wwPDB X-ray Structure Validation Summary Report (i)

Jun 26, 2024 – 07:38 AM EDT

PDB ID	:	6S09
Title	:	C-terminally extended and N-terminally truncated variant of FimA E. coli at 1.5 Angstrom resolution
Authors	:	Zyla, D.; Echeverria, B.; Glockshuber, R.
Deposited on	:	2019-06-14
Resolution	:	1.50 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 (i) 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 (i)) were used in the production of this report:

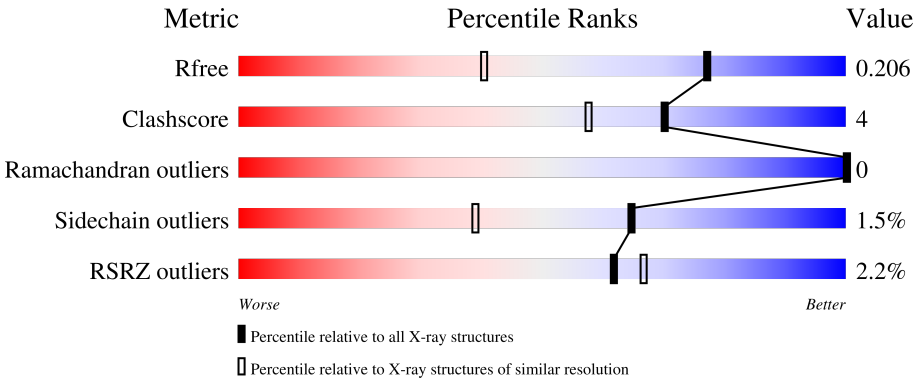
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 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 <=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	166	89% 8%
1	B	166	2% 88% 6% 6%
1	C	166	95%
1	D	166	4% 90% 7%
1	E	166	2% 90% 9%

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Mol	Chain	Length	Quality of chain
1	F	166	2% 93% 7%
1	G	166	% 93% 5%
1	H	166	3% 90% 10%

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
4	ACY	C	203	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19814 atoms, of which 8774 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 FimA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	F	166	Total	C	H	N	O	S	0	3	0
			2281	707	1127	203	242	2			
1	A	161	Total	C	H	N	O	S	0	2	0
			2205	684	1084	198	237	2			
1	B	156	Total	C	H	N	O	S	0	1	0
			2154	669	1059	192	232	2			
1	C	164	Total	C	H	N	O	S	0	0	0
			2221	689	1090	201	239	2			
1	D	161	Total	C	H	N	O	S	0	1	0
			2206	685	1085	197	237	2			
1	E	164	Total	C	H	N	O	S	0	2	0
			2233	694	1096	200	241	2			
1	G	163	Total	C	H	N	O	S	0	4	0
			2273	705	1126	200	240	2			
1	H	165	Total	C	H	N	O	S	0	1	0
			2246	697	1104	202	241	2			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	142	GLY	-	expression tag	UNP M4YRT1
F	143	GLY	-	expression tag	UNP M4YRT1
F	144	GLY	-	expression tag	UNP M4YRT1
F	145	GLY	-	expression tag	UNP M4YRT1
F	146	GLY	-	expression tag	UNP M4YRT1
F	147	GLY	-	expression tag	UNP M4YRT1
F	148	ALA	-	expression tag	UNP M4YRT1
F	149	ASN	-	expression tag	UNP M4YRT1
F	150	VAL	-	expression tag	UNP M4YRT1
F	151	VAL	-	expression tag	UNP M4YRT1
F	152	GLU	-	expression tag	UNP M4YRT1
F	153	GLY	-	expression tag	UNP M4YRT1
F	154	LYS	-	expression tag	UNP M4YRT1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	155	PHE	-	expression tag	UNP M4YRT1
F	156	HIS	-	expression tag	UNP M4YRT1
F	157	VAL	-	expression tag	UNP M4YRT1
F	158	THR	-	expression tag	UNP M4YRT1
F	159	GLY	-	expression tag	UNP M4YRT1
F	160	GLY	-	expression tag	UNP M4YRT1
F	161	ASN	-	expression tag	UNP M4YRT1
F	162	VAL	-	expression tag	UNP M4YRT1
F	163	THR	-	expression tag	UNP M4YRT1
F	164	THR	-	expression tag	UNP M4YRT1
F	165	ALA	-	expression tag	UNP M4YRT1
F	166	ALA	-	expression tag	UNP M4YRT1
A	142	GLY	-	expression tag	UNP M4YRT1
A	143	GLY	-	expression tag	UNP M4YRT1
A	144	GLY	-	expression tag	UNP M4YRT1
A	145	GLY	-	expression tag	UNP M4YRT1
A	146	GLY	-	expression tag	UNP M4YRT1
A	147	GLY	-	expression tag	UNP M4YRT1
A	148	ALA	-	expression tag	UNP M4YRT1
A	149	ASN	-	expression tag	UNP M4YRT1
A	150	VAL	-	expression tag	UNP M4YRT1
A	151	VAL	-	expression tag	UNP M4YRT1
A	152	GLU	-	expression tag	UNP M4YRT1
A	153	GLY	-	expression tag	UNP M4YRT1
A	154	LYS	-	expression tag	UNP M4YRT1
A	155	PHE	-	expression tag	UNP M4YRT1
A	156	HIS	-	expression tag	UNP M4YRT1
A	157	VAL	-	expression tag	UNP M4YRT1
A	158	THR	-	expression tag	UNP M4YRT1
A	159	GLY	-	expression tag	UNP M4YRT1
A	160	GLY	-	expression tag	UNP M4YRT1
A	161	ASN	-	expression tag	UNP M4YRT1
A	162	VAL	-	expression tag	UNP M4YRT1
A	163	THR	-	expression tag	UNP M4YRT1
A	164	THR	-	expression tag	UNP M4YRT1
A	165	ALA	-	expression tag	UNP M4YRT1
A	166	ALA	-	expression tag	UNP M4YRT1
B	142	GLY	-	expression tag	UNP M4YRT1
B	143	GLY	-	expression tag	UNP M4YRT1
B	144	GLY	-	expression tag	UNP M4YRT1
B	145	GLY	-	expression tag	UNP M4YRT1
B	146	GLY	-	expression tag	UNP M4YRT1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	147	GLY	-	expression tag	UNP M4YRT1
B	148	ALA	-	expression tag	UNP M4YRT1
B	149	ASN	-	expression tag	UNP M4YRT1
B	150	VAL	-	expression tag	UNP M4YRT1
B	151	VAL	-	expression tag	UNP M4YRT1
B	152	GLU	-	expression tag	UNP M4YRT1
B	153	GLY	-	expression tag	UNP M4YRT1
B	154	LYS	-	expression tag	UNP M4YRT1
B	155	PHE	-	expression tag	UNP M4YRT1
B	156	HIS	-	expression tag	UNP M4YRT1
B	157	VAL	-	expression tag	UNP M4YRT1
B	158	THR	-	expression tag	UNP M4YRT1
B	159	GLY	-	expression tag	UNP M4YRT1
B	160	GLY	-	expression tag	UNP M4YRT1
B	161	ASN	-	expression tag	UNP M4YRT1
B	162	VAL	-	expression tag	UNP M4YRT1
B	163	THR	-	expression tag	UNP M4YRT1
B	164	THR	-	expression tag	UNP M4YRT1
B	165	ALA	-	expression tag	UNP M4YRT1
B	166	ALA	-	expression tag	UNP M4YRT1
C	142	GLY	-	expression tag	UNP M4YRT1
C	143	GLY	-	expression tag	UNP M4YRT1
C	144	GLY	-	expression tag	UNP M4YRT1
C	145	GLY	-	expression tag	UNP M4YRT1
C	146	GLY	-	expression tag	UNP M4YRT1
C	147	GLY	-	expression tag	UNP M4YRT1
C	148	ALA	-	expression tag	UNP M4YRT1
C	149	ASN	-	expression tag	UNP M4YRT1
C	150	VAL	-	expression tag	UNP M4YRT1
C	151	VAL	-	expression tag	UNP M4YRT1
C	152	GLU	-	expression tag	UNP M4YRT1
C	153	GLY	-	expression tag	UNP M4YRT1
C	154	LYS	-	expression tag	UNP M4YRT1
C	155	PHE	-	expression tag	UNP M4YRT1
C	156	HIS	-	expression tag	UNP M4YRT1
C	157	VAL	-	expression tag	UNP M4YRT1
C	158	THR	-	expression tag	UNP M4YRT1
C	159	GLY	-	expression tag	UNP M4YRT1
C	160	GLY	-	expression tag	UNP M4YRT1
C	161	ASN	-	expression tag	UNP M4YRT1
C	162	VAL	-	expression tag	UNP M4YRT1
C	163	THR	-	expression tag	UNP M4YRT1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	164	THR	-	expression tag	UNP M4YRT1
C	165	ALA	-	expression tag	UNP M4YRT1
C	166	ALA	-	expression tag	UNP M4YRT1
D	142	GLY	-	expression tag	UNP M4YRT1
D	143	GLY	-	expression tag	UNP M4YRT1
D	144	GLY	-	expression tag	UNP M4YRT1
D	145	GLY	-	expression tag	UNP M4YRT1
D	146	GLY	-	expression tag	UNP M4YRT1
D	147	GLY	-	expression tag	UNP M4YRT1
D	148	ALA	-	expression tag	UNP M4YRT1
D	149	ASN	-	expression tag	UNP M4YRT1
D	150	VAL	-	expression tag	UNP M4YRT1
D	151	VAL	-	expression tag	UNP M4YRT1
D	152	GLU	-	expression tag	UNP M4YRT1
D	153	GLY	-	expression tag	UNP M4YRT1
D	154	LYS	-	expression tag	UNP M4YRT1
D	155	PHE	-	expression tag	UNP M4YRT1
D	156	HIS	-	expression tag	UNP M4YRT1
D	157	VAL	-	expression tag	UNP M4YRT1
D	158	THR	-	expression tag	UNP M4YRT1
D	159	GLY	-	expression tag	UNP M4YRT1
D	160	GLY	-	expression tag	UNP M4YRT1
D	161	ASN	-	expression tag	UNP M4YRT1
D	162	VAL	-	expression tag	UNP M4YRT1
D	163	THR	-	expression tag	UNP M4YRT1
D	164	THR	-	expression tag	UNP M4YRT1
D	165	ALA	-	expression tag	UNP M4YRT1
D	166	ALA	-	expression tag	UNP M4YRT1
E	142	GLY	-	expression tag	UNP M4YRT1
E	143	GLY	-	expression tag	UNP M4YRT1
E	144	GLY	-	expression tag	UNP M4YRT1
E	145	GLY	-	expression tag	UNP M4YRT1
E	146	GLY	-	expression tag	UNP M4YRT1
E	147	GLY	-	expression tag	UNP M4YRT1
E	148	ALA	-	expression tag	UNP M4YRT1
E	149	ASN	-	expression tag	UNP M4YRT1
E	150	VAL	-	expression tag	UNP M4YRT1
E	151	VAL	-	expression tag	UNP M4YRT1
E	152	GLU	-	expression tag	UNP M4YRT1
E	153	GLY	-	expression tag	UNP M4YRT1
E	154	LYS	-	expression tag	UNP M4YRT1
E	155	PHE	-	expression tag	UNP M4YRT1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	156	HIS	-	expression tag	UNP M4YRT1
E	157	VAL	-	expression tag	UNP M4YRT1
E	158	THR	-	expression tag	UNP M4YRT1
E	159	GLY	-	expression tag	UNP M4YRT1
E	160	GLY	-	expression tag	UNP M4YRT1
E	161	ASN	-	expression tag	UNP M4YRT1
E	162	VAL	-	expression tag	UNP M4YRT1
E	163	THR	-	expression tag	UNP M4YRT1
E	164	THR	-	expression tag	UNP M4YRT1
E	165	ALA	-	expression tag	UNP M4YRT1
E	166	ALA	-	expression tag	UNP M4YRT1
G	142	GLY	-	expression tag	UNP M4YRT1
G	143	GLY	-	expression tag	UNP M4YRT1
G	144	GLY	-	expression tag	UNP M4YRT1
G	145	GLY	-	expression tag	UNP M4YRT1
G	146	GLY	-	expression tag	UNP M4YRT1
G	147	GLY	-	expression tag	UNP M4YRT1
G	148	ALA	-	expression tag	UNP M4YRT1
G	149	ASN	-	expression tag	UNP M4YRT1
G	150	VAL	-	expression tag	UNP M4YRT1
G	151	VAL	-	expression tag	UNP M4YRT1
G	152	GLU	-	expression tag	UNP M4YRT1
G	153	GLY	-	expression tag	UNP M4YRT1
G	154	LYS	-	expression tag	UNP M4YRT1
G	155	PHE	-	expression tag	UNP M4YRT1
G	156	HIS	-	expression tag	UNP M4YRT1
G	157	VAL	-	expression tag	UNP M4YRT1
G	158	THR	-	expression tag	UNP M4YRT1
G	159	GLY	-	expression tag	UNP M4YRT1
G	160	GLY	-	expression tag	UNP M4YRT1
G	161	ASN	-	expression tag	UNP M4YRT1
G	162	VAL	-	expression tag	UNP M4YRT1
G	163	THR	-	expression tag	UNP M4YRT1
G	164	THR	-	expression tag	UNP M4YRT1
G	165	ALA	-	expression tag	UNP M4YRT1
G	166	ALA	-	expression tag	UNP M4YRT1
H	142	GLY	-	expression tag	UNP M4YRT1
H	143	GLY	-	expression tag	UNP M4YRT1
H	144	GLY	-	expression tag	UNP M4YRT1
H	145	GLY	-	expression tag	UNP M4YRT1
H	146	GLY	-	expression tag	UNP M4YRT1
H	147	GLY	-	expression tag	UNP M4YRT1

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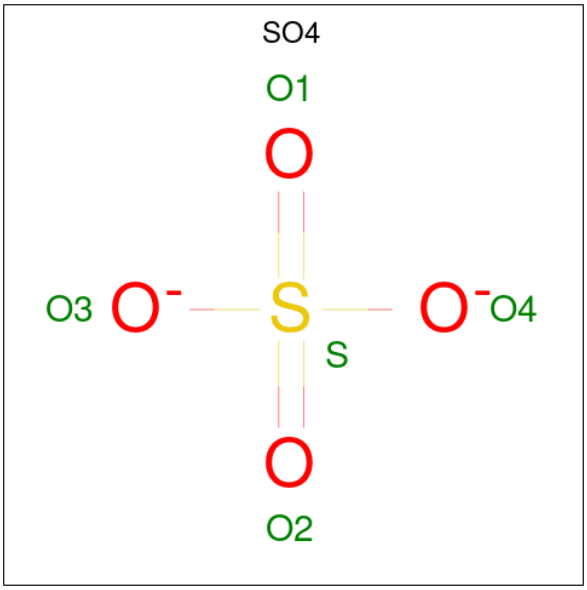
Chain	Residue	Modelled	Actual	Comment	Reference
H	148	ALA	-	expression tag	UNP M4YRT1
H	149	ASN	-	expression tag	UNP M4YRT1
H	150	VAL	-	expression tag	UNP M4YRT1
H	151	VAL	-	expression tag	UNP M4YRT1
H	152	GLU	-	expression tag	UNP M4YRT1
H	153	GLY	-	expression tag	UNP M4YRT1
H	154	LYS	-	expression tag	UNP M4YRT1
H	155	PHE	-	expression tag	UNP M4YRT1
H	156	HIS	-	expression tag	UNP M4YRT1
H	157	VAL	-	expression tag	UNP M4YRT1
H	158	THR	-	expression tag	UNP M4YRT1
H	159	GLY	-	expression tag	UNP M4YRT1
H	160	GLY	-	expression tag	UNP M4YRT1
H	161	ASN	-	expression tag	UNP M4YRT1
H	162	VAL	-	expression tag	UNP M4YRT1
H	163	THR	-	expression tag	UNP M4YRT1
H	164	THR	-	expression tag	UNP M4YRT1
H	165	ALA	-	expression tag	UNP M4YRT1
H	166	ALA	-	expression tag	UNP M4YRT1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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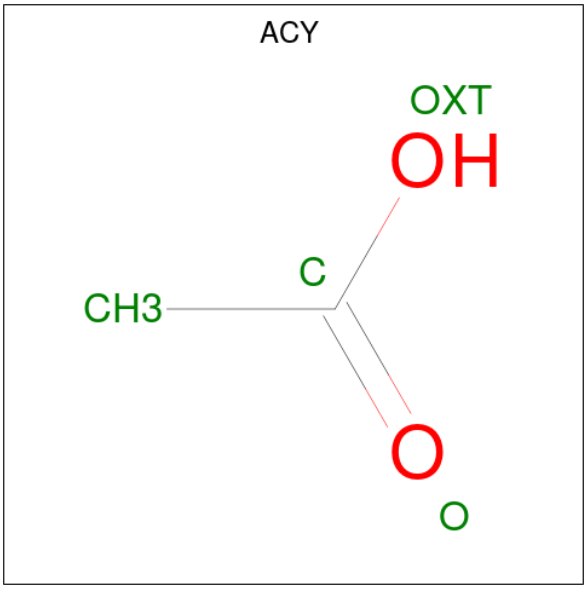
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Na 1 1	0	0

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C H O 7 2 3 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	234	Total O 234 234	0	0
5	A	250	Total O 250 250	0	0

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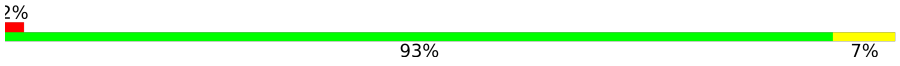
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	246	Total O 246 246	0	0
5	C	255	Total O 255 255	0	0
5	D	242	Total O 242 242	0	0
5	E	260	Total O 260 260	0	0
5	G	241	Total O 241 241	0	0
5	H	234	Total O 234 234	0	0

3 Residue-property plots (i)

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.

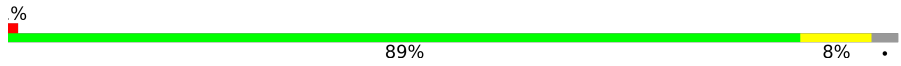
• Molecule 1: FimA

Chain F:



• Molecule 1: FimA

Chain A:

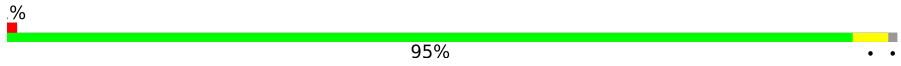


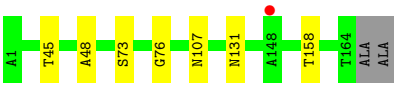
• Molecule 1: FimA

Chain B:

• Molecule 1: FimA

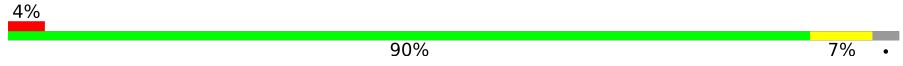
Chain C:





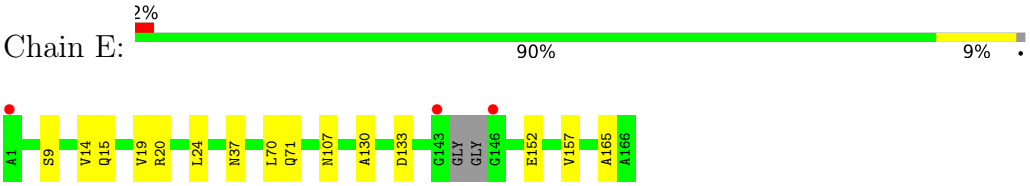
• Molecule 1: FimA

Chain D:



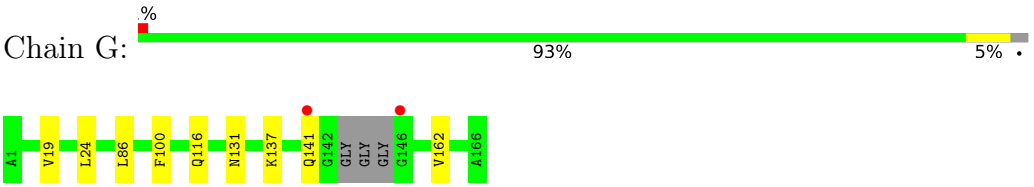
• Molecule 1: FimA

Chain E:



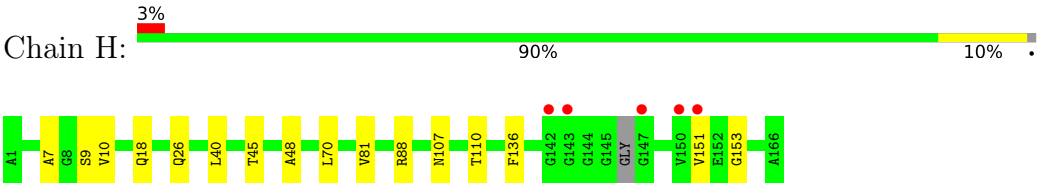
• Molecule 1: FimA

Chain G:



• Molecule 1: FimA

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.31Å 105.23Å 106.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.69 – 1.50 47.69 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.69-1.50) 100.0 (47.69-1.50)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.15-rc3	Depositor
R, R_{free}	0.169 , 0.206 0.169 , 0.206	Depositor DCC
R_{free} test set	3318 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	14.9	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	19814	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, ACY, 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	0.49	0/1138	0.69	0/1549
1	B	0.48	0/1109	0.66	0/1512
1	C	0.46	0/1143	0.67	0/1559
1	D	0.47	0/1135	0.68	0/1547
1	E	0.51	0/1154	0.71	0/1574
1	F	0.52	0/1175	0.70	0/1603
1	G	0.49	0/1170	0.66	0/1596
1	H	0.49	0/1156	0.68	0/1575
All	All	0.49	0/9180	0.68	0/12515

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	1121	1084	1082	12	0
1	B	1095	1059	1057	5	0
1	C	1131	1090	1088	3	0
1	D	1121	1085	1084	7	0
1	E	1137	1096	1094	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1154	1127	1125	7	0
1	G	1147	1126	1124	8	1
1	H	1142	1104	1103	10	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	1	0
2	H	5	0	0	1	0
3	C	1	0	0	0	0
4	C	4	3	3	3	0
5	A	250	0	0	7	2
5	B	246	0	0	3	0
5	C	255	0	0	2	1
5	D	242	0	0	2	1
5	E	260	0	0	3	2
5	F	234	0	0	4	0
5	G	241	0	0	5	1
5	H	234	0	0	4	2
All	All	11040	8774	8760	65	5

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 4.

The worst 5 of 65 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:E:152:GLU:OE1	5:E:301:HOH:O	1.88	0.91
4:C:203:ACY:O	5:C:301:HOH:O	1.87	0.90
1:E:15:GLN:NE2	5:E:302:HOH:O	2.12	0.83
1:B:74:ALA:O	5:B:301:HOH:O	1.99	0.80
1:C:76:GLY:O	5:C:302:HOH:O	1.98	0.79

All (5) 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)
5:D:353:HOH:O	5:G:362:HOH:O[3_554]	2.01	0.19
5:A:351:HOH:O	5:C:374:HOH:O[3_544]	2.10	0.10
5:A:245:HOH:O	5:E:472:HOH:O[3_545]	2.15	0.05
5:E:547:HOH:O	5:H:529:HOH:O[2_555]	2.15	0.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:116:GLN:HE21	5:H:302:HOH:O[3_544]	1.60	0.00

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	159/166 (96%)	156 (98%)	3 (2%)	0	100	100
1	B	153/166 (92%)	147 (96%)	6 (4%)	0	100	100
1	C	162/166 (98%)	160 (99%)	2 (1%)	0	100	100
1	D	158/166 (95%)	154 (98%)	4 (2%)	0	100	100
1	E	162/166 (98%)	158 (98%)	4 (2%)	0	100	100
1	F	167/166 (101%)	162 (97%)	5 (3%)	0	100	100
1	G	163/166 (98%)	159 (98%)	4 (2%)	0	100	100
1	H	162/166 (98%)	156 (96%)	6 (4%)	0	100	100
All	All	1286/1328 (97%)	1252 (97%)	34 (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	111/112 (99%)	110 (99%)	1 (1%)	78	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	110/112 (98%)	107 (97%)	3 (3%)	44 15
1	C	112/112 (100%)	110 (98%)	2 (2%)	59 30
1	D	112/112 (100%)	111 (99%)	1 (1%)	78 61
1	E	113/112 (101%)	111 (98%)	2 (2%)	59 30
1	F	115/112 (103%)	113 (98%)	2 (2%)	60 33
1	G	116/112 (104%)	116 (100%)	0	100 100
1	H	113/112 (101%)	111 (98%)	2 (2%)	59 30
All	All	902/896 (101%)	889 (99%)	13 (1%)	65 42

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	107	ASN
1	D	107	ASN
1	H	107	ASN
1	E	107	ASN
1	H	9	SER

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

Mol	Chain	Res	Type
1	G	139	GLN
1	H	26	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)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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	H	201	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	E	201	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	201	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	F	201	-	4,4,4	0.11	0	6,6,6	0.12	0
2	SO4	B	201	-	4,4,4	0.15	0	6,6,6	0.10	0
4	ACY	C	203	-	3,3,3	0.26	0	3,3,3	0.67	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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	201	SO4	1	0
2	F	201	SO4	1	0
4	C	203	ACY	3	0

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, 95^{th} 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	161/166 (96%)	-0.46	2 (1%)	79	82	10, 16, 31, 51	0
1	B	156/166 (93%)	-0.48	4 (2%)	56	61	11, 16, 29, 57	0
1	C	164/166 (98%)	-0.42	1 (0%)	89	91	11, 18, 33, 49	0
1	D	161/166 (96%)	-0.33	7 (4%)	35	39	11, 18, 32, 72	0
1	E	164/166 (98%)	-0.40	3 (1%)	68	73	9, 15, 35, 79	0
1	F	166/166 (100%)	-0.54	4 (2%)	59	63	10, 15, 30, 75	0
1	G	163/166 (98%)	-0.57	2 (1%)	79	82	11, 14, 28, 70	0
1	H	165/166 (99%)	-0.39	5 (3%)	50	55	10, 16, 45, 93	0
All	All	1300/1328 (97%)	-0.45	28 (2%)	62	67	9, 16, 34, 93	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	143	GLY	5.6
1	D	150	VAL	4.9
1	F	146	GLY	4.3
1	A	146	GLY	4.2
1	D	1	ALA	4.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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	F	201	5/5	0.80	0.18	54,70,74,80	0
4	ACY	C	203	4/4	0.84	0.11	24,29,30,37	0
2	SO4	E	201	5/5	0.86	0.15	60,66,69,70	0
2	SO4	C	201	5/5	0.88	0.14	63,66,67,73	0
2	SO4	B	201	5/5	0.92	0.12	58,60,65,65	0
2	SO4	H	201	5/5	0.94	0.15	59,59,63,65	0
3	NA	C	202	1/1	0.99	0.04	20,20,20,20	0

6.5 Other polymers

There are no such residues in this entry.