



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2021 – 12:01 PM GMT

PDB ID : 7NC7
Title : Crystal structure of fructose-bisphosphate aldolases FBAC from *Bacillus methanolicus*
Authors : Einsle, O.; Zhang, L.; Guetle, D.; Jacquot, J.P.
Deposited on : 2021-01-28
Resolution : 2.20 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.16

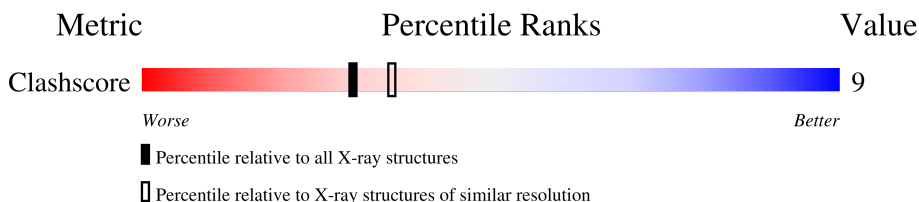
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	285	 80% 15% .
1	B	285	 77% 18% 5%

2 Entry composition [i](#)

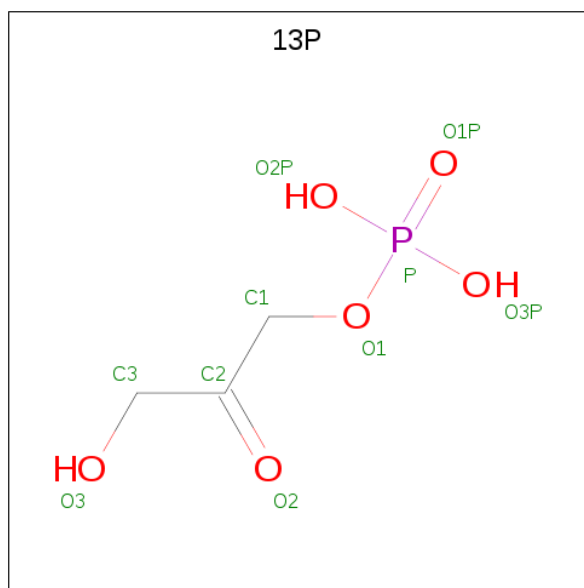
There are 3 unique types of molecules in this entry. The entry contains 4325 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fructose-bisphosphate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	Total 2086	C 1313	N 359	O 401	S 13	0	3	0
1	B	272	Total 2069	C 1302	N 355	O 399	S 13	0	2	0

- Molecule 2 is 1,3-DIHYDROXYACETONEPHOSPHATE (three-letter code: 13P) (formula: $C_3H_7O_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	Total 10	C 3	O 6	P 1	0	0
2	B	1	Total 10	C 3	O 6	P 1	0	0

- Molecule 3 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	79	Total 79	O 79	0	0
3	B	71	Total 71	O 71	0	0

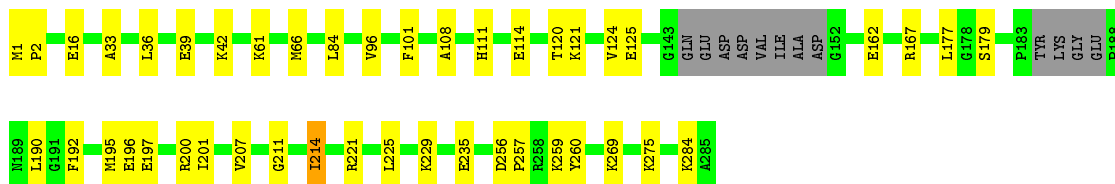
3 Residue-property plots

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.


Note EDS failed to run properly.

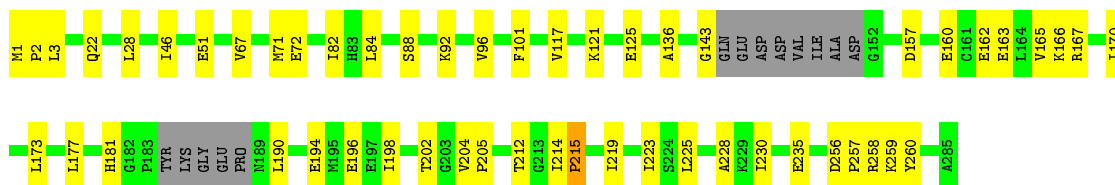
- Molecule 1: Fructose-bisphosphate aldolase

Chain A: 



- Molecule 1: Fructose-bisphosphate aldolase

Chain B: 



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	71.97Å 98.26Å 139.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.42 – 2.20	Depositor
% Data completeness (in resolution range)	71.2 (27.42-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.189 , 0.253	Depositor
Wilson B-factor (Å ²)	33.2	Xtrriage
Anisotropy	0.044	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4325	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 13P

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	0.71	1/2119 (0.0%)	0.71	0/2853
1	B	0.75	2/2100 (0.1%)	0.74	1/2827 (0.0%)
All	All	0.73	3/4219 (0.1%)	0.73	1/5680 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	215	PRO	N-CA	12.65	1.68	1.47
1	A	214	ILE	C-N	8.69	1.50	1.34
1	B	214	ILE	C-N	5.37	1.44	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	PRO	CA-N-CD	-7.08	101.59	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2086	0	2105	37	0
1	B	2069	0	2091	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	5	0	0
2	B	10	0	5	0	0
3	A	79	0	0	3	1
3	B	71	0	0	2	0
All	All	4325	0	4206	78	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 9.

All (78) 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:215:PRO:N	1:B:215:PRO:CA	1.68	1.36
1:A:195:MET:SD	3:A:477:HOH:O	2.28	0.91
1:A:1:MET:HE2	3:A:457:HOH:O	1.75	0.86
1:A:1:MET:CE	1:A:2:PRO:O	2.36	0.74
1:B:96:VAL:HG13	1:B:101:PHE:CG	2.24	0.72
1:A:196:GLU:HG3	1:A:225:LEU:HD22	1.71	0.71
1:A:1:MET:HE1	1:A:2:PRO:O	1.92	0.70
1:A:195:MET:HE1	1:A:225:LEU:HB2	1.74	0.68
1:B:235[B]:GLU:OE1	3:B:401:HOH:O	2.10	0.68
1:A:96:VAL:HG13	1:A:101:PHE:CG	2.30	0.65
1:B:165:VAL:HG21	1:B:202:THR:CG2	2.27	0.65
1:A:256:ASP:HB3	1:A:259:LYS:HG3	1.79	0.64
1:B:163:GLU:CG	1:B:167:ARG:HD2	2.30	0.61
1:B:196:GLU:HB2	1:B:225:LEU:HD13	1.84	0.60
1:A:1:MET:HE2	1:A:2:PRO:O	2.02	0.58
1:B:163:GLU:HG2	1:B:167:ARG:HD2	1.85	0.58
1:A:162:GLU:HB2	1:A:201:ILE:HD12	1.84	0.58
1:A:195:MET:CE	1:A:225:LEU:HB2	2.35	0.56
1:B:215:PRO:C	1:B:215:PRO:N	2.52	0.56
1:B:198:ILE:O	1:B:202:THR:OG1	2.18	0.55
1:B:202:THR:HG22	1:B:204:VAL:HG22	1.88	0.55
1:A:84:LEU:HB2	1:A:96:VAL:HG11	1.89	0.55
1:B:165:VAL:HG21	1:B:202:THR:HG23	1.90	0.54
1:B:51:GLU:OE2	1:B:92:LYS:HG2	2.08	0.54
1:A:114:GLU:CD	1:A:167:ARG:HH12	2.11	0.54
1:A:66:MET:HE1	1:B:28:LEU:HD22	1.90	0.54
1:A:39:GLU:O	1:A:42:LYS:HD3	2.08	0.52
1:A:221:ARG:NH1	3:A:408:HOH:O	2.43	0.52
1:B:219:ILE:O	1:B:223:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:GLU:HG2	1:B:166:LYS:HE3	1.91	0.52
1:A:197:GLU:O	1:A:201:ILE:HG12	2.10	0.51
1:A:196:GLU:O	1:A:200:ARG:HG2	2.10	0.51
1:A:235:GLU:OE2	1:A:275:LYS:HE3	2.11	0.49
1:B:84:LEU:HB2	1:B:96:VAL:HG11	1.95	0.48
1:B:212:THR:HG23	1:B:235[A]:GLU:HB2	1.95	0.48
1:A:207:VAL:HG22	1:A:229:LYS:HB3	1.95	0.48
1:B:88:SER:OG	3:B:402:HOH:O	2.20	0.47
1:A:36:LEU:HD12	1:A:269:LYS:HZ1	1.80	0.47
1:A:121:LYS:O	1:A:125:GLU:HG3	2.15	0.47
1:A:179:SER:N	1:A:190:LEU:HD21	2.30	0.47
1:B:117:VAL:HG11	1:B:167:ARG:HH21	1.79	0.47
1:B:96:VAL:HG13	1:B:101:PHE:CD2	2.49	0.47
1:A:96:VAL:HG13	1:A:101:PHE:CD2	2.50	0.46
1:B:194:GLU:OE2	1:B:194:GLU:N	2.46	0.46
1:B:67:VAL:HG11	1:B:82:ILE:HD11	1.98	0.46
1:A:177:LEU:O	1:A:190:LEU:HD23	2.16	0.46
1:B:257:PRO:HA	1:B:260:TYR:CE2	2.51	0.46
1:B:219:ILE:HD12	1:B:230:ILE:HD13	1.98	0.45
1:A:84:LEU:HD22	1:A:96:VAL:HG21	1.99	0.45
1:B:163:GLU:HG3	1:B:167:ARG:HD2	1.98	0.45
1:A:192:PHE:CD1	1:A:221:ARG:HG2	2.52	0.45
1:B:205:PRO:HB3	1:B:228:ALA:HB3	1.99	0.45
1:B:165:VAL:HG22	1:B:170:ILE:HD11	1.99	0.44
1:A:200:ARG:HA	1:A:200:ARG:HE	1.81	0.44
1:B:2:PRO:HD2	1:B:71:MET:HE3	1.98	0.44
1:B:1:MET:N	1:B:2:PRO:CD	2.80	0.44
1:A:120:THR:O	1:A:124:VAL:HG23	2.18	0.44
1:B:121:LYS:O	1:B:125:GLU:HG3	2.17	0.44
1:A:61:LYS:HD2	1:B:72:GLU:OE1	2.18	0.43
1:A:108:ALA:O	1:A:111:HIS:HB2	2.18	0.43
1:B:157:ASP:HB3	1:B:160:GLU:HB2	2.00	0.43
1:B:136:ALA:HB3	1:B:170:ILE:HD13	2.01	0.43
1:B:162:GLU:O	1:B:166:LYS:HG2	2.18	0.43
1:B:143:GLY:HA2	1:B:181:HIS:HB2	2.01	0.43
1:B:3:LEU:HD12	1:B:3:LEU:HA	1.76	0.43
1:B:136:ALA:O	1:B:173:LEU:HD12	2.18	0.42
1:B:256:ASP:HB3	1:B:259:LYS:HG3	2.02	0.42
1:B:92:LYS:HA	1:B:92:LYS:HD2	1.89	0.42
1:A:61:LYS:HD2	1:B:72:GLU:CD	2.40	0.42
1:B:256:ASP:OD1	1:B:258[A]:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:O	1:B:190:LEU:HA	2.19	0.41
1:A:211:GLY:HA2	1:A:214:ILE:HD12	2.02	0.41
1:A:257:PRO:HA	1:A:260:TYR:CE2	2.55	0.41
1:A:33:ALA:HA	1:A:269:LYS:NZ	2.35	0.41
1:A:61:LYS:HE3	1:B:72:GLU:OE2	2.21	0.41
1:B:196:GLU:HA	1:B:225:LEU:HB3	2.03	0.40
1:A:16:GLU:OE2	1:A:284:LYS:NZ	2.45	0.40
1:B:22:GLN:HA	1:B:46:ILE:HB	2.04	0.40

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)
3:A:454:HOH:O	3:A:454:HOH:O[3_655]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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 monosaccharides in this entry.

5.6 Ligand geometry

2 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	13P	B	301	-	9,9,9	0.57	0	10,12,12	0.63	0
2	13P	A	301	-	9,9,9	0.81	0	10,12,12	0.83	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
2	13P	B	301	-	-	4/7/8/8	-
2	13P	A	301	-	-	5/7/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

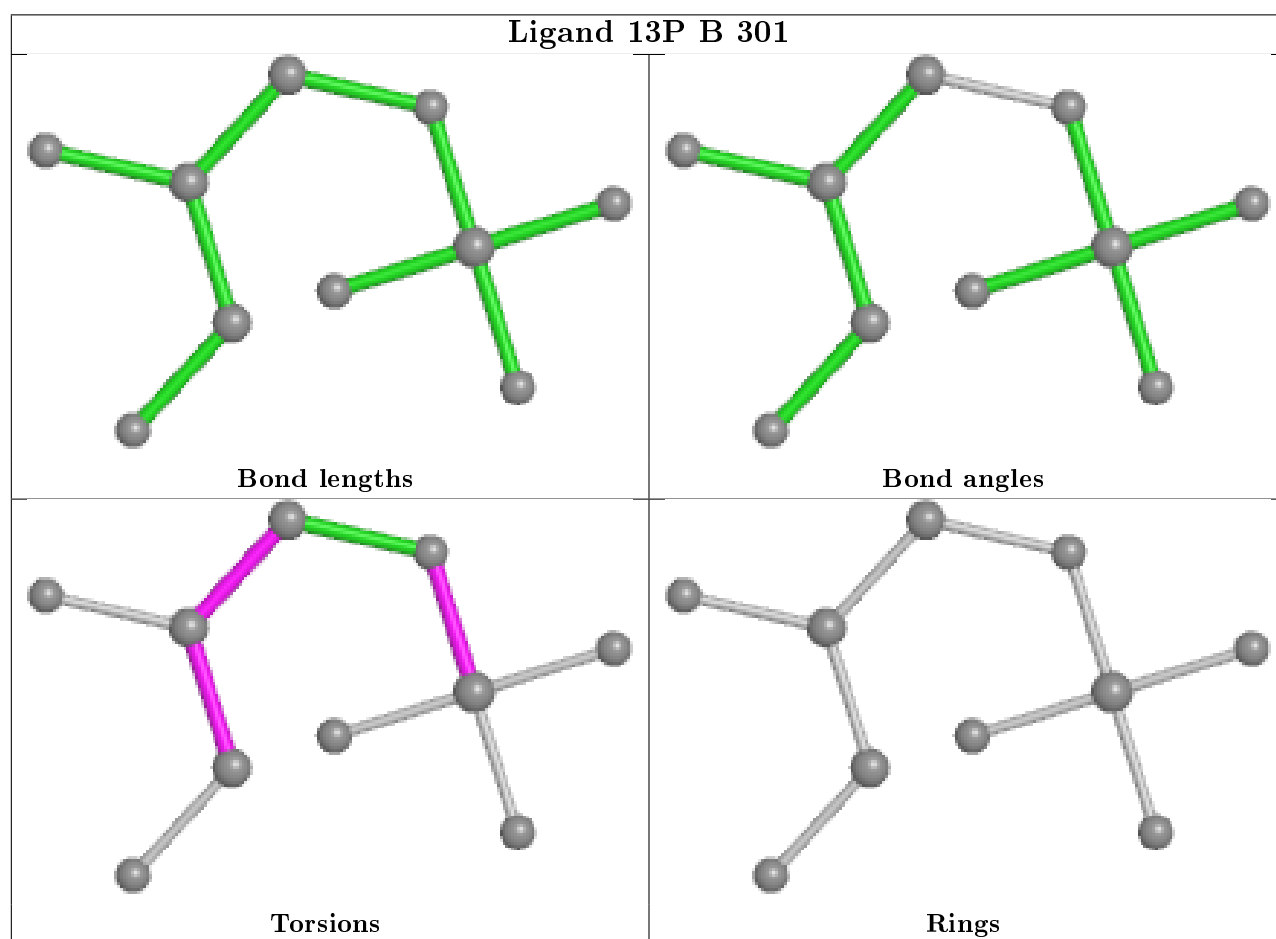
All (9) torsion outliers are listed below:

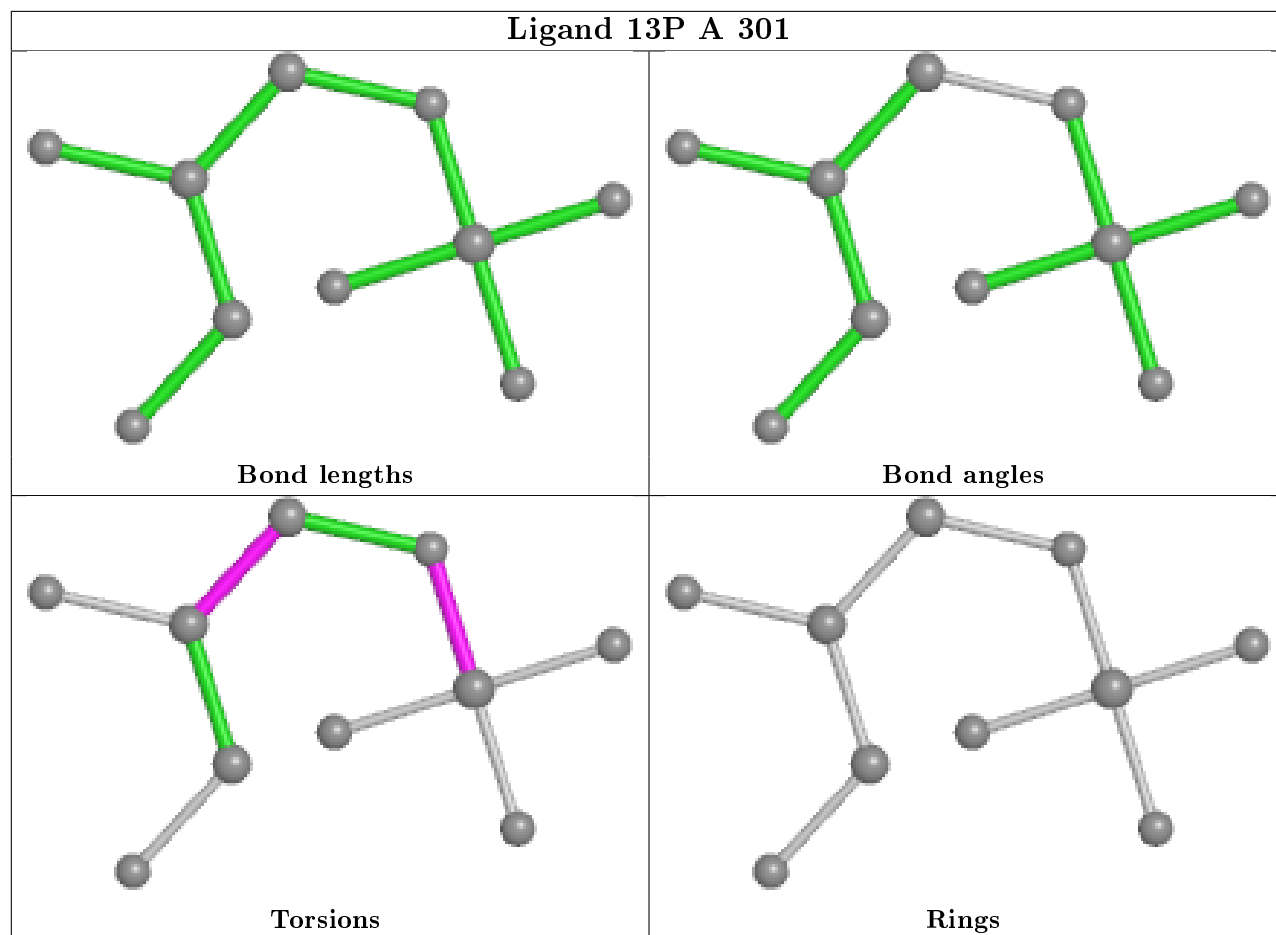
Mol	Chain	Res	Type	Atoms
2	B	301	13P	O2-C2-C3-O3
2	A	301	13P	C1-O1-P-O1P
2	A	301	13P	C1-O1-P-O2P
2	A	301	13P	C1-O1-P-O3P
2	B	301	13P	O1-C1-C2-O2
2	A	301	13P	O1-C1-C2-O2
2	B	301	13P	C1-O1-P-O1P
2	A	301	13P	O1-C1-C2-C3
2	B	301	13P	O1-C1-C2-C3

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.





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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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