

Full wwPDB X-ray Structure Validation Report (i)

Dec 28, 2023 – 06:03 PM EST

PDB ID : 8G50

Title : E. coli DHFR complex with NADP+ and folate: EF-X excited state model by

Laue diffraction (electric field along b axis; 8-fold extrapolation of structure

factor differences)

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Deposited on : 2023-02-10

Resolution : 1.70 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 (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: 4.02b-467

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)

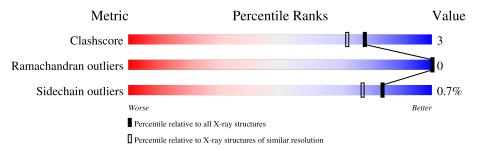
Validation Pipeline (wwPDB-VP) : 2.36

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 1.70 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	Similar resolution		
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(\mathring{A}))$		
Clashscore	141614	4695 (1.70-1.70)		
Ramachandran outliers	138981	4610 (1.70-1.70)		
Sidechain outliers	138945	4610 (1.70-1.70)		

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain	
1	A	159	94%	5% •
1	В	159	93%	7%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5828 atoms, of which 2701 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 Dihydrofolate reductase.

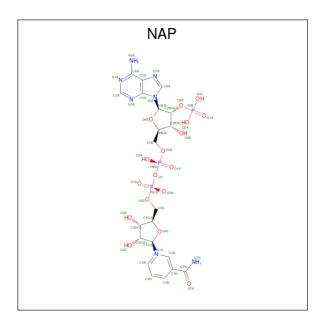
Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	A	159	Total 2642	_		N 232	O 256	S 9	0	18	0
1	В	159	Total 2676	_	H 1317	N 234	O 260	S 10	0	21	0

• Molecule 2 is FOLIC ACID (three-letter code: FOL) (formula: $C_{19}H_{19}N_7O_6$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
9	Λ	1	Total	С	Н	N	О	0	0	
2 A	1	49	19	17	7	6	0	0		
9	D	1	Total	С	Н	N	О	0	0	
	2 B	1	49	19	17	7	6	U	U	

• Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).





Mol	Chain	Residues	\mathbf{Atoms}				ZeroOcc	AltConf		
9	Λ	1	Total	С	Н	N	О	Р	0	0
3	3 A	1	73	21	25	7	17	3		0
9	D	1	Total	С	Н	N	О	Р	0	0
3 B	1	73	21	25	7	17	3	U	0	

• Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total Mn 6 6	0	0
4	В	4	Total Mn 4 4	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	125	Total O 131 131	0	9
5	В	124	Total O 125 125	0	4

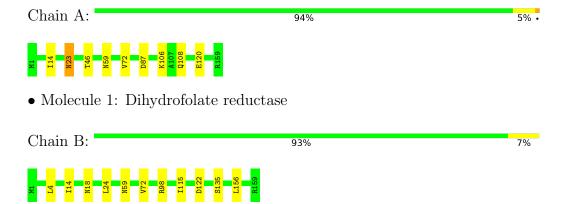


3 Residue-property plots (i)

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.

Note EDS failed to run properly.

• Molecule 1: Dihydrofolate reductase





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	34.29Å 45.53 Å 99.00 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.36 - 1.70	Depositor
% Data completeness	99.4 (41.36-1.70)	Depositor
(in resolution range)	,	-
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	0.86 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.306 , 0.350	Depositor
Wilson B-factor (A^2)	-5.1	Xtriage
Anisotropy	-0.514	Xtriage
L-test for twinning ²	$< L > = 0.53, < L^2> = 0.37$	Xtriage
Estimated twinning fraction	0.316 for h,-k,-l	Xtriage
Total number of atoms	5828	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	5.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 14.21% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: FOL, NAP, CSD, MN

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		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.45	0/1436	0.57	0/1950	
1	В	0.44	0/1462	0.58	0/1985	
All	All	0.45	0/2898	0.58	0/3935	

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 (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	1342	1300	1219	7	0
1	В	1359	1317	1226	9	0
2	A	32	17	17	0	0
2	В	32	17	17	0	0
3	A	48	25	25	2	0
3	В	48	25	25	1	0
4	A	6	0	0	0	0
4	В	4	0	0	0	0
5	A	131	0	0	1	0
5	В	125	0	0	3	0
All	All	3127	2701	2529	16	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 3.

All (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash	
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap (Å)	
1:B:98[B]:ARG:NH1	5:B:309:HOH:O	2.36	0.59	
1:A:14:ILE:O	3:A:202:NAP:H2N	2.07	0.54	
1:A:106:LYS:O	1:A:108[B]:GLN:NE2	2.43	0.52	
1:A:59:ASN:HB2	1:A:72:VAL:HG12	1.93	0.51	
1:B:59:ASN:HB2	1:B:72:VAL:HG12	1.93	0.50	
1:B:14:ILE:O	3:B:202:NAP:H2N	2.12	0.48	
1:B:122:ASP:OD2	5:B:301:HOH:O	2.20	0.48	
1:A:23:ASN:O	1:A:23:ASN:CG	2.54	0.46	
1:B:18:ASN:ND2	5:B:317:HOH:O	2.48	0.46	
1:B:24:LEU:HD12	1:B:115:ILE:HD13	1.97	0.46	
1:A:23:ASN:OD1	5:A:301:HOH:O	2.21	0.43	
1:A:46:THR:OG1	3:A:202:NAP:H6N	2.18	0.43	
1:B:135:SER:HA	1:B:156[A]:LEU:HD23	2.01	0.42	
1:B:24:LEU:HD12	1:B:115:ILE:CD1	2.49	0.42	

There are no symmetry-related clashes.

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 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	Perce	entiles
1	A	173/159 (109%)	172 (99%)	1 (1%)	0	100	100
1	В	176/159 (111%)	175 (99%)	1 (1%)	0	100	100
All	All	349/318 (110%)	347 (99%)	2 (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 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	Perce	ntiles
1	A	149/135 (110%)	147 (99%)	2 (1%)	69	56
1	В	152/135 (113%)	152 (100%)	0	100	100
All	All	301/270 (112%)	299 (99%)	2 (1%)	84	77

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	87	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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).

Г	Mol	Tuno	Chain	Res	Link	Bond lengths			В	ond ang	gles
	WIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
	1	CSD	A	152[B]	1	3,7,8	0.81	0	1,8,10	0.23	0
	1	CSD	В	152[A]	1	3,7,8	0.80	0	1,8,10	0.46	0
	1	CSD	В	152[B]	1	3,7,8	0.83	0	1,8,10	0.31	0



Mol	Type	Chain	Res	Link	Link Bond lengths		Bond angles		gles	
IVIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	A	152[A]	1	3,7,8	0.75	0	1,8,10	0.29	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
1	CSD	A	152[B]	1	-	1/2/6/8	-
1	CSD	В	152[A]	1	-	0/2/6/8	-
1	CSD	В	152[B]	1	-	1/2/6/8	-
1	CSD	A	152[A]	1	-	0/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	152[B]	CSD	CA-CB-SG-OD1
1	В	152[B]	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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	Trunc	Chain	Res	Link	Bo	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	FOL	A	201	-	34,34,34	1.14	2 (5%)	44,47,47	1.95	12 (27%)	
3	NAP	В	202	-	45,52,52	1.06	4 (8%)	56,80,80	0.92	2 (3%)	
2	FOL	В	201	-	34,34,34	1.04	2 (5%)	44,47,47	1.70	11 (25%)	
3	NAP	A	202	4	45,52,52	1.12	5 (11%)	56,80,80	1.00	2 (3%)	

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	FOL	A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	В	202	-	-	3/31/67/67	0/5/5/5
2	FOL	В	201	-	-	0/22/22/22	0/3/3/3
3	NAP	A	202	4	-	1/31/67/67	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
2	A	201	FOL	C8A-N8	-3.82	1.31	1.37
2	A	201	FOL	C4A-C4	3.65	1.47	1.41
2	В	201	FOL	C4A-C4	3.19	1.46	1.41
2	В	201	FOL	C8A-N8	-3.07	1.32	1.37
3	A	202	NAP	O4D-C1D	2.82	1.45	1.41
3	A	202	NAP	P2B-O2B	2.75	1.64	1.59
3	В	202	NAP	O4D-C1D	2.48	1.44	1.41
3	A	202	NAP	C3N-C7N	-2.13	1.47	1.50
3	В	202	NAP	C3N-C7N	-2.13	1.47	1.50
3	В	202	NAP	O4B-C1B	2.12	1.44	1.41
3	В	202	NAP	C2N-N1N	-2.08	1.32	1.35
3	A	202	NAP	C4A-N3A	-2.07	1.32	1.35
3	A	202	NAP	O4B-C1B	2.02	1.43	1.41

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	201	FOL	C4A-C4-N3	-5.27	116.22	123.43
2	A	201	FOL	C4A-C4-N3	-5.11	116.44	123.43
2	A	201	FOL	C2-N3-C4	4.41	122.93	115.93
2	A	201	FOL	C8A-C4A-C4	-4.21	117.17	119.95
2	A	201	FOL	N8-C8A-N1	4.06	120.45	115.82

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	201	FOL	C2-N3-C4	3.89	122.11	115.93
2	В	201	FOL	CT-CA-N	-3.52	102.22	110.55
2	В	201	FOL	N8-C8A-N1	3.27	119.55	115.82
2	A	201	FOL	CT-CA-N	-3.07	103.28	110.55
2	A	201	FOL	C9-C6-N5	2.85	121.72	116.66
2	A	201	FOL	CB-CA-CT	2.85	117.22	110.35
2	A	201	FOL	C2-N1-C8A	2.81	118.56	115.36
3	В	202	NAP	C3N-C7N-N7N	2.67	120.95	117.75
2	В	201	FOL	C2-N1-C8A	2.63	118.36	115.36
3	A	202	NAP	C3N-C7N-N7N	2.47	120.71	117.75
3	A	202	NAP	O7N-C7N-N7N	-2.46	119.08	122.58
2	В	201	FOL	O2-CT-O1	-2.45	118.53	124.09
2	A	201	FOL	C4-C4A-N5	2.43	121.38	118.60
2	В	201	FOL	C9-N10-C14	2.36	128.21	122.15
2	В	201	FOL	OE2-CD-CG	2.31	121.44	114.03
2	A	201	FOL	C9-N10-C14	2.28	128.00	122.15
2	A	201	FOL	N1-C2-N3	-2.25	124.23	127.22
2	A	201	FOL	O2-CT-O1	-2.19	119.11	124.09
2	В	201	FOL	C8A-C4A-C4	-2.17	118.52	119.95
2	В	201	FOL	O2-CT-CA	2.12	120.43	113.40
2	В	201	FOL	C9-C6-N5	2.04	120.29	116.66
3	В	202	NAP	O2B-C2B-C1B	-2.00	102.89	110.10

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	FOL	N-CA-CB-CG
2	A	201	FOL	CT-CA-CB-CG
3	A	202	NAP	O4D-C1D-N1N-C6N
3	В	202	NAP	C2B-O2B-P2B-O2X
3	В	202	NAP	O4D-C1D-N1N-C6N
3	В	202	NAP	PA-O3-PN-O5D

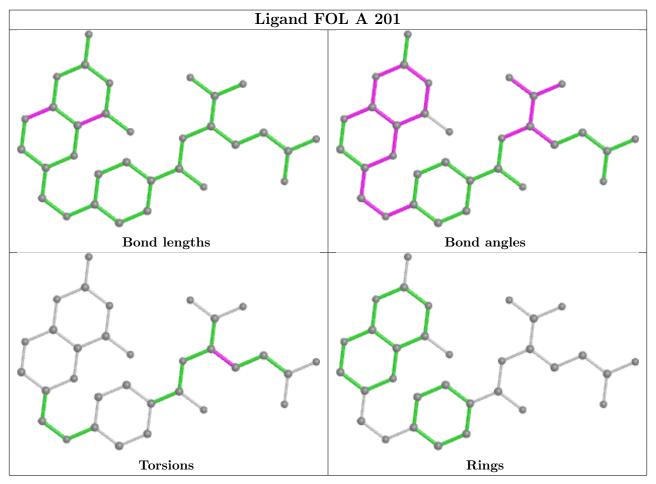
There are no ring outliers.

2 monomers are involved in 3 short contacts:

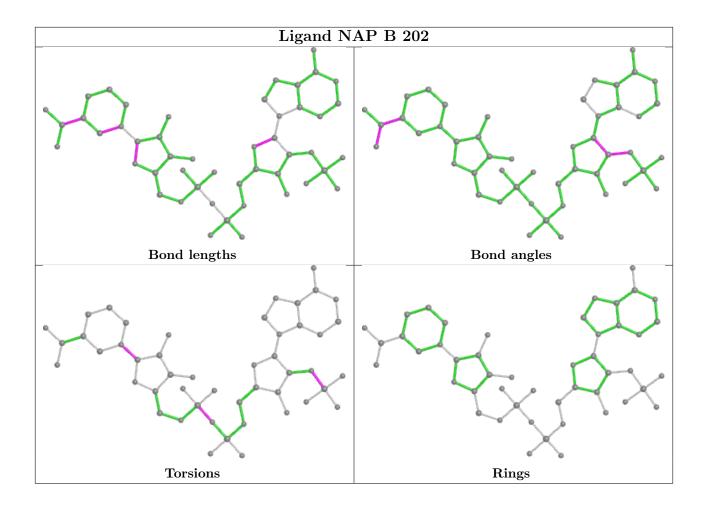
	Mol	Chain	Res	Type	Clashes	Symm-Clashes
	3	В	202	NAP	1	0
ĺ	3	A	202	NAP	2	0



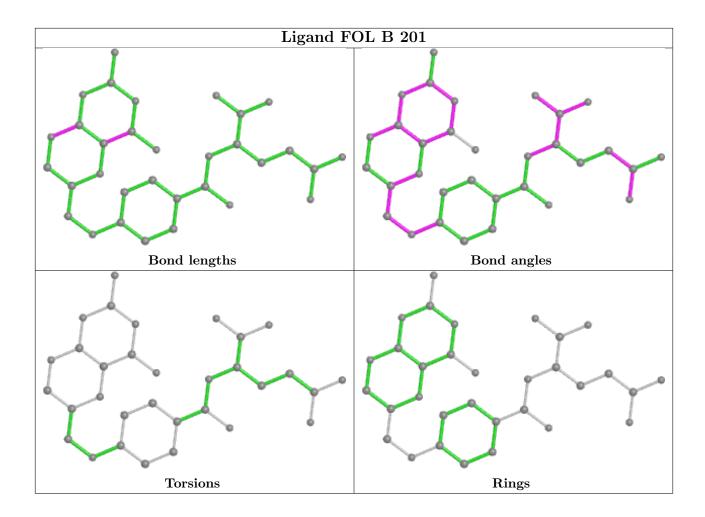
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



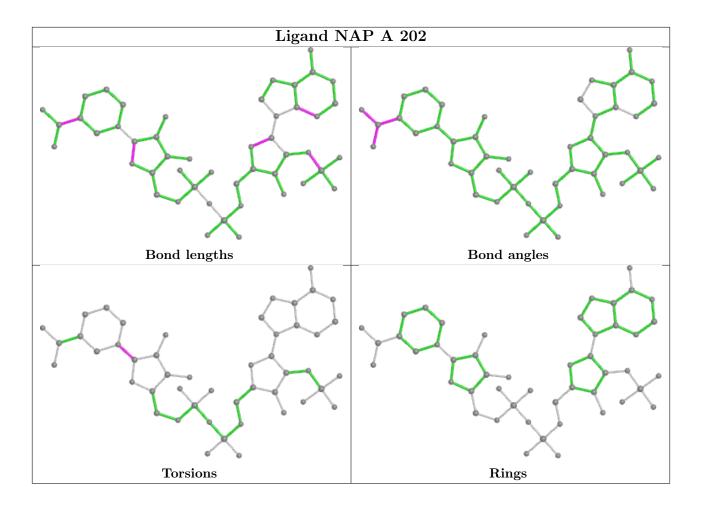












5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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

