Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 08:56 pm BST

PDB ID	:	2CD2
Title	:	LIGAND INDUCED CONFORMATIONAL CHANGES IN THE CRYSTAL STRUCTURES OF PNEUMOCYSTIS CARINII DIHYDROFOLATE REDUCTASE COMPLEXES WITH FOLATE AND NADP+
Authors	:	Cody, V.; Galitsky, N.; Rak, D.; Luft, J.; Pangborn, W.; Queener, S.
Deposited on	:	1999-03-15
Resolution	:	1.90 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:

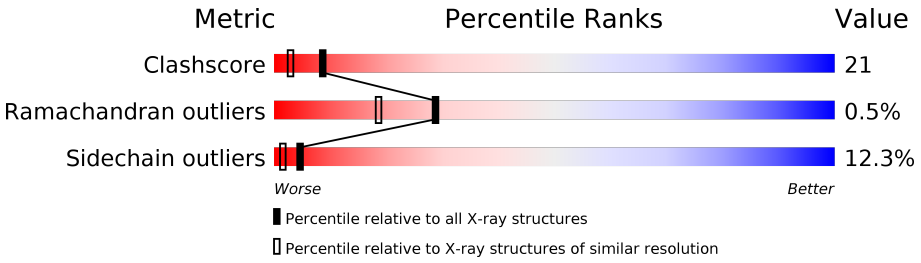
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.90 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	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 on 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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	206	53% 37% 9% .

2 Entry composition (i)

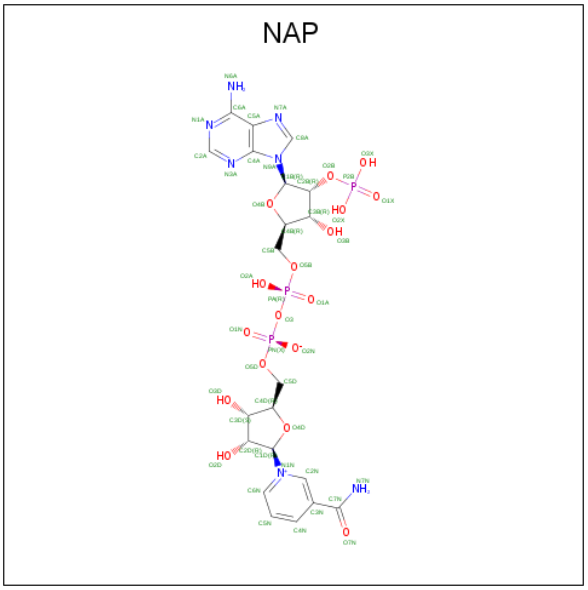
There are 4 unique types of molecules in this entry. The entry contains 1841 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

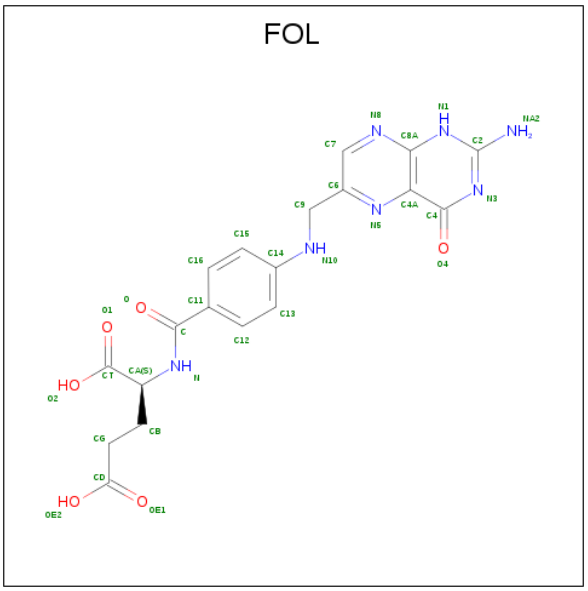
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	206	1686	1086	288	305	7	0	0	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0

- Molecule 3 is FOLIC ACID (three-letter code: FOL) (formula: $C_{19}H_{19}N_7O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 32 19 7 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	75	Total O 75 75	0	0

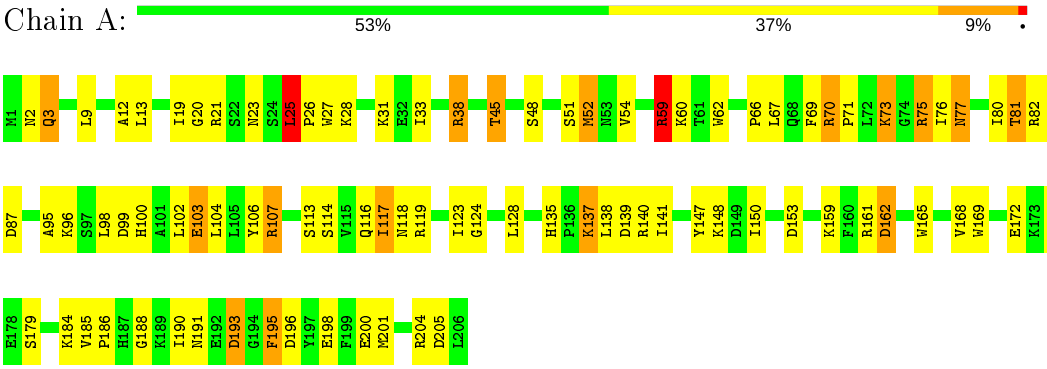
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	37.30Å 43.15Å 61.15Å 90.00° 94.77° 90.00°	Depositor
Resolution (Å)	8.00 – 1.90	Depositor
% Data completeness (in resolution range)	97.4 (8.00-1.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.196 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1841	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.89	1/1728 (0.1%)	1.95	47/2330 (2.0%)

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	LYS	C-N	6.63	1.45	1.33

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	140	ARG	NE-CZ-NH1	21.26	130.93	120.30
1	A	59	ARG	NE-CZ-NH2	15.16	127.88	120.30
1	A	176	ASP	CB-CA-C	12.81	136.02	110.40
1	A	107	ARG	NE-CZ-NH1	-11.61	114.49	120.30
1	A	205	ASP	CB-CG-OD1	11.37	128.53	118.30
1	A	204	ARG	NE-CZ-NH1	-11.31	114.64	120.30
1	A	119	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	A	140	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	A	38	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	A	161	ARG	CD-NE-CZ	8.30	135.22	123.60
1	A	162	ASP	CB-CG-OD1	8.16	125.65	118.30
1	A	139	ASP	CB-CG-OD1	7.93	125.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	12	ALA	N-CA-CB	7.84	121.07	110.10
1	A	153	ASP	CB-CG-OD2	7.68	125.21	118.30
1	A	59	ARG	NE-CZ-NH1	-7.61	116.50	120.30
1	A	162	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	A	124	GLY	C-N-CA	7.42	137.88	122.30
1	A	147	TYR	CB-CG-CD2	-7.28	116.63	121.00
1	A	103	GLU	CB-CG-CD	7.01	133.13	114.20
1	A	176	ASP	CB-CG-OD1	-6.98	112.02	118.30
1	A	184	LYS	CB-CA-C	6.92	124.23	110.40
1	A	198	GLU	CG-CD-OE2	-6.80	104.69	118.30
1	A	103	GLU	OE1-CD-OE2	6.67	131.30	123.30
1	A	147	TYR	CB-CG-CD1	6.50	124.90	121.00
1	A	70	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	A	95	ALA	CB-CA-C	6.49	119.84	110.10
1	A	107	ARG	CD-NE-CZ	-6.47	114.53	123.60
1	A	75	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	193	ASP	CB-CG-OD1	-6.07	112.84	118.30
1	A	75	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	176	ASP	OD1-CG-OD2	5.99	134.68	123.30
1	A	25	LEU	CA-CB-CG	5.89	128.86	115.30
1	A	161	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	140	ARG	NH1-CZ-NH2	-5.79	113.03	119.40
1	A	70	ARG	CD-NE-CZ	-5.76	115.54	123.60
1	A	200	GLU	CG-CD-OE2	-5.62	107.05	118.30
1	A	176	ASP	CB-CG-OD2	-5.58	113.27	118.30
1	A	196	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	21	ARG	CD-NE-CZ	-5.54	115.85	123.60
1	A	140	ARG	CD-NE-CZ	5.48	131.28	123.60
1	A	172	GLU	CG-CD-OE2	5.45	129.20	118.30
1	A	175	SER	C-N-CA	-5.41	108.18	121.70
1	A	87	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	196	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	A	59	ARG	CD-NE-CZ	-5.17	116.37	123.60
1	A	38	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
1	A	198	GLU	OE1-CD-OE2	5.01	129.31	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	73	LYS	Mainchain

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	1686	0	1693	70	0
2	A	48	0	25	10	0
3	A	32	0	17	3	0
4	A	75	0	0	5	0
All	All	1841	0	1735	72	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 21.

All (72) 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:81:THR:HG22	2:A:207:NAP:O2X	1.51	1.10
1:A:59:ARG:HH11	1:A:59:ARG:HG2	1.28	0.99
1:A:165:TRP:HE3	1:A:168:VAL:HG11	1.28	0.98
1:A:59:ARG:NH1	1:A:59:ARG:HG2	1.83	0.89
1:A:83:ASN:HB2	4:A:255:HOH:O	1.71	0.89
1:A:84:GLU:OE1	1:A:84:GLU:O	1.96	0.82
1:A:165:TRP:CE3	1:A:168:VAL:HG11	2.15	0.80
1:A:186:PRO:HB2	1:A:190:ILE:HD11	1.66	0.78
1:A:81:THR:CG2	2:A:207:NAP:O2X	2.32	0.75
1:A:45:THR:O	1:A:48:SER:HB2	1.87	0.74
1:A:52:MET:HG2	1:A:76:ILE:HG13	1.71	0.72
1:A:135:HIS:HD2	1:A:137:LYS:H	1.39	0.69
1:A:82:ARG:HG3	2:A:207:NAP:H2A	1.75	0.68
1:A:3:GLN:HG3	1:A:137:LYS:HG3	1.74	0.68
1:A:59:ARG:NH1	1:A:59:ARG:CG	2.50	0.68
1:A:117:ILE:N	1:A:117:ILE:HD13	2.11	0.65
1:A:165:TRP:HE3	1:A:168:VAL:CG1	2.08	0.63
1:A:107:ARG:NE	4:A:273:HOH:O	2.33	0.60
1:A:38:ARG:HH21	1:A:185:VAL:HG22	1.67	0.59
1:A:26:PRO:HG2	1:A:27:TRP:CE3	2.37	0.59
1:A:3:GLN:HB3	1:A:102:LEU:HD13	1.84	0.58
1:A:165:TRP:O	1:A:168:VAL:HG12	2.04	0.58
1:A:135:HIS:CD2	1:A:137:LYS:H	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASP:OD1	1:A:135:HIS:HE1	1.87	0.58
1:A:3:GLN:CG	1:A:137:LYS:HG3	2.35	0.56
1:A:70:ARG:HA	1:A:71:PRO:C	2.25	0.56
1:A:174:HIS:HD2	4:A:218:HOH:O	1.88	0.56
2:A:207:NAP:H4N	3:A:307:FOL:C7	2.35	0.56
1:A:19:ILE:O	2:A:207:NAP:H2N	2.05	0.56
1:A:103:GLU:HG3	1:A:104:LEU:N	2.22	0.54
1:A:60:LYS:NZ	4:A:266:HOH:O	2.37	0.54
1:A:2:ASN:HD21	1:A:99:ASP:HB3	1.73	0.54
1:A:69:PHE:CD1	3:A:307:FOL:HG2	2.43	0.53
1:A:62:TRP:CE2	1:A:70:ARG:HD3	2.43	0.53
1:A:59:ARG:HH12	2:A:207:NAP:P2B	2.32	0.51
1:A:159:LYS:NZ	1:A:162:ASP:OD2	2.43	0.51
1:A:104:LEU:C	1:A:104:LEU:HD23	2.32	0.50
1:A:23:ASN:OD1	2:A:207:NAP:H3D	2.12	0.50
1:A:80:ILE:O	2:A:207:NAP:H1B	2.10	0.50
1:A:38:ARG:NH2	1:A:185:VAL:HG22	2.26	0.50
1:A:107:ARG:NH2	4:A:273:HOH:O	2.19	0.50
1:A:116:GLN:C	1:A:117:ILE:HD13	2.32	0.50
1:A:59:ARG:HG3	1:A:60:LYS:N	2.27	0.50
1:A:185:VAL:HG13	1:A:186:PRO:HD2	1.94	0.49
1:A:150:ILE:HD11	1:A:195:PHE:CE2	2.47	0.49
1:A:168:VAL:HG13	1:A:169:TRP:N	2.28	0.49
1:A:185:VAL:CG1	1:A:186:PRO:HD2	2.43	0.48
1:A:86:LEU:HD12	1:A:86:LEU:C	2.33	0.48
1:A:177:LEU:HD13	1:A:201:MET:HB2	1.95	0.47
1:A:123:ILE:O	3:A:307:FOL:H7	2.15	0.47
1:A:100:HIS:O	1:A:103:GLU:HG3	2.15	0.46
1:A:25:LEU:HD12	1:A:27:TRP:CD1	2.52	0.45
1:A:66:PRO:HB2	1:A:69:PHE:HD2	1.81	0.45
1:A:62:TRP:HH2	1:A:71:PRO:HG3	1.81	0.45
1:A:3:GLN:HA	1:A:106:TYR:HE2	1.81	0.45
1:A:54:VAL:HG22	1:A:76:ILE:HB	1.99	0.44
1:A:159:LYS:CB	1:A:159:LYS:NZ	2.80	0.44
1:A:148:LYS:HG2	1:A:150:ILE:HG13	1.98	0.44
1:A:59:ARG:NH1	2:A:207:NAP:P2B	2.91	0.44
1:A:75:ARG:O	1:A:77:ASN:ND2	2.50	0.44
1:A:86:LEU:C	1:A:86:LEU:CD1	2.87	0.43
1:A:191:ASN:HA	1:A:195:PHE:O	2.18	0.42
1:A:20:GLY:HA2	1:A:26:PRO:HD3	2.01	0.42
1:A:77:ASN:N	1:A:77:ASN:HD22	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LEU:HD13	1:A:128:LEU:HD11	2.01	0.42
2:A:207:NAP:H71N	2:A:207:NAP:H2N	1.60	0.42
1:A:100:HIS:O	1:A:103:GLU:CG	2.68	0.42
1:A:138:LEU:HD13	1:A:138:LEU:C	2.39	0.42
1:A:51:SER:HB3	1:A:118:ASN:HB2	2.02	0.42
1:A:62:TRP:CZ2	1:A:70:ARG:HD3	2.55	0.41
1:A:9:LEU:HD22	1:A:141:ILE:HG23	2.03	0.41
1:A:168:VAL:HG13	1:A:169:TRP:H	1.86	0.40

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	Percentiles
1	A	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	29 18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	GLY

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	187/187 (100%)	164 (88%)	23 (12%)	4 1

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	13	LEU
1	A	25	LEU
1	A	28	LYS
1	A	31	LYS
1	A	33	ILE
1	A	45	THR
1	A	52	MET
1	A	59	ARG
1	A	67	LEU
1	A	77	ASN
1	A	81	THR
1	A	84	GLU
1	A	85	SER
1	A	86	LEU
1	A	96	LYS
1	A	113	SER
1	A	114	SER
1	A	117	ILE
1	A	137	LYS
1	A	179	SER
1	A	193	ASP
1	A	195	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	3	GLN
1	A	127	GLN
1	A	135	HIS
1	A	151	HIS
1	A	174	HIS
1	A	187	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates 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	$\#\|Z\| > 2$
3	FOL	A	307	-	28,34,34	1.16	4 (14%)	36,47,47	2.80	16 (44%)
2	NAP	A	207	-	45,52,52	3.16	19 (42%)	56,80,80	2.48	20 (35%)

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	FOL	A	307	-	-	2/16/22/22	0/3/3/3
2	NAP	A	207	-	-	2/31/67/67	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	207	NAP	O4B-C4B	-9.57	1.23	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	207	NAP	C4N-C3N	8.62	1.54	1.39
2	A	207	NAP	P2B-O2B	7.49	1.73	1.59
2	A	207	NAP	C5N-C4N	5.72	1.51	1.38
2	A	207	NAP	C2N-N1N	5.30	1.41	1.35
2	A	207	NAP	O4D-C1D	4.72	1.47	1.41
2	A	207	NAP	C3B-C4B	4.32	1.64	1.53
2	A	207	NAP	C6A-C5A	3.75	1.57	1.43
2	A	207	NAP	C5A-C4A	-3.68	1.31	1.40
2	A	207	NAP	O3B-C3B	3.14	1.50	1.43
3	A	307	FOL	C4-C4A	2.90	1.46	1.41
2	A	207	NAP	C2N-C3N	-2.90	1.34	1.39
2	A	207	NAP	C6N-C5N	-2.67	1.32	1.38
2	A	207	NAP	PN-O1N	-2.55	1.41	1.50
3	A	307	FOL	O4-C4	2.51	1.30	1.24
2	A	207	NAP	O4D-C4D	2.38	1.50	1.45
2	A	207	NAP	C6N-N1N	2.30	1.41	1.35
2	A	207	NAP	P2B-O2X	-2.23	1.46	1.54
2	A	207	NAP	PA-O5B	2.23	1.68	1.59
3	A	307	FOL	C2-NA2	-2.21	1.29	1.33
2	A	207	NAP	O4B-C1B	2.08	1.44	1.41
3	A	307	FOL	C8A-N8	-2.05	1.34	1.37
2	A	207	NAP	C8A-N7A	-2.04	1.31	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	307	FOL	C2-N1-C8A	8.35	124.89	115.36
2	A	207	NAP	C5N-C4N-C3N	-7.81	111.11	120.34
3	A	307	FOL	N1-C2-N3	-6.18	118.98	127.22
2	A	207	NAP	O3B-C3B-C4B	-5.78	94.34	111.05
2	A	207	NAP	C2N-C3N-C4N	5.62	124.62	118.26
3	A	307	FOL	C4-C4A-C8A	-5.41	116.37	119.95
2	A	207	NAP	N6A-C6A-N1A	5.01	128.98	118.57
3	A	307	FOL	CA-N-C	4.61	128.28	122.34
3	A	307	FOL	N8-C8A-N1	4.52	120.98	115.82
2	A	207	NAP	O3X-P2B-O2X	4.42	124.53	107.64
2	A	207	NAP	C3N-C7N-N7N	-4.07	112.86	117.75
2	A	207	NAP	C5A-C6A-N6A	-4.02	114.24	120.35
2	A	207	NAP	C4A-C5A-N7A	3.92	113.48	109.40
2	A	207	NAP	O7N-C7N-N7N	3.60	127.69	122.58
3	A	307	FOL	C15-C14-C13	-3.30	114.52	119.03
2	A	207	NAP	PN-O3-PA	3.27	144.04	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	207	NAP	C3N-C2N-N1N	-3.25	117.25	120.43
3	A	307	FOL	CB-CG-CD	-3.24	106.63	113.59
2	A	207	NAP	C5B-C4B-C3B	-3.09	103.59	115.18
3	A	307	FOL	NA2-C2-N1	3.08	122.81	117.79
3	A	307	FOL	C12-C13-C14	2.72	123.44	120.30
3	A	307	FOL	C7-N8-C8A	-2.70	113.98	116.69
2	A	207	NAP	O5B-PA-O1A	-2.63	98.80	109.07
3	A	307	FOL	C4A-C8A-N1	-2.62	117.41	121.80
2	A	207	NAP	C2B-C3B-C4B	-2.59	96.37	101.99
3	A	307	FOL	C4-C4A-N5	2.58	121.55	118.60
3	A	307	FOL	C15-C14-N10	2.50	126.16	120.97
3	A	307	FOL	C6-C7-N8	2.45	125.53	123.13
2	A	207	NAP	C6N-C5N-C4N	2.44	122.98	119.44
3	A	307	FOL	CG-CB-CA	-2.41	108.17	113.04
2	A	207	NAP	O5D-C5D-C4D	-2.41	100.70	108.99
2	A	207	NAP	O4B-C1B-C2B	-2.38	102.46	106.59
3	A	307	FOL	C4-N3-C2	2.25	119.50	115.93
2	A	207	NAP	O2B-P2B-O1X	-2.23	100.77	109.39
2	A	207	NAP	C3B-C2B-C1B	-2.20	98.74	102.89
2	A	207	NAP	O3B-C3B-C2B	2.13	117.22	111.17

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	307	FOL	CT-CA-CB-CG
2	A	207	NAP	O4D-C1D-N1N-C6N
2	A	207	NAP	PA-O3-PN-O5D
3	A	307	FOL	N-CA-CB-CG

There are no ring outliers.

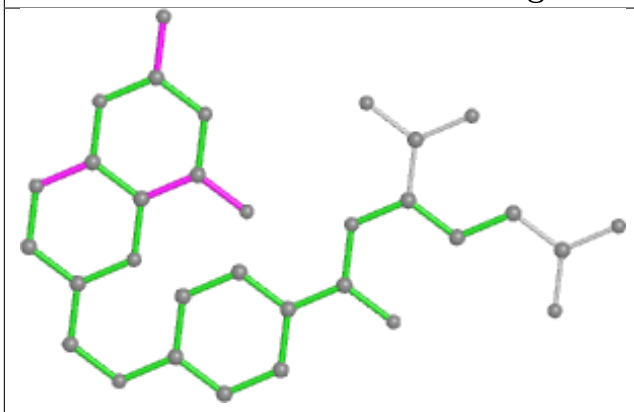
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	307	FOL	3	0
2	A	207	NAP	10	0

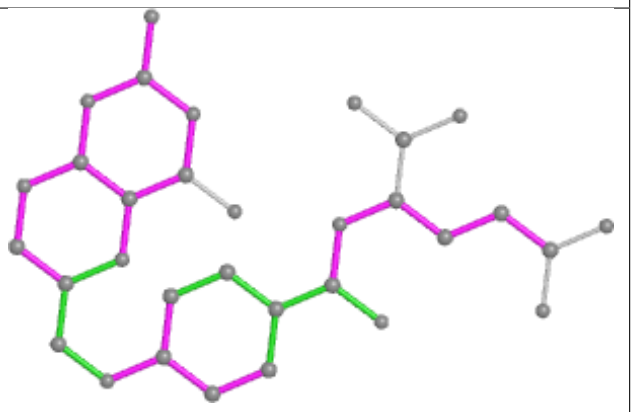
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

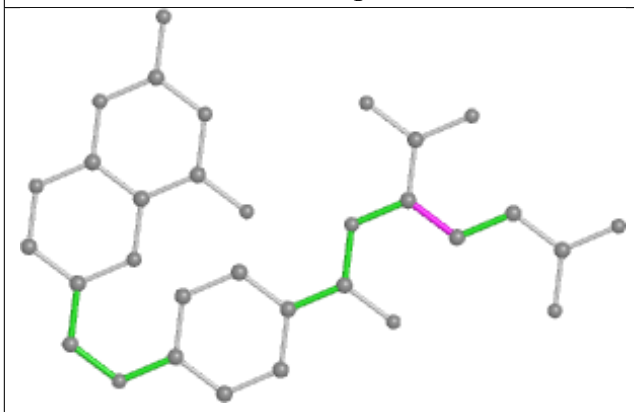
Ligand FOL A 307



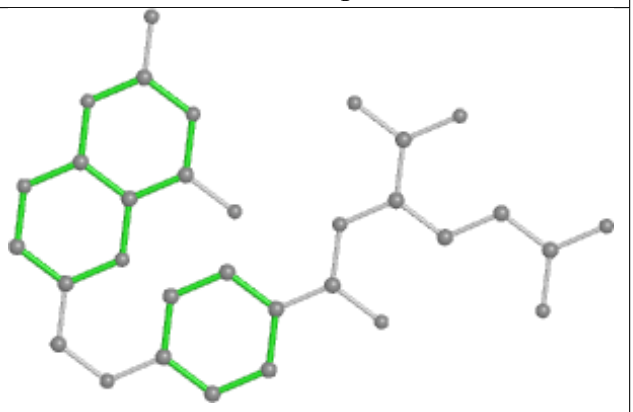
Bond lengths



Bond angles

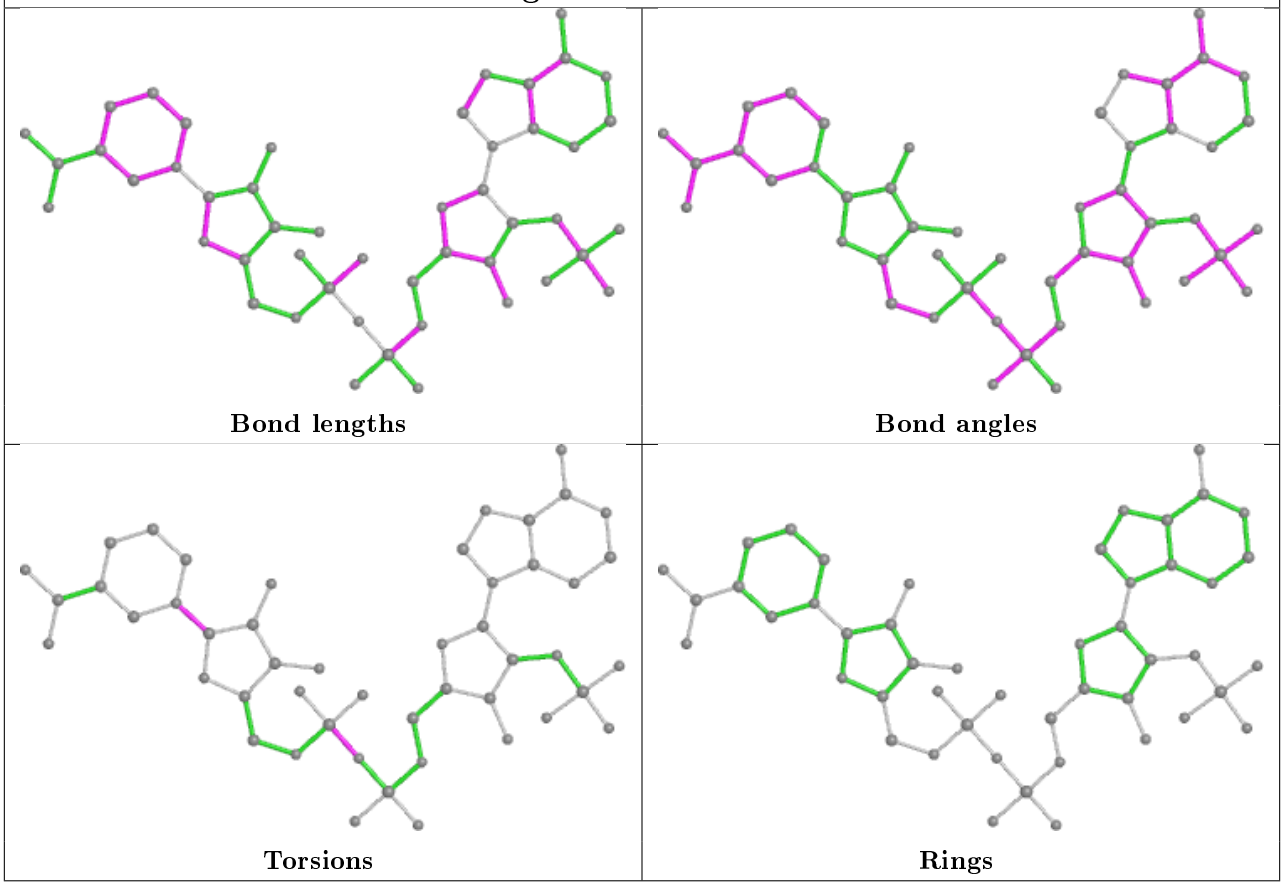


Torsions



Rings

Ligand NAP A 207



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.