

Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 07:53 AM EDT

PDB ID	:	11BG
Title	:	A POTENTIAL ALLOSTERIC SUBSITE GENERATED BY DOMAIN
		SWAPPING IN BOVINE SEMINAL RIBONUCLEASE
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Deposited on		
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 (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:

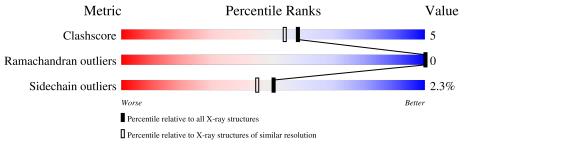
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	Similar resolution		
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
Clashscore	141614	6847 (1.90-1.90)		
Ramachandran outliers	138981	6760 (1.90-1.90)		
Sidechain outliers	138945	6760 (1.90-1.90)		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	А	124	91%	8%	•
1	В	124	87%	11%	•



2 Entry composition (i)

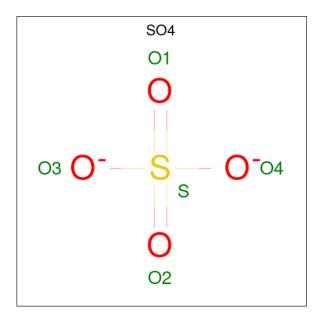
There are 4 unique types of molecules in this entry. The entry contains 2163 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (BOVINE SEMINAL RIBONUCLEASE).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	124	Total	С	Ν	0	S	0	0	0
	A	124	941	571	171	184	15	0		
1	В	124	Total	С	Ν	0	S	0	0	0
1	D	124	941	571	171	184	15	0	0	0

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



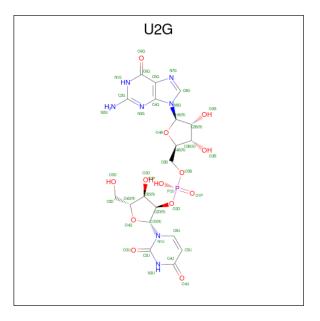
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is URIDYLYL-2'-5'-PHOSPHO-GUANOSINE (three-letter code: U2G) (formula: $C_{19}H_{24}N_7O_{13}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C N O P 33 15 6 11 1	0	0
3	А	1	Total C N O P 40 19 7 13 1	0	0
3	А	1	Total C N O 20 10 5 5	0	0
3	В	1	Total C N O P 24 10 5 8 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	72	TotalO7272	0	0



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Mol	Chain	Residues Atoms		ZeroOcc	AltConf
4	В	52	$\begin{array}{cc} \text{Total} & \text{O} \\ 52 & 52 \end{array}$	0	0

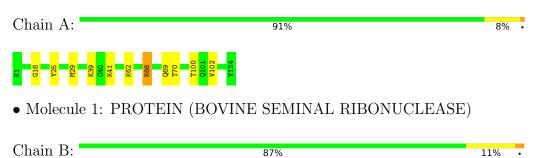


3 Residue-property plots (i)

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 (BOVINE SEMINAL RIBONUCLEASE)







4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants	36.40Å 66.70Å 107.70Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 - 1.90	Depositor
% Data completeness	92.1 (12.00-1.90)	Depositor
(in resolution range)	52.1 (12.00 1.50)	Depositor
R_{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2163	wwPDB-VP
Average B, all atoms $(Å^2)$	23.0	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: SO4, $\rm U2G$

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.75	0/956	0.81	0/1281	
1	В	0.69	0/956	0.80	1/1281~(0.1%)	
All	All	0.72	0/1912	0.81	1/2562~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
1	В	80	ARG	NE-CZ-NH2	-5.61	117.50	120.30

There are no chirality outliers.

There are no planarity outliers.

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	А	941	0	924	7	0
1	В	941	0	924	10	0
2	А	25	0	0	0	0
2	В	15	0	0	1	0
3	А	93	0	55	4	0
3	В	24	0	12	3	0
4	А	72	0	0	1	0
4	В	52	0	0	0	0



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Mol	Chain	Non-H H(model)		H(added)	Clashes	Symm-Clashes	
All	All	2163	0	1915	19	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 5.

All (19) 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:B:85:ARG:HH22	3:B:133:U2G:H5G2	1.37	0.90
1:B:85:ARG:NH2	3:B:133:U2G:H5G2	2.04	0.72
1:B:22:SER:N	2:B:129:SO4:O3	2.29	0.65
3:B:133:U2G:O5B	3:B:133:U2G:H8G	1.99	0.62
1:A:41:LYS:HE3	3:A:132:U2G:C2G	2.31	0.60
1:A:25:TYR:CZ	1:A:29:MET:HG3	2.38	0.58
1:A:66:LYS:HE3	3:A:130:U2G:O2B	2.05	0.56
3:A:130:U2G:O2P	3:A:130:U2G:H3G'	2.07	0.54
1:B:65:CYS:SG	1:B:69:GLN:HG3	2.49	0.52
1:B:92:TYR:CD1	1:B:93:PRO:HA	2.46	0.49
1:B:25:TYR:CZ	1:B:29:MET:HG3	2.47	0.49
1:A:62:LYS:NZ	1:A:70:THR:O	2.39	0.48
1:B:1:LYS:HD3	1:B:2:GLU:O	2.14	0.47
1:A:16:GLY:O	1:B:80:ARG:NH2	2.43	0.46
1:B:43:VAL:HG22	1:B:85:ARG:HG3	1.98	0.46
1:A:69:GLN:HG3	4:A:315:HOH:O	2.16	0.45
1:A:100:THR:HG22	1:A:102:VAL:HG13	1.99	0.43
3:A:130:U2G:N2G	3:A:132:U2G:H1G'	2.34	0.42
1:B:74:GLN:NE2	1:B:124:VAL:HG11	2.36	0.41

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	Perce	entiles
1	А	122/124~(98%)	118 (97%)	4(3%)	0	100	100
1	В	122/124~(98%)	115 (94%)	7~(6%)	0	100	100
All	All	244/248~(98%)	233~(96%)	11 (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 side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	110/110~(100%)	108~(98%)	2(2%)	59 55		
1	В	110/110 (100%)	107~(97%)	3(3%)	44 38		
All	All	220/220~(100%)	215~(98%)	5(2%)	50 45		

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	39	LYS
1	А	66	LYS
1	В	34	LYS
1	В	37	GLN
1	В	85	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such side chains are listed below:

Mol	Chain	Res	Type
1	А	11	GLN
1	А	74	GLN
1	В	11	GLN
1	В	17	ASN
1	В	71	ASN
1	В	74	GLN



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)

12 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	Trune	Chain	Res	Link	Bo	ond leng	ths	B	ond ang	les
10101	Type	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	U2G	А	132	-	18,22,44	1.10	2 (11%)	19,33,67	0.71	1 (5%)
2	SO4	А	128	-	4,4,4	0.44	0	6,6,6	1.14	1 (16%)
3	U2G	А	130	-	31,36,44	1.19	3 (9%)	37,55,67	0.90	1 (2%)
2	SO4	А	134	-	4,4,4	1.25	0	6,6,6	0.92	0
3	U2G	А	131	-	40,44,44	0.86	3 (7%)	52,67,67	0.95	2 (3%)
2	SO4	В	127	-	4,4,4	0.99	0	6,6,6	0.61	0
2	SO4	В	129	-	4,4,4	0.67	0	6,6,6	0.99	0
2	SO4	А	135	-	4,4,4	1.06	0	6,6,6	0.50	0
2	SO4	А	125	-	4,4,4	0.48	0	6,6,6	0.78	0
2	SO4	В	136	-	4,4,4	0.61	0	6,6,6	1.10	0
2	SO4	А	126	-	4,4,4	0.57	0	6,6,6	0.54	0
3	U2G	В	133	-	22,26,44	0.96	2 (9%)	26,40,67	1.02	2 (7%)

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.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	U2G	А	132	-	-	0/2/22/53	0/3/3/5
3	U2G	В	133	-	-	1/6/26/53	0/3/3/5
3	U2G	А	130	-	-	2/13/49/53	0/4/4/5
3	U2G	А	131	-	-	5/17/53/53	0/5/5/5

'-' means no outliers of that kind were identified.

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
3	А	130	U2G	C5G-C6G	-4.64	1.38	1.47
3	А	131	U2G	C5G-C6G	-2.89	1.41	1.47
3	А	132	U2G	C5G-C6G	-2.73	1.41	1.47
3	А	130	U2G	C8G-N7G	-2.50	1.30	1.35
3	А	132	U2G	C8G-N7G	-2.46	1.30	1.35
3	А	131	U2G	C8G-N7G	-2.37	1.31	1.35
3	А	130	U2G	C5G-C4G	-2.17	1.37	1.43
3	В	133	U2G	P-O2D	2.10	1.62	1.54
3	А	131	U2G	C5G-C4G	-2.08	1.37	1.43
3	В	133	U2G	C8G-N7G	-2.07	1.31	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	А	131	U2G	O2D-C2D-C3D	3.13	123.02	111.68
3	А	130	U2G	O2D-C2D-C3D	2.52	120.83	111.68
3	А	131	U2G	O4B-C1B-C2B	2.51	110.59	106.93
2	А	128	SO4	O4-S-O3	2.49	119.71	109.06
3	В	133	U2G	O6G-C6G-C5G	2.47	129.20	124.37
3	В	133	U2G	O2P-P-O1P	2.31	119.71	110.68
3	А	132	U2G	O6G-C6G-C5G	2.01	128.29	124.37

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	130	U2G	C2D-O2D-P-O5B
3	А	131	U2G	C3B-C4B-C5B-O5B
3	А	131	U2G	C5B-O5B-P-O1P
3	А	131	U2G	O4B-C4B-C5B-O5B
3	А	131	U2G	C5B-O5B-P-O2D
3	А	130	U2G	C4B-C5B-O5B-P



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Mol	Chain	Res	Type	Atoms
3	А	131	U2G	C5B-O5B-P-O2P
3	В	133	U2G	C4B-C5B-O5B-P

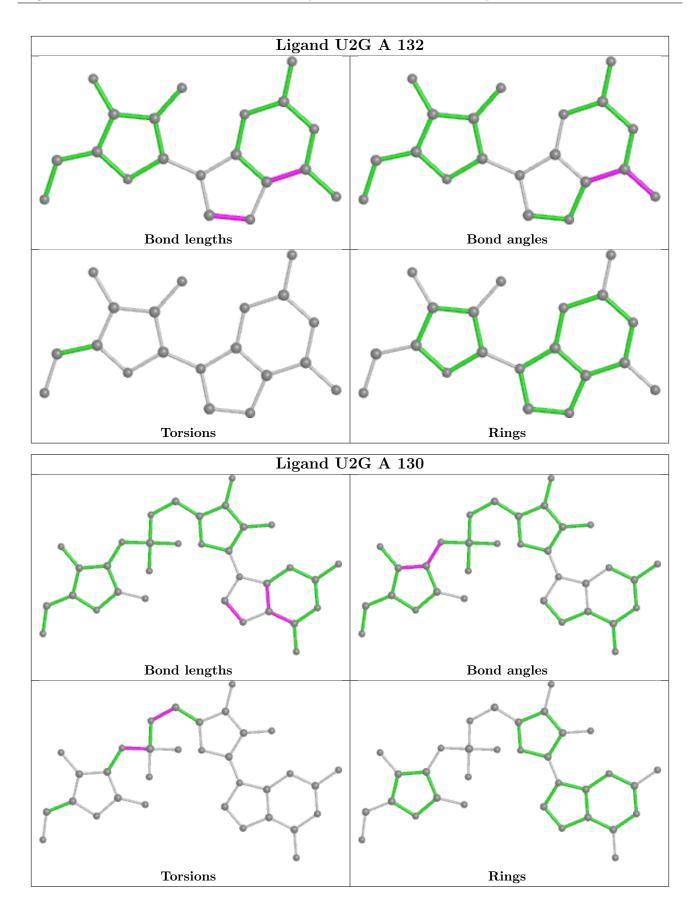
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	132	U2G	2	0
3	А	130	U2G	3	0
2	В	129	SO4	1	0
3	В	133	U2G	3	0

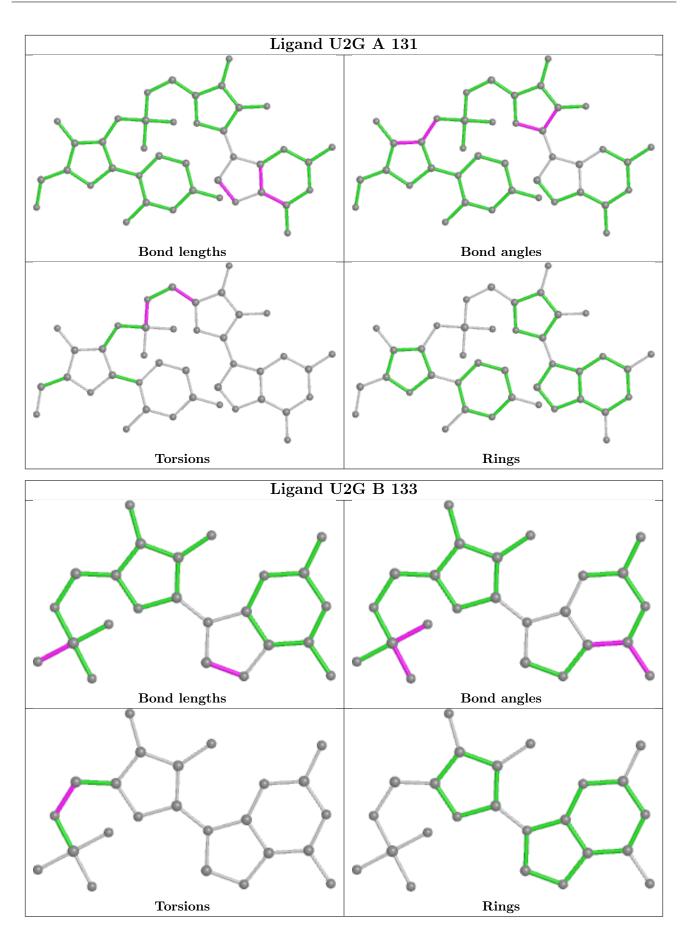
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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













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.

