



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:59 PM UTC

PDB ID : 3CVR / pdb_00003cvr
Title : Crystal structure of the full length IpaH3
Authors : Zhu, Y.; Shao, F.
Deposited on : 2008-04-19
Resolution : 2.80 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

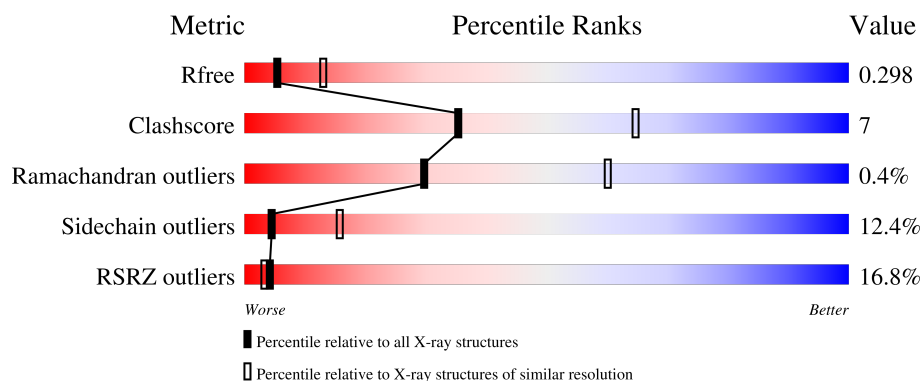
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	571	14% 65% 15% • 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3741 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 Invasion plasmid antigen.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	Se	0	0	0
			3702	2341	632	718	5	6			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	344	ALA	THR	SEE REMARK 999	UNP Q83RJ4
A	500	LEU	GLN	SEE REMARK 999	UNP Q83RJ4
A	514	PRO	SER	SEE REMARK 999	UNP Q83RJ4
A	552	LEU	VAL	SEE REMARK 999	UNP Q83RJ4
A	562	PRO	SER	SEE REMARK 999	UNP Q83RJ4

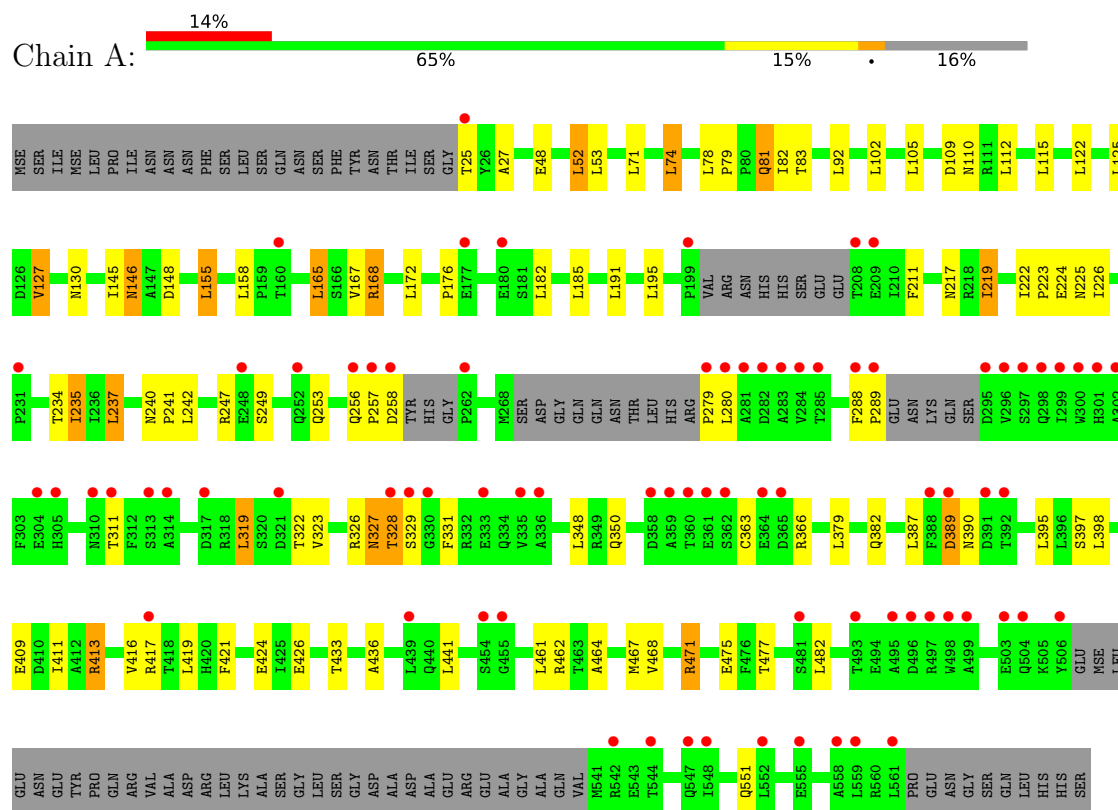
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	39	Total	O	0	0
			39	39		

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: Invasion plasmid antigen



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	154.19Å 154.19Å 85.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 2.80 48.76 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.76-2.80) 99.4 (48.76-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.76 (at 2.81Å)	Xtriage
Refinement program	CNS, REFMAC 5.2.0019	Depositor
R, R_{free}	0.251 , 0.277 0.274 , 0.298	Depositor DCC
R_{free} test set	1318 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3741	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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	0.46	0/3767	0.84	3/5125 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	ASN	N-CA-C	9.37	125.53	112.04
1	A	327	ASN	CA-C-N	6.07	132.62	121.70
1	A	327	ASN	C-N-CA	6.07	132.62	121.70

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	3702	0	3516	53	0
2	A	39	0	0	0	0
All	All	3741	0	3516	53	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 7.

All (53) 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:329:SER:HB3	1:A:331:PHE:H	1.15	1.09
1:A:288:PHE:HB3	1:A:289:PRO:HA	1.67	0.77
1:A:329:SER:HB3	1:A:331:PHE:N	1.98	0.76
1:A:319:LEU:O	1:A:322:THR:HG22	1.89	0.71
1:A:25:THR:HG22	1:A:27:ALA:H	1.58	0.69
1:A:411:ILE:HD11	1:A:467:MSE:HG2	1.75	0.68
1:A:366:ARG:CZ	1:A:413:ARG:HG3	2.24	0.66
1:A:224:GLU:HG3	1:A:419:LEU:HG	1.78	0.66
1:A:329:SER:CB	1:A:331:PHE:H	2.01	0.65
1:A:328:THR:HA	1:A:329:SER:C	2.23	0.64
1:A:110:ASN:HB2	1:A:130:ASN:HD21	1.68	0.58
1:A:146:ASN:ND2	1:A:148:ASP:H	2.03	0.56
1:A:81:GLN:NE2	1:A:81:GLN:H	2.06	0.54
1:A:155:LEU:HD13	1:A:172:LEU:HD21	1.89	0.53
1:A:471:ARG:NH1	1:A:475:GLU:OE1	2.42	0.53
1:A:112:LEU:H	1:A:130:ASN:HD22	1.57	0.52
1:A:222:ILE:HG13	1:A:421:PHE:HB3	1.93	0.51
1:A:235:ILE:HG22	1:A:237:LEU:HD13	1.91	0.51
1:A:219:ILE:H	1:A:240:ASN:HD22	1.57	0.51
1:A:79:PRO:HB2	1:A:82:ILE:HG23	1.92	0.51
1:A:222:ILE:HD12	1:A:226:ILE:HG21	1.94	0.50
1:A:48:GLU:O	1:A:52:LEU:HD22	2.12	0.49
1:A:115:LEU:HD11	1:A:127:VAL:HG21	1.95	0.48
1:A:319:LEU:HD11	1:A:331:PHE:HE2	1.78	0.48
1:A:146:ASN:HD22	1:A:146:ASN:C	2.21	0.48
1:A:366:ARG:NE	1:A:413:ARG:HG3	2.29	0.47
1:A:413:ARG:HG2	1:A:424:GLU:OE1	2.14	0.47
1:A:127:VAL:O	1:A:127:VAL:HG13	2.15	0.46
1:A:257:PRO:HA	1:A:258:ASP:HA	1.59	0.46
1:A:413:ARG:O	1:A:417:ARG:HB2	2.15	0.46
1:A:326:ARG:HH22	1:A:426:GLU:CD	2.24	0.46
1:A:222:ILE:HG21	1:A:237:LEU:HD21	1.98	0.45
1:A:240:ASN:C	1:A:242:LEU:H	2.25	0.45
1:A:148:ASP:CG	1:A:168:ARG:HG3	2.40	0.45
1:A:74:LEU:HD13	1:A:92:LEU:HD21	1.98	0.45
1:A:436:ALA:HA	1:A:441:LEU:HD12	1.99	0.44
1:A:92:LEU:H	1:A:110:ASN:HD22	1.64	0.44
1:A:327:ASN:N	1:A:328:THR:C	2.76	0.44
1:A:279:PRO:HA	1:A:280:LEU:HA	1.69	0.44
1:A:288:PHE:HB3	1:A:289:PRO:CA	2.43	0.43
1:A:195:LEU:HD13	1:A:237:LEU:HD11	2.00	0.43
1:A:110:ASN:HB2	1:A:130:ASN:ND2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ALA:O	1:A:468:VAL:HG23	2.19	0.42
1:A:217:ASN:HB2	1:A:240:ASN:HD21	1.84	0.42
1:A:389:ASP:HA	1:A:390:ASN:HA	1.81	0.42
1:A:256:GLN:HA	1:A:257:PRO:HD3	1.93	0.41
1:A:249:SER:O	1:A:253:GLN:HG2	2.20	0.41
1:A:327:ASN:H	1:A:328:THR:C	2.28	0.41
1:A:145:ILE:HB	1:A:165:LEU:HD23	2.03	0.41
1:A:223:PRO:HB2	1:A:225:ASN:OD1	2.21	0.41
1:A:158:LEU:HG	1:A:176:PRO:HG2	2.02	0.41
1:A:382:GLN:HB3	1:A:387:LEU:HD22	2.02	0.41
1:A:288:PHE:CB	1:A:289:PRO:HA	2.44	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	465/571 (81%)	434 (93%)	29 (6%)	2 (0%)	30 60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	THR
1	A	241	PRO

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	387/496 (78%)	339 (88%)	48 (12%)	4 16

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	53	LEU
1	A	71	LEU
1	A	74	LEU
1	A	78	LEU
1	A	81	GLN
1	A	83	THR
1	A	102	LEU
1	A	105	LEU
1	A	109	ASP
1	A	122	LEU
1	A	125	LEU
1	A	127	VAL
1	A	146	ASN
1	A	155	LEU
1	A	165	LEU
1	A	167	VAL
1	A	168	ARG
1	A	182	LEU
1	A	185	LEU
1	A	191	LEU
1	A	211	PHE
1	A	219	ILE
1	A	234	THR
1	A	235	ILE
1	A	237	LEU
1	A	247	ARG
1	A	311	THR
1	A	319	LEU
1	A	323	VAL
1	A	348	LEU
1	A	350	GLN
1	A	363	CYS
1	A	379	LEU
1	A	389	ASP
1	A	395	LEU

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Mol	Chain	Res	Type
1	A	397	SER
1	A	398	LEU
1	A	409	GLU
1	A	413	ARG
1	A	416	VAL
1	A	433	THR
1	A	461	LEU
1	A	462	ARG
1	A	471	ARG
1	A	477	THR
1	A	482	LEU
1	A	551	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	65	GLN
1	A	81	GLN
1	A	110	ASN
1	A	130	ASN
1	A	146	ASN
1	A	240	ASN
1	A	253	GLN
1	A	327	ASN
1	A	372	ASN
1	A	373	ASN
1	A	381	HIS
1	A	474	ASN

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 [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 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	469/571 (82%)	1.11	79 (16%) 4 3	40, 64, 99, 103	6 (1%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	SER	7.6
1	A	295	ASP	6.8
1	A	258	ASP	6.8
1	A	506	TYR	6.3
1	A	279	PRO	6.2
1	A	289	PRO	6.0
1	A	296	VAL	5.3
1	A	208	THR	4.9
1	A	285	THR	4.9
1	A	497	ARG	4.6
1	A	328	THR	4.5
1	A	329	SER	4.5
1	A	248	GLU	4.3
1	A	561	LEU	4.2
1	A	439	LEU	4.0
1	A	310	ASN	4.0
1	A	313	SER	4.0
1	A	317	ASP	4.0
1	A	542	ARG	4.0
1	A	365	ASP	3.9
1	A	392	THR	3.9
1	A	361	GLU	3.8
1	A	280	LEU	3.8
1	A	305	HIS	3.6
1	A	299	ILE	3.4
1	A	333	GLU	3.4
1	A	481	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	335	VAL	3.3
1	A	256	GLN	3.3
1	A	364	GLU	3.2
1	A	391	ASP	3.2
1	A	281	ALA	3.2
1	A	330	GLY	3.1
1	A	454	SER	3.0
1	A	231	PRO	3.0
1	A	362	SER	3.0
1	A	359	ALA	3.0
1	A	257	PRO	2.9
1	A	283	ALA	2.9
1	A	314	ALA	2.9
1	A	548	ILE	2.9
1	A	559	LEU	2.9
1	A	302	ALA	2.9
1	A	496	ASP	2.9
1	A	358	ASP	2.8
1	A	262	PRO	2.8
1	A	547	GLN	2.7
1	A	558	ALA	2.7
1	A	455	GLY	2.7
1	A	503	GLU	2.6
1	A	25	THR	2.6
1	A	360	THR	2.6
1	A	388	PHE	2.6
1	A	301	HIS	2.6
1	A	252	GLN	2.5
1	A	495	ALA	2.5
1	A	311	THR	2.4
1	A	282	ASP	2.4
1	A	284	VAL	2.4
1	A	555	GLU	2.3
1	A	304	GLU	2.3
1	A	504	GLN	2.3
1	A	209	GLU	2.3
1	A	288	PHE	2.2
1	A	177	GLU	2.2
1	A	552	LEU	2.2
1	A	160	THR	2.2
1	A	389	ASP	2.2
1	A	493	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	300	TRP	2.2
1	A	199	PRO	2.1
1	A	498	TRP	2.1
1	A	180	GLU	2.1
1	A	336	ALA	2.1
1	A	499	ALA	2.1
1	A	321	ASP	2.1
1	A	544	THR	2.1
1	A	298	GLN	2.0
1	A	417	ARG	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.