



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 9Y01 / pdb_00009y01
Title : QatB-QatC complex in qatABCD anti-phage defense
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Deposited on : 2025-08-28
Resolution : 1.31 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

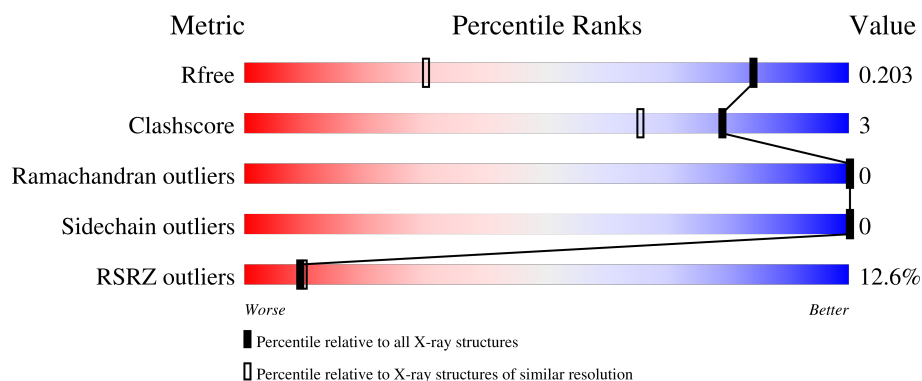
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.31 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}	164625	2202 (1.34-1.30)
Clashscore	180529	2378 (1.34-1.30)
Ramachandran outliers	177936	2325 (1.34-1.30)
Sidechain outliers	177891	2325 (1.34-1.30)
RSRZ outliers	164620	2199 (1.34-1.30)

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	287	<div> <div>10%</div> <div>72%</div> <div>25%</div> </div>
2	B	466	<div> <div>11%</div> <div>87%</div> <div>5%</div> <div>8%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5569 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 QatB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1591	978	289	318	6			

- Molecule 2 is a protein called QatC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	0	0
			3330	2090	596	627	17			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	178	Total	O	0	0
			178	178		
4	B	469	Total	O	0	0
			469	469		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.87Å 74.59Å 133.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.25 – 1.31 34.25 – 1.31	Depositor EDS
% Data completeness (in resolution range)	76.4 (34.25-1.31) 77.2 (34.25-1.31)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.31Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.183 , 0.203 0.183 , 0.203	Depositor DCC
R_{free} test set	6428 reflections (3.75%)	wwPDB-VP
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5569	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0/1609	0.61	0/2170
2	B	0.49	0/3397	0.68	0/4606
All	All	0.48	0/5006	0.66	0/6776

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	1591	0	1566	7	0
2	B	3330	0	3281	19	0
3	B	1	0	0	0	0
4	A	178	0	0	3	3
4	B	469	0	0	7	4
All	All	5569	0	4847	25	4

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 (25) 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:167:GLY:HA2	2:B:275:ALA:HB3	1.69	0.72
2:B:154:LEU:HD22	2:B:237:PHE:CE1	2.24	0.71
2:B:154:LEU:HD21	2:B:241:ALA:HB2	1.73	0.70
2:B:87:SER:OG	4:B:601:HOH:O	2.13	0.66
2:B:12:GLU:HG2	4:B:843:HOH:O	1.98	0.63
1:A:273:GLU:HG2	4:A:396:HOH:O	2.05	0.56
2:B:55:LEU:HB3	2:B:247:ALA:HB1	1.90	0.53
2:B:276:CYS:HA	4:B:863:HOH:O	2.10	0.52
2:B:187:THR:N	4:B:610:HOH:O	2.44	0.50
2:B:351:PRO:N	4:B:611:HOH:O	2.44	0.50
1:A:144:GLN:OE1	1:A:148:GLN:HG2	2.13	0.49
1:A:166:GLU:CD	4:A:303:HOH:O	2.56	0.49
2:B:306:PHE:CD2	2:B:314:MET:HE3	2.48	0.48
2:B:227:GLU:N	4:B:612:HOH:O	2.46	0.48
1:A:140:VAL:HG23	1:A:144:GLN:NE2	2.30	0.47
2:B:154:LEU:HD22	2:B:237:PHE:CD1	2.50	0.47
2:B:3:HIS:HB3	4:B:827:HOH:O	2.15	0.45
2:B:56:SER:HB3	2:B:141:PRO:HD3	1.98	0.45
2:B:267:PRO:CG	2:B:274:GLY:HA2	2.49	0.42
1:A:116:LYS:HD3	1:A:156:PHE:O	2.20	0.42
1:A:75:ARG:NH2	4:A:307:HOH:O	2.53	0.42
2:B:140:THR:HA	2:B:141:PRO:HD3	1.90	0.42
2:B:154:LEU:HD23	2:B:154:LEU:HA	1.85	0.42
2:B:6:ILE:HD13	2:B:28:THR:HB	2.02	0.41
2:B:54:GLY:HA3	2:B:145:ARG:HA	2.04	0.40

All (4) 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)
4:A:334:HOH:O	4:B:953:HOH:O[4_445]	2.02	0.18
4:A:410:HOH:O	4:B:636:HOH:O[4_445]	2.02	0.18
4:B:624:HOH:O	4:B:955:HOH:O[4_555]	2.06	0.14
4:A:448:HOH:O	4:B:982:HOH:O[4_455]	2.16	0.04

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	A	211/287 (74%)	209 (99%)	2 (1%)	0	100	100
2	B	420/466 (90%)	411 (98%)	9 (2%)	0	100	100
All	All	631/753 (84%)	620 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	163/217 (75%)	163 (100%)	0	100	100
2	B	360/392 (92%)	360 (100%)	0	100	100
All	All	523/609 (86%)	523 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	180	HIS
2	B	317	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

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	215/287 (74%)	0.70	28 (13%) 9 9	11, 25, 57, 76	0
2	B	428/466 (91%)	0.51	53 (12%) 9 10	11, 20, 48, 67	0
All	All	643/753 (85%)	0.57	81 (12%) 9 10	11, 22, 52, 76	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	VAL	8.2
1	A	230	VAL	6.9
1	A	229	ALA	6.4
1	A	185	GLY	5.8
2	B	456	ILE	5.4
2	B	390	THR	5.3
1	A	256	TRP	5.1
1	A	259	PRO	5.0
2	B	270	PRO	5.0
2	B	216	PHE	4.9
2	B	276	CYS	4.7
2	B	372	GLY	4.6
2	B	274	GLY	4.6
2	B	273	LEU	4.5
2	B	230	LEU	4.4
1	A	257	PRO	4.2
2	B	237	PHE	4.1
2	B	268	LEU	4.1
2	B	275	ALA	4.1
2	B	450	LEU	4.1
2	B	413	HIS	4.0
2	B	452	GLY	3.9
2	B	455	ALA	3.9
2	B	337	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	387	ALA	3.8
1	A	262	GLN	3.8
2	B	388	LEU	3.8
2	B	228	ASP	3.6
2	B	269	ASP	3.6
2	B	227	GLU	3.5
2	B	457	PRO	3.5
1	A	258	ALA	3.5
2	B	454	THR	3.3
2	B	280	THR	3.3
2	B	453	VAL	3.2
2	B	277	SER	3.2
2	B	187	THR	3.1
1	A	233	ILE	3.1
2	B	272	ARG	3.1
2	B	399	ARG	3.1
2	B	135	ASP	3.0
2	B	271	ARG	3.0
1	A	217	GLY	3.0
2	B	2	ARG	2.9
1	A	232	ARG	2.9
2	B	233	ARG	2.8
2	B	393	SER	2.8
2	B	335	SER	2.7
2	B	385	ALA	2.6
2	B	3	HIS	2.6
1	A	184	GLY	2.6
2	B	398	VAL	2.6
2	B	229	THR	2.5
1	A	286	LEU	2.5
2	B	107	THR	2.4
1	A	228	ASP	2.4
1	A	78	ARG	2.4
2	B	134	ILE	2.4
2	B	140	THR	2.3
1	A	255	GLN	2.3
2	B	206	SER	2.3
1	A	260	THR	2.2
2	B	142	GLU	2.2
1	A	75	ARG	2.2
2	B	391	ASN	2.2
2	B	267	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	336	SER	2.2
1	A	64	GLY	2.2
1	A	71	SER	2.2
2	B	36	TYR	2.2
2	B	449	TYR	2.2
2	B	394	ASP	2.1
1	A	234	GLN	2.1
2	B	386	GLN	2.1
1	A	254	GLU	2.1
1	A	261	ASP	2.1
2	B	395	GLY	2.1
1	A	231	GLU	2.0
1	A	67	ARG	2.0
1	A	68	GLY	2.0
1	A	250	ALA	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 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(\AA^2)	Q<0.9
3	ZN	B	501	1/1	0.96	0.07	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.