



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 9GVL / pdb_00009gvl
Title : type-I interferons autoantibody pmab15 in complex with Interferon alpha-2
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Deposited on : 2024-09-25
Resolution : 2.01 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 ⓘ 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

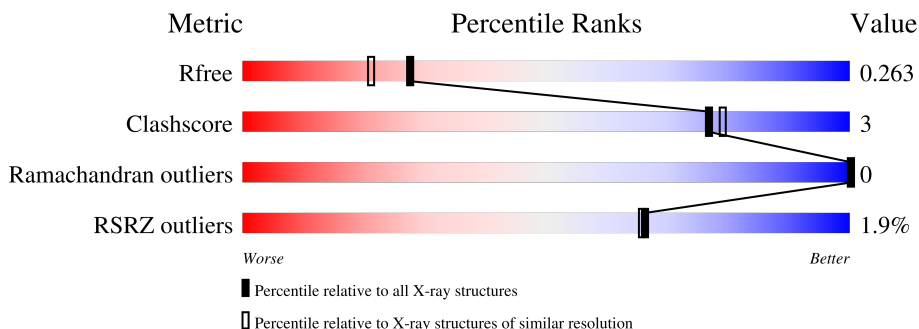
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	188	2% 61%7%32%
1	B	188	2% 63%6%31%
2	H	294	% 75%.21%
2	I	294	% 74%5%20%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5953 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-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			1046	674	176	190	6			
1	B	130	Total	C	N	O	S	0	0	0
			1046	673	174	193	6			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	GLY	-	expression tag	UNP P01563
A	167	GLY	-	expression tag	UNP P01563
A	168	GLY	-	expression tag	UNP P01563
A	169	GLY	-	expression tag	UNP P01563
A	170	SER	-	expression tag	UNP P01563
A	171	LEU	-	expression tag	UNP P01563
A	172	VAL	-	expression tag	UNP P01563
A	173	PRO	-	expression tag	UNP P01563
A	174	ARG	-	expression tag	UNP P01563
A	175	GLY	-	expression tag	UNP P01563
A	176	SER	-	expression tag	UNP P01563
A	177	GLY	-	expression tag	UNP P01563
A	178	GLY	-	expression tag	UNP P01563
A	179	GLY	-	expression tag	UNP P01563
A	180	SER	-	expression tag	UNP P01563
A	181	HIS	-	expression tag	UNP P01563
A	182	HIS	-	expression tag	UNP P01563
A	183	HIS	-	expression tag	UNP P01563
A	184	HIS	-	expression tag	UNP P01563
A	185	HIS	-	expression tag	UNP P01563
A	186	HIS	-	expression tag	UNP P01563
A	187	HIS	-	expression tag	UNP P01563
A	188	HIS	-	expression tag	UNP P01563
B	166	GLY	-	expression tag	UNP P01563
B	167	GLY	-	expression tag	UNP P01563

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Chain	Residue	Modelled	Actual	Comment	Reference
B	168	GLY	-	expression tag	UNP P01563
B	169	GLY	-	expression tag	UNP P01563
B	170	SER	-	expression tag	UNP P01563
B	171	LEU	-	expression tag	UNP P01563
B	172	VAL	-	expression tag	UNP P01563
B	173	PRO	-	expression tag	UNP P01563
B	174	ARG	-	expression tag	UNP P01563
B	175	GLY	-	expression tag	UNP P01563
B	176	SER	-	expression tag	UNP P01563
B	177	GLY	-	expression tag	UNP P01563
B	178	GLY	-	expression tag	UNP P01563
B	179	GLY	-	expression tag	UNP P01563
B	180	SER	-	expression tag	UNP P01563
B	181	HIS	-	expression tag	UNP P01563
B	182	HIS	-	expression tag	UNP P01563
B	183	HIS	-	expression tag	UNP P01563
B	184	HIS	-	expression tag	UNP P01563
B	185	HIS	-	expression tag	UNP P01563
B	186	HIS	-	expression tag	UNP P01563
B	187	HIS	-	expression tag	UNP P01563
B	188	HIS	-	expression tag	UNP P01563

- Molecule 2 is a protein called scFv type-I interferons autoantibody pmab15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	233	Total	C	N	O	S	0	0	0
			1769	1103	314	346	6			
2	I	235	Total	C	N	O	S	0	0	0
			1784	1111	316	351	6			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	33	Total 33	O 33	0	0
5	B	27	Total 27	O 27	0	0
5	H	124	Total 124	O 124	0	0
5	I	103	Total 103	O 103	0	0

- Molecule 1: Interferon alpha-2



GLY	PRO	PHE	GLU	ASP	ASP	ASP	LYS	ALA	GLY	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	GLY	GLY	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	SER	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.16Å 83.72Å 70.26Å 90.00° 113.80° 90.00°	Depositor
Resolution (Å)	14.97 – 2.01 14.97 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.5 (14.97-2.01) 99.2 (14.97-2.01)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.214 , 0.270 0.209 , 0.263	Depositor DCC
R_{free} test set	2428 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5953	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL

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	0.66	0/1066	0.99	0/1433
1	B	0.64	0/1065	1.01	0/1434
2	H	0.72	0/1812	1.04	3/2460 (0.1%)
2	I	0.76	0/1827	1.01	0/2480
All	All	0.71	0/5770	1.01	3/7807 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	30	THR	CA-C-N	6.59	129.40	120.38
2	H	30	THR	C-N-CA	6.59	129.40	120.38
2	H	230	PHE	CA-CB-CG	-5.48	108.32	113.80

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	1046	0	1034	11	0
1	B	1046	0	1023	7	0
2	H	1769	0	1654	7	0
2	I	1784	0	1668	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	0	0
4	B	5	0	0	0	0
4	H	5	0	0	0	0
4	I	5	0	0	0	0
5	A	33	0	0	0	0
5	B	27	0	0	0	0
5	H	124	0	0	0	0
5	I	103	0	0	0	0
All	All	5953	0	5387	32	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 3.

The worst 5 of 32 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)
2:H:173:GLN:NE2	2:I:3:GLU:OE1	2.27	0.68
1:A:57:HIS:CD2	1:A:92:LEU:HD22	2.31	0.64
1:B:57:HIS:CD2	1:B:92:LEU:HD22	2.32	0.64
1:B:57:HIS:CE1	1:B:61:GLN:HE21	2.16	0.63
1:B:57:HIS:CE1	1:B:61:GLN:NE2	2.71	0.58

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	121/188 (64%)	118 (98%)	3 (2%)	0	100	100
1	B	124/188 (66%)	121 (98%)	3 (2%)	0	100	100
2	H	229/294 (78%)	226 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	231/294 (79%)	227 (98%)	4 (2%)	0	100	100
All	All	705/964 (73%)	692 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	B	202	-	4,4,4	0.29	0	6,6,6	0.36	0
4	SO4	H	301	-	4,4,4	0.31	0	6,6,6	0.89	0
3	GOL	B	201	-	5,5,5	0.05	0	5,5,5	0.27	0
4	SO4	I	301	-	4,4,4	0.29	0	6,6,6	0.28	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	201	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	201	GOL	O1-C1-C2-O2
3	B	201	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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	A	127/188 (67%)	0.12	4 (3%) 51 50	33, 55, 83, 92	0
1	B	130/188 (69%)	0.21	3 (2%) 61 60	32, 56, 88, 97	0
2	H	233/294 (79%)	-0.33	3 (1%) 75 74	24, 38, 56, 65	0
2	I	235/294 (79%)	-0.23	4 (1%) 69 68	23, 41, 67, 75	0
All	All	725/964 (75%)	-0.12	14 (1%) 66 66	23, 45, 74, 97	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	127	GLY	3.3
2	H	27	SER	2.9
1	A	39	PRO	2.8
1	A	43	PHE	2.7
1	B	98	CYS	2.4

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	201	6/6	0.43	0.10	79,79,79,79	0
4	SO4	B	202	5/5	0.55	0.12	131,131,131,131	0
4	SO4	H	301	5/5	0.86	0.10	59,59,60,60	0
4	SO4	I	301	5/5	0.89	0.06	95,95,95,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.