Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2022 – 08:42 PM EST

PDB ID	:	1BOZ
Title	:	STRUCTURE-BASED DESIGN AND SYNTHESIS OF LIPOPHILIC 2,4-D IAMINO-6-SUBSTITUTED QUINAZOLINES AND THEIR EVALUATION AS INHIBITORS OF DIHYDROFOLATE REDUCTASE AND POTENTIAL ANTITUMOR AGENTS
Authors	:	Gangjee, A.; Vidwans, A.P.; Vasudevan, A.; Queener, S.F.; Kisliuk, R.L.; Cody, V.; Li, R.; Galitsky, N.; Luft, J.R.; Pangborn, W.
Deposited on	:	1998-08-06
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

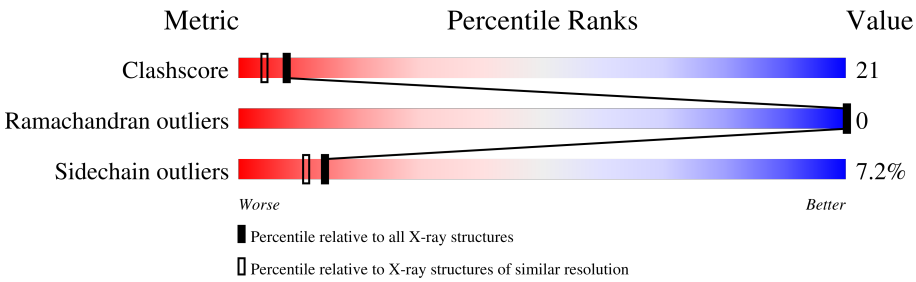
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	186	59% 31% 10% •

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	PRD	A	400	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1693 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.

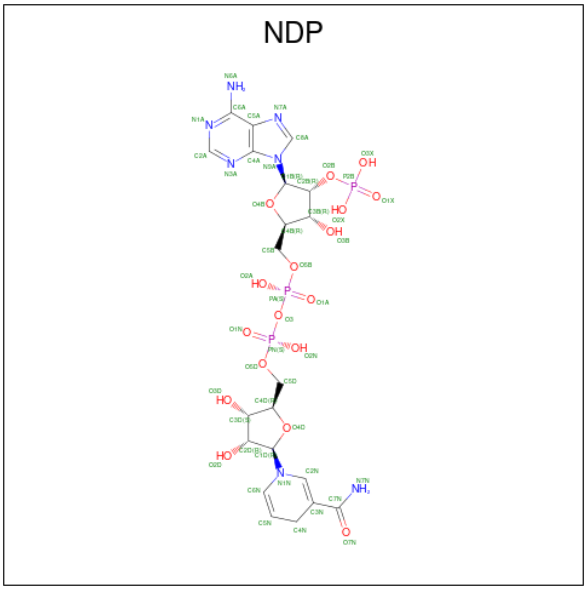
- Molecule 1 is a protein called PROTEIN (DIHYDROFOLATE REDUCTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1495	956	253	279	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLY	PHE	conflict	UNP P00374

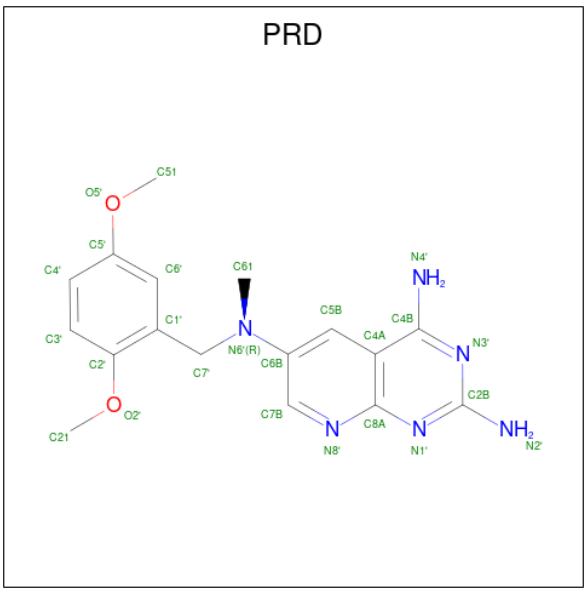
- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 3 is N6-(2,5-DIMETHOXY-BENZYL)-N6-METHYL-PYRIDO[2,3-D]PYRIMIDI

NE-2,4,6-TRIAMINE (three-letter code: PRD) (formula: $C_{17}H_{20}N_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	25	17	6	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	125	125	125	0	0

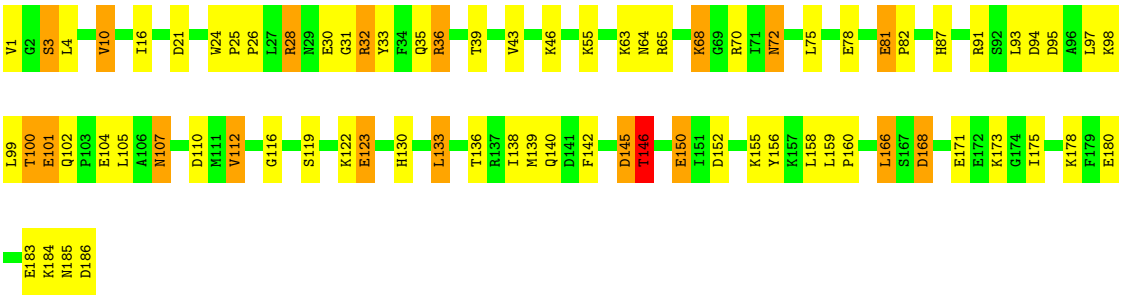
3 Residue-property plots (i)

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: PROTEIN (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	H 3	Depositor
Cell constants a, b, c, α, β, γ	86.26Å 86.26Å 77.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	95.0 (8.00-2.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1693	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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: PRD, NDP

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	0.90	1/1529 (0.1%)	1.85	26/2062 (1.3%)

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	119	SER	CB-OG	6.08	1.50	1.42

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	65	ARG	CD-NE-CZ	21.71	154.00	123.60
1	A	36	ARG	NE-CZ-NH2	-13.97	113.32	120.30
1	A	21	ASP	CB-CG-OD2	-10.46	108.89	118.30
1	A	70	ARG	NE-CZ-NH2	-9.21	115.70	120.30
1	A	145	ASP	CB-CG-OD1	8.93	126.34	118.30
1	A	78	GLU	CG-CD-OE1	7.80	133.91	118.30
1	A	65	ARG	NE-CZ-NH2	7.63	124.11	120.30
1	A	21	ASP	CB-CG-OD1	7.45	125.00	118.30
1	A	10	VAL	CA-CB-CG1	7.20	121.71	110.90
1	A	110	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	36	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	A	33	TYR	CB-CG-CD1	-6.94	116.84	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	138	ILE	CB-CG1-CD1	6.56	132.26	113.90
1	A	168	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	91	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	150	GLU	CB-CG-CD	6.39	131.45	114.20
1	A	3	SER	N-CA-CB	-6.31	101.04	110.50
1	A	28	ARG	CD-NE-CZ	6.28	132.39	123.60
1	A	32	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	A	123	GLU	CA-CB-CG	5.87	126.32	113.40
1	A	78	GLU	CA-CB-CG	5.44	125.37	113.40
1	A	65	ARG	CG-CD-NE	5.39	123.12	111.80
1	A	146	THR	CB-CA-C	5.38	126.12	111.60
1	A	81	GLU	CG-CD-OE1	5.22	128.74	118.30
1	A	33	TYR	CB-CG-CD2	5.09	124.06	121.00
1	A	133	LEU	CB-CG-CD1	5.00	119.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	36	ARG	Sidechain

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	1495	0	1505	66	0
2	A	48	0	26	4	0
3	A	25	0	20	2	0
4	A	125	0	0	3	1
All	All	1693	0	1551	67	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 21.

All (67) 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:139:MET:HE3	1:A:178:LYS:HD3	1.19	1.14
1:A:1:VAL:HG21	1:A:100:THR:HG23	1.32	1.11
1:A:139:MET:CE	1:A:178:LYS:HD3	1.88	1.01
1:A:72:ASN:H	1:A:87:HIS:HD2	1.20	0.88
1:A:99:LEU:HD23	1:A:105:LEU:HD12	1.55	0.87
1:A:107:ASN:ND2	1:A:107:ASN:H	1.76	0.81
1:A:145:ASP:OD1	1:A:146:THR:HG22	1.80	0.80
1:A:72:ASN:H	1:A:87:HIS:CD2	1.99	0.80
1:A:95:ASP:HA	1:A:98:LYS:HE3	1.65	0.79
1:A:99:LEU:CD2	1:A:105:LEU:HD12	2.18	0.73
1:A:122:LYS:HG3	4:A:263:HOH:O	1.90	0.71
1:A:4:LEU:HD12	1:A:112:VAL:HG22	1.73	0.71
1:A:99:LEU:HA	1:A:102:GLN:HG2	1.76	0.67
1:A:1:VAL:CG2	1:A:100:THR:HG23	2.19	0.67
1:A:107:ASN:H	1:A:107:ASN:HD22	1.43	0.66
1:A:166:LEU:HD13	4:A:306:HOH:O	1.96	0.64
1:A:140:GLN:HG3	1:A:142:PHE:CE2	2.35	0.62
1:A:116:GLY:HA3	2:A:187:NDP:H5N	1.82	0.61
1:A:97:LEU:O	1:A:100:THR:HB	2.00	0.61
1:A:26:PRO:O	1:A:173:LYS:NZ	2.31	0.58
1:A:75:LEU:O	2:A:187:NDP:H1B	2.03	0.57
1:A:93:LEU:HB2	1:A:123:GLU:OE2	2.05	0.57
1:A:1:VAL:HG11	1:A:100:THR:HG21	1.85	0.56
1:A:98:LYS:O	1:A:101:GLU:HB2	2.07	0.55
1:A:1:VAL:HG11	1:A:100:THR:CG2	2.37	0.54
1:A:102:GLN:HG3	1:A:104:GLU:OE2	2.07	0.54
1:A:31:GLY:O	1:A:35:GLN:HG2	2.07	0.53
1:A:35:GLN:HE22	3:A:400:PRD:C51	2.20	0.53
1:A:43:VAL:HG12	1:A:46:LYS:HG3	1.89	0.53
1:A:107:ASN:ND2	1:A:107:ASN:N	2.49	0.52
1:A:95:ASP:CA	1:A:98:LYS:HE3	2.36	0.52
1:A:186:ASP:OD1	1:A:186:ASP:C	2.49	0.51
1:A:55:LYS:HD3	2:A:187:NDP:H51N	1.92	0.51
1:A:28:ARG:O	1:A:32:ARG:HG3	2.11	0.51
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.93	0.51
1:A:130:HIS:HE1	1:A:183:GLU:OE2	1.94	0.50
1:A:152:ASP:OD2	1:A:155:LYS:HE2	2.13	0.49
1:A:122:LYS:HE2	4:A:263:HOH:O	2.13	0.48
1:A:130:HIS:CE1	1:A:183:GLU:OE2	2.67	0.48
1:A:139:MET:HE2	1:A:178:LYS:HD3	1.90	0.47
1:A:99:LEU:HD23	1:A:105:LEU:CD1	2.38	0.47
1:A:72:ASN:N	1:A:87:HIS:HD2	2.01	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:CD2	1:A:105:LEU:CD1	2.92	0.46
1:A:94:ASP:C	1:A:98:LYS:HE3	2.37	0.45
1:A:156:TYR:CZ	1:A:184:LYS:HD3	2.52	0.45
1:A:102:GLN:C	1:A:104:GLU:N	2.70	0.45
1:A:63:LYS:HE3	1:A:64:ASN:HD21	1.82	0.45
1:A:107:ASN:HD22	1:A:107:ASN:N	2.10	0.44
1:A:81:GLU:HB2	1:A:82:PRO:HD2	1.99	0.44
3:A:400:PRD:HC62	3:A:400:PRD:H5'	1.70	0.44
1:A:4:LEU:CD1	1:A:112:VAL:HG22	2.46	0.43
1:A:168:ASP:OD1	1:A:168:ASP:N	2.32	0.43
1:A:139:MET:CE	1:A:178:LYS:CD	2.78	0.43
1:A:171:GLU:HA	1:A:175:ILE:O	2.20	0.42
1:A:63:LYS:HG3	1:A:64:ASN:N	2.34	0.42
1:A:39:THR:HG22	1:A:39:THR:O	2.19	0.41
1:A:93:LEU:CB	1:A:123:GLU:OE2	2.67	0.41
1:A:158:LEU:HD11	1:A:180:GLU:HB3	2.03	0.41
1:A:30:GLU:HG2	1:A:136:THR:HG21	2.02	0.41
1:A:102:GLN:C	1:A:104:GLU:H	2.24	0.41
1:A:16:ILE:O	2:A:187:NDP:H2N	2.20	0.41
1:A:159:LEU:HA	1:A:160:PRO:HD3	1.80	0.41
1:A:63:LYS:HE3	1:A:64:ASN:ND2	2.35	0.40
1:A:10:VAL:HG12	1:A:16:ILE:HG23	2.03	0.40
1:A:94:ASP:O	1:A:98:LYS:HE3	2.21	0.40
1:A:158:LEU:CD1	1:A:180:GLU:HB3	2.51	0.40
1:A:68:LYS:NZ	1:A:68:LYS:HB3	2.36	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)
4:A:226:HOH:O	4:A:266:HOH:O[6_555]	2.10	0.10

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%)	177 (96%)	7 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/167 (100%)	155 (93%)	12 (7%)	14	11

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	68	LYS
1	A	72	ASN
1	A	100	THR
1	A	101	GLU
1	A	107	ASN
1	A	112	VAL
1	A	133	LEU
1	A	146	THR
1	A	150	GLU
1	A	166	LEU
1	A	185	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	87	HIS
1	A	107	ASN
1	A	185	ASN

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)

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	187	-	45,52,52	3.13	22 (48%)	53,80,80	2.90	23 (43%)
3	PRD	A	400	-	27,27,27	2.80	13 (48%)	36,38,38	3.89	21 (58%)

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	NDP	A	187	-	-	9/30/77/77	0/5/5/5
3	PRD	A	400	-	-	6/12/12/12	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	C7N-N7N	8.15	1.55	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	O4B-C1B	7.56	1.51	1.41
2	A	187	NDP	O7N-C7N	-6.95	1.08	1.24
3	A	400	PRD	C4B-C4A	-6.88	1.38	1.45
2	A	187	NDP	O4B-C4B	-6.18	1.31	1.45
3	A	400	PRD	C7'-N6'	-6.10	1.34	1.46
2	A	187	NDP	P2B-O3X	-5.31	1.34	1.54
3	A	400	PRD	C8A-N1'	5.11	1.46	1.36
2	A	187	NDP	O3B-C3B	4.77	1.54	1.43
2	A	187	NDP	O4D-C1D	4.45	1.52	1.42
2	A	187	NDP	P2B-O2B	4.35	1.67	1.59
3	A	400	PRD	O2'-C2'	3.98	1.43	1.37
3	A	400	PRD	C7B-N8'	3.58	1.37	1.31
2	A	187	NDP	PA-O5B	-3.52	1.45	1.59
2	A	187	NDP	P2B-O2X	-3.28	1.42	1.54
2	A	187	NDP	C5A-C4A	-3.13	1.32	1.40
2	A	187	NDP	C3D-C4D	3.04	1.60	1.53
2	A	187	NDP	O4D-C4D	2.98	1.51	1.45
3	A	400	PRD	C7B-C6B	2.97	1.44	1.38
2	A	187	NDP	PA-O1A	-2.92	1.40	1.50
3	A	400	PRD	C6'-C1'	2.90	1.44	1.39
2	A	187	NDP	C7N-C3N	2.87	1.54	1.48
2	A	187	NDP	C2N-C3N	2.86	1.42	1.34
2	A	187	NDP	C6A-C5A	2.73	1.53	1.43
3	A	400	PRD	C5B-C4A	-2.72	1.36	1.42
2	A	187	NDP	O2B-C2B	-2.71	1.34	1.44
2	A	187	NDP	C1D-N1N	2.70	1.54	1.46
3	A	400	PRD	C6B-N6'	2.62	1.46	1.39
3	A	400	PRD	O2'-C21	2.40	1.50	1.42
3	A	400	PRD	C7'-C1'	2.32	1.55	1.51
2	A	187	NDP	P2B-O1X	-2.29	1.43	1.50
2	A	187	NDP	PN-O2N	-2.22	1.44	1.55
3	A	400	PRD	C2'-C1'	-2.19	1.36	1.40
2	A	187	NDP	O5B-C5B	2.14	1.53	1.44
3	A	400	PRD	O5'-C5'	2.06	1.41	1.37

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	400	PRD	N1'-C2B-N3'	-9.68	114.30	127.22
3	A	400	PRD	C5B-C6B-N6'	-9.67	110.15	121.33
3	A	400	PRD	C21-O2'-C2'	-8.37	104.89	117.53
3	A	400	PRD	C2B-N1'-C8A	7.62	124.06	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	187	NDP	O3D-C3D-C4D	-6.87	91.18	111.05
2	A	187	NDP	O2X-P2B-O2B	-6.66	76.16	105.99
2	A	187	NDP	C3N-C2N-N1N	-6.51	113.81	123.10
3	A	400	PRD	C1'-C7'-N6'	6.19	123.99	114.48
2	A	187	NDP	O7N-C7N-C3N	5.34	130.95	120.90
3	A	400	PRD	N2'-C2B-N3'	5.33	125.54	117.25
2	A	187	NDP	O7N-C7N-N7N	-5.22	110.68	122.88
2	A	187	NDP	PN-O5D-C5D	5.17	152.02	121.68
2	A	187	NDP	O4B-C1B-C2B	-4.21	99.28	106.59
2	A	187	NDP	N6A-C6A-N1A	4.18	127.26	118.57
3	A	400	PRD	O2'-C2'-C3'	-4.16	117.24	124.37
2	A	187	NDP	O3B-C3B-C4B	-4.14	99.07	111.05
3	A	400	PRD	C2B-N3'-C4B	4.02	128.21	116.72
2	A	187	NDP	C5A-C6A-N6A	-4.02	114.25	120.35
3	A	400	PRD	C51-O5'-C5'	-3.90	109.04	117.51
2	A	187	NDP	C3B-C2B-C1B	-3.90	95.55	102.89
3	A	400	PRD	C4A-C4B-N3'	-3.87	117.90	121.93
2	A	187	NDP	O2A-PA-O5B	3.79	125.35	107.75
2	A	187	NDP	O4D-C1D-N1N	-3.67	100.88	108.06
2	A	187	NDP	O5D-C5D-C4D	-3.55	96.76	108.99
3	A	400	PRD	N8'-C8A-N1'	3.49	119.80	115.82
2	A	187	NDP	O3X-P2B-O1X	3.38	123.92	110.68
2	A	187	NDP	O3X-P2B-O2X	3.33	120.36	107.64
2	A	187	NDP	O2B-C2B-C3B	3.14	123.06	111.68
2	A	187	NDP	PN-O3-PA	2.87	142.68	132.83
3	A	400	PRD	C4A-C4B-N4'	2.82	125.90	121.54
2	A	187	NDP	C2B-C3B-C4B	-2.74	96.04	101.99
3	A	400	PRD	O5'-C5'-C4'	-2.60	107.39	119.82
3	A	400	PRD	C7'-C1'-C2'	-2.60	115.04	120.12
3	A	400	PRD	C7'-C1'-C6'	2.58	124.98	120.38
3	A	400	PRD	C5'-C6'-C1'	-2.51	116.98	120.47
3	A	400	PRD	C4A-C8A-N1'	-2.51	117.21	122.17
3	A	400	PRD	O2'-C2'-C1'	2.42	119.35	115.97
3	A	400	PRD	C61-N6'-C6B	-2.42	115.39	119.57
2	A	187	NDP	O5B-PA-O1A	2.39	118.39	109.07
3	A	400	PRD	C5B-C4A-C4B	-2.38	122.35	124.76
3	A	400	PRD	C4'-C5'-C6'	2.32	123.72	120.53
2	A	187	NDP	O2N-PN-O5D	2.12	117.61	107.75
2	A	187	NDP	C4A-C5A-N7A	2.06	111.55	109.40
2	A	187	NDP	C2D-C1D-N1N	2.01	118.33	113.30

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	187	NDP	C5D-O5D-PN-O3
3	A	400	PRD	C3'-C2'-O2'-C21
3	A	400	PRD	C1'-C2'-O2'-C21
3	A	400	PRD	C5B-C6B-N6'-C61
3	A	400	PRD	C7B-C6B-N6'-C61
2	A	187	NDP	C5D-O5D-PN-O1N
2	A	187	NDP	C5D-O5D-PN-O2N
2	A	187	NDP	C3B-C4B-C5B-O5B
3	A	400	PRD	C1'-C7'-N6'-C6B
2	A	187	NDP	O4D-C1D-N1N-C2N
2	A	187	NDP	C2D-C1D-N1N-C2N
2	A	187	NDP	C3D-C4D-C5D-O5D
3	A	400	PRD	C2'-C1'-C7'-N6'
2	A	187	NDP	O4D-C4D-C5D-O5D
2	A	187	NDP	C2N-C3N-C7N-N7N

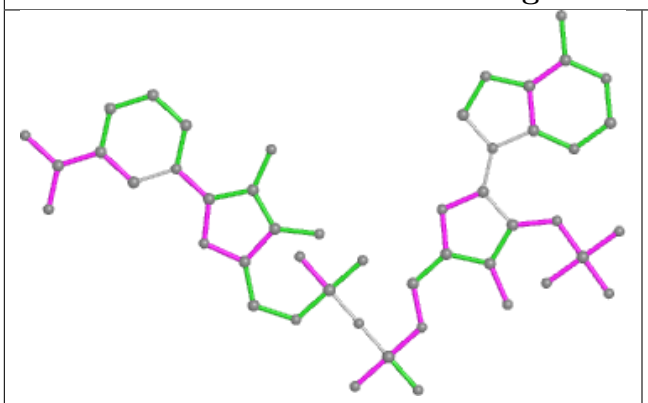
There are no ring outliers.

2 monomers are involved in 6 short contacts:

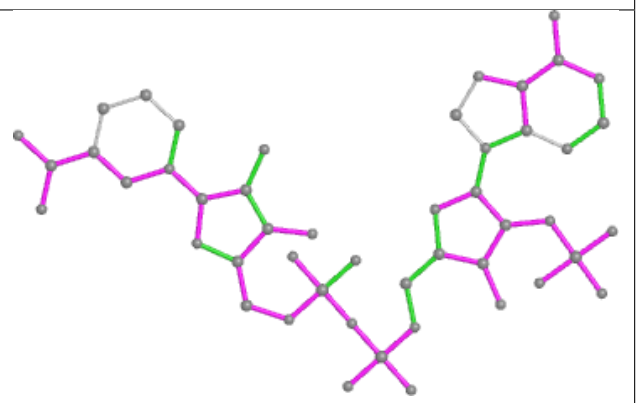
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	187	NDP	4	0
3	A	400	PRD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

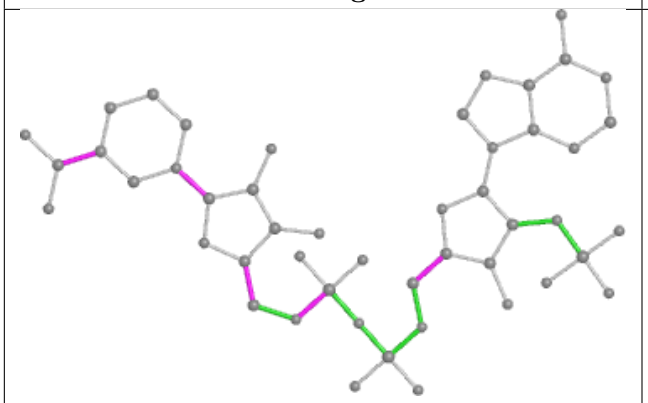
Ligand NDP A 187



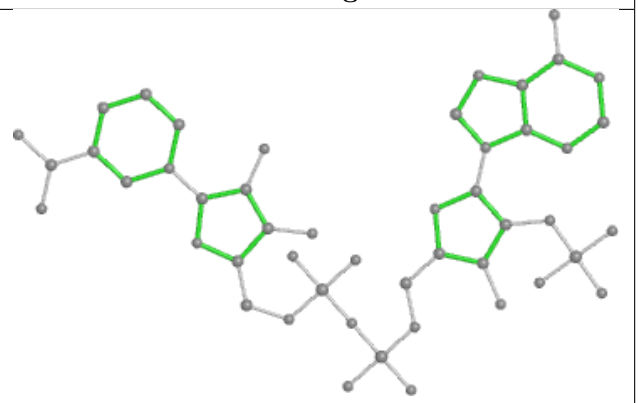
Bond lengths



Bond angles

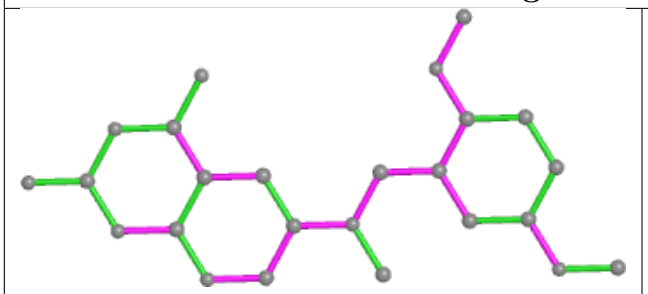


Torsions

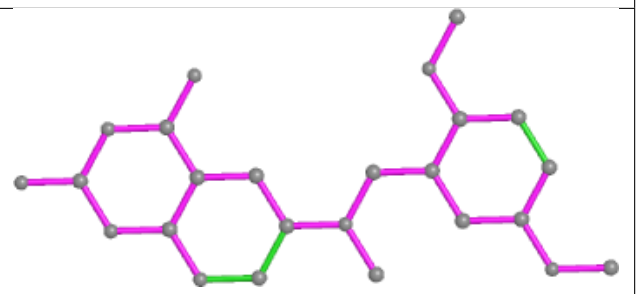


Rings

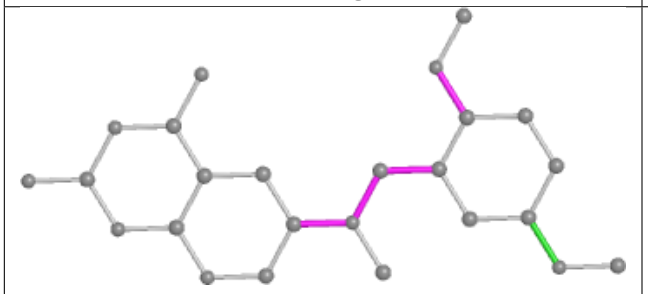
Ligand PRD A 400



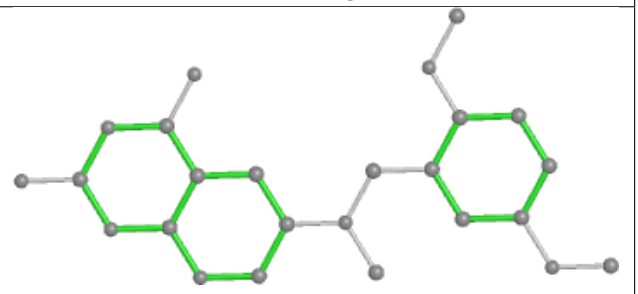
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.