



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:08 AM UTC

PDB ID : 2CD2 / pdb_00002cd2
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

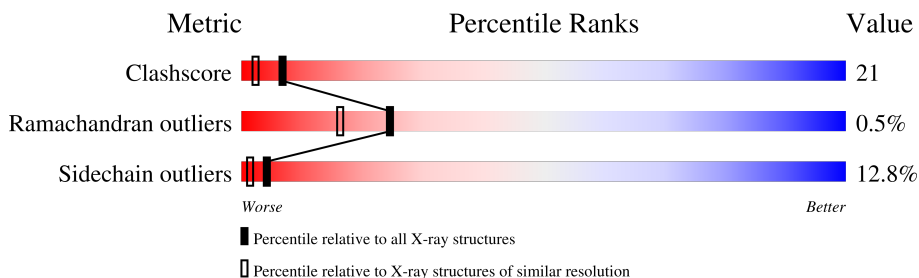
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	206	 44% 42% 12% .

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 (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

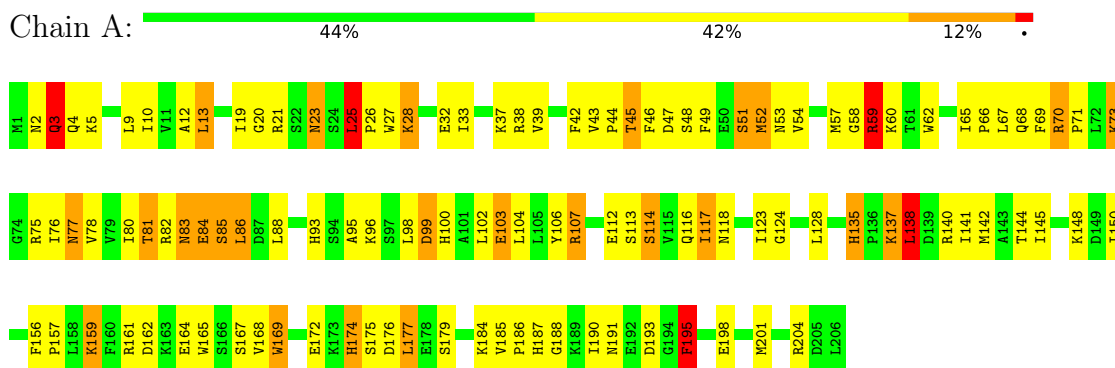
- Molecule 3 is FOLIC ACID (CCD ID: FOL) (formula: C₁₉H₁₉N₇O₆).

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



4 Data and refinement statistics

Xtrriage (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.	Xtrriage
Total number of atoms	1841	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: 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	1.12	2/1728 (0.1%)	2.23	83/2330 (3.6%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	LYS	C-N	8.14	1.45	1.33
1	A	144	THR	CA-CB	5.49	1.60	1.53

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ASP	CB-CA-C	13.10	136.02	109.95
1	A	103	GLU	CB-CG-CD	12.08	133.13	112.60
1	A	47	ASP	CA-CB-CG	9.74	122.34	112.60
1	A	59	ARG	NE-CZ-NH2	9.64	127.88	119.20
1	A	140	ARG	NE-CZ-NH1	9.43	130.93	121.50
1	A	124	GLY	CA-C-N	8.99	137.88	121.70
1	A	124	GLY	C-N-CA	8.99	137.88	121.70
1	A	85	SER	N-CA-C	-8.48	101.05	111.40
1	A	184	LYS	CB-CA-C	8.03	124.23	109.46
1	A	161	ARG	CD-NE-CZ	7.73	135.22	124.40
1	A	184	LYS	N-CA-C	-7.50	99.37	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	SER	N-CA-C	7.49	121.37	110.28
1	A	193	ASP	N-CA-C	7.47	121.82	111.74
1	A	78	VAL	CA-C-O	-7.09	112.70	120.43
1	A	174	HIS	CA-CB-CG	-7.06	106.74	113.80
1	A	107	ARG	CD-NE-CZ	-7.05	114.53	124.40
1	A	195	PHE	CA-CB-CG	7.01	120.81	113.80
1	A	177	LEU	N-CA-C	-7.01	103.57	111.14
1	A	107	ARG	NE-CZ-NH1	-7.01	114.49	121.50
1	A	175	SER	CA-C-N	-6.87	108.18	121.58
1	A	175	SER	C-N-CA	-6.87	108.18	121.58
1	A	204	ARG	NE-CZ-NH1	-6.86	114.64	121.50
1	A	49	PHE	N-CA-C	6.63	119.07	111.11
1	A	70	ARG	N-CA-C	6.63	120.16	110.14
1	A	23	ASN	CA-CB-CG	-6.58	106.02	112.60
1	A	12	ALA	N-CA-CB	6.56	121.07	110.77
1	A	193	ASP	N-CA-CB	-6.54	102.26	112.13
1	A	4	GLN	CB-CG-CD	6.52	123.69	112.60
1	A	99	ASP	CA-CB-CG	-6.40	106.20	112.60
1	A	95	ALA	CA-C-N	6.37	129.99	120.31
1	A	95	ALA	C-N-CA	6.37	129.99	120.31
1	A	57	MET	CA-C-N	6.34	128.63	120.64
1	A	57	MET	C-N-CA	6.34	128.63	120.64
1	A	42	PHE	N-CA-C	6.33	119.40	109.96
1	A	70	ARG	CD-NE-CZ	-6.33	115.54	124.40
1	A	39	VAL	O-C-N	6.29	128.07	121.91
1	A	83	ASN	OD1-CG-ND2	6.27	128.87	122.60
1	A	114	SER	N-CA-C	-6.25	104.00	111.69
1	A	25	LEU	N-CA-C	-6.25	102.18	109.93
1	A	156	PHE	CA-C-O	-6.14	113.66	119.80
1	A	21	ARG	CD-NE-CZ	-6.11	115.85	124.40
1	A	10	ILE	CA-C-O	6.06	126.75	120.39
1	A	145	ILE	O-C-N	6.04	130.31	122.94
1	A	59	ARG	CA-C-O	-6.00	114.70	121.00
1	A	5	LYS	N-CA-C	5.99	118.44	110.53
1	A	37	LYS	CA-C-N	5.97	128.53	120.65
1	A	37	LYS	C-N-CA	5.97	128.53	120.65
1	A	157	PRO	N-CA-C	5.96	121.31	113.86
1	A	198	GLU	CG-CD-OE2	-5.96	104.69	118.40
1	A	169	TRP	O-C-N	5.95	130.00	123.27
1	A	93	HIS	CA-C-O	5.93	128.72	121.72
1	A	95	ALA	CA-C-O	5.93	127.41	120.89
1	A	167	SER	N-CA-C	-5.83	106.17	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	GLU	CA-C-O	-5.79	114.36	120.55
1	A	59	ARG	CD-NE-CZ	-5.74	116.37	124.40
1	A	13	LEU	CA-C-O	-5.70	114.96	121.40
1	A	187	HIS	CA-C-O	-5.66	115.27	121.89
1	A	49	PHE	CA-CB-CG	-5.63	108.17	113.80
1	A	28	LYS	CB-CA-C	-5.62	101.78	111.23
1	A	46	PHE	CA-CB-CG	-5.62	108.18	113.80
1	A	13	LEU	O-C-N	5.56	129.90	123.17
1	A	3	GLN	CA-C-O	5.48	127.15	120.25
1	A	25	LEU	CB-CA-C	5.46	117.28	109.26
1	A	65	ILE	O-C-N	5.45	127.32	121.10
1	A	112	GLU	CB-CG-CD	5.37	121.73	112.60
1	A	172	GLU	CA-C-O	-5.35	115.41	121.72
1	A	53	ASN	N-CA-CB	5.32	119.05	110.85
1	A	44	PRO	CA-C-N	5.31	128.78	120.82
1	A	44	PRO	C-N-CA	5.31	128.78	120.82
1	A	95	ALA	CB-CA-C	5.29	119.84	110.16
1	A	47	ASP	O-C-N	5.22	130.12	122.39
1	A	43	VAL	O-C-N	5.22	127.05	121.10
1	A	58	GLY	N-CA-C	-5.17	105.68	112.82
1	A	37	LYS	O-C-N	-5.14	116.67	122.12
1	A	138	LEU	CB-CA-C	5.08	118.61	110.29
1	A	135	HIS	CB-CA-C	5.07	117.62	109.41
1	A	4	GLN	CB-CA-C	5.07	119.45	111.39
1	A	156	PHE	CA-CB-CG	-5.06	108.74	113.80
1	A	85	SER	CA-C-O	5.05	125.96	120.55
1	A	21	ARG	CA-CB-CG	-5.03	104.03	114.10
1	A	164	GLU	CB-CG-CD	5.02	121.13	112.60
1	A	3	GLN	N-CA-CB	5.01	118.72	110.90
1	A	59	ARG	NE-CZ-NH1	-5.00	116.50	121.50

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	73	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	75	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 (75) 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:HG2	1:A:59:ARG:NH1	1.83	0.89
1:A:83:ASN:HB2	4:A:255:HOH:O	1.71	0.89
1:A:84:GLU:O	1:A:84:GLU:OE1	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:70:ARG:HA	1:A:71:PRO:C	2.25	0.61
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
1:A:99:ASP:OD1	1:A:135:HIS:HE1	1.87	0.58
1:A:142:MET:HE1	1:A:177:LEU:CD1	2.34	0.57
1:A:3:GLN:CG	1:A:137:LYS:HG3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:104:LEU:HD23	1:A:104:LEU:C	2.32	0.55
1:A:116:GLN:C	1:A:117:ILE:HD13	2.32	0.55
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:103:GLU:HG3	1:A:104:LEU:N	2.22	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:86:LEU:HD12	1:A:86:LEU:C	2.33	0.52
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: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: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:C	1:A:86:LEU:CD1	2.87	0.47
1:A:123:ILE:O	3:A:307:FOL:H7	2.15	0.47
1:A:177:LEU:HD13	1:A:201:MET:HB2	1.95	0.47
1:A:138:LEU:C	1:A:138:LEU:HD13	2.39	0.46
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:NZ	1:A:159:LYS:CB	2.80	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:148:LYS:HG2	1:A:150:ILE:HG13	1.98	0.44
1:A:9:LEU:C	1:A:9:LEU:HD23	2.44	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
1:A:98:LEU:HD13	1:A:128:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:207:NAP:H2N	2:A:207:NAP:H71N	1.60	0.42
1:A:100:HIS:O	1:A:103:GLU:CG	2.68	0.42
1:A:51:SER:HB3	1:A:118:ASN:HB2	2.02	0.42
1:A:66:PRO:C	1:A:68:GLN:N	2.77	0.41
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%)	24 16

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%)	163 (87%)	24 (13%)	4 1

All (24) 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	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	88	LEU
1	A	96	LYS
1	A	113	SER
1	A	114	SER
1	A	117	ILE
1	A	137	LYS
1	A	138	LEU
1	A	159	LYS
1	A	179	SER
1	A	195	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) 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	174	HIS
1	A	187	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	NAP	A	207	-	50,52,52	3.40	22 (44%)	71,80,80	2.50	25 (35%)
3	FOL	A	307	-	34,34,34	1.38	5 (14%)	43,47,47	2.16	19 (44%)

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	NAP	A	207	-	-	3/35/67/67	0/5/5/5
3	FOL	A	307	-	-	4/22/22/22	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	207	NAP	C4N-C3N	9.66	1.54	1.39
2	A	207	NAP	O4B-C4B	-9.62	1.23	1.45
2	A	207	NAP	P2B-O2B	7.94	1.73	1.59
2	A	207	NAP	C5N-C4N	7.06	1.51	1.38
2	A	207	NAP	C2N-N1N	5.86	1.41	1.35
2	A	207	NAP	C5A-C6A	5.83	1.57	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	207	NAP	O4D-C1D	5.16	1.47	1.40
2	A	207	NAP	PA-O3	-4.84	1.54	1.59
2	A	207	NAP	C5A-C4A	-4.43	1.31	1.39
2	A	207	NAP	C3B-C4B	4.35	1.64	1.53
3	A	307	FOL	O4-C4	4.34	1.30	1.23
2	A	207	NAP	C5A-N7A	3.94	1.46	1.39
3	A	307	FOL	C4-N3	-3.48	1.31	1.38
2	A	207	NAP	C4A-N9A	-3.39	1.30	1.37
2	A	207	NAP	O3B-C3B	3.00	1.50	1.43
3	A	307	FOL	OE1-CD	2.87	1.31	1.22
2	A	207	NAP	C6N-C5N	-2.85	1.32	1.38
2	A	207	NAP	C2N-C3N	-2.83	1.34	1.39
2	A	207	NAP	PN-O1N	-2.58	1.41	1.50
2	A	207	NAP	C6A-N1A	-2.56	1.28	1.35
2	A	207	NAP	C6N-N1N	2.50	1.41	1.35
2	A	207	NAP	O4D-C4D	2.39	1.50	1.45
2	A	207	NAP	P2B-O2X	-2.30	1.46	1.54
2	A	207	NAP	PA-O5B	2.28	1.68	1.59
3	A	307	FOL	C8A-N1	-2.17	1.35	1.38
2	A	207	NAP	O2B-C2B	-2.04	1.37	1.44
3	A	307	FOL	C2-NA2	-2.00	1.29	1.34

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	207	NAP	C5N-C4N-C3N	-9.42	111.11	120.36
3	A	307	FOL	OE2-CD-OE1	-6.20	107.37	123.33
2	A	207	NAP	O3B-C3B-C4B	-5.83	94.34	111.08
2	A	207	NAP	C4D-O4D-C1D	-5.69	104.71	109.92
2	A	207	NAP	C2N-C3N-C4N	5.47	124.62	118.26
3	A	307	FOL	C8A-C4A-C4	-4.92	116.37	119.56
2	A	207	NAP	N6A-C6A-N1A	4.76	128.98	118.38
2	A	207	NAP	O3X-P2B-O2X	4.46	124.53	107.80
2	A	207	NAP	O2A-PA-O3	4.02	118.13	107.27
2	A	207	NAP	C3N-C7N-N7N	-3.96	112.86	117.74
2	A	207	NAP	C5A-C6A-N6A	-3.65	114.24	123.29
2	A	207	NAP	O7N-C7N-N7N	3.51	127.69	122.62
2	A	207	NAP	C4A-N9A-C8A	3.48	109.39	105.74
3	A	307	FOL	C15-C14-C13	-3.41	114.52	119.04
2	A	207	NAP	C4B-O4B-C1B	3.37	116.91	109.47
3	A	307	FOL	OE2-CD-CG	3.35	124.58	114.00
2	A	207	NAP	C5B-C4B-C3B	-3.23	103.59	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	307	FOL	N1-C8A-N8	3.09	120.98	116.38
2	A	207	NAP	C5A-N7A-C8A	-3.03	98.68	103.45
3	A	307	FOL	O2-CT-O1	2.90	130.67	124.08
3	A	307	FOL	NA2-C2-N1	2.87	122.81	116.77
2	A	207	NAP	O4B-C1B-N9A	2.84	113.55	108.09
2	A	207	NAP	C6N-N1N-C1D	-2.81	114.21	119.73
3	A	307	FOL	CA-N-C	2.80	128.28	121.56
3	A	307	FOL	C12-C13-C14	2.73	123.44	120.30
3	A	307	FOL	CG-CB-CA	-2.71	108.17	113.16
2	A	207	NAP	C2B-C3B-C4B	-2.61	96.37	101.99
2	A	207	NAP	O5B-PA-O1A	-2.56	98.80	108.94
2	A	207	NAP	C4A-C5A-N7A	2.54	113.48	110.58
3	A	307	FOL	C6-C7-N8	2.49	125.53	123.14
2	A	207	NAP	C6N-C5N-C4N	2.45	122.98	119.45
2	A	207	NAP	O5D-C5D-C4D	-2.44	100.70	108.99
2	A	207	NAP	O2B-P2B-O1X	-2.40	100.77	109.33
2	A	207	NAP	O4B-C1B-C2B	-2.40	102.46	106.59
3	A	307	FOL	N1-C2-N3	-2.37	118.98	123.32
3	A	307	FOL	O1-CT-CA	-2.32	114.79	122.26
3	A	307	FOL	C15-C14-N10	2.30	126.16	120.96
3	A	307	FOL	C4A-C8A-N1	-2.23	117.41	120.13
3	A	307	FOL	CB-CG-CD	-2.20	106.63	112.49
2	A	207	NAP	O3B-C3B-C2B	2.16	117.22	111.19
3	A	307	FOL	O4-C4-N3	-2.14	116.98	120.23
2	A	207	NAP	C3B-C2B-C1B	-2.12	98.74	102.81
3	A	307	FOL	C16-C11-C12	-2.12	115.88	118.57
3	A	307	FOL	C15-C16-C11	2.00	122.94	120.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

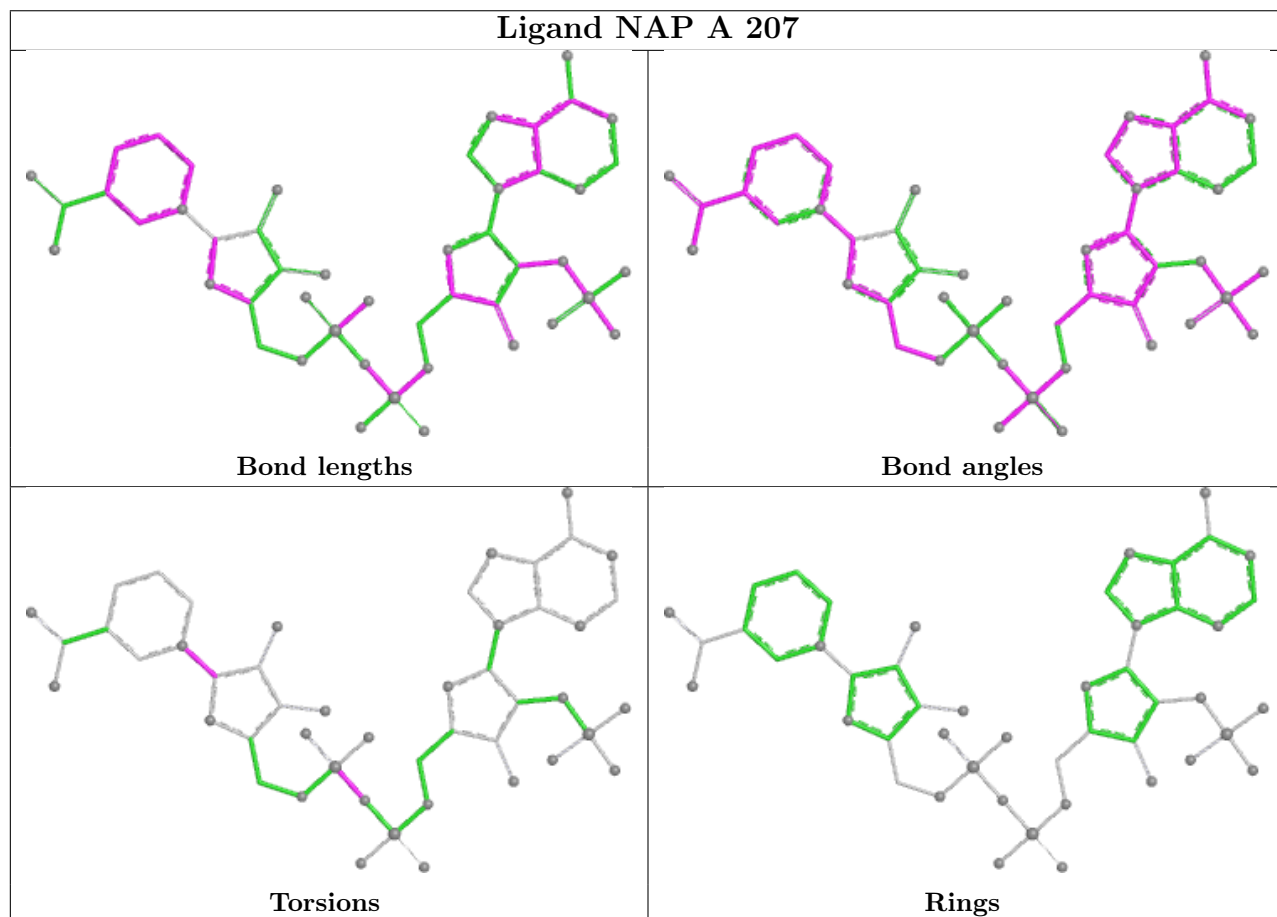
Mol	Chain	Res	Type	Atoms
2	A	207	NAP	O4D-C1D-N1N-C6N
3	A	307	FOL	CT-CA-CB-CG
2	A	207	NAP	PA-O3-PN-O5D
3	A	307	FOL	N-CA-CB-CG
3	A	307	FOL	OE2-CD-CG-CB
3	A	307	FOL	OE1-CD-CG-CB
2	A	207	NAP	O4D-C1D-N1N-C2N

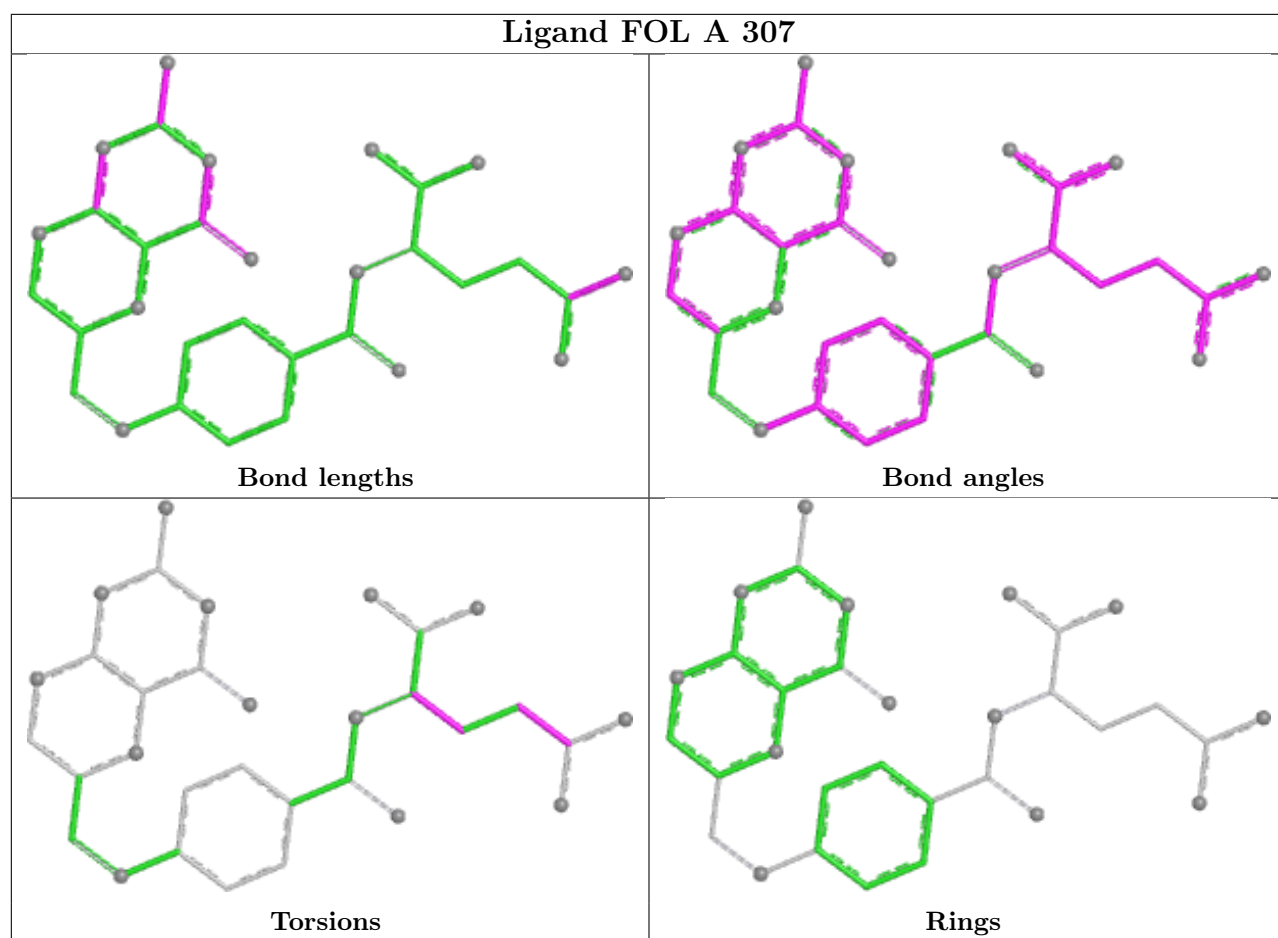
There are no ring outliers.

2 monomers are involved in 12 short contacts:

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