



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:19 am GMT

PDB ID : 4OLS
Title : The amidase-2 domain of LysGH15
Authors : Gu, J.; Ouyang, S.; Liu, Z.J.; Han, W.
Deposited on : 2014-01-24
Resolution : 2.27 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

<http://wwpdb.org/validation/2016/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) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

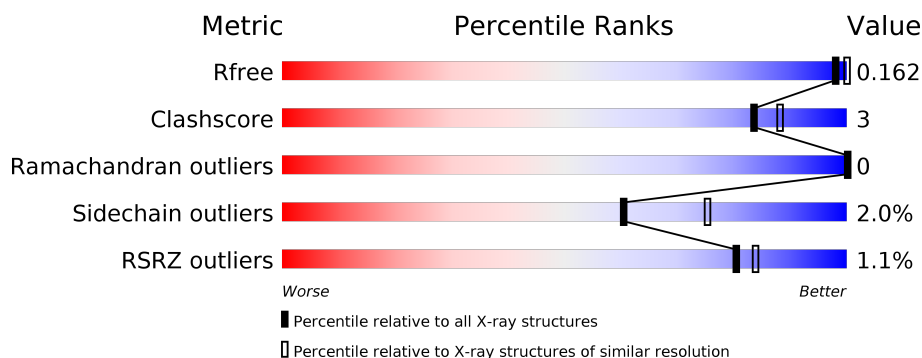
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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}	100719	5609 (2.30-2.26)
Clashscore	112137	6364 (2.30-2.26)
Ramachandran outliers	110173	6281 (2.30-2.26)
Sidechain outliers	110143	6281 (2.30-2.26)
RSRZ outliers	101464	5639 (2.30-2.26)

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. 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	242	<div> <div style="width: 72%;"></div> <div style="width: 24%;"></div> <div style="width: 4%;"></div> </div>
1	B	242	<div> <div style="width: 2%;"></div> <div style="width: 66%;"></div> <div style="width: 10%;"></div> <div style="width: 24%;"></div> </div>
1	C	242	<div> <div style="width: 0%;"></div> <div style="width: 69%;"></div> <div style="width: 7%;"></div> <div style="width: 24%;"></div> </div>
1	D	242	<div> <div style="width: 71%;"></div> <div style="width: 6%;"></div> <div style="width: 24%;"></div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	B	502	-	-	-	X
2	ZN	C	505	-	-	-	X
2	ZN	D	501	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6551 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 Endolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	1	0
			1473	927	266	271	9			
1	B	185	Total	C	N	O	S	0	1	0
			1473	927	266	271	9			
1	C	185	Total	C	N	O	S	0	1	0
			1473	927	266	271	9			
1	D	185	Total	C	N	O	S	0	1	0
			1473	927	266	271	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	SER	-	EXPRESSION TAG	UNP D6QY02
A	163	ASN	-	EXPRESSION TAG	UNP D6QY02
A	164	ALA	-	EXPRESSION TAG	UNP D6QY02
B	162	SER	-	EXPRESSION TAG	UNP D6QY02
B	163	ASN	-	EXPRESSION TAG	UNP D6QY02
B	164	ALA	-	EXPRESSION TAG	UNP D6QY02
C	162	SER	-	EXPRESSION TAG	UNP D6QY02
C	163	ASN	-	EXPRESSION TAG	UNP D6QY02
C	164	ALA	-	EXPRESSION TAG	UNP D6QY02
D	162	SER	-	EXPRESSION TAG	UNP D6QY02
D	163	ASN	-	EXPRESSION TAG	UNP D6QY02
D	164	ALA	-	EXPRESSION TAG	UNP D6QY02

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Zn	0	0
			5	5		
2	A	4	Total	Zn	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	3	Total	Zn	0	0
			3	3		
2	C	5	Total	Zn	0	0
			5	5		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		

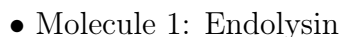
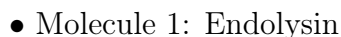
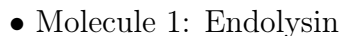
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Fe	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	177	Total	O	0	0
			177	177		
5	B	116	Total	O	0	0
			116	116		
5	C	167	Total	O	0	0
			167	167		
5	D	180	Total	O	0	0
			180	180		

- Molecule 1: Endolysin



SER	SER	SER	THR	VAL	LYS	ASP	GLY	LYS	THR	SER	SER	ALA	SER	THR	PRO	ALA	THR	ARG	PRO	VAL	THR	GLY	SER	TRP	LYS	LYS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	135.40Å 135.40Å 107.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.57 – 2.27 39.54 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.57-2.27) 99.8 (39.54-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	18.73 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.158 , 0.161 0.157 , 0.162	Depositor DCC
R_{free} test set	2595 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6551	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, FE

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	0.50	0/1512	0.54	0/2035
1	B	0.44	0/1512	0.50	0/2035
1	C	0.50	1/1512 (0.1%)	0.52	1/2035 (0.0%)
1	D	0.48	0/1512	0.56	0/2035
All	All	0.48	1/6048 (0.0%)	0.53	1/8140 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	351	PRO	N-CD	5.11	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	350	ARG	C-N-CD	5.40	139.74	128.40

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	1473	0	1427	4	0
1	B	1473	0	1427	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1473	0	1427	7	0
1	D	1473	0	1427	8	0
2	A	4	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	3	0	0	0	0
3	D	1	0	0	0	0
4	D	1	0	0	0	0
5	A	177	0	0	0	0
5	B	116	0	0	2	0
5	C	167	0	0	0	1
5	D	180	0	0	1	1
All	All	6551	0	5708	32	1

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 (32) 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:316:PRO:HG2	1:B:368:LYS:HG3	1.69	0.74
1:D:228:SER:OG	1:D:236:ARG:NH1	2.27	0.68
1:B:200:THR:OG1	5:B:692:HOH:O	2.15	0.65
1:C:372:ASP:O	1:C:373:LYS:HB2	1.98	0.62
1:D:330:THR:HG23	1:D:332:CYS:H	1.65	0.60
1:C:201:MET:HG3	1:C:255:ILE:HD13	1.85	0.58
1:C:328:VAL:HG23	1:C:330:THR:HG23	1.87	0.56
1:C:316:PRO:HG2	1:C:368:LYS:HG3	1.89	0.55
1:B:220:SER:O	1:B:284:CYS:HB3	2.10	0.51
1:D:228:SER:HG	1:D:236:ARG:HH12	1.55	0.51
1:D:220:SER:O	1:D:284:CYS:HB3	2.11	0.51
1:B:225:TYR:O	1:B:229:LEU:HB2	2.11	0.51
1:A:220:SER:O	1:A:284:CYS:HB3	2.12	0.50
1:B:223:GLN:HG2	1:B:250:TYR:CZ	2.47	0.49
1:A:372:ASP:O	1:A:373:LYS:HB2	2.13	0.49
1:C:220:SER:O	1:C:284:CYS:HB3	2.13	0.48
1:B:312:TRP:O	5:B:680:HOH:O	2.20	0.47
1:C:306:ALA:HB1	1:C:371:MET:HG3	1.98	0.46
1:D:223:GLN:HG2	1:D:250:TYR:CZ	2.53	0.44
1:B:201:MET:HG3	1:B:255:ILE:HD13	1.99	0.43
1:B:214:HIS:HB2	1:B:282:GLU:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:MET:HG3	1:D:255:ILE:HD13	2.01	0.42
1:B:283:VAL:HG22	1:B:301:VAL:HG21	2.01	0.42
1:D:236:ARG:NE	5:D:701:HOH:O	2.32	0.41
1:A:225:TYR:O	1:A:229:LEU:HB2	2.21	0.41
1:D:220:SER:HB2	1:D:225:TYR:CZ	2.55	0.41
1:B:330:THR:HG23	1:B:332:CYS:H	1.86	0.41
1:B:191:LYS:HE2	1:B:191:LYS:HB2	1.82	0.41
1:C:204:ARG:HD2	1:C:206:LYS:O	2.20	0.41
1:A:328:VAL:HG23	1:A:330:THR:HG23	2.03	0.41
1:B:334:HIS:CG	1:B:335:ARG:N	2.89	0.41
1:B:350:ARG:HG3	1:B:351:PRO:HD2	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:766:HOH:O	5:D:766:HOH:O[4_655]	1.94	0.26

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	184/242 (76%)	178 (97%)	6 (3%)	0	100	100
1	B	184/242 (76%)	177 (96%)	7 (4%)	0	100	100
1	C	184/242 (76%)	178 (97%)	6 (3%)	0	100	100
1	D	184/242 (76%)	179 (97%)	5 (3%)	0	100	100
All	All	736/968 (76%)	712 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	153/197 (78%)	150 (98%)	3 (2%)	60	75
1	B	153/197 (78%)	148 (97%)	5 (3%)	43	57
1	C	153/197 (78%)	151 (99%)	2 (1%)	73	85
1	D	153/197 (78%)	150 (98%)	3 (2%)	60	75
All	All	612/788 (78%)	599 (98%)	13 (2%)	60	73

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	SER
1	A	229	LEU
1	A	324	HIS
1	B	229	LEU
1	B	272	ASN
1	B	310	LYS
1	B	365[A]	LYS
1	B	365[B]	LYS
1	C	229	LEU
1	C	324	HIS
1	D	229	LEU
1	D	269	THR
1	D	368	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 19 ligands modelled in this entry, 19 are 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 [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	185/242 (76%)	-0.65	0 100 100	20, 30, 48, 76	0
1	B	185/242 (76%)	-0.29	4 (2%) 62 68	28, 41, 65, 108	0
1	C	185/242 (76%)	-0.49	3 (1%) 72 77	23, 33, 52, 89	0
1	D	185/242 (76%)	-0.63	1 (0%) 90 93	21, 31, 49, 88	0
All	All	740/968 (76%)	-0.52	8 (1%) 80 84	20, 33, 58, 108	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	372	ASP	3.2
1	B	205	GLY	3.0
1	B	373	LYS	2.6
1	D	372	ASP	2.5
1	C	373	LYS	2.4
1	C	372	ASP	2.4
1	B	189	THR	2.1
1	C	189	THR	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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	C	505	1/1	0.98	0.34	8.45	225,225,225,225	0
2	ZN	D	501	1/1	0.96	0.19	5.13	112,112,112,112	0
2	ZN	B	502	1/1	0.83	0.12	2.02	126,126,126,126	0
3	MG	D	504	1/1	1.00	0.12	1.91	18,18,18,18	0
4	FE	D	505	1/1	0.99	0.10	1.63	19,19,19,19	1
2	ZN	C	504	1/1	0.95	0.06	-	82,82,82,82	0
2	ZN	B	504	1/1	0.88	0.10	-	107,107,107,107	0
2	ZN	B	501	1/1	0.99	0.05	-	42,42,42,42	1
2	ZN	A	504	1/1	0.97	0.04	-	82,82,82,82	0
2	ZN	D	503	1/1	0.98	0.10	-	31,31,31,31	1
2	ZN	C	503	1/1	0.80	0.06	-	105,105,105,105	0
2	ZN	A	501	1/1	0.98	0.08	-	35,35,35,35	1
2	ZN	C	501	1/1	0.99	0.09	-	32,32,32,32	1
2	ZN	C	502	1/1	0.99	0.05	-	78,78,78,78	0
2	ZN	B	503	1/1	0.85	0.08	-	116,116,116,116	0
2	ZN	D	502	1/1	0.93	0.04	-	82,82,82,82	0
2	ZN	A	502	1/1	0.98	0.07	-	78,78,78,78	0
2	ZN	A	503	1/1	0.96	0.05	-	74,74,74,74	0
2	ZN	B	505	1/1	0.92	0.08	-	113,113,113,113	0

6.5 Other polymers

There are no such residues in this entry.