



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 01:06 AM BST

PDB ID : 6RUT
Title : Mycoplasma Genitalium Heterodimer Nap Complex (P140-P110 globular)
Authors : Fita, I.; Aparicio, D.
Deposited on : 2019-05-29
Resolution : 2.65 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

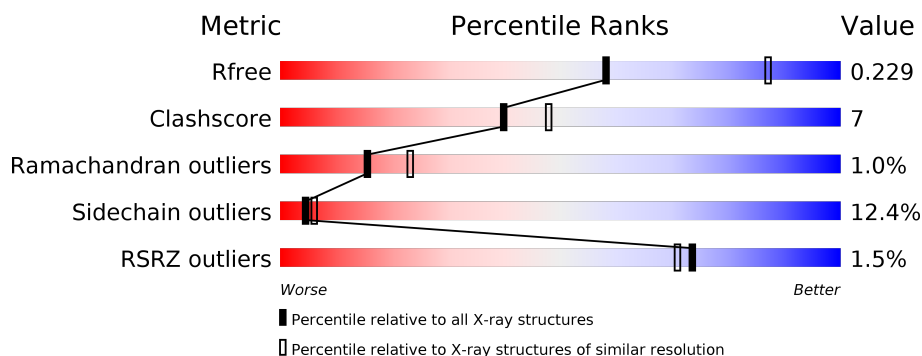
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	802	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>• •</div> </div> </div>
1	C	802	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
1	E	802	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>• •</div> </div> </div>
1	G	802	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>
2	B	1334	<div> <div></div> <div> <div>69%</div> <div>22%</div> <div>• 5%</div> </div> </div>
2	D	1334	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>22%</div> <div>• 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	1334	<div><div><div></div><div></div><div></div><div></div></div><div>3%67%22%6%</div></div>
2	H	1334	<div><div><div></div><div></div><div></div><div></div></div><div>3%67%23%7%</div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 64181 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 Mgp-operon protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	0	0
			6013	3758	1009	1240	6			
1	C	779	Total	C	N	O	S	0	0	0
			5999	3751	1006	1236	6			
1	E	783	Total	C	N	O	S	0	0	0
			6017	3760	1010	1241	6			
1	G	784	Total	C	N	O	S	0	0	0
			6023	3763	1011	1243	6			

- Molecule 2 is a protein called Adhesin P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1268	Total	C	N	O	S	0	0	0
			9938	6303	1679	1942	14			
2	D	1265	Total	C	N	O	S	0	0	0
			9918	6293	1676	1935	14			
2	F	1250	Total	C	N	O	S	0	0	0
			9822	6242	1658	1909	13			
2	H	1247	Total	C	N	O	S	0	0	0
			9798	6228	1654	1903	13			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	121	Total	O	0	0
			121	121		
3	C	87	Total	O	0	0
			87	87		
3	D	137	Total	O	0	0
			137	137		

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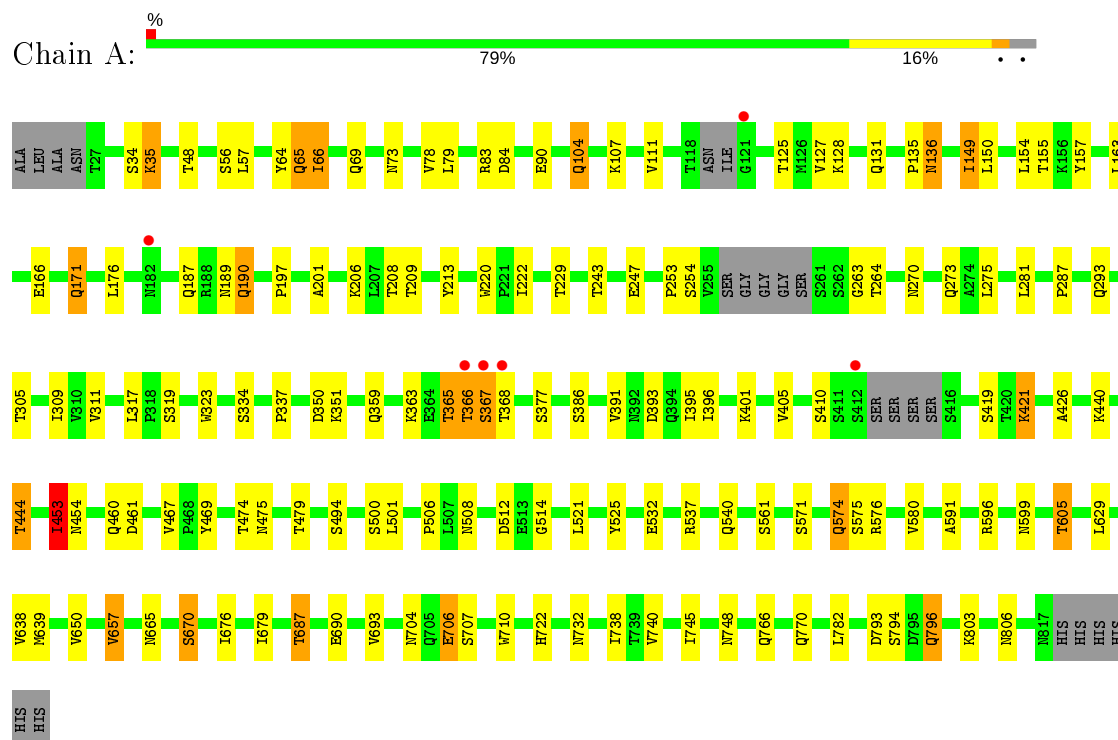
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	69	Total 69	O 69	0	0
3	F	70	Total 70	O 70	0	0
3	G	49	Total 49	O 49	0	0
3	H	58	Total 58	O 58	0	0

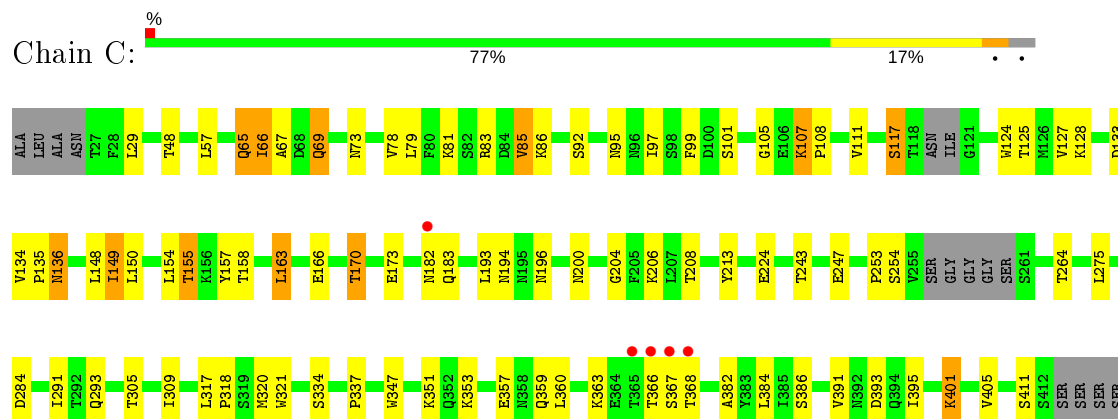
3 Residue-property plots [i](#)

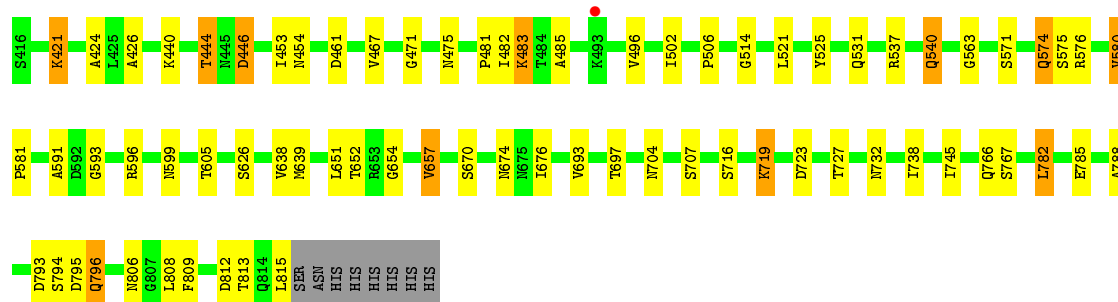
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Mgp-operon protein 3

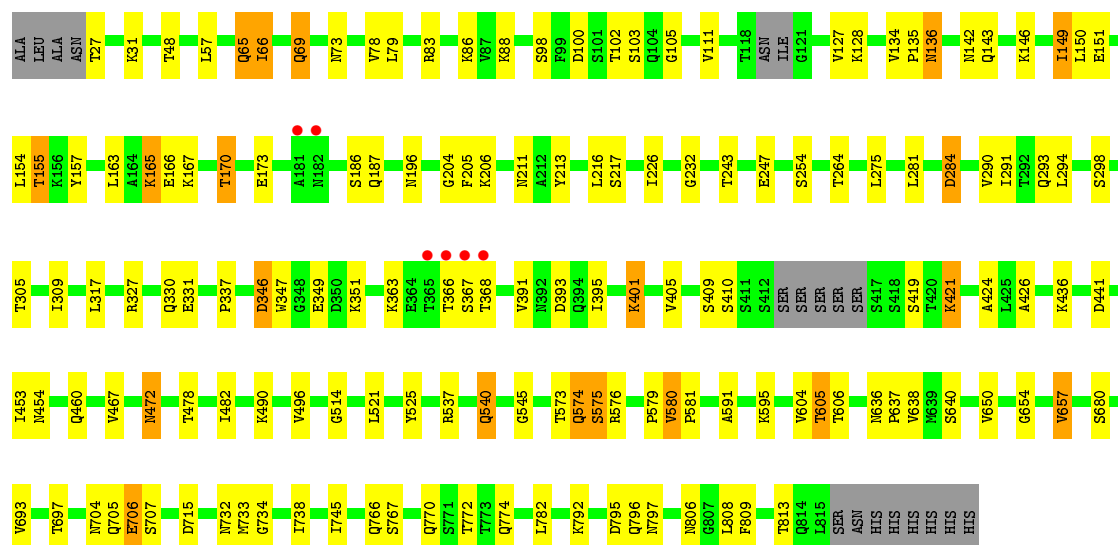
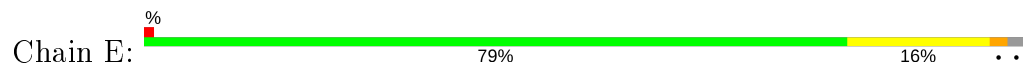


• Molecule 1: Mgp-operon protein 3

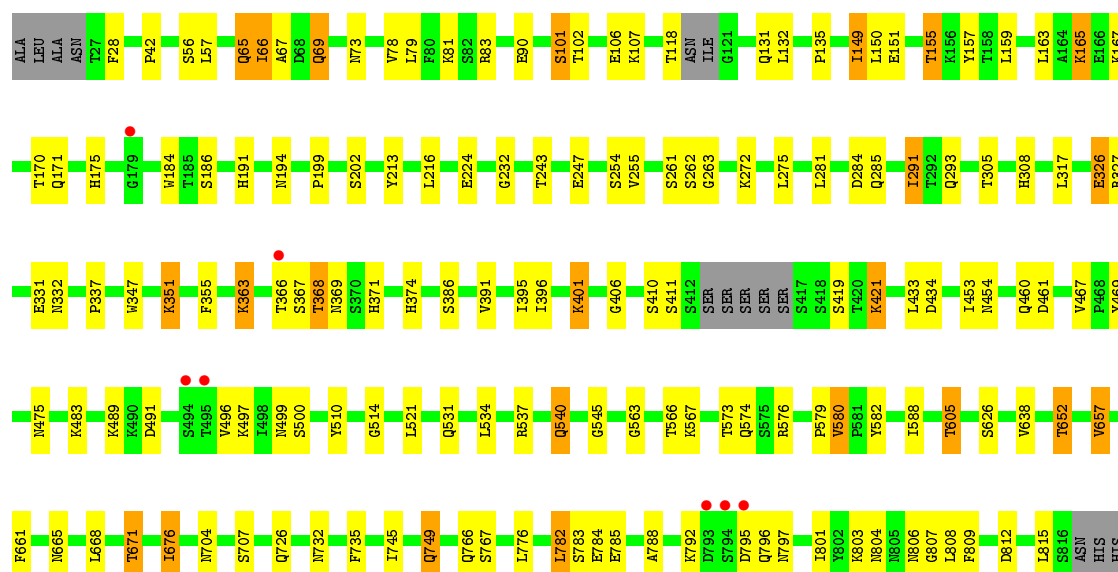
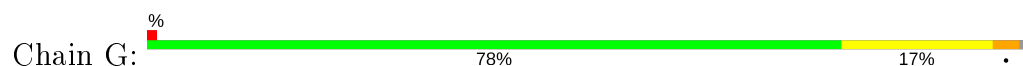




• Molecule 1: Mgp-operon protein 3



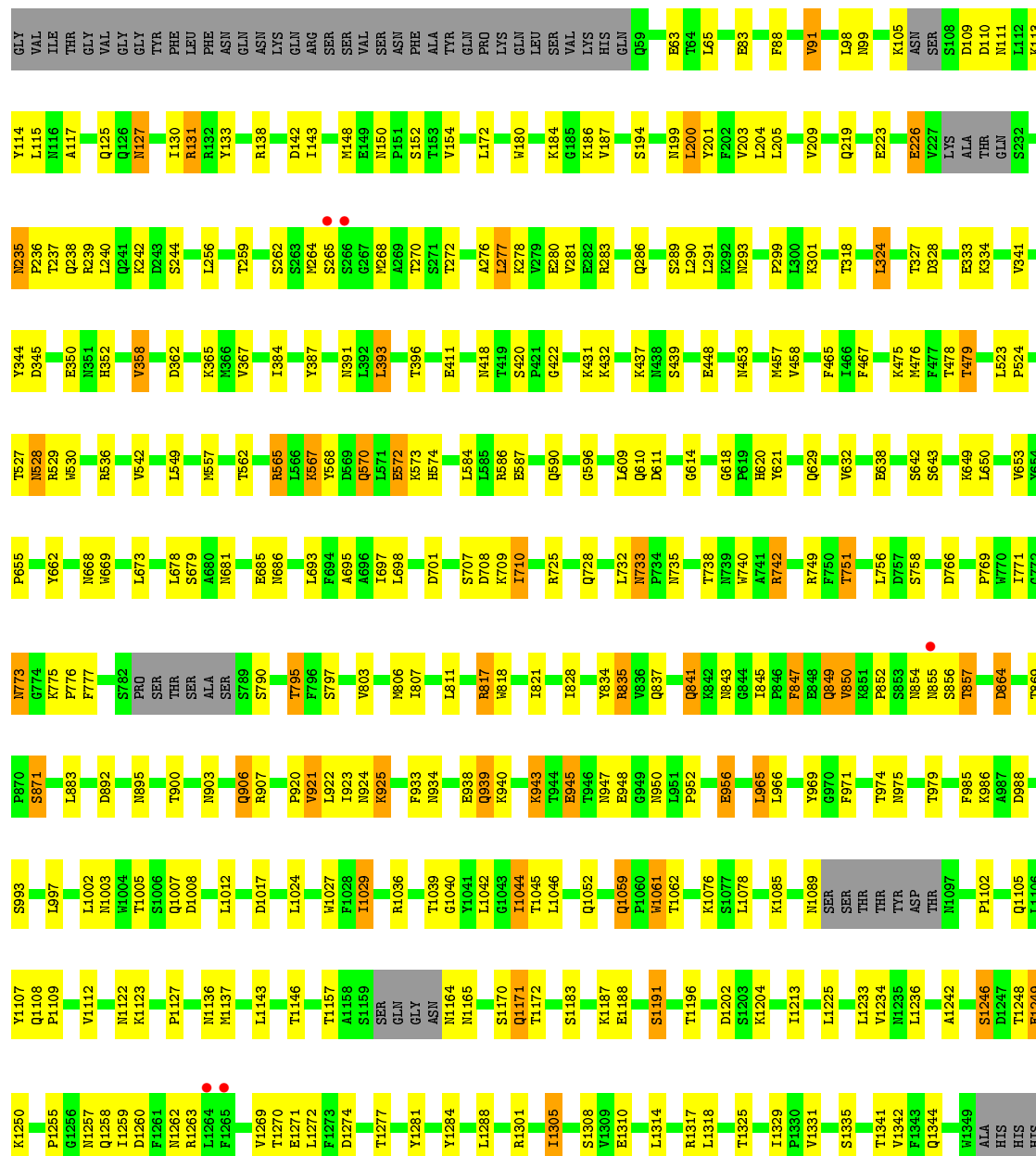
• Molecule 1: Mgp-operon protein 3



HIS
HIS
HIS

• Molecule 2: Adhesin P1

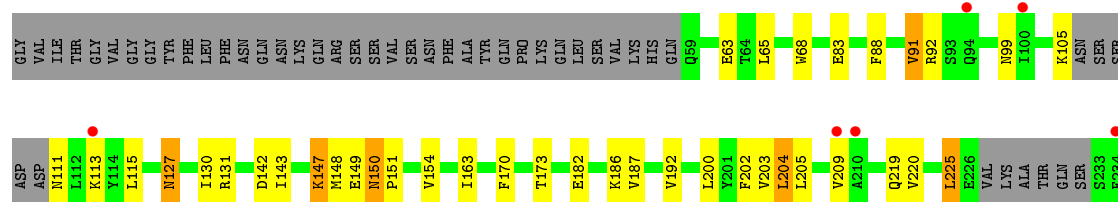
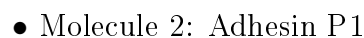
Chain B:  69% 22% 5%

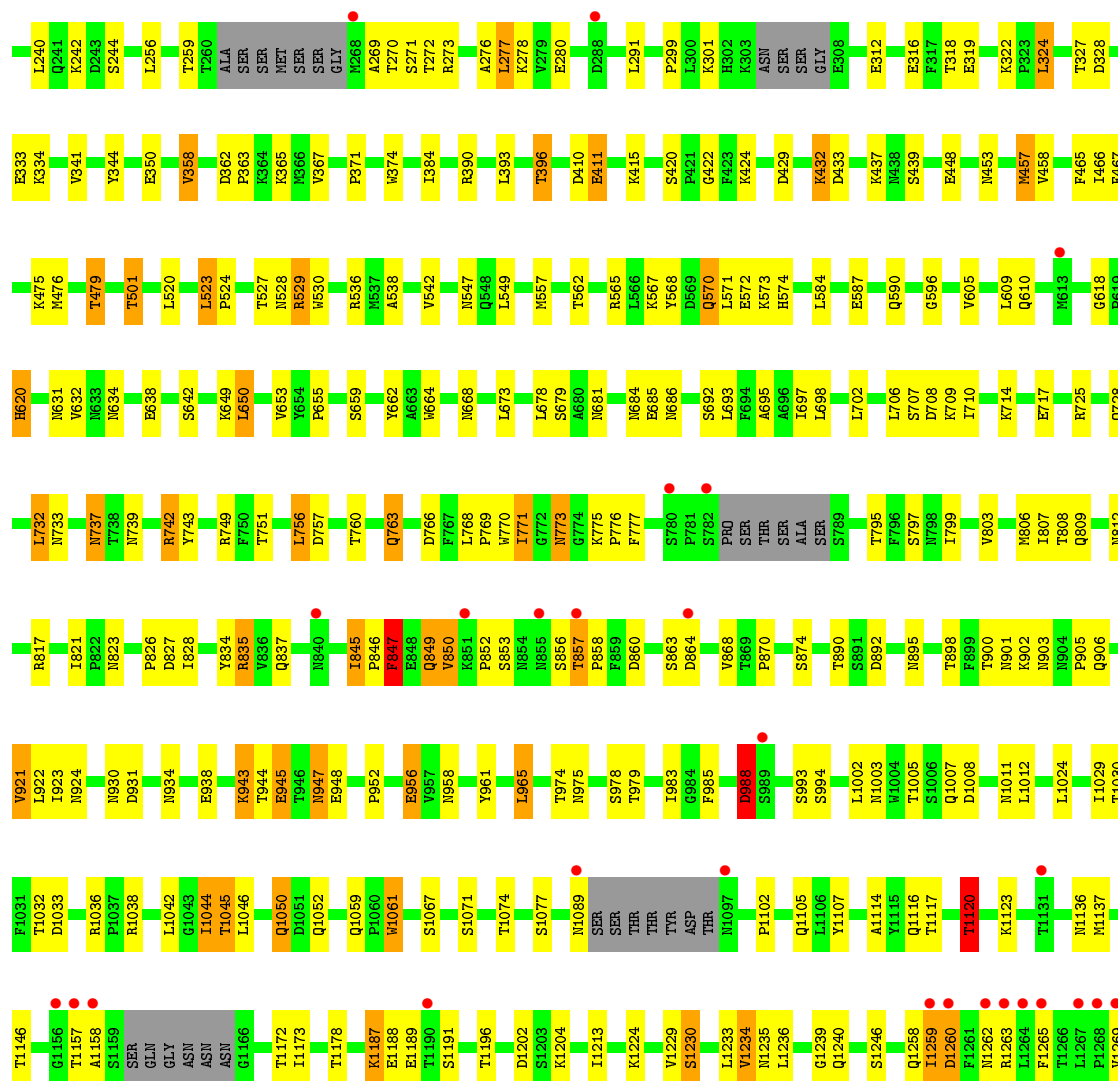


HIS
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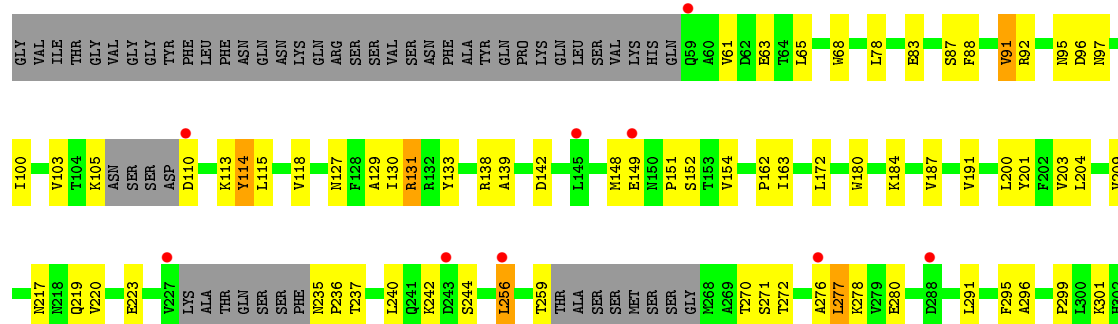
• Molecule 2: Adhesin P1

Chain D:  69% 22% 5%





• Molecule 2: Adhesin P1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	151.00Å 157.28Å 192.37Å 90.00° 93.81° 90.00°	Depositor
Resolution (Å)	121.66 – 2.65 150.67 – 2.65	Depositor EDS
% Data completeness (in resolution range)	73.2 (121.66-2.65) 73.3 (150.67-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.187 , 0.224 0.199 , 0.229	Depositor DCC
R_{free} test set	9457 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	64181	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.48	0/6136	0.74	0/8340
1	C	0.48	0/6122	0.74	0/8321
1	E	0.47	0/6141	0.74	0/8347
1	G	0.48	0/6147	0.74	1/8355 (0.0%)
2	B	0.50	0/10187	0.76	1/13863 (0.0%)
2	D	0.49	0/10167	0.76	4/13836 (0.0%)
2	F	0.46	0/10069	0.73	2/13701 (0.0%)
2	H	0.48	1/10044 (0.0%)	0.72	2/13668 (0.0%)
All	All	0.48	1/65013 (0.0%)	0.74	10/88431 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1115	TYR	CA-C	7.32	1.72	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	1165	ASN	C-N-CA	7.25	137.53	122.30
2	H	989	SER	CA-CB-OG	-5.95	95.13	111.20
2	D	530	TRP	N-CA-C	-5.77	95.43	111.00
1	G	367	SER	C-N-CA	5.75	136.09	121.70
2	B	856	SER	C-N-CA	5.64	135.79	121.70

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	6013	0	5805	61	0
1	C	5999	0	5794	71	0
1	E	6017	0	5809	62	0
1	G	6023	0	5814	90	0
2	B	9938	0	9645	145	0
2	D	9918	0	9631	163	0
2	F	9822	0	9548	155	0
2	H	9798	0	9529	199	0
3	A	62	0	0	0	0
3	B	121	0	0	2	0
3	C	87	0	0	0	0
3	D	137	0	0	5	0
3	E	69	0	0	0	0
3	F	70	0	0	1	0
3	G	49	0	0	0	0
3	H	58	0	0	2	0
All	All	64181	0	61575	915	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 7.

The worst 5 of 915 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:G:812:ASP:OD2	1:G:815:LEU:CD1	1.72	1.35
1:G:255:VAL:HG23	1:G:726:GLN:HB3	1.19	1.11
1:G:812:ASP:OD2	1:G:815:LEU:HD13	1.36	1.09
1:G:812:ASP:OD2	1:G:815:LEU:HD12	1.54	1.06
1:G:460:GLN:CA	2:H:812:ASN:HD21	1.68	1.05

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	773/802 (96%)	717 (93%)	50 (6%)	6 (1%)	19	29
1	C	771/802 (96%)	715 (93%)	48 (6%)	8 (1%)	15	23
1	E	777/802 (97%)	710 (91%)	60 (8%)	7 (1%)	17	26
1	G	778/802 (97%)	719 (92%)	50 (6%)	9 (1%)	13	19
2	B	1256/1334 (94%)	1162 (92%)	87 (7%)	7 (1%)	25	37
2	D	1253/1334 (94%)	1157 (92%)	84 (7%)	12 (1%)	15	23
2	F	1234/1334 (92%)	1139 (92%)	80 (6%)	15 (1%)	13	19
2	H	1231/1334 (92%)	1125 (91%)	91 (7%)	15 (1%)	13	19
All	All	8073/8544 (94%)	7444 (92%)	550 (7%)	79 (1%)	15	23

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	THR
1	A	367	SER
1	C	368	THR
2	D	618	GLY
2	D	1157	THR

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	685/701 (98%)	615 (90%)	70 (10%)	7	10
1	C	683/701 (97%)	616 (90%)	67 (10%)	8	11
1	E	684/701 (98%)	612 (90%)	72 (10%)	7	10
1	G	685/701 (98%)	624 (91%)	61 (9%)	9	14
2	B	1112/1171 (95%)	955 (86%)	157 (14%)	3	4
2	D	1109/1171 (95%)	949 (86%)	160 (14%)	3	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	1097/1171 (94%)	938 (86%)	159 (14%)	3	3
2	H	1093/1171 (93%)	951 (87%)	142 (13%)	4	5
All	All	7148/7488 (96%)	6260 (88%)	888 (12%)	4	6

5 of 888 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	974	THR
1	E	419	SER
2	H	768	LEU
2	D	1059	GLN
2	D	1341	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 188 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	631	ASN
1	E	454	ASN
2	H	634	ASN
2	D	728	GLN
2	D	1119	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	781/802 (97%)	-0.55	6 (0%) 86 85	8, 29, 71, 112	0
1	C	779/802 (97%)	-0.55	6 (0%) 86 85	9, 28, 73, 99	0
1	E	783/802 (97%)	-0.58	6 (0%) 86 85	7, 29, 68, 109	0
1	G	784/802 (97%)	-0.53	7 (0%) 84 83	8, 32, 69, 105	0
2	B	1268/1334 (95%)	-0.51	5 (0%) 92 93	7, 29, 76, 130	0
2	D	1265/1334 (94%)	-0.57	7 (0%) 89 89	6, 27, 73, 118	0
2	F	1250/1334 (93%)	-0.19	42 (3%) 45 41	9, 44, 103, 136	0
2	H	1247/1334 (93%)	-0.03	46 (3%) 41 38	14, 55, 115, 149	0
All	All	8157/8544 (95%)	-0.41	125 (1%) 73 71	6, 34, 91, 149	0

The worst 5 of 125 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	856	SER	7.1
1	A	367	SER	6.8
2	F	1265	PHE	6.1
2	H	855	ASN	6.0
2	H	1294	GLY	6.0

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.