



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2016 – 01:38 PM EDT

PDB ID : 5K1Y
Title : P2(1) Structure of pNOB8 AspA-DNA complex
Authors : Schumacher, M.
Deposited on : 2016-05-18
Resolution : 2.97 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

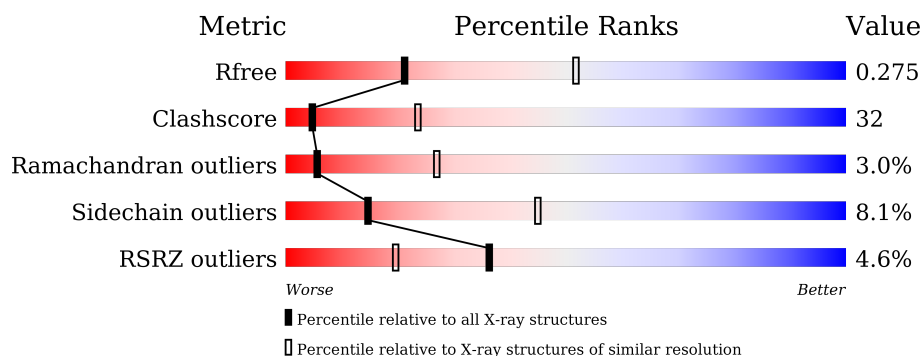
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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}	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	92	<div> <div>5%</div> <div>42%</div> <div>48%</div> <div>• 5%</div> </div>
1	B	92	<div> <div>5%</div> <div>34%</div> <div>60%</div> <div>7%</div> </div>
1	C	92	<div> <div>2%</div> <div>41%</div> <div>54%</div> <div>...</div> </div>
1	D	92	<div> <div>3%</div> <div>43%</div> <div>50%</div> <div>7%</div> </div>
1	E	92	<div> <div>2%</div> <div>50%</div> <div>37%</div> <div>12%</div> <div>•</div> </div>
1	F	92	<div> <div>8%</div> <div>52%</div> <div>39%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
2	P	33	<div><div></div><div>6%</div><div>15%</div><div>76%</div><div>9%</div></div>
3	N	33	<div><div></div><div>6%</div><div>12%</div><div>76%</div><div>12%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5772 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 AspA.

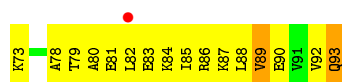
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	C	91	Total	C	N	O	0	0	0
			738	481	122	135			
1	D	92	Total	C	N	O	0	0	0
			748	486	124	138			
1	A	87	Total	C	N	O	0	0	0
			711	464	117	130			
1	B	92	Total	C	N	O	0	0	0
			748	486	124	138			
1	E	91	Total	C	N	O	0	0	0
			738	481	122	135			
1	F	92	Total	C	N	O	0	0	0
			748	486	124	138			

- Molecule 2 is a DNA chain called DNA (33-MER).

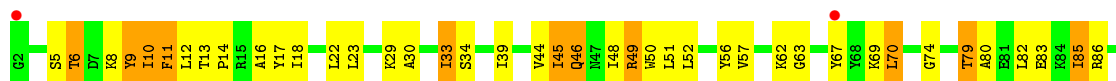
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	33	Total	C	N	O	P	0	0	0
			665	320	115	198	32			

- Molecule 3 is a DNA chain called DNA (33-MER).

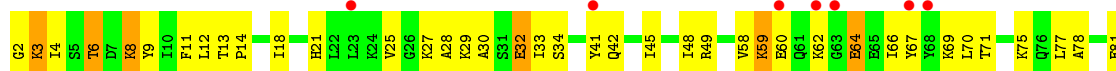
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	33	Total	C	N	O	P	0	0	0
			676	324	126	194	32			



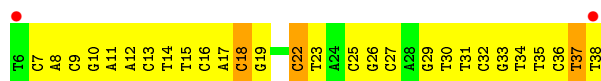
- Molecule 1: AspA



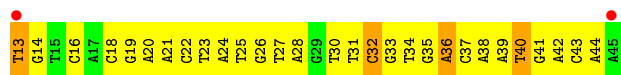
- Molecule 1: AspA



- Molecule 2: DNA (33-MER)



- Molecule 3: DNA (33-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.37Å 72.31Å 90.51Å 90.00° 114.72° 90.00°	Depositor
Resolution (Å)	39.46 – 2.97 39.46 – 2.97	Depositor EDS
% Data completeness (in resolution range)	89.3 (39.46-2.97) 89.2 (39.46-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.95Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.210 , 0.280 0.203 , 0.275	Depositor DCC
R_{free} test set	1825 reflections (9.90%)	DCC
Wilson B-factor (Å ²)	96.2	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5772	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.26	0/722	0.44	0/974
1	B	0.27	0/759	0.46	0/1021
1	C	0.25	0/749	0.43	0/1009
1	D	0.27	0/759	0.43	0/1021
1	E	0.29	0/749	0.46	0/1009
1	F	0.25	0/759	0.44	0/1021
2	P	0.54	0/743	1.32	5/1143 (0.4%)
3	N	0.56	0/759	1.31	9/1170 (0.8%)
All	All	0.36	0/5999	0.79	14/8368 (0.2%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	32	DC	C3'-C2'-C1'	-6.42	94.80	102.50
3	N	13	DT	O4'-C1'-N1	6.39	112.47	108.00
3	N	40	DT	N3-C4-O4	5.76	123.36	119.90
3	N	36	DA	C3'-C2'-C1'	-5.69	95.67	102.50
2	P	25	DC	C1'-O4'-C4'	-5.68	104.42	110.10

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	711	0	753	50	0
1	B	748	0	793	65	0
1	C	738	0	785	45	0
1	D	748	0	793	59	0
1	E	738	0	785	42	0
1	F	748	0	793	52	0
2	P	665	0	375	67	0
3	N	676	0	374	61	0
All	All	5772	0	5451	354	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 32.

The worst 5 of 354 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)
2:P:35:DT:H2"	2:P:36:DC:H5"	1.27	1.09
1:C:84:LYS:HA	1:C:87:LYS:HE2	1.35	1.08
1:F:28:ALA:HB1	1:F:32:GLU:HG2	1.41	1.01
1:B:41:TYR:OH	1:B:45:ILE:HD11	1.64	0.95
1:E:9:TYR:HB3	1:E:12:LEU:O	1.67	0.94

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	85/92 (92%)	67 (79%)	15 (18%)	3 (4%)	4	23
1	B	90/92 (98%)	75 (83%)	11 (12%)	4 (4%)	3	17
1	C	89/92 (97%)	69 (78%)	16 (18%)	4 (4%)	3	16
1	D	90/92 (98%)	74 (82%)	15 (17%)	1 (1%)	17	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	89/92 (97%)	70 (79%)	16 (18%)	3 (3%)	5	23
1	F	90/92 (98%)	73 (81%)	16 (18%)	1 (1%)	17	57
All	All	533/552 (97%)	428 (80%)	89 (17%)	16 (3%)	5	27

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	6	THR
1	B	25	VAL
1	E	6	THR
1	E	91	VAL
1	F	3	LYS

5.3.2 Protein sidechains ⓘ

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	77/81 (95%)	74 (96%)	3 (4%)	39	76
1	B	81/81 (100%)	75 (93%)	6 (7%)	17	50
1	C	80/81 (99%)	75 (94%)	5 (6%)	22	58
1	D	81/81 (100%)	76 (94%)	5 (6%)	23	59
1	E	80/81 (99%)	68 (85%)	12 (15%)	3	15
1	F	81/81 (100%)	73 (90%)	8 (10%)	10	34
All	All	480/486 (99%)	441 (92%)	39 (8%)	15	45

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	79	THR
1	E	11	PHE
1	F	82	LEU
1	B	93	GLN
1	E	9	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	42	GLN
1	B	61	GLN
1	B	93	GLN
1	E	21	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 ⓘ

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(Å²)	Q<0.9
1	A	87/92 (94%)	0.52	5 (5%)	27	14	63, 95, 142, 155	0
1	B	92/92 (100%)	0.26	5 (5%)	29	15	63, 100, 130, 152	0
1	C	91/92 (98%)	0.32	2 (2%)	65	42	66, 93, 132, 145	0
1	D	92/92 (100%)	0.52	3 (3%)	50	29	71, 97, 130, 148	0
1	E	91/92 (98%)	0.35	2 (2%)	65	42	63, 85, 126, 143	0
1	F	92/92 (100%)	0.63	7 (7%)	17	8	65, 95, 120, 151	0
2	P	33/33 (100%)	-0.09	2 (6%)	25	12	69, 83, 134, 149	0
3	N	33/33 (100%)	0.22	2 (6%)	25	12	69, 84, 138, 182	0
All	All	611/618 (98%)	0.39	28 (4%)	36	19	63, 94, 134, 182	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	62	LYS	14.5
3	N	45	DA	8.0
1	F	63	GLY	5.6
3	N	13	DT	4.5
1	C	91	VAL	4.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.