



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 07:37 pm GMT

PDB ID : 2BJ6  
Title : CRYSTAL STRUCTURE OF A DECAMERIC HNA-RNA HYBRID  
Authors : Maier, T.; Przytylski, I.; Straeter, N.; Herdewijn, P.; Saenger, W.  
Deposited on : 2005-01-30  
Resolution : 2.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

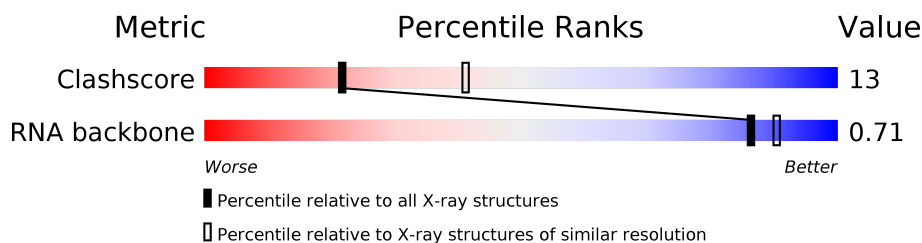
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	112137	2895 (2.60-2.60)
RNA backbone	2435	1140 (3.00-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	10	
1	B	10	
1	C	10	
1	D	10	
2	E	10	
2	F	10	
2	G	10	
2	H	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
1	6HC	B	10	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1876 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 SYNTHETIC HNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	10	Total	C	N	O	P	0	0	0
			209	106	36	58	9			
1	B	10	Total	C	N	O	P	0	0	0
			209	106	36	58	9			
1	C	10	Total	C	N	O	P	0	0	0
			209	106	36	58	9			
1	D	10	Total	C	N	O	P	0	0	0
			209	106	36	58	9			

- Molecule 2 is a RNA chain called 5'-R(\*GP\*GP\*CP\*AP\*UP\*UP\*AP\*CP\*GP\*GP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	10	Total	C	N	O	P	0	0	0
			213	96	40	68	9			
2	F	10	Total	C	N	O	P	0	0	0
			213	96	40	68	9			
2	G	10	Total	C	N	O	P	0	0	0
			213	96	40	68	9			
2	H	10	Total	C	N	O	P	0	0	0
			213	96	40	68	9			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total	O	0	0
			36	36		
4	B	16	Total	O	0	0
			16	16		
4	C	20	Total	O	0	0
			20	20		
4	D	13	Total	O	0	0
			13	13		
4	E	26	Total	O	0	0
			26	26		
4	F	17	Total	O	0	0
			17	17		
4	G	28	Total	O	0	0
			28	28		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	7	Total	O	0	0
			7	7		

### 3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

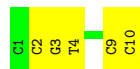
- Molecule 1: SYNTHETIC HNA

Chain A: 



- Molecule 1: SYNTHETIC HNA

Chain B: 



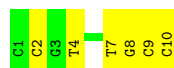
- Molecule 1: SYNTHETIC HNA

Chain C: 




- Molecule 1: SYNTHETIC HNA

Chain D: 



- Molecule 2: 5'-R(\*GP\*GP\*CP\*AP\*UP\*UP\*AP\*CP\*GP\*GP)-3'

Chain E: 



- Molecule 2: 5'-R(\*GP\*GP\*CP\*AP\*UP\*UP\*AP\*CP\*GP\*GP)-3'

Chain F: 



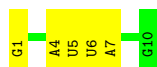
- Molecule 2: 5'-R(\*GP\*GP\*CP\*AP\*UP\*UP\*AP\*CP\*GP\*GP)-3'

Chain G: 



- Molecule 2: 5'-R(\*GP\*GP\*CP\*AP\*UP\*UP\*AP\*CP\*GP\*GP)-3'

Chain H: 





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.91Å 113.91Å 55.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.60	Depositor
% Data completeness (in resolution range)	99.8 (35.00-2.60)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.217 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1876	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	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: 6HT, 6HG, 6HA, SO4, 6HC

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	$\# Z  > 5$
2	E	0.78	0/238	0.88	0/370
2	F	0.67	0/238	0.79	0/370
2	G	0.68	0/238	0.81	0/370
2	H	0.52	0/238	0.66	0/370
All	All	0.67	0/952	0.79	0/1480

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
2	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	5	U	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	209	0	133	3	0
1	B	209	0	133	12	0
1	C	209	0	133	5	0
1	D	209	0	133	8	0
2	E	213	0	110	0	0
2	F	213	0	110	1	0
2	G	213	0	110	4	0
2	H	213	0	110	5	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	E	5	0	0	0	0
3	G	10	0	0	0	0
4	A	36	0	0	0	0
4	B	16	0	0	0	0
4	C	20	0	0	2	0
4	D	13	0	0	1	0
4	E	26	0	0	0	0
4	F	17	0	0	0	0
4	G	28	0	0	0	0
4	H	7	0	0	0	0
All	All	1876	0	972	36	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 13.

All (36) 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:9:6HC:H2''	1:B:10:6HC:O5'	1.84	0.77
1:D:4:6HT:H72	4:D:2005:HOH:O	1.94	0.66
1:B:10:6HC:H3'	1:B:10:6HC:C6	2.26	0.66
1:B:10:6HC:H3'	1:B:10:6HC:H6	1.84	0.59
1:D:2:6HC:H6	1:D:2:6HC:O4'	2.07	0.54
1:C:4:6HT:P	4:C:2004:HOH:O	2.66	0.54
1:B:9:6HC:O4'	1:B:9:6HC:H6	2.09	0.53
2:G:8:C:H2'	2:G:9:G:O4'	2.09	0.53
1:B:9:6HC:C2'	1:B:10:6HC:O5'	2.56	0.52
1:D:7:6HT:O4'	1:D:7:6HT:H6	2.11	0.51
2:H:4:A:O2'	2:H:5:U:H5'	2.12	0.50
2:H:5:U:O2'	2:H:6:U:H5'	2.12	0.49
1:A:9:6HC:O4'	1:A:9:6HC:H6	2.12	0.48
1:D:4:6HT:O4'	1:D:4:6HT:H6	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:6HC:H5	4:C:2002:HOH:O	2.13	0.47
2:H:6:U:H2'	2:H:7:A:H8	1.80	0.47
1:D:7:6HT:H71	1:D:7:6HT:OP2	2.14	0.46
2:G:9:G:O2'	2:G:10:G:H5'	2.15	0.46
1:C:9:6HC:H6	1:C:9:6HC:O4'	2.15	0.46
1:B:10:6HC:O4'	1:B:10:6HC:H6	2.15	0.46
1:B:4:6HT:H6	1:B:4:6HT:O4'	2.16	0.45
1:B:10:6HC:C3'	1:B:10:6HC:C6	2.95	0.45
1:B:10:6HC:C3'	1:B:10:6HC:H6	2.47	0.45
1:A:10:6HC:H6	1:A:10:6HC:O4'	2.18	0.44
1:B:2:6HC:H6	1:B:2:6HC:O4'	2.17	0.44
1:D:8:6HG:H2''	1:D:9:6HC:O4'	2.16	0.44
1:D:9:6HC:H6	1:D:9:6HC:O4'	2.18	0.44
1:B:10:6HC:C2	2:F:1:G:H1	2.30	0.44
1:C:4:6HT:O4'	1:C:4:6HT:H6	2.18	0.44
2:H:6:U:H2'	2:H:7:A:C8	2.54	0.43
1:A:1:6HC:O4'	1:A:1:6HC:H6	2.17	0.43
2:G:7:A:O2'	2:G:8:C:H5'	2.20	0.42
1:D:10:6HC:C2	2:H:1:G:H22	2.32	0.41
1:C:4:6HT:H2''	1:C:5:6HA:O4'	2.20	0.41
1:B:3:6HG:O4'	1:B:3:6HG:H8	2.21	0.41
2:G:4:A:O2'	2:G:5:U:H5'	2.21	0.40

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](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	9/10 (90%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	9/10 (90%)	0	0
2	G	9/10 (90%)	0	0
2	H	9/10 (90%)	0	0
All	All	36/40 (90%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains

40 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	6HC	A	1	1,2	15,18,22	0.84	0	14,25,32	0.72	0
1	6HC	A	10	1,2	15,21,22	0.91	0	16,29,32	0.90	0
1	6HC	A	2	1,2	15,21,22	0.83	0	16,29,32	0.99	1 (6%)
1	6HG	A	3	1,2	18,25,26	1.22	1 (5%)	18,36,39	2.72	4 (22%)
1	6HT	A	4	1,2	14,22,23	1.17	2 (14%)	15,31,34	4.39	3 (20%)
1	6HA	A	5	1,2	18,24,25	0.82	0	16,34,37	0.83	0
1	6HA	A	6	1,2	18,24,25	0.64	0	16,34,37	0.66	0
1	6HT	A	7	1,2	14,22,23	1.23	1 (7%)	15,31,34	4.39	3 (20%)
1	6HG	A	8	1,2	18,25,26	1.08	1 (5%)	18,36,39	2.76	4 (22%)
1	6HC	A	9	1,2	15,21,22	0.79	0	16,29,32	0.85	0
1	6HC	B	1	1,2	15,18,22	0.96	1 (6%)	14,25,32	0.87	0
1	6HC	B	10	1,2	15,21,22	0.81	0	16,29,32	1.07	1 (6%)
1	6HC	B	2	1,2	15,21,22	1.04	2 (13%)	16,29,32	0.82	0
1	6HG	B	3	1,2	18,25,26	1.16	3 (16%)	18,36,39	2.75	4 (22%)
1	6HT	B	4	1,2	14,22,23	1.27	2 (14%)	15,31,34	4.28	3 (20%)
1	6HA	B	5	1,2	18,24,25	0.62	0	16,34,37	0.89	0
1	6HA	B	6	1,2	18,24,25	0.66	0	16,34,37	0.90	0
1	6HT	B	7	1,2	14,22,23	1.02	2 (14%)	15,31,34	4.45	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	6HG	B	8	1,2	18,25,26	1.09	2 (11%)	18,36,39	2.67	4 (22%)
1	6HC	B	9	1,2	15,21,22	0.95	0	16,29,32	0.87	0
1	6HC	C	1	1,2	15,18,22	0.84	1 (6%)	14,25,32	0.84	0
1	6HC	C	10	1,2	15,21,22	0.89	0	16,29,32	0.96	1 (6%)
1	6HC	C	2	1,2	15,21,22	0.88	0	16,29,32	0.71	0
1	6HG	C	3	1,2	18,25,26	1.24	1 (5%)	18,36,39	2.72	5 (27%)
1	6HT	C	4	1,2	14,22,23	1.28	3 (21%)	15,31,34	4.43	3 (20%)
1	6HA	C	5	1,2	18,24,25	0.67	0	16,34,37	0.74	0
1	6HA	C	6	1,2	18,24,25	0.67	0	16,34,37	0.80	0
1	6HT	C	7	1,2	14,22,23	1.12	2 (14%)	15,31,34	4.32	3 (20%)
1	6HG	C	8	1,2	18,25,26	1.16	1 (5%)	18,36,39	2.76	5 (27%)
1	6HC	C	9	1,2	15,21,22	1.05	0	16,29,32	1.00	0
1	6HC	D	1	1,2	15,18,22	0.84	0	14,25,32	0.67	0
1	6HC	D	10	1,2	15,21,22	0.83	0	16,29,32	0.76	0
1	6HC	D	2	1,2	15,21,22	1.03	1 (6%)	16,29,32	0.69	0
1	6HG	D	3	1,2	18,25,26	1.16	2 (11%)	18,36,39	2.77	5 (27%)
1	6HT	D	4	1,2	14,22,23	1.21	2 (14%)	15,31,34	4.41	5 (33%)
1	6HA	D	5	1,2	18,24,25	0.75	0	16,34,37	0.71	0
1	6HA	D	6	1,2	18,24,25	0.76	0	16,34,37	0.85	0
1	6HT	D	7	1,2	14,22,23	1.14	2 (14%)	15,31,34	4.44	3 (20%)
1	6HG	D	8	1,2	18,25,26	1.18	1 (5%)	18,36,39	2.79	5 (27%)
1	6HC	D	9	1,2	15,21,22	0.89	0	16,29,32	0.64	0

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	6HC	A	1	1,2	-	0/4/19/23	0/2/2/2
1	6HC	A	10	1,2	-	0/5/22/23	0/2/2/2
1	6HC	A	2	1,2	-	0/5/22/23	0/2/2/2
1	6HG	A	3	1,2	-	0/3/22/23	0/3/3/3
1	6HT	A	4	1,2	-	0/5/22/23	0/2/2/2
1	6HA	A	5	1,2	-	0/3/22/23	0/3/3/3
1	6HA	A	6	1,2	-	0/3/22/23	0/3/3/3
1	6HT	A	7	1,2	-	0/5/22/23	0/2/2/2
1	6HG	A	8	1,2	-	0/3/22/23	0/3/3/3
1	6HC	A	9	1,2	-	0/5/22/23	0/2/2/2
1	6HC	B	1	1,2	-	0/4/19/23	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	6HC	B	10	1,2	-	0/5/22/23	0/2/2/2
1	6HC	B	2	1,2	-	0/5/22/23	0/2/2/2
1	6HG	B	3	1,2	-	0/3/22/23	0/3/3/3
1	6HT	B	4	1,2	-	0/5/22/23	0/2/2/2
1	6HA	B	5	1,2	-	0/3/22/23	0/3/3/3
1	6HA	B	6	1,2	-	0/3/22/23	0/3/3/3
1	6HT	B	7	1,2	-	0/5/22/23	0/2/2/2
1	6HG	B	8	1,2	-	0/3/22/23	0/3/3/3
1	6HC	B	9	1,2	-	0/5/22/23	0/2/2/2
1	6HC	C	1	1,2	-	0/4/19/23	0/2/2/2
1	6HC	C	10	1,2	-	0/5/22/23	0/2/2/2
1	6HC	C	2	1,2	-	0/5/22/23	0/2/2/2
1	6HG	C	3	1,2	-	0/3/22/23	0/3/3/3
1	6HT	C	4	1,2	-	0/5/22/23	0/2/2/2
1	6HA	C	5	1,2	-	0/3/22/23	0/3/3/3
1	6HA	C	6	1,2	-	0/3/22/23	0/3/3/3
1	6HT	C	7	1,2	-	0/5/22/23	0/2/2/2
1	6HG	C	8	1,2	-	0/3/22/23	0/3/3/3
1	6HC	C	9	1,2	-	0/5/22/23	0/2/2/2
1	6HC	D	1	1,2	-	0/4/19/23	0/2/2/2
1	6HC	D	10	1,2	-	0/5/22/23	0/2/2/2
1	6HC	D	2	1,2	-	0/5/22/23	0/2/2/2
1	6HG	D	3	1,2	-	0/3/22/23	0/3/3/3
1	6HT	D	4	1,2	-	0/5/22/23	0/2/2/2
1	6HA	D	5	1,2	-	0/3/22/23	0/3/3/3
1	6HA	D	6	1,2	-	0/3/22/23	0/3/3/3
1	6HT	D	7	1,2	-	0/5/22/23	0/2/2/2
1	6HG	D	8	1,2	-	0/3/22/23	0/3/3/3
1	6HC	D	9	1,2	-	0/5/22/23	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	2	6HC	O5'-C5'	-2.45	1.41	1.44
1	C	4	6HT	C6-C5	-2.38	1.33	1.40
1	D	7	6HT	C6-C5	-2.33	1.33	1.40
1	C	4	6HT	O5'-C5'	-2.31	1.41	1.44
1	B	4	6HT	C6-C5	-2.30	1.34	1.40
1	B	3	6HG	C8-N7	-2.25	1.30	1.34
1	C	7	6HT	C6-C5	-2.22	1.34	1.40
1	B	1	6HC	C6-C5	-2.18	1.33	1.38
1	B	8	6HG	C8-N7	-2.14	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4	6HT	C6-C5	-2.14	1.34	1.40
1	B	2	6HC	C6-C5	-2.12	1.33	1.38
1	A	4	6HT	C6-C5	-2.12	1.34	1.40
1	D	3	6HG	C8-N7	-2.09	1.30	1.34
1	B	3	6HG	O5'-C5'	-2.09	1.41	1.44
1	B	2	6HC	O5'-C5'	-2.08	1.41	1.44
1	B	7	6HT	C6-C5	-2.07	1.34	1.40
1	C	1	6HC	C6-C5	-2.05	1.33	1.38
1	B	7	6HT	C4-N3	2.65	1.37	1.33
1	C	7	6HT	C4-N3	2.87	1.38	1.33
1	D	7	6HT	C4-N3	2.92	1.38	1.33
1	A	7	6HT	C4-N3	3.04	1.38	1.33
1	C	4	6HT	C4-N3	3.07	1.38	1.33
1	A	8	6HG	C6-N1	3.10	1.38	1.33
1	A	4	6HT	C4-N3	3.14	1.38	1.33
1	B	3	6HG	C6-N1	3.19	1.38	1.33
1	D	4	6HT	C4-N3	3.24	1.38	1.33
1	B	4	6HT	C4-N3	3.42	1.39	1.33
1	B	8	6HG	C6-N1	3.46	1.39	1.33
1	D	3	6HG	C6-N1	3.55	1.39	1.33
1	C	8	6HG	C6-N1	3.55	1.39	1.33
1	C	3	6HG	C6-N1	3.60	1.39	1.33
1	D	8	6HG	C6-N1	3.77	1.39	1.33
1	A	3	6HG	C6-N1	3.77	1.39	1.33

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	6HT	C5-C4-N3	-9.23	115.07	125.24
1	C	4	6HT	C5-C4-N3	-9.15	115.16	125.24
1	D	4	6HT	C5-C4-N3	-9.06	115.26	125.24
1	B	7	6HT	C5-C4-N3	-9.01	115.31	125.24
1	D	7	6HT	C5-C4-N3	-8.97	115.36	125.24
1	B	4	6HT	C5-C4-N3	-8.93	115.40	125.24
1	C	7	6HT	C5-C4-N3	-8.77	115.57	125.24
1	A	7	6HT	C5-C4-N3	-8.64	115.72	125.24
1	D	8	6HG	C5-C6-N1	-8.60	111.24	123.48
1	C	3	6HG	C5-C6-N1	-8.53	111.34	123.48
1	A	3	6HG	C5-C6-N1	-8.43	111.47	123.48
1	D	3	6HG	C5-C6-N1	-8.43	111.48	123.48
1	C	8	6HG	C5-C6-N1	-8.42	111.50	123.48
1	B	3	6HG	C5-C6-N1	-8.37	111.56	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	6HG	C5-C6-N1	-8.22	111.78	123.48
1	A	8	6HG	C5-C6-N1	-8.07	111.99	123.48
1	B	3	6HG	C2-N3-C4	-2.88	111.80	115.16
1	D	3	6HG	C2-N3-C4	-2.82	111.86	115.16
1	D	8	6HG	C2-N3-C4	-2.81	111.88	115.16
1	A	8	6HG	C2-N3-C4	-2.80	111.89	115.16
1	C	3	6HG	C2-N3-C4	-2.73	111.97	115.16
1	B	8	6HG	C2-N3-C4	-2.70	112.01	115.16
1	C	8	6HG	C2-N3-C4	-2.67	112.04	115.16
1	A	3	6HG	C2-N3-C4	-2.63	112.09	115.16
1	A	8	6HG	N3-C2-N1	-2.57	123.71	127.46
1	A	3	6HG	N3-C2-N1	-2.52	123.78	127.46
1	B	8	6HG	N3-C2-N1	-2.34	124.04	127.46
1	C	8	6HG	N3-C2-N1	-2.33	124.06	127.46
1	D	3	6HG	N3-C2-N1	-2.30	124.11	127.46
1	D	8	6HG	N3-C2-N1	-2.28	124.13	127.46
1	D	4	6HT	O3'-C3'-C2'	-2.27	104.53	110.02
1	B	3	6HG	N3-C2-N1	-2.27	124.14	127.46
1	C	3	6HG	N3-C2-N1	-2.25	124.17	127.46
1	A	2	6HC	C5'-C4'-C3'	-2.19	110.64	113.81
1	C	3	6HG	C6-C5-C4	-2.12	118.74	120.84
1	C	8	6HG	C6-C5-C4	-2.12	118.74	120.84
1	C	10	6HC	C5'-C4'-C3'	-2.06	110.82	113.81
1	D	8	6HG	C6-C5-C4	-2.02	118.83	120.84
1	D	3	6HG	C6-C5-C4	-2.02	118.83	120.84
1	B	7	6HT	C5M-C5-C6	2.06	122.78	118.67
1	B	4	6HT	C5M-C5-C6	2.07	122.80	118.67
1	C	4	6HT	C5M-C5-C6	2.09	122.84	118.67
1	D	7	6HT	C5M-C5-C6	2.10	122.87	118.67
1	D	4	6HT	C5M-C5-C6	2.13	122.92	118.67
1	A	4	6HT	C5M-C5-C6	2.18	123.02	118.67
1	C	7	6HT	C5M-C5-C6	2.28	123.21	118.67
1	D	4	6HT	C6'-O4'-C4'	2.31	115.35	112.17
1	A	7	6HT	C5M-C5-C6	2.59	123.84	118.67
1	B	10	6HC	O3'-C3'-C2'	3.09	117.49	110.02
1	B	8	6HG	C6-N1-C2	6.03	124.73	116.06
1	B	3	6HG	C6-N1-C2	6.19	124.96	116.06
1	A	3	6HG	C6-N1-C2	6.19	124.97	116.06
1	C	3	6HG	C6-N1-C2	6.20	124.98	116.06
1	C	8	6HG	C6-N1-C2	6.21	125.00	116.06
1	D	8	6HG	C6-N1-C2	6.33	125.16	116.06
1	D	3	6HG	C6-N1-C2	6.37	125.22	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	6HG	C6-N1-C2	6.38	125.23	116.06
1	B	4	6HT	C4-N3-C2	13.55	127.01	115.16
1	D	4	6HT	C4-N3-C2	13.58	127.04	115.16
1	C	7	6HT	C4-N3-C2	13.75	127.18	115.16
1	A	4	6HT	C4-N3-C2	13.76	127.19	115.16
1	A	7	6HT	C4-N3-C2	13.89	127.30	115.16
1	C	4	6HT	C4-N3-C2	14.02	127.42	115.16
1	D	7	6HT	C4-N3-C2	14.24	127.61	115.16
1	B	7	6HT	C4-N3-C2	14.25	127.62	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	6HC	1	0
1	A	10	6HC	1	0
1	A	9	6HC	1	0
1	B	10	6HC	8	0
1	B	2	6HC	1	0
1	B	3	6HG	1	0
1	B	4	6HT	1	0
1	B	9	6HC	3	0
1	C	2	6HC	1	0
1	C	4	6HT	3	0
1	C	5	6HA	1	0
1	C	9	6HC	1	0
1	D	10	6HC	1	0
1	D	2	6HC	1	0
1	D	4	6HT	2	0
1	D	7	6HT	2	0
1	D	8	6HG	1	0
1	D	9	6HC	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

5 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$
3	SO4	B	1011	-	4,4,4	1.88	1 (25%)	6,6,6	0.97	0
3	SO4	C	1011	-	4,4,4	1.96	1 (25%)	6,6,6	0.93	0
3	SO4	E	1011	-	4,4,4	1.85	1 (25%)	6,6,6	1.01	0
3	SO4	G	1011	-	4,4,4	1.91	2 (50%)	6,6,6	0.91	0
3	SO4	G	1012	-	4,4,4	1.97	1 (25%)	6,6,6	0.92	0

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	SO4	B	1011	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1011	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1011	-	-	0/0/0/0	0/0/0/0
3	SO4	G	1011	-	-	0/0/0/0	0/0/0/0
3	SO4	G	1012	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1011	SO4	O3-S	-2.03	1.30	1.47
3	E	1011	SO4	O1-S	3.20	1.63	1.45
3	G	1011	SO4	O1-S	3.22	1.63	1.45
3	B	1011	SO4	O1-S	3.24	1.63	1.45
3	C	1011	SO4	O1-S	3.40	1.64	1.45
3	G	1012	SO4	O1-S	3.42	1.64	1.45

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.