



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:05 AM UTC

PDB ID : 4JPP / pdb_00004jpp
Title : Bacteriophage phiX174 H protein residues 143-282
Authors : Sun, L.; Young, L.N.; Boudko, S.B.; Fokine, A.; Zhang, X.; Rossmann, M.G.;
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Deposited on : 2013-03-19
Resolution : 2.40 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

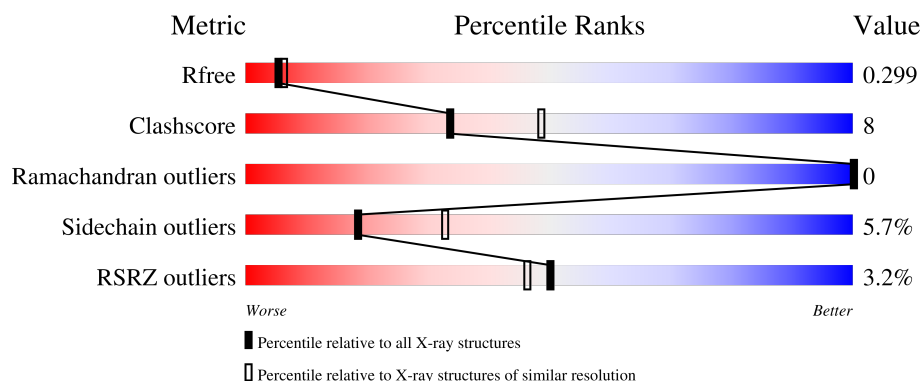
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	140	 71% 16% • 9%
1	B	140	 72% 15% • 9%
1	C	140	 71% 14% • 13%
1	D	140	 75% 15% • 8%
1	E	140	 71% 14% • 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5545 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 Minor spike protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			1018	612	185	214	7			
1	B	127	Total	C	N	O	S	0	0	0
			1023	616	185	215	7			
1	C	122	Total	C	N	O	S	0	0	0
			978	589	176	206	7			
1	D	129	Total	C	N	O	S	0	0	0
			1034	623	187	217	7			
1	E	121	Total	C	N	O	S	0	0	0
			974	587	175	205	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	115	Total	O	0	0
			115	115		
2	B	98	Total	O	0	0
			98	98		
2	C	95	Total	O	0	0
			95	95		
2	D	103	Total	O	0	0
			103	103		
2	E	107	Total	O	0	0
			107	107		

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 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.

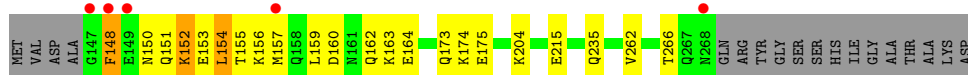
- Molecule 1: Minor spike protein H



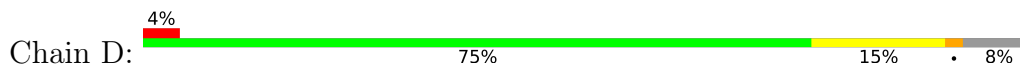
- Molecule 1: Minor spike protein H



- Molecule 1: Minor spike protein H



- Molecule 1: Minor spike protein H



- Molecule 1: Minor spike protein H



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	68.70Å 68.70Å 372.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40 8.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.8 (8.00-2.40) 92.9 (8.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.16 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.245 , 0.290 0.258 , 0.299	Depositor DCC
R_{free} test set	1737 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.48 , 79.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5545	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.31% 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	0.82	2/1023 (0.2%)	0.94	3/1371 (0.2%)
1	B	0.68	0/1029	0.92	2/1379 (0.1%)
1	C	0.74	0/983	0.88	0/1317
1	D	0.74	0/1040	0.86	0/1394
1	E	0.73	0/979	0.89	0/1312
All	All	0.74	2/5054 (0.0%)	0.90	5/6773 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	GLU	C-O	7.52	1.32	1.24
1	A	196	ASN	C-O	5.59	1.30	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	GLU	N-CA-C	-6.11	104.62	111.28
1	A	199	LEU	CA-C-N	-5.75	112.58	120.28
1	A	199	LEU	C-N-CA	-5.75	112.58	120.28
1	B	158	GLN	N-CA-C	5.34	117.10	111.28
1	A	145	ASP	N-CA-C	5.03	116.68	108.63

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	1018	0	997	15	0
1	B	1023	0	997	25	0
1	C	978	0	958	18	0
1	D	1034	0	1009	20	0
1	E	974	0	955	18	0
2	A	115	0	0	5	0
2	B	98	0	0	4	0
2	C	95	0	0	1	0
2	D	103	0	0	4	0
2	E	107	0	0	5	0
All	All	5545	0	4916	77	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 8.

All (77) 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:165:ILE:HA	1:A:168:MET:HE2	1.58	0.86
1:B:150:ASN:OD1	1:B:151:GLN:N	2.08	0.86
2:A:395:HOH:O	1:B:229:MET:SD	2.37	0.82
1:A:154:LEU:HA	1:A:157:MET:HE2	1.67	0.74
1:B:155:THR:HG21	1:C:154:LEU:HD23	1.70	0.71
1:D:157:MET:HG3	2:D:383:HOH:O	1.95	0.65
1:D:270:ARG:HE	1:E:264:GLN:NE2	1.94	0.65
1:D:230:ARG:NH2	2:D:364:HOH:O	2.30	0.64
1:B:148:PHE:CE1	1:C:150:ASN:HB3	2.33	0.64
1:C:163:LYS:NZ	1:D:164:GLU:OE1	2.28	0.62
1:E:154:LEU:O	1:E:157:MET:HG2	2.00	0.61
1:C:159:LEU:HD13	1:D:161:ASN:HB2	1.81	0.61
1:E:174:LYS:NZ	2:E:380:HOH:O	2.32	0.61
1:C:159:LEU:O	1:D:161:ASN:ND2	2.34	0.60
1:A:196:ASN:O	1:A:199:LEU:HB3	2.02	0.60
1:C:148:PHE:O	1:C:151:GLN:HB2	2.04	0.58
2:B:357:HOH:O	1:C:164:GLU:HB2	2.03	0.58
1:E:148:PHE:N	1:E:151:GLN:HE21	2.03	0.56
1:C:173:GLN:HB3	1:D:176:ILE:HD11	1.88	0.55
1:C:151:GLN:HB3	1:D:154:LEU:HD11	1.88	0.55
2:A:367:HOH:O	1:B:204:LYS:HD2	2.07	0.54
1:A:235:GLN:HB2	2:A:395:HOH:O	2.07	0.54
1:A:163:LYS:NZ	1:A:167:GLU:OE2	2.41	0.54
1:A:205:GLU:HG2	1:A:209:ARG:NH1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LEU:O	1:B:158:GLN:HG3	2.08	0.53
1:B:155:THR:HG21	1:C:154:LEU:CD2	2.39	0.53
1:B:160:ASP:O	1:B:164:GLU:HG2	2.10	0.52
1:D:265:GLN:HA	2:D:390:HOH:O	2.10	0.52
1:A:162:GLN:NE2	2:A:386:HOH:O	2.42	0.52
1:D:150:ASN:OD1	1:D:151:GLN:HG2	2.09	0.52
1:E:161:ASN:O	1:E:165:ILE:HD12	2.10	0.51
1:E:214:MET:SD	2:E:321:HOH:O	2.59	0.51
1:E:161:ASN:O	1:E:164:GLU:HG2	2.10	0.51
1:A:174:LYS:HA	1:B:176:ILE:HD11	1.93	0.50
1:B:147:GLY:O	1:B:150:ASN:CG	2.55	0.50
1:B:270:ARG:HG2	1:B:271:TYR:CZ	2.46	0.50
1:E:161:ASN:HA	1:E:164:GLU:HG2	1.94	0.50
1:B:221:LYS:NZ	2:B:322:HOH:O	2.44	0.49
1:B:152:LYS:O	1:B:155:THR:HB	2.13	0.49
1:C:159:LEU:HD11	1:D:158:GLN:HA	1.93	0.49
1:D:185:ARG:HD2	1:E:187:ASN:OD1	2.12	0.49
1:D:268:ASN:HB2	2:D:390:HOH:O	2.11	0.49
1:A:231:GLN:HB3	1:B:229:MET:HE3	1.95	0.49
1:B:270:ARG:HG2	1:B:271:TYR:CE1	2.50	0.47
1:D:148:PHE:CD1	1:E:150:ASN:HB3	2.49	0.47
1:C:148:PHE:HZ	1:D:153:GLU:OE2	1.98	0.47
1:B:147:GLY:O	1:B:150:ASN:ND2	2.49	0.47
1:A:163:LYS:NZ	1:B:168:MET:SD	2.87	0.46
1:E:230:ARG:HD3	2:E:401:HOH:O	2.15	0.46
1:D:225:VAL:O	1:D:229:MET:HG2	2.16	0.45
1:B:152:LYS:HB3	1:B:152:LYS:HE2	1.32	0.45
1:E:250:GLU:OE2	2:E:310:HOH:O	2.21	0.45
1:B:172:THR:O	1:B:176:ILE:HG12	2.17	0.45
1:A:156:LYS:NZ	1:A:160:ASP:OD2	2.50	0.44
1:D:254:LYS:HE2	1:D:258:GLU:OE2	2.17	0.44
1:A:174:LYS:HG2	1:B:176:ILE:HD11	2.00	0.43
1:C:235:GLN:HG2	2:C:377:HOH:O	2.18	0.43
1:E:157:MET:HE2	1:E:157:MET:HB3	1.80	0.43
1:B:174:LYS:NZ	1:C:175:GLU:OE1	2.50	0.43
1:E:204:LYS:HE2	1:E:204:LYS:HB3	1.86	0.43
1:E:205:GLU:HG2	1:E:209:ARG:NH1	2.34	0.43
1:E:244:THR:O	1:E:248:ILE:HG13	2.18	0.43
1:C:152:LYS:HE2	1:C:152:LYS:HB3	1.77	0.42
1:B:202:GLN:HA	2:B:358:HOH:O	2.18	0.42
1:A:255:VAL:O	1:A:259:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLU:OE1	2:B:390:HOH:O	2.22	0.42
1:B:270:ARG:HE	1:B:270:ARG:HB2	1.52	0.42
1:A:169:GLN:HB2	2:A:378:HOH:O	2.20	0.42
1:C:262:VAL:O	1:C:266:THR:HG23	2.20	0.41
1:C:204:LYS:HE2	1:C:204:LYS:HB3	1.83	0.41
1:A:153:GLU:O	1:A:157:MET:HG3	2.20	0.41
1:D:193:TYR:O	1:D:197:GLU:HG2	2.21	0.41
1:E:162:GLN:NE2	2:E:400:HOH:O	2.52	0.41
1:D:270:ARG:HE	1:E:264:GLN:HE22	1.64	0.41
1:D:229:MET:HG2	1:D:229:MET:H	1.72	0.41
1:C:160:ASP:O	1:C:164:GLU:HG2	2.21	0.40
1:B:192:VAL:O	1:B:195:GLN:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	125/140 (89%)	124 (99%)	1 (1%)	0	100	100
1	B	125/140 (89%)	123 (98%)	2 (2%)	0	100	100
1	C	120/140 (86%)	120 (100%)	0	0	100	100
1	D	127/140 (91%)	125 (98%)	2 (2%)	0	100	100
1	E	119/140 (85%)	116 (98%)	3 (2%)	0	100	100
All	All	616/700 (88%)	608 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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 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	113/122 (93%)	106 (94%)	7 (6%)	16	29
1	B	113/122 (93%)	107 (95%)	6 (5%)	20	36
1	C	109/122 (89%)	99 (91%)	10 (9%)	8	14
1	D	114/122 (93%)	108 (95%)	6 (5%)	20	36
1	E	109/122 (89%)	106 (97%)	3 (3%)	38	60
All	All	558/610 (92%)	526 (94%)	32 (6%)	18	33

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	VAL
1	A	151	GLN
1	A	154	LEU
1	A	162	GLN
1	A	164	GLU
1	A	179	ILE
1	A	267	GLN
1	B	148	PHE
1	B	149	GLU
1	B	152	LYS
1	B	163	LYS
1	B	167	GLU
1	B	270	ARG
1	C	148	PHE
1	C	152	LYS
1	C	153	GLU
1	C	154	LEU
1	C	155	THR
1	C	156	LYS
1	C	157	MET
1	C	162	GLN
1	C	174	LYS
1	C	215	GLU

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Mol	Chain	Res	Type
1	D	150	ASN
1	D	154	LEU
1	D	155	THR
1	D	215	GLU
1	D	229	MET
1	D	267	GLN
1	E	151	GLN
1	E	154	LEU
1	E	215	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	B	247	GLN
1	B	268	ASN
1	C	151	GLN
1	C	161	ASN
1	C	162	GLN
1	C	169	GLN
1	C	173	GLN
1	C	247	GLN
1	D	158	GLN
1	D	241	GLN
1	D	247	GLN
1	E	158	GLN
1	E	162	GLN
1	E	241	GLN
1	E	247	GLN
1	E	264	GLN

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	127/140 (90%)	0.08	2 (1%) 70 66	26, 42, 78, 90	0
1	B	127/140 (90%)	0.09	5 (3%) 43 39	27, 40, 81, 124	0
1	C	122/140 (87%)	0.19	5 (4%) 41 37	27, 42, 96, 139	0
1	D	129/140 (92%)	0.16	6 (4%) 36 32	27, 42, 82, 109	0
1	E	121/140 (86%)	0.12	2 (1%) 69 65	27, 42, 79, 103	0
All	All	626/700 (89%)	0.13	20 (3%) 50 46	26, 42, 82, 139	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	147	GLY	4.0
1	C	268	ASN	3.7
1	D	150	ASN	3.3
1	C	149	GLU	3.3
1	B	150	ASN	3.3
1	B	146	ALA	3.0
1	A	145	ASP	2.9
1	C	147	GLY	2.8
1	B	148	PHE	2.5
1	C	148	PHE	2.5
1	D	149	GLU	2.4
1	E	155	THR	2.4
1	B	151	GLN	2.4
1	C	157	MET	2.3
1	D	144	VAL	2.3
1	B	147	GLY	2.1
1	D	146	ALA	2.1
1	A	150	ASN	2.1
1	E	268	ASN	2.1
1	D	172	THR	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.