



wwPDB EM Validation Summary Report ⓘ

Jun 7, 2026 – 12:09 AM JST

PDB ID : 9LN6 / pdb_00009ln6
EMDB ID : EMD-63227
Title : Structure of human NLRP14-UHRF1 complex
Authors : Qi, Q.; Chi, P.; Liu, S.; Lu, Y.; Li, J.; Li, J.; Wang, X.; Jiang, Y.; Deng, D.
Deposited on : 2025-01-20
Resolution : 3.49 Å(reported)

This is a wwPDB EM 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/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 : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

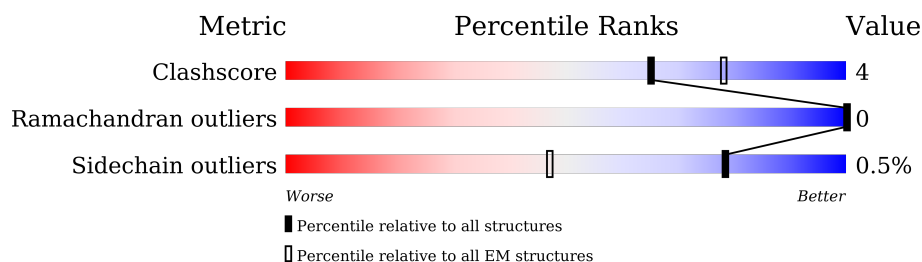
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.49 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	1506	
2	B	495	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8130 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 Maltose/maltodextrin-binding periplasmic protein,NACHT, LRR and PYD domains-containing protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	937	Total	C	N	O	S	0	0
			7491	4755	1274	1389	73		

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-412	MET	-	initiating methionine	UNP P0AEX9
A	-411	TRP	-	expression tag	UNP P0AEX9
A	-410	SER	-	expression tag	UNP P0AEX9
A	-409	HIS	-	expression tag	UNP P0AEX9
A	-408	PRO	-	expression tag	UNP P0AEX9
A	-407	GLN	-	expression tag	UNP P0AEX9
A	-406	PHE	-	expression tag	UNP P0AEX9
A	-405	GLU	-	expression tag	UNP P0AEX9
A	-404	LYS	-	expression tag	UNP P0AEX9
A	-403	ASP	-	expression tag	UNP P0AEX9
A	-402	GLU	-	expression tag	UNP P0AEX9
A	-401	VAL	-	expression tag	UNP P0AEX9
A	-400	ASP	-	expression tag	UNP P0AEX9
A	-399	ALA	-	expression tag	UNP P0AEX9
A	-398	GLY	-	expression tag	UNP P0AEX9
A	-397	SER	-	expression tag	UNP P0AEX9
A	-396	GLY	-	expression tag	UNP P0AEX9
A	-395	HIS	-	expression tag	UNP P0AEX9
A	-394	MET	-	expression tag	UNP P0AEX9
A	-27	ASN	-	linker	UNP P0AEX9
A	-26	SER	-	linker	UNP P0AEX9
A	-25	SER	-	linker	UNP P0AEX9
A	-24	SER	-	linker	UNP P0AEX9
A	-23	ASN	-	linker	UNP P0AEX9
A	-22	ASN	-	linker	UNP P0AEX9
A	-21	ASN	-	linker	UNP P0AEX9
A	-20	ASN	-	linker	UNP P0AEX9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	ASN	-	linker	UNP P0AEX9
A	-18	ASN	-	linker	UNP P0AEX9
A	-17	ASN	-	linker	UNP P0AEX9
A	-16	ASN	-	linker	UNP P0AEX9
A	-15	ASN	-	linker	UNP P0AEX9
A	-14	ASN	-	linker	UNP P0AEX9
A	-13	LEU	-	linker	UNP P0AEX9
A	-12	GLY	-	linker	UNP P0AEX9
A	-11	ILE	-	linker	UNP P0AEX9
A	-10	ASP	-	linker	UNP P0AEX9
A	-9	LEU	-	linker	UNP P0AEX9
A	-8	GLU	-	linker	UNP P0AEX9
A	-7	VAL	-	linker	UNP P0AEX9
A	-6	LEU	-	linker	UNP P0AEX9
A	-5	PHE	-	linker	UNP P0AEX9
A	-4	GLN	-	linker	UNP P0AEX9
A	-3	GLY	-	linker	UNP P0AEX9
A	-2	PRO	-	linker	UNP P0AEX9
A	-1	GLY	-	linker	UNP P0AEX9
A	0	THR	-	linker	UNP P0AEX9

- Molecule 2 is a protein called Maltose/maltodextrin-binding periplasmic protein,E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	75	Total	C	N	O	S	0	0
			639	401	120	115	3		

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-416	MET	-	initiating methionine	UNP P0AEX9
B	-415	HIS	-	expression tag	UNP P0AEX9
B	-414	HIS	-	expression tag	UNP P0AEX9
B	-413	HIS	-	expression tag	UNP P0AEX9
B	-412	HIS	-	expression tag	UNP P0AEX9
B	-411	HIS	-	expression tag	UNP P0AEX9
B	-410	HIS	-	expression tag	UNP P0AEX9
B	-409	HIS	-	expression tag	UNP P0AEX9
B	-408	HIS	-	expression tag	UNP P0AEX9
B	-407	HIS	-	expression tag	UNP P0AEX9
B	-406	HIS	-	expression tag	UNP P0AEX9

Continued on next page...

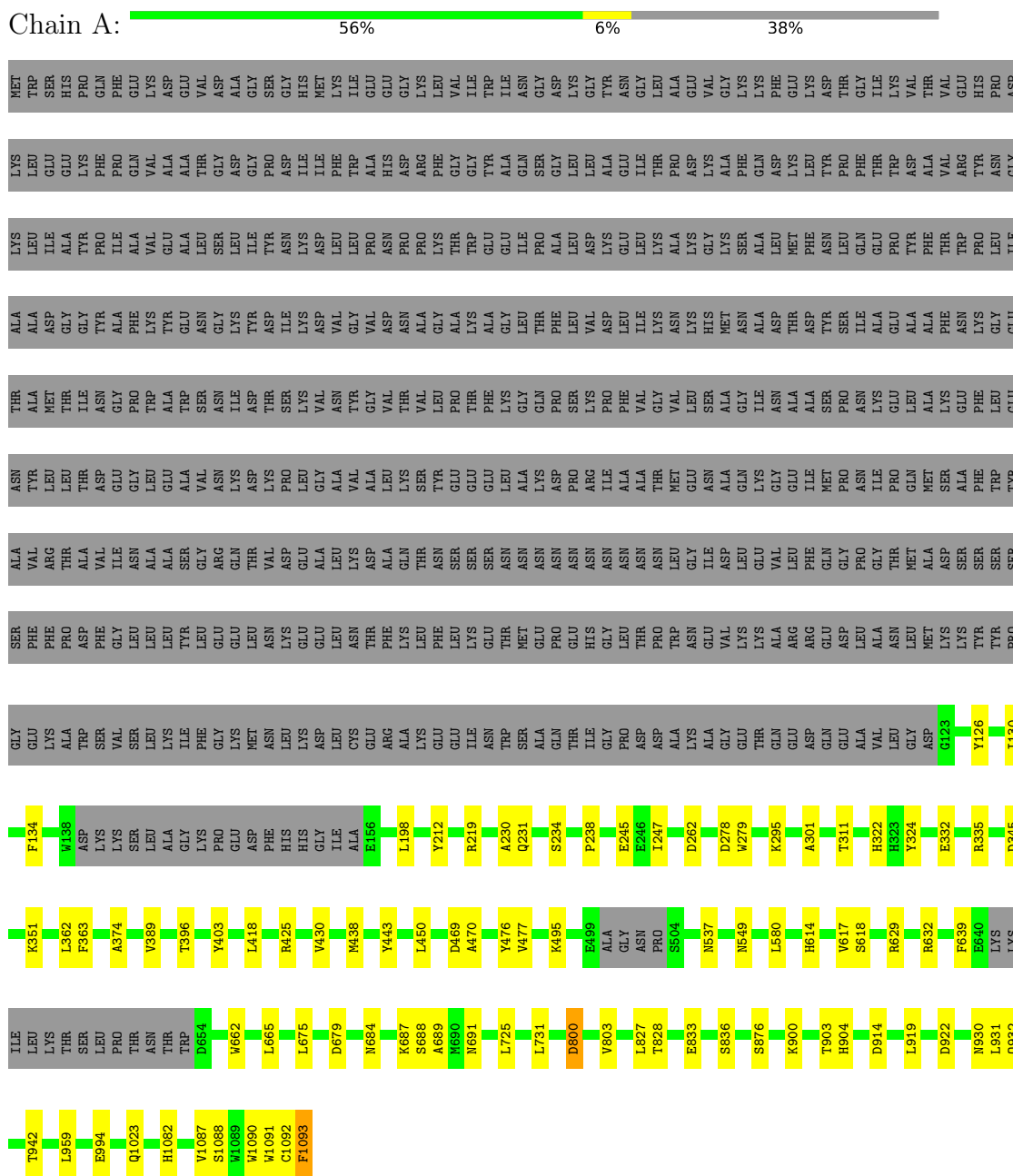
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-405	SER	-	expression tag	UNP P0AEX9
B	-404	GLY	-	expression tag	UNP P0AEX9
B	-403	ASP	-	expression tag	UNP P0AEX9
B	-402	GLU	-	expression tag	UNP P0AEX9
B	-401	VAL	-	expression tag	UNP P0AEX9
B	-400	ASP	-	expression tag	UNP P0AEX9
B	-399	ALA	-	expression tag	UNP P0AEX9
B	-398	GLY	-	expression tag	UNP P0AEX9
B	-397	SER	-	expression tag	UNP P0AEX9
B	-396	GLY	-	expression tag	UNP P0AEX9
B	-395	HIS	-	expression tag	UNP P0AEX9
B	-394	MET	-	expression tag	UNP P0AEX9
B	-27	ASN	-	linker	UNP P0AEX9
B	-26	SER	-	linker	UNP P0AEX9
B	-25	SER	-	linker	UNP P0AEX9
B	-24	SER	-	linker	UNP P0AEX9
B	-23	ASN	-	linker	UNP P0AEX9
B	-22	ASN	-	linker	UNP P0AEX9
B	-21	ASN	-	linker	UNP P0AEX9
B	-20	ASN	-	linker	UNP P0AEX9
B	-19	ASN	-	linker	UNP P0AEX9
B	-18	ASN	-	linker	UNP P0AEX9
B	-17	ASN	-	linker	UNP P0AEX9
B	-16	ASN	-	linker	UNP P0AEX9
B	-15	ASN	-	linker	UNP P0AEX9
B	-14	ASN	-	linker	UNP P0AEX9
B	-13	LEU	-	linker	UNP P0AEX9
B	-12	GLY	-	linker	UNP P0AEX9
B	-11	ILE	-	linker	UNP P0AEX9
B	-10	ASP	-	linker	UNP P0AEX9
B	-9	LEU	-	linker	UNP P0AEX9
B	-8	GLU	-	linker	UNP P0AEX9
B	-7	VAL	-	linker	UNP P0AEX9
B	-6	LEU	-	linker	UNP P0AEX9
B	-5	PHE	-	linker	UNP P0AEX9
B	-4	GLN	-	linker	UNP P0AEX9
B	-3	GLY	-	linker	UNP P0AEX9
B	-2	PRO	-	linker	UNP P0AEX9
B	-1	GLY	-	linker	UNP P0AEX9
B	0	THR	-	linker	UNP P0AEX9

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: Maltose/maltodextrin-binding periplasmic protein,NACHT, LRR and PYD domains-containing protein 14



- Chain B:  14% 85%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73160	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.13	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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	0.26	0/7634	0.39	0/10308
2	B	0.20	0/649	0.32	0/871
All	All	0.26	0/8283	0.38	0/11179

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

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	7491	0	7507	61	0
2	B	639	0	647	4	0
All	All	8130	0	8154	65	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.

The worst 5 of 65 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:322:HIS:NE2	1:A:324:TYR:CE2	2.31	0.98
1:A:322:HIS:HE2	1:A:324:TYR:HE2	0.99	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLU:N	1:A:245:GLU:OE1	2.07	0.87
1:A:322:HIS:NE2	1:A:324:TYR:HE2	1.75	0.81
1:A:322:HIS:CD2	1:A:324:TYR:CE2	2.70	0.79

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	929/1506 (62%)	896 (96%)	33 (4%)	0	100	100
2	B	73/495 (15%)	70 (96%)	3 (4%)	0	100	100
All	All	1002/2001 (50%)	966 (96%)	36 (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 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	857/1325 (65%)	852 (99%)	5 (1%)	78	79
2	B	71/411 (17%)	71 (100%)	0	100	100
All	All	928/1736 (54%)	923 (100%)	5 (0%)	78	80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	418	LEU
1	A	639	PHE
1	A	688	SER
1	A	800	ASP
1	A	1093	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	4	GLN
1	A	1083	ASN
1	A	694	HIS
1	A	660	HIS
1	A	733	HIS

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 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.