wwPDB X-ray Structure Validation Summary Report (i)

Oct 27, 2026 – 06:03 PM EDT

PDB ID	:	37IR / pdb_000037ir
Title	:	Crystal structure of Interferon alpha8 bound to IFA003 ScFv
Authors	:	Vasquez, S.; Rubio, A.A.; Barnes, C.O.
Deposited on	:	2026-07-22
Resolution	:	2.08 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

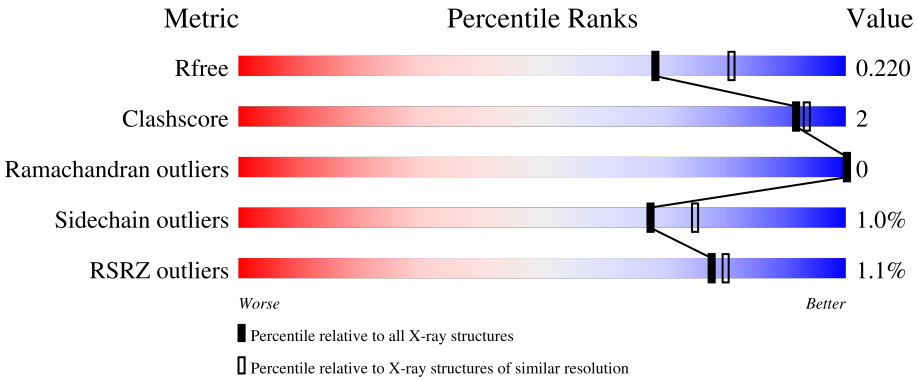
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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 <=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	206	% 71% . 27%
2	H	138	80% 6% 14%
3	L	118	% 86% 6% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3118 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 alpha-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1164	747	193	216	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	167	GLU	-	expression tag	UNP P32881
A	168	ASN	-	expression tag	UNP P32881
A	169	LEU	-	expression tag	UNP P32881
A	170	TYR	-	expression tag	UNP P32881
A	171	PHE	-	expression tag	UNP P32881
A	172	GLN	-	expression tag	UNP P32881
A	173	GLY	-	expression tag	UNP P32881
A	174	GLY	-	expression tag	UNP P32881
A	175	GLY	-	expression tag	UNP P32881
A	176	GLY	-	expression tag	UNP P32881
A	177	GLY	-	expression tag	UNP P32881
A	178	SER	-	expression tag	UNP P32881
A	179	GLY	-	expression tag	UNP P32881
A	180	GLY	-	expression tag	UNP P32881
A	181	GLY	-	expression tag	UNP P32881
A	182	GLY	-	expression tag	UNP P32881
A	183	SER	-	expression tag	UNP P32881
A	184	HIS	-	expression tag	UNP P32881
A	185	HIS	-	expression tag	UNP P32881
A	186	HIS	-	expression tag	UNP P32881
A	187	HIS	-	expression tag	UNP P32881
A	188	HIS	-	expression tag	UNP P32881
A	189	HIS	-	expression tag	UNP P32881
A	190	HIS	-	expression tag	UNP P32881
A	191	HIS	-	expression tag	UNP P32881
A	192	GLY	-	expression tag	UNP P32881
A	193	LEU	-	expression tag	UNP P32881

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	ASN	-	expression tag	UNP P32881
A	195	ASP	-	expression tag	UNP P32881
A	196	ILE	-	expression tag	UNP P32881
A	197	PHE	-	expression tag	UNP P32881
A	198	GLU	-	expression tag	UNP P32881
A	199	ALA	-	expression tag	UNP P32881
A	200	GLN	-	expression tag	UNP P32881
A	201	LYS	-	expression tag	UNP P32881
A	202	ILE	-	expression tag	UNP P32881
A	203	GLU	-	expression tag	UNP P32881
A	204	TRP	-	expression tag	UNP P32881
A	205	HIS	-	expression tag	UNP P32881
A	206	GLU	-	expression tag	UNP P32881

- Molecule 2 is a protein called IFA003 variable heavy chain ScFv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	118	Total	C	N	O	S	0	1	0
			913	574	161	173	5			

- Molecule 3 is a protein called IFA003 variable light chain ScFv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	109	Total	C	N	O	S	0	0	0
			808	502	141	162	3			

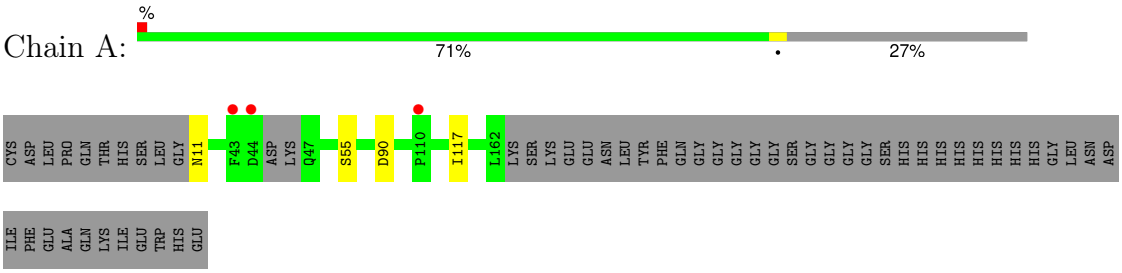
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total	O	0	0
			70	70		
4	H	95	Total	O	0	0
			95	95		
4	L	68	Total	O	0	0
			68	68		

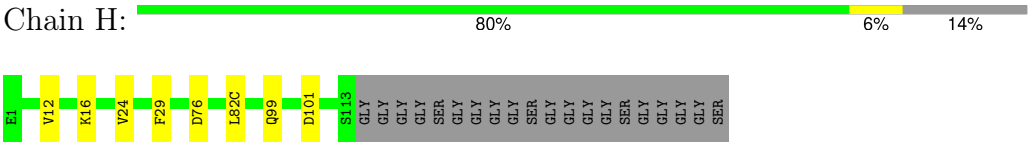
3 Residue-property plots (i)

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.

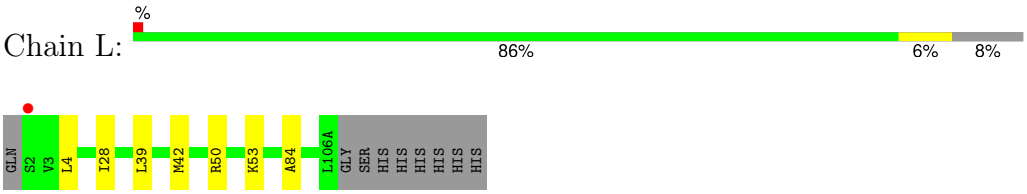
• Molecule 1: Interferon alpha-8



• Molecule 2: IFA003 variable heavy chain ScFv



• Molecule 3: IFA003 variable light chain ScFv



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	37.83Å 66.31Å 164.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.91 – 2.08 34.91 – 2.08	Depositor EDS
% Data completeness (in resolution range)	98.6 (34.91-2.08) 98.6 (34.91-2.08)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.180 , 0.219 0.181 , 0.220	Depositor DCC
R_{free} test set	1268 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	21.3	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3118	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	A	0.24	0/1183	0.39	0/1598
2	H	0.30	0/935	0.52	0/1265
3	L	0.31	0/827	0.49	0/1126
All	All	0.28	0/2945	0.46	0/3989

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	1164	0	1102	1	0
2	H	913	0	859	4	0
3	L	808	0	767	4	0
4	A	70	0	0	0	0
4	H	95	0	0	1	0
4	L	68	0	0	1	0
All	All	3118	0	2728	9	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 2.

The worst 5 of 9 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:55:SER:HB3	1:A:117:ILE:HD11	1.69	0.74
3:L:39:LEU:HD23	3:L:84:ALA:HB2	1.91	0.53
2:H:12:VAL:HG11	2:H:82(C):LEU:HD13	1.91	0.52
3:L:42:MET:HE3	4:L:251:HOH:O	2.12	0.49
2:H:16:LYS:HD2	4:H:258:HOH:O	2.17	0.44

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	146/206 (71%)	144 (99%)	2 (1%)	0	100	100
2	H	117/138 (85%)	116 (99%)	1 (1%)	0	100	100
3	L	107/118 (91%)	104 (97%)	3 (3%)	0	100	100
All	All	370/462 (80%)	364 (98%)	6 (2%)	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 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	119/184 (65%)	117 (98%)	2 (2%)	53	60
2	H	96/104 (92%)	95 (99%)	1 (1%)	68	75
3	L	88/98 (90%)	88 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	303/386 (78%)	300 (99%)	3 (1%)	68 75

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	90	ASP
2	H	24	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
2	H	13	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

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, 95^{th} 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	150/206 (72%)	0.19	3 (2%) 65 67	14, 28, 47, 55	0
2	H	118/138 (85%)	-0.29	0 100 100	8, 20, 36, 50	1 (0%)
3	L	109/118 (92%)	-0.08	1 (0%) 81 83	10, 23, 39, 57	0
All	All	377/462 (81%)	-0.04	4 (1%) 78 80	8, 23, 44, 57	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	110	PRO	2.8
1	A	44	ASP	2.5
1	A	43	PHE	2.2
3	L	2	SER	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.