



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:19 PM EDT

PDB ID : 6LOL / pdb_00006lol
Title : The crystal structure of full length IpaH9.8
Authors : Ye, Y.; Huang, H.
Deposited on : 2020-01-06
Resolution : 2.75 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 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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

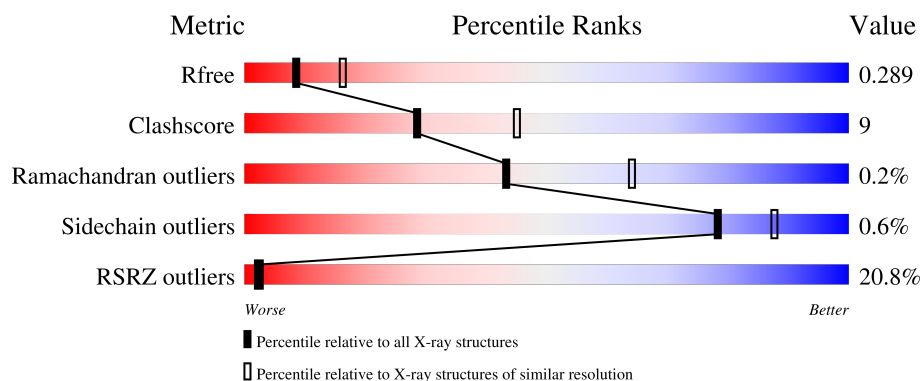
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	526	18% 73% 16% 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3460 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 E3 ubiquitin-protein ligase ipaH9.8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3460	2185	598	670	7			

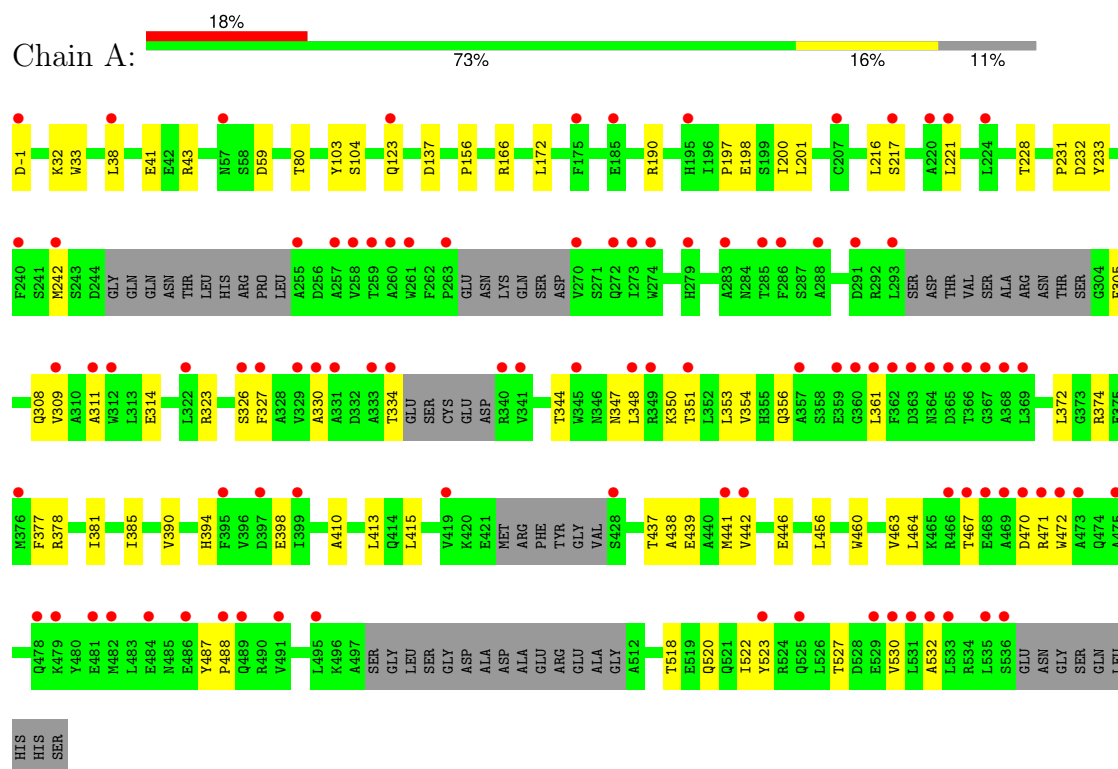
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	expression tag	UNP D2AJU0
A	0	PRO	-	expression tag	UNP D2AJU0

3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: E3 ubiquitin-protein ligase ipaH9.8



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	106.64Å 122.25Å 149.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.91 – 2.75 86.91 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (86.91-2.75) 99.6 (86.91-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.246 , 0.285 0.252 , 0.289	Depositor DCC
R_{free} test set	1319 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	80.1	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 96.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3460	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.18	0/3523	0.44	0/4818

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 [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	A	3460	0	3216	59	0
All	All	3460	0	3216	59	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 9.

All (59) 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:33:TRP:NE1	1:A:43:ARG:HH11	1.71	0.88
1:A:33:TRP:CD1	1:A:43:ARG:HH11	1.91	0.87
1:A:518:THR:O	1:A:522:ILE:HD12	1.86	0.75
1:A:456:LEU:HD11	1:A:520:GLN:HA	1.68	0.75
1:A:330:ALA:HB2	1:A:348:LEU:HD11	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TRP:NE1	1:A:43:ARG:NH1	2.35	0.73
1:A:200:ILE:HD12	1:A:201:LEU:HG	1.77	0.66
1:A:200:ILE:HD12	1:A:201:LEU:N	2.11	0.65
1:A:200:ILE:CD1	1:A:201:LEU:HG	2.29	0.63
1:A:385:ILE:CD1	1:A:441:MET:HE2	2.28	0.63
1:A:410:ALA:HA	1:A:415:LEU:HD12	1.81	0.62
1:A:530:VAL:HG23	1:A:532:ALA:H	1.66	0.60
1:A:216:LEU:HB2	1:A:221:LEU:HD11	1.84	0.59
1:A:308:GLN:HA	1:A:311:ALA:H	1.67	0.59
1:A:472:TRP:HZ3	1:A:523:TYR:HE1	1.50	0.58
1:A:385:ILE:HD11	1:A:441:MET:HE2	1.85	0.58
1:A:413:LEU:HD21	1:A:439:GLU:HG3	1.84	0.58
1:A:217:SER:O	1:A:221:LEU:HD13	2.04	0.57
1:A:472:TRP:HZ3	1:A:523:TYR:CE1	2.22	0.57
1:A:231:PRO:O	1:A:232:ASP:HB3	2.04	0.56
1:A:353:LEU:HD21	1:A:372:LEU:HD21	1.89	0.55
1:A:166:ARG:CZ	1:A:190:ARG:HE	2.22	0.53
1:A:38:LEU:O	1:A:41:GLU:HG2	2.09	0.53
1:A:527:THR:HA	1:A:530:VAL:HG12	1.91	0.52
1:A:323:ARG:HA	1:A:326:SER:H	1.75	0.52
1:A:390:VAL:HG11	1:A:398:GLU:HA	1.91	0.52
1:A:530:VAL:HG23	1:A:532:ALA:N	2.25	0.51
1:A:104:SER:O	1:A:104:SER:OG	2.30	0.50
1:A:347:ASN:O	1:A:351:THR:HG23	2.12	0.49
1:A:103:TYR:CD1	1:A:123:GLN:HG3	2.48	0.49
1:A:166:ARG:NH1	1:A:190:ARG:HE	2.11	0.49
1:A:305:PHE:O	1:A:309:VAL:HG13	2.13	0.49
1:A:311:ALA:HA	1:A:314:GLU:HB2	1.94	0.48
1:A:-1:ASP:OD1	1:A:-1:ASP:N	2.37	0.48
1:A:323:ARG:HB2	1:A:327:PHE:CZ	2.48	0.48
1:A:197:PRO:O	1:A:200:ILE:HG13	2.16	0.46
1:A:200:ILE:HD12	1:A:201:LEU:H	1.81	0.45
1:A:166:ARG:HA	1:A:190:ARG:O	2.16	0.45
1:A:350:LYS:O	1:A:354:VAL:HG13	2.16	0.45
1:A:377:PHE:O	1:A:381:ILE:HG12	2.18	0.44
1:A:198:GLU:OE2	1:A:394:HIS:ND1	2.46	0.43
1:A:242:MET:HE3	1:A:242:MET:HB2	1.65	0.43
1:A:527:THR:C	1:A:530:VAL:HG12	2.44	0.43
1:A:487:TYR:N	1:A:488:PRO:HD2	2.34	0.43
1:A:374:ARG:O	1:A:378:ARG:HG3	2.19	0.43
1:A:463:VAL:O	1:A:467:THR:N	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:GLN:HB3	1:A:361:LEU:HD23	2.02	0.42
1:A:460:TRP:O	1:A:464:LEU:HG	2.19	0.42
1:A:442:VAL:O	1:A:446:GLU:HB2	2.19	0.42
1:A:59:ASP:HB3	1:A:80:THR:OG1	2.21	0.41
1:A:172:LEU:HB3	1:A:197:PRO:HD3	2.02	0.41
1:A:228:THR:HG22	1:A:233:TYR:CZ	2.56	0.41
1:A:438:ALA:O	1:A:442:VAL:HG12	2.21	0.41
1:A:437:THR:O	1:A:441:MET:HG3	2.20	0.41
1:A:137:ASP:HA	1:A:156:PRO:HB3	2.02	0.41
1:A:232:ASP:O	1:A:232:ASP:CG	2.64	0.40
1:A:32:LYS:O	1:A:32:LYS:HD2	2.22	0.40
1:A:103:TYR:HD1	1:A:123:GLN:HG3	1.84	0.40
1:A:344:THR:O	1:A:348:LEU:HD22	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 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	452/526 (86%)	414 (92%)	37 (8%)	1 (0%)	43	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	470	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	344/462 (74%)	342 (99%)	2 (1%)	78	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	334	THR
1	A	471	ARG

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

Mol	Chain	Res	Type
1	A	36	GLN
1	A	192	GLN
1	A	195	HIS
1	A	205	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 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	466/526 (88%)	1.13	97 (20%) 2 2	46, 91, 180, 203	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	ILE	6.4
1	A	366	THR	6.2
1	A	330	ALA	6.0
1	A	469	ALA	5.9
1	A	329	VAL	5.8
1	A	293	LEU	5.3
1	A	367	GLY	4.9
1	A	312	TRP	4.9
1	A	270	VAL	4.8
1	A	472	TRP	4.5
1	A	291	ASP	4.4
1	A	495	LEU	4.3
1	A	255	ALA	4.2
1	A	536	SER	4.2
1	A	428	SER	4.0
1	A	175	PHE	3.9
1	A	220	ALA	3.8
1	A	530	VAL	3.8
1	A	466	ARG	3.7
1	A	361	LEU	3.6
1	A	309	VAL	3.6
1	A	471	ARG	3.5
1	A	531	LEU	3.4
1	A	362	PHE	3.4
1	A	340	ARG	3.3
1	A	363	ASP	3.3
1	A	481	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	345	TRP	3.3
1	A	368	ALA	3.3
1	A	341	VAL	3.3
1	A	38	LEU	3.2
1	A	468	GLU	3.2
1	A	274	TRP	3.2
1	A	532	ALA	3.2
1	A	331	ALA	3.1
1	A	473	ALA	3.1
1	A	334	THR	3.1
1	A	467	THR	3.1
1	A	529	GLU	3.0
1	A	349	ARG	3.0
1	A	272	GLN	3.0
1	A	365	ASP	3.0
1	A	258	VAL	3.0
1	A	207	CYS	2.9
1	A	470	ASP	2.9
1	A	224	LEU	2.9
1	A	475	ALA	2.9
1	A	488	PRO	2.9
1	A	419	VAL	2.9
1	A	359	GLU	2.8
1	A	263	PRO	2.7
1	A	525	GLN	2.7
1	A	326	SER	2.7
1	A	491	VAL	2.7
1	A	533	LEU	2.6
1	A	311	ALA	2.6
1	A	376	MET	2.6
1	A	221	LEU	2.6
1	A	351	THR	2.6
1	A	322	LEU	2.6
1	A	288	ALA	2.6
1	A	489	GLN	2.5
1	A	482	MET	2.5
1	A	123	GLN	2.5
1	A	260	ALA	2.5
1	A	242	MET	2.5
1	A	397	ASP	2.5
1	A	478	GLN	2.5
1	A	364	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	217	SER	2.5
1	A	360	GLY	2.5
1	A	283	ALA	2.5
1	A	259	THR	2.4
1	A	327	PHE	2.4
1	A	357	ALA	2.4
1	A	535	LEU	2.4
1	A	257	ALA	2.4
1	A	57	ASN	2.3
1	A	369	LEU	2.3
1	A	185	GLU	2.3
1	A	-1	ASP	2.3
1	A	286	PHE	2.3
1	A	333	ALA	2.2
1	A	195	HIS	2.2
1	A	442	VAL	2.2
1	A	261	TRP	2.2
1	A	348	LEU	2.2
1	A	523	TYR	2.2
1	A	441	MET	2.2
1	A	395	PHE	2.1
1	A	486	GLU	2.1
1	A	399	ILE	2.1
1	A	484	GLU	2.0
1	A	479	LYS	2.0
1	A	285	THR	2.0
1	A	279	HIS	2.0
1	A	240	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.