



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 29, 2026 – 01:44 pm BST

PDB ID : 9TUX / pdb_00009tux
Title : PfrIPR bound to monoclonal antibody MAD8-66
Authors : Farrell, B.; Higgins, M.K.
Deposited on : 2026-01-10
Resolution : 2.25 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
Xtrriage (Phenix) : 2.0
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) : 2.50

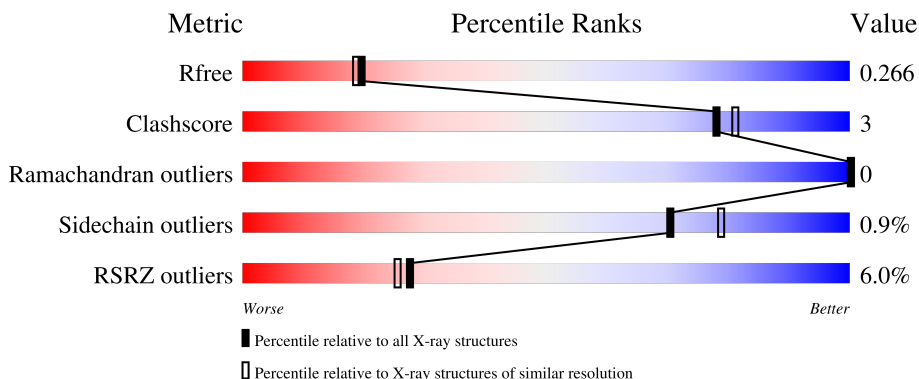
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

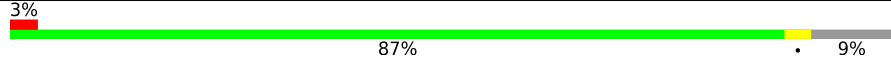
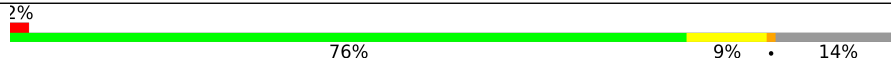
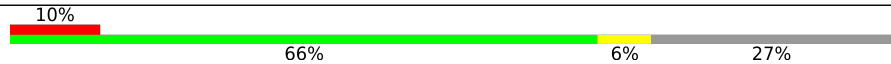
The reported resolution of this entry is 2.25 Å.

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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	239	
2	B	255	
3	C	231	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4810 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 MAD8-66 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	217	1681	1055	282	339	5	0	0	0

- Molecule 2 is a protein called MAD8-66 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	220	1657	1051	281	319	6	0	0	0

- Molecule 3 is a protein called Rh5-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	168	1379	880	214	271	14	0	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	879	MET	-	initiating methionine	UNP O97302
C	880	LYS	-	expression tag	UNP O97302
C	881	LEU	-	expression tag	UNP O97302
C	882	CYS	-	expression tag	UNP O97302
C	883	ILE	-	expression tag	UNP O97302
C	884	LEU	-	expression tag	UNP O97302
C	885	LEU	-	expression tag	UNP O97302
C	886	ALA	-	expression tag	UNP O97302
C	887	VAL	-	expression tag	UNP O97302
C	888	VAL	-	expression tag	UNP O97302
C	889	ALA	-	expression tag	UNP O97302
C	890	PHE	-	expression tag	UNP O97302
C	891	VAL	-	expression tag	UNP O97302
C	892	GLY	-	expression tag	UNP O97302

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Chain	Residue	Modelled	Actual	Comment	Reference
C	893	LEU	-	expression tag	UNP O97302
C	894	SER	-	expression tag	UNP O97302
C	895	LEU	-	expression tag	UNP O97302
C	896	GLY	-	expression tag	UNP O97302
C	897	GLY	-	expression tag	UNP O97302
C	898	THR	-	expression tag	UNP O97302
C	964	GLN	ASN	conflict	UNP O97302
C	1021	GLN	ASN	conflict	UNP O97302
C	1087	GLY	-	expression tag	UNP O97302
C	1088	SER	-	expression tag	UNP O97302
C	1089	ALA	-	expression tag	UNP O97302
C	1090	SER	-	expression tag	UNP O97302
C	1091	GLY	-	expression tag	UNP O97302
C	1092	LEU	-	expression tag	UNP O97302
C	1093	ASN	-	expression tag	UNP O97302
C	1094	ASP	-	expression tag	UNP O97302
C	1095	ILE	-	expression tag	UNP O97302
C	1096	PHE	-	expression tag	UNP O97302
C	1097	GLU	-	expression tag	UNP O97302
C	1098	ALA	-	expression tag	UNP O97302
C	1099	GLN	-	expression tag	UNP O97302
C	1100	LYS	-	expression tag	UNP O97302
C	1101	ILE	-	expression tag	UNP O97302
C	1102	GLU	-	expression tag	UNP O97302
C	1103	TRP	-	expression tag	UNP O97302
C	1104	HIS	-	expression tag	UNP O97302
C	1105	GLU	-	expression tag	UNP O97302
C	1106	GLU	-	expression tag	UNP O97302
C	1107	PRO	-	expression tag	UNP O97302
C	1108	GLU	-	expression tag	UNP O97302
C	1109	ALA	-	expression tag	UNP O97302

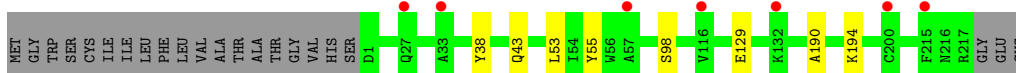
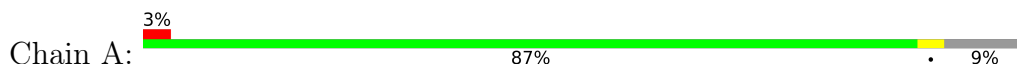
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	37	Total O 37 37	0	0
4	B	39	Total O 39 39	0	0
4	C	17	Total O 17 17	0	0

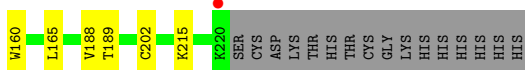
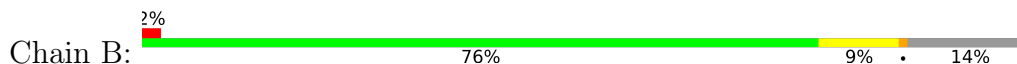
3 Residue-property plots [i](#)

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.

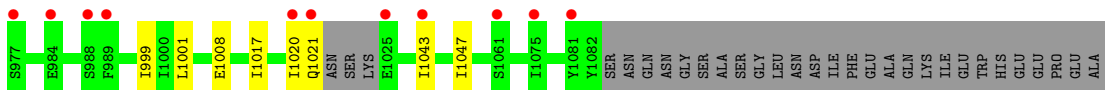
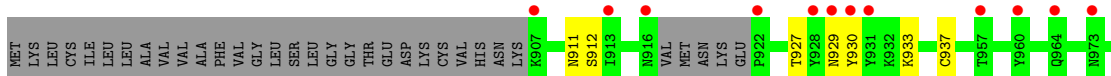
- Molecule 1: MAD8-66 light chain



- Molecule 2: MAD8-66 heavy chain



- Molecule 3: Rh5-interacting protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.79Å 63.24Å 250.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.68 – 2.25 62.68 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (62.68-2.25) 99.9 (62.68-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.25Å)	Xtrriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.230 , 0.262 0.238 , 0.266	Depositor DCC
R_{free} test set	2037 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtrriage
Anisotropy	0.464	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4810	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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](#)

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	0.12	0/1719	0.31	0/2338
2	B	0.22	0/1698	0.39	0/2311
3	C	0.13	0/1410	0.31	0/1905
All	All	0.16	0/4827	0.34	0/6554

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	A	1681	0	1628	4	0
2	B	1657	0	1645	14	0
3	C	1379	0	1286	10	0
4	A	37	0	0	0	0
4	B	39	0	0	0	0
4	C	17	0	0	0	0
All	All	4810	0	4559	26	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 26 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)
3:C:1020:ILE:HG13	3:C:1021:GLN:HG3	1.66	0.76
2:B:60:TYR:H	2:B:65:ARG:NH1	1.92	0.66
2:B:100:HIS:CE1	2:B:102:VAL:HB	2.32	0.65
2:B:103:THR:HG23	2:B:105:ALA:H	1.64	0.62
1:A:55:TYR:HB2	2:B:103:THR:HG21	1.86	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	215/239 (90%)	211 (98%)	4 (2%)	0	100	100
2	B	218/255 (86%)	215 (99%)	3 (1%)	0	100	100
3	C	162/231 (70%)	157 (97%)	5 (3%)	0	100	100
All	All	595/725 (82%)	583 (98%)	12 (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	191/208 (92%)	190 (100%)	1 (0%)	81	87
2	B	187/217 (86%)	183 (98%)	4 (2%)	47	58
3	C	158/211 (75%)	158 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	536/636 (84%)	531 (99%)	5 (1%)	70 79

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	GLU
2	B	79	VAL
2	B	99	VAL
2	B	102	VAL
2	B	141	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	44	GLN
2	B	39	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

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	217/239 (90%)	0.50	7 (3%) 50 50	24, 52, 67, 74	1 (0%)
2	B	220/255 (86%)	0.49	6 (2%) 56 57	40, 51, 65, 72	0
3	C	168/231 (72%)	1.14	23 (13%) 6 6	46, 63, 91, 121	0
All	All	605/725 (83%)	0.67	36 (5%) 27 25	24, 54, 77, 121	1 (0%)

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	ALA	8.5
3	C	931	TYR	5.8
3	C	928	TYR	5.5
3	C	1081	TYR	5.4
3	C	1021	GLN	4.9

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.