



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:02 PM UTC

PDB ID : 8RZ2 / pdb_00008rz2
Title : PfRH5 bound to monoclonal antibody R5.034
Authors : Farrell, B.; Higgins, M.K.
Deposited on : 2024-02-11
Resolution : 2.40 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	:	NOT EXECUTED
Xtriage (Phenix)	:	2.0
EDS	:	NOT EXECUTED
Buster-report	:	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

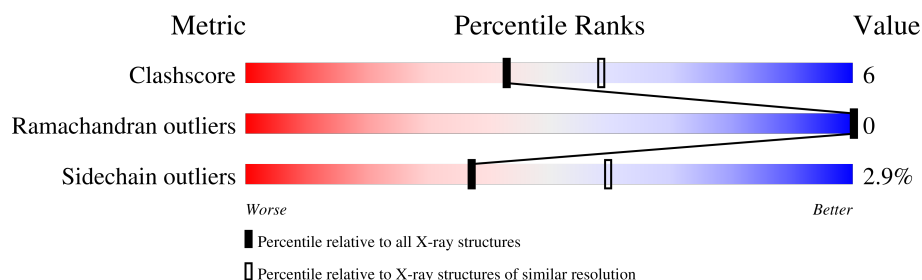
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	A	526	
2	B	256	
3	C	235	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5650 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 Reticulocyte binding protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2396	1548	401	434	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	216	ALA	THR	conflict	UNP B2L3N7

- Molecule 2 is a protein called R5.034 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1612	1015	277	313	7			

- Molecule 3 is a protein called R5.034 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	211	Total	C	N	O	S	0	0	0
			1577	987	265	321	4			

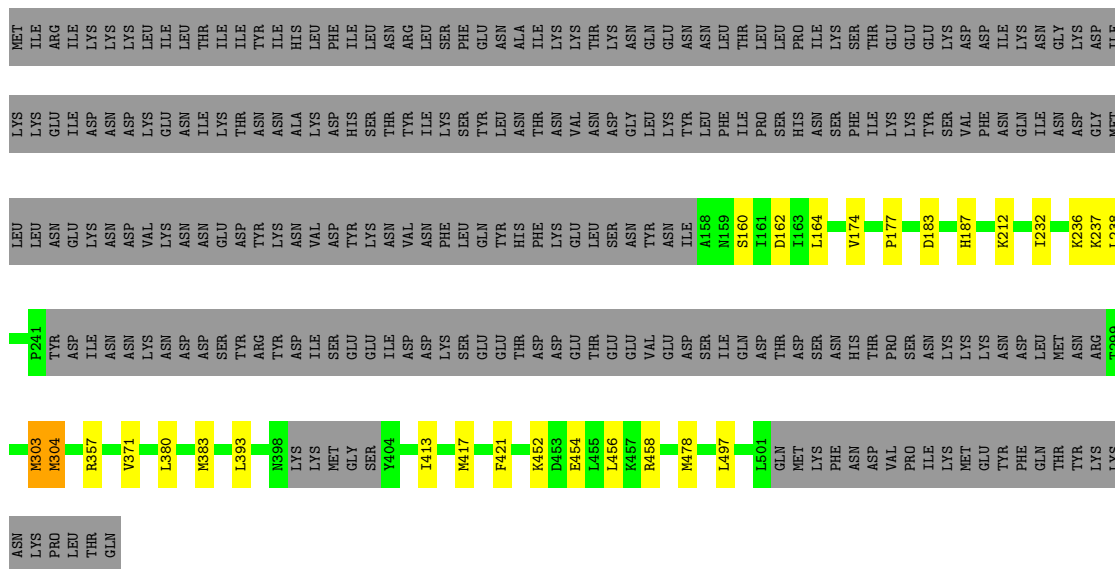
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	B	21	Total	O	0	0
			21	21		
4	C	15	Total	O	0	0
			15	15		

Note EDS was not executed.

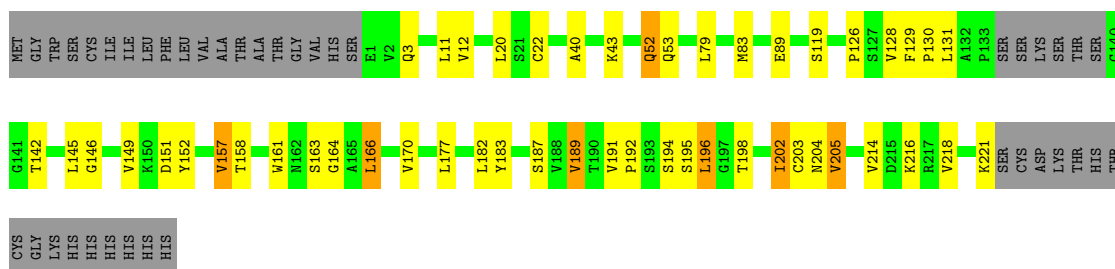
- Molecule 1: Reticulocyte binding protein 5

46%



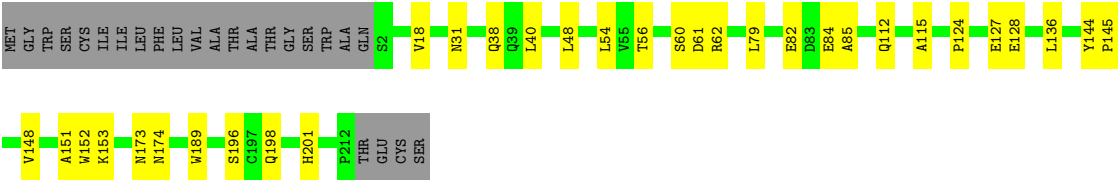
- Molecule 2: R5.034 heavy chain

16%



- Molecule 3: R5.034 light chain

10%



4 Data and refinement statistics

EDS was not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.75Å 82.99Å 118.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.03 – 2.40	Depositor
% Data completeness (in resolution range)	100.0 (68.03-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.40Å)	Xtriage
Refinement program	BUSTER 2.10.4 (26-JUL-2023)	Depositor
R, R_{free}	0.255 , 0.305	Depositor
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.665	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
Total number of atoms	5650	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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 [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	0.58	0/2446	0.98	0/3283
2	B	0.63	0/1649	0.92	0/2245
3	C	0.61	0/1614	0.89	0/2202
All	All	0.60	0/5709	0.94	0/7730

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	2396	0	2412	16	0
2	B	1612	0	1577	33	0
3	C	1577	0	1532	23	0
4	A	29	0	0	0	0
4	B	21	0	0	0	0
4	C	15	0	0	0	0
All	All	5650	0	5521	69	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 (69) 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:A:454:GLU:O	1:A:458:ARG:HG2	1.90	0.72
3:C:40:LEU:HD23	3:C:85:ALA:HB2	1.73	0.70
2:B:128:VAL:HG11	2:B:205:VAL:HG11	1.75	0.68
2:B:126:PRO:HB3	2:B:152:TYR:HB3	1.76	0.67
1:A:237:LYS:HB3	1:A:303:MET:HE2	1.76	0.66
3:C:127:GLU:O	3:C:128:GLU:HB3	1.95	0.66
2:B:166:LEU:HD22	2:B:192:PRO:HD3	1.79	0.65
3:C:112:GLN:HB2	3:C:144:TYR:CZ	2.31	0.65
3:C:153:LYS:HB2	3:C:196:SER:HB3	1.79	0.62
2:B:164:GLY:HA3	2:B:202:ILE:H	1.64	0.62
2:B:198:THR:HG22	2:B:221:LYS:HB3	1.89	0.54
1:A:238:LEU:HD13	1:A:303:MET:HG2	1.88	0.54
3:C:112:GLN:HB2	3:C:144:TYR:CE1	2.42	0.53
2:B:22:CYS:HB3	2:B:79:LEU:HB3	1.90	0.53
1:A:383:MET:HE3	1:A:421:PHE:HD2	1.73	0.53
2:B:20:LEU:HG	2:B:83:MET:HE2	1.90	0.53
2:B:195:SER:O	2:B:196:LEU:C	2.51	0.53
3:C:144:TYR:CD2	3:C:145:PRO:HD3	2.44	0.52
2:B:40:ALA:HB3	2:B:43:LYS:HD2	1.91	0.52
2:B:130:PRO:HB2	2:B:218:VAL:HG23	1.94	0.49
3:C:115:ALA:HB3	3:C:144:TYR:H	1.78	0.49
2:B:146:GLY:HA3	2:B:187:SER:O	2.13	0.48
2:B:198:THR:CG2	2:B:221:LYS:HB3	2.43	0.48
2:B:129:PHE:CD2	3:C:128:GLU:HB2	2.48	0.48
2:B:191:VAL:HB	2:B:194:SER:OG	2.14	0.48
3:C:124:PRO:HD2	3:C:189:TRP:CE2	2.48	0.48
2:B:89:GLU:H	2:B:89:GLU:CD	2.22	0.48
3:C:84:GLU:OE1	3:C:174:ASN:OD1	2.32	0.47
1:A:160:SER:HB3	1:A:177:PRO:HD3	1.96	0.47
1:A:164:LEU:HG	1:A:478:MET:HB3	1.95	0.47
1:A:380:LEU:HA	1:A:383:MET:HE2	1.96	0.47
2:B:151:ASP:HB3	2:B:182:LEU:HD13	1.98	0.46
3:C:152:TRP:C	3:C:153:LYS:HD2	2.41	0.46
1:A:413:ILE:O	1:A:417:MET:HG3	2.16	0.46
3:C:145:PRO:HD2	3:C:201:HIS:CE1	2.51	0.46
2:B:149:VAL:HG11	2:B:157:VAL:HG11	1.97	0.46
2:B:161:TRP:CH2	2:B:203:CYS:HB3	2.52	0.45
2:B:170:VAL:HG12	2:B:189:VAL:CG1	2.46	0.45
3:C:145:PRO:HB2	3:C:201:HIS:NE2	2.31	0.45
2:B:214:VAL:HG12	2:B:216:LYS:HG2	1.99	0.44
1:A:174:VAL:HG21	1:A:478:MET:HE1	1.98	0.44
2:B:166:LEU:CD2	2:B:192:PRO:HD3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:LEU:HD11	2:B:119:SER:HB3	1.99	0.44
3:C:38:GLN:HB2	3:C:48:LEU:HD11	2.00	0.44
1:A:383:MET:HE3	1:A:421:PHE:CD2	2.52	0.44
2:B:166:LEU:HD23	2:B:189:VAL:HG23	1.99	0.44
1:A:304:MET:HE3	1:A:304:MET:HB2	1.85	0.44
3:C:124:PRO:HD3	3:C:136:LEU:CD2	2.48	0.44
3:C:151:ALA:HB3	3:C:198:GLN:HB2	1.99	0.43
3:C:18:VAL:CG2	3:C:79:LEU:HD22	2.48	0.43
2:B:129:PHE:CE2	3:C:128:GLU:HB2	2.54	0.43
1:A:183:ASP:OD2	1:A:187:HIS:NE2	2.50	0.43
3:C:148:VAL:HG12	3:C:201:HIS:HB2	2.01	0.43
2:B:177:LEU:HD13	2:B:183:TYR:CE1	2.54	0.42
1:A:357:ARG:HH11	1:A:357:ARG:HG2	1.83	0.42
3:C:173:ASN:O	3:C:174:ASN:HB2	2.20	0.42
3:C:82:GLU:H	3:C:82:GLU:CD	2.28	0.41
1:A:232:ILE:O	1:A:236:LYS:HG2	2.21	0.41
2:B:158:THR:O	2:B:205:VAL:HA	2.20	0.41
2:B:52:GLN:HG2	2:B:53:GLN:OE1	2.21	0.41
2:B:131:LEU:O	2:B:145:LEU:HB2	2.19	0.41
2:B:142:THR:HA	2:B:194:SER:HB2	2.04	0.40
2:B:163:SER:HB3	2:B:204:ASN:OD1	2.20	0.40
1:A:212:LYS:HG3	3:C:54:LEU:HD11	2.02	0.40
2:B:216:LYS:HD2	2:B:216:LYS:HA	1.91	0.40
1:A:452:LYS:O	1:A:456:LEU:HG	2.21	0.40
2:B:52:GLN:HG2	2:B:53:GLN:H	1.87	0.40
2:B:128:VAL:CG1	2:B:205:VAL:HG11	2.47	0.40
3:C:60:SER:OG	3:C:62:ARG:HG3	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	276/526 (52%)	273 (99%)	3 (1%)	0	100	100
2	B	211/256 (82%)	200 (95%)	11 (5%)	0	100	100
3	C	209/235 (89%)	198 (95%)	11 (5%)	0	100	100
All	All	696/1017 (68%)	671 (96%)	25 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	273/511 (53%)	267 (98%)	6 (2%)	45	67
2	B	177/213 (83%)	168 (95%)	9 (5%)	21	37
3	C	177/196 (90%)	174 (98%)	3 (2%)	53	74
All	All	627/920 (68%)	609 (97%)	18 (3%)	37	60

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ASP
1	A	303	MET
1	A	304	MET
1	A	371	VAL
1	A	393	LEU
1	A	497	LEU
2	B	3	GLN
2	B	12	VAL
2	B	52	GLN
2	B	157	VAL
2	B	166	LEU
2	B	189	VAL
2	B	196	LEU
2	B	202	ILE
2	B	205	VAL

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Mol	Chain	Res	Type
3	C	31	ASN
3	C	56	THR
3	C	61	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	82	GLN
2	B	112	GLN
2	B	178	GLN
3	C	198	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](#)

Mogul was not executed - this section is therefore empty.

5.5 Carbohydrates [i](#)

Mogul was not executed - this section is therefore empty.

5.6 Ligand geometry [i](#)

Mogul was not executed - this section is therefore empty.

5.7 Other polymers [i](#)

Mogul was not executed - this section is therefore empty.

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.