W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 06:53 AM GMT

PDB ID	:	2YPF
Title	:	Structure of the AvrBs3-DNA complex provides new insights into the initial thymine-recognition mechanism
Authors	:	Stella, S.; Molina, R.; Yefimenko, I.; Prieto, J.; Silva, G.H.; Bertonati, C.; Juillerat, A.; Duchateau, P.; Montoya, G.
Deposited on	:	2012-10-30
Resolution	:	2.55 Å(reported)

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

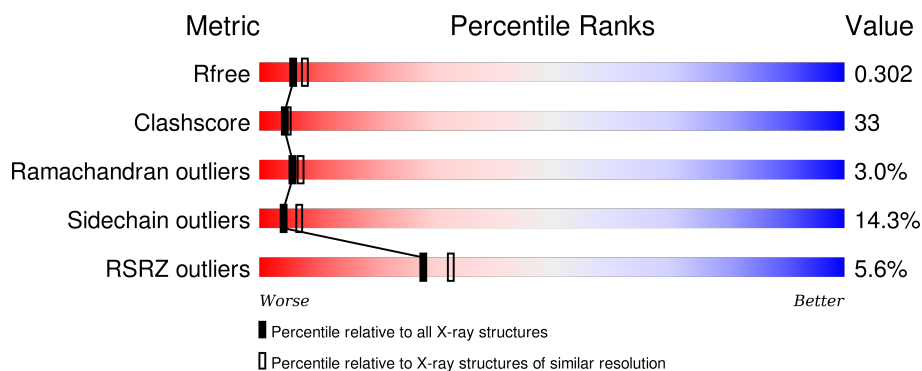|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.55 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	Percentile Ranks	Value
Rfree		0.302
Clashscore		33
Ramachandran outliers		3.0%
Sidechain outliers		14.3%
RSRZ outliers		5.6%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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. 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% 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.

Mol	Chain	Length	Quality of chain
1	A	758	5% 41% 41% 6% · 11%
2	B	22	5% 59% 36% 5%
3	C	21	5% 43% 57%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5822 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 AVRBS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	675	Total 4772	C 2988	N 871	O 897	S 16	0	0	0

- Molecule 2 is a DNA chain called 5'-D(*TP*TP*TP*AP*TP*AP*TP*AP*AP*AP*CP*CP*TP*AP *AP*CP*CP*CP*TP*CP*TP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	22	Total 439	C 214	N 74	O 130	P 21	0	0	0

- Molecule 3 is a DNA chain called 5'-D(*TP*AP*GP*AP*GP*GP*GP*TP*TP*AP*GP*G P*TP*TP *TP*AP*TP*AP*TP*AP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	21	Total 436	C 210	N 81	O 125	P 20	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total 139	O 139	0	0
4	B	17	Total 17	O 17	0	0
4	C	19	Total 19	O 19	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 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: AVRBS3
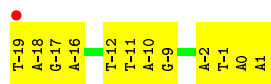
• Molecule 2: 5'-D(*TP*TP*TP*AP*TP*AP*TP*AP*AP*AP*CP*CP*TP*AP *AP*CP*CP*C P*TP*CP*TP*AP)-3'

Chain B:
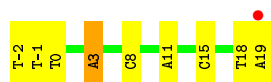
• Molecule 3: 5'-D(*TP*AP*GP*AP*GP*GP*GP*TP*TP*AP*GP*GP*TP*TP *TP*AP*TP* AP*TP*AP*AP)-3'

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	151.11Å 100.25Å 61.37Å 90.00° 102.55° 90.00°	Depositor
Resolution (Å)	32.29 – 2.55 32.29 – 2.55	Depositor EDS
% Data completeness (in resolution range)	93.3 (32.29-2.55) 93.3 (32.29-2.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.236 , 0.290 0.246 , 0.302	Depositor DCC
R_{free} test set	1475 reflections (5.73%)	DCC
Wilson B-factor (Å²)	67.8	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.28 , 74.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Outliers	2 of 27137 reflections (0.007%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5822	wwPDB-VP
Average B, all atoms (Å²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.62	0/4831	0.91	13/6609 (0.2%)
2	B	0.80	1/490 (0.2%)	1.11	1/752 (0.1%)
3	C	0.52	0/490	0.94	0/757
All	All	0.63	1/5811 (0.0%)	0.93	14/8118 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	DA	O3'-P	-7.05	1.52	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	314	LEU	CA-CB-CG	7.26	132.01	115.30
1	A	200	PRO	N-CA-CB	6.35	110.92	103.30
1	A	218	PRO	N-CA-CB	6.16	110.69	103.30
1	A	647	LEU	CB-CG-CD1	-5.97	100.86	111.00
1	A	579	LEU	CB-CG-CD2	-5.58	101.52	111.00

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	A	4772	0	4877	347	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	439	0	252	10	0
3	C	436	0	241	12	0
4	A	139	0	0	35	0
4	B	17	0	0	0	0
4	C	19	0	0	4	0
All	All	5822	0	5370	361	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 33.

The worst 5 of 361 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:266:ARG:NH1	1:A:267:GLY:H	1.41	1.17
1:A:278:TRP:HB3	1:A:282:LEU:HD21	1.19	1.17
1:A:244:VAL:HB	4:A:2028:HOH:O	1.41	1.17
1:A:604:ALA:HB2	4:A:2104:HOH:O	1.42	1.15
1:A:289:LEU:HB3	1:A:293:GLN:NE2	1.63	1.13

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	Percentiles	
1	A	670/758 (88%)	551 (82%)	99 (15%)	20 (3%)	5	7

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	ALA
1	A	235	ALA

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Mol	Chain	Res	Type
1	A	236	ARG
1	A	288	ASN
1	A	810	ASN

5.3.2   Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	483/584 (83%)	414 (86%)	69 (14%)	4 7

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	515	GLN
1	A	583	GLN
1	A	821	GLN
1	A	525	HIS
1	A	549	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	463	GLN
1	A	509	GLN
1	A	645	GLN
1	A	457	HIS
1	A	708	HIS

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)

There are no ligands in this entry.

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)

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(Å²)	Q<0.9
1	A	675/758 (89%)	0.24	38 (5%)	28	33	34, 71, 112, 164	0
2	B	22/22 (100%)	-0.33	1 (4%)	37	43	32, 41, 70, 147	0
3	C	21/21 (100%)	-0.24	1 (4%)	34	40	34, 55, 99, 197	0
All	All	718/801 (89%)	0.21	40 (5%)	28	33	32, 70, 115, 197	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	857	LEU	6.9
1	A	832	GLY	5.3
1	A	284	GLY	5.2
1	A	838	VAL	5.0
1	A	859	PRO	4.7

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.