

Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 - 02:55 am BST

PDB ID	:	296D
Title	:	SEQUENCE-DEPENDENT EFFECTS IN DRUG-DNA INTERACTION:
		THE CRYSTAL STRUCTURE OF HOECHST 33258 BOUND TO THE
		D(CGCAAATTTGCG)2 DUPLEX
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Deposited on		
Resolution	:	2.25 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 following versions of software and data (see references (1)) were used in the production of this report:

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 2.25 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	Percent	tile Ranks	Value
Clashscore 📕			23
Wa	orse		Better
P	ercentile relative to all X-ray stru	uctures	
0 P	ercentile relative to X-ray structu	ures of similar resolution	
Metric	Whole archive	Similar re	solution

Metric	Whole archive	Similar resolution
Metric	$(\# {\it Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	1487 (2.26-2.26)

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 on 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	12	33%	67%	
1	В	12	50%	33%	17%



2 Entry composition (i)

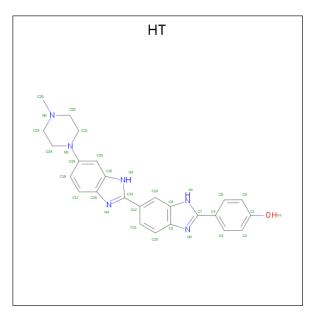
There are 3 unique types of molecules in this entry. The entry contains 583 atoms, of which 0 are hydrogens and 0 are deuteriums.

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(*CP*GP*CP*AP*AP*AP*TP*TP*TP*GP* CP*G)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	12	Total	С	Ν	Ο	Р	0	0	0
1	Л	12	244	117	45	70	12	0	0	0
1	В	12	Total	С	Ν	Ο	Р	0	0	0
1	D	12	244	117	45	70	12	0	0	0

• Molecule 2 is 2'-(4-HYDROXYPHENYL)-5-(4-METHYL-1-PIPERAZINYL)-2,5'-BI-BENZ IMIDAZOLE (three-letter code: HT) (formula: C₂₅H₂₄N₆O).



Mol	Chain	Residues	A	Aton	ıs		ZeroOcc	AltConf
2	В	1	Total 32	$\begin{array}{c} \mathrm{C} \\ 25 \end{array}$		0 1	0	0

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	33	Total O 33 33	0	0
3	В	30	Total O 30 30	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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 colorcoded 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(*CP*GP*CP*AP*AP*AP*TP*TP*TP*GP*CP*G)-3')

Chain A:	33%	67%	
C1 C3 C3 C3 C3 C3 C3 C3 C10 C11 C11 C12 C12			
• Molecule 1: DNA	A $(5'-D(*CP*GP*CP*AP*$	AP*AP*TP*TP*TP*GI	₽*CP*G)-3')

Chain B:	50%	33%	17%
C13 G14 G15 A16 A17 A17 A17 T20 T20 G22 C23 C23 C23			



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	25.27Å 41.32 Å 65.11 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 - 2.25	Depositor
% Data completeness	(Not available) (8.00-2.25)	Depositor
(in resolution range)	(1000 available) (0.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	NUCLSQ	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	583	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: HT

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).

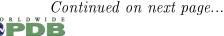
Mol	Chain	Bo	nd lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	4.35	10/273~(3.7%)	3.21	46/419~(11.0%)	
1	В	4.38	11/273~(4.0%)	3.45	50/419~(11.9%)	
All	All	4.36	21/546~(3.8%)	3.33	96/838~(11.5%)	

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	В	0	2

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(A)	Ideal(Å)
1	А	1	DC	P-O5'	-63.56	0.96	1.59
1	В	13	DC	P-O5'	-63.17	0.96	1.59
1	А	7	DT	N1-C6	-8.23	1.32	1.38
1	А	12	DG	P-O5'	7.47	1.67	1.59
1	В	17	DA	N3-C4	7.04	1.39	1.34
1	В	22	DG	C5'-C4'	6.53	1.58	1.51
1	А	9	DT	C5-C7	5.95	1.53	1.50
1	А	9	DT	N1-C6	-5.82	1.34	1.38
1	В	19	DT	C5'-C4'	-5.66	1.45	1.51
1	А	9	DT	C5'-C4'	-5.61	1.45	1.51
1	В	20	DT	C4-C5	-5.60	1.40	1.45
1	А	1	DC	C4'-C3'	-5.59	1.47	1.52
1	В	17	DA	C4'-C3'	-5.47	1.47	1.52
1	В	17	DA	C5'-C4'	-5.32	1.45	1.51
1	В	22	DG	C5-C4	-5.32	1.34	1.38
1	В	22	DG	C4'-C3'	5.30	1.58	1.53

All (21) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	В	14	DG	C4'- $C3$ '	-5.26	1.47	1.52
1	В	20	DT	C5'-C4'	5.25	1.57	1.51
1	А	9	DT	C5-C6	-5.22	1.30	1.34
1	А	12	DG	N7-C5	5.22	1.42	1.39
1	А	6	DA	O3'-P	-5.04	1.55	1.61

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All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	23	DC	O4'-C1'-N1	18.53	120.97	108.00
1	В	19	DT	O4'-C1'-C2'	-15.62	93.41	105.90
1	В	20	DT	O4'-C1'-C2'	-15.30	93.66	105.90
1	А	1	DC	P-O3'-C3'	12.99	135.29	119.70
1	В	21	DT	N3-C2-O2	-12.86	114.58	122.30
1	В	21	DT	C6-C5-C7	-11.94	115.73	122.90
1	В	21	DT	N1-C2-N3	11.93	121.76	114.60
1	А	9	DT	C6-C5-C7	-11.75	115.85	122.90
1	А	7	DT	O4'-C1'-C2'	-10.73	97.31	105.90
1	А	1	DC	P-O5'-C5'	-10.63	103.89	120.90
1	А	7	DT	C4-C5-C6	10.43	124.26	118.00
1	А	5	DA	C4'-C3'-C2'	-10.36	93.77	103.10
1	В	19	DT	O4'-C1'-N1	10.12	115.08	108.00
1	В	16	DA	P-O3'-C3'	9.62	131.24	119.70
1	А	4	DA	P-O3'-C3'	9.55	131.17	119.70
1	В	19	DT	C1'-O4'-C4'	-9.51	100.59	110.10
1	А	7	DT	N3-C2-O2	-9.36	116.69	122.30
1	А	1	DC	O4'-C1'-C2'	-9.32	98.44	105.90
1	В	20	DT	O4'-C1'-N1	9.32	114.53	108.00
1	А	4	DA	O4'-C1'-C2'	-9.13	98.60	105.90
1	В	20	DT	N3-C4-O4	8.90	125.24	119.90
1	В	14	DG	O4'-C1'-N9	8.90	114.23	108.00
1	А	4	DA	N1-C2-N3	8.60	133.60	129.30
1	А	8	DT	C6-C5-C7	-8.57	117.76	122.90
1	В	21	DT	C5-C4-O4	8.49	130.84	124.90
1	В	19	DT	C6-C5-C7	-8.49	117.81	122.90
1	В	13	DC	P-O5'-C5'	-8.44	107.40	120.90
1	А	2	DG	O4'-C1'-N9	8.40	113.88	108.00
1	В	13	DC	P-O3'-C3'	8.36	129.73	119.70
1	В	24	DG	O4'-C4'-C3'	-8.36	100.98	106.00
1	А	3	DC	O4'-C1'-C2'	-8.27	99.28	105.90
1	В	21	DT	N3-C4-O4	-8.27	114.94	119.90
1	В	17	DA	P-O5'-C5'	-8.11	107.92	120.90

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Mol	nuea fron Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	1	DC	O4'-C4'-C3'	-8.00	101.20	106.00
1	А	6	DA	O4'-C1'-N9	7.97	113.58	108.00
1	А	5	DA	P-O3'-C3'	7.95	129.25	119.70
1	В	19	DT	C4-C5-C6	7.93	122.76	118.00
1	А	2	DG	P-O3'-C3'	7.76	129.02	119.70
1	В	16	DA	O4'-C1'-N9	7.60	113.32	108.00
1	А	10	DG	P-O5'-C5'	-7.53	108.85	120.90
1	А	7	DT	N1-C2-N3	7.50	119.10	114.60
1	В	13	DC	N3-C4-N4	7.48	123.23	118.00
1	В	20	DT	C4'-C3'-C2'	-7.47	96.38	103.10
1	А	4	DA	O4'-C1'-N9	7.34	113.14	108.00
1	В	18	DA	O4'-C1'-C2'	-7.15	100.18	105.90
1	В	23	DC	C4'-C3'-C2'	-7.09	96.72	103.10
1	А	5	DA	O4'-C1'-C2'	-7.06	100.25	105.90
1	А	3	DC	O4'-C1'-N1	7.04	112.93	108.00
1	А	9	DT	C4-C5-C7	6.92	123.16	119.00
1	В	15	DC	P-O3'-C3'	6.88	127.95	119.70
1	В	21	DT	C4-C5-C7	6.66	123.00	119.00
1	А	10	DG	P-O3'-C3'	6.66	127.69	119.70
1	В	13	DC	C4'-C3'-C2'	-6.64	97.12	103.10
1	А	9	DT	O4'-C4'-C3'	6.62	109.97	106.00
1	А	5	DA	O4'-C1'-N9	6.57	112.60	108.00
1	А	2	DG	P-O5'-C5'	6.46	131.24	120.90
1	В	19	DT	O4'-C4'-C3'	-6.33	101.97	104.50
1	В	13	DC	C5-C4-N4	-6.26	115.82	120.20
1	В	21	DT	O4'-C1'-C2'	-6.24	100.91	105.90
1	В	17	DA	N7-C8-N9	-6.12	110.74	113.80
1	А	8	DT	O5'-P-OP2	-6.10	100.21	105.70
1	А	10	DG	O4'-C1'-C2'	-6.10	101.02	105.90
1	В	22	DG	O4'-C1'-N9	6.08	112.25	108.00
1	А	6	DA	N7-C8-N9	6.05	116.83	113.80
1	В	21	DT	C2-N3-C4	-6.03	123.58	127.20
1	А	8	DT	C4-C5-C6	5.91	121.55	118.00
1	В	17	DA	O3'-P-O5'	-5.91	92.77	104.00
1	А	8	DT	O4'-C1'-N1	5.90	112.13	108.00
1	А	4	DA	C6-N1-C2	-5.89	115.07	118.60
1	В	23	DC	N3-C4-C5	5.85	124.24	121.90
1	В	14	DG	C5-C6-N1	-5.84	108.58	111.50
1	А	10	DG	O4'-C4'-C3'	-5.83	102.17	104.50
1	В	14	DG	N1-C6-O6	5.80	123.38	119.90
1	А	7	DT	N3-C4-C5	-5.80	111.72	115.20
1	А	7	DT	C6-C5-C7	-5.72	119.47	122.90

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	22	DG	C1'-O4'-C4'	-5.58	104.52	110.10
1	В	21	DT	C6-N1-C2	-5.55	118.53	121.30
1	А	10	DG	C4'-C3'-O3'	-5.55	95.84	109.70
1	А	2	DG	O4'-C1'-C2'	-5.52	101.48	105.90
1	А	8	DT	O4'-C1'-C2'	-5.50	101.50	105.90
1	В	23	DC	C5-C4-N4	-5.46	116.38	120.20
1	В	14	DG	N3-C2-N2	-5.44	116.09	119.90
1	В	21	DT	C4-C5-C6	5.44	121.27	118.00
1	А	6	DA	C4'-C3'-C2'	-5.39	98.24	103.10
1	В	16	DA	N1-C2-N3	5.32	131.96	129.30
1	В	21	DT	O4'-C4'-C3'	-5.29	102.39	104.50
1	В	17	DA	C5-N7-C8	5.27	106.54	103.90
1	А	1	DC	C1'-O4'-C4'	5.26	115.36	110.10
1	В	20	DT	C4-C5-C6	5.23	121.14	118.00
1	А	7	DT	C6-N1-C2	-5.22	118.69	121.30
1	А	9	DT	P-O3'-C3'	5.19	125.93	119.70
1	А	2	DG	N3-C4-C5	-5.15	126.02	128.60
1	В	15	DC	N3-C4-N4	5.09	121.56	118.00
1	А	2	DG	C4-C5-C6	5.05	121.83	118.80
1	В	21	DT	C5-C6-N1	-5.03	120.68	123.70
1	В	20	DT	C5-C4-O4	-5.00	121.40	124.90

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There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	14	DG	Sidechain
1	В	15	DC	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	А	244	0	137	12	0
1	В	244	0	137	7	0
2	В	32	0	24	4	0
3	А	33	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	30	0	0	0	0
All	All	583	0	298	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 23.

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:A:1:DC:C6	1:A:1:DC:P	2.32	1.22
1:A:1:DC:N1	1:A:1:DC:P	2.41	0.93
1:A:1:DC:P	1:A:1:DC:C1'	2.58	0.90
1:A:8:DT:H2"	1:A:9:DT:H5'	1.63	0.80
1:A:6:DA:H8	3:A:72:HOH:O	1.77	0.68
1:A:11:DC:O4'	2:B:25:HT:H252	1.98	0.64
1:B:18:DA:H5'	2:B:25:HT:H241	1.81	0.61
1:A:1:DC:P	1:A:1:DC:C2'	2.89	0.60
1:A:5:DA:H2"	3:A:72:HOH:O	2.05	0.56
1:B:15:DC:H2'	1:B:16:DA:C8	2.44	0.53
1:A:3:DC:H2"	1:A:4:DA:C8	2.45	0.52
1:A:9:DT:H2"	1:A:10:DG:C8	2.45	0.51
1:B:13:DC:H2"	1:B:14:DG:C8	2.45	0.50
1:A:1:DC:H2'	1:A:1:DC:P	2.54	0.47
1:B:17:DA:N3	2:B:25:HT:H20	2.32	0.44
1:B:17:DA:H2'	1:B:17:DA:O5'	2.18	0.44
1:A:9:DT:H2'	1:A:9:DT:H6	1.67	0.43
1:B:13:DC:H6	1:B:13:DC:C5'	2.32	0.42
1:B:17:DA:C2	2:B:25:HT:H20	2.56	0.41

There are no symmetry-related clashes.

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)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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		
			nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HT	В	25	-	37,37,37	1.31	3 (8%)	43,54,54	1.66	10 (23%)

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	ΗT	В	25	-	-	2/12/22/22	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	В	25	ΗT	C4-C7	-4.08	1.37	1.48
2	В	25	ΗT	C12-C14	-3.36	1.39	1.48
2	В	25	ΗT	C10-C11	2.19	1.41	1.36



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	25	ΗT	C14-N3-C15	4.69	113.08	103.78
2	В	25	ΗT	C7-N1-C8	4.19	112.08	103.78
2	В	25	ΗT	C12-C13-C8	-3.38	118.48	121.44
2	В	25	ΗT	C25-N6-C22	2.90	115.00	110.66
2	В	25	ΗT	C20-C15-N3	2.58	138.21	130.83
2	В	25	ΗT	C19-C20-C15	-2.57	119.22	121.02
2	В	25	ΗT	C18-C17-C16	2.16	123.56	120.84
2	В	25	ΗT	C7-N2-C9	-2.09	99.63	103.78
2	В	25	ΗT	C13-C8-N1	2.08	136.79	130.83
2	В	25	ΗT	C11-C10-C9	2.04	123.41	120.84

All (10) bond angle outliers are listed below:

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	25	HT	C20-C19-N5-C24
2	В	25	HT	C18-C19-N5-C24

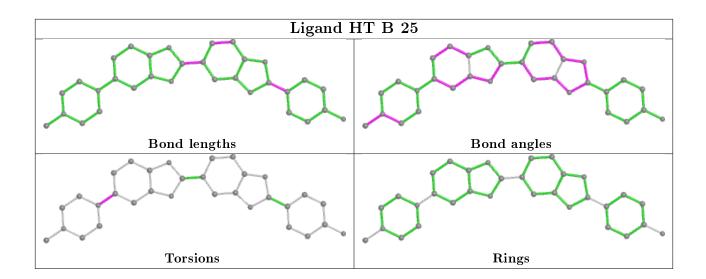
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	25	HT	4	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.

