

Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 07:28 PM EDT

PDB ID	:	60JF
Title	:	Dimeric structure of LRRK2 GTPase domain
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Deposited on		
Resolution	:	1.60 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
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)	:	2.35.1

Clashscore

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 1.60 Å.

141614

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.

3665(1.60-1.60)

Metric	Percent	ile Ranks Value
Clashscore		2
W	orse	Better
I	Percentile relative to all X-ray structures	
0	Percentile relative to X-ray structures of sin	nilar resolution
ЪЛани	Whole archive	Similar resolution
Metric	(# Entries)	(# Entries, resolution range(Å))



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3252 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.

M	ol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	1	٨	100	Total	С	Ν	0	S	0	0 0	0
1	I A	188	1477	936	264	270	$\overline{7}$	0	Z	0	
1	I	р	100	Total	С	Ν	0	S	0		0
1	L	В	186	1400	0.40	000	070	10	0	3	0

263

273

10

• Molecule 1 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

Chain	Residue	Modelled	Actual	Comment	Reference
А	1315	MET	-	initiating methionine	UNP Q5S007
А	1316	GLY	- expression tag		UNP Q5S007
А	1317	SER	-	expression tag	UNP Q5S007
А	1318	SER	-	expression tag	UNP $Q5S007$
А	1319	HIS	-	expression tag	UNP Q5S007
А	1320	HIS	-	expression tag	UNP $Q5S007$
А	1321	HIS	-	expression tag	UNP Q5S007
А	1322	HIS	-	expression tag	UNP $Q5S007$
А	1323	HIS	-	expression tag	UNP $Q5S007$
A	1324	HIS	-	expression tag	UNP $Q5S007$
А	1325	SER	-	expression tag	UNP $Q5S007$
А	1326	GLN	-	expression tag	UNP $Q5S007$
А	1327	ASP	-	expression tag	UNP $Q5S007$
А	1328	PRO	-	expression tag	UNP $Q5S007$
А	1460	ALA	LYS	engineered mutation	UNP Q5S007
А	1463	ALA	LYS	engineered mutation	UNP $Q5S007$
В	1315	MET	-	initiating methionine	UNP $Q5S007$
В	1316	GLY	-	expression tag	UNP $Q5S007$
В	1317	SER	-	expression tag	UNP $Q5S007$
В	1318	SER	-	expression tag	UNP $Q5S007$
В	1319	HIS	-	expression tag	UNP $Q5S007$
В	1320	HIS	-	expression tag	UNP $Q5S007$
В	1321	HIS	-	expression tag	UNP $Q5S007$
В	1322	HIS	-	expression tag	UNP $Q5S007$
В	1323	HIS	-	expression tag	UNP $Q5S007$
				Continued	on nert nage

There are 32 discrepancies between the modelled and reference sequences:

942

1488

Continued on next page...



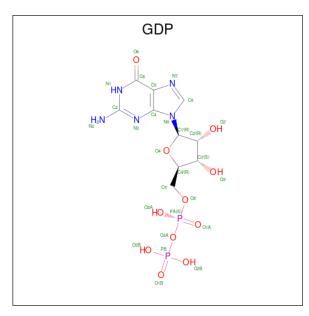
Chain	Residue	Modelled	Actual	Comment	Reference
В	1324	HIS	-	expression tag	UNP Q5S007
В	1325	SER	-	expression tag	UNP $Q5S007$
В	1326	GLN	-	expression tag	UNP $Q5S007$
В	1327	ASP	-	expression tag	UNP $Q5S007$
В	1328	PRO	-	expression tag	UNP $Q5S007$
В	1460	ALA	LYS	engineered mutation	UNP $Q5S007$
В	1463	ALA	LYS	engineered mutation	UNP $Q5S007$

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• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Mg 2 2	0	0
2	В	2	Total Mg 2 2	0	0

• Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
9	Δ	1	Total	С	Ν	0	Р	0	0	
0	3 A	1	28	10	5	11	2	0	0	
9	D	1	Total	С	Ν	Ο	Р	0	0	
0	D	B I		10	5	11	2	0	0	

• Molecule 4 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	97	Total O 102 102	0	5
4	В	121	Total O 125 125	0	4

SEQUENCE-PLOTS INFOmissingINFO



3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	44.63Å 101.88Å 44.61 Å	Depositor
a, b, c, α , β , γ	90.00° 100.95° 90.00°	Depositor
Resolution (Å)	43.82 - 1.60	Depositor
% Data completeness	97.4 (43.82-1.60)	Depositor
(in resolution range)		-
R _{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	226.39 (at 1.59 Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.143 , 0.158	Depositor
Wilson B-factor ($Å^2$)	31.1	Xtriage
Anisotropy	0.101	Xtriage
L-test for twinning ²	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.089 for l,-k,h	Xtriage
Total number of atoms	3252	wwPDB-VP
Average B, all atoms $(Å^2)$	40.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.77% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

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

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.65	0/1509	0.72	0/2037	
1	В	0.64	0/1514	0.71	0/2040	
All	All	0.64	0/3023	0.72	0/4077	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	А	1477	0	1476	5	0
1	В	1488	0	1494	9	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
3	А	28	0	12	0	0
3	В	28	0	12	0	0
4	А	102	0	0	0	0
4	В	125	0	0	1	0
All	All	3252	0	2994	11	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.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1389:VAL:HB	1:B:1333:ASN:HB2	1.84	0.59
1:A:1505:ILE:HG12	1:B:1378:ILE:HG21	1.86	0.57
1:B:1332:TYR:CE2	1:B:1399:GLU:HG2	2.40	0.56
1:B:1379:GLN:HA	1:B:1386:ARG:NH2	2.24	0.53
1:B:1334:ARG:HH12	1:B:1412:ARG:HG3	1.75	0.51
1:A:1368:THR:HG21	4:B:1742:HOH:O	2.12	0.49
1:A:1380:ILE:HD13	1:B:1509:LEU:HD11	1.95	0.48
1:A:1340:VAL:HB	1:A:1434:TRP:CZ3	2.51	0.46
1:B:1432:LYS:N	1:B:1433:PRO:HD2	2.34	0.43
1:B:1414:LEU:HD13	1:B:1446:PRO:HG2	2.00	0.42
1:B:1416:LEU:HD21	1:B:1450:VAL:HG21	2.01	0.42

All (11) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

4.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

4.3.3 RNA (i)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.



4.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

