



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:32 PM UTC

PDB ID : 9YY0 / pdb_00009yy0
Title : IGHV4-34 germline-reverted antibody pre166
Authors : Langley, D.B.; Christ, D.
Deposited on : 2025-10-28
Resolution : 1.34 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

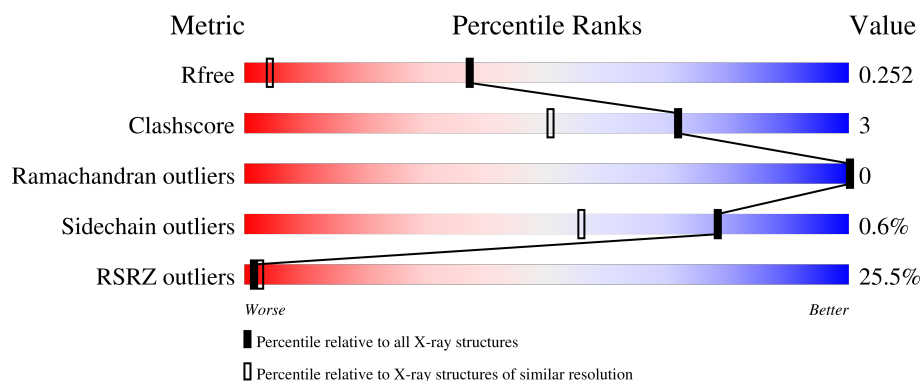
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.34 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	2194 (1.36-1.32)
Clashscore	190562	2222 (1.36-1.32)
Ramachandran outliers	187476	2197 (1.36-1.32)
Sidechain outliers	187428	2197 (1.36-1.32)
RSRZ outliers	180081	2193 (1.36-1.32)

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	H	229	
2	L	214	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6676 atoms, of which 3079 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 Heavy chain Fab of pre166 antibody.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	209	Total	C	H	N	O	S	0	4	0
			3097	1006	1515	262	310	4			

- Molecule 2 is a protein called Light chain Fab of pre166 antibody.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	211	Total	C	H	N	O	S	0	5	0
			3193	1019	1564	276	330	4			

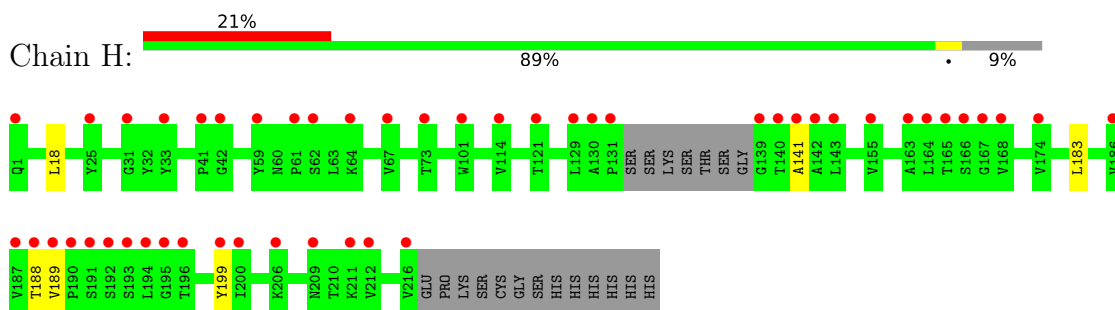
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	207	Total	O	0	0
			207	207		
3	L	179	Total	O	0	0
			179	179		

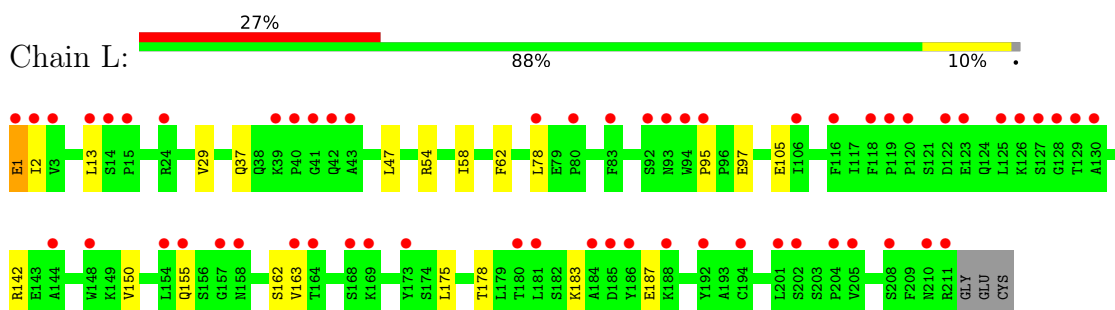
3 Residue-property plots [i](#)

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: Heavy chain Fab of pre166 antibody



- Molecule 2: Light chain Fab of pre166 antibody



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.46Å 47.09Å 71.15Å 90.00° 114.38° 90.00°	Depositor
Resolution (Å)	38.10 – 1.34 38.10 – 1.34	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.10-1.34) 99.7 (38.10-1.34)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.34Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.224 , 0.253 0.224 , 0.252	Depositor DCC
R_{free} test set	4144 reflections (3.74%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6676	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6592e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	H	0.43	0/1639	0.62	0/2245
2	L	0.39	0/1698	0.62	0/2317
All	All	0.41	0/3337	0.62	0/4562

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 [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	H	1582	1515	1510	4	0
2	L	1629	1564	1536	17	0
3	H	207	0	0	0	0
3	L	179	0	0	5	0
All	All	3597	3079	3046	21	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.

All (21) 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:L:2:ILE:HD13	2:L:29:VAL:HG12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:178:THR:HB	3:L:427:HOH:O	1.99	0.61
2:L:155:GLN:HB2	3:L:301:HOH:O	2.00	0.60
2:L:142:ARG:NH2	2:L:163[A]:VAL:HG21	2.23	0.53
2:L:13:LEU:HD12	2:L:78:LEU:HD11	1.94	0.49
1:H:18:LEU:C	1:H:18:LEU:HD23	2.38	0.48
2:L:2:ILE:HD13	2:L:29:VAL:CG1	2.44	0.48
2:L:54:ARG:HD3	2:L:62:PHE:O	2.15	0.47
1:H:183:LEU:C	1:H:183:LEU:HD12	2.40	0.47
2:L:13:LEU:CD1	2:L:78:LEU:HD11	2.46	0.46
2:L:54:ARG:HG2	2:L:58:ILE:HB	1.97	0.46
2:L:162:SER:CB	3:L:316:HOH:O	2.64	0.46
2:L:162:SER:HB3	3:L:316:HOH:O	2.15	0.46
2:L:163[A]:VAL:HG22	2:L:175:LEU:HD12	1.99	0.45
1:H:141:ALA:O	1:H:188:THR:HA	2.17	0.45
2:L:37:GLN:HB2	2:L:47:LEU:HD11	2.01	0.43
1:H:189:VAL:HG11	1:H:199:TYR:CE1	2.54	0.43
2:L:150:VAL:HB	3:L:301:HOH:O	2.20	0.42
2:L:183:LYS:HE3	2:L:187:GLU:OE1	2.19	0.42
2:L:1:GLU:HG3	2:L:97:GLU:OE2	2.22	0.40

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	H	209/229 (91%)	204 (98%)	5 (2%)	0	100	100
2	L	214/214 (100%)	210 (98%)	4 (2%)	0	100	100
All	All	423/443 (96%)	414 (98%)	9 (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	H	179/196 (91%)	179 (100%)	0	100	100
2	L	185/186 (100%)	183 (99%)	2 (1%)	65	33
All	All	364/382 (95%)	362 (100%)	2 (0%)	78	61

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	1	GLU
2	L	105	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	58	ASN
2	L	42	GLN
2	L	93	ASN
2	L	100	GLN
2	L	160	GLN
2	L	189	HIS

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

There are no ligands in this entry.

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	H	209/229 (91%)	1.44	49 (23%)  	7, 16, 33, 41	2 (0%)
2	L	211/214 (98%)	1.49	58 (27%)  	8, 18, 30, 40	2 (0%)
All	All	420/443 (94%)	1.47	107 (25%)  	7, 17, 30, 41	4 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	94[A]	TRP	7.0
1	H	189	VAL	5.8
1	H	131	PRO	5.3
1	H	140	THR	5.0
1	H	139	GLY	4.9
1	H	195	GLY	4.5
1	H	141	ALA	4.4
2	L	184	ALA	4.4
1	H	1	GLN	4.4
2	L	83	PHE	4.3
2	L	181	LEU	4.3
1	H	192	SER	4.3
1	H	209	ASN	4.2
2	L	168	SER	4.2
1	H	190	PRO	4.1
1	H	42	GLY	4.1
1	H	194	LEU	4.0
1	H	130	ALA	3.9
1	H	191	SER	3.8
1	H	101	TRP	3.8
1	H	165	THR	3.7
1	H	143	LEU	3.7
2	L	201	LEU	3.6
2	L	41	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
2	L	185	ASP	3.5
2	L	158	ASN	3.5
1	H	193	SER	3.4
2	L	157	GLY	3.4
1	H	142	ALA	3.4
2	L	106	ILE	3.3
2	L	42	GLN	3.2
2	L	80	PRO	3.2
2	L	15	PRO	3.1
1	H	166	SER	3.1
2	L	40	PRO	3.0
2	L	120	PRO	3.0
2	L	123[A]	GLU	3.0
2	L	122	ASP	2.9
1	H	167	GLY	2.9
2	L	148	TRP	2.9
2	L	194	CYS	2.9
1	H	196	THR	2.9
1	H	164	LEU	2.8
2	L	180	THR	2.8
2	L	93	ASN	2.8
2	L	163[A]	VAL	2.8
1	H	188	THR	2.8
2	L	192	TYR	2.8
2	L	155	GLN	2.7
2	L	1	GLU	2.7
1	H	155	VAL	2.7
2	L	119	PRO	2.7
1	H	199	TYR	2.7
2	L	13	LEU	2.7
2	L	92	SER	2.7
2	L	2	ILE	2.6
1	H	168	VAL	2.6
1	H	206	LYS	2.6
1	H	31	GLY	2.6
1	H	64	LYS	2.6
1	H	200	ILE	2.6
1	H	73	THR	2.5
2	L	128	GLY	2.5
2	L	186	TYR	2.5
2	L	14	SER	2.5
1	H	41	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	L	95	PRO	2.5
2	L	204	PRO	2.4
2	L	202	SER	2.4
2	L	169	LYS	2.4
1	H	62	SER	2.4
1	H	163	ALA	2.4
1	H	67	VAL	2.4
2	L	188	LYS	2.4
1	H	211	LYS	2.3
1	H	25	TYR	2.3
1	H	212	VAL	2.3
2	L	39	LYS	2.3
1	H	129	LEU	2.3
2	L	125	LEU	2.3
2	L	154	LEU	2.3
1	H	174	VAL	2.3
1	H	187	VAL	2.3
1	H	216	VAL	2.3
2	L	205	VAL	2.3
2	L	78	LEU	2.2
2	L	126	LYS	2.2
2	L	144	ALA	2.2
2	L	164[A]	THR	2.2
2	L	118	PHE	2.2
1	H	114	VAL	2.2
2	L	127	SER	2.2
1	H	61	PRO	2.2
2	L	173	TYR	2.1
2	L	130	ALA	2.1
2	L	3	VAL	2.1
2	L	211	ARG	2.1
2	L	116	PHE	2.1
2	L	210	ASN	2.1
2	L	43	ALA	2.1
1	H	186	VAL	2.1
2	L	24	ARG	2.1
1	H	121	THR	2.1
2	L	129	THR	2.1
1	H	59	TYR	2.1
2	L	208	SER	2.0
1	H	33	TYR	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.