

Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 10:10 AM EDT

PDB ID 3N26

> Title Cpn0482: the arginine binding protein from the periplasm of chlamydia Pneu-

> > moniae

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Deposited on 2010-05-17

Resolution 2.10 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 (i) 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 (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13

EDS 2.36

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)

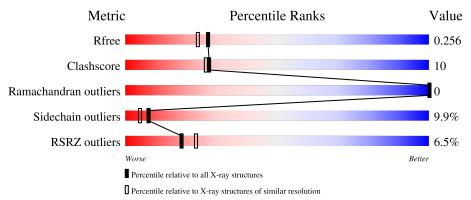
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.10 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	
			6%	
1	A	246	76%	13% • • 6%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2044 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 Amino acid ABC transporter, periplasmic amino acid-binding protein.

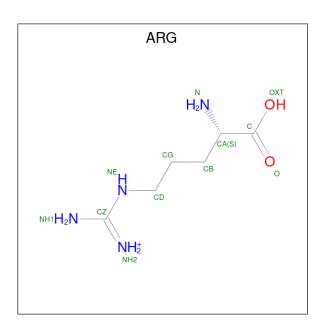
I	Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
	1	A	231	Total 1829	C 1172	N 309	O 342	S 6	17	2	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual Comment		Reference
A	22	MET	-	initiating methionine	UNP Q9JS59
A	260	LEU	-	expression tag	UNP Q9JS59
A	261	GLU	-	expression tag	UNP Q9JS59
A	262	HIS	-	expression tag	UNP Q9JS59
A	263	HIS	-	expression tag	UNP Q9JS59
A	264	HIS	-	expression tag	UNP Q9JS59
A	265	HIS	-	expression tag	UNP Q9JS59
A	266	HIS	-	expression tag	UNP Q9JS59
A	267	HIS	-	expression tag	UNP Q9JS59

• Molecule 2 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 12 6 4 2	0	0

• Molecule 3 is water.

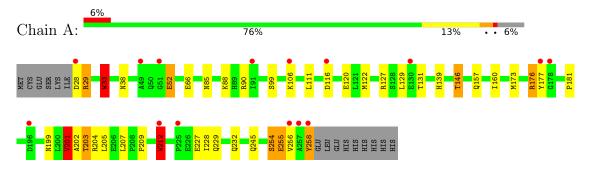
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	203	Total O 203 203	0	0



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: Amino acid ABC transporter, periplasmic amino acid-binding protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	51.60Å 51.60Å 206.30Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 - 2.10	Depositor
Resolution (A)	34.40 - 2.10	EDS
% Data completeness	100.0 (20.00-2.10)	Depositor
(in resolution range)	99.6 (34.40-2.10)	EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	4.51 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
P. P.	0.190 , 0.251	Depositor
R, R_{free}	0.197 , 0.256	DCC
R_{free} test set	858 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.40 , 72.6	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	0.94	EDS
Total number of atoms	2044	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 5.03% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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	Boı	Bond lengths		ond angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	1.12	5/1870 (0.3%)	0.92	$6/2539 \ (0.2\%)$

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$Ideal(\AA)$
1	A	229	GLN	CB-CG	-12.31	1.19	1.52
1	A	33	TRP	CE3-CZ3	-7.49	1.25	1.38
1	A	52	GLU	CB-CG	-7.41	1.38	1.52
1	A	245	GLN	CG-CD	6.18	1.65	1.51
1	A	212	TRP	CE3-CZ3	-6.11	1.28	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	212	TRP	CA-CB-CG	5.81	124.75	113.70
1	A	29	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	146	THR	CB-CA-C	-5.36	97.14	111.60
1	A	201	VAL	CB-CA-C	-5.14	101.63	111.40
1	A	229	GLN	CA-CB-CG	5.13	124.68	113.40
1	A	212	TRP	CB-CA-C	-5.05	100.31	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	254	SER	Peptide

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	1829	0	1876	37	0
2	A	12	0	12	3	0
3	A	203	0	0	8	0
All	All	2044	0	1888	37	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 10.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance } (\text{\AA}) \end{array}$	Clash overlap (Å)
1:A:255:GLU:HB3	3:A:681:HOH:O	1.47	1.15
1:A:255:GLU:HA	3:A:684:HOH:O	1.62	1.00
1:A:173:MET:CE	1:A:177:TYR:CE2	2.57	0.87
1:A:173:MET:HE3	1:A:177:TYR:CE2	2.12	0.83
1:A:38:ASN:HD22	2:A:500:ARG:HH12	1.26	0.79
1:A:173:MET:CE	1:A:177:TYR:HE2	1.96	0.77
1:A:33:TRP:HZ3	3:A:683:HOH:O	1.71	0.73
1:A:203:THR:HG23	3:A:503:HOH:O	1.90	0.71
1:A:120:GLU:OE2	1:A:204[B]:ARG:HD2	1.93	0.69
1:A:173:MET:HE1	1:A:177:TYR:CE2	2.27	0.68
1:A:207:LEU:O	1:A:212:TRP:HZ3	1.80	0.63
1:A:255:GLU:CB	3:A:681:HOH:O	2.20	0.63
1:A:127:ARG:CZ	1:A:201:VAL:HG13	2.31	0.60
1:A:207:LEU:O	1:A:212:TRP:CZ3	2.55	0.60
1:A:85:ASN:ND2	1:A:90:ARG:HG2	2.18	0.59
1:A:203:THR:CG2	3:A:503:HOH:O	2.46	0.58
1:A:85:ASN:HD22	1:A:90:ARG:HG2	1.68	0.58
1:A:127:ARG:NH2	1:A:201:VAL:HG13	2.19	0.57
1:A:122:MET:HE2	1:A:204[A]:ARG:HH22	1.76	0.49
1:A:176[B]:ARG:HH12	1:A:199:ASN:HD22	1.58	0.49

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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap (Å)
1:A:90:ARG:O	1:A:90:ARG:HG3	2.11	0.49
1:A:122:MET:HG3	1:A:202:ALA:HB1	1.95	0.48
1:A:176[B]:ARG:CZ	1:A:199:ASN:HB2	2.44	0.47
1:A:255:GLU:HG2	1:A:258:TYR:CE2	2.51	0.46
1:A:38:ASN:HD22	2:A:500:ARG:NH1	2.06	0.46
1:A:99:SER:HG	2:A:500:ARG:N	2.14	0.46
1:A:227:GLU:OE1	3:A:683:HOH:O	2.21	0.46
1:A:139:HIS:HB3	1:A:181:PRO:HG2	1.96	0.45
1:A:176[A]:ARG:NH1	3:A:685:HOH:O	2.50	0.44
1:A:204[A]:ARG:HD3	1:A:204[A]:ARG:HA	1.31	0.42
1:A:176[B]:ARG:NH1	1:A:199:ASN:HB2	2.33	0.42
1:A:157:GLN:HB2	1:A:160:ILE:HD12	2.01	0.42
1:A:122:MET:CE	1:A:204[A]:ARG:HH22	2.34	0.41
1:A:228:ILE:O	1:A:232:GLN:HB2	2.20	0.41
1:A:116:ASP:OD2	1:A:116:ASP:N	2.54	0.41
1:A:209:PRO:HA	1:A:212:TRP:CD2	2.55	0.41
1:A:85:ASN:HD22	1:A:90:ARG:CG	2.34	0.40

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	lysed Favoured Allow		Outliers	Percei	ntiles
1	A	231/246 (94%)	225 (97%)	6 (3%)	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	204/217 (94%)	183 (90%)	21 (10%)	7 4	

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	29	ARG
1	A	33	TRP
1	A	52	GLU
1	A	66	GLU
1	A	88	LYS
1	A	106	LYS
1	A	111	LEU
1	A	129	LEU
1	A	131	THR
1	A	146	THR
1	A	176[A]	ARG
1	A	176[B]	ARG
1	A	201	VAL
1	A	203	THR
1	A	205	LEU
1	A	212	TRP
1	A	254	SER
1	A	255	GLU
1	A	256	VAL
1	A	258	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	85	ASN
1	A	152	HIS
1	A	199	ASN
1	A	233	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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Type	Chain	Pog	Res Link Bond lengths		Bond angles		les		
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ARG	A	500	-	10,11,11	0.94	1 (10%)	11,13,13	1.16	2 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ARG	A	500	-	-	0/11/11/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
2	A	500	ARG	OXT-C	-2.20	1.23	1.30

All (2) bond angle outliers are listed below:

	Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
Ī	2	A	500	ARG	OXT-C-O	-2.49	118.43	124.09
Ī	2	A	500	ARG	OXT-C-CA	2.39	121.52	113.38



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	ARG	3	0

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, 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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	231/246 (93%)	0.22	15 (6%) 18 23	7, 17, 37, 51	6 (2%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	TYR	6.3
1	A	91	ILE	4.9
1	A	28	ASP	4.6
1	A	49	ALA	4.4
1	A	212	TRP	3.5
1	A	225	PRO	3.3
1	A	256	VAL	3.2
1	A	130	GLU	3.1
1	A	106	LYS	2.6
1	A	51	GLY	2.4
1	A	177	TYR	2.3
1	A	178	GLY	2.3
1	A	116	ASP	2.1
1	A	257	ALA	2.1
1	A	196	ASP	2.1

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	ARG	A	500	12/12	0.97	0.13	8,10,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.

