



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2025 – 11:05 am BST

PDB ID : 9GVO / pdb_00009gvo
Title : type-I interferons autoantibodies pmab15 and pmab14 in complex with Interferon alpha-2
Authors : Duquerroy, S.; Rey, F.; Ahouzi, O.; Mahevas, M.; Chappert, P.
Deposited on : 2024-09-25
Resolution : 1.81 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

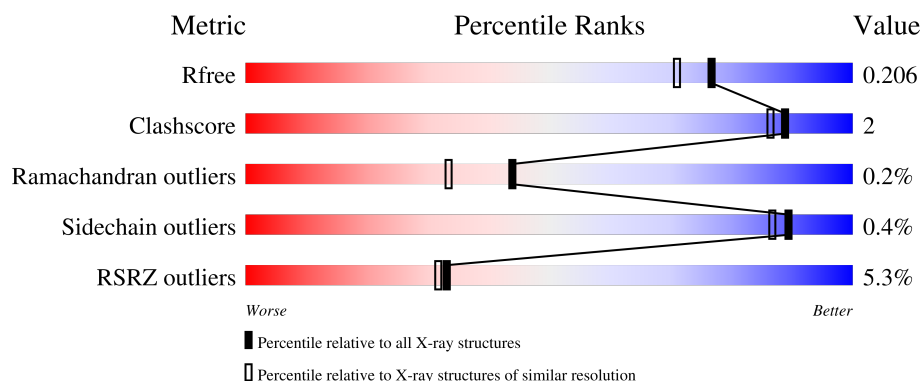
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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}	164625	9242 (1.84-1.80)
Clashscore	180529	1080 (1.82-1.82)
Ramachandran outliers	177936	1073 (1.82-1.82)
Sidechain outliers	177891	1073 (1.82-1.82)
RSRZ outliers	164620	9241 (1.84-1.80)

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	290	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>19%</div> </div> </div>
2	B	188	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>28%</div> </div> </div>
3	H	294	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>19%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5172 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 scFv type-I interferons autoantibody pmab14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	5	0
			1780	1117	299	357	7			

- Molecule 2 is a protein called Interferon alpha-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	135	Total	C	N	O	S	0	3	0
			1137	730	191	208	8			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	166	GLY	-	expression tag	UNP P01563
B	167	GLY	-	expression tag	UNP P01563
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

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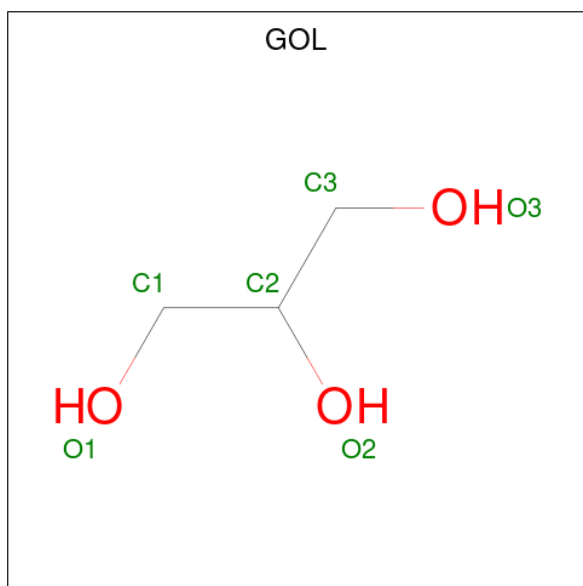
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Chain	Residue	Modelled	Actual	Comment	Reference
B	186	HIS	-	expression tag	UNP P01563
B	187	HIS	-	expression tag	UNP P01563
B	188	HIS	-	expression tag	UNP P01563

- Molecule 3 is a protein called scFv type-I interferons autoantibody pmab15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	237	Total	C	N	O	S	0	4	0
			1824	1138	320	359	7			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	K	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	132	Total	O	0	0
			132	132		
7	B	86	Total	O	0	0
			86	86		
7	H	166	Total	O	0	0
			166	166		

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.93Å 112.93Å 155.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.99 – 1.81 14.99 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.7 (14.99-1.81) 99.5 (14.99-1.81)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.81Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.193 , 0.215 0.182 , 0.206	Depositor DCC
R_{free} test set	5205 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5172	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, GOL, PO4

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	0.71	1/1831 (0.1%)	0.94	1/2487 (0.0%)
2	B	0.77	0/1167	0.95	0/1568
3	H	0.70	0/1878	0.95	0/2547
All	All	0.72	1/4876 (0.0%)	0.94	1/6602 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	PRO	CA-C	5.65	1.54	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	PHE	CA-CB-CG	5.05	118.85	113.80

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	1780	0	1726	5	0
2	B	1137	0	1143	8	0
3	H	1824	0	1715	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	6	0	8	0	0
4	B	24	0	32	2	0
4	H	6	0	8	0	0
5	B	5	0	0	1	0
5	H	5	0	0	0	0
6	B	1	0	0	0	0
7	A	132	0	0	0	0
7	B	86	0	0	0	0
7	H	166	0	0	0	0
All	All	5172	0	4632	17	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.

All (17) 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)
4:B:201:GOL:H2	4:B:202:GOL:H32	1.37	1.04
4:B:201:GOL:C2	4:B:202:GOL:H32	2.15	0.75
2:B:33[B]:ARG:HH12	3:H:244:TRP:HE1	1.34	0.72
1:A:166:THR:HG22	1:A:216[B]:THR:HG22	1.81	0.63
2:B:33[B]:ARG:NH1	3:H:244:TRP:HE1	1.97	0.61
2:B:108:THR:HG22	2:B:111:MET:H	1.65	0.61
1:A:85:MET:HE2	1:A:88:LEU:HD21	1.83	0.61
2:B:34:HIS:ND1	5:B:205:PO4:O4	2.23	0.60
2:B:33[B]:ARG:HH12	3:H:244:TRP:NE1	2.00	0.60
1:A:14:VAL:HG11	1:A:88:LEU:HD13	1.87	0.56
3:H:184:GLN:HB2	3:H:194:LEU:HD11	1.98	0.46
2:B:33[B]:ARG:NH1	3:H:240:SER:O	2.52	0.43
1:A:181:GLN:HB2	1:A:191:LEU:HD11	2.01	0.43
3:H:6:LEU:HB3	3:H:98[A]:CYS:SG	2.60	0.42
2:B:22:ARG:NE	3:H:105:ASN:HB3	2.36	0.41
1:A:238:THR:HA	1:A:239:PRO:C	2.46	0.41
2:B:87:GLU:O	2:B:91[A]:GLN:HG2	2.21	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	235/290 (81%)	228 (97%)	6 (3%)	1 (0%)	30	19
2	B	132/188 (70%)	132 (100%)	0	0	100	100
3	H	237/294 (81%)	233 (98%)	4 (2%)	0	100	100
All	All	604/772 (78%)	593 (98%)	10 (2%)	1 (0%)	44	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLY

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	197/225 (88%)	195 (99%)	2 (1%)	73	62
2	B	128/167 (77%)	127 (99%)	1 (1%)	79	72
3	H	194/221 (88%)	194 (100%)	0	100	100
All	All	519/613 (85%)	516 (99%)	3 (1%)	89	78

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

Mol	Chain	Res	Type
1	A	91[A]	GLU
1	A	91[B]	GLU

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Mol	Chain	Res	Type
2	B	108	THR

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	41	GLN
1	A	182	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](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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	GOL	A	301	-	5,5,5	0.04	0	5,5,5	0.27	0
4	GOL	B	202	-	5,5,5	0.15	0	5,5,5	0.32	0
4	GOL	B	203	-	5,5,5	0.06	0	5,5,5	0.25	0
4	GOL	B	204	-	5,5,5	0.04	0	5,5,5	0.20	0
4	GOL	B	201	-	5,5,5	0.12	0	5,5,5	0.29	0
5	PO4	H	302	-	4,4,4	0.26	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	H	301	-	5,5,5	0.03	0	5,5,5	0.25	0
5	PO4	B	205	-	4,4,4	0.22	0	6,6,6	0.33	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
4	GOL	A	301	-	-	2/4/4/4	-
4	GOL	B	202	-	-	0/4/4/4	-
4	GOL	B	203	-	-	2/4/4/4	-
4	GOL	B	204	-	-	0/4/4/4	-
4	GOL	B	201	-	-	0/4/4/4	-
4	GOL	H	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	203	GOL	C1-C2-C3-O3
4	A	301	GOL	O1-C1-C2-C3
4	B	203	GOL	O2-C2-C3-O3
4	A	301	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	GOL	2	0
4	B	201	GOL	2	0
5	B	205	PO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	234/290 (80%)	0.02	14 (5%) 29 27	21, 49, 69, 87	5 (2%)
2	B	135/188 (71%)	0.07	11 (8%) 19 18	23, 45, 78, 97	3 (2%)
3	H	237/294 (80%)	-0.11	7 (2%) 52 52	23, 46, 66, 79	4 (1%)
All	All	606/772 (78%)	-0.02	32 (5%) 33 32	21, 47, 70, 97	12 (1%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	PHE	4.8
1	A	17	GLY	4.3
2	B	157	LEU	3.9
1	A	4	VAL	3.8
2	B	108	THR	3.5
2	B	97	ALA	3.4
1	A	3	GLU	3.3
1	A	252	GLY	3.2
1	A	90	ALA	3.0
3	H	224	ARG	2.9
3	H	258	PHE	2.8
2	B	51	GLU	2.7
2	B	43	PHE	2.6
2	B	98	CYS	2.6
1	A	143	ALA	2.6
1	A	253	PRO	2.6
2	B	156	ASN	2.5
1	A	123	SER	2.5
2	B	50	ALA	2.3
3	H	188	GLY	2.3
1	A	122	VAL	2.3
1	A	18	GLY	2.2
3	H	153	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	154	SER	2.1
1	A	15	GLN	2.1
3	H	126	SER	2.1
2	B	96	GLU	2.1
3	H	210	ARG	2.1
3	H	30	THR	2.1
1	A	124	SER	2.0
2	B	12	ARG	2.0
1	A	145	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](#)

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(Å ²)	Q<0.9
4	GOL	B	204	6/6	0.71	0.25	90,90,91,91	0
6	K	B	206	1/1	0.71	0.30	119,119,119,119	0
5	PO4	H	302	5/5	0.75	0.13	137,137,137,137	0
4	GOL	H	301	6/6	0.78	0.25	97,97,97,98	0
4	GOL	A	301	6/6	0.81	0.15	81,82,82,82	0
4	GOL	B	201	6/6	0.81	0.14	54,55,56,56	0
4	GOL	B	202	6/6	0.83	0.14	52,56,56,57	0
4	GOL	B	203	6/6	0.87	0.14	82,82,82,82	0
5	PO4	B	205	5/5	0.93	0.09	67,67,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.