



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 10:00 AM UTC

PDB ID : 1QUN / pdb_00001qun
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)

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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

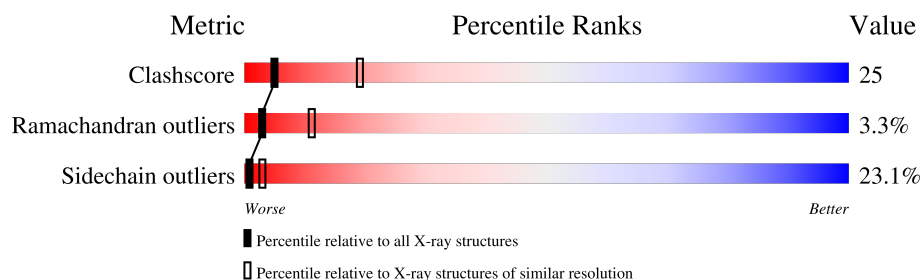
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

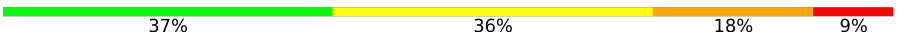
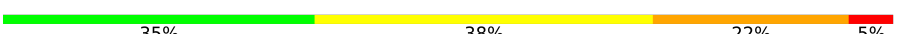
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	205	
1	C	205	
1	E	205	
1	G	205	
1	I	205	
1	K	205	
1	M	205	
1	O	205	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	279	 36%40%16%9%
2	D	279	 37%36%18%9%
2	F	279	 36%37%18%9%
2	H	279	 36%39%16%9%
2	J	279	 35%38%22%5%
2	L	279	 35%37%23%5%
2	N	279	 35%38%23%5%
2	P	279	 35%37%23%5%

2 Entry composition

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	C	N	O	S	5	0	0
			1553	985	268	294	6			
1	C	200	Total	C	N	O	S	5	0	0
			1553	985	268	294	6			
1	E	200	Total	C	N	O	S	5	0	0
			1553	985	268	294	6			
1	G	200	Total	C	N	O	S	5	0	0
			1553	985	268	294	6			
1	I	198	Total	C	N	O	S	177	0	0
			1543	979	266	292	6			
1	K	198	Total	C	N	O	S	176	0	0
			1543	979	266	292	6			
1	M	198	Total	C	N	O	S	177	0	0
			1543	979	266	292	6			
1	O	198	Total	C	N	O	S	177	0	0
			1543	979	266	292	6			

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

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

Continued on next page...

Continued from previous page...

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.

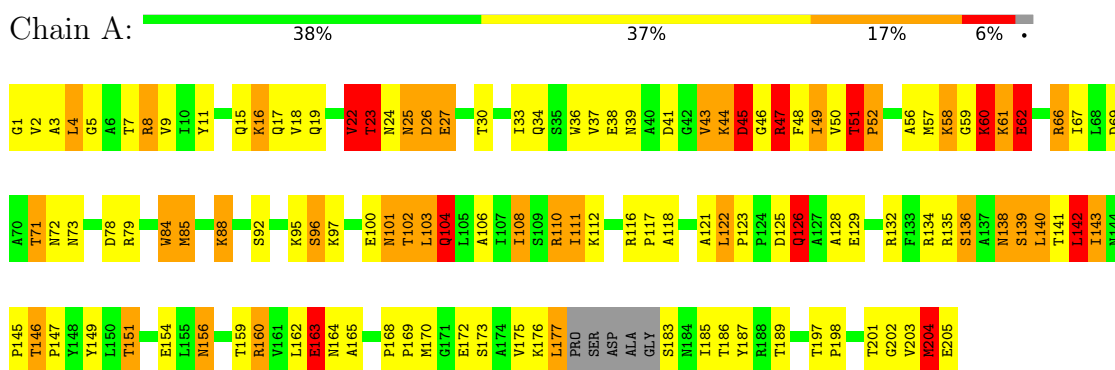
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total 5	O 5	0	0
3	B	10	Total 10	O 10	0	0
3	C	6	Total 6	O 6	0	0
3	D	11	Total 11	O 11	0	0
3	E	5	Total 5	O 5	0	0
3	F	12	Total 12	O 12	0	0
3	G	5	Total 5	O 5	0	0
3	H	10	Total 10	O 10	0	0

3 Residue-property plots

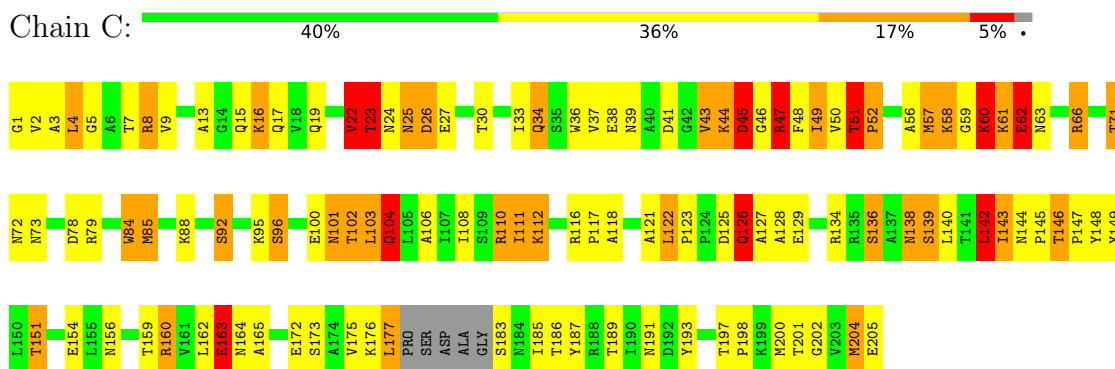
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

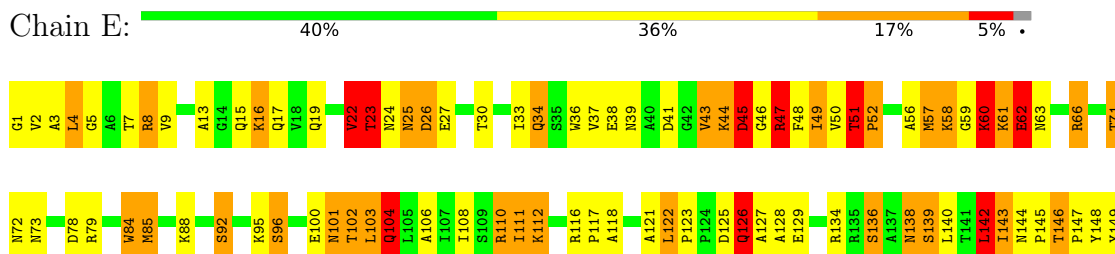
• Molecule 1: PAPD-LIKE CHAPERONE FIMC

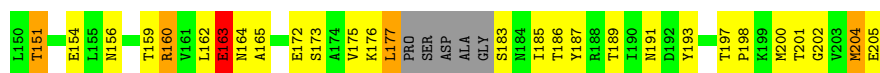


• Molecule 1: PAPD-LIKE CHAPERONE FIMC



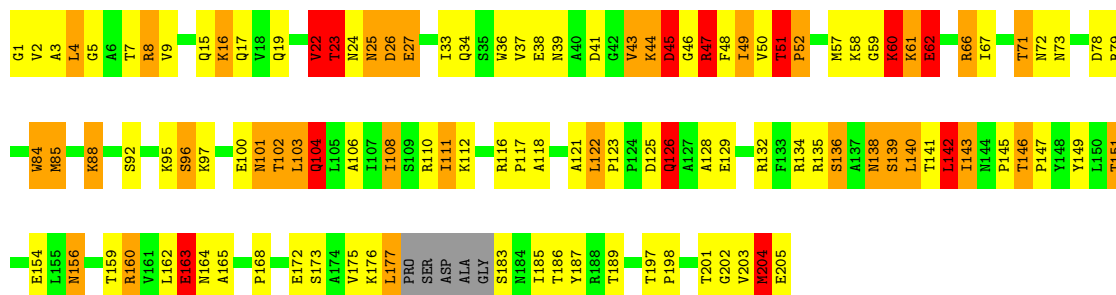
• Molecule 1: PAPD-LIKE CHAPERONE FIMC





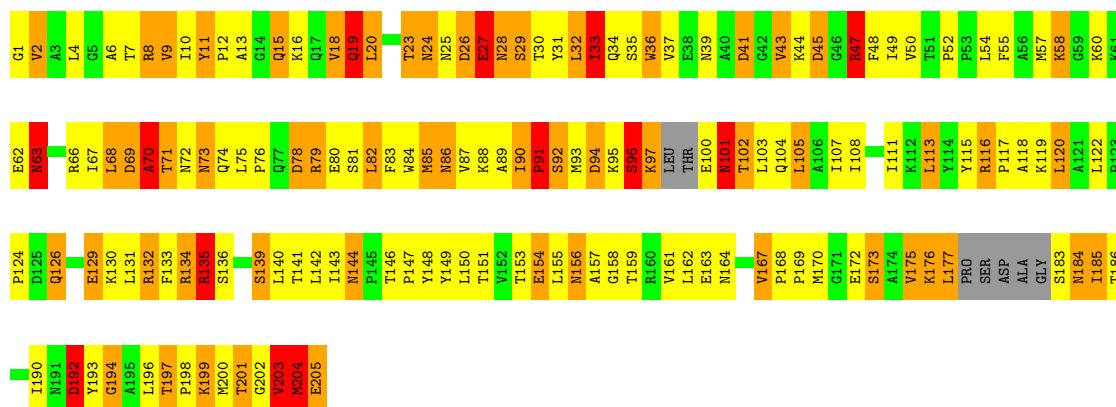
• Molecule 1: PAPD-LIKE CHAPERONE FIMC

Chain G: 41% 35% 16% 6% .



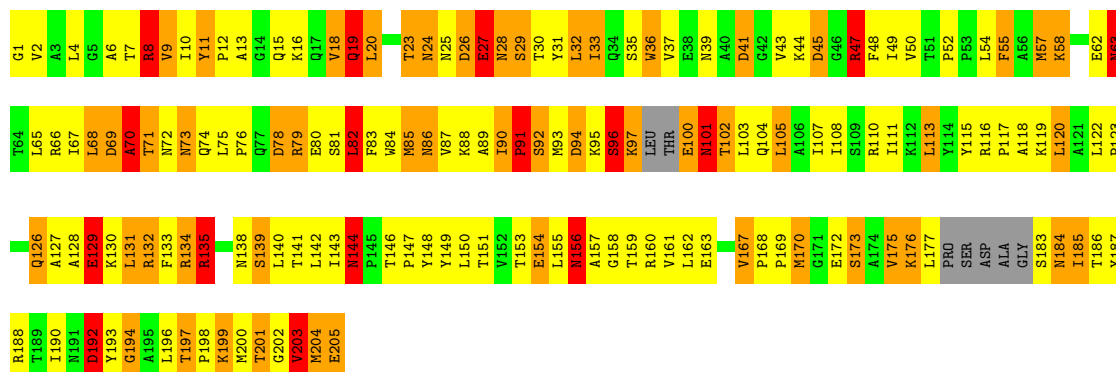
• Molecule 1: PAPD-LIKE CHAPERONE FIMC

Chain I: 20% 42% 27% 6% .

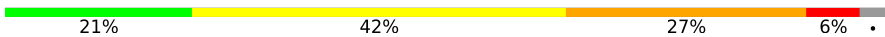


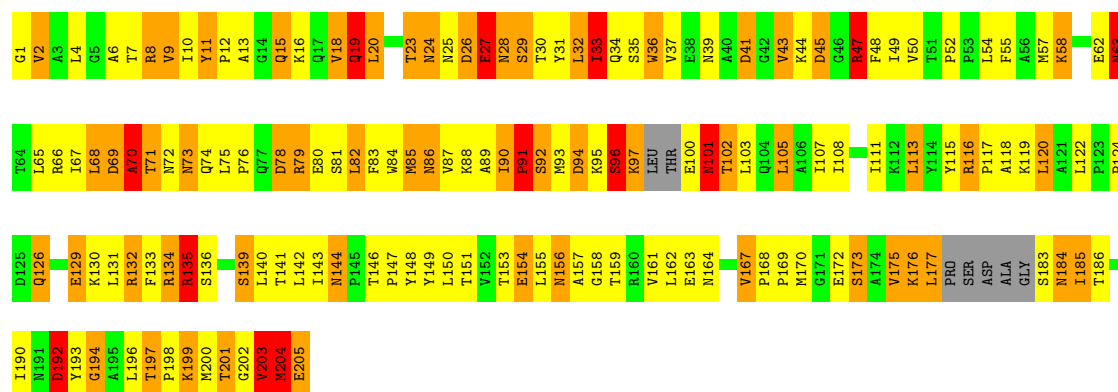
• Molecule 1: PAPD-LIKE CHAPERONE FIMC

Chain K: 19% 44% 26% 8% .



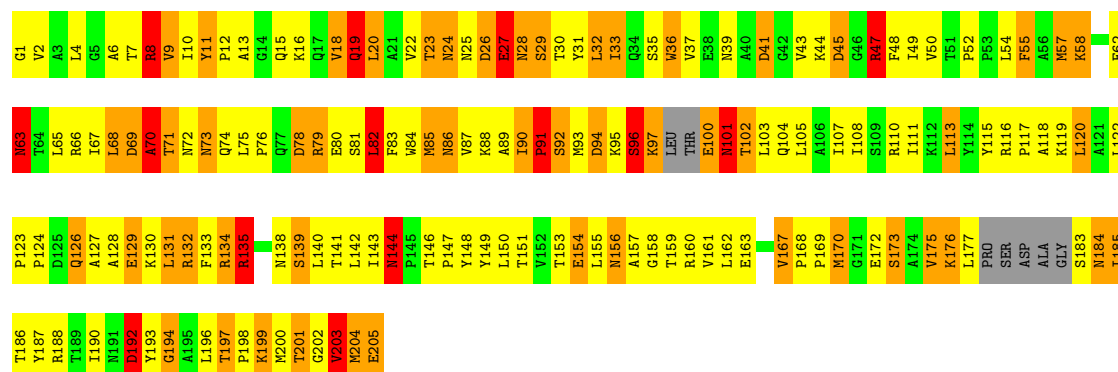
• Molecule 1: PAPD-LIKE CHAPERONE FIMC

Chain M: 

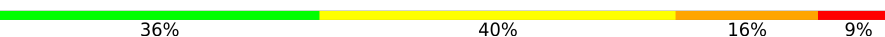


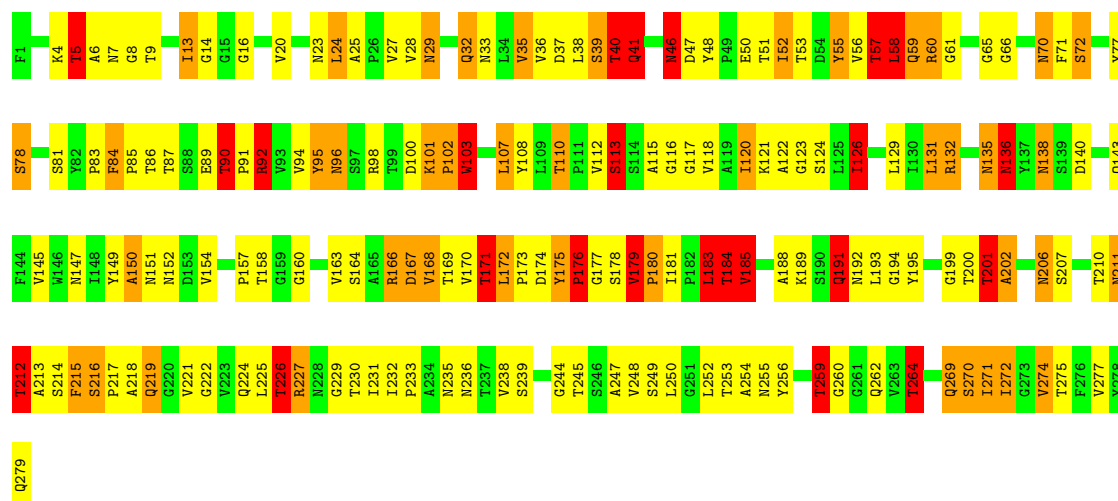
• Molecule 1: PAPD-LIKE CHAPERONE FIMC

Chain O: 

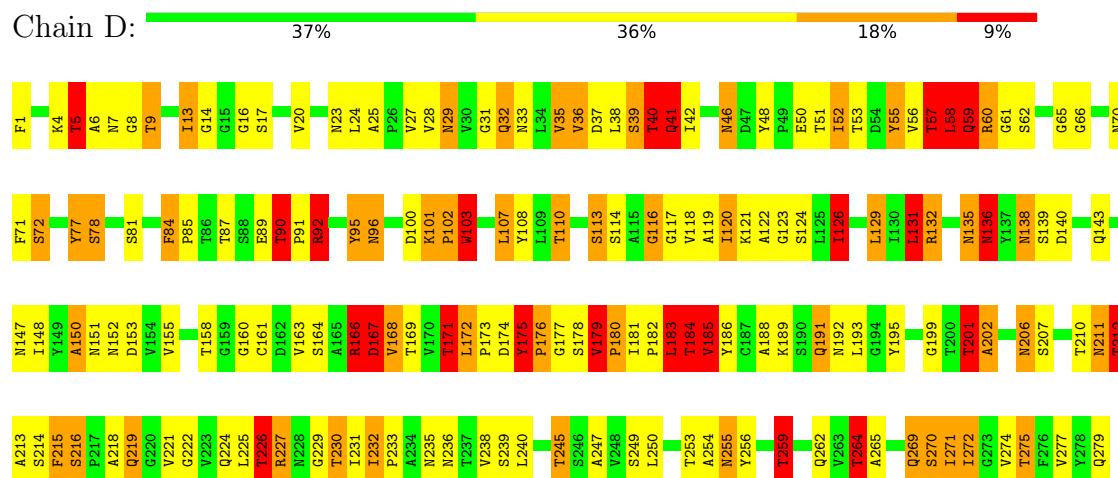


• Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

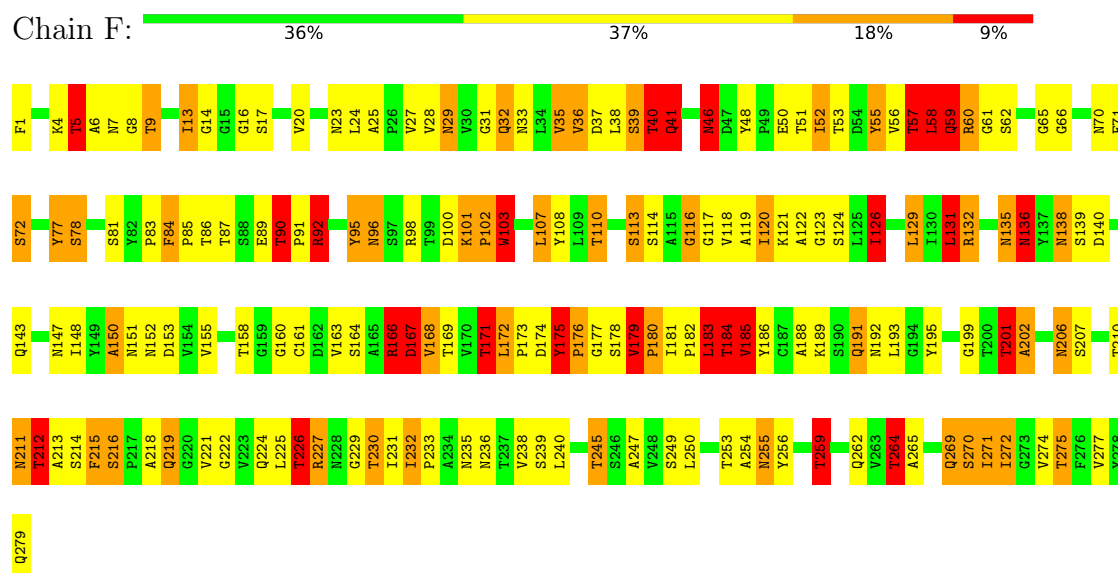
Chain B: 



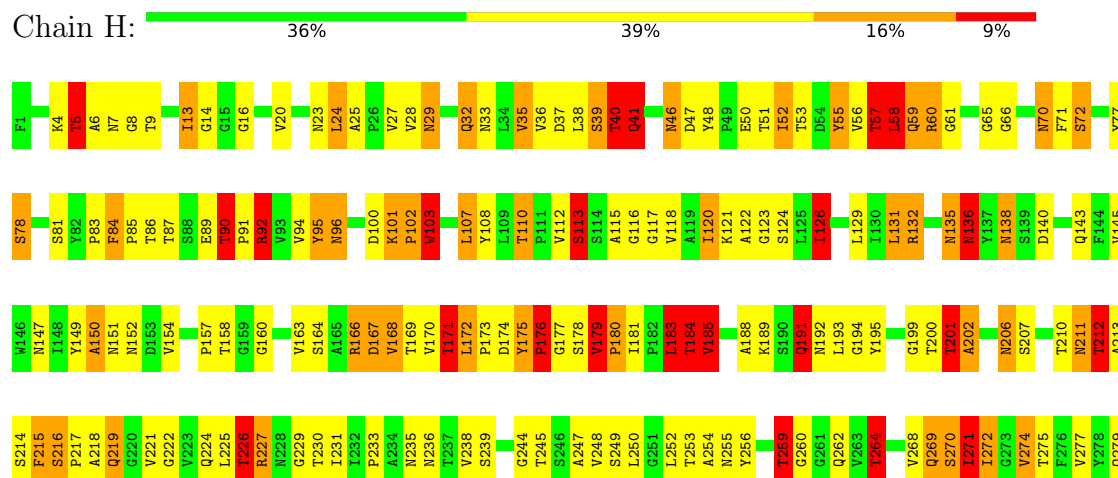
• Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH



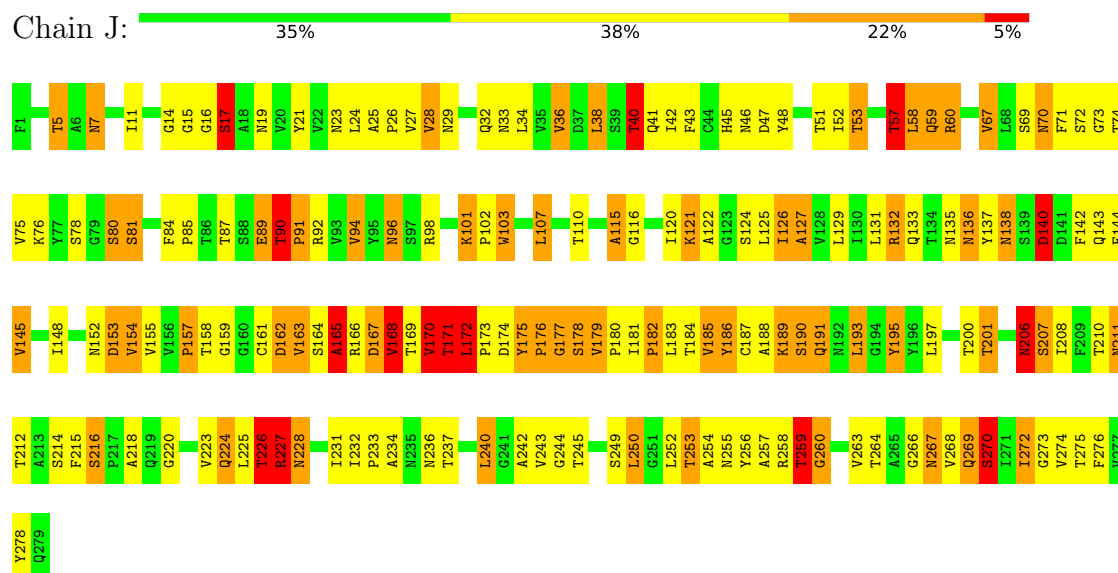
• Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH



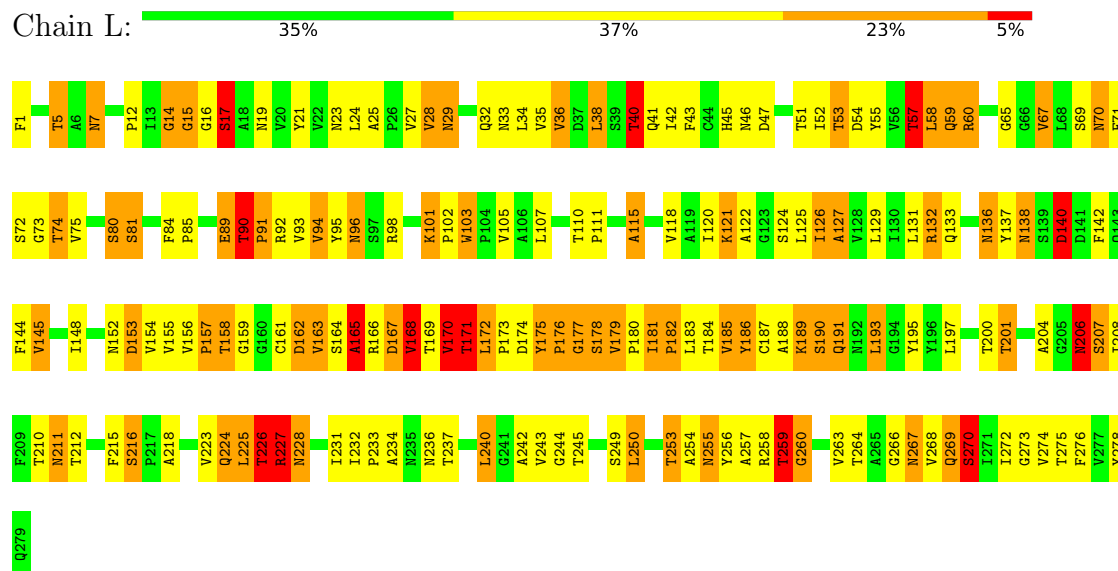
• Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH



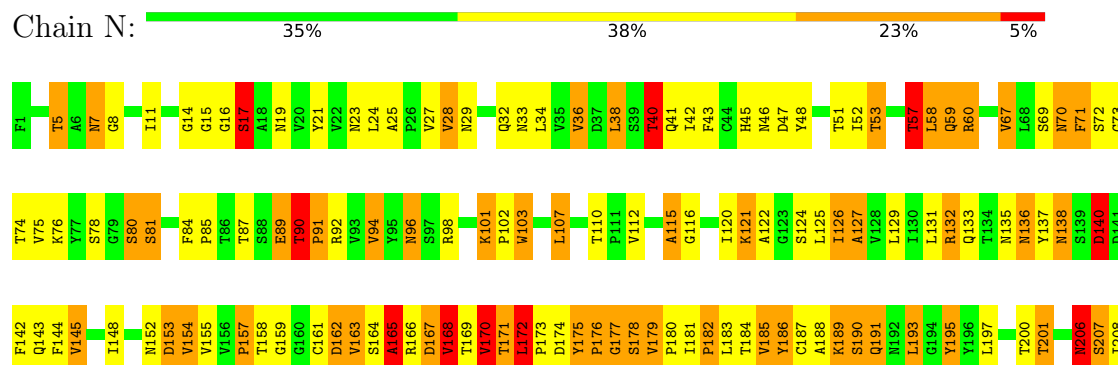
• Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

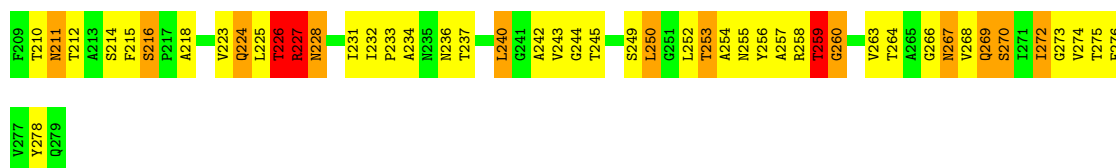


• Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH



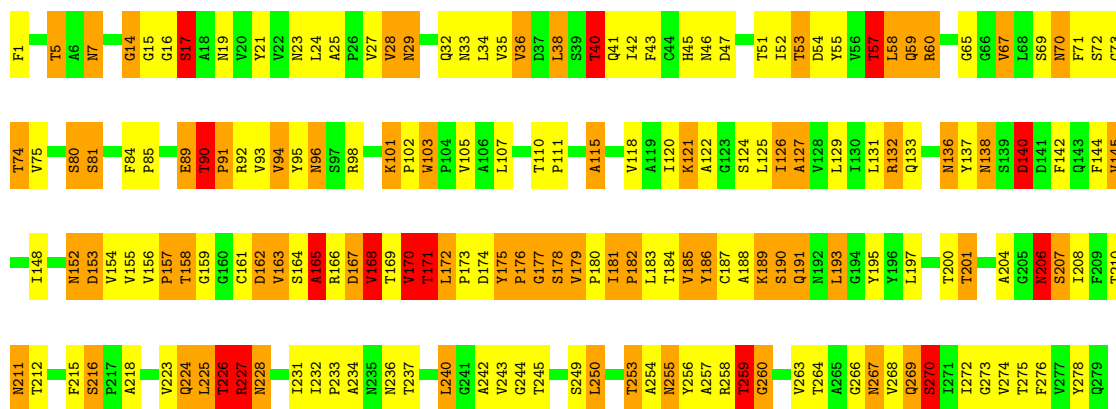
• Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH





• Molecule 2: MANNOSE-SPECIFIC ADHESIN FIMH

Chain P: 35% 37% 23% 5%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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 (Å ²)	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	1.18	3/1580 (0.2%)	3.14	143/2146 (6.7%)
1	C	1.21	4/1580 (0.3%)	3.19	155/2146 (7.2%)
1	E	1.21	4/1580 (0.3%)	3.19	155/2146 (7.2%)
1	G	1.18	3/1580 (0.2%)	3.14	141/2146 (6.6%)
1	I	2.83	14/1568 (0.9%)	3.45	115/2126 (5.4%)
1	K	2.84	16/1568 (1.0%)	3.37	119/2126 (5.6%)
1	M	2.83	14/1568 (0.9%)	3.45	116/2126 (5.5%)
1	O	2.84	16/1568 (1.0%)	3.37	119/2126 (5.6%)
2	B	1.89	7/2097 (0.3%)	3.33	269/2881 (9.3%)
2	D	1.82	8/2097 (0.4%)	3.31	271/2881 (9.4%)
2	F	1.82	8/2097 (0.4%)	3.31	271/2881 (9.4%)
2	H	1.89	7/2097 (0.3%)	3.33	269/2881 (9.3%)
2	J	1.64	5/2096 (0.2%)	3.28	177/2878 (6.2%)
2	L	1.78	5/2097 (0.2%)	3.19	163/2881 (5.7%)
2	N	1.64	5/2096 (0.2%)	3.28	177/2878 (6.2%)
2	P	1.78	5/2097 (0.2%)	3.19	164/2881 (5.7%)
All	All	1.96	124/29366 (0.4%)	3.28	2824/40130 (7.0%)

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

Continued on next page...

Continued from previous page...

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 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	167	ASP	C-O	-57.28	0.55	1.23
2	P	167	ASP	C-O	-57.28	0.55	1.23
1	I	26	ASP	CG-OD1	52.96	2.25	1.25
1	M	26	ASP	CG-OD1	52.95	2.25	1.25
1	K	135	ARG	C-N	-51.93	0.58	1.33

The worst 5 of 2824 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	165	ALA	O-C-N	-73.91	24.29	122.59
2	N	165	ALA	O-C-N	-73.91	24.30	122.59
2	L	165	ALA	O-C-N	-72.82	25.74	122.59
2	P	165	ALA	O-C-N	-72.82	25.74	122.59
1	C	51	THR	CA-C-O	-71.53	60.10	120.19

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	Peptide,Mainchain

Continued on next page...

Continued from previous page...

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

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	1553	0	1587	58	0
1	C	1553	0	1587	50	0
1	E	1553	0	1587	48	0
1	G	1553	0	1587	51	0
1	I	1543	0	1576	115	0
1	K	1543	0	1576	115	0
1	M	1543	0	1576	113	0
1	O	1543	0	1576	115	0
2	B	2052	0	2006	86	0
2	D	2052	0	2006	81	0
2	F	2052	0	2006	86	0
2	H	2052	0	2006	85	0
2	J	2052	0	2004	116	0
2	L	2052	0	2004	120	0
2	N	2052	0	2004	115	0
2	P	2052	0	2004	115	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	28692	1387	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 25.

The worst 5 of 1387 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%)	0	1
1	K	190/205 (93%)	134 (70%)	37 (20%)	19 (10%)	0	1
1	M	190/205 (93%)	135 (71%)	37 (20%)	18 (10%)	0	1
1	O	190/205 (93%)	134 (70%)	37 (20%)	19 (10%)	0	1
2	B	277/279 (99%)	253 (91%)	23 (8%)	1 (0%)	30	60
2	D	277/279 (99%)	254 (92%)	22 (8%)	1 (0%)	30	60
2	F	277/279 (99%)	254 (92%)	22 (8%)	1 (0%)	30	60
2	H	277/279 (99%)	253 (91%)	23 (8%)	1 (0%)	30	60
2	J	275/279 (99%)	238 (86%)	25 (9%)	12 (4%)	2	7
2	L	277/279 (99%)	242 (87%)	24 (9%)	11 (4%)	2	8
2	N	275/279 (99%)	238 (86%)	25 (9%)	12 (4%)	2	7
2	P	277/279 (99%)	242 (87%)	24 (9%)	11 (4%)	2	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3756/3872 (97%)	3250 (86%)	382 (10%)	124 (3%)	3	11

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 ⓘ

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%)	130 (77%)	39 (23%)	1	3
1	C	169/175 (97%)	128 (76%)	41 (24%)	1	2
1	E	169/175 (97%)	128 (76%)	41 (24%)	1	2
1	G	169/175 (97%)	130 (77%)	39 (23%)	1	3
1	I	169/175 (97%)	117 (69%)	52 (31%)	0	1
1	K	169/175 (97%)	118 (70%)	51 (30%)	0	1
1	M	169/175 (97%)	117 (69%)	52 (31%)	0	1
1	O	169/175 (97%)	118 (70%)	51 (30%)	0	1
2	B	226/226 (100%)	179 (79%)	47 (21%)	1	4
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%)	179 (79%)	47 (21%)	1	4
2	J	226/226 (100%)	181 (80%)	45 (20%)	1	5
2	L	226/226 (100%)	181 (80%)	45 (20%)	1	5
2	N	226/226 (100%)	181 (80%)	45 (20%)	1	5
2	P	226/226 (100%)	181 (80%)	45 (20%)	1	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3160/3208 (98%)	2430 (77%)	730 (23%)	1 3

5 of 730 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	92	SER
1	M	143	ILE
1	K	144	ASN
1	K	91	PRO
2	L	179	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	101	ASN
2	P	41	GLN
2	P	267	ASN
1	G	156	ASN
1	G	126	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 ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	5
1	M	5
1	K	5
1	O	5
2	J	2
2	N	2
2	L	2
2	P	2
2	B	2
2	H	2
2	D	2
2	F	2

The worst 5 of 36 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	173:PRO	C	174:ASP	N	2.75
1	N	173:PRO	C	174:ASP	N	2.75
1	I	74:GLN	C	75:LEU	N	2.13
1	M	74:GLN	C	75:LEU	N	2.13
1	K	74:GLN	C	75:LEU	N	2.05

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.