



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2026 – 01:35 pm BST

PDB ID : 9HMH / pdb_00009hmh
Title : Crystal structure of the Calf domains of Integrin Alpha5
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Deposited on : 2024-12-09
Resolution : 1.92 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

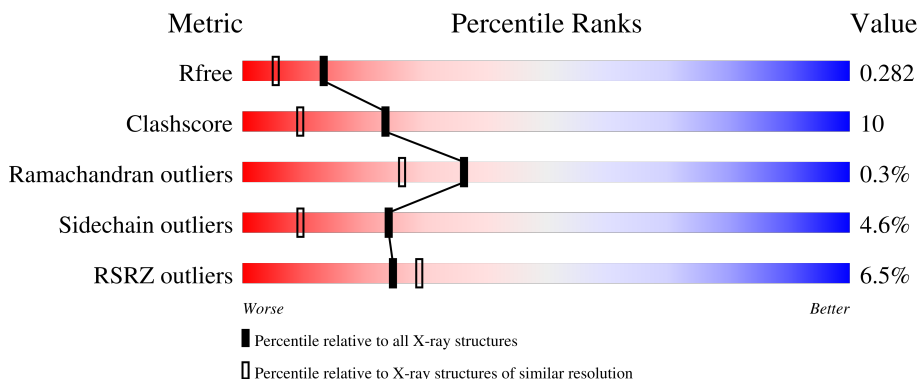
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	359	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5204 atoms, of which 2488 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 Integrin alpha-5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	321	5016	1595	2488	445	476	12	73	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	HIS	-	expression tag	UNP P08648
A	25	HIS	-	expression tag	UNP P08648
A	26	HIS	-	expression tag	UNP P08648
A	27	HIS	-	expression tag	UNP P08648
A	28	HIS	-	expression tag	UNP P08648
A	29	HIS	-	expression tag	UNP P08648

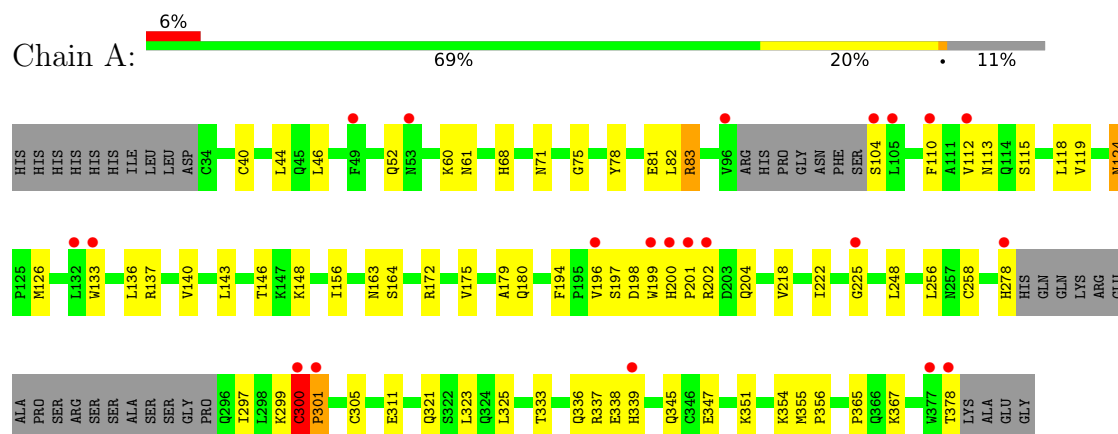
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	188	Total	O	0	0
			188	188		

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: Integrin alpha-5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.02Å 71.44Å 121.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.28 – 1.92 46.28 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.28-1.92) 99.5 (46.28-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.222 , 0.282 0.222 , 0.282	Depositor DCC
R_{free} test set	2000 reflections (5.86%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5204	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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

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	A	0.80	0/2585	1.28	12/3512 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	300	CYS	CA-CB-SG	-6.91	98.51	114.40
1	A	110	PHE	CA-CB-CG	6.39	120.19	113.80
1	A	278	HIS	CA-CB-CG	5.92	119.72	113.80
1	A	378	THR	CA-CB-OG1	-5.35	101.57	109.60
1	A	347	GLU	CB-CG-CD	5.34	121.68	112.60
1	A	339	HIS	CB-CA-C	5.30	120.96	110.42
1	A	194	PHE	CB-CA-C	5.20	116.63	108.63
1	A	124	ASN	O-C-N	-5.16	117.05	121.23
1	A	301	PRO	CB-CA-C	5.10	121.81	113.20
1	A	200	HIS	N-CA-C	-5.03	102.84	110.39
1	A	200	HIS	CA-CB-CG	5.02	118.82	113.80
1	A	301	PRO	CA-N-CD	5.02	119.03	112.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	SER	Peptide

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Mol	Chain	Res	Type	Group
1	A	137	ARG	Sidechain
1	A	172	ARG	Sidechain
1	A	197	SER	Peptide
1	A	199	TRP	Peptide
1	A	201	PRO	Peptide
1	A	202	ARG	Sidechain
1	A	299	LYS	Peptide
1	A	83	ARG	Sidechain

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	A	2528	2488	2472	47	0
2	A	188	0	0	34	0
All	All	2716	2488	2472	47	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 10.

All (47) 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:126:MET:SD	2:A:817:HOH:O	2.25	0.92
1:A:258:CYS:HB3	2:A:712:HOH:O	1.82	0.79
1:A:146:THR:OG1	2:A:701:HOH:O	2.03	0.76
1:A:323:LEU:HD13	2:A:803:HOH:O	1.87	0.73
1:A:345:GLN:CD	2:A:704:HOH:O	2.33	0.71
1:A:367:LYS:HD2	2:A:766:HOH:O	1.92	0.69
1:A:68:HIS:CD2	2:A:755:HOH:O	2.49	0.65
1:A:78:TYR:HD2	2:A:702:HOH:O	1.80	0.65
1:A:124:ASN:OD1	2:A:702:HOH:O	2.15	0.65
1:A:119:VAL:HG13	2:A:703:HOH:O	1.99	0.63
1:A:218:VAL:HG23	2:A:734:HOH:O	2.00	0.62
1:A:365:PRO:HD3	2:A:710:HOH:O	2.02	0.60
1:A:156:ILE:HG23	2:A:713:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLU:N	2:A:713:HOH:O	2.37	0.58
1:A:140:VAL:HG23	2:A:709:HOH:O	2.05	0.55
1:A:133:TRP:CD1	2:A:755:HOH:O	2.60	0.54
1:A:179:ALA:N	2:A:710:HOH:O	2.34	0.53
1:A:354:LYS:NZ	2:A:716:HOH:O	2.43	0.52
1:A:82:LEU:C	2:A:703:HOH:O	2.52	0.52
1:A:333:THR:O	1:A:337:ARG:NH1	2.42	0.51
1:A:355:MET:HE1	2:A:710:HOH:O	2.08	0.51
1:A:61:ASN:ND2	2:A:718:HOH:O	2.43	0.50
1:A:180:GLN:H	1:A:225:GLY:HA3	1.77	0.49
1:A:323:LEU:CD1	2:A:803:HOH:O	2.52	0.49
1:A:44:LEU:CD2	1:A:126:MET:CE	2.90	0.49
1:A:82:LEU:O	2:A:703:HOH:O	2.19	0.49
1:A:300:CYS:HG	1:A:305:CYS:CB	2.22	0.49
1:A:297:ILE:CG2	2:A:704:HOH:O	2.61	0.49
1:A:118:LEU:HD22	2:A:886:HOH:O	2.13	0.48
1:A:124:ASN:C	2:A:702:HOH:O	2.57	0.48
1:A:345:GLN:NE2	2:A:704:HOH:O	2.49	0.44
1:A:222:ILE:HD12	2:A:721:HOH:O	2.17	0.44
1:A:256:LEU:HD21	1:A:321:GLN:HB3	1.99	0.44
1:A:367:LYS:CE	2:A:766:HOH:O	2.66	0.43
1:A:143:LEU:HD12	2:A:769:HOH:O	2.18	0.43
1:A:300:CYS:O	1:A:301:PRO:C	2.59	0.43
1:A:248:LEU:C	1:A:248:LEU:HD12	2.44	0.42
1:A:136:LEU:HB3	2:A:886:HOH:O	2.19	0.42
1:A:71:ASN:HB2	1:A:126:MET:HE3	2.02	0.42
1:A:60:LYS:HE3	2:A:869:HOH:O	2.20	0.41
1:A:83:ARG:HD2	1:A:119:VAL:HG22	2.02	0.41
1:A:40:CYS:O	1:A:75:GLY:HA3	2.21	0.41
1:A:325:LEU:N	2:A:725:HOH:O	2.53	0.41
1:A:113:ASN:HD22	1:A:113:ASN:N	2.19	0.40
1:A:143:LEU:HD21	1:A:175:VAL:HG13	2.03	0.40
1:A:163:ASN:O	1:A:164:SER:C	2.64	0.40
1:A:179:ALA:HB3	2:A:710:HOH:O	2.21	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	A	315/359 (88%)	305 (97%)	9 (3%)	1 (0%)	36	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	VAL

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	280/313 (90%)	267 (95%)	13 (5%)	24	9

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	52	GLN
1	A	112	VAL
1	A	115	SER
1	A	148	LYS
1	A	198	ASP
1	A	204	GLN
1	A	300	CYS
1	A	311	GLU
1	A	336	GLN

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Mol	Chain	Res	Type
1	A	338	GLU
1	A	351	LYS
1	A	356	PRO

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

Mol	Chain	Res	Type
1	A	113	ASN
1	A	178	GLN
1	A	321	GLN
1	A	326	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 [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 [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	321/359 (89%)	0.38	21 (6%) 25 29	30, 49, 82, 160	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	TRP	6.7
1	A	201	PRO	5.7
1	A	378	THR	4.7
1	A	278	HIS	3.9
1	A	104	SER	3.7
1	A	200	HIS	3.1
1	A	96	VAL	3.1
1	A	202	ARG	2.9
1	A	225	GLY	2.6
1	A	133	TRP	2.5
1	A	132	LEU	2.5
1	A	49	PHE	2.4
1	A	339	HIS	2.4
1	A	110	PHE	2.2
1	A	112	VAL	2.2
1	A	196	VAL	2.2
1	A	300	CYS	2.2
1	A	301	PRO	2.1
1	A	377	TRP	2.1
1	A	105	LEU	2.1
1	A	53	ASN	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.