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P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:52 PM GMT

PDB ID	:	1QUN
Title	:	X-RAY STRUCTURE OF THE FIMC-FIMH CHAPERONE ADHESIN COMPLEX FROM UROPATHOGENIC E.COLI
Authors	:	Choudhury, D.; Thompson, A.; Stojanoff, V.; Langerman, S.; Pinkner, J.; Hultgren, S.J.; Knight, S.
Deposited on	:	1999-07-01
Resolution	:	2.80 Å(reported)

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

http://wwpdb.org/validation/2016/XrayValidationReportHelp

with specific help available everywhere you see the (i) symbol.

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

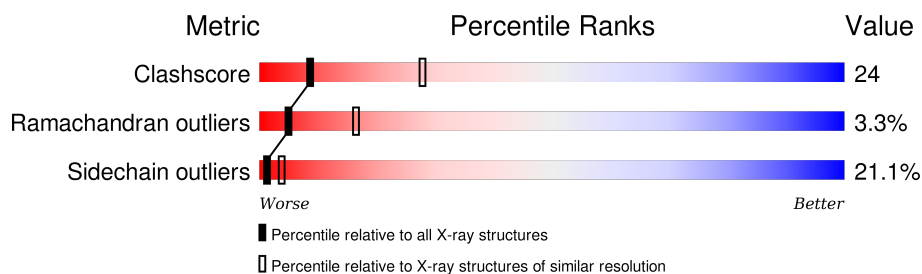|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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	Percentile Ranks	Value
Clashscore		24
Ramachandran outliers		3.3%
Sidechain outliers		21.1%

Worse　　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	205	51% ・ 35% ・ 11% ・・
1	C	205	53% ・ 34% ・ 9% ・・
1	E	205	53% ・ 34% ・ 9% ・・
1	G	205	52% ・ 35% ・ 9% ・・
1	I	205	29% ・ 41% ・ 21% ・ 5% ・
1	K	205	30% ・ 41% ・ 20% ・ 6% ・
1	M	205	30% ・ 40% ・ 21% ・ 5% ・

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Mol	Chain	Length	Quality of chain
1	O	205	28% 43% 21% • •
2	B	279	50% 35% 8% 8%
2	D	279	49% 35% 8% 7%
2	F	279	49% 36% 8% 8%
2	H	279	50% 35% 8% 7%
2	J	279	49% 32% 15% •
2	L	279	48% 33% 16% •
2	N	279	48% 33% 15% •
2	P	279	48% 33% 16% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 28864 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 PAPD-LIKE CHAPERONE FIMC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total 1553	C 985	N 268	O 294	S 6	5	0	0
1	C	200	Total 1553	C 985	N 268	O 294	S 6	5	0	0
1	E	200	Total 1553	C 985	N 268	O 294	S 6	5	0	0
1	G	200	Total 1553	C 985	N 268	O 294	S 6	5	0	0
1	I	198	Total 1543	C 979	N 266	O 292	S 6	177	0	0
1	K	198	Total 1543	C 979	N 266	O 292	S 6	176	0	0
1	M	198	Total 1543	C 979	N 266	O 292	S 6	177	0	0
1	O	198	Total 1543	C 979	N 266	O 292	S 6	177	0	0

- Molecule 2 is a protein called MANNOSE-SPECIFIC ADHESIN FIMH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	279	Total 2052	C 1297	N 342	O 409	S 4	42	0	0
2	D	279	Total 2052	C 1297	N 342	O 409	S 4	42	0	0
2	F	279	Total 2052	C 1297	N 342	O 409	S 4	42	0	0
2	H	279	Total 2052	C 1297	N 342	O 409	S 4	42	0	0
2	J	279	Total 2052	C 1297	N 342	O 409	S 4	67	0	0
2	L	279	Total 2052	C 1297	N 342	O 409	S 4	67	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	279	Total 2052	C 1297	N 342	O 409	S 4	67	0	0
2	P	279	Total 2052	C 1297	N 342	O 409	S 4	67	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total 5	O 5	0	0
3	B	10	Total 10	O 10	0	0
3	C	6	Total 6	O 6	0	0
3	D	11	Total 11	O 11	0	0
3	E	5	Total 5	O 5	0	0
3	F	12	Total 12	O 12	0	0
3	G	5	Total 5	O 5	0	0
3	H	10	Total 10	O 10	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.

Note EDS was not executed.

• Molecule 1: PAPD-LIKE CHAPERONE FIMC
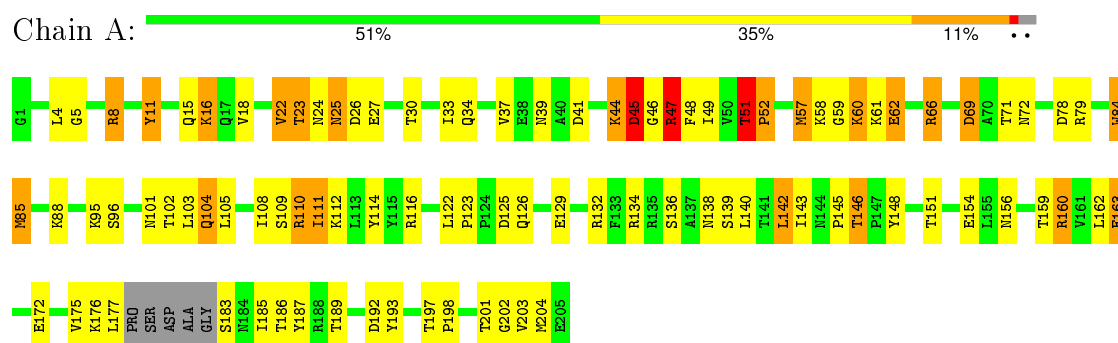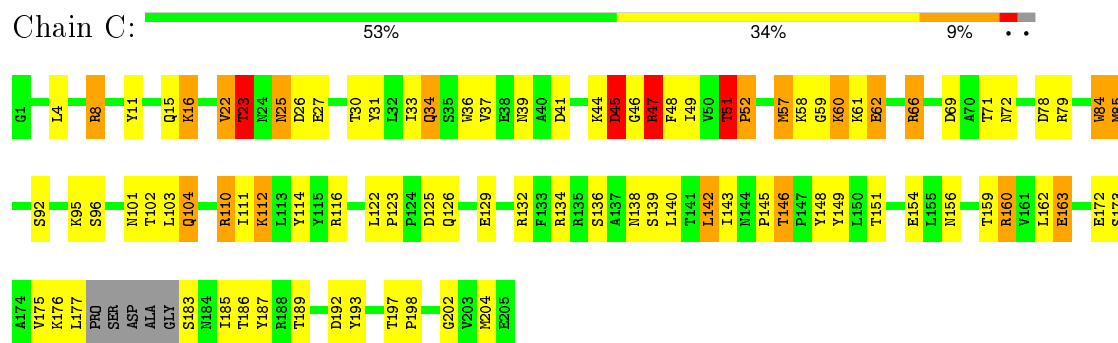
• Molecule 1: PAPD-LIKE CHAPERONE FIMC

• Molecule 1: PAPD-LIKE CHAPERONE FIMC

● Molecule 1: PAPD-LIKE CHAPERONE FIMC

Chain G:

● Molecule 1: PAPD-LIKE CHAPERONE FIMC

Chain I:

● Molecule 1: PAPD-LIKE CHAPERONE FIMC

Chain K:

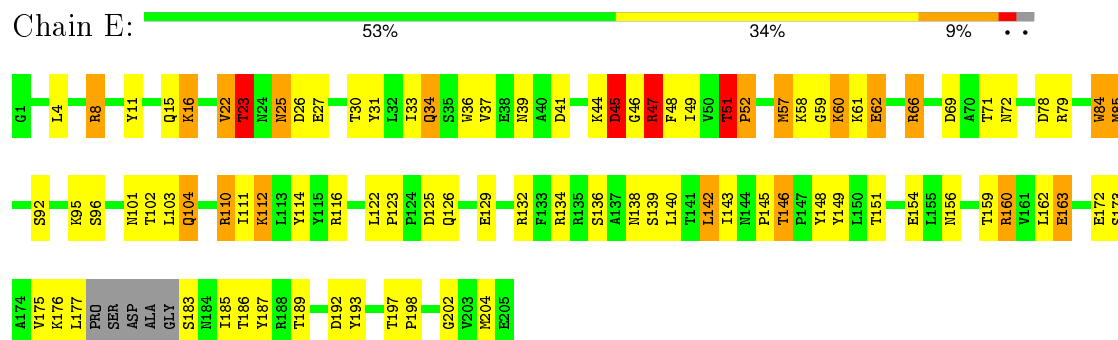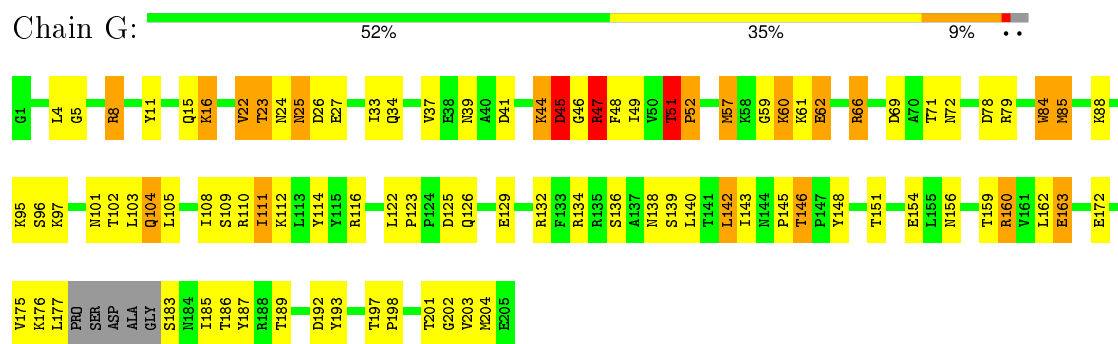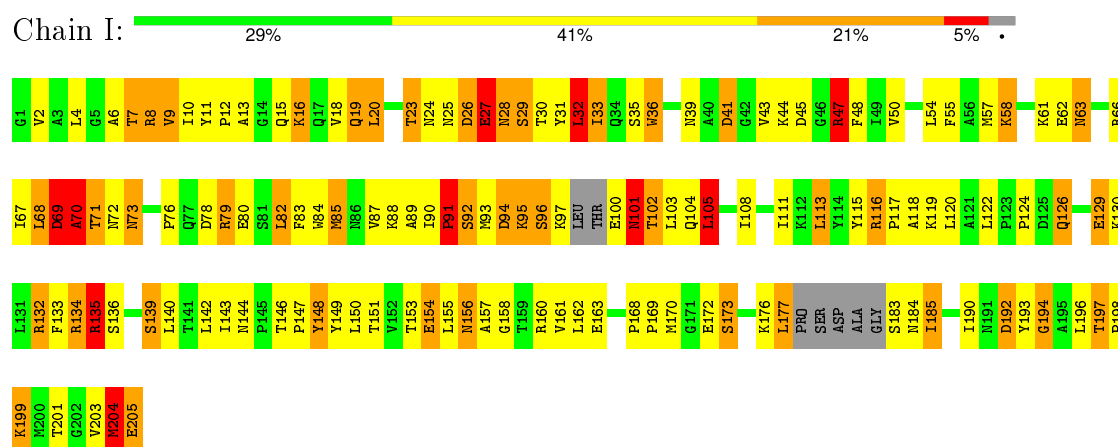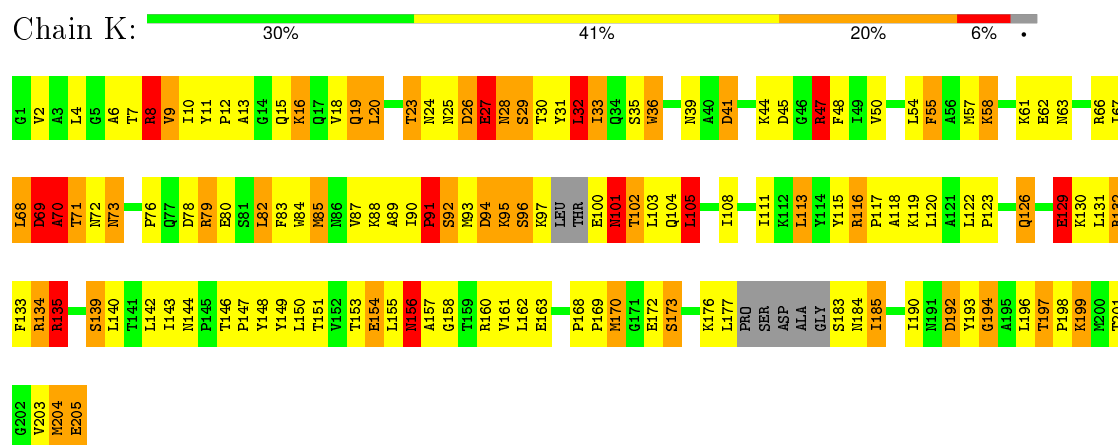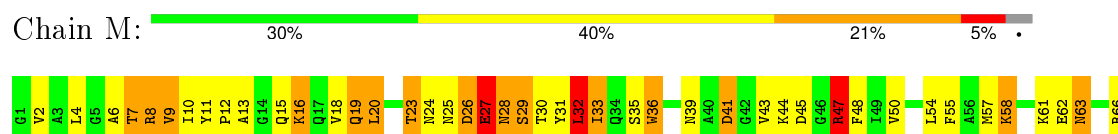● Molecule 1: PAPD-LIKE CHAPERONE FIMC

Chain M:

I67 L68 D69 A70 T71 N72 N73 P76 Q77 D78 R79 E80 S81 L82 F83 W84 M85 N86 V87 K88 A89 I90 P91 S92 M93 D94 K95 S96 K97 LEU THR E100 N101 T102 L103 Q104 L105 I108 I111 K112 L113 Y114 Y115 R116 P117 A118 K119 L120 A121 L122 P123 P124 D125 Q126 E129 K130

L131 R132 F133 R134 R135 S136 S139 L140 T141 L142 I143 N144 P145 T146 P147 Y148 Y149 L150 T151 V152 T153 E154 L155 N156 A157 G158 T159 R160 V161 L162 E163 P168 P169 M170 G171 E172 S173 K176 L177 PRO SER ASP ALA GLY S183 N184 I185 I190 N191 D192 Y193 G194 A195 L196 T197 P198

K199 M200 T201 G202 V203 M204 E205

● Molecule 1: PAPD-LIKE CHAPERONE FIMC

Chain O: 28%   43%   21%   • •

G1 V2 A3 L4 G5 A6 T7 R8 V9 I10 Y11 P12 A13 G14 Q15 K16 Q17 V18 Q19 L20 A21 V22 T23 N24 N25 D26 E27 N28 S29 T30 Y31 L32 I33 Q34 S35 W36 N39 A40 D41 K44 D45 G46 H47 F48 I49 V50 L54 F55 A56 M57 K58 K61 E62 N63 R66

I67 L68 D69 A70 T71 N72 N73 P76 Q77 D78 R79 E80 S81 L82 F83 W84 M85 N86 V87 K88 A89 I90 P91 S92 M93 D94 K95 S96 K97 LEU THR E100 N101 T102 L103 Q104 L105 I108 I111 K112 L113 Y114 Y115 R116 P117 A118 K119 L120 A121 L122 P123 P124 D125 Q126 A127 A128 E129

K130 L131 R132 F133 R134 R135 S139 L140 T141 L142 I143 N144 P145 T146 P147 Y148 Y149 L150 T151 V152 T153 E154 L155 N156 A157 G158 T159 R160 V161 L162 E163 P168 P169 M170 G171 E172 S173 K176 L177 PRO SER ASP ALA GLY S183 N184 I185 T186 Y187 I190 N191 D192 Y193 G194 A195 L196

T197 P198 K199 M200 T201 G202 V203 M204 E205

● Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

Chain B: 50%   35%   8%   8%

F1 A2 C3 K4 T5 A6 T9 I13 V20 Y21 L24 V27 V28 N29 Q32 V35 V36 D37 L38 S39 T40 Q41 N46 D47 Y48 T51 I52 T53 D54 Y55 V56 T57 L58 Q59 R60 Y64 L68 S69 N70 F71 S72 Y77 S78 Y82 P83 F84 P85

T86 T87 S88 E89 T90 P91 R92 Y95 N96 S97 R98 T99 D100 K101 P102 N103 L107 Y108 L109 T110 P111 V112 S113 S114 A115 V118 A119 I120 K121 A122 G123 I126 L129 I130 L131 R132 N135 N136 Y137 N138 S139 D140 D141 Y149 A150 D153 T158 D162 V163 S164

A165 R166 D167 V168 T169 V170 T171 L172 P173 D174 Y175 P176 G177 S178 V179 P180 I183 T184 V185 A188 K189 S190 Q191 N192 L193 G194 Y195 Y196 G199 T200 T201 A202 N206 F209 T210 N211 T212 A213 F215 S216 P217 A218 Q219 T226 R227 N228 G229 I232 N235 N236

S239 T245 S246 A247 L250 G251 L252 T253 A254 N255 Y256 A257 R258 T259 Q262 V263 T264 Q269 S270 I271 I272 G273 V274 T275 Q279

● Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

Chain D: 49%   35%   8%   7%

F1 A2 C3 K4 T5 A6 T9 I13 G14 V20 Y21 L24 N29 Q32 V35 V36 D37 L38 S39 T40 Q41 I42 N46 D47 Y48 T51 I52 T53 D54 V55 V56 T57 L58 Q59 R60 Y64 G65 L68 S69 N70 F71 S72 Y77 S78 Y82 P83 F84

P85 T86 T87 S88 E89 T90 P91 R92 V93 V94 Y95 N96 K101 P102 N103 L107 T110 S113 V118 A119 I120 K121 A122 G123 I126 L129 I130 L131 R132 N135 N136 Y137 N138 S139 D140 I148 Y149 A150 D153 T158 C161 D162 V163 S164 A165 R166 D167 V168

T169 V170 I171 L172 P173 D174 Y175 P176 G177 S178 V179 P180 L183 T184 V185 Y186 C187 A188 K189 S190 Q191 N192 L193 G194 Y195 Y196 T201 A202 D203 A204 G205 N206 T210 N211 T212 A213 S214 F215 S216 P217 A218 Q219 T226 R227 N228 G229 T230 I231 I232 P233 A234 N235 N236 S239 L240

G241 A242 T245 S246 A247 L250 T253 A254 N255 Y256 A257 R258 T259 Q262 V263 T264 Q269 S270 I271 I272 G273 V274 T275 Q279

• Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

Chain F: `[49% | 36% | 8% | 8%]`

F1 A2 C3 K4 T5 A6 T9 I13 G14 V20 Y21 L24 N29 Q32 V35 V36 D37 L38 S39 T40 Q41 N46 D47 Y48 T51 I52 T53 D54 Y55 V56 I57 L58 Q59 R60 Y64 G65 L68 S69 N70 F71 S72 Y77 S78 Y82 P83 F84 P85

T86 T87 S88 E89 T90 P91 R92 V93 V94 Y95 N96 S97 R98 K101 P102 W103 L107 T110 S113 V118 A119 I120 K121 A122 G123 I126 L129 I130 L131 R132 N135 N136 Y137 N138 S139 D140 I148 Y149 A150 D153 T158 C161 D162 V163 S164 A165 R166 D167

V168 T169 I169 V170 T171 L172 P173 D174 Y175 P176 G177 S178 V179 P180 L183 T184 V185 Y186 C187 A188 K189 S190 Q191 N192 L193 G194 Y195 Y196 T201 A202 D203 A204 G205 N206 T210 N211 T212 A213 S214 F215 S216 P217 A218 Q219 T226 R227 N228 G229 T230 I231 I232 P233 A234 N235 N236 S239

L240 G241 A242 T245 S246 A247 L250 T253 A254 N255 Y256 A257 R258 T259 Q262 V263 T264 Q269 S270 I271 I272 G273 V274 T275 Q279

• Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

Chain H: `[50% | 35% | 8% | 7%]`

F1 A2 C3 K4 T5 A6 T9 I13 V20 Y21 L24 V27 V28 N29 Q32 V35 V36 D37 L38 S39 T40 D41 N46 D47 Y48 T51 I52 T53 D54 Y55 V56 T57 L58 Q59 R60 Y64 L68 S69 N70 F71 S72 Y77 S78 Y82 P83 F84 P85

T86 T87 S88 E89 T90 P91 R92 Y95 N96 D100 K101 P102 W103 L107 Y108 L109 T110 P111 V112 S113 S114 A115 V118 A119 I120 K121 A122 G123 I126 L129 I130 L131 R132 N135 N136 Y137 N138 S139 D140 D141 Y149 A150 D153 T158 D162 V163 S164 A165 R166

D167 V168 T169 V170 T171 L172 P173 D174 Y175 P176 G177 S178 V179 P180 L183 T184 V185 A188 K189 S190 Q191 N192 L193 G194 Y195 Y196 G199 T200 T201 A202 N206 F209 T210 N211 T212 A213 S214 F215 S216 P217 A218 Q219 T226 R227 N228 G229 N235 N236 S239 T245 S246

A247 L250 G251 L252 T253 A254 N255 Y256 A257 R258 T259 Q262 V263 T264 V268 Q269 S270 I271 I272 G273 V274 T275 Q279

• Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

Chain J: `[49% | 32% | 15% | •]`

F1 T5 A6 N7 G14 G15 G16 S17 L24 A25 P26 V27 V28 N29 Q32 L38 S39 T40 Q41 I42 D47 T51 I52 T53 D54 T57 L58 Q59 R60 Y64 V67 L68 S69 N70 F71 S72 V75 K76 Y77 S80 S81 E89 T90 P91 R92 V93 V94

Y95 N96 S97 R98 K101 P102 W103 L107 Y108 L109 T110 A115 G116 K121 A122 I126 A127 V128 L129 I130 L131 R132 N135 N136 Y137 N138 S139 D140 D141 F142 V145 I148 D153 V154 V155 V156 P157 T158 G159 G160 C161 D162 V163 S164 A165 R166 D167 T169 V170 I171

L172 P173 D174 Y175 P176 G177 S178 V179 P182 L183 T184 V185 Y186 C187 A188 K189 S190 Q191 N192 L193 G194 Y195 Y196 L197 T201 N206 S207 I208 N211 T212 F215 S216 P217 A218 Q224 L225 T226 R227 N228 I231 I232 P233 N236 L240 G241 A242 V243 G244 T245 S249

L250 G251 L252 T253 A254 N255 Y256 A257 R258 T259 G260 V263 T264 N267 V268 Q269 S270 I271 I272 T275 Y278 Q279

● Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

Chain L: 48% 33% 16% •

F1 T5 A6 N7 P12 I13 G14 G15 G16 S17 L24 A25 V28 N29 Q32 L38 S39 T40 Q41 I42 D47 T51 I52 T53 D54 V56 Y55 T57 L58 Q59 R60 Y64 V67 L68 S69 N70 F71 S72 G73 T74 V75 S80 S81 E89 T90 P91 Q92 V93

V94 Y95 N96 S97 R98 K101 P102 W103 P104 V105 A106 L107 Y108 L109 T110 A115 K121 A122 I126 A127 V128 L129 I130 L131 R132 Q133 N136 Y137 N138 S139 D140 D141 F142 V145 I148 D153 V154 V155 V156 P157 T158 G159 G160 C161 D162 V163 S164 A165 R166 D167 T168 T169

V170 T171 L172 P173 D174 Y175 P176 G177 S178 V179 P180 I181 P182 L183 T184 V185 Y186 K189 S190 Q191 N192 L193 G194 Y195 T201 A204 G205 N206 S207 I208 N211 T212 F215 S216 P217 A218 L225 T226 R227 N228 I231 I232 P233 N236 L240 G241 A242 V243 G244 T245

L250 T253 A254 N255 Y256 A257 R258 T259 G260 V263 T264 N267 V268 Q269 S270 I271 I272 T275 Y278 Q279

● Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

Chain N: 48% 33% 15% •

F1 T5 A6 N7 G8 G14 G15 G16 S17 L24 A25 V28 N29 Q32 L38 S39 T40 Q41 I42 D47 T51 I52 T53 D54 T57 L58 Q59 R60 Y64 V67 L68 S69 N70 F71 S72 V75 K76 Y77 S80 S81 E89 T90 P91 R92 V93 V94

Y95 N96 S97 R98 K101 P102 W103 L107 Y108 L109 T110 P111 V112 A115 G116 K121 A122 I126 A127 V128 L129 I130 L131 R132 N135 N136 Y137 N138 S139 D140 D141 F142 V145 I148 D153 V154 V155 V156 P157 T158 G159 G160 C161 D162 S164 A165 R166 D167 V168 T169

V170 T171 L172 P173 D174 Y175 P176 G177 S178 V179 P182 L183 T184 V185 Y186 C187 A188 K189 S190 Q191 N192 L193 G194 Y195 V196 L197 T201 N206 S207 I208 N211 T212 F215 S216 P217 A218 Q224 L225 T226 R227 N228 I231 I232 P233 N236 L240 G241 A242 V243 G244 T245

S249 L250 G251 L252 T253 A254 N255 Y256 A257 R258 T259 G260 V263 T264 N267 V268 Q269 S270 I271 I272 T275 Y278 Q279

● Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

Chain P: 48% 33% 16% •

F1 T5 A6 N7 G14 G15 G16 S17 L24 A25 V28 N29 Q32 L38 S39 T40 Q41 I42 D47 T51 I52 T53 D54 Y55 V56 T57 L58 Q59 R60 Y64 V67 L68 S69 N70 F71 S72 G73 T74 V75 S80 S81 E89 T90 P91 R92 V93 V94 Y95

N96 S97 R98 K101 P102 W103 P104 V105 A106 L107 Y108 L109 T110 A115 K121 A122 I126 A127 V128 L129 I130 L131 R132 Q133 N136 Y137 N138 S139 D140 D141 F142 V145 I148 N152 D153 V154 V155 V156 P157 T158 G159 G160 C161 D162 V163 S164 A165 R166 D167 V168 T169 V170

T171 L172 P173 D174 Y175 P176 G177 S178 V179 P180 I181 P182 L183 T184 V185 Y186 C187 A188 K189 S190 Q191 N192 L193 G194 Y195 T201 A204 G205 N206 S207 I208 N211 T212 F215 S216 P217 A218 Q224 L225 T226 R227 N228 I231 I232 P233 N236 L240 G241 A242 V243 G244 T245

L250 T253 A254 N255 Y256 A257 R258 T259 G260 V263 T264 N267 V268 Q269 S270 I271 I272 T275 Y278 Q279

4   Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.41Å 139.57Å 215.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.240 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28864	wwPDB-VP
Average B, all atoms (Å²)	45.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.92	3/1580 (0.2%)	2.40	60/2146 (2.8%)
1	C	0.94	3/1580 (0.2%)	2.43	65/2146 (3.0%)
1	E	0.94	3/1580 (0.2%)	2.43	65/2146 (3.0%)
1	G	0.92	3/1580 (0.2%)	2.40	60/2146 (2.8%)
1	I	2.03	14/1568 (0.9%)	2.88	63/2126 (3.0%)
1	K	2.17	13/1568 (0.8%)	2.87	63/2126 (3.0%)
1	M	2.03	14/1568 (0.9%)	2.88	64/2126 (3.0%)
1	O	2.17	13/1568 (0.8%)	2.87	63/2126 (3.0%)
2	B	1.44	6/2097 (0.3%)	2.57	116/2881 (4.0%)
2	D	1.39	7/2097 (0.3%)	2.57	117/2881 (4.1%)
2	F	1.39	7/2097 (0.3%)	2.57	117/2881 (4.1%)
2	H	1.44	6/2097 (0.3%)	2.57	116/2881 (4.0%)
2	J	1.14	6/2096 (0.3%)	2.54	63/2878 (2.2%)
2	L	1.20	4/2097 (0.2%)	2.45	56/2881 (1.9%)
2	N	1.14	6/2096 (0.3%)	2.54	64/2878 (2.2%)
2	P	1.20	4/2097 (0.2%)	2.45	56/2881 (1.9%)
All	All	1.45	112/29366 (0.4%)	2.58	1208/40130 (3.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	4
1	E	0	4
1	G	0	4
1	I	1	9
1	K	0	10
1	M	1	9
1	O	0	10
2	B	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	1	7
2	F	1	7
2	H	0	7
2	J	1	4
2	L	1	3
2	N	1	4
2	P	1	3
All	All	8	96

The worst 5 of 112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	26	ASP	CG-OD1	43.75	2.25	1.25
1	M	26	ASP	CG-OD1	43.74	2.25	1.25
1	K	26	ASP	CG-OD1	40.57	2.18	1.25
1	O	26	ASP	CG-OD1	40.57	2.18	1.25
2	L	167	ASP	C-O	-35.59	0.55	1.23

The worst 5 of 1208 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	165	ALA	O-C-N	-61.51	24.29	122.70
2	N	165	ALA	O-C-N	-61.50	24.30	122.70
1	K	26	ASP	CB-CG-OD1	-61.39	63.05	118.30
1	O	26	ASP	CB-CG-OD1	-61.38	63.06	118.30
2	L	165	ALA	O-C-N	-60.60	25.74	122.70

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	176	PRO	CA
2	F	176	PRO	CA
1	I	156	ASN	CA
2	J	215	PHE	CA
2	L	215	PHE	CA

5 of 96 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	ASN	Mainchain
1	A	45	ASP	Mainchain
1	A	51	THR	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
2	B	24	LEU	Mainchain
2	B	35	VAL	Mainchain

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	1553	0	1587	48	0
1	C	1553	0	1587	42	0
1	E	1553	0	1587	41	0
1	G	1553	0	1587	44	0
1	I	1543	0	1576	110	0
1	K	1543	0	1576	107	0
1	M	1543	0	1576	109	0
1	O	1543	0	1576	105	0
2	B	2052	0	2006	83	0
2	D	2052	0	2006	80	0
2	F	2052	0	2006	82	0
2	H	2052	0	2006	81	0
2	J	2052	0	2003	114	0
2	L	2052	0	2004	118	0
2	N	2052	0	2003	114	0
2	P	2052	0	2004	114	0
3	A	5	0	0	0	0
3	B	10	0	0	1	0
3	C	6	0	0	0	0
3	D	11	0	0	1	0
3	E	5	0	0	0	0
3	F	12	0	0	1	0
3	G	5	0	0	0	0
3	H	10	0	0	1	0
All	All	28864	0	28690	1311	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 24.

The worst 5 of 1311 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:O:197:THR:HB	1:O:198:PRO:HD2	1.45	0.98
2:N:53:THR:H	2:N:136:ASN:HD21	1.08	0.98
2:J:53:THR:H	2:J:136:ASN:HD21	1.08	0.98
2:B:226:THR:HG22	2:B:253:THR:HB	1.45	0.98
1:I:197:THR:HB	1:I:198:PRO:HD2	1.46	0.98

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	196/205 (96%)	185 (94%)	11 (6%)	0	100	100
1	C	196/205 (96%)	184 (94%)	12 (6%)	0	100	100
1	E	196/205 (96%)	184 (94%)	12 (6%)	0	100	100
1	G	196/205 (96%)	185 (94%)	11 (6%)	0	100	100
1	I	190/205 (93%)	135 (71%)	37 (20%)	18 (10%)	1	1
1	K	190/205 (93%)	134 (70%)	37 (20%)	19 (10%)	1	1
1	M	190/205 (93%)	135 (71%)	37 (20%)	18 (10%)	1	1
1	O	190/205 (93%)	134 (70%)	37 (20%)	19 (10%)	1	1
2	B	277/279 (99%)	253 (91%)	23 (8%)	1 (0%)	39	74
2	D	277/279 (99%)	254 (92%)	22 (8%)	1 (0%)	39	74
2	F	277/279 (99%)	254 (92%)	22 (8%)	1 (0%)	39	74
2	H	277/279 (99%)	253 (91%)	23 (8%)	1 (0%)	39	74
2	J	275/279 (99%)	238 (86%)	25 (9%)	12 (4%)	3	10
2	L	277/279 (99%)	242 (87%)	24 (9%)	11 (4%)	4	12
2	N	275/279 (99%)	238 (86%)	25 (9%)	12 (4%)	3	10
2	P	277/279 (99%)	242 (87%)	24 (9%)	11 (4%)	4	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3756/3872 (97%)	3250 (86%)	382 (10%)	124 (3%)	5 16

5 of 124 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	176	PRO
2	D	176	PRO
2	F	176	PRO
2	H	176	PRO
1	I	68	LEU

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	169/175 (97%)	134 (79%)	35 (21%)	1 4
1	C	169/175 (97%)	132 (78%)	37 (22%)	1 3
1	E	169/175 (97%)	132 (78%)	37 (22%)	1 3
1	G	169/175 (97%)	134 (79%)	35 (21%)	1 4
1	I	169/175 (97%)	121 (72%)	48 (28%)	0 1
1	K	169/175 (97%)	121 (72%)	48 (28%)	0 1
1	M	169/175 (97%)	121 (72%)	48 (28%)	0 1
1	O	169/175 (97%)	121 (72%)	48 (28%)	0 1
2	B	226/226 (100%)	181 (80%)	45 (20%)	1 5
2	D	226/226 (100%)	181 (80%)	45 (20%)	1 5
2	F	226/226 (100%)	181 (80%)	45 (20%)	1 5
2	H	226/226 (100%)	181 (80%)	45 (20%)	1 5
2	J	226/226 (100%)	188 (83%)	38 (17%)	2 8
2	L	226/226 (100%)	189 (84%)	37 (16%)	3 8
2	N	226/226 (100%)	188 (83%)	38 (17%)	2 8
2	P	226/226 (100%)	189 (84%)	37 (16%)	3 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3160/3208 (98%)	2494 (79%)	666 (21%)	1 4

5 of 666 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	138	ASN
2	J	17	SER
1	O	132	ARG
2	H	183	LEU
1	I	61	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	144	ASN
1	K	24	ASN
2	P	96	ASN
2	J	41	GLN
2	J	206	ASN

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 carbohydrates 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)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.