



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:47 PM UTC

PDB ID : 1XQ4 / pdb_00001xq4
Title : Crystal Structure of the Putative ApaA Protein from Bordetella pertussis, Northeast Structural Genomics Target BeR40
Authors : Forouhar, F.; Yong, W.; Vorobiev, S.M.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2004-10-11
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

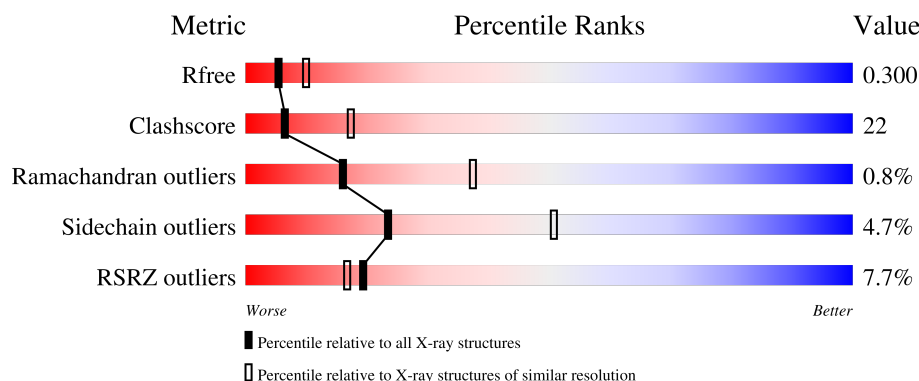
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	139	6% 53% 33% 12%
1	B	139	9% 58% 28% 13%
1	C	139	5% 53% 32% 12%
1	D	139	6% 59% 24% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	401	-	X	-	-
2	PO4	B	402	-	X	-	-
2	PO4	C	403	-	X	-	-
2	PO4	D	404	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4122 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 Protein apaG.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	Se	0	0	0
			957	610	162	181	2	2			
1	B	121	Total	C	N	O	S	Se	0	0	0
			939	600	157	178	2	2			
1	C	122	Total	C	N	O	S	Se	0	0	0
			950	606	161	179	2	2			
1	D	122	Total	C	N	O	S	Se	0	0	0
			950	606	161	179	2	2			

There are 40 discrepancies between the modelled and reference sequences:

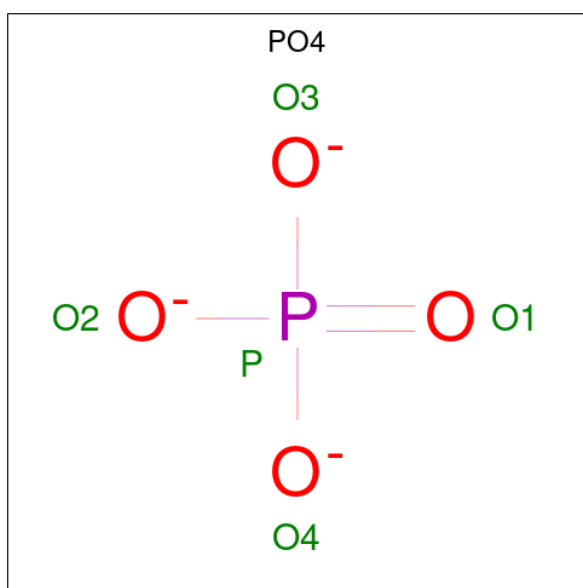
Chain	Residue	Modelled	Actual	Comment	Reference
A	101	MSE	MET	modified residue	UNP Q7VU61
A	126	MSE	MET	modified residue	UNP Q7VU61
A	132	LEU	-	cloning artifact	UNP Q7VU61
A	133	GLU	-	cloning artifact	UNP Q7VU61
A	134	HIS	-	cloning artifact	UNP Q7VU61
A	135	HIS	-	cloning artifact	UNP Q7VU61
A	136	HIS	-	cloning artifact	UNP Q7VU61
A	137	HIS	-	cloning artifact	UNP Q7VU61
A	138	HIS	-	cloning artifact	UNP Q7VU61
A	139	HIS	-	cloning artifact	UNP Q7VU61
B	101	MSE	MET	modified residue	UNP Q7VU61
B	126	MSE	MET	modified residue	UNP Q7VU61
B	132	LEU	-	cloning artifact	UNP Q7VU61
B	133	GLU	-	cloning artifact	UNP Q7VU61
B	134	HIS	-	cloning artifact	UNP Q7VU61
B	135	HIS	-	cloning artifact	UNP Q7VU61
B	136	HIS	-	cloning artifact	UNP Q7VU61
B	137	HIS	-	cloning artifact	UNP Q7VU61
B	138	HIS	-	cloning artifact	UNP Q7VU61
B	139	HIS	-	cloning artifact	UNP Q7VU61
C	101	MSE	MET	modified residue	UNP Q7VU61

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	126	MSE	MET	modified residue	UNP Q7VU61
C	132	LEU	-	cloning artifact	UNP Q7VU61
C	133	GLU	-	cloning artifact	UNP Q7VU61
C	134	HIS	-	cloning artifact	UNP Q7VU61
C	135	HIS	-	cloning artifact	UNP Q7VU61
C	136	HIS	-	cloning artifact	UNP Q7VU61
C	137	HIS	-	cloning artifact	UNP Q7VU61
C	138	HIS	-	cloning artifact	UNP Q7VU61
C	139	HIS	-	cloning artifact	UNP Q7VU61
D	101	MSE	MET	modified residue	UNP Q7VU61
D	126	MSE	MET	modified residue	UNP Q7VU61
D	132	LEU	-	cloning artifact	UNP Q7VU61
D	133	GLU	-	cloning artifact	UNP Q7VU61
D	134	HIS	-	cloning artifact	UNP Q7VU61
D	135	HIS	-	cloning artifact	UNP Q7VU61
D	136	HIS	-	cloning artifact	UNP Q7VU61
D	137	HIS	-	cloning artifact	UNP Q7VU61
D	138	HIS	-	cloning artifact	UNP Q7VU61
D	139	HIS	-	cloning artifact	UNP Q7VU61

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

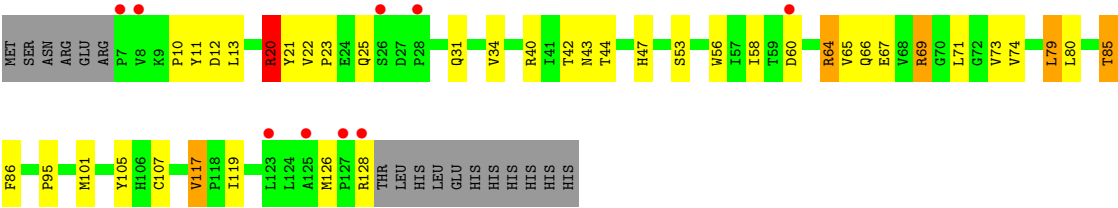
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	87	Total	O	0	0
			87	87		
3	C	71	Total	O	0	0
			71	71		
3	D	67	Total	O	0	0
			67	67		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.56Å 100.26Å 108.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.73 – 2.70 29.73 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.1 (29.73-2.70) 96.0 (29.73-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.286 0.259 , 0.300	Depositor DCC
R_{free} test set	5453 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.705	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4122	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.19 % 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 3.7833e-05. 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.44	0/983	0.97	1/1344 (0.1%)
1	B	0.47	0/965	0.99	1/1320 (0.1%)
1	C	0.46	0/976	0.96	3/1334 (0.2%)
1	D	0.47	0/976	0.95	0/1334
All	All	0.46	0/3900	0.97	5/5332 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	GLY	N-CA-C	-6.39	107.64	114.67
1	A	61	GLY	N-CA-C	-5.33	108.81	114.67
1	C	61	GLY	N-CA-C	-5.32	107.19	113.99
1	C	94	LEU	CA-C-N	5.01	124.50	119.19
1	C	94	LEU	C-N-CA	5.01	124.50	119.19

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	957	0	936	49	0
1	B	939	0	916	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	950	0	929	48	0
1	D	950	0	929	37	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	81	0	0	5	0
3	B	87	0	0	4	0
3	C	71	0	0	1	0
3	D	67	0	0	2	0
All	All	4122	0	3710	165	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 22.

The worst 5 of 165 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:38:THR:HG23	1:A:89:THR:HG22	1.51	0.92
1:B:38:THR:HG23	1:B:89:THR:HG22	1.56	0.87
1:D:20:ARG:HH11	1:D:20:ARG:HB2	1.42	0.83
1:D:69:ARG:HG3	1:D:69:ARG:HH11	1.47	0.80
1:B:111:ASN:OD1	1:B:113:ILE:HG12	1.82	0.78

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	121/139 (87%)	113 (93%)	5 (4%)	3 (2%)	4	11
1	B	119/139 (86%)	115 (97%)	4 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	120/139 (86%)	115 (96%)	5 (4%)	0	100	100
1	D	120/139 (86%)	114 (95%)	5 (4%)	1 (1%)	16	37
All	All	480/556 (86%)	457 (95%)	19 (4%)	4 (1%)	16	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ARG
1	A	8	VAL
1	D	20	ARG
1	A	127	PRO

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	A	107/121 (88%)	105 (98%)	2 (2%)	50	77
1	B	105/121 (87%)	101 (96%)	4 (4%)	29	58
1	C	106/121 (88%)	100 (94%)	6 (6%)	18	43
1	D	106/121 (88%)	98 (92%)	8 (8%)	12	31
All	All	424/484 (88%)	404 (95%)	20 (5%)	23	51

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	64	ARG
1	D	79	LEU
1	D	117	VAL
1	D	85	THR
1	C	22	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	43	ASN
1	D	25	GLN
1	C	77	GLN
1	D	30	GLN
1	B	31	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	D	404	-	4,4,4	2.52	3 (75%)	6,6,6	1.49	1 (16%)
2	PO4	B	402	-	4,4,4	2.55	3 (75%)	6,6,6	1.54	1 (16%)
2	PO4	A	401	-	4,4,4	2.47	3 (75%)	6,6,6	1.51	1 (16%)
2	PO4	C	403	-	4,4,4	2.46	3 (75%)	6,6,6	1.55	1 (16%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	PO4	P-O2	-3.20	1.45	1.54
2	D	404	PO4	P-O2	-3.17	1.45	1.54
2	C	403	PO4	P-O2	-3.11	1.45	1.54
2	D	404	PO4	P-O1	-3.11	1.43	1.50
2	B	402	PO4	P-O1	-3.11	1.43	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	PO4	O4-P-O3	-3.23	97.86	107.91
2	C	403	PO4	O4-P-O3	-3.15	98.11	107.91
2	A	401	PO4	O4-P-O3	-3.08	98.32	107.91
2	D	404	PO4	O4-P-O3	-3.00	98.58	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	121/139 (87%)	0.50	9 (7%) 20 18	12, 30, 59, 85	0
1	B	119/139 (85%)	0.51	12 (10%) 12 10	12, 29, 58, 69	0
1	C	120/139 (86%)	0.45	7 (5%) 29 25	12, 31, 59, 79	0
1	D	120/139 (86%)	0.39	9 (7%) 20 17	13, 29, 56, 78	0
All	All	480/556 (86%)	0.46	37 (7%) 19 17	12, 30, 59, 85	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	THR	6.7
1	C	7	PRO	5.3
1	D	7	PRO	4.6
1	B	123	LEU	4.1
1	A	7	PRO	3.7

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 oligosaccharides 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, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	A	401	5/5	0.91	0.13	60,60,61,63	0
2	PO4	B	402	5/5	0.92	0.12	51,51,51,52	0
2	PO4	C	403	5/5	0.93	0.12	51,51,51,52	0
2	PO4	D	404	5/5	0.95	0.12	47,48,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.