Full wwPDB X-ray Structure Validation Report (i)

Nov 28, 2016 – 03:58 PM EST

PDB ID	:	5B11
Title	:	A mutation of OspA
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Deposited on	:	2015-11-17
Resolution	:	1.20 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
http://wwpdb.org/validation/2016/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:

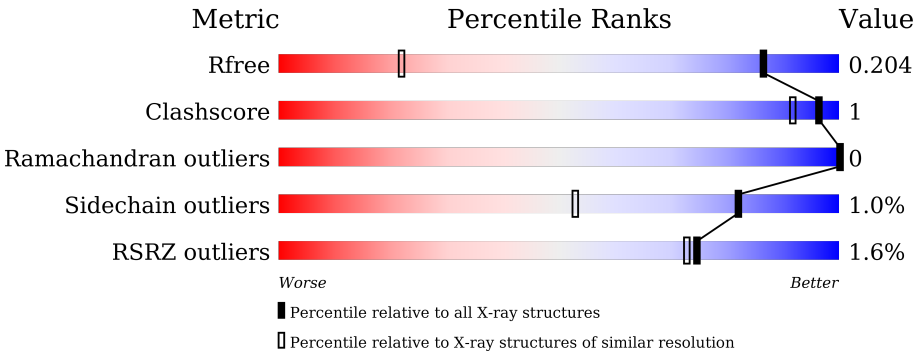
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 1.20 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	1495 (1.26-1.14)
Clashscore	102246	1607 (1.26-1.14)
Ramachandran outliers	100387	1540 (1.26-1.14)
Sidechain outliers	100360	1538 (1.26-1.14)
RSRZ outliers	91569	1500 (1.26-1.14)

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	O	251	2% 84% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2165 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 Outer surface protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	246	Total	C	N	O	S	0	3	0
			1822	1118	301	402	1			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	23	GLY	-	expression tag	UNP P0CL66
O	24	SER	-	expression tag	UNP P0CL66
O	25	HIS	-	expression tag	UNP P0CL66
O	26	MET	-	expression tag	UNP P0CL66
O	37	SER	GLU	engineered mutation	UNP P0CL66
O	45	SER	GLU	engineered mutation	UNP P0CL66
O	46	SER	LYS	engineered mutation	UNP P0CL66
O	48	ALA	LYS	engineered mutation	UNP P0CL66
O	60	ALA	LYS	engineered mutation	UNP P0CL66
O	64	SER	LYS	engineered mutation	UNP P0CL66
O	83	ALA	LYS	engineered mutation	UNP P0CL66
O	104	SER	GLU	engineered mutation	UNP P0CL66
O	107	SER	LYS	engineered mutation	UNP P0CL66
O	122	GLY	THR	engineered mutation	UNP P0CL66
O	196	ALA	GLU	engineered mutation	UNP P0CL66
O	239	SER	LYS	engineered mutation	UNP P0CL66
O	240	SER	GLU	engineered mutation	UNP P0CL66
O	254	SER	LYS	engineered mutation	UNP P0CL66

- Molecule 2 is water.

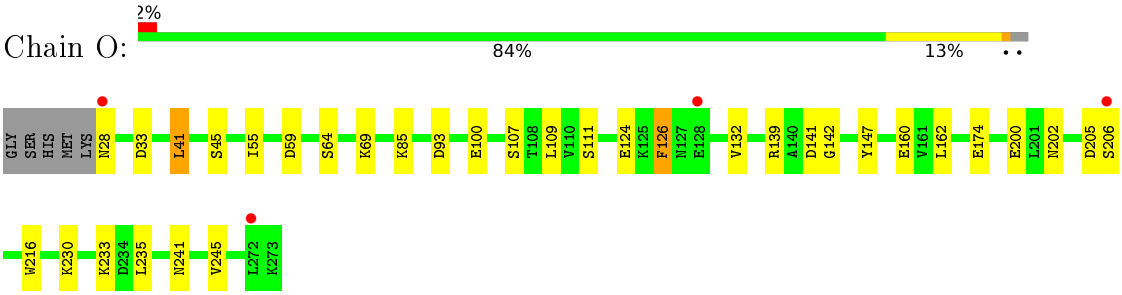
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	O	343	Total	O	0	0
			343	343		

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: Outer surface protein A

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	33.04Å 54.45Å 66.07Å 90.00° 100.39° 90.00°	Depositor
Resolution (Å)	20.00 – 1.20 19.74 – 1.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-1.20) 98.5 (19.74-1.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.42 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.176 , 0.199 0.183 , 0.204	Depositor DCC
R_{free} test set	3575 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	12.6	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2165	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	O	1.61	20/1835 (1.1%)	1.30	13/2470 (0.5%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	111	SER	CB-OG	-10.34	1.28	1.42
1	O	200	GLU	CB-CG	-9.12	1.34	1.52
1	O	64	SER	CB-OG	-8.18	1.31	1.42
1	O	33	ASP	CB-CG	-7.14	1.36	1.51
1	O	233	LYS	CB-CG	-6.77	1.34	1.52
1	O	45	SER	CB-OG	-6.40	1.33	1.42
1	O	216	TRP	CB-CG	-6.04	1.39	1.50
1	O	147	TYR	CE2-CZ	-5.96	1.30	1.38
1	O	241	ASN	CG-ND2	-5.85	1.18	1.32
1	O	245	VAL	CB-CG2	-5.83	1.40	1.52
1	O	126	PHE	CG-CD1	5.74	1.47	1.38
1	O	107	SER	C-N	-5.49	1.21	1.34
1	O	139	ARG	CZ-NH1	-5.46	1.25	1.33
1	O	124	GLU	CG-CD	-5.36	1.44	1.51
1	O	142	GLY	N-CA	-5.29	1.38	1.46
1	O	109	LEU	CA-C	-5.28	1.39	1.52
1	O	100	GLU	CD-OE1	-5.24	1.19	1.25
1	O	216	TRP	CZ3-CH2	-5.16	1.31	1.40
1	O	235	LEU	C-O	5.11	1.33	1.23
1	O	160	GLU	CG-CD	-5.09	1.44	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	139	ARG	NE-CZ-NH1	10.93	125.76	120.30
1	O	139	ARG	NE-CZ-NH2	-9.45	115.58	120.30
1	O	206[A]	SER	CB-CA-C	-8.37	94.21	110.10
1	O	206[B]	SER	CB-CA-C	-8.37	94.21	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	141	ASP	CB-CG-OD1	8.33	125.80	118.30
1	O	41	LEU	CB-CG-CD1	7.90	124.43	111.00
1	O	174	GLU	OE1-CD-OE2	-7.11	114.76	123.30
1	O	93	ASP	CB-CG-OD1	6.71	124.34	118.30
1	O	59[A]	ASP	CB-CG-OD2	-6.70	112.28	118.30
1	O	59[B]	ASP	CB-CG-OD2	-6.70	112.28	118.30
1	O	205	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	O	85	LYS	CD-CE-NZ	-5.44	99.18	111.70
1	O	230	LYS	CD-CE-NZ	5.24	123.76	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	O	1822	0	1861	5	0
2	O	343	0	0	2	0
All	All	2165	0	1861	5	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 1.

All (5) 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:O:202:ASN:HB3	2:O:560:HOH:O	1.51	1.06
1:O:126:PHE:CE2	1:O:132:VAL:HG22	2.26	0.70
1:O:69:LYS:HE3	2:O:579:HOH:O	1.96	0.66
1:O:55:ILE:HG21	1:O:55:ILE:HD13	1.79	0.45
1:O:162:LEU:N	1:O:162:LEU:HD22	2.35	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	O	247/251 (98%)	243 (98%)	4 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	O	212/214 (99%)	210 (99%)	2 (1%)	84 56

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	28	ASN
1	O	41	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	270	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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	O	246/251 (98%)	0.11	4 (1%)	74	73	10, 14, 24, 48	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	28	ASN	3.3
1	O	206[A]	SER	3.2
1	O	128	GLU	2.7
1	O	272	LEU	2.5

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.