



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2024 – 08:23 PM EST

PDB ID : 1JOL  
Title : THE CRYSTAL STRUCTURE OF THE BINARY COMPLEX BETWEEN FOLINIC ACID (LEUCOVORIN) AND E. COLI DIHYDROFOLATE REDUCTASE  
Authors : Lee, H.; Reyes, V.M.; Kraut, J.  
Deposited on : 1996-02-25  
Resolution : 1.96 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](mailto: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 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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

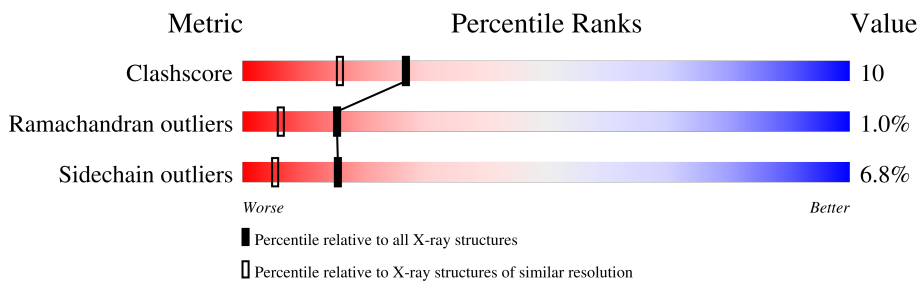
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)

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  $\geq 3$ , 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	159	
1	B	159	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3004 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 DIHYDROFOLATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	159	1246	793	211	235	7	0	0	0
1	B	159	1262	803	216	236	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	ASP	ASN	conflict	UNP P0ABQ4
B	37	ASP	ASN	conflict	UNP P0ABQ4

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is N-[4-({[(6S)-2-amino-5-formyl-4-oxo-3,4,5,6,7,8-hexahydropteridin-6-yl]methyl}amino)benzoyl]-L-glutamic acid (three-letter code: FFO) (formula: C<sub>20</sub>H<sub>23</sub>N<sub>7</sub>O<sub>7</sub>).

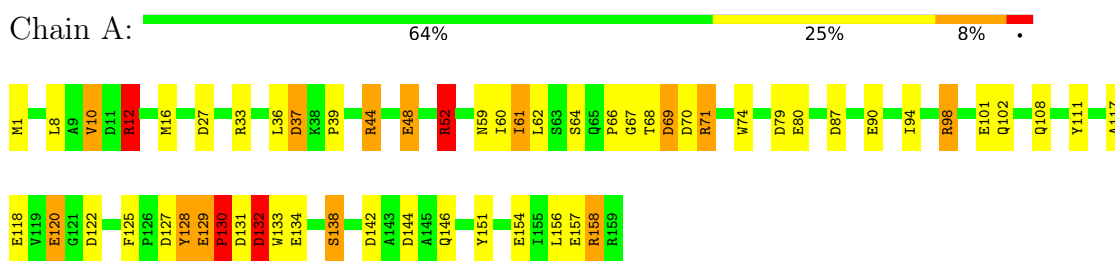


### 3 Residue-property plots [i](#)

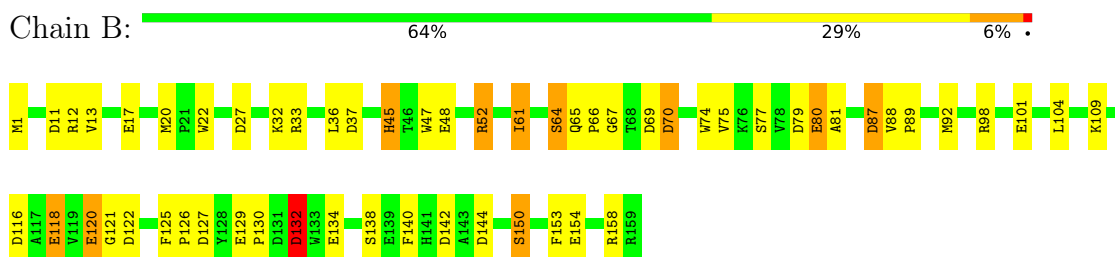
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 was not executed.

#### • Molecule 1: DIHYDROFOLATE REDUCTASE



#### • Molecule 1: DIHYDROFOLATE REDUCTASE



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.58Å 92.58Å 73.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.96	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.96)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.142 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3004	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 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: CA, CL, FFO

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	1.15	7/1279 (0.5%)	1.70	36/1740 (2.1%)
1	B	1.22	8/1296 (0.6%)	1.70	30/1762 (1.7%)
All	All	1.19	15/2575 (0.6%)	1.70	66/3502 (1.9%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	GLU	CD-OE2	7.73	1.34	1.25
1	B	134	GLU	CD-OE2	7.58	1.33	1.25
1	B	48	GLU	CD-OE2	7.48	1.33	1.25
1	B	17	GLU	CD-OE2	7.46	1.33	1.25
1	A	120	GLU	CD-OE2	7.06	1.33	1.25
1	A	90	GLU	CD-OE2	6.77	1.33	1.25
1	A	134	GLU	CD-OE2	6.35	1.32	1.25
1	A	118	GLU	CD-OE2	6.29	1.32	1.25
1	A	157	GLU	CD-OE2	6.11	1.32	1.25
1	B	120	GLU	CD-OE2	6.09	1.32	1.25
1	B	118	GLU	CD-OE2	5.97	1.32	1.25
1	B	101	GLU	CD-OE1	5.55	1.31	1.25
1	B	154	GLU	CD-OE1	5.51	1.31	1.25
1	A	48	GLU	CD-OE2	5.37	1.31	1.25
1	A	80	GLU	CD-OE1	5.27	1.31	1.25

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ASP	CB-CG-OD2	-11.28	108.15	118.30
1	B	144	ASP	CB-CG-OD1	11.14	128.33	118.30
1	B	144	ASP	CB-CG-OD2	-10.01	109.29	118.30
1	B	98	ARG	NE-CZ-NH2	-9.66	115.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	B	122	ASP	CB-CG-OD2	-8.86	110.32	118.30
1	A	12	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	B	127	ASP	CB-CG-OD2	-8.61	110.55	118.30
1	B	87	ASP	CB-CG-OD2	-8.40	110.74	118.30
1	A	128	TYR	CB-CG-CD2	8.33	126.00	121.00
1	B	158	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	B	116	ASP	CB-CG-OD2	-7.85	111.24	118.30
1	A	127	ASP	CB-CG-OD2	-7.73	111.35	118.30
1	B	37	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	B	150	SER	CB-CA-C	7.23	123.84	110.10
1	B	122	ASP	CB-CG-OD1	7.22	124.80	118.30
1	B	132	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	B	52	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	12	ARG	CD-NE-CZ	6.73	133.02	123.60
1	A	127	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	128	TYR	CB-CG-CD1	-6.64	117.01	121.00
1	A	44	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	69	ASP	CB-CG-OD1	6.55	124.20	118.30
1	A	79	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	79	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	98	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	B	27	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	B	27	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	111	TYR	CB-CG-CD2	-6.21	117.28	121.00
1	B	69	ASP	CB-CG-OD1	6.19	123.87	118.30
1	B	79	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	158	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	1	MET	CA-CB-CG	-6.10	102.93	113.30
1	B	132	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	45	HIS	CA-CB-CG	-6.09	103.24	113.60
1	B	127	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	12	ARG	CG-CD-NE	5.99	124.37	111.80
1	A	151	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	A	108	GLN	N-CA-CB	5.96	121.33	110.60
1	A	142	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	37	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	B	116	ASP	CB-CG-OD1	5.85	123.57	118.30
1	A	70	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	B	70	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	144	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	130	PRO	N-CA-CB	5.76	110.21	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	SER	CB-CA-C	5.60	120.73	110.10
1	A	122	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	27	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	79	ASP	CB-CG-OD2	-5.37	113.46	118.30
1	B	101	GLU	CA-CB-CG	-5.37	101.58	113.40
1	B	92	MET	CG-SD-CE	5.37	108.79	100.20
1	A	70	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	52	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	146	GLN	CB-CA-C	-5.21	99.98	110.40
1	A	16	MET	CG-SD-CE	5.20	108.52	100.20
1	B	120	GLU	C-N-CA	-5.20	111.39	122.30
1	A	144	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	B	109	LYS	N-CA-CB	-5.14	101.35	110.60
1	B	98	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	37	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	39	PRO	N-CA-CB	5.06	109.38	103.30
1	A	132	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	A	27	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	B	11	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	A	142	ASP	CB-CG-OD1	5.00	122.81	118.30

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	1246	0	1178	24	3
1	B	1262	0	1217	26	4
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	34	0	21	1	0
3	B	32	0	21	1	0
4	B	1	0	0	0	0
5	A	229	0	0	4	3
5	B	198	0	0	6	7

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3004	0	2437	51	9

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 10.

All (51) 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:A:66:PRO:N	5:A:508:HOH:O	2.17	0.76
1:B:150:SER:HB3	5:B:644:HOH:O	1.84	0.76
1:B:129:GLU:HB3	1:B:132:ASP:OD2	1.85	0.75
1:A:69:ASP:OD1	1:A:71:ARG:HG3	1.91	0.70
1:A:129:GLU:O	1:A:131:ASP:N	2.26	0.69
1:B:12:ARG:NH1	1:B:125:PHE:O	2.26	0.68
3:B:361:FFO:H5A	5:B:648:HOH:O	1.93	0.68
1:B:77:SER:OG	1:B:80:GLU:HG3	1.98	0.63
1:A:44:ARG:O	1:A:48:GLU:HG2	2.00	0.61
1:A:132:ASP:OD1	1:A:132:ASP:N	2.32	0.61
1:B:45:HIS:HB3	5:B:800:HOH:O	2.00	0.61
1:B:142:ASP:HA	1:B:150:SER:HB2	1.84	0.60
1:B:45:HIS:HD2	5:B:808:HOH:O	1.84	0.60
1:A:61:ILE:HD13	1:A:61:ILE:N	2.18	0.59
1:A:128:TYR:CD2	1:A:130:PRO:HD3	2.37	0.58
1:B:67:GLY:HA3	1:B:74:TRP:CD2	2.38	0.57
1:A:67:GLY:HA3	1:A:74:TRP:CD2	2.41	0.55
1:A:98:ARG:O	1:A:102:GLN:NE2	2.28	0.55
1:B:52:ARG:O	1:B:52:ARG:HG3	2.04	0.55
1:B:132:ASP:HB3	5:B:690:HOH:O	2.07	0.54
1:A:10:VAL:HG13	1:A:117:ALA:O	2.09	0.53
1:A:130:PRO:O	1:A:133:TRP:O	2.27	0.52
1:B:65:GLN:HB3	1:B:66:PRO:HD2	1.91	0.52
1:B:67:GLY:HA3	1:B:74:TRP:CE2	2.46	0.51
1:B:32:LYS:HE3	5:B:717:HOH:O	2.10	0.51
1:A:60:ILE:C	1:A:61:ILE:HD13	2.32	0.50
1:A:12:ARG:HD3	5:A:541:HOH:O	2.11	0.49
1:B:138:SER:HA	1:B:153:PHE:O	2.13	0.49
1:B:20:MET:HE3	1:B:22:TRP:CZ3	2.48	0.48
1:B:75:VAL:HG21	1:B:81:ALA:HB2	1.95	0.48
1:B:104:LEU:HD22	1:B:126:PRO:HG2	1.95	0.48
1:A:98:ARG:NH1	1:A:101:GLU:OE1	2.43	0.48
1:B:129:GLU:HB3	1:B:132:ASP:CG	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLU:HG2	1:A:156:LEU:CD1	2.43	0.47
1:B:36:LEU:HA	1:B:36:LEU:HD12	1.59	0.46
1:A:94:ILE:O	3:A:161:FFO:H7	2.16	0.46
1:A:154:GLU:HG2	1:A:156:LEU:HD11	1.97	0.46
1:A:36:LEU:O	1:A:37:ASP:HB2	2.16	0.46
1:B:47:TRP:HB2	1:B:61:ILE:HD12	1.96	0.46
1:B:20:MET:CE	1:B:22:TRP:CH2	2.99	0.45
1:B:75:VAL:HB	1:B:80:GLU:HB2	1.97	0.45
1:A:8:LEU:HD22	1:A:125:PHE:HB2	1.99	0.44
1:B:13:VAL:HG13	1:B:121:GLY:HA3	1.99	0.44
1:A:128:TYR:O	1:A:130:PRO:HD3	2.17	0.44
1:B:20:MET:HE2	1:B:22:TRP:CH2	2.53	0.44
1:B:129:GLU:HA	1:B:130:PRO:HD3	1.71	0.43
1:A:61:ILE:N	1:A:61:ILE:CD1	2.82	0.42
1:A:52:ARG:NH2	5:A:551:HOH:O	2.33	0.42
1:A:158:ARG:NH2	5:A:438:HOH:O	2.51	0.40
1:B:88:VAL:HA	1:B:89:PRO:HD3	1.82	0.40
1:A:59:ASN:HD22	1:A:59:ASN:N	2.19	0.40

All (9) 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)
1:A:64:SER:OG	5:B:799:HOH:O[3_564]	1.14	1.06
1:A:130:PRO:CB	5:A:462:HOH:O[6_655]	1.23	0.97
1:B:140:PHE:O	5:A:610:HOH:O[2_665]	1.60	0.60
1:B:64:SER:CB	5:B:786:HOH:O[6_655]	1.92	0.28
5:B:817:HOH:O	5:B:818:HOH:O[5_564]	1.95	0.25
1:B:70:ASP:OD2	5:B:789:HOH:O[5_564]	1.96	0.24
1:B:65:GLN:NE2	5:B:786:HOH:O[6_655]	2.01	0.19
1:A:64:SER:CB	5:B:799:HOH:O[3_564]	2.12	0.08
5:A:601:HOH:O	5:B:768:HOH:O[6_654]	2.15	0.05

## 5.3 Torsion angles

### 5.3.1 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	157/159 (99%)	150 (96%)	4 (2%)	3 (2%)	8	2
1	B	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
All	All	314/318 (99%)	304 (97%)	7 (2%)	3 (1%)	15	6

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	THR
1	A	130	PRO
1	A	129	GLU

### 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	Percentiles	
1	A	129/136 (95%)	118 (92%)	11 (8%)	10	3
1	B	134/136 (98%)	127 (95%)	7 (5%)	23	10
All	All	263/272 (97%)	245 (93%)	18 (7%)	16	5

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	12	ARG
1	A	33	ARG
1	A	52	ARG
1	A	61	ILE
1	A	62	LEU
1	A	71	ARG
1	A	87	ASP
1	A	120	GLU
1	A	132	ASP

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Mol	Chain	Res	Type
1	A	138	SER
1	B	1	MET
1	B	61	ILE
1	B	64	SER
1	B	87	ASP
1	B	118	GLU
1	B	120	GLU
1	B	132	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	B	124	HIS

### 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 [i](#)

Of 5 ligands modelled in this entry, 3 are 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
3	FFO	B	361	-	31,34,36	2.93	7 (22%)	33,47,50	2.96	14 (42%)
3	FFO	A	161	-	33,36,36	2.95	8 (24%)	36,50,50	2.67	15 (41%)

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	FFO	B	361	-	-	5/22/35/37	0/3/3/3
3	FFO	A	161	-	-	8/24/37/37	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	161	FFO	C7-N8	-12.78	1.33	1.46
3	B	361	FFO	C7-N8	-12.72	1.33	1.46
3	A	161	FFO	C7-C6	-6.18	1.44	1.52
3	B	361	FFO	C7-C6	-6.05	1.45	1.52
3	B	361	FFO	C15-C14	-3.59	1.33	1.39
3	A	161	FFO	C9-N10	3.45	1.52	1.45
3	A	161	FFO	C15-C14	-3.10	1.34	1.39
3	B	361	FFO	C9-N10	2.98	1.51	1.45
3	A	161	FFO	CA-N	2.96	1.52	1.45
3	A	161	FFO	CB-CG	2.89	1.61	1.52
3	B	361	FFO	CG-CB	2.57	1.65	1.51
3	B	361	FFO	C16-C11	-2.38	1.35	1.39
3	A	161	FFO	C2-N3	2.23	1.43	1.37
3	B	361	FFO	C13-C14	2.18	1.42	1.39
3	A	161	FFO	C5A-N5	-2.17	1.32	1.36

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	161	FFO	CB-CG-CD	-8.22	90.68	112.51
3	A	161	FFO	CG-CB-CA	-6.42	101.15	113.16
3	B	361	FFO	C15-C14-C13	6.42	127.82	119.03
3	B	361	FFO	NA2-C2-N1	6.15	131.71	119.73
3	B	361	FFO	C2-N1-C8A	5.75	123.82	113.43
3	B	361	FFO	C16-C15-C14	-5.48	113.97	120.30
3	B	361	FFO	N3-C2-N1	-4.93	114.12	123.32

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	161	FFO	C2-N1-C8A	4.92	122.31	113.43
3	A	161	FFO	O5B-C5A-N5	-4.67	116.69	124.63
3	B	361	FFO	O5B-C5A-N5	-4.32	117.28	124.63
3	B	361	FFO	C12-C13-C14	-4.24	115.40	120.30
3	A	161	FFO	OE2-CD-OE1	4.13	133.58	123.30
3	A	161	FFO	CT-CA-N	-3.52	102.20	110.55
3	B	361	FFO	C13-C14-N10	-3.33	114.08	120.97
3	B	361	FFO	C11-C-N	3.17	123.14	117.06
3	A	161	FFO	OE1-CD-CG	-3.02	113.39	123.08
3	B	361	FFO	O-C-C11	-2.87	115.81	120.94
3	A	161	FFO	C13-C12-C11	2.66	123.87	120.78
3	B	361	FFO	C4A-C4-N3	2.63	115.63	110.99
3	A	161	FFO	C11-C-N	2.55	121.95	117.06
3	B	361	FFO	CD-CG-CB	2.45	125.11	113.29
3	A	161	FFO	CA-N-C	2.40	127.48	121.60
3	B	361	FFO	O4-C4-C4A	-2.36	121.75	127.54
3	A	161	FFO	N3-C2-N1	-2.35	118.93	123.32
3	A	161	FFO	C4A-C4-N3	2.32	115.09	110.99
3	B	361	FFO	CB-CA-CT	-2.28	104.86	110.35
3	A	161	FFO	C12-C13-C14	-2.26	117.69	120.30
3	A	161	FFO	C9-N10-C14	-2.15	116.58	122.14
3	A	161	FFO	C16-C11-C12	-2.13	115.55	118.59

There are no chirality outliers.

All (13) torsion outliers are listed below:

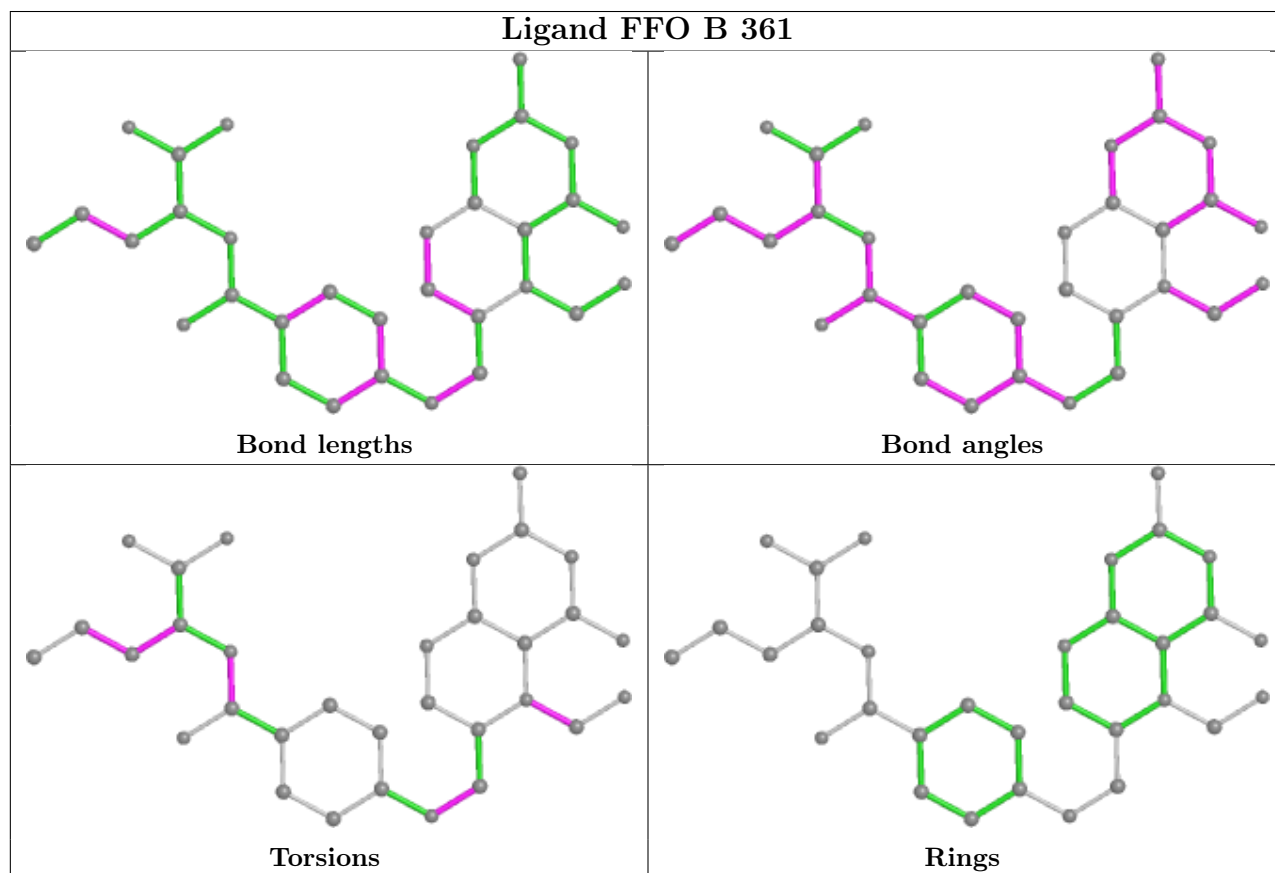
Mol	Chain	Res	Type	Atoms
3	A	161	FFO	O5B-C5A-N5-C4A
3	A	161	FFO	O5B-C5A-N5-C6
3	A	161	FFO	N-CA-CB-CG
3	B	361	FFO	O5B-C5A-N5-C6
3	A	161	FFO	CT-CA-CB-CG
3	B	361	FFO	O-C-N-CA
3	A	161	FFO	CA-CB-CG-CD
3	B	361	FFO	CA-CB-CG-CD
3	B	361	FFO	N-CA-CB-CG
3	A	161	FFO	OE1-CD-CG-CB
3	A	161	FFO	C6-C9-N10-C14
3	B	361	FFO	C6-C9-N10-C14
3	A	161	FFO	OE2-CD-CG-CB

There are no ring outliers.

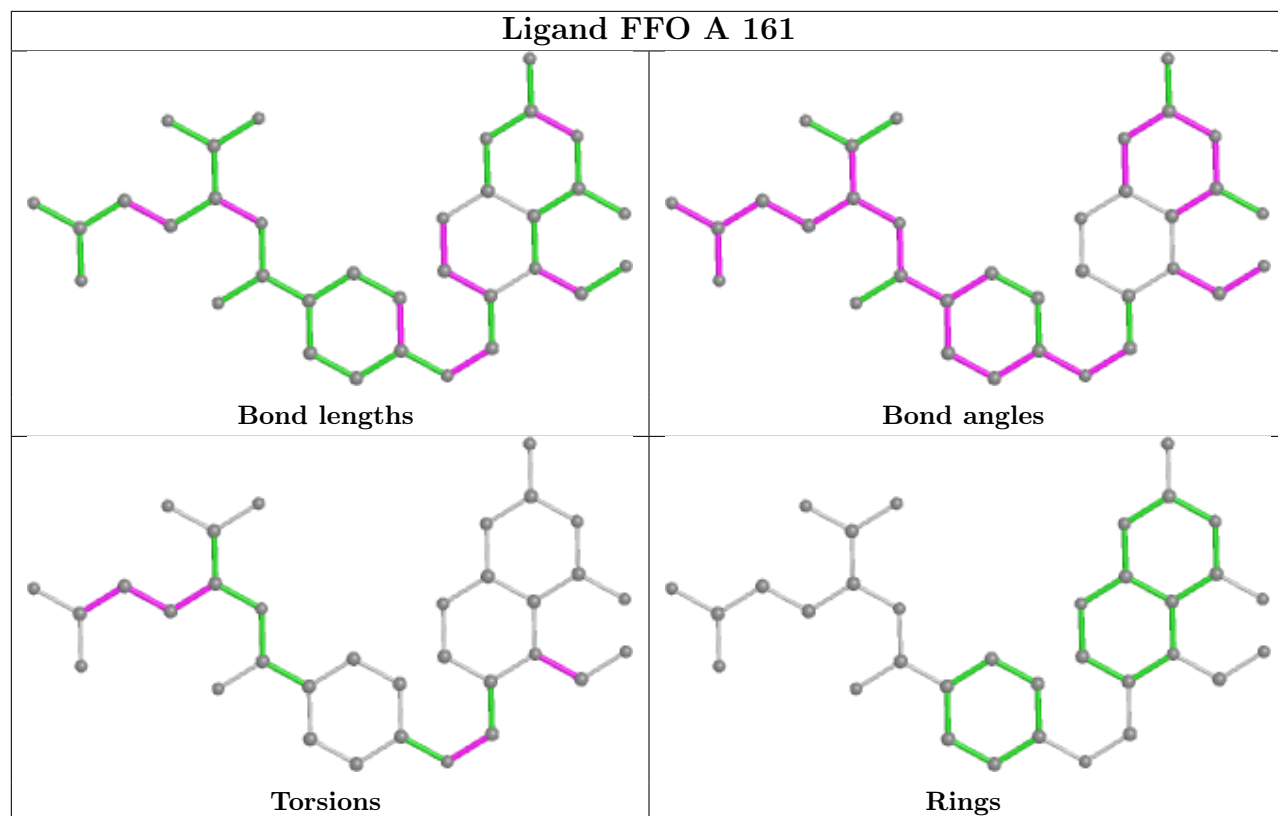
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	361	FFO	1	0
3	A	161	FFO	1	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.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.