



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:22 PM GMT

PDB ID : 3V06
Title : Crystal structure of S-6'-Me-3'-fluoro hexitol nucleic acid
Authors : Pallan, P.S.; Egli, M.
Deposited on : 2011-12-07
Resolution : 1.53 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

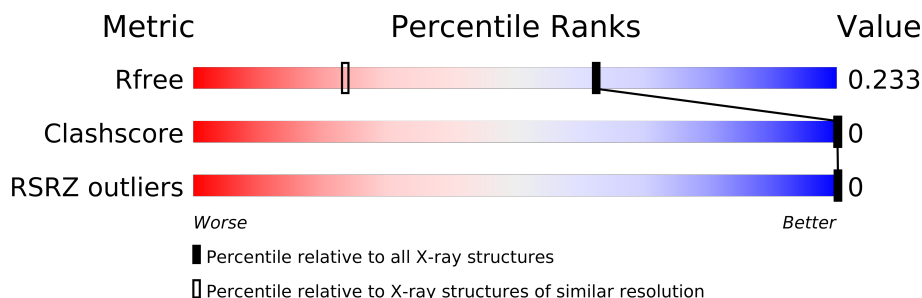
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.53 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))
R_{free}	66092	1031 (1.56-1.52)
Clashscore	79885	1155 (1.56-1.52)
RSRZ outliers	66119	1031 (1.56-1.52)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	10	
1	B	10	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SR	A	201	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 488 atoms, of which 0 are hydrogen and 0 are deuterium.

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(*GP*CP*GP*TP*AP*(F5H)P*AP*CP*GP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	10	Total	C	F	N	O	P	0	0	0
			205	99	1	38	58	9			
1	B	10	Total	C	F	N	O	P	0	0	0
			205	99	1	38	58	9			

- Molecule 2 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Sr	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	30	Total	O	0	0
			30	30		

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 errors 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.

- Molecule 1: DNA (5'-D(*GP*CP*GP*TP*AP*(F5H)P*AP*CP*GP*C)-3')

Chain A: 

G101	G102	G103	T104	A105	A106	A107	C108	G109	C110
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- Molecule 1: DNA (5'-D(*GP*CP*GP*TP*AP*(F5H)P*AP*CP*GP*C)-3')

Chain B: 

G201	G202	G203	T204	A207	C208	G209	C210
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	24.88Å 45.22Å 46.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.45 – 1.53 23.30 – 1.53	Depositor EDS
% Data completeness (in resolution range)	97.0 (32.45-1.53) 97.0 (23.30-1.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.86 (at 1.53Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.167 , 0.227 0.172 , 0.233	Depositor DCC
R_{free} test set	377 reflections (4.85%)	DCC
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 50.2	EDS
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 8157 reflections (0.012%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	488	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: SR, F5H

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	2.17	4/203 (2.0%)	2.62	21/309 (6.8%)
1	B	2.02	7/203 (3.4%)	2.48	16/309 (5.2%)
All	All	2.10	11/406 (2.7%)	2.55	37/618 (6.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	DG	C8-N7	-7.95	1.26	1.30
1	A	105	DA	N9-C4	7.47	1.42	1.37
1	B	204	DT	N1-C2	6.56	1.43	1.38
1	B	208	DC	C4-C5	6.25	1.48	1.43
1	B	207	DA	N7-C5	5.26	1.42	1.39
1	B	208	DC	N1-C6	5.20	1.40	1.37
1	B	209	DG	N9-C4	5.16	1.42	1.38
1	A	110	DC	N1-C6	5.15	1.40	1.37
1	A	107	DA	C8-N7	-5.13	1.27	1.31
1	B	201	DG	O3'-P	-5.08	1.55	1.61
1	B	208	DC	C2-O2	-5.06	1.19	1.24

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	DA	N1-C2-N3	-12.34	123.13	129.30
1	B	203	DG	O4'-C4'-C3'	-10.22	99.87	106.00
1	A	109	DG	C5-N7-C8	-9.28	99.66	104.30
1	B	209	DG	O4'-C1'-C2'	8.79	112.94	105.90
1	A	101	DG	C8-N9-C4	-8.79	102.88	106.40
1	A	104	DT	O4'-C4'-C3'	-8.52	100.89	106.00
1	B	207	DA	C2-N3-C4	8.43	114.81	110.60
1	A	109	DG	O4'-C4'-C3'	-8.32	101.01	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	DG	C4-C5-N7	8.23	114.09	110.80
1	B	210	DC	O4'-C4'-C3'	-8.14	101.11	106.00
1	A	101	DG	N9-C4-C5	7.68	108.47	105.40
1	A	105	DA	C6-N1-C2	7.41	123.05	118.60
1	A	104	DT	C6-C5-C7	-7.28	118.53	122.90
1	B	208	DC	C4'-C3'-C2'	-7.21	96.61	103.10
1	A	108	DC	O4'-C4'-C3'	-7.17	101.63	104.50
1	A	110	DC	C6-N1-C2	6.83	123.03	120.30
1	A	102	DC	N1-C2-O2	-6.74	114.86	118.90
1	A	105	DA	N1-C2-N3	-6.68	125.96	129.30
1	A	109	DG	C6-C5-N7	-6.26	126.65	130.40
1	B	209	DG	C5-N7-C8	6.20	107.40	104.30
1	B	207	DA	C6-N1-C2	6.14	122.29	118.60
1	A	105	DA	C5-C6-N1	-6.13	114.63	117.70
1	B	210	DC	O4'-C1'-N1	-5.98	103.82	108.00
1	A	102	DC	O4'-C4'-C3'	-5.89	102.14	104.50
1	A	108	DC	N1-C2-O2	-5.79	115.42	118.90
1	B	210	DC	C6-N1-C2	5.76	122.60	120.30
1	A	109	DG	N7-C8-N9	5.72	115.96	113.10
1	A	103	DG	C5-C6-N1	-5.68	108.66	111.50
1	B	208	DC	C4-C5-C6	-5.40	114.70	117.40
1	A	103	DG	C4-C5-N7	-5.37	108.65	110.80
1	B	209	DG	C4-C5-N7	-5.29	108.69	110.80
1	B	203	DG	C4-C5-N7	5.28	112.91	110.80
1	A	101	DG	N7-C8-N9	5.23	115.72	113.10
1	B	210	DC	O4'-C1'-C2'	5.16	110.03	105.90
1	A	101	DG	OP2-P-O3'	5.15	116.52	105.20
1	B	204	DT	O4'-C4'-C3'	-5.08	102.47	104.50
1	B	209	DG	C1'-O4'-C4'	-5.07	105.03	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	205	0	0	0	0
1	B	205	0	0	0	0
2	A	1	0	0	0	0
3	A	47	0	0	0	1
3	B	30	0	0	0	1
All	All	488	0	0	0	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 0.

There are no clashes within the asymmetric unit.

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	Distance(Å)	Clash(Å)
3:A:345:HOH:O	3:B:327:HOH:O[4_454]	1.98	0.22

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

There are no protein chains in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein chains in this entry.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 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	F5H	A	106	1	22,24,25	2.06	6 (27%)	27,35,38	2.71	11 (40%)
1	F5H	B	206	1	22,24,25	1.13	2 (9%)	27,35,38	3.43	5 (18%)

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	F5H	A	106	1	-	0/7/29/30	0/2/2/2
1	F5H	B	206	1	-	0/7/29/30	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	F5H	O4-C4	5.48	1.35	1.24
1	A	106	F5H	C3'-C4'	4.10	1.55	1.52
1	A	106	F5H	C1'-C2'	3.40	1.57	1.52
1	B	206	F5H	O4-C4	3.13	1.30	1.24
1	A	106	F5H	C3'-C2'	2.83	1.56	1.51
1	B	206	F5H	P-O2P	2.52	1.49	1.46
1	A	106	F5H	C2-N1	-2.23	1.36	1.38
1	A	106	F5H	O5'-C5'	2.13	1.45	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	F5H	C6-N1-C2	-14.79	118.21	122.41
1	A	106	F5H	C6-N1-C2	-7.54	120.27	122.41
1	A	106	F5H	O5'-C1'-C2'	-5.71	107.57	111.69
1	B	206	F5H	N3-C2-N1	5.69	120.72	115.97
1	B	206	F5H	C7-C5-C4	5.01	126.16	121.04
1	A	106	F5H	C1'-O5'-C5'	4.68	119.37	111.73
1	A	106	F5H	N3-C2-N1	4.61	119.82	115.97
1	A	106	F5H	O6'-C6'-C7'	3.67	116.27	110.13
1	B	206	F5H	C1'-O5'-C5'	3.37	117.23	111.73
1	A	106	F5H	O4'-C4'-C5'	-2.74	103.46	109.85
1	A	106	F5H	C3'-C2'-N1	-2.53	107.98	111.88
1	A	106	F5H	F3'-C3'-C4'	2.49	110.53	108.55
1	A	106	F5H	C4-N3-C2	-2.31	120.64	125.39
1	A	106	F5H	C1'-C2'-N1	2.22	114.99	112.02
1	B	206	F5H	C5-C6-N1	2.13	123.66	121.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	F5H	C7-C5-C6	2.07	122.99	118.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	10/10 (100%)	-0.50	0 100 100	14, 16, 18, 22	0
1	B	10/10 (100%)	-0.54	0 100 100	16, 17, 19, 23	0
All	All	20/20 (100%)	-0.52	0 100 100	14, 17, 22, 23	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	F5H	A	106	23/24	0.06	1.10	12,15,18,20	0
1	F5H	B	206	23/24	0.05	-1.15	13,16,21,21	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SR	A	201	1/1	0.22	119.50	28,28,28,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.