



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 11:17 AM EDT

PDB ID : 5H5V
Title : Crystal structure of the flagellar cap protein FliD D1-D2-D3 domains from Escherichia coli
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Deposited on : 2016-11-09
Resolution : 3.00 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

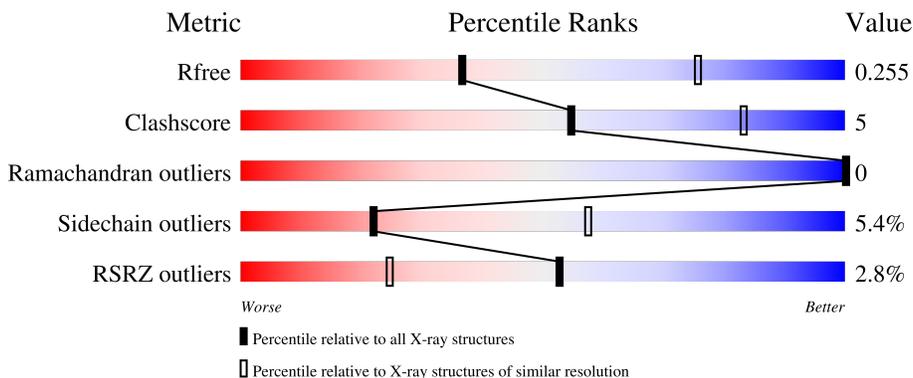
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	380	 79% 13% • 7%
1	B	380	 77% 11% • 11%
1	C	380	 80% 12% • 6%
1	D	380	 82% 8% • 9%
1	E	380	 74% • • 21%

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Mol	Chain	Length	Quality of chain
1	F	380	 <p>2% 76% 9% ** 13%</p>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13919 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 Flagellar hook-associated protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	352	2497	1524	423	546	4	0	0	0
1	B	339	2345	1424	399	518	4	0	0	0
1	C	356	2513	1536	425	548	4	0	0	0
1	D	345	2363	1438	400	521	4	0	0	0
1	E	299	1921	1151	344	423	3	0	0	0
1	F	330	2280	1386	392	498	4	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	GLY	-	expression tag	UNP A0A094VPA5
A	38	SER	-	expression tag	UNP A0A094VPA5
A	39	ALA	-	expression tag	UNP A0A094VPA5
A	40	LYS	-	expression tag	UNP A0A094VPA5
A	41	ASP	-	expression tag	UNP A0A094VPA5
A	42	LEU	-	expression tag	UNP A0A094VPA5
B	37	GLY	-	expression tag	UNP A0A094VPA5
B	38	SER	-	expression tag	UNP A0A094VPA5
B	39	ALA	-	expression tag	UNP A0A094VPA5
B	40	LYS	-	expression tag	UNP A0A094VPA5
B	41	ASP	-	expression tag	UNP A0A094VPA5
B	42	LEU	-	expression tag	UNP A0A094VPA5
C	37	GLY	-	expression tag	UNP A0A094VPA5
C	38	SER	-	expression tag	UNP A0A094VPA5
C	39	ALA	-	expression tag	UNP A0A094VPA5
C	40	LYS	-	expression tag	UNP A0A094VPA5
C	41	ASP	-	expression tag	UNP A0A094VPA5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	42	LEU	-	expression tag	UNP A0A094VPA5
D	37	GLY	-	expression tag	UNP A0A094VPA5
D	38	SER	-	expression tag	UNP A0A094VPA5
D	39	ALA	-	expression tag	UNP A0A094VPA5
D	40	LYS	-	expression tag	UNP A0A094VPA5
D	41	ASP	-	expression tag	UNP A0A094VPA5
D	42	LEU	-	expression tag	UNP A0A094VPA5
E	37	GLY	-	expression tag	UNP A0A094VPA5
E	38	SER	-	expression tag	UNP A0A094VPA5
E	39	ALA	-	expression tag	UNP A0A094VPA5
E	40	LYS	-	expression tag	UNP A0A094VPA5
E	41	ASP	-	expression tag	UNP A0A094VPA5
E	42	LEU	-	expression tag	UNP A0A094VPA5
F	37	GLY	-	expression tag	UNP A0A094VPA5
F	38	SER	-	expression tag	UNP A0A094VPA5
F	39	ALA	-	expression tag	UNP A0A094VPA5
F	40	LYS	-	expression tag	UNP A0A094VPA5
F	41	ASP	-	expression tag	UNP A0A094VPA5
F	42	LEU	-	expression tag	UNP A0A094VPA5

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.06Å 181.58Å 110.46Å 90.00° 105.23° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.79 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-3.00) 99.2 (29.79-2.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 3.00Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.228 , 0.258 0.227 , 0.255	Depositor DCC
R_{free} test set	3134 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtrriage
Anisotropy	0.129	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13919	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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](#)

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	0.67	0/2509	0.74	0/3415
1	B	0.60	0/2356	0.70	0/3218
1	C	0.68	0/2526	0.74	0/3439
1	D	0.64	0/2375	0.71	0/3249
1	E	0.54	0/1922	0.66	0/2631
1	F	0.67	2/2290 (0.1%)	0.80	7/3127 (0.2%)
All	All	0.64	2/13978 (0.0%)	0.73	7/19079 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	216	MSE	CG-SE	-8.62	1.66	1.95
1	F	216	MSE	CB-CG	-7.43	1.30	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	216	MSE	CB-CG-SE	16.46	162.07	112.70
1	F	115	ASP	CB-CG-OD1	7.71	125.24	118.30
1	F	115	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	F	188	ASP	CB-CG-OD1	5.92	123.63	118.30
1	F	198	ASP	CB-CG-OD1	-5.17	113.64	118.30

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	2497	0	2459	35	0
1	B	2345	0	2208	28	0
1	C	2513	0	2459	35	0
1	D	2363	0	2186	21	0
1	E	1921	0	1629	8	0
1	F	2280	0	2132	19	0
All	All	13919	0	13073	141	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 5.

The worst 5 of 141 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:C:339:LYS:H	1:C:343:GLN:HE22	1.22	0.88
1:C:54:LEU:HD11	1:C:321:ILE:HD13	1.68	0.75
1:F:321:ILE:HG23	1:F:397:TRP:CZ3	2.23	0.73
1:D:145:ALA:O	1:D:148:SER:HB3	1.91	0.71
1:F:325:LEU:HD23	1:F:328:MSE:HE3	1.72	0.71

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	348/380 (92%)	335 (96%)	13 (4%)	0	100	100
1	B	335/380 (88%)	326 (97%)	9 (3%)	0	100	100
1	C	352/380 (93%)	342 (97%)	10 (3%)	0	100	100
1	D	341/380 (90%)	333 (98%)	8 (2%)	0	100	100
1	E	293/380 (77%)	287 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	326/380 (86%)	318 (98%)	8 (2%)	0	100	100
All	All	1995/2280 (88%)	1941 (97%)	54 (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	272/302 (90%)	258 (95%)	14 (5%)	24	60
1	B	242/302 (80%)	228 (94%)	14 (6%)	20	55
1	C	270/302 (89%)	255 (94%)	15 (6%)	21	56
1	D	235/302 (78%)	224 (95%)	11 (5%)	26	63
1	E	161/302 (53%)	152 (94%)	9 (6%)	21	56
1	F	229/302 (76%)	216 (94%)	13 (6%)	20	56
All	All	1409/1812 (78%)	1333 (95%)	76 (5%)	22	57

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	114	ARG
1	F	216	MSE
1	E	238	SER
1	F	79	THR
1	F	276	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	104	GLN
1	F	104	GLN
1	F	343	GLN

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Mol	Chain	Res	Type
1	F	272	GLN
1	C	343	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](#)

There are no ligands in this entry.

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	348/380 (91%)	-0.52	0 100 100	34, 51, 83, 104	0
1	B	335/380 (88%)	-0.36	4 (1%) 79 54	32, 60, 134, 197	0
1	C	352/380 (92%)	-0.51	0 100 100	33, 48, 87, 111	0
1	D	341/380 (89%)	-0.23	8 (2%) 60 31	27, 62, 149, 188	0
1	E	295/380 (77%)	0.31	37 (12%) 3 1	37, 77, 289, 348	0
1	F	326/380 (85%)	-0.26	6 (1%) 68 40	34, 66, 145, 189	0
All	All	1997/2280 (87%)	-0.28	55 (2%) 53 25	27, 57, 223, 348	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	278	TRP	5.6
1	D	46	ALA	5.4
1	E	402	GLY	4.7
1	E	399	SER	4.7
1	E	406	ALA	4.6

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.