



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:22 AM UTC

PDB ID : 7FAB / pdb_00007fab
Title : CRYSTAL STRUCTURE OF HUMAN IMMUNOGLOBULIN FRAGMENT
FAB NEW REFINED AT 2.0 ANGSTROMS RESOLUTION
Authors : Saul, F.; Poljak, R.J.
Deposited on : 1991-11-20
Resolution : 2.00 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

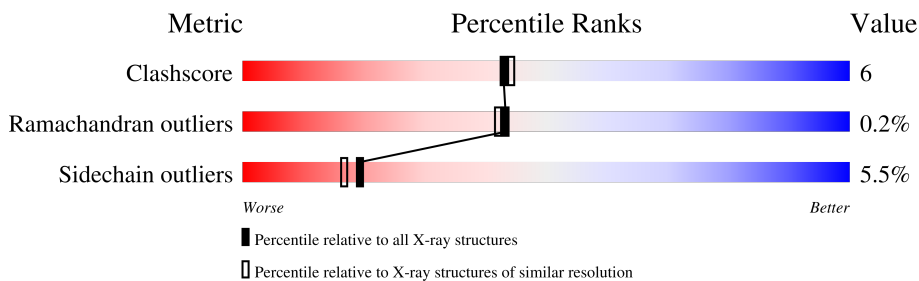
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	208	
2	H	217	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3313 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 IGG1-LAMBDA NEW FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	204	Total	C	N	O	S	0	0	0
			1514	950	258	302	4			

- Molecule 2 is a protein called IGG1-LAMBDA NEW FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	209	Total	C	N	O	S	0	0	0
			1570	1000	261	304	5			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	133	Total	O	0	0
			133	133		
3	H	96	Total	O	0	0
			96	96		

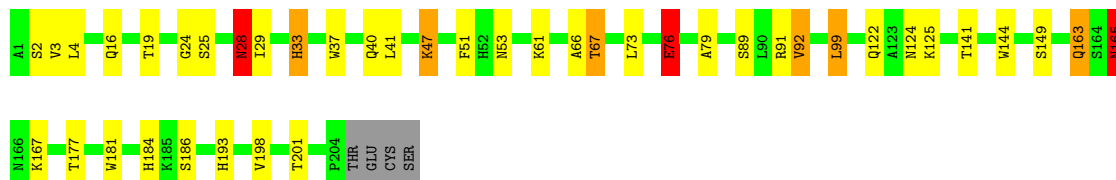
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

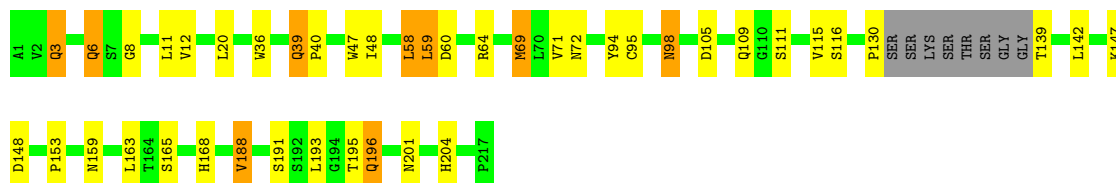
• Molecule 1: IGG1-LAMBDA NEW FAB (LIGHT CHAIN)

Chain L:  78% 16% . . .



• Molecule 2: IGG1-LAMBDA NEW FAB (HEAVY CHAIN)

Chain H:  76% 16% . .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.43Å 56.68Å 90.30Å 90.00° 116.46° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3313	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

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	0.99	4/1550 (0.3%)	1.65	28/2115 (1.3%)
2	H	0.98	3/1609 (0.2%)	1.65	21/2205 (1.0%)
All	All	0.98	7/3159 (0.2%)	1.65	49/4320 (1.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	204	HIS	CD2-NE2	-7.01	1.30	1.37
1	L	184	HIS	CD2-NE2	-6.62	1.30	1.37
1	L	193	HIS	CD2-NE2	-6.27	1.30	1.37
2	H	168	HIS	CD2-NE2	-6.08	1.31	1.37
1	L	33	HIS	CD2-NE2	-5.80	1.31	1.37
2	H	40	PRO	CA-CB	-5.77	1.48	1.53
1	L	184	HIS	CG-ND1	-5.08	1.32	1.38

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	163	GLN	OE1-CD-NE2	-8.39	114.21	122.60
2	H	48	ILE	N-CA-C	-8.16	104.55	111.56
1	L	28	ASN	OD1-CG-ND2	-7.90	114.70	122.60
1	L	165	ASN	OD1-CG-ND2	-7.60	115.00	122.60
2	H	148	ASP	N-CA-C	7.54	120.45	111.02
2	H	39	GLN	CA-C-N	7.52	125.15	119.66
2	H	39	GLN	C-N-CA	7.52	125.15	119.66
2	H	201	ASN	OD1-CG-ND2	-7.36	115.24	122.60
2	H	98	ASN	OD1-CG-ND2	-7.12	115.48	122.60
1	L	76	GLU	CA-CB-CG	7.06	128.22	114.10
1	L	122	GLN	OE1-CD-NE2	-6.68	115.92	122.60
1	L	51	PHE	CA-CB-CG	-6.41	107.39	113.80
1	L	144	TRP	CG-CD2-CE3	6.11	140.01	133.90
2	H	147	LYS	CA-CB-CG	5.95	126.01	114.10
2	H	105	ASP	CA-CB-CG	5.87	118.47	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	159	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	L	149	SER	CA-C-N	5.85	125.61	119.76
1	L	149	SER	C-N-CA	5.85	125.61	119.76
1	L	181	TRP	CG-CD2-CE3	5.84	139.74	133.90
1	L	33	HIS	CB-CG-CD2	-5.83	123.62	131.20
1	L	53	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	L	181	TRP	CB-CG-CD1	-5.79	118.21	126.90
1	L	2	SER	N-CA-C	-5.76	98.54	110.80
2	H	204	HIS	CB-CG-CD2	-5.67	123.82	131.20
2	H	6	GLN	OE1-CD-NE2	-5.67	116.93	122.60
1	L	16	GLN	CA-CB-CG	5.61	125.31	114.10
1	L	165	ASN	CB-CG-ND2	5.58	124.77	116.40
2	H	69	MET	CA-CB-CG	-5.58	102.95	114.10
2	H	40	PRO	CA-C-O	-5.53	116.92	120.90
2	H	72	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	L	198	VAL	N-CA-C	-5.46	100.46	108.11
1	L	177	THR	N-CA-C	-5.43	103.09	110.36
1	L	163	GLN	CG-CD-NE2	5.42	124.53	116.40
1	L	141	THR	N-CA-C	-5.33	100.72	109.40
1	L	37	TRP	CE2-CD2-CG	-5.31	100.83	107.20
1	L	92	VAL	O-C-N	-5.26	117.57	123.26
1	L	28	ASN	CB-CG-ND2	5.24	124.27	116.40
2	H	47	TRP	CG-CD1-NE1	-5.22	103.41	110.20
2	H	188	VAL	CA-C-N	5.21	125.46	119.83
2	H	188	VAL	C-N-CA	5.21	125.46	119.83
1	L	122	GLN	CG-CD-NE2	5.17	124.15	116.40
2	H	3	GLN	OE1-CD-NE2	-5.16	117.44	122.60
2	H	40	PRO	N-CA-CB	5.16	106.08	103.19
2	H	60	ASP	CA-CB-CG	5.10	117.70	112.60
1	L	181	TRP	CG-CD1-NE1	-5.08	103.60	110.20
1	L	193	HIS	CB-CG-CD2	-5.07	124.61	131.20
2	H	196	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	L	144	TRP	CE2-CD2-CG	-5.04	101.15	107.20
1	L	124	ASN	OD1-CG-ND2	-5.02	117.58	122.60

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	1514	0	1486	24	0
2	H	1570	0	1557	17	0
3	H	96	0	0	0	0
3	L	133	0	0	3	0
All	All	3313	0	3043	38	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 6.

All (38) 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:L:28:ASN:HD22	1:L:29:ILE:H	1.30	0.79
1:L:41:LEU:H	1:L:47:LYS:HZ1	1.33	0.75
1:L:19:THR:HG23	1:L:67:THR:HG23	1.77	0.65
1:L:40:GLN:HE22	2:H:39:GLN:HE22	1.45	0.64
1:L:165:ASN:ND2	1:L:167:LYS:H	1.95	0.63
1:L:91:ARG:HE	2:H:98:ASN:ND2	1.97	0.62
1:L:76:GLU:HG3	3:L:306:HOH:O	1.99	0.62
2:H:6:GLN:HE21	2:H:95:CYS:H	1.48	0.62
2:H:8:GLY:HA3	2:H:20:LEU:HD23	1.82	0.60
1:L:163:GLN:HB2	1:L:165:ASN:ND2	2.20	0.57
2:H:58:LEU:HD12	2:H:59:LEU:H	1.70	0.56
2:H:59:LEU:HD21	2:H:64:ARG:HD3	1.90	0.54
2:H:36:TRP:HD1	2:H:69:MET:HE3	1.72	0.54
1:L:3:VAL:HB	1:L:92:VAL:HG13	1.90	0.53
1:L:25:SER:H	1:L:28:ASN:ND2	2.08	0.52
2:H:36:TRP:CD1	2:H:69:MET:HE3	2.45	0.52
1:L:19:THR:HG23	1:L:67:THR:CG2	2.39	0.52
1:L:163:GLN:HE21	1:L:165:ASN:HD21	1.59	0.51
1:L:91:ARG:HE	2:H:98:ASN:HD21	1.59	0.50
2:H:130:PRO:HD3	2:H:142:LEU:HB3	1.93	0.50
2:H:109:GLN:N	2:H:109:GLN:CD	2.70	0.49
1:L:33:HIS:HE1	3:L:229:HOH:O	1.95	0.49
1:L:41:LEU:HD23	1:L:79:ALA:HB2	1.94	0.49
2:H:139:THR:HA	2:H:188:VAL:O	2.16	0.46
2:H:6:GLN:HE21	2:H:94:TYR:HA	1.81	0.46
1:L:3:VAL:HB	1:L:92:VAL:CG1	2.45	0.46
1:L:67:THR:HG22	3:L:218:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:61:LYS:HA	1:L:66:ALA:HA	1.99	0.44
2:H:11:LEU:HD11	2:H:116:SER:HB3	1.99	0.44
2:H:12:VAL:O	2:H:115:VAL:HA	2.17	0.44
2:H:6:GLN:NE2	2:H:95:CYS:H	2.13	0.44
1:L:25:SER:H	1:L:28:ASN:HD21	1.66	0.43
1:L:73:LEU:HD11	1:L:99:LEU:HD11	2.00	0.43
2:H:6:GLN:HE21	2:H:95:CYS:N	2.15	0.43
1:L:24:GLY:HA3	1:L:28:ASN:HD21	1.83	0.43
1:L:186:SER:HB2	1:L:201:THR:CG2	2.49	0.43
1:L:163:GLN:HE21	1:L:165:ASN:ND2	2.17	0.43
1:L:4:LEU:HG	1:L:92:VAL:HG12	2.03	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	L	202/208 (97%)	194 (96%)	8 (4%)	0	100	100
2	H	205/217 (94%)	200 (98%)	4 (2%)	1 (0%)	24	21
All	All	407/425 (96%)	394 (97%)	12 (3%)	1 (0%)	43	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	193	LEU

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	L	168/174 (97%)	160 (95%)	8 (5%)	23	21
2	H	179/185 (97%)	168 (94%)	11 (6%)	17	14
All	All	347/359 (97%)	328 (94%)	19 (6%)	19	17

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	28	ASN
1	L	47	LYS
1	L	67	THR
1	L	76	GLU
1	L	89	SER
1	L	99	LEU
1	L	125	LYS
1	L	165	ASN
2	H	3	GLN
2	H	58	LEU
2	H	59	LEU
2	H	71	VAL
2	H	111	SER
2	H	153	PRO
2	H	163	LEU
2	H	165	SER
2	H	191	SER
2	H	195	THR
2	H	196	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	28	ASN
1	L	34	ASN
1	L	39	GLN
1	L	40	GLN
1	L	53	ASN
1	L	84	GLN
1	L	165	ASN
2	H	16	GLN

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Mol	Chain	Res	Type
2	H	77	GLN
2	H	168	HIS
2	H	203	ASN

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.