



Full wwPDB EM Validation Report ⓘ

Nov 9, 2024 – 12:05 PM EST

PDB ID : 6VP8
EMDB ID : EMD-21250
Title : Cryo-EM structure of the C-terminal half of the Parkinson's Disease-linked protein Leucine Rich Repeat Kinase 2 (LRRK2)
Authors : Leschziner, A.; Deniston, C.; Lahiri, I.
Deposited on : 2020-02-01
Resolution : 3.50 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

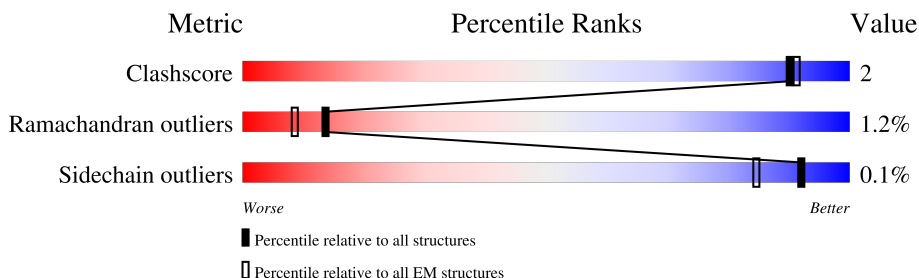
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




The reported resolution of this entry is 3.50 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1198	 85% . . 10%
2	B	281	 91% . 6%
3	C	359	 86% . 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13158 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1084	Total	C	N	O	P	S	0	0
			8531	5473	1455	1551	1	51		

- Molecule 2 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	265	Total	C	N	O	S	0	0
			2147	1387	360	386	14		

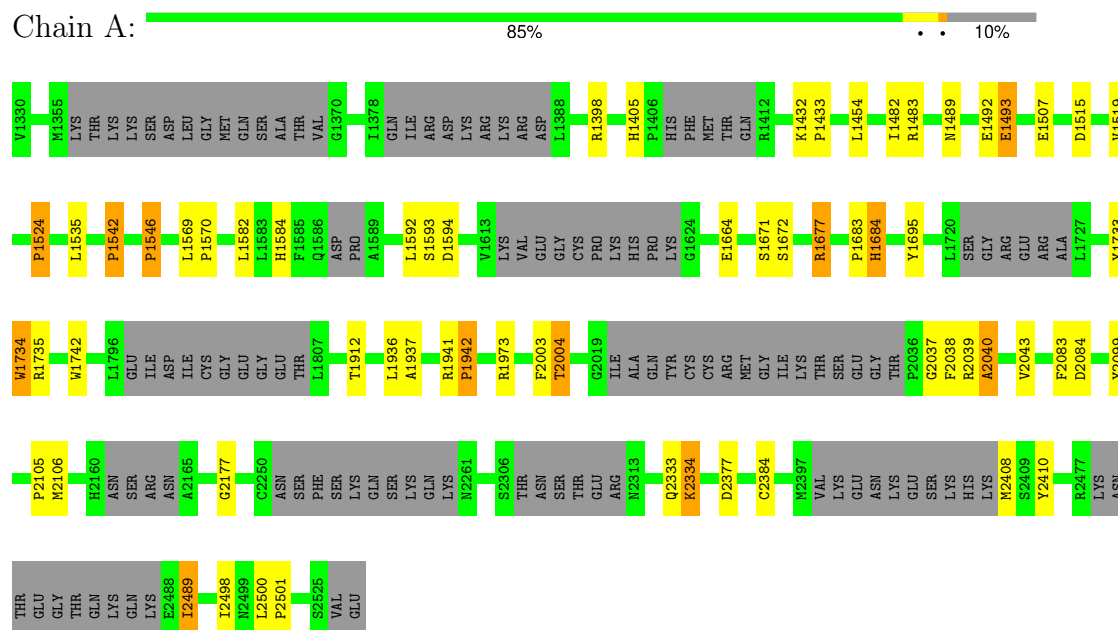
- Molecule 3 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	319	Total	C	N	O	S	0	0
			2480	1580	420	459	21		

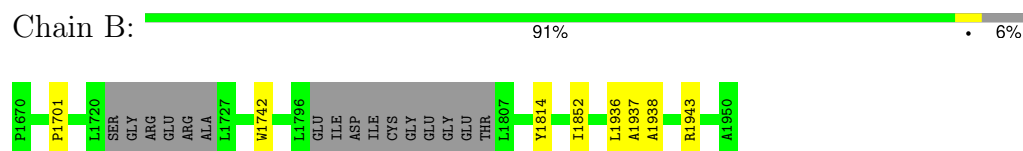
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

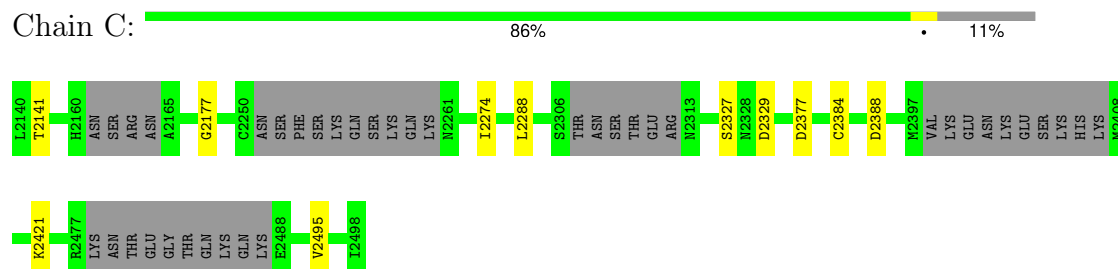
- Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2



- Molecule 2: Leucine-rich repeat serine/threonine-protein kinase 2



- Molecule 3: Leucine-rich repeat serine/threonine-protein kinase 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	70953	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Per-particle CTF values	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	6.65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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: TPO

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	0.80	1/8682 (0.0%)	0.72	9/11746 (0.1%)
2	B	0.76	0/2200	0.69	0/2983
3	C	0.69	0/2515	0.71	0/3397
All	All	0.77	1/13397 (0.0%)	0.71	9/18126 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2040	ALA	C-N	5.95	1.45	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1524	PRO	N-CA-CB	6.54	111.15	103.30
1	A	1734	TRP	CB-CA-C	-6.53	97.34	110.40
1	A	1546	PRO	N-CA-CB	6.49	111.09	103.30
1	A	2410	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	A	1542	PRO	N-CA-CB	6.20	110.74	103.30
1	A	1973	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	1695	TYR	CB-CG-CD2	-5.34	117.79	121.00
1	A	2099	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	A	1733	TYR	CB-CG-CD2	-5.19	117.89	121.00

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	8531	0	8567	36	0
2	B	2147	0	2156	2	0
3	C	2480	0	2549	5	0
All	All	13158	0	13272	43	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 2.

All (43) 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:2037:GLY:O	1:A:2083:PHE:CE2	2.44	0.70
1:A:1677:ARG:O	1:A:1677:ARG:HG3	1.94	0.68
1:A:2037:GLY:O	1:A:2083:PHE:HE2	1.81	0.64
1:A:1398:ARG:O	1:A:1398:ARG:HG3	2.01	0.59
1:A:2408:MET:O	1:A:2408:MET:SD	2.62	0.58
1:A:1483:ARG:NE	1:A:1483:ARG:HA	2.22	0.55
1:A:1582:LEU:C	1:A:1582:LEU:HD12	2.26	0.55
1:A:1912:THR:HG22	1:A:1912:THR:O	2.07	0.54
1:A:2105:PRO:O	1:A:2106:MET:HB2	2.09	0.53
1:A:2489:ILE:HG22	1:A:2489:ILE:O	2.08	0.53
1:A:1592:LEU:HD23	1:A:1592:LEU:O	2.10	0.52
1:A:1569:LEU:HB3	1:A:1570:PRO:HD3	1.92	0.50
1:A:1683:PRO:O	1:A:1684:HIS:HB2	2.11	0.50
1:A:2004:THR:O	1:A:2004:THR:HG23	2.12	0.50
1:A:2040:ALA:HB3	1:A:2043:VAL:HG22	1.94	0.49
1:A:1492:GLU:O	1:A:1493:GLU:CB	2.63	0.46
3:C:2377:ASP:HB2	3:C:2384:CYS:SG	2.55	0.46
1:A:1936:LEU:O	1:A:1937:ALA:HB3	2.16	0.46
1:A:1535:LEU:C	1:A:1535:LEU:HD23	2.36	0.45
1:A:2377:ASP:HB2	1:A:2384:CYS:SG	2.56	0.45
1:A:1454:LEU:HB3	1:A:1489:ASN:HA	1.98	0.45
1:A:1515:ASP:O	1:A:1519:VAL:N	2.50	0.45
1:A:2333:GLN:O	1:A:2334:LYS:HB3	2.17	0.45
1:A:2498:ILE:O	1:A:2498:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2039:ARG:NH2	1:A:2084:ASP:OD1	2.38	0.44
3:C:2141:THR:N	3:C:2495:VAL:O	2.51	0.44
3:C:2388:ASP:OD1	3:C:2388:ASP:C	2.56	0.43
3:C:2327:SER:OG	3:C:2329:ASP:OD1	2.35	0.43
1:A:1734:TRP:O	1:A:1735:ARG:HB3	2.18	0.43
1:A:1492:GLU:O	1:A:1493:GLU:HB2	2.19	0.42
1:A:1671:SER:O	1:A:1672:SER:CB	2.67	0.42
1:A:2500:LEU:HB3	1:A:2501:PRO:HD3	2.00	0.42
3:C:2274:ILE:O	3:C:2288:LEU:N	2.52	0.42
1:A:1664:GLU:OE1	1:A:1664:GLU:N	2.40	0.42
1:A:1593:SER:OG	1:A:1594:ASP:N	2.51	0.42
1:A:2003:PHE:O	1:A:2004:THR:HB	2.19	0.41
1:A:1584:HIS:ND1	1:A:1584:HIS:C	2.73	0.41
1:A:1405:HIS:CG	1:A:1405:HIS:O	2.73	0.41
1:A:1507:GLU:OE1	1:A:1507:GLU:HA	2.20	0.41
2:B:1814:TYR:CD2	2:B:1814:TYR:C	2.93	0.41
1:A:1432:LYS:HB2	1:A:1433:PRO:HD3	2.02	0.41
1:A:1941:ARG:HB3	1:A:1942:PRO:HD3	2.02	0.41
2:B:1936:LEU:O	2:B:1937:ALA:HB3	2.22	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 PDB entries followed by that with respect to all EM entries.

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	1055/1198 (88%)	977 (93%)	64 (6%)	14 (1%)	10	41
2	B	259/281 (92%)	232 (90%)	23 (9%)	4 (2%)	8	39
3	C	307/359 (86%)	294 (96%)	11 (4%)	2 (1%)	19	53
All	All	1621/1838 (88%)	1503 (93%)	98 (6%)	20 (1%)	14	43

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1493	GLU
1	A	2004	THR
2	B	1852	ILE
1	A	2334	LYS
2	B	1742	TRP
3	C	2421	LYS
1	A	1524	PRO
1	A	1542	PRO
1	A	1942	PRO
1	A	2177	GLY
1	A	2489	ILE
2	B	1938	ALA
3	C	2177	GLY
1	A	1482	ILE
1	A	2038	PHE
2	B	1701	PRO
1	A	1742	TRP
1	A	1684	HIS
1	A	1677	ARG
1	A	1546	PRO

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 PDB entries followed by that with respect to all EM entries.

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	926/1071 (86%)	926 (100%)	0	100	100
2	B	240/252 (95%)	239 (100%)	1 (0%)	89	95
3	C	283/322 (88%)	283 (100%)	0	100	100
All	All	1449/1645 (88%)	1448 (100%)	1 (0%)	92	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1943	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	2333	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
1	TPO	A	1343	1	8,10,11	0.93	0	10,14,16	0.76	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
1	TPO	A	1343	1	-	1/9/11/13	-

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
1	A	1343	TPO	CB-OG1-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 Map visualisation

This section contains visualisations of the EMDB entry EMD-21250. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section was not generated.