



Full wwPDB X-ray Structure Validation Report

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PDB ID : 2PI3
Title : The crystal structure of OspA mutant
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Deposited on : 2007-04-12
Resolution : 1.40 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>

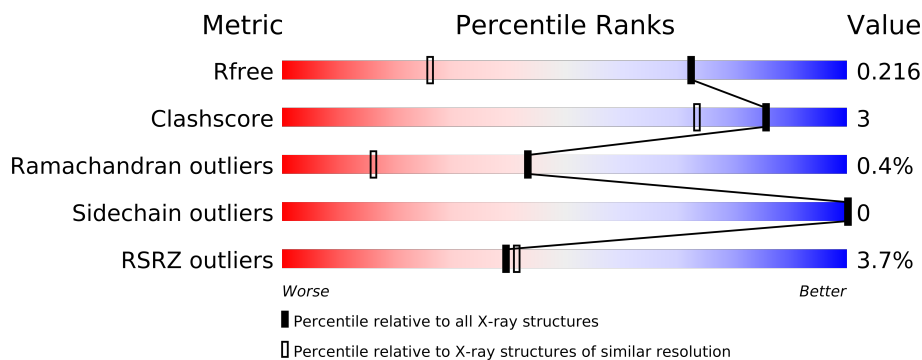
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.40 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	1097 (1.42-1.38)
Clashscore	79885	1246 (1.42-1.38)
Ramachandran outliers	78287	1206 (1.42-1.38)
Sidechain outliers	78261	1205 (1.42-1.38)
RSRZ outliers	66119	1097 (1.42-1.38)

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	O	251	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2278 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 protein called Outer surface protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	246	Total	C	N	O	S	0	6	0
			1848	1145	300	401	2			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	23	GLY	-	EXPRESSION TAG	UNP Q45040
O	24	SER	-	EXPRESSION TAG	UNP Q45040
O	25	HIS	-	EXPRESSION TAG	UNP Q45040
O	26	MET	-	EXPRESSION TAG	UNP Q45040
O	37	SER	GLU	ENGINEERED	UNP Q45040
O	45	SER	GLU	ENGINEERED	UNP Q45040
O	46	SER	LYS	ENGINEERED	UNP Q45040
O	48	ALA	LYS	ENGINEERED	UNP Q45040
O	60	ALA	LYS	ENGINEERED	UNP Q45040
O	64	SER	LYS	ENGINEERED	UNP Q45040
O	83	ALA	LYS	ENGINEERED	UNP Q45040
O	104	SER	GLU	ENGINEERED	UNP Q45040
O	107	SER	LYS	ENGINEERED	UNP Q45040
O	113	PHE	LYS	ENGINEERED	UNP Q45040
O	123	PHE	GLU	ENGINEERED	UNP Q45040
O	136	PHE	ILE	ENGINEERED	UNP Q45040
O	239	SER	LYS	ENGINEERED	UNP Q45040
O	240	SER	GLU	ENGINEERED	UNP Q45040
O	254	SER	LYS	ENGINEERED	UNP Q45040

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	O	430	Total	O	0	0
			430	430		

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- Molecule 1: Outer surface protein A

Relative frequencies of amino acids in the N-terminal region of the protein. The chart shows the relative frequency of each amino acid, with red dots indicating specific amino acids.

Amino Acid	Relative Frequency (approx.)
GLY	0.15
SER	0.15
HIS	0.15
MET	0.15
LYS	0.15
N28	0.85
S29	0.85
V30	0.85
K80	0.85
A81	0.85
D82	0.85
A83	0.85
K129	0.85
K135	0.85
A173	0.85
E174	0.85
L187	0.85
K193	0.85
V199	0.85
S206	0.85
K273	0.85

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.13Å 55.62Å 66.12Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	20.00 – 1.40 28.76 – 1.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.40) 98.7 (28.76-1.39)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.81 (at 1.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.169 , 0.207 0.180 , 0.216	Depositor DCC
R_{free} test set	2600 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 51033 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2278	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.46	0/1878	0.66	0/2526

There are no bond length outliers.

There are no bond angle outliers.

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	O	1848	0	7	5	0
2	O	430	0	0	3	0
All	All	2278	0	7	5	0

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 3.

All (5) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:135[B]:LYS:NZ	2:O:532:HOH:O	2.47	0.48
1:O:82:ASP:O	1:O:83:ALA:CB	2.63	0.46
1:O:187:LEU:HD11	1:O:199:VAL:CG1	2.50	0.41
1:O:82:ASP:N	2:O:640:HOH:O	2.54	0.41
1:O:80:LYS:NZ	2:O:578:HOH:O	2.55	0.40

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	250/251 (100%)	245 (98%)	4 (2%)	1 (0%)	43 16

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	82	ASP

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	218/216 (101%)	218 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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, 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	O	246/251 (98%)	0.05	9 (3%) 39 41	14, 19, 27, 32	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	81	ALA	4.8
1	O	174	GLU	4.6
1	O	206	SER	3.8
1	O	173	ALA	3.7
1	O	28	ASN	3.2
1	O	193	LYS	2.3
1	O	30	VAL	2.1
1	O	129	LYS	2.1
1	O	83	ALA	2.0

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.