



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:28 pm BST

PDB ID : 5LQI
Title : W288A mutant of GlxA from Streptomyces lividans: apo form
Authors : Chaplin, A.K.; Hough, M.A.; Worrall, J.A.R.
Deposited on : 2016-08-17
Resolution : 1.92 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 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	:	2.11
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)	:	2.11

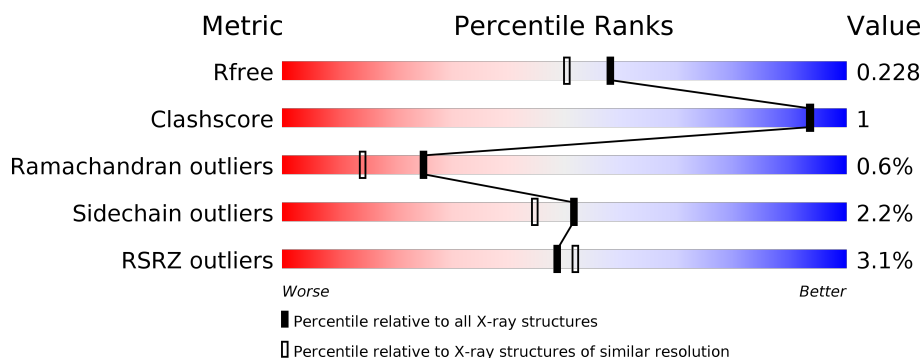
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	609	
1	B	609	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10008 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 Secreted protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	599	Total	C	N	O	S	32	2	0
			4657	2932	811	903	11			
1	B	609	Total	C	N	O	S	74	0	0
			4708	2966	816	915	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	ALA	TRP	engineered mutation	UNP D6EWM0
B	288	ALA	TRP	engineered mutation	UNP D6EWM0

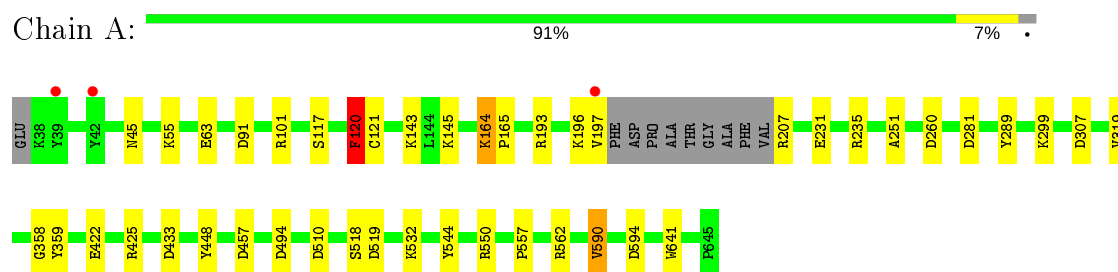
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	464	Total	O	0	2
			464	464		
2	B	179	Total	O	0	0
			179	179		

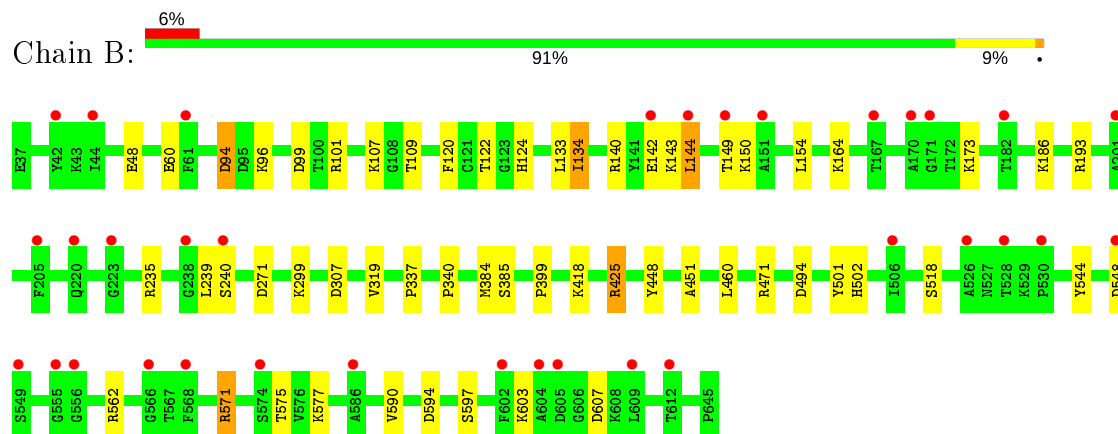
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Secreted protein



- Molecule 1: Secreted protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.54Å 126.29Å 106.94Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	35.60 – 1.92 35.61 – 1.92	Depositor EDS
% Data completeness (in resolution range)	97.4 (35.60-1.92) 97.4 (35.61-1.92)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.182 , 0.224 0.189 , 0.228	Depositor DCC
R_{free} test set	4974 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10008	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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

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	0.87	5/4761 (0.1%)	1.02	24/6446 (0.4%)
1	B	0.91	9/4815 (0.2%)	0.93	21/6525 (0.3%)
All	All	0.89	14/9576 (0.1%)	0.97	45/12971 (0.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	235	ARG	NE-CZ	33.05	1.76	1.33
1	B	48	GLU	CB-CG	-18.38	1.17	1.52
1	B	607	ASP	CB-CG	-15.95	1.18	1.51
1	B	186	LYS	CE-NZ	10.36	1.75	1.49
1	A	532	LYS	CD-CE	7.79	1.70	1.51
1	B	107	LYS	CG-CD	-7.70	1.26	1.52
1	A	63	GLU	CG-CD	-7.61	1.40	1.51
1	B	418	LYS	CG-CD	-7.56	1.26	1.52
1	B	173	LYS	CB-CG	-6.21	1.35	1.52
1	A	145	LYS	CB-CG	-5.88	1.36	1.52
1	B	143	LYS	CA-CB	5.79	1.66	1.53
1	A	143	LYS	CG-CD	-5.63	1.33	1.52
1	B	96	LYS	C-O	5.29	1.33	1.23
1	A	422	GLU	CD-OE1	5.06	1.31	1.25

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	603	LYS	CB-CG-CD	14.18	148.48	111.60
1	B	164	LYS	CB-CG-CD	13.53	146.78	111.60
1	A	164	LYS	CB-CG-CD	12.74	144.74	111.60
1	B	235	ARG	NE-CZ-NH1	-11.15	114.72	120.30
1	A	562	ARG	NE-CZ-NH1	10.99	125.80	120.30
1	A	120[A]	PHE	C-N-CA	9.84	146.31	121.70
1	A	120[B]	PHE	C-N-CA	9.84	146.31	121.70
1	B	425	ARG	NE-CZ-NH1	9.21	124.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	607	ASP	CB-CG-OD2	9.18	126.56	118.30
1	B	235	ARG	NE-CZ-NH2	8.73	124.67	120.30
1	B	48	GLU	CA-CB-CG	8.61	132.33	113.40
1	B	607	ASP	CB-CG-OD1	-8.30	110.83	118.30
1	A	235	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	A	562	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	B	607	ASP	CA-CB-CG	7.79	130.54	113.40
1	A	235	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	B	150	LYS	CA-CB-CG	6.96	128.71	113.40
1	B	577	LYS	CA-CB-CG	6.89	128.55	113.40
1	B	425	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	B	186	LYS	CD-CE-NZ	-6.81	96.04	111.70
1	A	101	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	519	ASP	CB-CG-OD1	6.77	124.39	118.30
1	A	494	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	B	562	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	457	ASP	CB-CG-OD1	6.45	124.10	118.30
1	A	307	ASP	CB-CG-OD1	6.23	123.91	118.30
1	B	164	LYS	CG-CD-CE	6.21	130.53	111.90
1	B	101	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	494	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	510	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	193	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	143	LYS	CB-CG-CD	5.64	126.28	111.60
1	A	63	GLU	CG-CD-OE1	5.59	129.47	118.30
1	A	164	LYS	CG-CD-CE	5.55	128.55	111.90
1	B	193	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	134	ILE	CB-CA-C	5.38	122.35	111.60
1	A	63	GLU	CG-CD-OE2	-5.36	107.57	118.30
1	A	260	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	A	281	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	145	LYS	CA-CB-CG	5.25	124.95	113.40
1	B	494	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	91	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	550	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	271	ASP	CB-CG-OD1	5.06	122.85	118.30
1	B	307	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

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	4657	0	4596	11	0
1	B	4708	0	4641	15	0
2	A	464	0	0	0	0
2	B	179	0	0	0	0
All	All	10008	0	9237	26	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 1.

All (26) 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:B:571:ARG:HH21	1:B:571:ARG:HG2	1.26	0.98
1:B:94:ASP:OD1	1:B:140:ARG:NH2	2.10	0.85
1:B:384:MET:SD	1:B:425:ARG:HD2	2.20	0.80
1:A:45:ASN:OD1	1:A:55:LYS:HE3	1.90	0.72
1:B:571:ARG:CG	1:B:571:ARG:HH21	2.04	0.70
1:A:45:ASN:OD1	1:A:55:LYS:CE	2.46	0.63
1:A:120[A]:PHE:C	1:A:120[A]:PHE:CD1	2.79	0.55
1:B:571:ARG:HG2	1:B:571:ARG:NH2	2.06	0.55
1:A:164:LYS:HG2	1:A:165:PRO:O	2.08	0.53
1:A:299:LYS:HB3	1:A:319:VAL:CG1	2.43	0.48
1:B:451:ALA:HA	1:B:460:LEU:O	2.13	0.48
1:B:571:ARG:CG	1:B:571:ARG:NH2	2.68	0.47
1:B:144:LEU:HD11	1:B:154:LEU:CD1	2.44	0.47
1:B:122:THR:HG21	1:B:134:ILE:HD11	1.97	0.46
1:B:399:PRO:HB3	1:B:597:SER:HB3	1.97	0.46
1:A:358:GLY:O	1:A:359:TYR:HB2	2.16	0.45
1:B:299:LYS:HB3	1:B:319:VAL:CG1	2.47	0.45
1:A:196:LYS:O	1:A:197:VAL:C	2.56	0.44
1:A:231:GLU:HA	1:A:251:ALA:O	2.19	0.43
1:A:121:CYS:HB2	1:A:289:TYR:CD1	2.54	0.42
1:B:337:PRO:O	1:B:340:PRO:HD3	2.20	0.42
1:A:196:LYS:O	1:A:207:ARG:O	2.37	0.41
1:A:557:PRO:HA	1:A:641:TRP:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:HIS:HA	1:B:133:LEU:O	2.20	0.41
1:B:385:SER:O	1:B:425:ARG:HD3	2.21	0.41
1:B:501:TYR:CE2	1:B:502:HIS:CE1	3.10	0.40

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	597/609 (98%)	578 (97%)	16 (3%)	3 (0%)	29	18
1	B	607/609 (100%)	576 (95%)	27 (4%)	4 (1%)	22	11
All	All	1204/1218 (99%)	1154 (96%)	43 (4%)	7 (1%)	25	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	SER
1	B	518	SER
1	B	448	TYR
1	A	448	TYR
1	B	240	SER
1	A	590	VAL
1	B	590	VAL

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	499/504 (99%)	491 (98%)	8 (2%)	62	58
1	B	504/504 (100%)	489 (97%)	15 (3%)	41	31
All	All	1003/1008 (100%)	980 (98%)	23 (2%)	52	43

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	SER
1	A	120[A]	PHE
1	A	120[B]	PHE
1	A	425	ARG
1	A	433	ASP
1	A	544	TYR
1	A	590	VAL
1	A	594	ASP
1	B	60	GLU
1	B	94	ASP
1	B	99	ASP
1	B	109	THR
1	B	120	PHE
1	B	142	GLU
1	B	144	LEU
1	B	149	THR
1	B	239	LEU
1	B	471	ARG
1	B	544	TYR
1	B	548	ASP
1	B	571	ARG
1	B	575	THR
1	B	594	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	89	ASN

5.3.3 RNA ⓘ

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 ⓘ

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	599/609 (98%)	-0.18	3 (0%) 91 92	12, 23, 39, 61	34 (5%)
1	B	609/609 (100%)	0.32	34 (5%) 24 27	21, 43, 71, 86	63 (10%)
All	All	1208/1218 (99%)	0.07	37 (3%) 49 52	12, 31, 66, 86	97 (8%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	238	GLY	4.3
1	A	197	VAL	4.3
1	B	149	THR	4.1
1	B	566	GLY	4.1
1	B	220	GLN	3.6
1	B	604	ALA	3.5
1	B	568	PHE	3.0
1	B	42	TYR	3.0
1	B	586	ALA	3.0
1	B	223	GLY	2.9
1	B	240	SER	2.9
1	A	39	TYR	2.9
1	A	42	TYR	2.9
1	B	526	ALA	2.7
1	B	170	ALA	2.7
1	B	528	THR	2.6
1	B	151	ALA	2.6
1	B	602	PHE	2.5
1	B	201	ALA	2.5
1	B	574	SER	2.5
1	B	556	GLY	2.4
1	B	144	LEU	2.4
1	B	530	PRO	2.4
1	B	142	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	605	ASP	2.3
1	B	549	SER	2.3
1	B	548	ASP	2.3
1	B	609	LEU	2.2
1	B	205	PHE	2.2
1	B	44	ILE	2.2
1	B	182	THR	2.2
1	B	61	PHE	2.1
1	B	555	GLY	2.1
1	B	167	THR	2.1
1	B	506	ILE	2.1
1	B	612	THR	2.0
1	B	171	GLY	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.