



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 01:31 am BST

PDB ID : 6N8Q
Title : Crystal structure of the human cell polarity protein Lethal Giant Larvae 2 (Lgl2). Unphosphorylated, crystal form 2.
Authors : Almagor, L.; Weis, W.I.
Deposited on : 2018-11-30
Resolution : 2.20 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

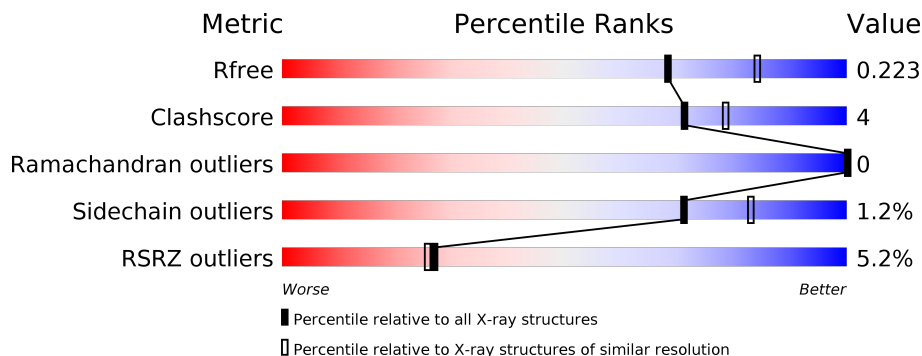
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	979	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6680 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 Lethal(2) giant larvae protein homolog 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	829	6450	4123	1127	1176	24	0	1	0

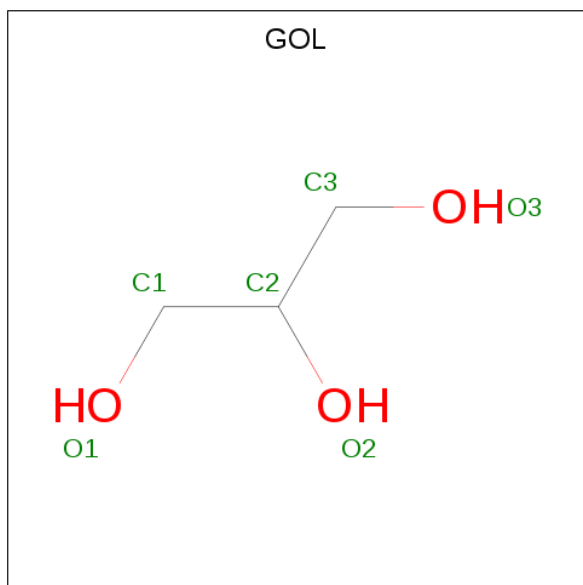
There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP Q6P1M3
A	979	GLU	-	expression tag	UNP Q6P1M3
A	980	PHE	-	expression tag	UNP Q6P1M3
A	981	THR	-	expression tag	UNP Q6P1M3
A	982	THR	-	expression tag	UNP Q6P1M3
A	983	ALA	-	expression tag	UNP Q6P1M3
A	984	SER	-	expression tag	UNP Q6P1M3
A	985	GLU	-	expression tag	UNP Q6P1M3
A	986	ASN	-	expression tag	UNP Q6P1M3
A	987	LEU	-	expression tag	UNP Q6P1M3
A	988	TYR	-	expression tag	UNP Q6P1M3
A	989	PHE	-	expression tag	UNP Q6P1M3
A	990	GLN	-	expression tag	UNP Q6P1M3

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0

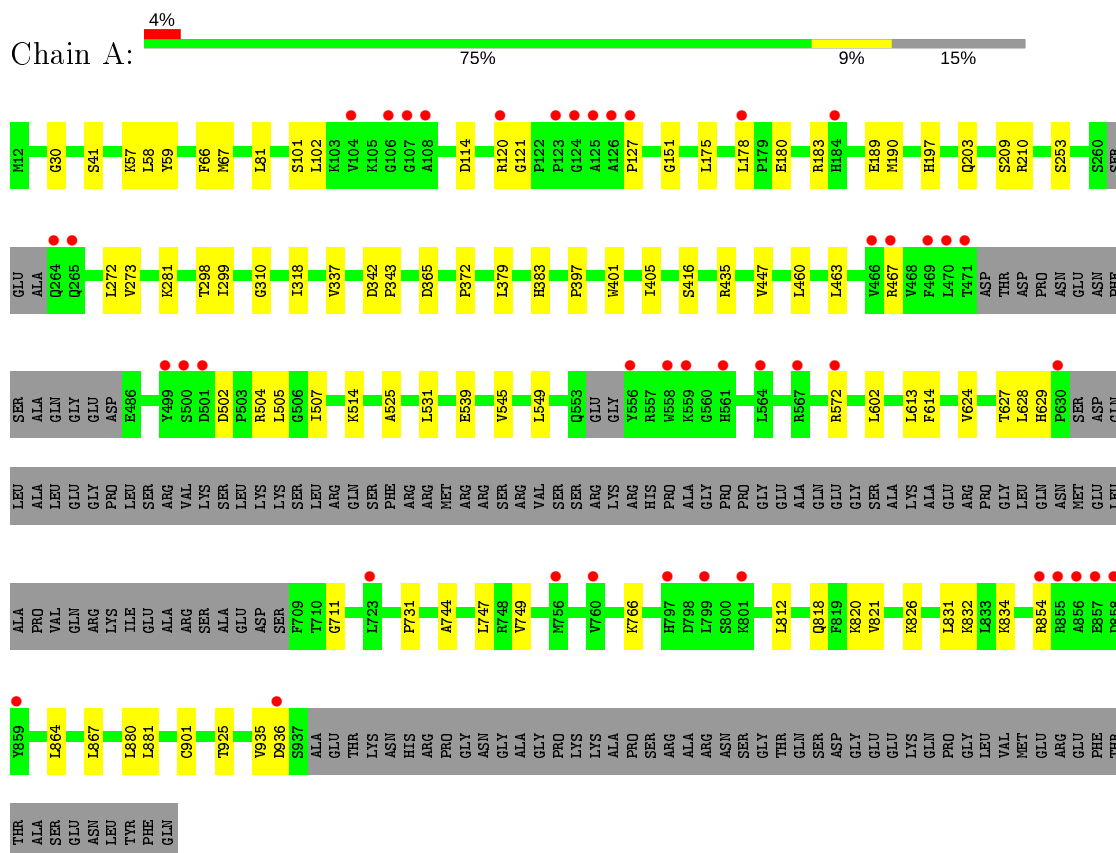
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	223	Total O 223 223	0	0

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: Lethal(2) giant larvae protein homolog 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.53Å 46.76Å 137.69Å 90.00° 116.00° 90.00°	Depositor
Resolution (Å)	39.22 – 2.20 39.22 – 2.20	Depositor EDS
% Data completeness (in resolution range)	66.5 (39.22-2.20) 66.6 (39.22-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.206 , 0.226 0.203 , 0.223	Depositor DCC
R_{free} test set	1706 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtrriage
Anisotropy	0.142	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6680	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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: GOL, CL

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	0.25	0/6618	0.45	0/9021

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	6450	0	6312	45	0
2	A	1	0	0	0	0
3	A	6	0	8	2	0
4	A	223	0	0	0	0
All	All	6680	0	6320	45	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 4.

All (45) 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:30:GLY:H	3:A:1002:GOL:H32	1.31	0.94
1:A:379:LEU:H	3:A:1002:GOL:H31	1.52	0.75
1:A:281:LYS:HD2	1:A:310:GLY:HA2	1.72	0.71
1:A:504:ARG:HB2	1:A:525:ALA:HB2	1.78	0.65
1:A:447:VAL:HG23	1:A:507:ILE:HD13	1.80	0.63
1:A:854:ARG:HD3	1:A:925:THR:HB	1.81	0.62
1:A:463:LEU:HD11	1:A:531:LEU:HD22	1.83	0.61
1:A:731:PRO:HB2	1:A:747:LEU:HB2	1.83	0.61
1:A:102:LEU:HD13	1:A:935:VAL:HG21	1.82	0.60
1:A:744:ALA:HB3	1:A:766:LYS:HB2	1.84	0.60
1:A:821:VAL:HG23	1:A:881:LEU:HD11	1.87	0.57
1:A:549:LEU:HD23	1:A:624:VAL:HG13	1.87	0.56
1:A:627:THR:O	1:A:711:GLY:HA3	2.05	0.56
1:A:299:ILE:HD13	1:A:337:VAL:HG21	1.87	0.56
1:A:58:LEU:HB2	1:A:66:PHE:HB2	1.88	0.56
1:A:151:GLY:HA3	1:A:189:GLU:HB2	1.86	0.56
1:A:405:ILE:HG12	1:A:460:LEU:HD22	1.89	0.54
1:A:175:LEU:HA	1:A:178:LEU:HD12	1.89	0.54
1:A:298:THR:HB	1:A:318:ILE:HB	1.92	0.52
1:A:253:SER:HB3	1:A:273:VAL:HG22	1.90	0.52
1:A:101:SER:HB2	1:A:114:ASP:OD2	2.10	0.52
1:A:180:GLU:HA	1:A:183:ARG:HD2	1.92	0.51
1:A:602:LEU:HB3	1:A:613:LEU:HD11	1.92	0.51
1:A:401:TRP:CG	1:A:435:ARG:HD2	2.47	0.50
1:A:59:TYR:CZ	1:A:379:LEU:HD21	2.46	0.49
1:A:342:ASP:HB2	1:A:343:PRO:HD2	1.94	0.48
1:A:545:VAL:HG11	1:A:614:PHE:HE1	1.79	0.48
1:A:397:PRO:HD3	1:A:514:LYS:HD2	1.96	0.48
1:A:812:LEU:HD21	1:A:864:LEU:HD11	1.96	0.48
1:A:820:LYS:HE2	1:A:832:LYS:HE2	1.95	0.47
1:A:731:PRO:HG2	1:A:749:VAL:HG12	1.97	0.46
1:A:197:HIS:HB2	1:A:203:GLN:HB2	1.99	0.45
1:A:120:ARG:HD3	1:A:121:GLY:N	2.32	0.44
1:A:190:MET:HB3	1:A:209:SER:HB2	1.99	0.44
1:A:372:PRO:HG2	1:A:416:SER:HB2	1.98	0.44
1:A:539:GLU:HG3	1:A:572:ARG:HB2	2.01	0.43
1:A:831:LEU:HD13	1:A:880:LEU:HA	1.99	0.43
1:A:41:SER:HB2	1:A:81:LEU:HD22	2.00	0.42
1:A:120:ARG:HH22	1:A:127:PRO:HB3	1.85	0.42
1:A:867:LEU:HD22	1:A:901:CYS:HB3	2.00	0.42
1:A:502:ASP:HB3	1:A:505:LEU:HD13	2.01	0.42
1:A:818:GLN:HG2	1:A:834:LYS:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:GLU:HA	1:A:572:ARG:HA	2.03	0.41
1:A:57:LYS:HE2	1:A:67:MET:HG3	2.02	0.41
1:A:365:ASP:HB3	1:A:372:PRO:HD2	2.04	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	820/979 (84%)	783 (96%)	37 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	693/837 (83%)	685 (99%)	8 (1%)	71 83

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	ARG
1	A	272	LEU
1	A	383	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	467	ARG
1	A	628	LEU
1	A	629	HIS
1	A	826	LYS
1	A	936	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	A	412	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	GOL	A	1002	-	5,5,5	0.85	0	5,5,5	1.00	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	GOL	A	1002	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	GOL	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

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	829/979 (84%)	-0.03	43 (5%) 27 26	15, 42, 88, 131	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	GLY	5.3
1	A	104	VAL	4.4
1	A	855	ARG	4.4
1	A	859	TYR	4.4
1	A	561	HIS	4.2
1	A	858	ASP	4.2
1	A	854	ARG	4.1
1	A	123	PRO	4.0
1	A	856	ALA	4.0
1	A	760	VAL	4.0
1	A	499	TYR	4.0
1	A	630	PRO	3.6
1	A	466	VAL	3.5
1	A	799	LEU	3.4
1	A	471	THR	3.2
1	A	127	PRO	3.1
1	A	556	TYR	3.0
1	A	125	ALA	3.0
1	A	264	GLN	2.9
1	A	756	MET	2.9
1	A	184	HIS	2.8
1	A	469	PHE	2.7
1	A	857	GLU	2.7
1	A	501	ASP	2.6
1	A	936	ASP	2.5
1	A	126	ALA	2.4
1	A	467	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	178	LEU	2.3
1	A	567	ARG	2.3
1	A	108	ALA	2.3
1	A	106	GLY	2.2
1	A	797	HIS	2.2
1	A	801	LYS	2.2
1	A	470	LEU	2.2
1	A	723	LEU	2.2
1	A	265	GLN	2.2
1	A	559	LYS	2.1
1	A	500	SER	2.1
1	A	564	LEU	2.1
1	A	558	TRP	2.0
1	A	107	GLY	2.0
1	A	120	ARG	2.0
1	A	572	ARG	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](#)

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(\AA^2)	Q<0.9
3	GOL	A	1002	6/6	0.92	0.16	24,26,27,28	0
2	CL	A	1001	1/1	1.00	0.28	44,44,44,44	1

6.5 Other polymers [i](#)

There are no such residues in this entry.