



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:43 pm BST

PDB ID : 1LRV
Title : A LEUCINE-RICH REPEAT VARIANT WITH A NOVEL REPETITIVE
PROTEIN STRUCTURAL MOTIF
Authors : Peters, J.W.; Stowell, M.H.B.; Rees, D.C.
Deposited on : 1996-11-05
Resolution : 2.60 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

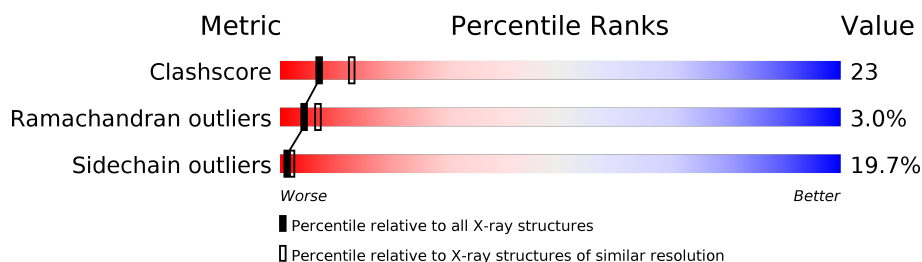
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	244	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1887 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-RICH REPEAT VARIANT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	233	1887	1179	355	344	9	0	0	0

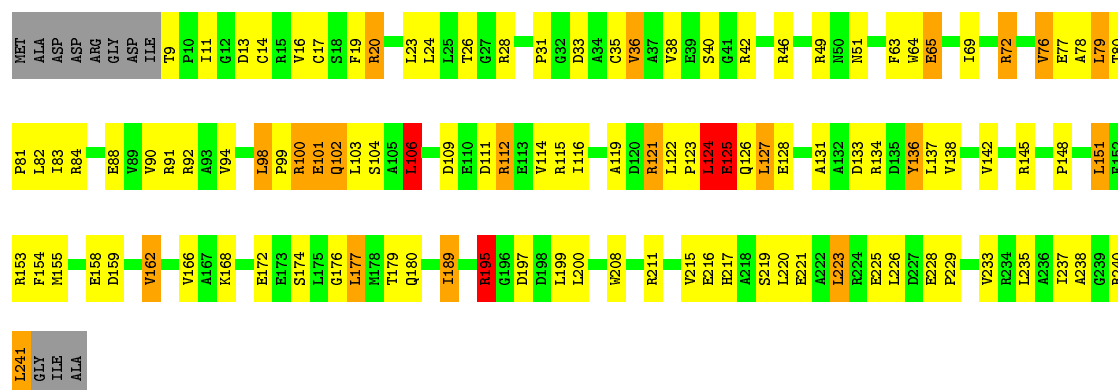
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

• Molecule 1: LEUCINE-RICH REPEAT VARIANT

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	69.80 Å 69.80 Å 159.80 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	92.0 (8.00-2.60)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.204 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1887	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

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	0.73	0/1921	0.98	5/2604 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	195	ARG	O-C-N	-8.12	109.40	123.20
1	A	36	VAL	CB-CA-C	-7.25	97.63	111.40
1	A	195	ARG	CA-C-N	5.75	127.71	116.20
1	A	121	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	106	LEU	CA-CB-CG	5.38	127.67	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	ARG	Mainchain

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	1887	0	1904	87	2
All	All	1887	0	1904	87	2

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 23.

All (87) 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:124:LEU:O	1:A:127:LEU:N	1.97	0.98
1:A:104:SER:OG	1:A:126:GLN:NE2	2.04	0.91
1:A:148:PRO:HA	1:A:151:LEU:HD22	1.52	0.89
1:A:65:GLU:O	1:A:69:ILE:HG12	1.75	0.87
1:A:72:ARG:HB2	1:A:72:ARG:HH11	1.49	0.75
1:A:83:ILE:HD11	1:A:98:LEU:HD21	1.69	0.74
1:A:76:VAL:HA	1:A:79:LEU:HD22	1.69	0.73
1:A:237:ILE:HG22	1:A:240:ARG:NH2	2.07	0.69
1:A:20:ARG:HH11	1:A:20:ARG:HB2	1.57	0.69
1:A:101:GLU:O	1:A:103:LEU:N	2.28	0.67
1:A:83:ILE:CD1	1:A:98:LEU:HD21	2.26	0.66
1:A:159:ASP:HB3	1:A:162:VAL:HG13	1.81	0.63
1:A:90:VAL:O	1:A:94:VAL:HG23	1.99	0.62
1:A:94:VAL:HG12	1:A:98:LEU:HD22	1.82	0.62
1:A:124:LEU:O	1:A:127:LEU:HB2	1.99	0.62
1:A:211:ARG:O	1:A:215:VAL:HG23	2.00	0.61
1:A:124:LEU:O	1:A:125:GLU:C	2.40	0.60
1:A:99:PRO:O	1:A:100:ARG:C	2.41	0.59
1:A:101:GLU:HG3	1:A:102:GLN:H	1.65	0.59
1:A:124:LEU:O	1:A:127:LEU:CB	2.49	0.59
1:A:123:PRO:O	1:A:124:LEU:C	2.39	0.59
1:A:176:GLY:HA2	1:A:179:THR:HG23	1.85	0.59
1:A:197:ASP:HA	1:A:200:LEU:HD13	1.85	0.58
1:A:148:PRO:HA	1:A:151:LEU:CD2	2.31	0.58
1:A:112:ARG:O	1:A:116:ILE:HG13	2.04	0.57
1:A:80:THR:HA	1:A:83:ILE:HD13	1.86	0.57
1:A:80:THR:O	1:A:83:ILE:HD13	2.05	0.57
1:A:174:SER:O	1:A:177:LEU:HB2	2.05	0.57
1:A:223:LEU:O	1:A:226:LEU:HB2	2.05	0.56
1:A:46:ARG:HA	1:A:49:ARG:HG3	1.85	0.56
1:A:72:ARG:HB2	1:A:72:ARG:NH1	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:NH2	1:A:137:LEU:HD12	2.20	0.56
1:A:101:GLU:C	1:A:103:LEU:H	2.10	0.56
1:A:19:PHE:CD1	1:A:23:LEU:HD22	2.41	0.55
1:A:100:ARG:O	1:A:103:LEU:HB2	2.07	0.55
1:A:112:ARG:NE	1:A:116:ILE:HD11	2.22	0.54
1:A:80:THR:HB	1:A:81:PRO:HD3	1.89	0.54
1:A:98:LEU:O	1:A:121:ARG:NH2	2.37	0.54
1:A:123:PRO:O	1:A:124:LEU:O	2.26	0.53
1:A:124:LEU:HD12	1:A:127:LEU:HD12	1.88	0.53
1:A:112:ARG:HE	1:A:116:ILE:HD11	1.75	0.52
1:A:77:GLU:H	1:A:77:GLU:CD	2.14	0.51
1:A:100:ARG:O	1:A:101:GLU:C	2.49	0.50
1:A:33:ASP:HA	1:A:46:ARG:NH2	2.27	0.49
1:A:88:GLU:O	1:A:92:ARG:HG3	2.11	0.49
1:A:98:LEU:HD12	1:A:99:PRO:HD3	1.95	0.49
1:A:233:VAL:O	1:A:237:ILE:HG13	2.12	0.49
1:A:28:ARG:HB3	1:A:51:ASN:HD21	1.77	0.49
1:A:35:CYS:SG	1:A:38:VAL:HG23	2.53	0.49
1:A:64:TRP:CD2	1:A:65:GLU:N	2.81	0.48
1:A:127:LEU:CD2	1:A:142:VAL:HG22	2.43	0.48
1:A:189:ILE:HD12	1:A:189:ILE:O	2.14	0.48
1:A:91:ARG:NH1	1:A:109:ASP:OD1	2.46	0.47
1:A:122:LEU:HA	1:A:123:PRO:HD3	1.72	0.47
1:A:20:ARG:HH11	1:A:20:ARG:CB	2.25	0.47
1:A:42:ARG:O	1:A:46:ARG:HD3	2.14	0.47
1:A:19:PHE:HB3	1:A:23:LEU:HB2	1.97	0.47
1:A:98:LEU:HD12	1:A:98:LEU:HA	1.65	0.47
1:A:168:LYS:HA	1:A:189:ILE:HD11	1.97	0.46
1:A:125:GLU:O	1:A:126:GLN:C	2.53	0.46
1:A:14:CYS:SG	1:A:31:PRO:HG3	2.55	0.46
1:A:125:GLU:HG2	1:A:126:GLN:H	1.81	0.46
1:A:115:ARG:NH1	1:A:133:ASP:OD1	2.48	0.46
1:A:82:LEU:HB3	1:A:94:VAL:HG21	1.98	0.46
1:A:111:ASP:OD2	1:A:114:VAL:HG23	2.15	0.45
1:A:219:SER:O	1:A:223:LEU:HD22	2.17	0.45
1:A:79:LEU:O	1:A:82:LEU:HB2	2.17	0.45
1:A:116:ILE:CD1	1:A:137:LEU:HD13	2.47	0.44
1:A:220:LEU:O	1:A:223:LEU:HB2	2.17	0.44
1:A:63:PHE:CE2	1:A:65:GLU:HB3	2.52	0.44
1:A:20:ARG:HH11	1:A:20:ARG:CG	2.31	0.44
1:A:136:TYR:C	1:A:136:TYR:CD1	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:LEU:O	1:A:241:LEU:HD13	2.18	0.43
1:A:238:ALA:C	1:A:240:ARG:H	2.22	0.42
1:A:64:TRP:CG	1:A:65:GLU:N	2.87	0.42
1:A:106:LEU:O	1:A:109:ASP:HB2	2.19	0.42
1:A:162:VAL:O	1:A:166:VAL:HG23	2.20	0.42
1:A:220:LEU:HD22	1:A:240:ARG:HG3	2.01	0.42
1:A:241:LEU:HA	1:A:241:LEU:HD22	1.88	0.42
1:A:98:LEU:HD12	1:A:99:PRO:CD	2.49	0.41
1:A:131:ALA:HB1	1:A:154:PHE:CZ	2.56	0.41
1:A:116:ILE:HD13	1:A:137:LEU:HD13	2.03	0.41
1:A:115:ARG:NH1	1:A:138:VAL:HG21	2.36	0.41
1:A:228:GLU:HA	1:A:229:PRO:HD2	1.97	0.41
1:A:119:ALA:O	1:A:145:ARG:NH1	2.52	0.40
1:A:91:ARG:HH11	1:A:91:ARG:HD2	1.74	0.40
1:A:78:ALA:O	1:A:81:PRO:HD2	2.22	0.40

All (2) 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)
1:A:100:ARG:NH2	1:A:208:TRP:CZ2[5_675]	1.52	0.68
1:A:100:ARG:NH2	1:A:208:TRP:CH2[5_675]	1.95	0.25

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	231/244 (95%)	209 (90%)	15 (6%)	7 (3%)	4 7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	124	LEU
1	A	125	GLU
1	A	13	ASP
1	A	101	GLU
1	A	128	GLU
1	A	100	ARG

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	203 / 210 (97%)	163 (80%)	40 (20%)	1 2

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	11	ILE
1	A	16	VAL
1	A	17	CYS
1	A	20	ARG
1	A	24	LEU
1	A	26	THR
1	A	36	VAL
1	A	40	SER
1	A	65	GLU
1	A	72	ARG
1	A	76	VAL
1	A	79	LEU
1	A	84	ARG
1	A	98	LEU
1	A	106	LEU
1	A	112	ARG
1	A	124	LEU
1	A	125	GLU
1	A	127	LEU

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Mol	Chain	Res	Type
1	A	134	ARG
1	A	136	TYR
1	A	151	LEU
1	A	153	ARG
1	A	155	MET
1	A	158	GLU
1	A	162	VAL
1	A	172	GLU
1	A	177	LEU
1	A	180	GLN
1	A	189	ILE
1	A	195	ARG
1	A	199	LEU
1	A	216	GLU
1	A	217	HIS
1	A	221	GLU
1	A	223	LEU
1	A	225	GLU
1	A	235	LEU
1	A	241	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	50	ASN
1	A	51	ASN
1	A	126	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.