.57
1:A:118:SER:HA	1:A:208:ILE:HD12	1.87	0.56
1:A:125:PRO:HA	1:A:155:SER:HB3	1.90	0.53
1:A:16:TRP:N	1:A:28:GLN:OE1	2.28	0.53
1:B:116:ARG:HD3	1:B:117:ARG:NE	2.24	0.52
1:B:158:LEU:HD22	1:B:193:ARG:NH2	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LEU:HD22	1:B:218:ILE:HD13	1.92	0.52
1:A:102:GLN:NE2	3:A:410:HOH:O	2.42	0.52
1:B:14:GLY:H	1:B:17:ASN:HB2	1.76	0.51
1:A:52:PHE:CE1	1:A:184:LEU:HB2	2.45	0.51
1:A:196:LEU:HD21	1:A:220:LEU:HD21	1.89	0.51
1:A:159:LYS:NZ	3:A:411:HOH:O	2.42	0.51
1:A:114:LEU:HD13	1:A:118:SER:HB2	1.94	0.49
1:A:140:ARG:HA	1:A:143:LYS:HG3	1.95	0.49
1:B:162:LEU:HB2	1:B:194:ALA:HB1	1.94	0.48
1:B:222:LEU:HD23	1:B:228:ALA:HA	1.96	0.47
1:B:196:LEU:HD12	1:B:212:LEU:HD11	1.95	0.47
1:A:51:GLU:HB3	1:B:140:ARG:CZ	2.45	0.45
1:A:90:ARG:NH2	1:A:115:TRP:O	2.39	0.45
1:B:74:LEU:HB3	1:B:76:GLN:NE2	2.31	0.45
1:A:24:SER:HB3	1:A:96:ILE:HG12	1.98	0.45
1:B:219:LEU:HB2	1:B:235:LEU:HD11	1.98	0.45
1:A:5:LYS:HD3	1:A:219:LEU:HD11	1.99	0.44
1:B:140:ARG:HA	1:B:143:LYS:HE2	1.99	0.44
1:B:162:LEU:HD11	1:B:198:HIS:HB2	1.99	0.44
1:B:174:ALA:HA	1:B:177:VAL:CG1	2.47	0.44
1:B:86:ARG:HD3	1:B:164:ARG:O	2.18	0.43
1:B:143:LYS:HB2	1:B:143:LYS:HE3	1.67	0.43
1:B:53:ASP:O	1:B:54:LEU:HD22	2.18	0.43
1:B:159:LYS:O	1:B:163:GLU:HG3	2.19	0.43
1:A:19:GLU:OE1	1:A:21:ARG:HD2	2.19	0.43
1:B:114:LEU:CD1	1:B:121:VAL:HG11	2.48	0.43
1:B:220:LEU:HD21	1:B:222:LEU:HD21	2.01	0.43
1:A:203:SER:OG	1:A:206:ASP:OD2	2.31	0.42
1:B:91:HIS:NE2	1:B:137:TYR:OH	2.49	0.42
1:B:74:LEU:HB3	1:B:76:GLN:HE21	1.84	0.42
1:B:173:ILE:O	1:B:176:GLU:N	2.50	0.42
1:B:4:TYR:HE2	1:B:224:GLU:HA	1.84	0.42
1:B:172:ARG:O	1:B:172:ARG:NH1	2.53	0.42
1:B:114:LEU:C	1:B:114:LEU:HD13	2.41	0.41
1:A:139:ASP:CG	1:A:141:ARG:HE	2.23	0.41
1:A:59:VAL:O	1:A:141:ARG:NH1	2.53	0.41
1:A:3:LYS:HZ1	1:A:221:GLU:HB3	1.85	0.41
1:B:241:ILE:HG22	1:B:241:ILE:O	2.22	0.40
1:A:119:TYR:HA	1:A:158:LEU:HB3	2.04	0.40

There are no symmetry-related clashes.

4.3 Torsion angles

4.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	252/267 (94%)	240 (95%)	11 (4%)	1 (0%)	34	52
1	B	241/267 (90%)	221 (92%)	20 (8%)	0	100	100
All	All	493/534 (92%)	461 (94%)	31 (6%)	1 (0%)	47	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LYS

4.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	224/238 (94%)	219 (98%)	5 (2%)	52	75
1	B	216/238 (91%)	211 (98%)	5 (2%)	50	74
All	All	440/476 (92%)	430 (98%)	10 (2%)	50	74

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	28	GLN
1	A	103	MET
1	A	129	SER
1	A	220	LEU

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Mol	Chain	Res	Type
1	B	6	LEU
1	B	28	GLN
1	B	50	PHE
1	B	159	LYS
1	B	223	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

3 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

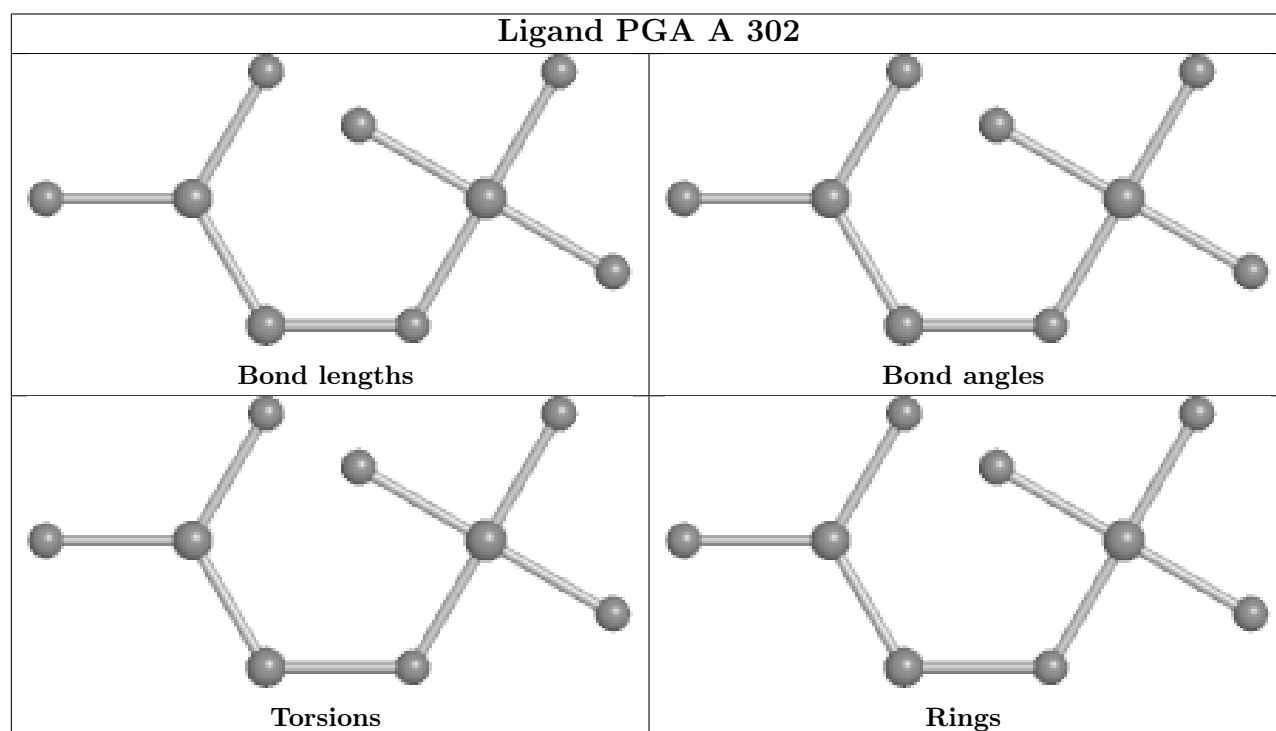
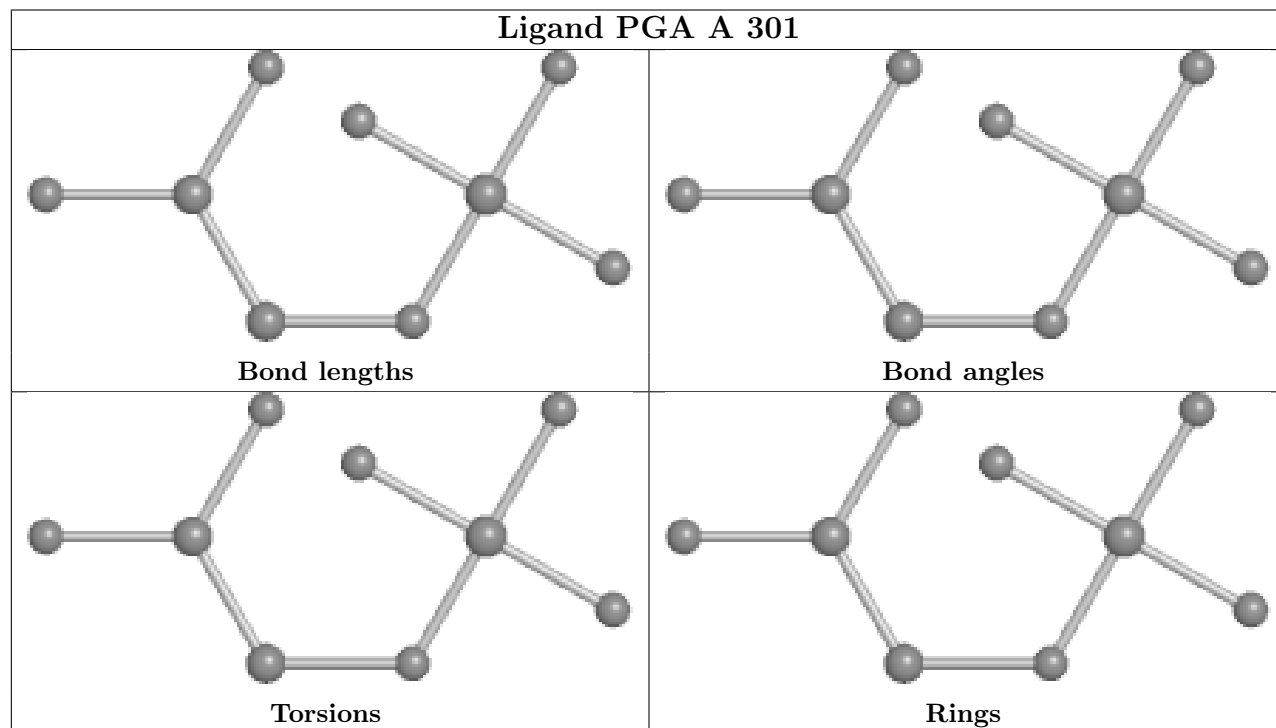
There are no torsion outliers.

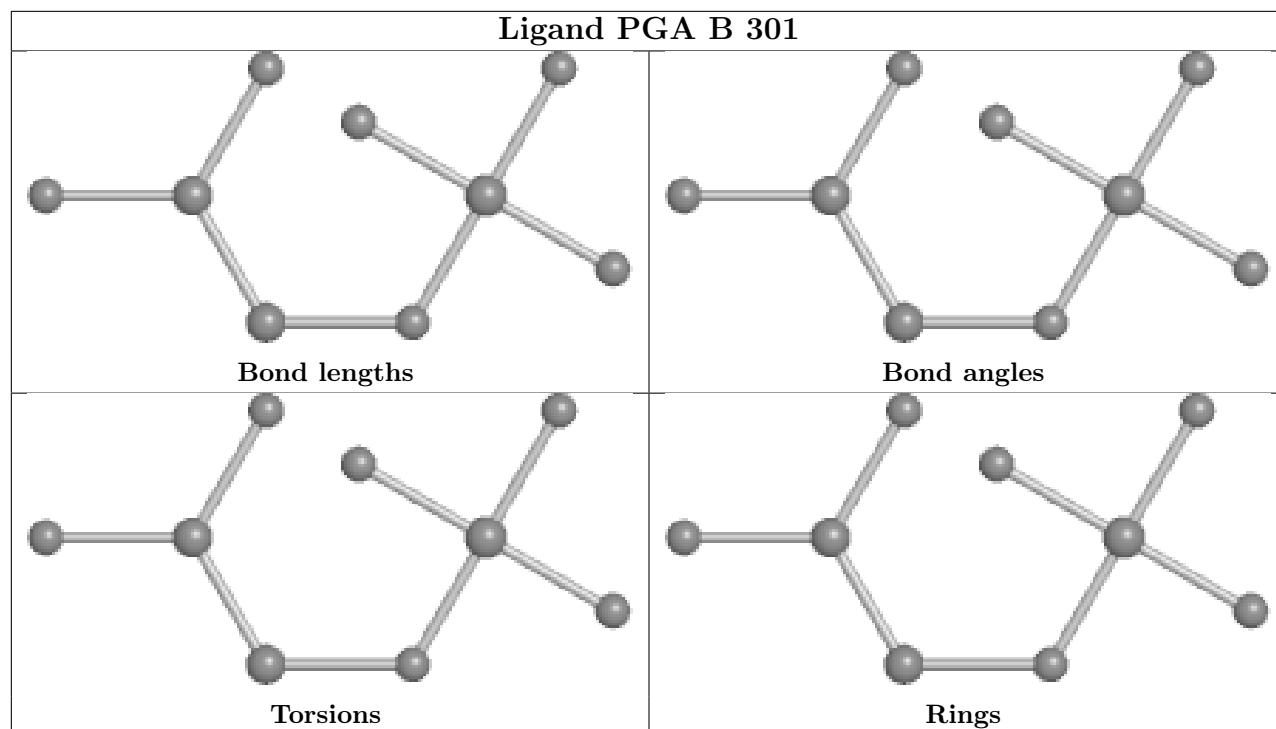
There are no ring outliers.

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 [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.