wwPDB X-ray Structure Validation Summary Report (i)

Sep 14, 2026 – 04:02 PM EDT

PDB ID	:	1D22 / pdb_00001d22
Title	:	BINDING OF THE ANTITUMOR DRUG NOGALAMYCIN AND ITS DERIVATIVES TO DNA: STRUCTURAL COMPARISON
Authors	:	Gao, Y.-G.; Liaw, Y.-C.; Robinson, H.; Wang, A.H.-J.
Deposited on	:	1990-08-08
Resolution	:	1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

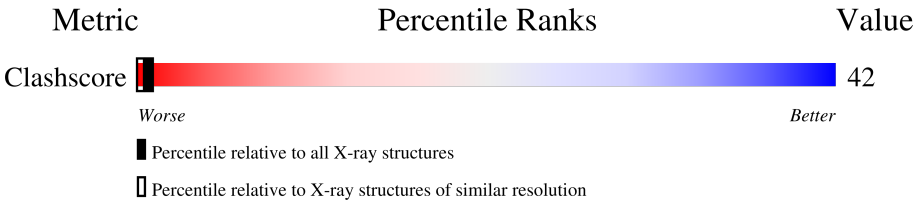
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.80 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	8479 (1.80-1.80)

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	6	50% 50%
1	B	6	33% 67%

2 Entry composition

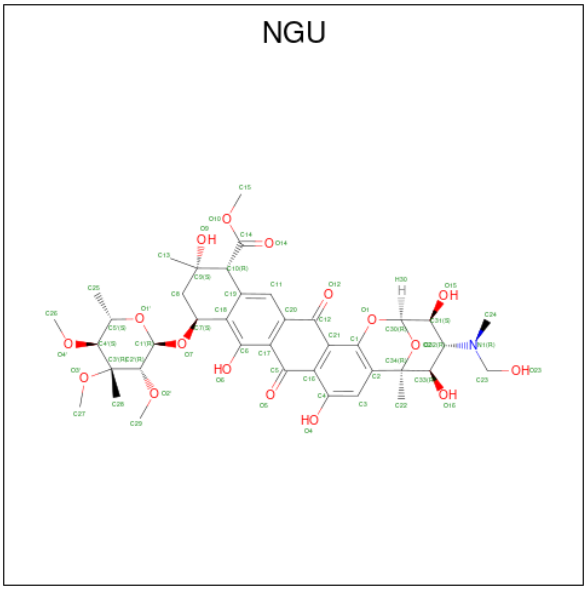
There are 3 unique types of molecules in this entry. The entry contains 433 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA chain called DNA (5'-D(*(5CM)P*GP*TP*(AS)P*(5CM)P*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	6	Total	C	N	O	P	S	0	0	0
			122	60	23	33	5	1			
1	B	6	Total	C	N	O	P	S	0	0	0
			122	60	23	33	5	1			

- Molecule 2 is U-58872, HYDROXY DERIVATIVE OF NOGALAMYCIN (CCD ID: NGU) (formula: $C_{39}H_{49}NO_{17}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			57	39	1	17		
2	B	1	Total	C	N	O	0	0
			57	39	1	17		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	27	Total O 27 27	0	0
3	B	48	Total O 48 48	0	0

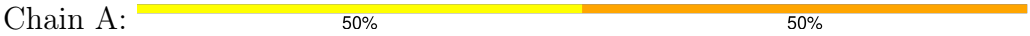
3 Residue-property plots (i)

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: DNA (5'-D(*(5CM)P*GP*TP*(AS)P*(5CM)P*G)-3')

Chain A:

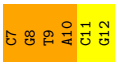




- Molecule 1: DNA (5'-D(*(5CM)P*GP*TP*(AS)P*(5CM)P*G)-3')

Chain B:





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	26.27Å 26.27Å 100.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	NUCLSQ	Depositor
R, R_{free}	0.196 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	433	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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: 5CM, NGU, AS

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	1.70	1/70 (1.4%)	4.21	11/104 (10.6%)
1	B	1.53	0/70	2.53	5/104 (4.8%)
All	All	1.62	1/140 (0.7%)	3.47	16/208 (7.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	DT	P-OP2	5.75	1.59	1.48

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3	DT	P-O5'-C5'	26.06	159.08	120.00
1	A	2	DG	P-O3'-C3'	20.54	151.01	120.20
1	A	2	DG	O3'-P-O5'	8.89	117.34	104.00
1	B	8	DG	P-O3'-C3'	8.76	133.34	120.20
1	B	8	DG	P-O5'-C5'	-8.04	107.94	120.00

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	122	0	71	7	5
1	B	122	0	72	6	2
2	B	114	0	94	17	1
3	A	27	0	0	3	0
3	B	48	0	0	5	9
All	All	433	0	237	25	9

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

The worst 5 of 25 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:4:AS:P	1:A:4:AS:S2P	1.52	1.52
1:A:3:DT:O3'	1:A:4:AS:S2P	2.22	0.98
3:A:47:HOH:O	2:B:13:NGU:H273	1.79	0.82
2:B:13:NGU:H271	3:B:74:HOH:O	1.84	0.77
2:B:13:NGU:H262	3:B:61:HOH:O	1.89	0.72

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:NGU:C26	3:B:87:HOH:O[6_555]	1.61	0.59
1:A:6:DG:N3	3:B:62:HOH:O[1_455]	1.62	0.58
1:A:6:DG:C1'	3:B:62:HOH:O[1_455]	1.75	0.45
1:A:6:DG:C4	3:B:62:HOH:O[1_455]	1.87	0.33
1:A:6:DG:N2	3:B:25:HOH:O[1_455]	1.89	0.31

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein molecules in this entry.

5.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	AS	A	4	1	20,23,24	0.94	1 (5%)	28,33,36	1.47	5 (17%)
1	5CM	A	5	1	18,21,22	0.95	1 (5%)	24,30,33	1.87	9 (37%)
1	5CM	B	7	1	18,18,22	1.31	3 (16%)	25,26,33	1.32	3 (12%)
1	AS	B	10	1	20,23,24	1.05	2 (10%)	28,33,36	1.17	2 (7%)
1	5CM	A	1	1	18,18,22	1.62	4 (22%)	25,26,33	2.22	10 (40%)
1	5CM	B	11	1	18,21,22	1.33	3 (16%)	24,30,33	3.24	6 (25%)

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
1	AS	A	4	1	-	0/7/21/22	0/3/3/3
1	5CM	A	5	1	-	0/7/21/22	0/2/2/2
1	5CM	B	7	1	-	4/6/18/22	0/2/2/2
1	AS	B	10	1	-	0/7/21/22	0/3/3/3
1	5CM	A	1	1	-	2/6/18/22	0/2/2/2
1	5CM	B	11	1	-	2/7/21/22	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	5CM	C5-C4	-4.38	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	11	5CM	C5-C4	-3.35	1.41	1.44
1	B	10	AS	O4'-C1'	2.72	1.48	1.42
1	A	5	5CM	C5-C4	-2.69	1.42	1.44
1	B	7	5CM	O4'-C1'	2.57	1.48	1.42

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	11	5CM	O4'-C1'-N1	13.85	132.45	107.86
1	A	1	5CM	C2'-C1'-N1	4.85	125.94	113.81
1	A	1	5CM	C5'-C4'-C3'	4.56	126.19	114.82
1	A	5	5CM	O4'-C1'-N1	4.41	115.68	107.86
1	A	4	AS	C2-N1-C6	4.27	125.74	118.73

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	7	5CM	C3'-C4'-C5'-O5'
1	B	7	5CM	O4'-C4'-C5'-O5'
1	B	11	5CM	C3'-C4'-C5'-O5'
1	B	11	5CM	O4'-C4'-C5'-O5'
1	A	1	5CM	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	4	AS	6	0
1	B	7	5CM	2	0
1	B	10	AS	3	0

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	NGU	B	14	-	60,63,63	2.32	21 (35%)	72,102,102	1.88	16 (22%)
2	NGU	B	13	-	60,63,63	2.22	21 (35%)	72,102,102	1.96	19 (26%)

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	NGU	B	14	-	-	9/21/115/115	0/1/7/7
2	NGU	B	13	-	-	5/21/115/115	0/1/7/7

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	14	NGU	C13-C9	-6.21	1.42	1.52
2	B	14	NGU	C28-C3'	5.87	1.65	1.52
2	B	14	NGU	O2-C30	5.27	1.51	1.42
2	B	13	NGU	C13-C9	-5.15	1.44	1.52
2	B	13	NGU	O23-C23	-5.00	1.25	1.40

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	14	NGU	O10-C14-O14	-6.85	110.50	123.85
2	B	13	NGU	O10-C14-O14	-6.35	111.48	123.85
2	B	13	NGU	C27-O3'-C3'	5.23	131.00	117.70
2	B	14	NGU	O14-C14-C10	4.79	133.31	125.22
2	B	14	NGU	C26-O4'-C4'	4.26	121.67	114.46

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	13	NGU	C31-C32-N1-C24
2	B	14	NGU	C10-C14-O10-C15
2	B	14	NGU	C5'-C4'-O4'-C26
2	B	14	NGU	C31-C32-N1-C23
2	B	14	NGU	C33-C32-N1-C23

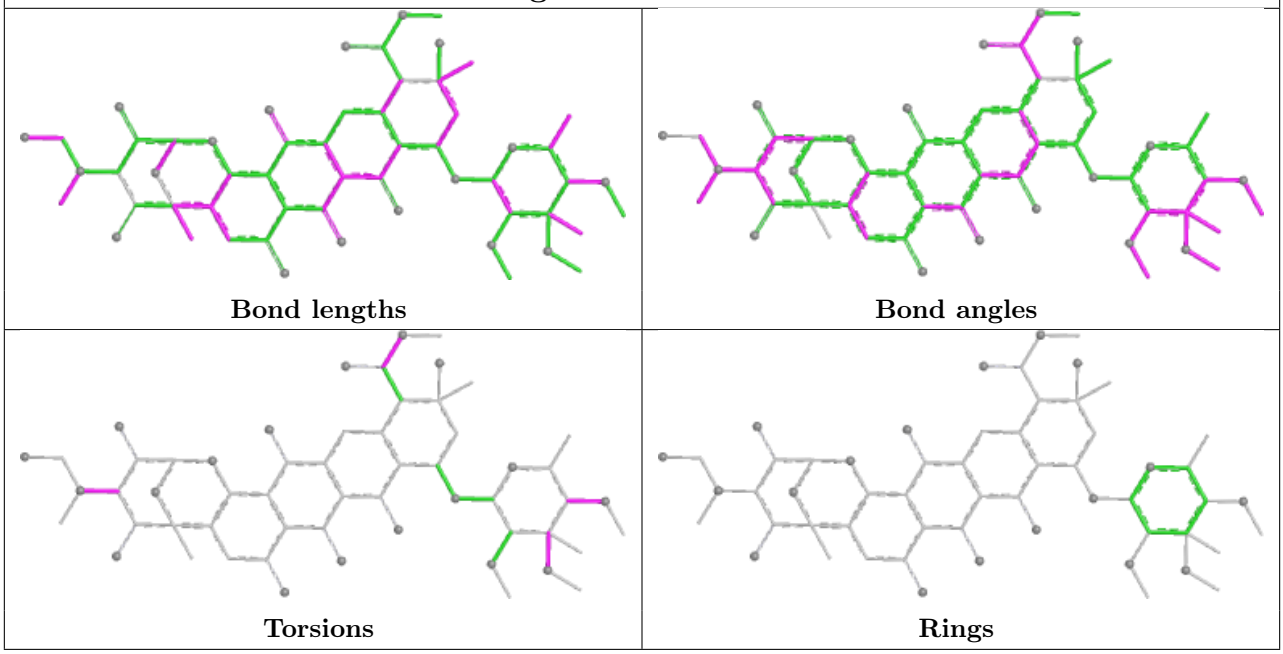
There are no ring outliers.

2 monomers are involved in 18 short contacts:

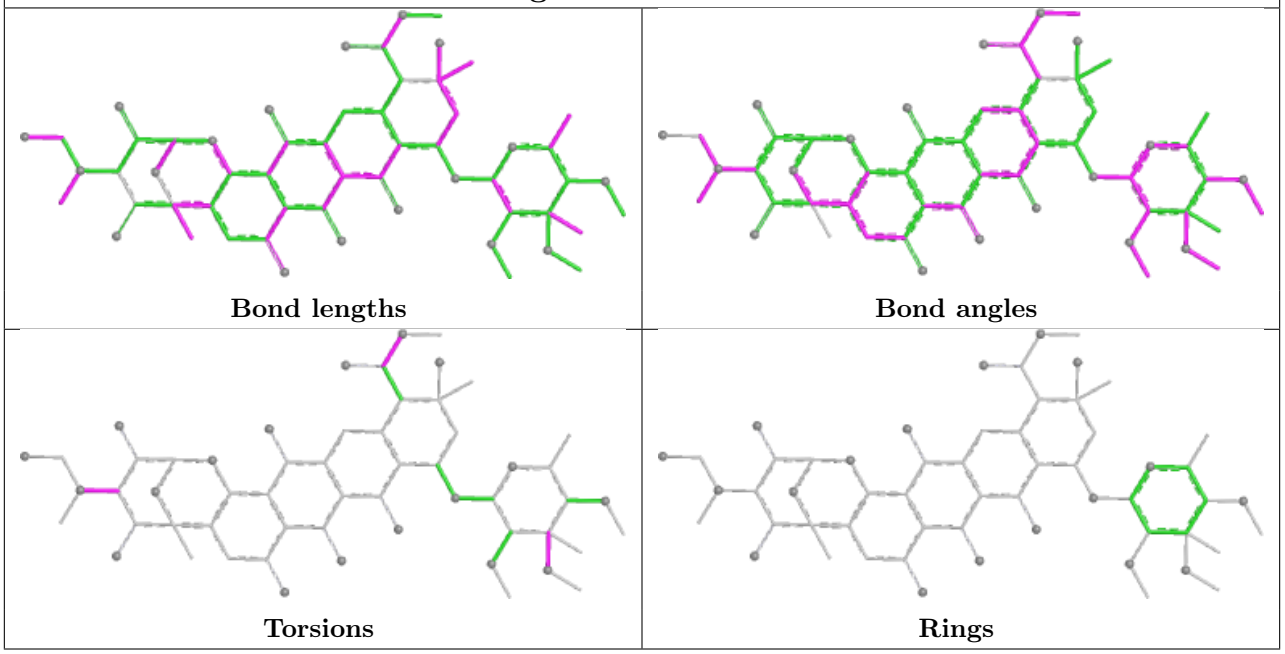
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	14	NGU	5	1
2	B	13	NGU	12	0

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 NGU B 14



Ligand NGU B 13



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.