



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:12 AM UTC

PDB ID : 9VNP / pdb_00009vnp
Title : The complexes of IFN-gamma and A01BM-03 Fab
Authors : Wang, X.; Zhang, L.; Wang, H.; Yu, J.
Deposited on : 2025-06-30
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
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

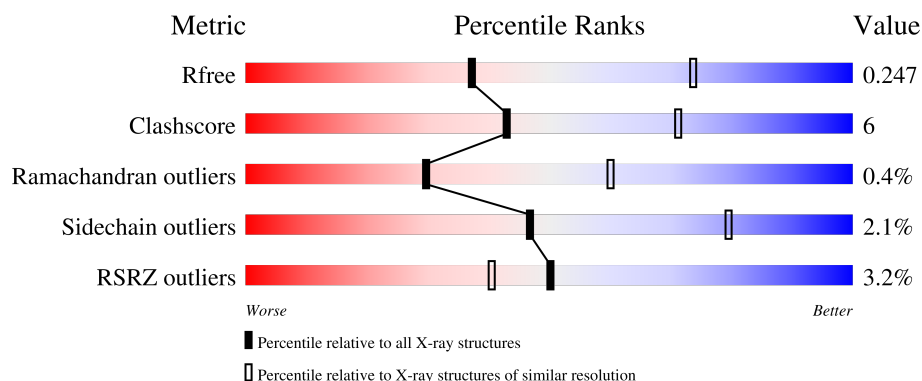
1 Overall quality at a glance

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	L	192	2% 45% 5% 50%
2	A	218	3% 86% 13% .
3	C	223	4% 83% 12% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4117 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 Interferon gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	96	Total	C	N	O	S	0	0	0
			804	515	135	151	3			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	137	GLN	ARG	variant	UNP P01579
L	144	HIS	-	expression tag	UNP P01579
L	145	HIS	-	expression tag	UNP P01579
L	146	HIS	-	expression tag	UNP P01579
L	147	HIS	-	expression tag	UNP P01579
L	148	HIS	-	expression tag	UNP P01579
L	149	HIS	-	expression tag	UNP P01579
L	150	HIS	-	expression tag	UNP P01579
L	151	HIS	-	expression tag	UNP P01579
L	152	SER	-	expression tag	UNP P01579
L	153	ALA	-	expression tag	UNP P01579
L	154	TRP	-	expression tag	UNP P01579
L	155	SER	-	expression tag	UNP P01579
L	156	HIS	-	expression tag	UNP P01579
L	157	PRO	-	expression tag	UNP P01579
L	158	GLN	-	expression tag	UNP P01579
L	159	PHE	-	expression tag	UNP P01579
L	160	GLU	-	expression tag	UNP P01579
L	161	LYS	-	expression tag	UNP P01579
L	162	GLY	-	expression tag	UNP P01579
L	163	GLY	-	expression tag	UNP P01579
L	164	GLY	-	expression tag	UNP P01579
L	165	SER	-	expression tag	UNP P01579
L	166	GLY	-	expression tag	UNP P01579
L	167	GLY	-	expression tag	UNP P01579
L	168	GLY	-	expression tag	UNP P01579
L	169	GLY	-	expression tag	UNP P01579

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Chain	Residue	Modelled	Actual	Comment	Reference
L	170	SER	-	expression tag	UNP P01579
L	171	GLY	-	expression tag	UNP P01579
L	172	GLY	-	expression tag	UNP P01579
L	173	SER	-	expression tag	UNP P01579
L	174	ALA	-	expression tag	UNP P01579
L	175	TRP	-	expression tag	UNP P01579
L	176	SER	-	expression tag	UNP P01579
L	177	HIS	-	expression tag	UNP P01579
L	178	PRO	-	expression tag	UNP P01579
L	179	GLN	-	expression tag	UNP P01579
L	180	PHE	-	expression tag	UNP P01579
L	181	GLU	-	expression tag	UNP P01579
L	182	LYS	-	expression tag	UNP P01579
L	183	GLY	-	expression tag	UNP P01579
L	184	SER	-	expression tag	UNP P01579
L	185	ASP	-	expression tag	UNP P01579
L	186	TYR	-	expression tag	UNP P01579
L	187	LYS	-	expression tag	UNP P01579
L	188	ASP	-	expression tag	UNP P01579
L	189	ASP	-	expression tag	UNP P01579
L	190	ASP	-	expression tag	UNP P01579
L	191	ASP	-	expression tag	UNP P01579
L	192	LYS	-	expression tag	UNP P01579

- Molecule 2 is a protein called Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	216	Total	C	N	O	S	0	0	0
			1631	1020	268	338	5			

- Molecule 3 is a protein called Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	216	Total	C	N	O	S	0	0	0
			1639	1033	279	319	8			

- Molecule 4 is water.

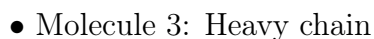
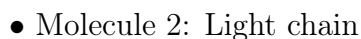
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	C	16	Total	O	0	0
			16	16		

- Molecule 1: Interferon gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	127.33Å 59.10Å 77.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.00 – 2.80 32.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (32.00-2.80) 99.6 (32.00-2.80)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.76Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.229 , 0.248 0.228 , 0.247	Depositor DCC
R_{free} test set	725 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4117	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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

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	L	0.86	0/816	1.17	0/1088
2	A	0.92	0/1672	1.14	0/2284
3	C	0.93	0/1677	1.17	0/2281
All	All	0.91	0/4165	1.16	0/5653

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	L	804	0	817	5	2
2	A	1631	0	1558	22	0
3	C	1639	0	1621	23	1
4	A	22	0	0	1	0
4	C	16	0	0	3	0
4	L	5	0	0	3	0
All	All	4117	0	3996	50	3

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 6.

All (50) 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)
3:C:200:THR:HG22	3:C:217:ARG:NH2	1.62	1.14
2:A:29:ILE:HD11	2:A:74:ALA:HB2	1.42	0.99
3:C:200:THR:CG2	3:C:217:ARG:NH2	2.43	0.82
3:C:200:THR:HG22	3:C:217:ARG:HH21	1.46	0.80
3:C:13:GLN:HB2	3:C:16:LYS:HG3	1.64	0.80
2:A:29:ILE:CD1	2:A:74:ALA:HB2	2.15	0.76
2:A:145:PHE:CE2	2:A:150:VAL:HG23	2.22	0.74
2:A:29:ILE:HD11	2:A:74:ALA:CB	2.19	0.72
3:C:13:GLN:HB2	3:C:16:LYS:CG	2.21	0.71
2:A:145:PHE:CE2	2:A:150:VAL:CG2	2.73	0.70
2:A:64:SER:OG	2:A:77:ILE:HB	1.92	0.68
3:C:97:GLY:HA3	3:C:107:LEU:HD23	1.75	0.68
3:C:119:SER:C	4:C:301:HOH:O	2.43	0.62
1:L:82:PHE:O	1:L:84:SER:N	2.33	0.61
1:L:121:SER:C	4:L:201:HOH:O	2.46	0.57
2:A:86:GLU:HG3	2:A:111:VAL:HG23	1.86	0.56
2:A:145:PHE:CE2	2:A:150:VAL:HG21	2.41	0.55
3:C:119:SER:CB	4:C:301:HOH:O	2.56	0.52
3:C:11:VAL:HA	3:C:117:THR:O	2.10	0.52
3:C:200:THR:HG22	3:C:217:ARG:CZ	2.38	0.51
3:C:87:ARG:O	3:C:118:VAL:HG11	2.11	0.51
2:A:213:ALA:O	2:A:216:GLU:HG3	2.11	0.50
2:A:157:ASP:CG	2:A:195:ARG:HE	2.19	0.50
1:L:97:ASN:C	4:L:202:HOH:O	2.55	0.49
2:A:36:TRP:HB2	2:A:49:ILE:HB	1.96	0.48
3:C:91:THR:OG1	3:C:118:VAL:HG12	2.13	0.48
3:C:99:ASP:O	3:C:100:SER:CB	2.61	0.48
2:A:29:ILE:HD13	2:A:73:SER:C	2.39	0.47
3:C:91:THR:HG23	3:C:117:THR:HA	1.97	0.47
2:A:64:SER:HG	2:A:77:ILE:HB	1.80	0.46
2:A:145:PHE:CZ	2:A:150:VAL:HG21	2.51	0.46
1:L:97:ASN:HB3	4:L:202:HOH:O	2.16	0.45
2:A:4:LEU:HB3	2:A:22:CYS:SG	2.58	0.44
2:A:126:PRO:HD3	2:A:138:LEU:HD23	2.00	0.44
3:C:53:PRO:CG	3:C:102:VAL:HG13	2.48	0.43
2:A:215:THR:HA	4:A:303:HOH:O	2.18	0.43
2:A:60:PRO:HB2	2:A:62:ARG:HG2	2.01	0.43
3:C:36:TRP:CD1	3:C:81:LEU:HD13	2.53	0.43
2:A:150:VAL:CG1	2:A:201:VAL:HG13	2.48	0.43
3:C:53:PRO:HA	3:C:72:ARG:HH22	1.84	0.43
2:A:108:LYS:HE2	2:A:108:LYS:HB3	1.91	0.42
2:A:114:GLN:HE21	2:A:114:GLN:HB3	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:53:PRO:HG2	3:C:102:VAL:HG13	2.02	0.41
3:C:119:SER:CA	4:C:301:HOH:O	2.69	0.41
1:L:115:GLN:O	1:L:119:GLU:HG2	2.21	0.41
3:C:12:VAL:HG13	3:C:118:VAL:HB	2.03	0.41
2:A:151:THR:OG1	2:A:202:THR:HB	2.20	0.40
3:C:50:LEU:HD11	3:C:104:ILE:HG23	2.03	0.40
3:C:99:ASP:HA	3:C:106:GLY:O	2.21	0.40
3:C:121:ALA:HB3	3:C:153:PHE:CE2	2.57	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:142:THR:OG1	3:C:142:THR:OG1[2_465]	1.98	0.22
1:L:80:LYS:CE	1:L:117:MET:O[2_555]	2.18	0.02
1:L:46:GLN:NE2	1:L:119:GLU:O[2_555]	2.19	0.01

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	L	94/192 (49%)	89 (95%)	4 (4%)	1 (1%)	11	36
2	A	214/218 (98%)	211 (99%)	3 (1%)	0	100	100
3	C	212/223 (95%)	204 (96%)	7 (3%)	1 (0%)	24	55
All	All	520/633 (82%)	504 (97%)	14 (3%)	2 (0%)	30	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	83	ASN
3	C	100	SER

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	L	92/167 (55%)	92 (100%)	0	100	100
2	A	185/187 (99%)	182 (98%)	3 (2%)	55	83
3	C	189/196 (96%)	182 (96%)	7 (4%)	30	65
All	All	466/550 (85%)	456 (98%)	10 (2%)	47	79

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	32	TYR
2	A	86	GLU
2	A	208	VAL
3	C	118	VAL
3	C	119	SER
3	C	142	THR
3	C	147	CYS
3	C	157	VAL
3	C	188	VAL
3	C	203	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	54	GLN
2	A	114	GLN
2	A	200	GLN
3	C	3	GLN
3	C	13	GLN
3	C	84	HIS
3	C	199	GLN

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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	L	96/192 (50%)	0.60	3 (3%)	51	41	40, 58, 97, 104	0
2	A	216/218 (99%)	0.36	6 (2%)	55	45	34, 47, 64, 76	0
3	C	216/223 (96%)	0.55	8 (3%)	45	36	30, 50, 77, 105	0
All	All	528/633 (83%)	0.48	17 (3%)	50	40	30, 50, 76, 105	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	119	SER	6.1
2	A	158	SER	3.7
1	L	97	ASN	3.2
3	C	62	ASP	3.0
3	C	72	ARG	2.8
3	C	123	THR	2.6
1	L	66	ILE	2.6
2	A	51	GLU	2.5
3	C	223	CYS	2.5
3	C	197	GLY	2.3
1	L	83	ASN	2.3
2	A	162	LYS	2.3
2	A	195	ARG	2.1
3	C	71	SER	2.1
3	C	1	GLN	2.1
2	A	52	ASP	2.0
2	A	97	ASP	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.