



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 04:21 PM UTC

PDB ID : 4QQ0 / pdb_00004qq0
Title : CdsD - The structural protein of the Type III secretion system of Chlamydia trachomatis: C-terminal domain
Authors : Merilainen, G.; Wierenga, R.K.
Deposited on : 2014-06-26
Resolution : 2.00 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

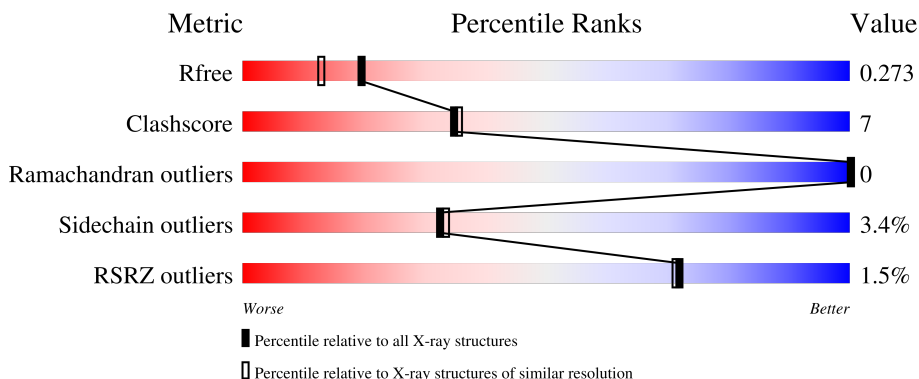
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	280	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1688 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 Adenylate cyclase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	3	0
			1597	1024	268	300	5			

There are 31 discrepancies between the modelled and reference sequences:

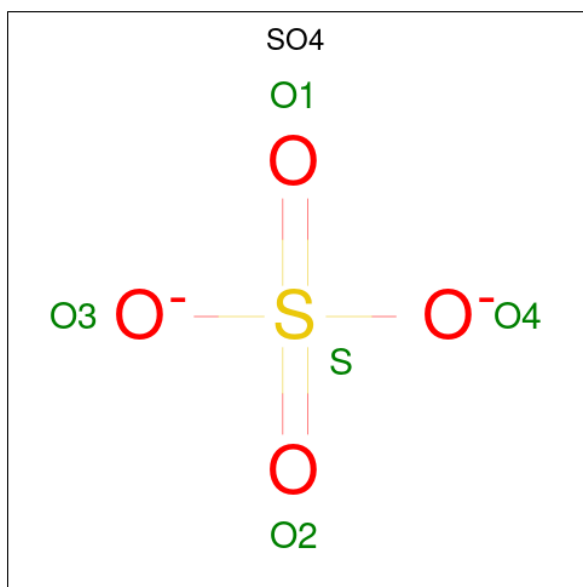
Chain	Residue	Modelled	Actual	Comment	Reference
A	509	MET	-	expression tag	UNP O84671
A	510	GLY	-	expression tag	UNP O84671
A	511	GLY	-	expression tag	UNP O84671
A	512	SER	-	expression tag	UNP O84671
A	513	HIS	-	expression tag	UNP O84671
A	514	HIS	-	expression tag	UNP O84671
A	515	HIS	-	expression tag	UNP O84671
A	516	HIS	-	expression tag	UNP O84671
A	517	HIS	-	expression tag	UNP O84671
A	518	HIS	-	expression tag	UNP O84671
A	519	GLY	-	expression tag	UNP O84671
A	520	MET	-	expression tag	UNP O84671
A	521	ALA	-	expression tag	UNP O84671
A	522	SER	-	expression tag	UNP O84671
A	523	MET	-	expression tag	UNP O84671
A	524	THR	-	expression tag	UNP O84671
A	525	GLY	-	expression tag	UNP O84671
A	526	GLY	-	expression tag	UNP O84671
A	527	GLN	-	expression tag	UNP O84671
A	528	GLN	-	expression tag	UNP O84671
A	529	MET	-	expression tag	UNP O84671
A	530	GLY	-	expression tag	UNP O84671
A	531	ARG	-	expression tag	UNP O84671
A	532	ASP	-	expression tag	UNP O84671
A	533	LEU	-	expression tag	UNP O84671
A	534	TYR	-	expression tag	UNP O84671
A	535	ASP	-	expression tag	UNP O84671

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	536	ASP	-	expression tag	UNP O84671
A	537	ASP	-	expression tag	UNP O84671
A	538	ASP	-	expression tag	UNP O84671
A	539	LYS	-	expression tag	UNP O84671

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

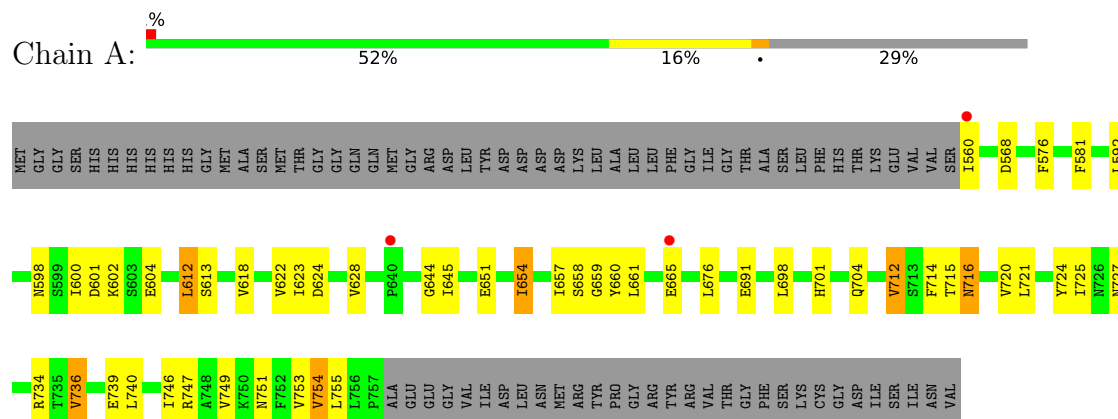
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		

3 Residue-property plots

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: Adenylate cyclase-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	23.51Å 49.43Å 76.93Å 90.00° 92.79° 90.00°	Depositor
Resolution (Å)	30.30 – 2.00 30.30 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.0 (30.30-2.00) 99.5 (30.30-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.192 , 0.245 (Not available) , 0.273	Depositor DCC
R_{free} test set	582 reflections (4.20%)	wwPDB-VP
Wilson B-factor (Å ²)	10.0	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
Reported twinning fraction	0.158 for H, K, L 0.842 for -h,-k,l	Depositor
Outliers	0 of 12405 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	1688	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.48% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.20	4/1626 (0.2%)	1.31	12/2202 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	613	SER	N-CA	8.54	1.56	1.46
1	A	628	VAL	CA-C	5.61	1.59	1.52
1	A	657	ILE	CA-C	5.47	1.59	1.52
1	A	592	LEU	N-CA	5.29	1.52	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	691	GLU	N-CA-C	6.14	117.98	111.28
1	A	623	ILE	N-CA-C	5.96	116.69	107.99
1	A	658	SER	N-CA-C	5.72	116.92	108.86
1	A	751	ASN	N-CA-C	5.66	117.87	108.20
1	A	701	HIS	N-CA-C	5.60	117.38	111.28

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	1597	0	1597	24	0
2	A	10	0	0	0	0
3	A	81	0	0	3	0
All	All	1688	0	1597	24	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 7.

The worst 5 of 24 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:712:VAL:CG1	1:A:721:LEU:HD23	2.05	0.87
1:A:712:VAL:HG12	1:A:721:LEU:HD23	1.61	0.78
1:A:651:GLU:HB3	1:A:654:ILE:HD12	1.85	0.59
1:A:734:ARG:NH2	3:A:923:HOH:O	2.34	0.58
1:A:600:ILE:HG13	3:A:934:HOH:O	2.06	0.55

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	153/280 (55%)	151 (99%)	2 (1%)	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	179/242 (74%)	173 (97%)	6 (3%)	32	33

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	715	THR
1	A	736	VAL
1	A	754	VAL
1	A	676	LEU
1	A	665	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	574	GLN
1	A	711	HIS
1	A	727	ASN
1	A	741	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	SO4	A	801	-	4,4,4	0.41	0	6,6,6	0.57	0
2	SO4	A	802	-	4,4,4	0.40	0	6,6,6	0.24	0

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 [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	198/280 (70%)	0.34	3 (1%) 72 71	1, 9, 23, 37	3 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	560	ILE	4.8
1	A	640	PRO	2.5
1	A	665	GLU	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 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(Å ²)	Q<0.9
2	SO4	A	802	5/5	0.66	0.19	69,71,71,72	0
2	SO4	A	801	5/5	0.90	0.12	23,25,25,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.