



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:13 PM GMT

PDB ID : 3TCH
Title : Crystal structure of E. coli OppA in an open conformation
Authors : Klepsch, M.M.; Kovermann, M.; Low, C.; Balbach, J.; de Gier, J.W.; Slotboom, D.J.; Berntsson, R.P.-A.
Deposited on : 2011-08-09
Resolution : 1.98 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

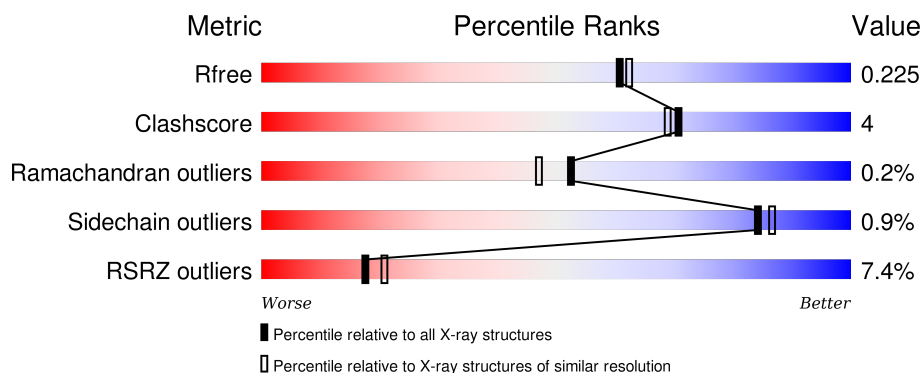
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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	524	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4655 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 Periplasmic oligopeptide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	7	0
			4175	2658	702	804	11			

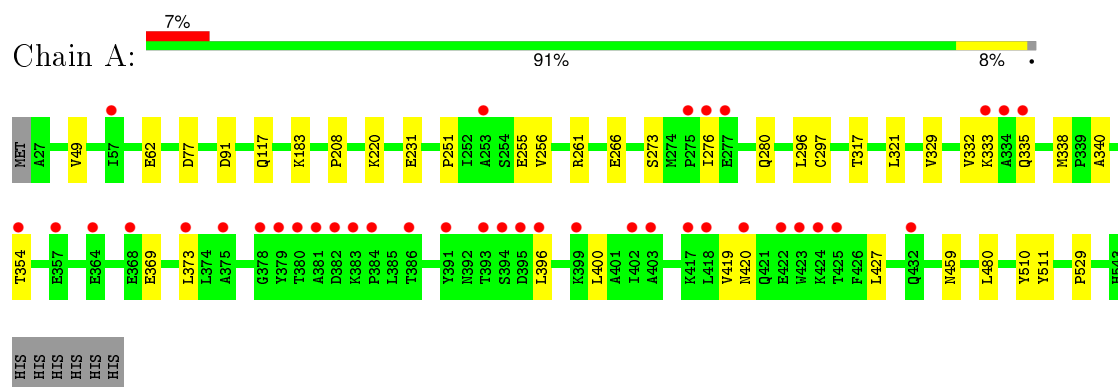
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	EXPRESSION TAG	UNP P23843
A	544	HIS	-	EXPRESSION TAG	UNP P23843
A	545	HIS	-	EXPRESSION TAG	UNP P23843
A	546	HIS	-	EXPRESSION TAG	UNP P23843
A	547	HIS	-	EXPRESSION TAG	UNP P23843
A	548	HIS	-	EXPRESSION TAG	UNP P23843
A	549	HIS	-	EXPRESSION TAG	UNP P23843

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	480	Total	O	0	0
			480	480		

- Molecule 1: Periplasmic oligopeptide-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.41Å 82.28Å 125.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.39 – 1.98 37.39 – 1.98	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.39-1.98) 98.5 (37.39-1.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.178 , 0.219 0.184 , 0.225	Depositor DCC
R_{free} test set	2081 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 41615 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4655	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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, 0.375 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	0.53	0/4284	0.60	1/5843 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ASP	CB-CG-OD2	5.50	123.25	118.30

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	4175	0	4077	36	0
2	A	480	0	0	12	0
All	All	4655	0	4077	36	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 4.

All (36) 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:369:GLU:O	1:A:373:LEU:HD13	1.62	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:THR:HG23	2:A:965:HOH:O	1.82	0.78
1:A:338[A]:MET:HE3	2:A:909:HOH:O	1.86	0.75
1:A:276:ILE:HD12	1:A:335:GLN:CG	2.17	0.74
1:A:317:THR:O	1:A:321:LEU:HD23	1.90	0.70
1:A:276:ILE:O	1:A:280:GLN:HG2	1.97	0.65
1:A:333:LYS:HZ3	1:A:396:LEU:HD21	1.63	0.63
1:A:373:LEU:HD11	2:A:974:HOH:O	2.01	0.60
1:A:183:LYS:HE2	2:A:753:HOH:O	2.01	0.59
1:A:480:LEU:HD13	2:A:953:HOH:O	2.02	0.59
1:A:333:LYS:NZ	1:A:396:LEU:HD21	2.17	0.58
1:A:256:VAL:HG23	2:A:962:HOH:O	2.04	0.57
1:A:276:ILE:HG21	1:A:333:LYS:O	2.05	0.56
1:A:396:LEU:O	1:A:400:LEU:HD13	2.05	0.56
1:A:117:GLN:HB2	2:A:1006:HOH:O	2.07	0.54
1:A:276:ILE:N	1:A:276:ILE:HD13	2.23	0.53
1:A:276:ILE:HD12	1:A:335:GLN:CD	2.28	0.53
1:A:317:THR:O	1:A:321:LEU:CD2	2.56	0.53
1:A:419:VAL:HG12	2:A:999:HOH:O	2.09	0.52
1:A:419:VAL:CG1	2:A:999:HOH:O	2.57	0.52
1:A:396:LEU:CD1	1:A:400:LEU:HD22	2.40	0.52
1:A:276:ILE:HD12	1:A:335:GLN:HG2	1.89	0.51
1:A:220:LYS:HD2	1:A:231:GLU:HG3	1.96	0.48
1:A:261:ARG:HD3	1:A:266:GLU:OE2	2.13	0.48
1:A:49:VAL:HB	1:A:62:GLU:HG2	1.96	0.47
1:A:332:VAL:O	1:A:332:VAL:HG12	2.16	0.46
1:A:340:ALA:HA	1:A:510:TYR:CE2	2.51	0.46
1:A:296:LEU:HG	1:A:529:PRO:HB2	1.99	0.44
1:A:297:CYS:HB2	1:A:511:TYR:CG	2.53	0.44
1:A:396:LEU:HD13	1:A:400:LEU:HD22	2.00	0.44
1:A:231:GLU:HG3	2:A:1005:HOH:O	2.18	0.43
1:A:459:ASN:H	1:A:459:ASN:ND2	2.17	0.42
1:A:255:GLU:OE1	1:A:273:SER:OG	2.35	0.42
1:A:317:THR:HG22	1:A:321:LEU:HD23	2.02	0.42
1:A:208:PRO:O	2:A:736:HOH:O	2.22	0.41
1:A:338[A]:MET:CE	2:A:909:HOH:O	2.56	0.41

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	522/524 (100%)	506 (97%)	15 (3%)	1 (0%)	52	47

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	PRO

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	458/458 (100%)	454 (99%)	4 (1%)	84	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ASP
1	A	329	VAL
1	A	420	ASN
1	A	427	LEU

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

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(Å ²)	Q<0.9
1	A	517/524 (98%)	0.44	38 (7%) 17 21	14, 27, 56, 73	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	381	ALA	5.3
1	A	396	LEU	5.1
1	A	276	ILE	5.1
1	A	393	THR	4.8
1	A	364	GLU	4.3
1	A	334	ALA	4.1
1	A	417	LYS	3.9
1	A	395	ASP	3.9
1	A	382	ASP	3.7
1	A	277	GLU	3.4
1	A	422	GLU	3.4
1	A	391	TYR	3.3
1	A	384	PRO	3.2
1	A	399	LYS	3.2
1	A	380	THR	3.2
1	A	394	SER	3.1
1	A	424	LYS	2.9
1	A	333	LYS	2.9
1	A	420	ASN	2.7
1	A	418	LEU	2.7
1	A	386	THR	2.6
1	A	425	THR	2.5
1	A	378	GLY	2.5
1	A	253	ALA	2.5
1	A	402	ILE	2.5
1	A	57	ILE	2.5
1	A	275	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	375	ALA	2.4
1	A	335	GLN	2.3
1	A	354	THR	2.3
1	A	383	LYS	2.3
1	A	423	TRP	2.2
1	A	368	GLU	2.2
1	A	432	GLN	2.1
1	A	373	LEU	2.1
1	A	403	ALA	2.1
1	A	379	TYR	2.1
1	A	357	GLU	2.0

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.