



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2023 – 06:25 pm GMT

PDB ID : 8ARN
Title : Crystal structure of the peptide binding protein, OppA, from Bacillus subtilis
in complex with an endogenous tetrapeptide
Authors : Hughes, A.; Dodson, E.J.; Wilkinson, A.J.
Deposited on : 2022-08-17
Resolution : 1.50 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.32.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.1

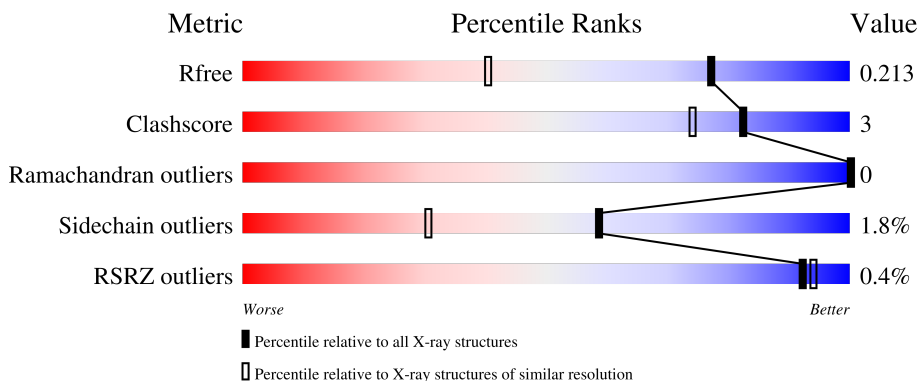
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

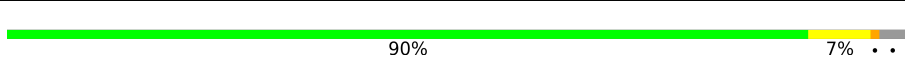
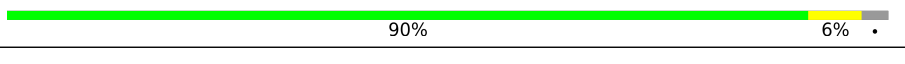
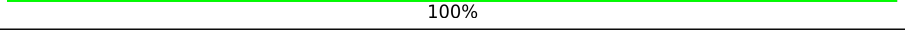
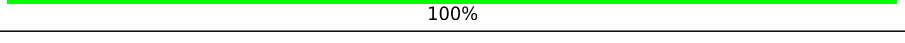
The reported resolution of this entry is 1.50 Å.

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}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	525	 90% 7% . .
1	B	525	 90% 6% .
2	C	4	 100%
2	D	4	 100%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 17047 atoms, of which 7978 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 Oligopeptide-binding protein OppA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	509	8051	2591	3978	673	796	13	225	1	0
1	B	508	8012	2582	3954	668	795	13	226	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	SER	THR	variant	UNP P24141
A	175	LYS	GLU	variant	UNP P24141
A	320	ILE	MET	variant	UNP P24141
B	6	SER	THR	variant	UNP P24141
B	175	LYS	GLU	variant	UNP P24141
B	320	ILE	MET	variant	UNP P24141

- Molecule 2 is a protein called Endogenous tetrapeptide (SER-ASN-SER-SER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	C	4	50	13	23	5	9	5	0	0
2	D	4	50	13	23	5	9	5	0	0


- Molecule 3 is water.

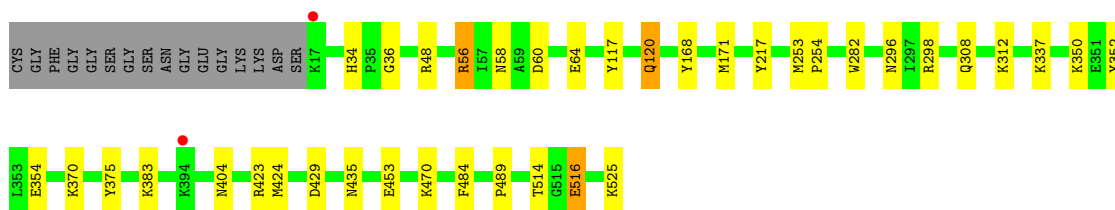
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	425	Total	O	0	0
			425	425		
3	B	458	Total	O	0	0
			458	458		
3	C	1	Total	O	0	0
			1	1		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

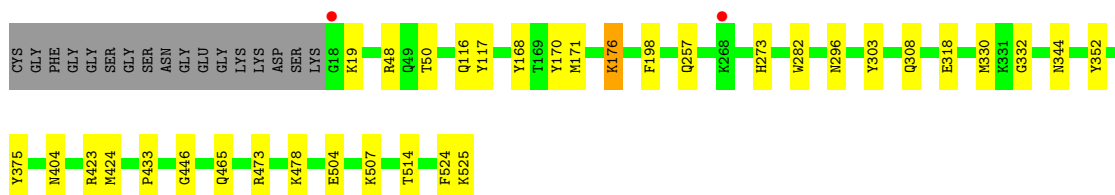
- Molecule 1: Oligopeptide-binding protein OppA

Chain A:  90% 7% ..



- Molecule 1: Oligopeptide-binding protein OppA

Chain B:  90% 6% •



- Molecule 2: Endogenous tetrapeptide (SER-ASN-SER-SER)

Chain C:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Endogenous tetrapeptide (SER-ASN-SER-SER)

Chain D:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.52Å 65.89Å 153.29Å 90.00° 100.97° 90.00°	Depositor
Resolution (Å)	55.02 – 1.50 54.96 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (55.02-1.50) 97.9 (54.96-1.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.50Å)	Xtrriage
Refinement program	REFMAC 5.8.0352, REFMAC 5.8.0352	Depositor
R, R_{free}	0.177 , 0.207 0.186 , 0.213	Depositor DCC
R_{free} test set	7692 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtrriage
Anisotropy	0.252	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17047	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1563e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.48	1/4168 (0.0%)	0.80	6/5641 (0.1%)
1	B	0.54	0/4153	0.86	3/5623 (0.1%)
2	C	0.83	0/26	0.75	0/32
2	D	0.94	0/26	1.10	0/32
All	All	0.51	1/8373 (0.0%)	0.83	9/11328 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	453	GLU	CD-OE1	6.59	1.32	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	298	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	298	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	48	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	B	48	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	56	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	170	TYR	CB-CG-CD1	5.50	124.30	121.00
1	B	48	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	516	GLU	CB-CA-C	-5.05	100.29	110.40

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	4073	3978	3967	25	0
1	B	4058	3954	3939	17	0
2	C	27	23	23	0	0
2	D	27	23	23	0	0
3	A	425	0	0	6	1
3	B	458	0	0	3	1
3	C	1	0	0	0	0
All	All	9069	7978	7952	41	1

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 3.

All (41) 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:56:ARG:NH1	3:A:601:HOH:O	1.91	1.03
1:A:58[B]:ASN:HD22	1:A:60:ASP:H	1.16	0.92
1:A:34:HIS:HD2	1:A:36:GLY:H	1.27	0.82
1:B:176:LYS:HE3	3:B:969:HOH:O	1.80	0.81
1:A:217:TYR:OH	3:A:601:HOH:O	1.99	0.80
1:A:525:LYS:O	3:A:602:HOH:O	2.02	0.77
1:B:176:LYS:CE	3:B:969:HOH:O	2.36	0.74
1:A:308:GLN:HE21	1:A:312:LYS:HD2	1.53	0.73
1:B:273:HIS:HE1	1:B:504:GLU:OE2	1.78	0.67
1:B:332:GLY:O	1:B:478:LYS:NZ	2.27	0.67
1:A:470:LYS:NZ	1:B:525:LYS:OXT	2.25	0.66
1:B:465:GLN:HE22	1:B:473:ARG:HH21	1.44	0.64
1:A:34:HIS:CD2	1:A:36:GLY:H	2.16	0.56
1:A:429:ASP:H	1:A:435:ASN:ND2	2.06	0.54
1:A:120:GLN:HE21	1:A:120:GLN:HA	1.74	0.53
1:A:58[B]:ASN:ND2	1:A:60:ASP:H	1.97	0.52
1:B:303:TYR:HE2	1:B:352:TYR:CE2	2.28	0.51
1:A:58[A]:ASN:OD1	1:A:60:ASP:OD1	2.29	0.51
1:B:296:ASN:HD22	1:B:352:TYR:HD1	1.61	0.49
1:A:58[B]:ASN:HD22	1:A:60:ASP:N	1.98	0.49
1:A:375:TYR:O	1:A:404:ASN:HA	2.12	0.49
1:B:168:TYR:HA	1:B:171:MET:HG2	1.94	0.48
1:B:507:LYS:HG3	1:B:525:LYS:HE2	1.97	0.47
1:B:375:TYR:O	1:B:404:ASN:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58[A]:ASN:HB3	1:A:64:GLU:CD	2.35	0.46
1:B:465:GLN:NE2	1:B:473:ARG:HH21	2.13	0.46
1:A:168:TYR:HA	1:A:171:MET:HG2	1.98	0.45
1:A:308:GLN:NE2	1:A:312:LYS:HD2	2.28	0.45
1:A:296:ASN:HD22	1:A:352:TYR:HD1	1.65	0.44
1:A:484:PHE:CE1	1:A:489:PRO:HG2	2.53	0.44
1:A:516:GLU:CG	3:A:805:HOH:O	2.64	0.44
1:B:257:GLN:NE2	3:B:615:HOH:O	2.51	0.43
1:B:19:LYS:HE3	1:B:524:PHE:CZ	2.55	0.41
1:A:34:HIS:HD2	1:A:36:GLY:N	2.07	0.41
1:A:253:MET:HB3	1:A:254:PRO:HA	2.02	0.41
1:A:350:LYS:O	1:A:354:GLU:HG2	2.21	0.41
1:B:50:THR:HA	1:B:198:PHE:O	2.21	0.41
1:B:116:GLN:O	1:B:446:GLY:HA3	2.22	0.40
1:A:514:THR:HG22	3:A:793:HOH:O	2.21	0.40
1:B:330:MET:HE2	1:B:433:PRO:HD3	2.03	0.40
1:A:383:LYS:HE3	3:A:866:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:997:HOH:O	3:B:1022:HOH:O[1_545]	1.91	0.29

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	508/525 (97%)	500 (98%)	8 (2%)	0	100	100
1	B	507/525 (97%)	496 (98%)	11 (2%)	0	100	100
2	C	2/4 (50%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1019/1058 (96%)	1000 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	437/448 (98%)	430 (98%)	7 (2%)	62	36
1	B	434/448 (97%)	425 (98%)	9 (2%)	53	23
2	C	4/4 (100%)	4 (100%)	0	100	100
2	D	4/4 (100%)	4 (100%)	0	100	100
All	All	879/904 (97%)	863 (98%)	16 (2%)	59	30

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	TYR
1	A	120	GLN
1	A	282	TRP
1	A	337	LYS
1	A	370	LYS
1	A	423	ARG
1	A	424	MET
1	B	117	TYR
1	B	176	LYS
1	B	282	TRP
1	B	308	GLN
1	B	318	GLU
1	B	344	ASN
1	B	423	ARG
1	B	424	MET
1	B	514	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	34	HIS
1	A	113	ASN
1	A	116	GLN
1	A	120	GLN
1	A	131	ASN
1	A	155	ASN
1	A	187	ASN
1	A	234	ASN
1	A	296	ASN
1	A	308	GLN
1	A	344	ASN
1	A	435	ASN
1	A	447	ASN
1	B	23	ASN
1	B	234	ASN
1	B	236	ASN
1	B	237	ASN
1	B	257	GLN
1	B	273	HIS
1	B	296	ASN
1	B	308	GLN
1	B	313	ASN
1	B	344	ASN
1	B	417	GLN
1	B	431	ASN
1	B	447	ASN
1	B	463	GLN
1	B	465	GLN

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 monosaccharides 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(Å ²)	Q<0.9
1	A	509/525 (96%)	-0.31	2 (0%) 92 94	16, 24, 39, 60	0
1	B	508/525 (96%)	-0.25	2 (0%) 92 94	13, 23, 37, 50	0
2	C	4/4 (100%)	-0.29	0 100 100	21, 23, 24, 28	0
2	D	4/4 (100%)	-0.29	0 100 100	20, 20, 21, 22	0
All	All	1025/1058 (96%)	-0.28	4 (0%) 92 94	13, 23, 38, 60	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	LYS	3.0
1	B	18	GLY	2.2
1	A	394	LYS	2.1
1	B	268	LYS	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 monosaccharides 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.