



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:14 AM UTC

PDB ID : 6SE5 / pdb_00006se5
Title : Y830A mutant from Mycoplasma genitalium P110 adhesin
Authors : Fita, I.; Aparicio, D.
Deposited on : 2019-07-29
Resolution : 2.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

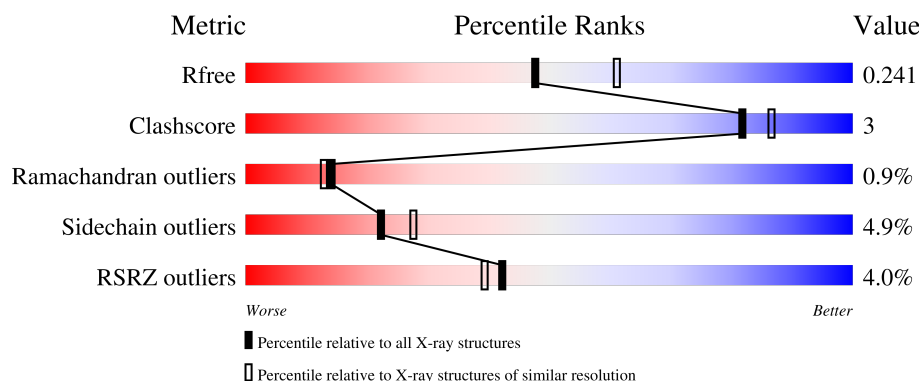
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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 $\leq 5\%$. 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	923	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7104 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	885	Total	C	N	O	S	0	1	0
			6812	4273	1137	1396	6			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	830	ALA	TYR	engineered mutation	UNP P22747
A	939	HIS	-	expression tag	UNP P22747
A	940	HIS	-	expression tag	UNP P22747
A	941	HIS	-	expression tag	UNP P22747
A	942	HIS	-	expression tag	UNP P22747
A	943	HIS	-	expression tag	UNP P22747
A	944	HIS	-	expression tag	UNP P22747

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		

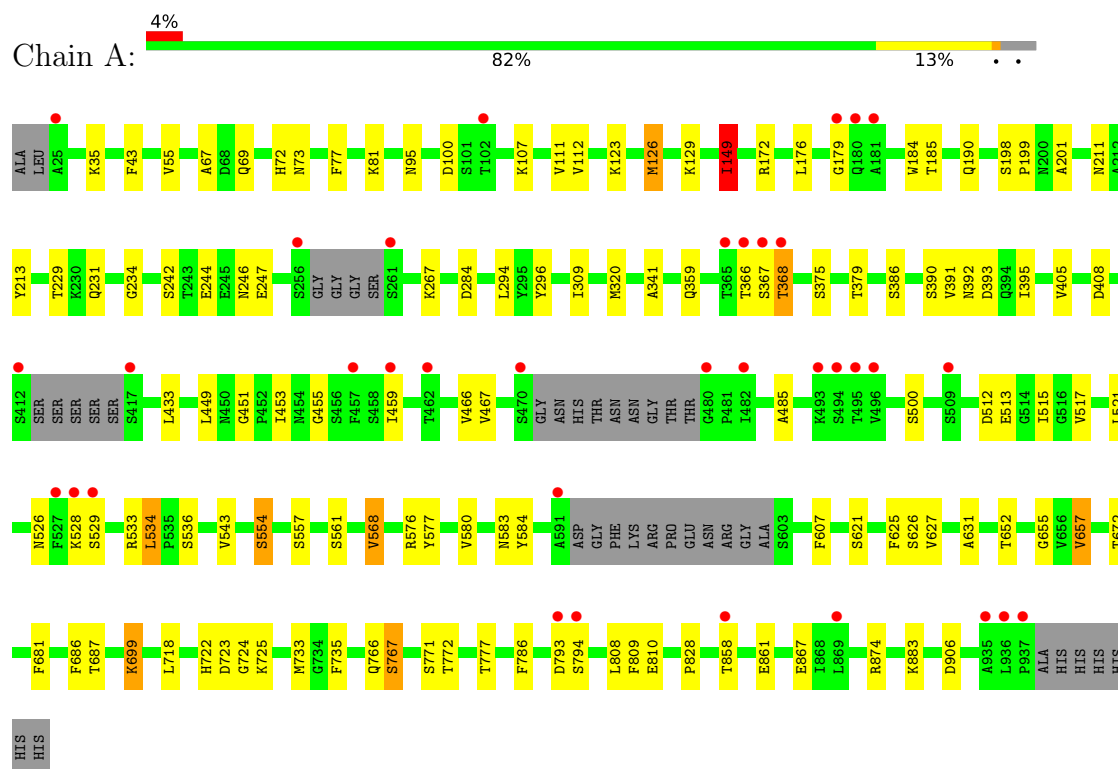
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	291	Total	O	0	0
			291	291		

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



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	109.32Å 153.12Å 169.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.30 – 2.21 32.30 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.8 (32.30-2.21) 98.7 (32.30-2.21)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.192 , 0.227 0.205 , 0.241	Depositor DCC
R_{free} test set	3571 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7104	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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](#)

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

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	0.85	1/6954 (0.0%)	1.26	33/9459 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	MET	SD-CE	-8.96	1.57	1.79

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	686	PHE	CA-CB-CG	8.18	121.97	113.80
1	A	766	GLN	CA-C-N	7.74	136.32	121.54
1	A	766	GLN	C-N-CA	7.74	136.32	121.54
1	A	722	HIS	CA-C-N	7.43	134.18	120.95
1	A	722	HIS	C-N-CA	7.43	134.18	120.95
1	A	657	VAL	N-CA-CB	6.53	118.83	110.99
1	A	625	PHE	CA-CB-CG	6.50	120.30	113.80
1	A	73	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	681	PHE	CA-CB-CG	5.75	119.55	113.80
1	A	95	ASN	CA-C-N	5.68	127.83	120.44
1	A	95	ASN	C-N-CA	5.68	127.83	120.44
1	A	100	ASP	CA-C-N	5.67	127.88	120.28
1	A	100	ASP	C-N-CA	5.67	127.88	120.28
1	A	244	GLU	CB-CG-CD	5.54	122.02	112.60
1	A	246	ASN	CA-C-N	5.46	127.54	120.44
1	A	246	ASN	C-N-CA	5.46	127.54	120.44
1	A	687	THR	N-CA-C	-5.44	101.95	110.17
1	A	607	PHE	CA-CB-CG	5.43	119.23	113.80
1	A	149	ILE	CB-CA-C	5.42	118.24	110.33
1	A	584	TYR	N-CA-C	-5.40	106.37	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	SER	CA-C-N	5.37	131.80	121.54
1	A	367	SER	C-N-CA	5.37	131.80	121.54
1	A	408	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	536	SER	N-CA-C	-5.31	102.66	110.52
1	A	724	GLY	N-CA-C	-5.27	108.87	114.67
1	A	777	THR	N-CA-C	-5.27	105.92	112.93
1	A	655	GLY	N-CA-C	5.21	118.30	110.18
1	A	786	PHE	N-CA-C	5.18	117.26	109.23
1	A	906	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	526	ASN	CA-CB-CG	5.15	117.75	112.60
1	A	583	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	513	GLU	CA-C-N	5.02	126.41	120.14
1	A	513	GLU	C-N-CA	5.02	126.41	120.14

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	6812	0	6598	34	0
2	A	1	0	0	0	0
3	A	291	0	0	0	0
All	All	7104	0	6598	34	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 3.

All (34) 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:A:554:SER:HB2	1:A:568:VAL:HG13	1.59	0.84
1:A:391:VAL:CG2	1:A:631:ALA:HB1	2.32	0.59
1:A:294:LEU:HD13	1:A:320:MET:HE2	1.85	0.58
1:A:231:GLN:HG2	1:A:267:LYS:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:TRP:CD2	1:A:199:PRO:HB3	2.43	0.54
1:A:392[A]:ASN:CG	1:A:393:ASP:H	2.16	0.53
1:A:111:VAL:HG11	1:A:309:ILE:HG21	1.92	0.51
1:A:126:MET:HE1	1:A:129:LYS:HD2	1.92	0.51
1:A:390:SER:HB3	1:A:395:ILE:HD13	1.94	0.49
1:A:528:LYS:HD3	1:A:529:SER:H	1.76	0.49
1:A:72:HIS:HB3	1:A:77:PHE:CE1	2.47	0.49
1:A:126:MET:HE2	1:A:129:LYS:HB2	1.96	0.47
1:A:580:VAL:HG21	1:A:621:SER:O	2.15	0.46
1:A:723:ASP:HB3	1:A:725:LYS:H	1.82	0.45
1:A:35:LYS:HG2	1:A:55:VAL:HG21	1.99	0.45
1:A:517:VAL:O	1:A:521:LEU:HG	2.17	0.45
1:A:626:SER:HB3	1:A:652:THR:HG22	1.99	0.44
1:A:211:ASN:O	1:A:234:GLY:HA2	2.18	0.44
1:A:433:LEU:HD23	1:A:534:LEU:HD21	2.00	0.43
1:A:341:ALA:O	1:A:379:THR:HG22	2.18	0.43
1:A:858:THR:HG23	1:A:861:GLU:H	1.83	0.43
1:A:767:SER:O	1:A:809:PHE:HB2	2.19	0.43
1:A:172:ARG:HG3	1:A:176:LEU:HD12	2.00	0.43
1:A:451:GLY:HA3	1:A:485:ALA:O	2.19	0.43
1:A:81:LYS:HE3	1:A:296:TYR:CE2	2.54	0.42
1:A:198:SER:HB3	1:A:201:ALA:HB2	2.02	0.41
1:A:43:PHE:HB3	1:A:828:PRO:HD3	2.03	0.41
1:A:699:LYS:HE2	1:A:718:LEU:HD11	2.02	0.41
1:A:67:ALA:HB2	1:A:81:LYS:HD3	2.03	0.41
1:A:533:ARG:HD3	1:A:577:TYR:HE2	1.85	0.41
1:A:735:PHE:CE2	1:A:771:SER:HB3	2.56	0.41
1:A:359:GLN:HG2	1:A:405:VAL:HG12	2.02	0.40
1:A:149:ILE:HG23	1:A:213:TYR:HB3	2.04	0.40
1:A:112:VAL:HG22	1:A:129:LYS:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	876/923 (95%)	837 (96%)	31 (4%)	8 (1%)	14	13

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	GLY
1	A	512	ASP
1	A	767	SER
1	A	284	ASP
1	A	368	THR
1	A	453	ILE
1	A	794	SER
1	A	455	GLY

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	774/801 (97%)	736 (95%)	38 (5%)	22	27

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	107	LYS
1	A	123	LYS
1	A	149	ILE
1	A	185	THR
1	A	190	GLN
1	A	229	THR
1	A	242	SER
1	A	247	GLU
1	A	366	THR
1	A	368	THR

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Mol	Chain	Res	Type
1	A	375	SER
1	A	386	SER
1	A	449	LEU
1	A	459	ILE
1	A	466	VAL
1	A	467	VAL
1	A	500	SER
1	A	515	ILE
1	A	534	LEU
1	A	543	VAL
1	A	554	SER
1	A	557	SER
1	A	561	SER
1	A	568	VAL
1	A	576	ARG
1	A	627	VAL
1	A	657	VAL
1	A	672	THR
1	A	699	LYS
1	A	733	MET
1	A	772	THR
1	A	793	ASP
1	A	808	LEU
1	A	810	GLU
1	A	867	GLU
1	A	874	ARG
1	A	883	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	73	ASN
1	A	131	GLN
1	A	231	GLN
1	A	246	ASN
1	A	285	GLN
1	A	352	GLN
1	A	380	GLN
1	A	492	GLN
1	A	660	ASN
1	A	662	ASN

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Mol	Chain	Res	Type
1	A	674	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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, 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	885/923 (95%)	0.18	35 (3%) 42 39	52, 79, 130, 186	1 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	591	ALA	5.9
1	A	470	SER	4.6
1	A	937	PRO	4.3
1	A	459	ILE	4.3
1	A	936	LEU	4.1
1	A	935	ALA	3.9
1	A	181	ALA	3.7
1	A	256	SER	3.3
1	A	480	GLY	3.2
1	A	25	ALA	3.1
1	A	261	SER	3.0
1	A	367	SER	3.0
1	A	496	VAL	2.9
1	A	529	SER	2.9
1	A	462	THR	2.8
1	A	366	THR	2.8
1	A	412	SER	2.8
1	A	417	SER	2.7
1	A	495	THR	2.6
1	A	102	THR	2.6
1	A	527	PHE	2.5
1	A	365	THR	2.5
1	A	368	THR	2.4
1	A	793	ASP	2.4
1	A	179	GLY	2.4
1	A	493	LYS	2.3
1	A	509	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	869	LEU	2.3
1	A	482	ILE	2.2
1	A	457	PHE	2.1
1	A	494	SER	2.1
1	A	794	SER	2.1
1	A	528	LYS	2.1
1	A	858	THR	2.0
1	A	180	GLN	2.0

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	K	A	1001	1/1	0.99	0.07	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.