



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:35 PM UTC

PDB ID : 1PD8 / pdb_00001pd8
Title : Analysis of Three Crystal Structure Determinations of a 5-Methyl-6-N-Methyl-5,6,7,8-tetrahydro-2H-pyrido[4,3-b]pyrimidin-2-one Antifolate Complex with Human Dihydrofolate Reductase
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Deposited on : 2003-05-19
Resolution : 2.10 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)
Xtriage (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

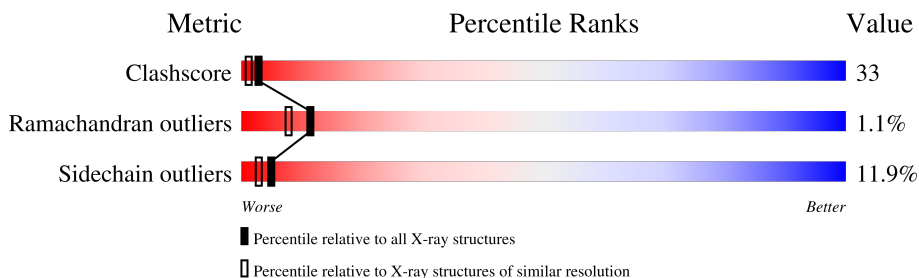
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	186	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CO4	A	301	X	-	X	-

2 Entry composition [i](#)

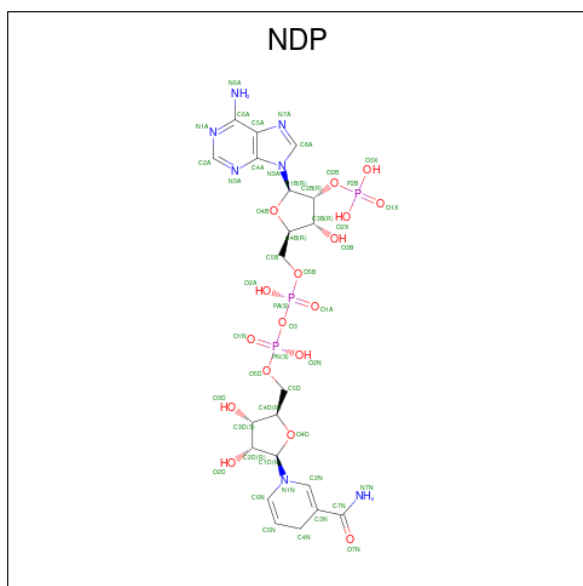
There are 4 unique types of molecules in this entry. The entry contains 1645 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

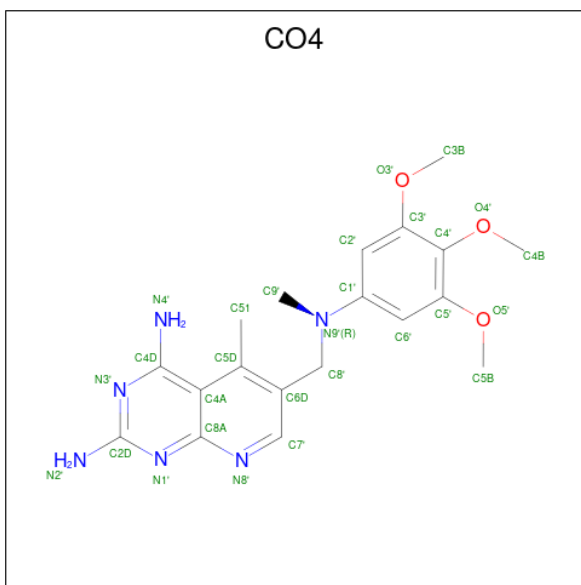
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1502	963	253	279	7	0	0	0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

- Molecule 3 is 2,4-DIAMINO-5-METHYL-6-[(3,4,5-TRIMETHOXY-N-METHYLANILINO) METHYL]PYRIDO[2,3-D]PYRIMIDINE (CCD ID: CO4) (formula: C₁₉H₂₄N₆O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	19	6	3		

- Molecule 4 is water.

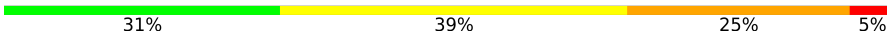
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	67	Total O 67 67	0	0

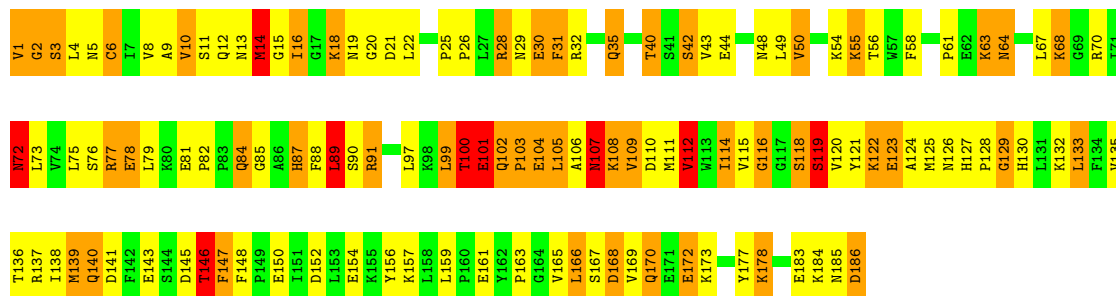
3 Residue-property plots

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 was not executed.

• Molecule 1: Dihydrofolate reductase

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	85.87Å 85.87Å 77.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.10	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.173 , 0.197	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1645	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: NDP, CO4

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	1.29	2/1537 (0.1%)	2.79	161/2073 (7.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	MET	C-N	-5.78	1.28	1.33
1	A	40	THR	CA-CB	5.53	1.61	1.53

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	GLY	CA-C-O	-12.74	112.01	122.33
1	A	12	GLN	CG-CD-NE2	-12.04	98.33	116.40
1	A	48	ASN	CA-CB-CG	11.77	124.36	112.60
1	A	22	LEU	CA-C-O	-11.45	109.57	119.76
1	A	126	ASN	CA-CB-CG	11.16	123.76	112.60
1	A	87	HIS	CA-C-O	-10.80	107.04	119.24
1	A	35	GLN	CB-CG-CD	10.57	130.57	112.60
1	A	70	ARG	NE-CZ-NH2	-10.00	110.20	119.20
1	A	12	GLN	CB-CG-CD	-9.60	96.28	112.60
1	A	68	LYS	CA-CB-CG	9.35	132.79	114.10
1	A	82	PRO	CB-CA-C	-9.29	102.66	111.39
1	A	88	PHE	O-C-N	9.17	133.69	123.33
1	A	109	VAL	N-CA-C	9.12	121.72	108.58
1	A	12	GLN	OE1-CD-NE2	9.10	131.69	122.60
1	A	161	GLU	CA-C-O	9.02	130.94	121.28
1	A	119	SER	O-C-N	8.69	132.39	122.22
1	A	141	ASP	CA-CB-CG	-8.63	103.97	112.60
1	A	118	SER	O-C-N	8.41	130.84	122.09
1	A	32	ARG	CD-NE-CZ	8.39	136.14	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	GLN	OE1-CD-NE2	8.34	130.94	122.60
1	A	50	VAL	N-CA-CB	8.15	121.73	111.46
1	A	84	GLN	OE1-CD-NE2	8.14	130.75	122.60
1	A	137	ARG	NE-CZ-NH2	8.02	126.42	119.20
1	A	186	ASP	CA-CB-CG	-8.01	104.59	112.60
1	A	35	GLN	CG-CD-OE1	7.97	136.74	120.80
1	A	22	LEU	O-C-N	7.89	129.78	121.42
1	A	127	HIS	N-CA-C	-7.88	99.63	109.64
1	A	128	PRO	CB-CA-C	7.75	121.40	110.17
1	A	19	ASN	OD1-CG-ND2	7.66	130.26	122.60
1	A	140	GLN	O-C-N	7.54	131.17	123.26
1	A	25	PRO	CB-CA-C	7.45	120.01	110.92
1	A	107	ASN	N-CA-CB	-7.43	98.79	110.46
1	A	91	ARG	CA-C-O	-7.38	111.08	119.79
1	A	78	GLU	CG-CD-OE1	7.34	135.29	118.40
1	A	148	PHE	CA-C-O	-7.31	114.05	120.19
1	A	16	ILE	CB-CA-C	7.30	118.51	110.62
1	A	10	VAL	CB-CA-C	-7.30	99.27	110.50
1	A	90	SER	N-CA-CB	7.24	124.15	111.55
1	A	140	GLN	N-CA-CB	7.15	122.47	111.46
1	A	168	ASP	CB-CA-C	7.04	121.42	109.80
1	A	58	PHE	CA-CB-CG	-7.03	106.77	113.80
1	A	3	SER	CA-C-O	-6.99	113.51	121.19
1	A	157	LYS	CA-C-O	-6.93	112.87	120.43
1	A	138	ILE	N-CA-C	-6.91	96.95	107.73
1	A	109	VAL	N-CA-CB	-6.88	103.22	110.72
1	A	165	VAL	CA-C-O	-6.78	113.02	120.48
1	A	120	VAL	O-C-N	6.78	128.95	121.90
1	A	143	GLU	CA-CB-CG	6.77	127.63	114.10
1	A	112	VAL	CB-CA-C	6.76	120.90	110.83
1	A	2	GLY	CA-C-N	6.74	130.28	120.71
1	A	2	GLY	C-N-CA	6.74	130.28	120.71
1	A	56	THR	CA-CB-OG1	-6.73	99.51	109.60
1	A	123	GLU	CA-CB-CG	-6.68	100.74	114.10
1	A	64	ASN	CA-CB-CG	-6.66	105.94	112.60
1	A	82	PRO	CA-C-O	-6.64	116.12	120.90
1	A	135	VAL	CA-C-O	-6.63	113.45	120.48
1	A	140	GLN	CB-CG-CD	-6.63	101.33	112.60
1	A	102	GLN	N-CA-C	-6.62	101.78	110.39
1	A	129	GLY	O-C-N	6.62	129.13	122.85
1	A	35	GLN	CG-CD-NE2	-6.61	106.48	116.40
1	A	172	GLU	CG-CD-OE2	-6.60	103.21	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	ARG	CA-C-O	6.60	127.50	120.70
1	A	105	LEU	N-CA-CB	-6.59	99.33	110.41
1	A	15	GLY	CA-C-O	-6.58	114.79	120.98
1	A	137	ARG	NE-CZ-NH1	-6.49	115.01	121.50
1	A	138	ILE	CA-CB-CG1	6.47	121.40	110.40
1	A	72	ASN	CA-CB-CG	6.42	119.02	112.60
1	A	165	VAL	O-C-N	6.36	129.79	122.99
1	A	88	PHE	CA-C-O	-6.36	113.87	120.99
1	A	169	VAL	CB-CA-C	6.36	121.95	111.59
1	A	129	GLY	N-CA-C	-6.35	103.83	112.52
1	A	18	LYS	CA-CB-CG	-6.31	101.48	114.10
1	A	16	ILE	N-CA-C	-6.29	107.11	113.47
1	A	121	TYR	O-C-N	6.26	128.52	122.07
1	A	68	LYS	N-CA-CB	6.26	119.17	109.97
1	A	178	LYS	CA-C-N	6.26	131.01	122.19
1	A	178	LYS	C-N-CA	6.26	131.01	122.19
1	A	157	LYS	CB-CA-C	-6.24	99.45	109.75
1	A	122	LYS	N-CA-CB	6.23	119.41	110.06
1	A	8	VAL	N-CA-C	6.18	116.41	107.88
1	A	115	VAL	N-CA-C	6.02	117.89	112.17
1	A	159	LEU	N-CA-C	-5.96	102.54	109.93
1	A	78	GLU	CG-CD-OE2	-5.93	104.75	118.40
1	A	166	LEU	CA-C-N	5.92	132.07	121.66
1	A	166	LEU	C-N-CA	5.92	132.07	121.66
1	A	107	ASN	CA-C-O	5.91	126.21	119.18
1	A	30	GLU	N-CA-C	-5.90	104.93	111.36
1	A	163	PRO	CA-C-N	5.87	131.58	121.07
1	A	163	PRO	C-N-CA	5.87	131.58	121.07
1	A	30	GLU	CG-CD-OE1	5.85	131.85	118.40
1	A	35	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	A	21	ASP	N-CA-CB	-5.82	102.08	110.87
1	A	103	PRO	N-CA-C	-5.81	106.48	113.98
1	A	91	ARG	O-C-N	5.77	130.06	122.33
1	A	135	VAL	O-C-N	5.74	129.21	123.18
1	A	91	ARG	CA-CB-CG	-5.74	102.62	114.10
1	A	148	PHE	N-CA-C	-5.72	102.87	110.07
1	A	64	ASN	CA-C-O	-5.69	112.55	119.43
1	A	125	MET	O-C-N	5.68	129.99	122.43
1	A	31	PHE	CB-CA-C	-5.68	99.76	110.67
1	A	161	GLU	CG-CD-OE2	-5.64	105.42	118.40
1	A	170	GLN	N-CA-CB	5.64	119.36	110.56
1	A	14	MET	CA-C-N	5.62	126.39	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	MET	C-N-CA	5.62	126.39	120.43
1	A	147	PHE	CA-CB-CG	-5.62	108.18	113.80
1	A	140	GLN	CB-CA-C	-5.59	100.21	111.17
1	A	107	ASN	CA-C-N	5.58	133.52	121.64
1	A	107	ASN	C-N-CA	5.58	133.52	121.64
1	A	44	GLU	N-CA-C	5.57	118.52	110.28
1	A	73	LEU	CA-C-O	-5.55	114.16	120.32
1	A	100	THR	CA-C-N	5.53	133.36	122.31
1	A	100	THR	C-N-CA	5.53	133.36	122.31
1	A	114	ILE	N-CA-CB	-5.51	104.71	111.00
1	A	89	LEU	CA-C-O	-5.51	114.20	120.32
1	A	25	PRO	N-CA-C	-5.50	103.99	110.70
1	A	101	GLU	CB-CA-C	-5.50	100.19	110.36
1	A	42	SER	CA-CB-OG	-5.48	100.13	111.10
1	A	40	THR	N-CA-C	5.47	118.11	109.96
1	A	85	GLY	CA-C-O	-5.46	113.66	119.55
1	A	167	SER	CA-C-N	-5.41	112.90	122.74
1	A	167	SER	C-N-CA	-5.41	112.90	122.74
1	A	107	ASN	CA-CB-CG	5.40	118.00	112.60
1	A	150	GLU	CB-CG-CD	5.39	121.77	112.60
1	A	78	GLU	CA-C-O	-5.38	113.31	119.60
1	A	40	THR	CA-CB-OG1	-5.37	101.54	109.60
1	A	11	SER	O-C-N	5.36	129.25	122.65
1	A	9	ALA	N-CA-C	-5.36	100.45	109.07
1	A	123	GLU	N-CA-C	5.36	118.98	112.23
1	A	99	LEU	CA-C-N	5.35	127.40	120.44
1	A	99	LEU	C-N-CA	5.35	127.40	120.44
1	A	159	LEU	CB-CA-C	5.34	117.12	109.26
1	A	31	PHE	N-CA-CB	5.32	118.53	110.28
1	A	82	PRO	O-C-N	5.32	123.76	121.31
1	A	120	VAL	CA-C-O	-5.32	115.15	121.05
1	A	177	TYR	CA-C-O	-5.31	115.60	121.33
1	A	139	MET	N-CA-C	5.30	122.10	110.80
1	A	87	HIS	N-CA-CB	5.29	117.63	110.59
1	A	73	LEU	O-C-N	5.29	129.49	123.31
1	A	6	CYS	O-C-N	5.28	130.10	123.23
1	A	152	ASP	CA-C-O	-5.28	114.95	121.02
1	A	146	THR	CB-CA-C	5.27	120.11	109.68
1	A	81	GLU	O-C-N	5.25	125.07	121.71
1	A	90	SER	O-C-N	5.25	129.98	123.15
1	A	90	SER	N-CA-C	-5.23	101.41	109.52
1	A	72	ASN	CB-CG-ND2	5.20	124.21	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	GLU	CB-CA-C	-5.20	99.22	109.67
1	A	172	GLU	OE1-CD-OE2	5.19	135.36	122.90
1	A	14	MET	N-CA-CB	-5.17	104.72	113.15
1	A	120	VAL	CB-CA-C	5.16	118.78	112.02
1	A	79	LEU	CA-C-O	-5.14	115.40	121.16
1	A	122	LYS	CA-C-O	-5.13	115.08	120.63
1	A	3	SER	O-C-N	5.10	129.14	122.87
1	A	161	GLU	CB-CG-CD	5.09	121.26	112.60
1	A	9	ALA	CA-C-O	-5.08	114.84	120.38
1	A	48	ASN	CB-CG-ND2	5.08	124.02	116.40
1	A	107	ASN	CB-CG-ND2	5.06	123.99	116.40
1	A	42	SER	CA-C-N	5.05	131.06	121.97
1	A	42	SER	C-N-CA	5.05	131.06	121.97
1	A	49	LEU	CA-C-O	-5.02	114.96	120.43
1	A	123	GLU	OE1-CD-OE2	5.01	134.92	122.90
1	A	108	LYS	N-CA-C	5.01	119.41	112.45

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	1502	0	1511	93	1
2	A	48	0	26	12	0
3	A	28	0	24	10	0
4	A	67	0	0	9	1
All	All	1645	0	1561	103	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 33.

All (103) 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:102:GLN:O	1:A:106:ALA:HB2	1.48	1.11
3:A:301:CO4:C4B	3:A:301:CO4:O3'	2.15	0.95
1:A:105:LEU:HA	1:A:108:LYS:HD2	1.48	0.93
1:A:26:PRO:O	1:A:173:LYS:HE3	1.70	0.91
1:A:107:ASN:ND2	1:A:107:ASN:H	1.66	0.90
1:A:40:THR:HG22	4:A:247:HOH:O	1.71	0.89
1:A:139:MET:HE1	1:A:178:LYS:HD3	1.54	0.89
3:A:301:CO4:O3'	3:A:301:CO4:H4B3	1.74	0.88
1:A:139:MET:CE	1:A:178:LYS:HD3	2.06	0.86
1:A:72:ASN:H	1:A:87:HIS:HD2	1.21	0.84
2:A:300:NDP:H42N	3:A:301:CO4:H512	1.60	0.83
1:A:111:MET:HE1	4:A:213:HOH:O	1.81	0.80
1:A:55:LYS:HD3	4:A:226:HOH:O	1.81	0.80
1:A:55:LYS:HD2	2:A:300:NDP:H51N	1.64	0.78
1:A:28:ARG:HH12	1:A:173:LYS:NZ	1.85	0.74
1:A:184:LYS:HA	4:A:234:HOH:O	1.87	0.73
1:A:1:VAL:HG22	1:A:109:VAL:HG12	1.70	0.73
3:A:301:CO4:H4'2	3:A:301:CO4:H513	1.53	0.72
1:A:107:ASN:H	1:A:107:ASN:HD22	1.35	0.71
1:A:91:ARG:O	2:A:300:NDP:H2A	1.90	0.71
1:A:72:ASN:H	1:A:87:HIS:CD2	2.08	0.71
1:A:139:MET:HE3	1:A:178:LYS:CD	2.21	0.70
1:A:186:ASP:OD1	1:A:186:ASP:C	2.34	0.70
1:A:99:LEU:HG	1:A:105:LEU:HD12	1.74	0.69
1:A:139:MET:CE	1:A:178:LYS:CD	2.70	0.68
1:A:102:GLN:O	1:A:106:ALA:CB	2.35	0.67
1:A:4:LEU:HD12	1:A:112:VAL:HG22	1.76	0.67
1:A:63:LYS:HD2	1:A:64:ASN:ND2	2.10	0.66
1:A:139:MET:HE3	1:A:178:LYS:CE	2.26	0.66
1:A:28:ARG:H	1:A:28:ARG:HH21	1.44	0.65
1:A:13:ASN:O	1:A:14:MET:HB2	1.96	0.65
1:A:139:MET:HE3	1:A:178:LYS:HE2	1.77	0.65
1:A:99:LEU:HA	1:A:102:GLN:HG2	1.79	0.64
1:A:114:ILE:HD13	1:A:124:ALA:HB2	1.82	0.62
1:A:166:LEU:HD22	1:A:166:LEU:H	1.64	0.62
3:A:301:CO4:O3'	3:A:301:CO4:H4B2	1.98	0.62
1:A:1:VAL:HG22	1:A:109:VAL:CG1	2.30	0.61
1:A:99:LEU:HG	1:A:105:LEU:CD1	2.30	0.61
1:A:16:ILE:O	2:A:300:NDP:H2N	2.00	0.60
1:A:105:LEU:HD23	1:A:108:LYS:HD2	1.84	0.59
1:A:129:GLY:O	1:A:184:LYS:NZ	2.36	0.58
1:A:61:PRO:HB3	4:A:252:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:HG3	2:A:300:NDP:P2B	2.46	0.56
1:A:119:SER:HA	1:A:122:LYS:HG2	1.88	0.56
1:A:3:SER:HB3	1:A:5:ASN:HD21	1.71	0.55
1:A:147:PHE:CD1	1:A:147:PHE:N	2.75	0.55
1:A:168:ASP:O	1:A:170:GLN:NE2	2.39	0.54
1:A:20:GLY:HA2	2:A:300:NDP:H3D	1.89	0.54
2:A:300:NDP:H42N	3:A:301:CO4:C51	2.35	0.54
1:A:107:ASN:HD22	1:A:107:ASN:N	2.05	0.54
1:A:166:LEU:H	1:A:166:LEU:CD2	2.21	0.53
1:A:97:LEU:O	1:A:100:THR:HB	2.09	0.53
1:A:6:CYS:HB2	1:A:133:LEU:HD12	1.91	0.52
1:A:28:ARG:HH12	1:A:173:LYS:HZ3	1.55	0.52
1:A:99:LEU:HA	1:A:102:GLN:CG	2.39	0.52
1:A:99:LEU:O	1:A:102:GLN:HG2	2.10	0.52
1:A:63:LYS:HD2	1:A:64:ASN:HD21	1.74	0.52
1:A:99:LEU:C	1:A:102:GLN:HG2	2.36	0.51
1:A:102:GLN:C	1:A:106:ALA:HB2	2.28	0.51
1:A:75:LEU:O	2:A:300:NDP:H1B	2.10	0.51
1:A:105:LEU:O	1:A:108:LYS:HB2	2.10	0.51
1:A:166:LEU:HD22	1:A:166:LEU:N	2.26	0.51
1:A:63:LYS:CD	1:A:64:ASN:ND2	2.74	0.51
3:A:301:CO4:H4'2	3:A:301:CO4:C51	2.23	0.50
1:A:50:VAL:HG21	1:A:67:LEU:HD12	1.94	0.50
1:A:130:HIS:HE1	1:A:183:GLU:OE1	1.94	0.49
1:A:132:LYS:HE3	4:A:212:HOH:O	2.12	0.49
1:A:130:HIS:CE1	1:A:183:GLU:OE1	2.66	0.49
2:A:300:NDP:C4N	3:A:301:CO4:H512	2.39	0.49
1:A:139:MET:HE3	1:A:178:LYS:HG2	1.95	0.48
1:A:2:GLY:HA3	4:A:250:HOH:O	2.14	0.48
3:A:301:CO4:H9'1	3:A:301:CO4:H2'	1.35	0.48
1:A:63:LYS:HD3	1:A:64:ASN:CG	2.39	0.47
3:A:301:CO4:H513	3:A:301:CO4:N4'	2.24	0.47
1:A:76:SER:HB3	1:A:89:LEU:HD11	1.97	0.47
1:A:116:GLY:HA3	2:A:300:NDP:H5N	1.97	0.47
1:A:13:ASN:O	1:A:14:MET:CB	2.63	0.46
1:A:102:GLN:C	1:A:104:GLU:N	2.72	0.46
1:A:42:SER:OG	1:A:110:ASP:OD1	2.34	0.46
1:A:105:LEU:HA	1:A:108:LYS:CD	2.33	0.46
1:A:29:ASN:HB2	1:A:172:GLU:OE1	2.15	0.46
1:A:103:PRO:HA	1:A:106:ALA:CB	2.47	0.45
1:A:54:LYS:HE2	2:A:300:NDP:O1X	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:CD1	1:A:112:VAL:HG22	2.44	0.45
1:A:18:LYS:HE2	1:A:18:LYS:HB3	1.74	0.45
1:A:30:GLU:HG2	1:A:136:THR:HG21	1.99	0.45
1:A:77:ARG:N	2:A:300:NDP:O3X	2.44	0.45
1:A:123:GLU:O	1:A:123:GLU:HG2	2.18	0.44
1:A:1:VAL:HG21	1:A:100:THR:CG2	2.48	0.44
1:A:133:LEU:HD22	1:A:156:TYR:CE2	2.53	0.44
1:A:28:ARG:HH12	1:A:173:LYS:HZ1	1.65	0.43
1:A:139:MET:CE	1:A:178:LYS:CE	2.95	0.43
1:A:20:GLY:CA	1:A:55:LYS:HE2	2.49	0.43
1:A:156:TYR:CZ	1:A:184:LYS:HD3	2.54	0.43
1:A:139:MET:HE3	1:A:178:LYS:CG	2.49	0.42
1:A:100:THR:HG22	1:A:101:GLU:N	2.34	0.42
1:A:28:ARG:NH1	4:A:245:HOH:O	2.52	0.42
1:A:31:PHE:O	1:A:35:GLN:HG2	2.20	0.41
1:A:130:HIS:HB2	4:A:210:HOH:O	2.20	0.41
1:A:133:LEU:HD22	1:A:156:TYR:CD2	2.55	0.41
1:A:99:LEU:CA	1:A:102:GLN:HG2	2.48	0.41
1:A:185:ASN:HD22	1:A:185:ASN:HA	1.67	0.40
1:A:145:ASP:OD1	1:A:146:THR:HG22	2.22	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)
1:A:154:GLU:OE2	4:A:207:HOH:O[8_544]	1.87	0.33

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	184/186 (99%)	176 (96%)	6 (3%)	2 (1%)	11 8

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	GLU
1	A	43	VAL

5.3.2 Protein sidechains ⓘ

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	168/168 (100%)	148 (88%)	20 (12%)	5 3

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	10	VAL
1	A	14	MET
1	A	28	ARG
1	A	55	LYS
1	A	63	LYS
1	A	68	LYS
1	A	72	ASN
1	A	77	ARG
1	A	84	GLN
1	A	89	LEU
1	A	100	THR
1	A	101	GLU
1	A	107	ASN
1	A	112	VAL
1	A	118	SER
1	A	119	SER
1	A	133	LEU
1	A	140	GLN
1	A	146	THR

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

Mol	Chain	Res	Type
1	A	5	ASN
1	A	12	GLN
1	A	47	GLN
1	A	87	HIS
1	A	102	GLN
1	A	107	ASN
1	A	185	ASN

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 oligosaccharides 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	NDP	A	300	-	51,52,52	3.17	28 (54%)	71,80,80	2.97	32 (45%)
3	CO4	A	301	-	29,30,30	1.30	5 (17%)	40,43,43	3.05	16 (40%)

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	CO4	A	301	-	1/1/1/1	2/14/14/14	0/3/3/3
2	NDP	A	300	-	-	6/34/77/77	0/5/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	NDP	C7N-N7N	7.27	1.54	1.33
2	A	300	NDP	PN-O3	7.05	1.67	1.59
2	A	300	NDP	O7N-C7N	-6.99	1.08	1.24
2	A	300	NDP	P2B-O3X	-5.65	1.33	1.54
2	A	300	NDP	O4B-C4B	-5.28	1.33	1.45
2	A	300	NDP	O4D-C1D	5.20	1.54	1.42
2	A	300	NDP	PA-O3	4.87	1.64	1.59
2	A	300	NDP	C5A-C6A	4.57	1.53	1.41
2	A	300	NDP	O3B-C3B	4.41	1.53	1.43
2	A	300	NDP	P2B-O2B	3.97	1.66	1.59
2	A	300	NDP	C3D-C4D	3.88	1.62	1.53
2	A	300	NDP	PA-O5B	-3.87	1.44	1.59
2	A	300	NDP	C2B-C1B	3.48	1.61	1.53
2	A	300	NDP	O4B-C1B	3.47	1.50	1.42
2	A	300	NDP	C7N-C3N	3.32	1.55	1.48
2	A	300	NDP	O2B-C2B	-3.17	1.33	1.44
2	A	300	NDP	O4D-C4D	3.08	1.51	1.45
2	A	300	NDP	C2N-C3N	2.99	1.43	1.35
2	A	300	NDP	C5A-C4A	-2.98	1.33	1.39
3	A	301	CO4	C8A-N8'	2.95	1.41	1.37
2	A	300	NDP	PA-O1A	-2.85	1.41	1.50
2	A	300	NDP	C8A-N7A	2.84	1.37	1.31
2	A	300	NDP	C1D-N1N	2.73	1.53	1.46
2	A	300	NDP	P2B-O2X	-2.61	1.45	1.54
3	A	301	CO4	C7'-C6D	2.55	1.42	1.37
2	A	300	NDP	C1B-N9A	-2.52	1.39	1.46
3	A	301	CO4	O4'-C4'	2.48	1.42	1.38
2	A	300	NDP	C4A-N9A	-2.45	1.32	1.37
2	A	300	NDP	C6A-N6A	2.40	1.40	1.34
2	A	300	NDP	P2B-O1X	-2.39	1.43	1.50
3	A	301	CO4	C8'-C6D	2.38	1.55	1.51
2	A	300	NDP	C6N-N1N	2.16	1.42	1.37
3	A	301	CO4	C6'-C1'	2.01	1.43	1.39

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	NDP	O2B-P2B-O1X	-9.03	77.16	109.33
2	A	300	NDP	O3D-C3D-C4D	-7.89	88.42	111.08
3	A	301	CO4	C6D-C8'-N9'	7.57	125.85	114.49
3	A	301	CO4	N2'-C2D-N3'	7.22	128.05	117.22
2	A	300	NDP	C3N-C2N-N1N	-6.30	113.95	123.20
2	A	300	NDP	O7N-C7N-C3N	5.73	131.69	120.90
3	A	301	CO4	O5'-C5'-C6'	-5.47	114.66	124.08
3	A	301	CO4	C6'-C5'-C4'	5.46	126.30	120.22
2	A	300	NDP	PN-O5D-C5D	5.27	151.54	121.35
2	A	300	NDP	O7N-C7N-N7N	-5.17	111.31	122.89
3	A	301	CO4	N2'-C2D-N1'	-5.08	109.85	117.79
3	A	301	CO4	C9'-N9'-C1'	-4.98	111.35	119.59
2	A	300	NDP	O3X-P2B-O2X	4.89	126.16	107.80
2	A	300	NDP	C4A-N9A-C8A	4.86	110.84	105.74
2	A	300	NDP	O3B-C3B-C4B	-4.85	97.15	111.08
3	A	301	CO4	C1'-C6'-C5'	-4.70	113.16	120.39
3	A	301	CO4	C5B-O5'-C5'	-4.50	110.92	117.51
2	A	300	NDP	O2A-PA-O5B	4.20	126.59	107.57
2	A	300	NDP	N6A-C6A-N1A	4.17	127.66	118.38
3	A	301	CO4	N1'-C2D-N3'	-4.05	122.06	127.21
3	A	301	CO4	C9'-N9'-C8'	3.95	125.39	115.11
2	A	300	NDP	C5A-C6A-N6A	-3.83	113.81	123.29
2	A	300	NDP	N9A-C8A-N7A	-3.81	108.53	113.94
2	A	300	NDP	C3B-C2B-C1B	-3.78	95.57	102.81
2	A	300	NDP	O4B-C1B-C2B	-3.70	100.21	106.59
2	A	300	NDP	C6N-N1N-C2N	3.56	123.13	119.32
2	A	300	NDP	C2D-C3D-C4D	-3.42	96.00	102.61
2	A	300	NDP	O3-PA-O1A	-3.38	100.55	110.70
2	A	300	NDP	O2N-PN-O3	-3.33	98.28	107.27
2	A	300	NDP	O3D-C3D-C2D	3.25	122.22	111.82
2	A	300	NDP	O5D-C5D-C4D	-3.18	98.17	108.99
2	A	300	NDP	O5D-PN-O1N	3.13	121.35	108.94
2	A	300	NDP	O2B-C2B-C3B	3.06	122.64	111.68
3	A	301	CO4	C8'-C6D-C7'	-3.03	116.97	121.30
3	A	301	CO4	C8'-C6D-C5D	3.00	125.89	120.54
2	A	300	NDP	C2D-C1D-N1N	2.97	120.62	113.31
2	A	300	NDP	C2B-C3B-C4B	-2.97	95.60	101.99
2	A	300	NDP	O3X-P2B-O1X	2.78	121.66	110.83
3	A	301	CO4	C3B-O3'-C3'	-2.68	113.58	117.51
2	A	300	NDP	O2A-PA-O1A	-2.66	100.08	112.44
2	A	300	NDP	O2X-P2B-O1X	-2.57	100.84	110.83
2	A	300	NDP	C1B-N9A-C8A	-2.50	121.55	127.09
2	A	300	NDP	C6A-C5A-C4A	-2.46	113.82	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	CO4	C3'-C4'-C5'	-2.34	117.28	119.56
2	A	300	NDP	O4D-C1D-N1N	-2.33	103.63	108.08
3	A	301	CO4	C1'-C2'-C3'	-2.28	116.89	120.39
3	A	301	CO4	O5'-C5'-C4'	2.21	118.92	115.14
2	A	300	NDP	P2B-O2B-C2B	-2.14	117.72	123.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	301	CO4	N9'

All (8) torsion outliers are listed below:

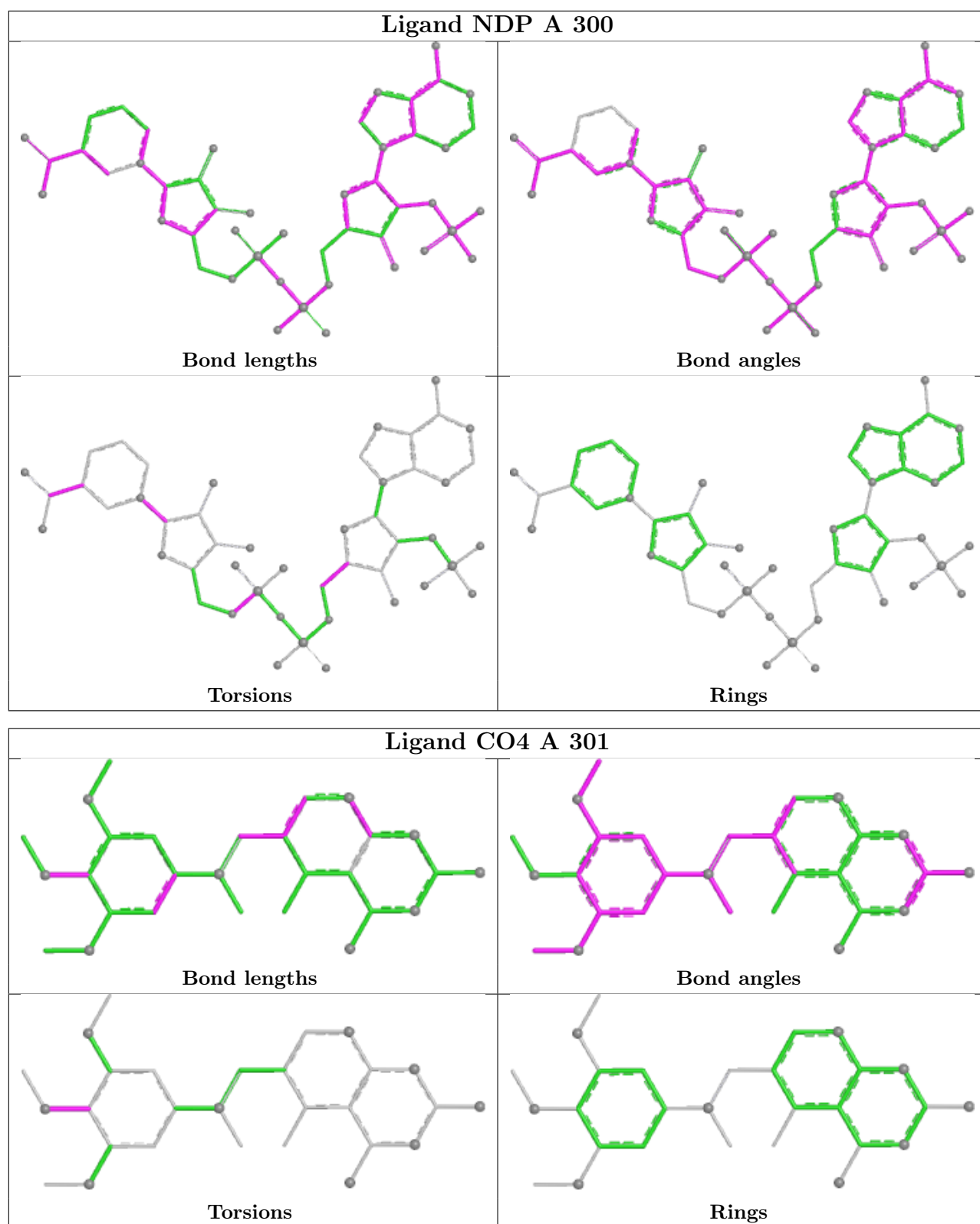
Mol	Chain	Res	Type	Atoms
2	A	300	NDP	C5D-O5D-PN-O3
3	A	301	CO4	C5'-C4'-O4'-C4B
3	A	301	CO4	C3'-C4'-O4'-C4B
2	A	300	NDP	C3B-C4B-C5B-O5B
2	A	300	NDP	O4B-C4B-C5B-O5B
2	A	300	NDP	O4D-C1D-N1N-C2N
2	A	300	NDP	C2N-C3N-C7N-N7N
2	A	300	NDP	C2D-C1D-N1N-C2N

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	NDP	12	0
3	A	301	CO4	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 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 ⓘ

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.