



Full wwPDB X-ray Structure Validation Report

Jun 17, 2014 – 09:14 AM EDT

PDB ID : 4HSS
Title : Structure of the Full-Length Major Pilin SpaD from *Corynebacterium diphtheriae*
Authors : Paterson, N.G.; Kang, H.J.; Baker, E.N.
Deposited on : 2012-10-30
Resolution : 2.50 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

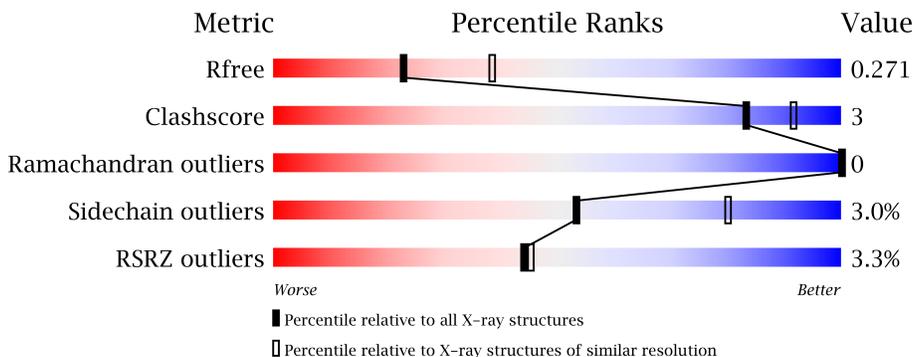
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : **FAILED**
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	431	
1	B	431	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6491 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Putative fimbrial subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	411	Total 3175	C 1996	N 528	O 646	S 5	0	0	0
1	B	393	Total 3034	C 1911	N 503	O 616	S 4	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Ca 1	0	0
2	A	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

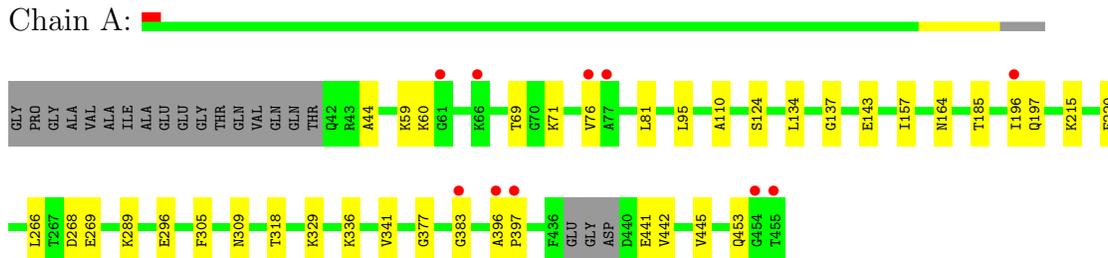
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	160	Total 160	O 160	0	0
3	B	120	Total 120	O 120	0	0

3 Residue-property plots

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

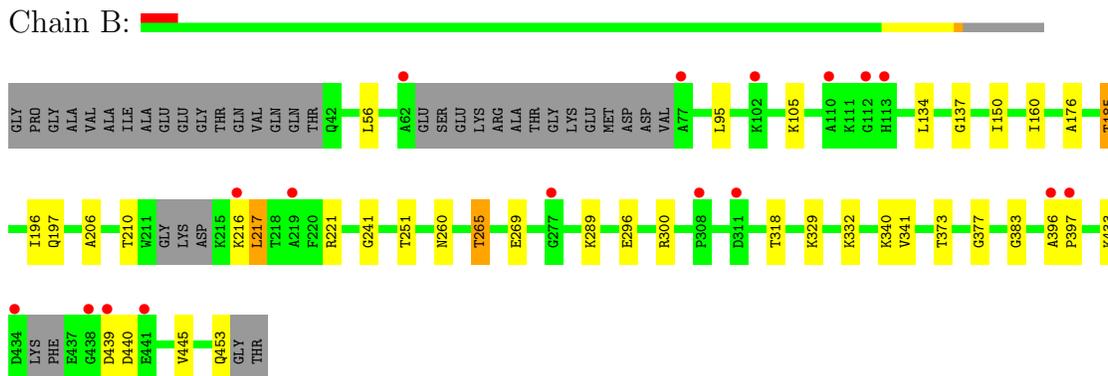
- Molecule 1: Putative fimbrial subunit

Chain A:



- Molecule 1: Putative fimbrial subunit

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	32.83Å 56.79Å 435.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.36 – 2.50 28.34 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (28.36-2.50) 94.0 (28.34-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.51Å)	Xtrriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.187 , 0.250 0.198 , 0.271	Depositor DCC
R_{free} test set	1405 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	44.9	Xtrriage
Anisotropy	0.703	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.0	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Outliers	0 of 27924 reflections	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6491	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: CA

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	0.51	0/3225	0.72	0/4350
1	B	0.51	0/3081	0.70	0/4159
All	All	0.51	0/6306	0.71	0/8509

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3175	0	3158	19	0
1	B	3034	0	3014	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	160	0	0	1	0
3	B	120	0	0	3	0
All	All	6491	0	6172	37	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (37) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:110:ALA:HB2	1:A:157:ILE:HD11	1.72	0.72
1:A:44:ALA:HB2	1:B:340:LYS:HB3	1.84	0.60
1:A:185:THR:HG22	1:A:318:THR:HG22	1.83	0.59
1:B:95:LEU:HD13	1:B:137:GLY:HA2	1.84	0.58
1:B:185:THR:HG22	1:B:318:THR:HG22	1.86	0.56
1:B:216:LYS:HG2	1:B:217:LEU:H	1.70	0.56
1:A:95:LEU:HD13	1:A:137:GLY:HA2	1.88	0.55
1:B:134:LEU:HD23	1:B:160:ILE:HD13	1.89	0.54
1:A:59:LYS:HE3	1:A:76:VAL:HA	1.90	0.53
1:B:216:LYS:HG2	1:B:217:LEU:N	2.23	0.53
1:A:215:LYS:HD2	1:A:309:ASN:HA	1.92	0.51
1:B:185:THR:HG23	1:B:206:ALA:HB2	1.92	0.51
1:A:60:LYS:HD3	1:A:81:LEU:HD13	1.94	0.50
1:A:441:GLU:HG3	1:A:442:VAL:HG13	1.93	0.50
1:B:329:LYS:HB3	1:B:445:VAL:HG22	1.95	0.49
1:A:329:LYS:HB3	1:A:445:VAL:HG22	1.96	0.48
1:B:241:GLY:HA2	3:B:653:HOH:O	2.14	0.48
1:B:185:THR:CG2	1:B:318:THR:HG22	2.44	0.47
1:A:143:GLU:HG3	3:A:603:HOH:O	2.13	0.47
1:B:221:ARG:HB3	1:B:265:THR:HG23	1.98	0.46
1:A:220:PHE:CD2	1:A:305:PHE:HB3	2.52	0.44
1:A:220:PHE:HB3	1:A:266:LEU:HD12	2.00	0.43
1:A:69:THR:O	1:A:164:ASN:HB2	2.19	0.43
1:B:341:VAL:HB	1:B:377:GLY:HA3	2.01	0.42
1:B:296:GLU:HG2	3:B:655:HOH:O	2.19	0.42
1:B:396:ALA:HA	1:B:397:PRO:HA	1.92	0.42
1:A:341:VAL:HB	1:A:377:GLY:HA3	2.01	0.42
1:A:110:ALA:CB	1:A:157:ILE:HD11	2.46	0.41
1:A:396:ALA:HA	1:A:397:PRO:HA	1.91	0.41
1:A:197:GLN:NE2	1:A:289:LYS:HA	2.36	0.41
1:B:197:GLN:NE2	1:B:289:LYS:HA	2.36	0.41
1:B:332:LYS:HB2	1:B:373:THR:HG21	2.03	0.41
1:B:56:LEU:HD23	1:B:176:ALA:HB3	2.03	0.41
1:B:196:ILE:HB	1:B:383:GLY:H	1.86	0.41
1:A:196:ILE:HB	1:A:383:GLY:H	1.86	0.40
1:A:69:THR:HB	1:A:71:LYS:HE3	2.03	0.40
1:B:210:THR:HG23	3:B:703:HOH:O	2.22	0.40

There are no symmetry-related clashes.

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	407/431 (94%)	393 (97%)	14 (3%)	0	100	100
1	B	385/431 (89%)	371 (96%)	14 (4%)	0	100	100
All	All	792/862 (92%)	764 (96%)	28 (4%)	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	346/359 (96%)	339 (98%)	7 (2%)	68	89
1	B	331/359 (92%)	318 (96%)	13 (4%)	43	70
All	All	677/718 (94%)	657 (97%)	20 (3%)	53	80

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	SER
1	A	134	LEU
1	A	268	ASP
1	A	269	GLU
1	A	296	GLU
1	A	336	LYS
1	A	453	GLN
1	B	105	LYS
1	B	150	ILE
1	B	185	THR
1	B	217	LEU

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Mol	Chain	Res	Type
1	B	251	THR
1	B	260	ASN
1	B	265	THR
1	B	269	GLU
1	B	300	ARG
1	B	433	LYS
1	B	439	ASP
1	B	440	ASP
1	B	453	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	197	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.8 Polymer linkage issues

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	411/431 (95%)	-0.11	10 (2%) 56 58	26, 46, 74, 114	0
1	B	393/431 (91%)	0.08	17 (4%) 34 35	35, 57, 85, 102	0
All	All	804/862 (93%)	-0.02	27 (3%) 44 44	26, 51, 82, 114	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	112	GLY	5.1
1	A	66	LYS	4.9
1	A	77	ALA	4.5
1	B	77	ALA	4.4
1	A	397	PRO	4.1
1	A	396	ALA	3.8
1	B	438	GLY	3.6
1	B	219	ALA	3.3
1	B	396	ALA	3.3
1	A	455	THR	3.1
1	A	76	VAL	3.0
1	B	113	HIS	2.8
1	A	454	GLY	2.8
1	B	62	ALA	2.8
1	B	434	ASP	2.7
1	A	61	GLY	2.6
1	B	102	LYS	2.6
1	B	439	ASP	2.6
1	B	216	LYS	2.5
1	B	397	PRO	2.4
1	B	311	ASP	2.3
1	B	110	ALA	2.2
1	B	308	PRO	2.2
1	B	441	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	383	GLY	2.1
1	A	196	ILE	2.0
1	B	277	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q < 0.9
2	CA	B	501	1/1	0.16	-0.14	87,87,87,87	0
2	CA	A	501	1/1	0.09	-1.80	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.