wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2021 – 07:03 AM EDT

PDB ID	:	1KIU
Title	:	FimH adhesin Q133N mutant-FimC chaperone complex with methyl-alpha-D -mannose
Authors	:	Hung, C.S.; Bouckaert, J.
Deposited on	:	2001-12-03
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 (i) symbol.

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

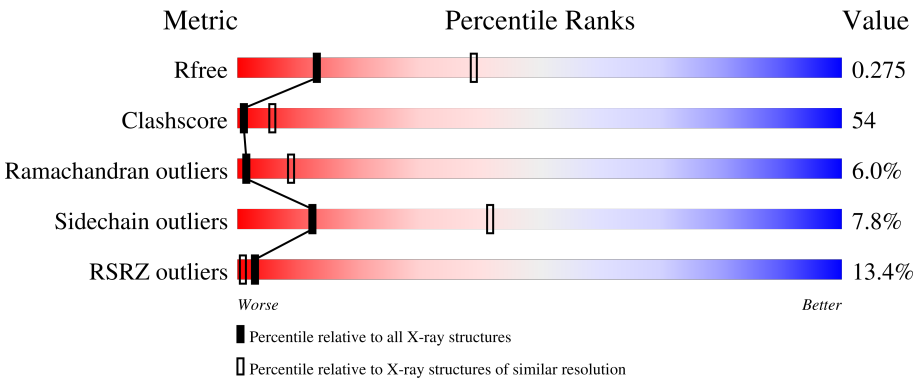
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 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 <=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	205	38% 53% 8% •
1	C	205	38% 53% 8% •
1	E	205	37% 55% 8% •
1	G	205	39% 53% 8% •
1	I	205	32% 22% 66% 12%

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Mol	Chain	Length	Quality of chain
1	K	205	42% 24% 65% 11%
1	M	205	37% 23% 65% 12%
1	O	205	35% 23% 65% 12%
2	B	279	49% 42% 10%
2	D	279	49% 42% 9%
2	F	279	48% 44% 8%
2	H	279	49% 42% 9%
2	J	279	19% 30% 62% 7%
2	L	279	20% 30% 62% 7%
2	N	279	19% 31% 62% 7%
2	P	279	20% 32% 61% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 29657 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 CHAPERONE PROTEIN FimC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	205	1596	1010	276	304	6	0	0	0
1	C	205	1596	1010	276	304	6	0	0	0
1	E	205	1596	1010	276	304	6	0	0	0
1	G	205	1596	1010	276	304	6	0	0	0
1	I	205	1596	1010	276	304	6	0	0	0
1	K	205	1596	1010	276	304	6	0	0	0
1	M	205	1596	1010	276	304	6	0	0	0
1	O	205	1596	1010	276	304	6	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	VAL	GLU	conflict	UNP P31697
C	18	VAL	GLU	conflict	UNP P31697
E	18	VAL	GLU	conflict	UNP P31697
G	18	VAL	GLU	conflict	UNP P31697
I	18	VAL	GLU	conflict	UNP P31697
K	18	VAL	GLU	conflict	UNP P31697
M	18	VAL	GLU	conflict	UNP P31697
O	18	VAL	GLU	conflict	UNP P31697

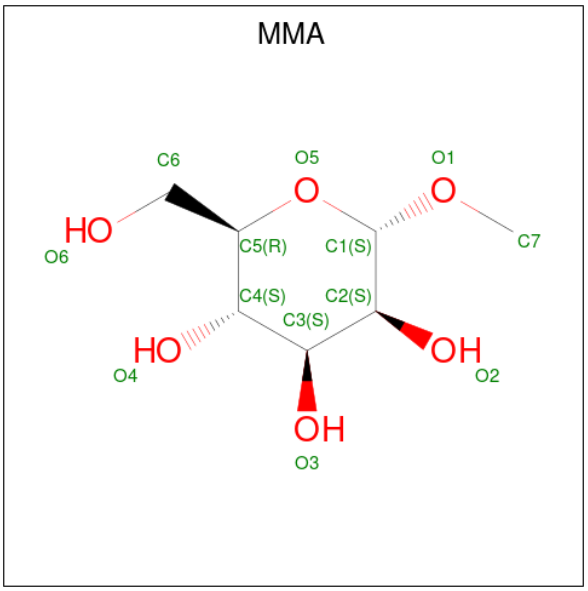
- Molecule 2 is a protein called FimH PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	279	2051	1296	342	409	4	0	0	0
2	D	279	2051	1296	342	409	4	0	0	0
2	F	279	2051	1296	342	409	4	0	0	0
2	H	279	2051	1296	342	409	4	0	0	0
2	J	279	2051	1296	342	409	4	0	0	0
2	L	279	2051	1296	342	409	4	0	0	0
2	N	279	2051	1296	342	409	4	0	0	0
2	P	279	2051	1296	342	409	4	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	133	ASN	GLN	engineered mutation	UNP P08191
D	133	ASN	GLN	engineered mutation	UNP P08191
F	133	ASN	GLN	engineered mutation	UNP P08191
H	133	ASN	GLN	engineered mutation	UNP P08191
J	133	ASN	GLN	engineered mutation	UNP P08191
L	133	ASN	GLN	engineered mutation	UNP P08191
N	133	ASN	GLN	engineered mutation	UNP P08191
P	133	ASN	GLN	engineered mutation	UNP P08191

- Molecule 3 is methyl alpha-D-mannopyranoside (three-letter code: MMA) (formula: $C_7H_{14}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 13 7 6	0	0
3	D	1	Total C O 13 7 6	0	0
3	F	1	Total C O 13 7 6	0	0
3	H	1	Total C O 13 7 6	0	0
3	J	1	Total C O 13 7 6	0	0
3	L	1	Total C O 13 7 6	0	0
3	N	1	Total C O 13 7 6	0	0
3	P	1	Total C O 13 7 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	19	Total O 19 19	0	0
4	B	58	Total O 58 58	0	0
4	C	20	Total O 20 20	0	0
4	D	54	Total O 54 54	0	0

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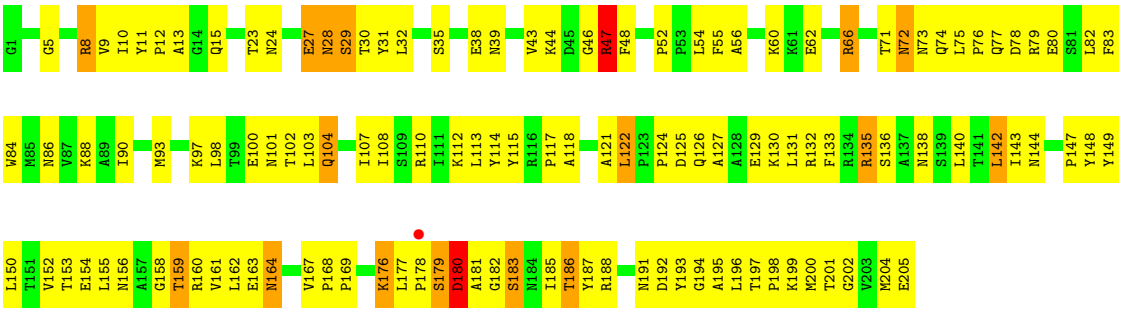
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	28	Total O 28 28	0	0
4	F	47	Total O 47 47	0	0
4	G	20	Total O 20 20	0	0
4	H	54	Total O 54 54	0	0
4	I	5	Total O 5 5	0	0
4	J	12	Total O 12 12	0	0
4	K	8	Total O 8 8	0	0
4	L	13	Total O 13 13	0	0
4	M	5	Total O 5 5	0	0
4	N	13	Total O 13 13	0	0
4	O	7	Total O 7 7	0	0
4	P	14	Total O 14 14	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.

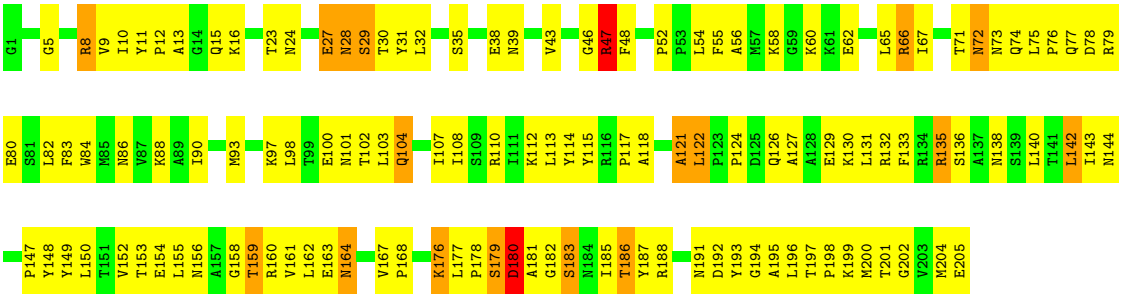
- Molecule 1: CHAPERONE PROTEIN FimC

Chain A:



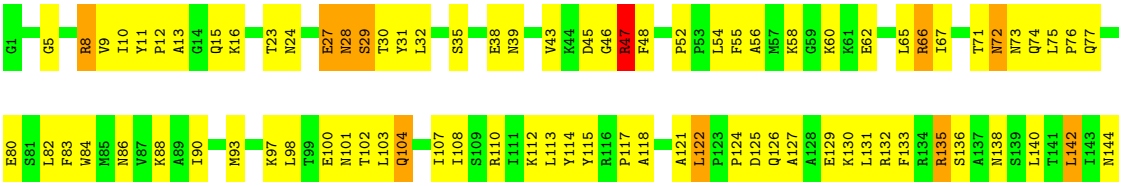
- Molecule 1: CHAPERONE PROTEIN FimC

Chain C:



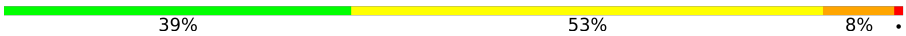
- Molecule 1: CHAPERONE PROTEIN FimC

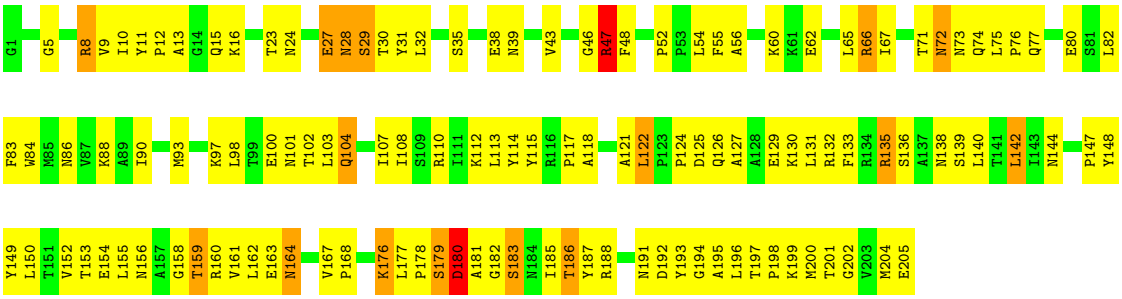
Chain E:



• Molecule 1: CHAPERONE PROTEIN FimC

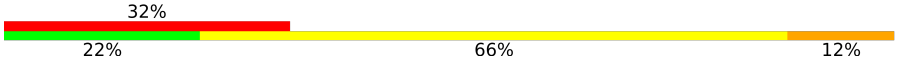
Chain G:

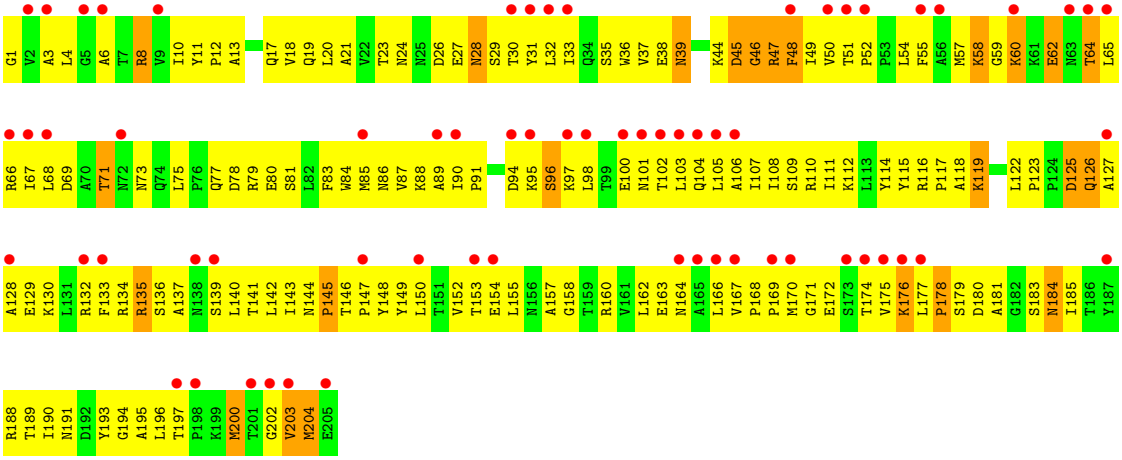




• Molecule 1: CHAPERONE PROTEIN FimC

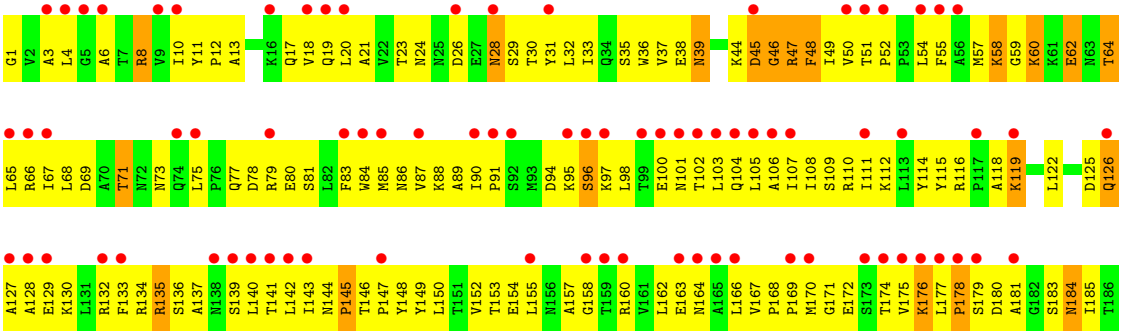
Chain I:

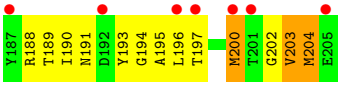




• Molecule 1: CHAPERONE PROTEIN FimC

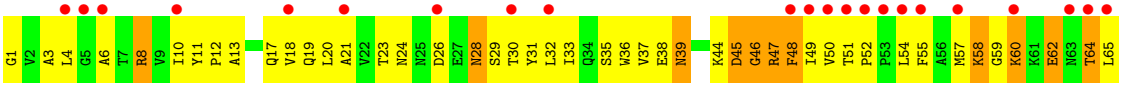
Chain K:

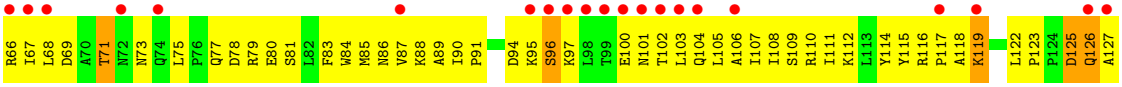


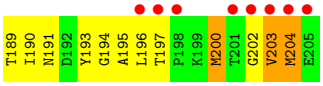


• Molecule 1: CHAPERONE PROTEIN FimC

Chain M:

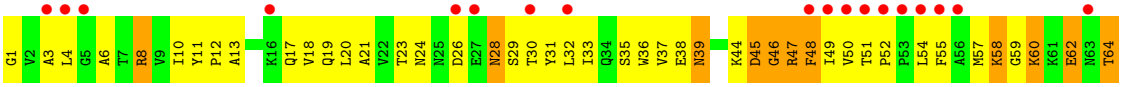


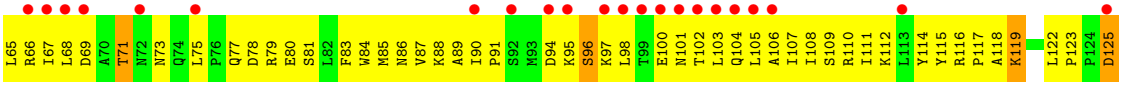


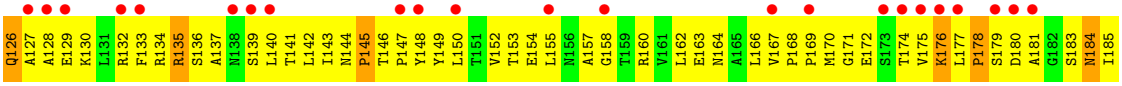


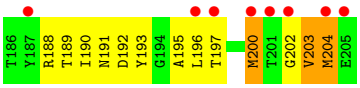
• Molecule 1: CHAPERONE PROTEIN FimC

Chain O:



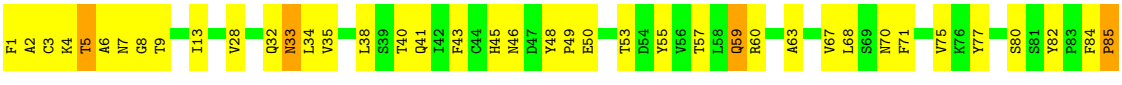


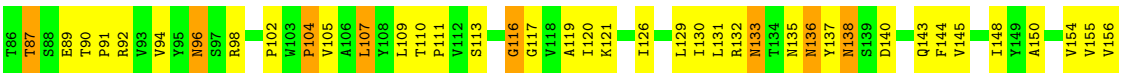


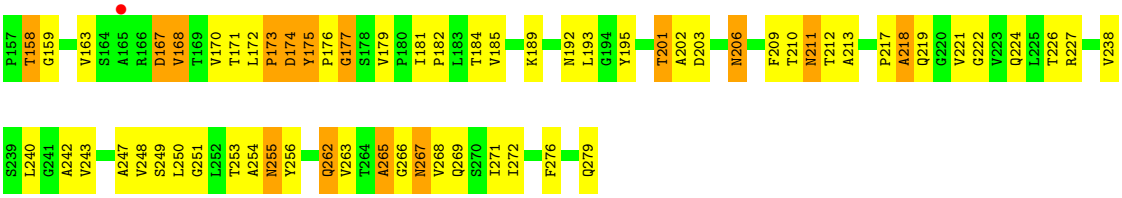


• Molecule 2: FimH PROTEIN

Chain B:

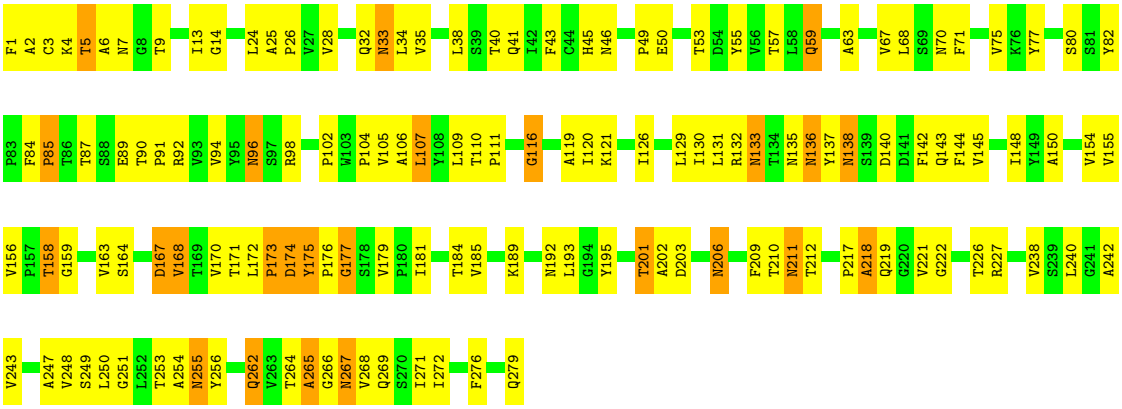






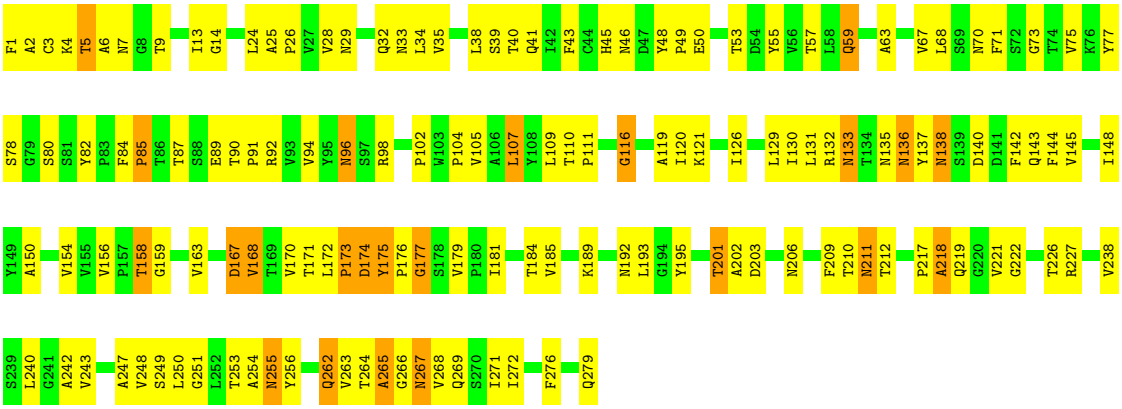
- Molecule 2: FimH PROTEIN

Chain D:



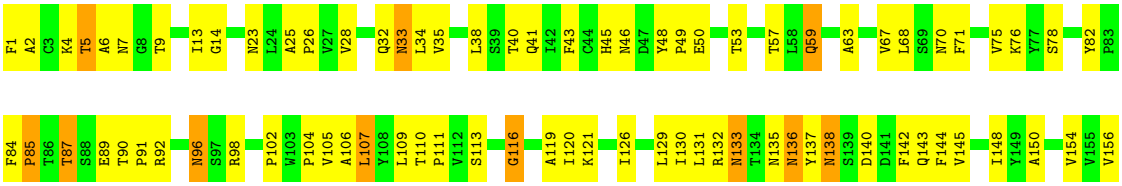
- Molecule 2: FimH PROTEIN

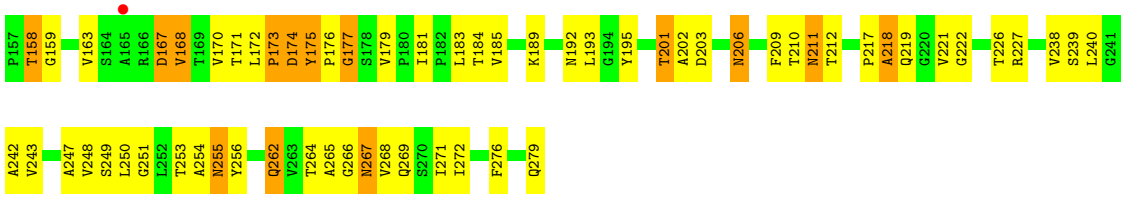
Chain F:



- Molecule 2: FimH PROTEIN

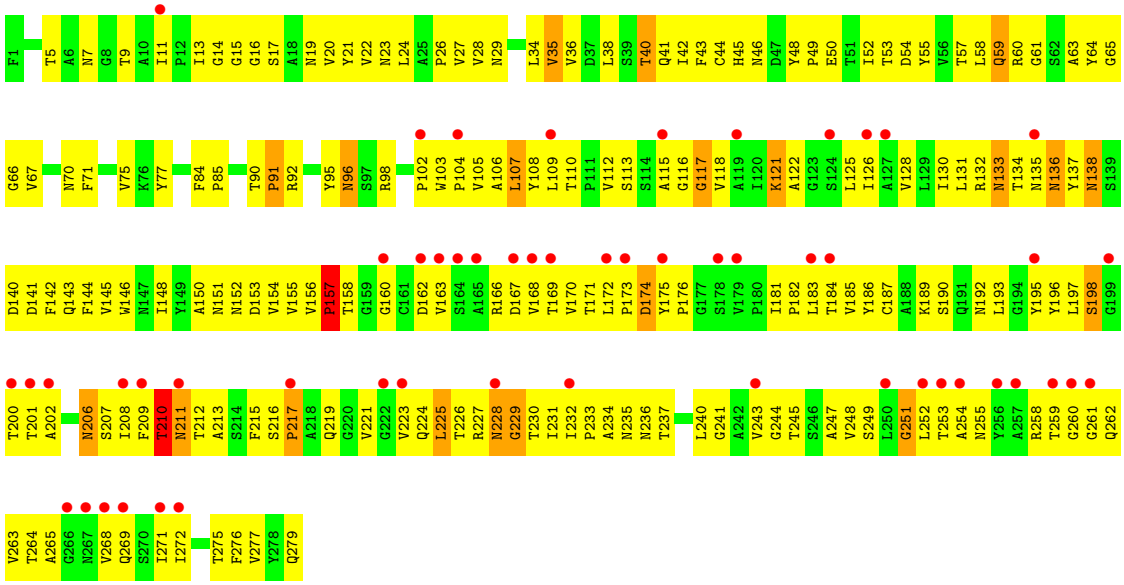
Chain H:





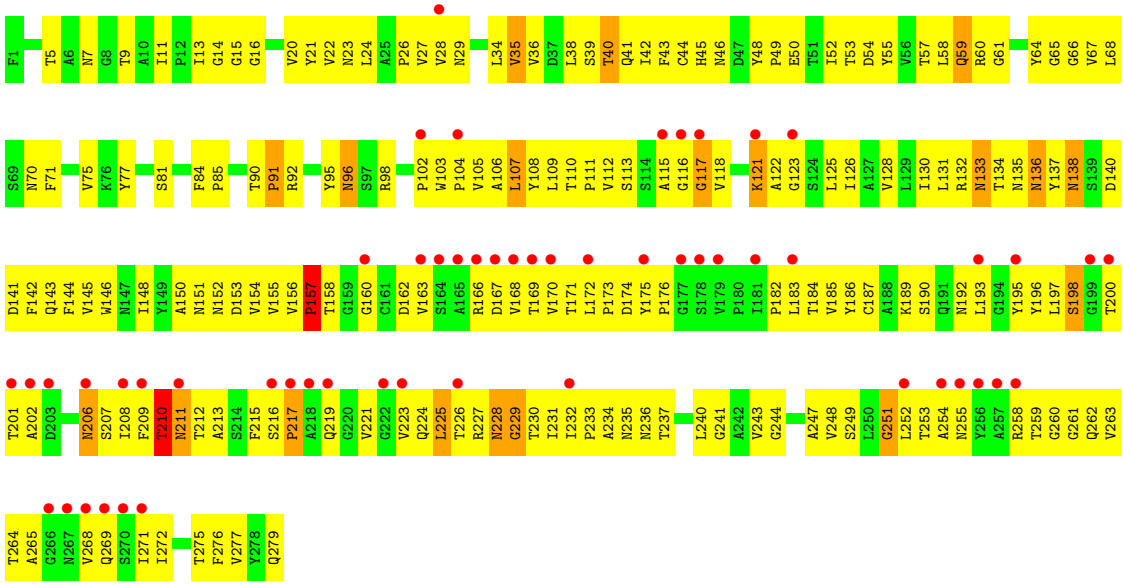
- Molecule 2: FimH PROTEIN

Chain J:



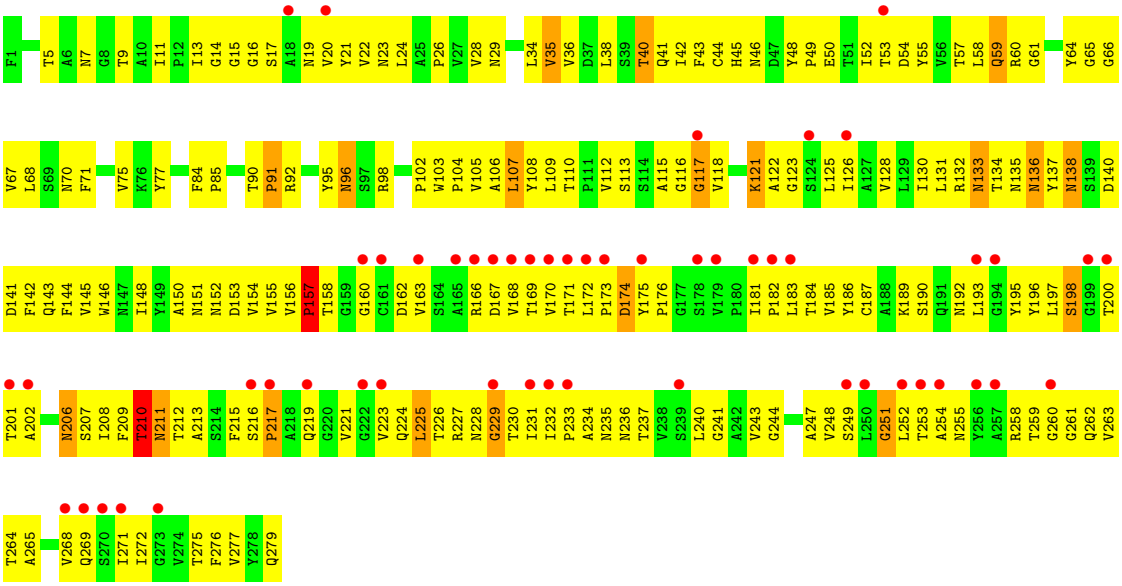
- Molecule 2: FimH PROTEIN

Chain L:



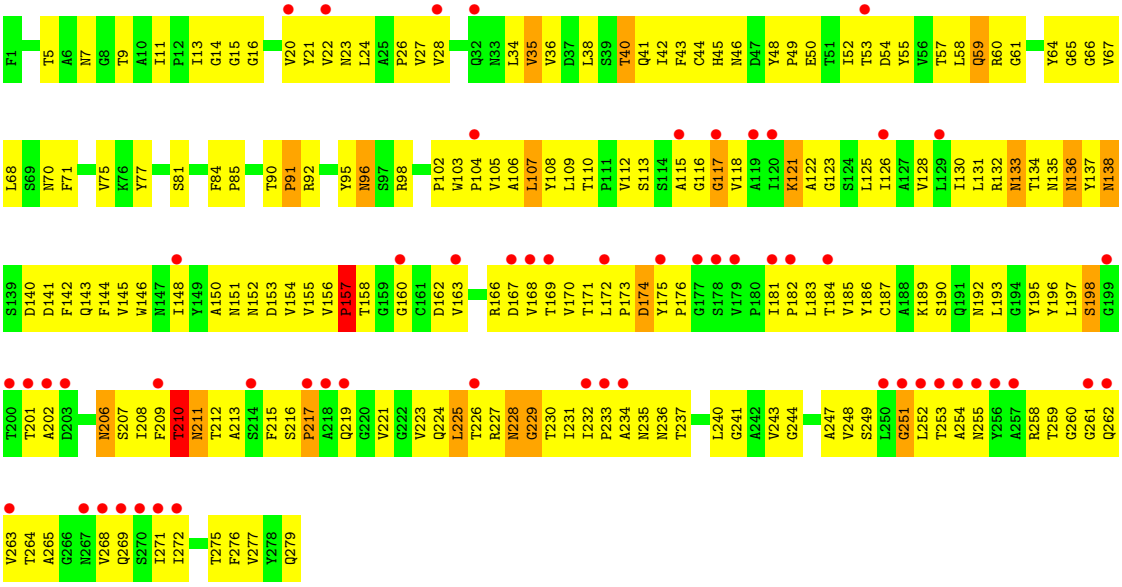
- Molecule 2: FimH PROTEIN

Chain N:



- Molecule 2: FimH PROTEIN

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	138.35Å 138.33Å 213.21Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	45.00 – 3.00 44.46 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.1 (45.00-3.00) 89.2 (44.46-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.278 0.233 , 0.275	Depositor DCC
R_{free} test set	7267 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å^2)	59.9	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 62.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.457 for k,h,-l 0.457 for -k,-h,-l 0.447 for -h,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	29657	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.15% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MMA

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	0.42	0/1625	0.71	0/2209
1	C	0.42	0/1625	0.71	0/2209
1	E	0.42	0/1625	0.70	0/2209
1	G	0.42	0/1625	0.71	0/2209
1	I	0.29	0/1625	0.54	0/2209
1	K	0.29	0/1625	0.54	0/2209
1	M	0.29	0/1625	0.54	0/2209
1	O	0.29	0/1625	0.54	0/2209
2	B	0.48	0/2096	0.76	0/2880
2	D	0.49	0/2096	0.76	0/2880
2	F	0.49	0/2096	0.76	0/2880
2	H	0.49	0/2096	0.76	0/2880
2	J	0.33	0/2096	0.60	0/2880
2	L	0.33	0/2096	0.60	0/2880
2	N	0.33	0/2096	0.60	0/2880
2	P	0.33	0/2096	0.59	0/2880
All	All	0.39	0/29768	0.66	0/40712

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 (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	1596	0	1639	151	0
1	C	1596	0	1639	158	0
1	E	1596	0	1639	157	0
1	G	1596	0	1639	148	0
1	I	1596	0	1639	242	0
1	K	1596	0	1639	246	0
1	M	1596	0	1639	240	0
1	O	1596	0	1639	243	0
2	B	2051	0	2005	182	0
2	D	2051	0	2005	173	0
2	F	2051	0	2005	180	0
2	H	2051	0	2005	183	0
2	J	2051	0	2005	262	0
2	L	2051	0	2005	264	0
2	N	2051	0	2005	255	0
2	P	2051	0	2005	263	0
3	B	13	0	14	2	0
3	D	13	0	14	0	0
3	F	13	0	14	2	0
3	H	13	0	14	3	0
3	J	13	0	14	1	0
3	L	13	0	14	1	0
3	N	13	0	14	1	0
3	P	13	0	14	1	0
4	A	19	0	0	4	0
4	B	58	0	0	11	0
4	C	20	0	0	9	0
4	D	54	0	0	6	0
4	E	28	0	0	9	0
4	F	47	0	0	10	0
4	G	20	0	0	3	0
4	H	54	0	0	9	0
4	I	5	0	0	2	0
4	J	12	0	0	5	0
4	K	8	0	0	2	0
4	L	13	0	0	5	0
4	M	5	0	0	1	0
4	N	13	0	0	0	0
4	O	7	0	0	2	0
4	P	14	0	0	2	0
All	All	29657	0	29264	3137	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 54.

The worst 5 of 3137 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:K:141:THR:HA	1:K:174:THR:CG2	1.33	1.59
1:M:141:THR:HA	1:M:174:THR:CG2	1.32	1.55
1:O:141:THR:HA	1:O:174:THR:CG2	1.33	1.54
1:I:141:THR:HA	1:I:174:THR:CG2	1.33	1.54
1:O:141:THR:HA	1:O:174:THR:HG21	1.26	1.16

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	203/205 (99%)	164 (81%)	27 (13%)	12 (6%)	1 9
1	C	203/205 (99%)	163 (80%)	28 (14%)	12 (6%)	1 9
1	E	203/205 (99%)	163 (80%)	29 (14%)	11 (5%)	2 11
1	G	203/205 (99%)	164 (81%)	28 (14%)	11 (5%)	2 11
1	I	203/205 (99%)	138 (68%)	47 (23%)	18 (9%)	1 3
1	K	203/205 (99%)	138 (68%)	47 (23%)	18 (9%)	1 3
1	M	203/205 (99%)	138 (68%)	47 (23%)	18 (9%)	1 3
1	O	203/205 (99%)	138 (68%)	47 (23%)	18 (9%)	1 3
2	B	277/279 (99%)	248 (90%)	18 (6%)	11 (4%)	3 17
2	D	277/279 (99%)	248 (90%)	18 (6%)	11 (4%)	3 17
2	F	277/279 (99%)	248 (90%)	18 (6%)	11 (4%)	3 17
2	H	277/279 (99%)	249 (90%)	18 (6%)	10 (4%)	3 19
2	J	277/279 (99%)	203 (73%)	57 (21%)	17 (6%)	1 8
2	L	277/279 (99%)	204 (74%)	56 (20%)	17 (6%)	1 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	277/279 (99%)	204 (74%)	56 (20%)	17 (6%)	1	8
2	P	277/279 (99%)	203 (73%)	57 (21%)	17 (6%)	1	8
All	All	3840/3872 (99%)	3013 (78%)	598 (16%)	229 (6%)	1	9

5 of 229 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	72	ASN
1	A	159	THR
1	A	179	SER
1	A	180	ASP

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	176/176 (100%)	160 (91%)	16 (9%)	9	34
1	C	176/176 (100%)	160 (91%)	16 (9%)	9	34
1	E	176/176 (100%)	160 (91%)	16 (9%)	9	34
1	G	176/176 (100%)	160 (91%)	16 (9%)	9	34
1	I	176/176 (100%)	163 (93%)	13 (7%)	13	44
1	K	176/176 (100%)	163 (93%)	13 (7%)	13	44
1	M	176/176 (100%)	163 (93%)	13 (7%)	13	44
1	O	176/176 (100%)	163 (93%)	13 (7%)	13	44
2	B	226/226 (100%)	206 (91%)	20 (9%)	10	36
2	D	226/226 (100%)	207 (92%)	19 (8%)	11	38
2	F	226/226 (100%)	208 (92%)	18 (8%)	12	40
2	H	226/226 (100%)	207 (92%)	19 (8%)	11	38
2	J	226/226 (100%)	211 (93%)	15 (7%)	16	49
2	L	226/226 (100%)	211 (93%)	15 (7%)	16	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	226/226 (100%)	211 (93%)	15 (7%)	16	49
2	P	226/226 (100%)	211 (93%)	15 (7%)	16	49
All	All	3216/3216 (100%)	2964 (92%)	252 (8%)	12	42

5 of 252 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	122	LEU
2	N	210	THR
1	I	45	ASP
2	N	187	CYS
1	O	176	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 215 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	45	HIS
2	L	41	GLN
2	P	41	GLN
2	J	151	ASN
1	K	19	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)

8 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
3	MMA	H	603	-	13,13,13	1.62	3 (23%)	18,18,18	0.89	0
3	MMA	D	601	-	13,13,13	1.53	3 (23%)	18,18,18	0.91	0
3	MMA	N	506	-	13,13,13	1.44	2 (15%)	18,18,18	0.86	0
3	MMA	B	500	-	13,13,13	1.57	3 (23%)	18,18,18	0.94	0
3	MMA	L	504	-	13,13,13	1.48	2 (15%)	18,18,18	0.85	0
3	MMA	P	607	-	13,13,13	1.48	2 (15%)	18,18,18	0.87	0
3	MMA	J	605	-	13,13,13	1.37	2 (15%)	18,18,18	0.93	0
3	MMA	F	502	-	13,13,13	1.51	3 (23%)	18,18,18	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MMA	H	603	-	-	2/4/24/24	0/1/1/1
3	MMA	D	601	-	-	2/4/24/24	0/1/1/1
3	MMA	N	506	-	-	3/4/24/24	0/1/1/1
3	MMA	B	500	-	-	2/4/24/24	0/1/1/1
3	MMA	L	504	-	-	1/4/24/24	0/1/1/1
3	MMA	P	607	-	-	4/4/24/24	0/1/1/1
3	MMA	J	605	-	-	4/4/24/24	0/1/1/1
3	MMA	F	502	-	-	2/4/24/24	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	MMA	O1-C1	3.94	1.47	1.40
3	H	603	MMA	O1-C1	3.91	1.46	1.40
3	D	601	MMA	O1-C1	3.64	1.46	1.40
3	L	504	MMA	O1-C1	3.58	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	502	MMA	O1-C1	3.46	1.46	1.40

There are no bond angle outliers.

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	601	MMA	C2-C1-O1-C7
3	D	601	MMA	O5-C1-O1-C7
3	F	502	MMA	C2-C1-O1-C7
3	F	502	MMA	O5-C1-O1-C7
3	B	500	MMA	O5-C1-O1-C7

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	603	MMA	3	0
3	N	506	MMA	1	0
3	B	500	MMA	2	0
3	L	504	MMA	1	0
3	P	607	MMA	1	0
3	J	605	MMA	1	0
3	F	502	MMA	2	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 (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	205/205 (100%)	-0.20	1 (0%) 91 75	15, 44, 85, 105	0
1	C	205/205 (100%)	-0.21	0 100 100	12, 44, 86, 105	0
1	E	205/205 (100%)	-0.21	0 100 100	16, 43, 87, 103	0
1	G	205/205 (100%)	-0.26	0 100 100	12, 44, 85, 102	0
1	I	205/205 (100%)	1.77	65 (31%) 0 0	20, 133, 152, 161	0
1	K	205/205 (100%)	1.95	87 (42%) 0 0	20, 133, 149, 161	0
1	M	205/205 (100%)	1.85	75 (36%) 0 0	20, 133, 149, 159	0
1	O	205/205 (100%)	1.86	71 (34%) 0 0	20, 133, 149, 162	0
2	B	279/279 (100%)	-0.30	1 (0%) 92 79	11, 35, 66, 97	0
2	D	279/279 (100%)	-0.35	0 100 100	11, 35, 70, 97	0
2	F	279/279 (100%)	-0.29	0 100 100	11, 35, 66, 96	0
2	H	279/279 (100%)	-0.28	1 (0%) 92 79	12, 33, 68, 97	0
2	J	279/279 (100%)	0.98	54 (19%) 1 0	52, 98, 154, 164	0
2	L	279/279 (100%)	1.11	55 (19%) 1 0	51, 97, 156, 163	0
2	N	279/279 (100%)	0.99	53 (18%) 1 0	53, 98, 154, 163	0
2	P	279/279 (100%)	1.04	57 (20%) 1 0	52, 100, 154, 160	0
All	All	3872/3872 (100%)	0.56	520 (13%) 3 1	11, 71, 148, 164	0

The worst 5 of 520 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	104	GLN	15.6
1	I	103	LEU	13.7
1	O	104	GLN	13.6
1	I	104	GLN	13.3
1	M	104	GLN	9.6

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)

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, 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MMA	L	504	13/13	0.76	0.28	102,108,111,112	0
3	MMA	B	500	13/13	0.82	0.36	36,56,63,64	0
3	MMA	N	506	13/13	0.84	0.28	93,96,98,100	0
3	MMA	D	601	13/13	0.86	0.29	39,65,67,68	0
3	MMA	J	605	13/13	0.86	0.35	116,117,120,121	0
3	MMA	P	607	13/13	0.87	0.26	112,115,117,117	0
3	MMA	F	502	13/13	0.88	0.31	34,54,58,58	0
3	MMA	H	603	13/13	0.90	0.31	32,55,58,59	0

6.5 Other polymers (i)

There are no such residues in this entry.