



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2021 – 07:04 PM EDT

PDB ID : 2HB6
Title : Structure of *Caenorhabditis elegans* leucine aminopeptidase (LAP1)
Authors : Patskovsky, Y.; Zhan, C.; Wengerter, B.C.; Ramagopal, U.; Milstein, S.; Vidal, M.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2006-06-13
Resolution : 2.00 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

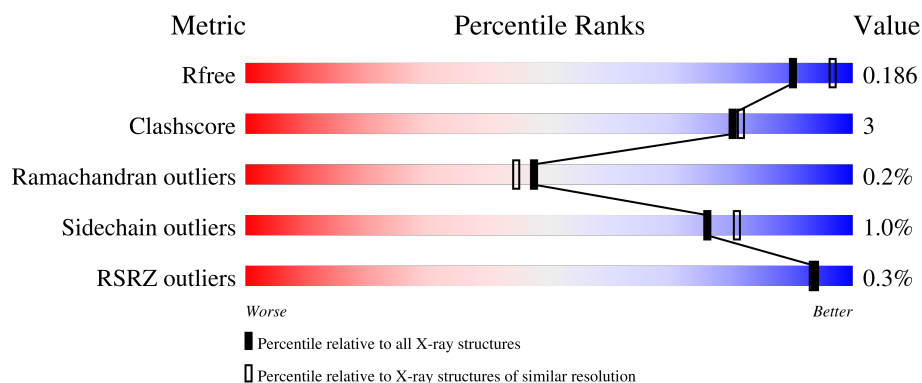
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

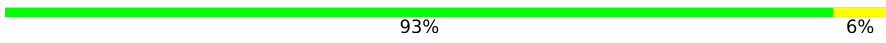
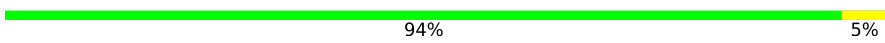
The reported resolution of this entry is 2.00 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	491	 93% 6%
1	B	491	 94% 5%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	2001	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8566 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 Leucine aminopeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	15	0
			3743	2385	629	711	18			
1	B	489	Total	C	N	O	S	0	20	0
			3764	2400	632	714	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	440	LEU	PHE	engineered mutation	UNP P34629
B	440	LEU	PHE	engineered mutation	UNP P34629

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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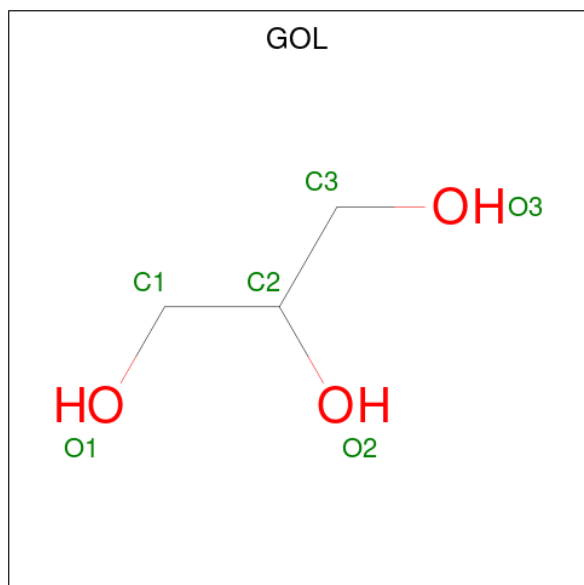
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Na	0	0
			3	3		
3	B	3	Total	Na	0	0
			3	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	493	Total	O	0	0
			493	493		
5	B	458	Total	O	0	0
			458	458		

- Molecule 1: Leucine aminopeptidase 1

- Molecule 1: Leucine aminopeptidase 1

MET
T2
K25
G36
R64
H65
P66
I75
T76
V77
I100
Y117
A125
R129
L171
N198
M276
K291
N314
K315
P316
D317
D318
I319
T333
E336
V345
I357
T364
A395
D413
I418
M429
T478
K490
CN

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	131.82Å 131.82Å 125.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.00 39.30 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.00) 99.9 (39.30-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.147 , 0.183 0.151 , 0.186	Depositor DCC
R_{free} test set	2495 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.490 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8566	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NA, GOL

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	0.56	2/3857 (0.1%)	0.66	6/5228 (0.1%)
1	B	0.53	0/3893	0.65	3/5275 (0.1%)
All	All	0.54	2/7750 (0.0%)	0.65	9/10503 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	386	GLU	CD-OE2	-6.25	1.18	1.25
1	A	386	GLU	CD-OE1	-5.50	1.19	1.25

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	171	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	A	386	GLU	OE1-CD-OE2	-6.22	115.84	123.30
1	A	129	ARG	NE-CZ-NH2	6.17	123.38	120.30
1	B	129	ARG	NE-CZ-NH1	5.48	123.04	120.30

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	3743	0	3833	18	0
1	B	3764	0	3873	22	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	42	0	56	5	0
4	B	30	0	40	8	0
5	A	493	0	0	3	0
5	B	458	0	0	2	0
All	All	8566	0	7802	41	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.

The worst 5 of 41 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:64[B]:ARG:NH1	4:B:2001:GOL:H32	1.70	1.04
1:B:64[B]:ARG:HH12	4:B:2001:GOL:H32	1.31	0.94
1:A:452:ARG:HH22	4:A:2012:GOL:H12	1.40	0.82
1:B:64[B]:ARG:CZ	4:B:2001:GOL:H32	2.14	0.78
1:B:36:GLY:H	4:B:2003:GOL:H2	1.50	0.76

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	502/491 (102%)	491 (98%)	10 (2%)	1 (0%)	47	44
1	B	507/491 (103%)	496 (98%)	10 (2%)	1 (0%)	47	44
All	All	1009/982 (103%)	987 (98%)	20 (2%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	ASP
1	B	317	ASP

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	409/396 (103%)	404 (99%)	5 (1%)	71	76
1	B	414/396 (104%)	411 (99%)	3 (1%)	84	88
All	All	823/792 (104%)	815 (99%)	8 (1%)	76	81

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	490	LYS
1	B	276	MET
1	A	490	LYS
1	A	276	MET
1	B	117	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	43	GLN
1	B	53	ASN
1	B	384	GLN
1	B	198	ASN
1	A	198	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](#)

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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	$\# Z > 2$
4	GOL	A	2010	-	5,5,5	0.36	0	5,5,5	0.50	0
4	GOL	A	2012	-	5,5,5	0.29	0	5,5,5	0.63	0
4	GOL	B	2001	-	5,5,5	0.54	0	5,5,5	0.33	0
4	GOL	B	2006	-	5,5,5	0.32	0	5,5,5	0.26	0
2	SO4	A	492	3	4,4,4	0.21	0	6,6,6	0.61	0
4	GOL	A	2005	-	5,5,5	0.29	0	5,5,5	0.38	0
4	GOL	B	2011	-	5,5,5	0.36	0	5,5,5	0.66	0
4	GOL	A	2004	-	5,5,5	0.33	0	5,5,5	0.31	0
2	SO4	B	494	-	4,4,4	0.17	0	6,6,6	0.17	0
4	GOL	A	2008	-	5,5,5	0.36	0	5,5,5	0.29	0
2	SO4	B	493	3	4,4,4	0.11	0	6,6,6	0.11	0
2	SO4	A	494	3	4,4,4	0.14	0	6,6,6	0.08	0
4	GOL	A	2007	-	5,5,5	0.31	0	5,5,5	0.53	0
4	GOL	B	2003	-	5,5,5	0.33	0	5,5,5	0.30	0
4	GOL	A	2002	-	5,5,5	0.40	0	5,5,5	0.43	0
4	GOL	B	2009	-	5,5,5	0.35	0	5,5,5	0.36	0
2	SO4	A	493	-	4,4,4	0.18	0	6,6,6	0.15	0
2	SO4	B	492	3	4,4,4	0.24	0	6,6,6	0.45	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
4	GOL	A	2010	-	-	4/4/4/4	-
4	GOL	A	2012	-	-	0/4/4/4	-
4	GOL	B	2001	-	-	0/4/4/4	-
4	GOL	B	2006	-	-	4/4/4/4	-
4	GOL	B	2011	-	-	0/4/4/4	-
4	GOL	A	2005	-	-	3/4/4/4	-
4	GOL	A	2004	-	-	2/4/4/4	-
4	GOL	A	2007	-	-	2/4/4/4	-
4	GOL	B	2003	-	-	0/4/4/4	-
4	GOL	A	2002	-	-	1/4/4/4	-
4	GOL	B	2009	-	-	4/4/4/4	-
4	GOL	A	2008	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2004	GOL	C1-C2-C3-O3
4	A	2010	GOL	O1-C1-C2-C3
4	B	2006	GOL	O1-C1-C2-C3
4	B	2009	GOL	O1-C1-C2-O2
4	B	2009	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2012	GOL	3	0
4	B	2001	GOL	7	0
4	A	2004	GOL	1	0
4	A	2008	GOL	1	0
4	B	2003	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	489/491 (99%)	-0.82	2 (0%) 92 92	17, 22, 41, 56	0
1	B	489/491 (99%)	-0.81	1 (0%) 95 94	17, 22, 41, 56	0
All	All	978/982 (99%)	-0.82	3 (0%) 94 93	17, 22, 41, 56	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	364	THR	2.5
1	A	270	PRO	2.0
1	A	364	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 monosaccharides 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(Å ²)	Q<0.9
4	GOL	A	2010	6/6	0.80	0.15	45,64,69,72	0
4	GOL	A	2004	6/6	0.82	0.17	53,60,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	2009	6/6	0.82	0.23	43,67,69,82	0
4	GOL	B	2011	6/6	0.83	0.24	41,61,69,73	0
4	GOL	B	2003	6/6	0.84	0.18	59,67,72,73	0
4	GOL	A	2012	6/6	0.88	0.22	35,51,60,60	0
4	GOL	B	2006	6/6	0.88	0.23	44,54,68,72	0
3	NA	B	3006	1/1	0.90	0.39	67,67,67,67	0
4	GOL	A	2005	6/6	0.90	0.20	46,47,67,76	0
4	GOL	A	2007	6/6	0.91	0.24	44,54,58,67	0
4	GOL	A	2008	6/6	0.91	0.20	52,66,71,79	0
3	NA	A	3002	1/1	0.93	0.08	31,31,31,31	0
3	NA	B	3003	1/1	0.94	0.10	28,28,28,28	0
3	NA	A	3005	1/1	0.94	0.30	58,58,58,58	0
4	GOL	A	2002	6/6	0.96	0.09	41,54,63,69	0
4	GOL	B	2001	6/6	0.96	0.13	38,48,56,70	0
3	NA	A	3001	1/1	0.96	0.14	28,28,28,28	0
2	SO4	B	493	5/5	0.97	0.11	62,64,71,73	0
3	NA	B	3004	1/1	0.97	0.11	31,31,31,31	0
2	SO4	A	494	5/5	0.97	0.10	66,68,71,73	0
2	SO4	A	493	5/5	0.99	0.10	32,44,46,50	0
2	SO4	B	494	5/5	0.99	0.12	35,45,49,50	0
2	SO4	A	492	5/5	0.99	0.08	22,23,26,28	0
2	SO4	B	492	5/5	0.99	0.07	21,22,26,28	0

6.5 Other polymers

There are no such residues in this entry.