



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 9HMI / pdb_00009hmi
Title : Crystal structure of the Calf domains of Integrin Alpha5 in complex with angiopoietin2 peptide
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Deposited on : 2024-12-09
Resolution : 2.87 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
Xtriage (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

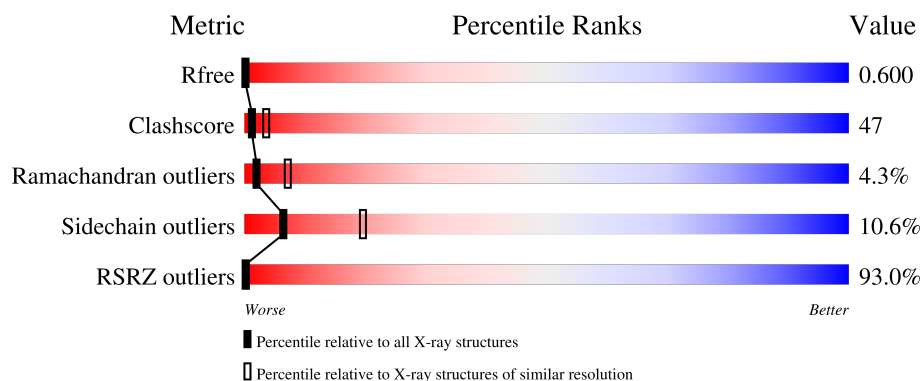
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	346	93% 33% 52% 13% .
2	P	9	89% 33% 67%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2903 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 Integrin alpha-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2721	1707	487	515	12			

- Molecule 2 is a protein called Angiopoietin-2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	9	Total	C	N	O	0	0	0
			74	46	12	16			

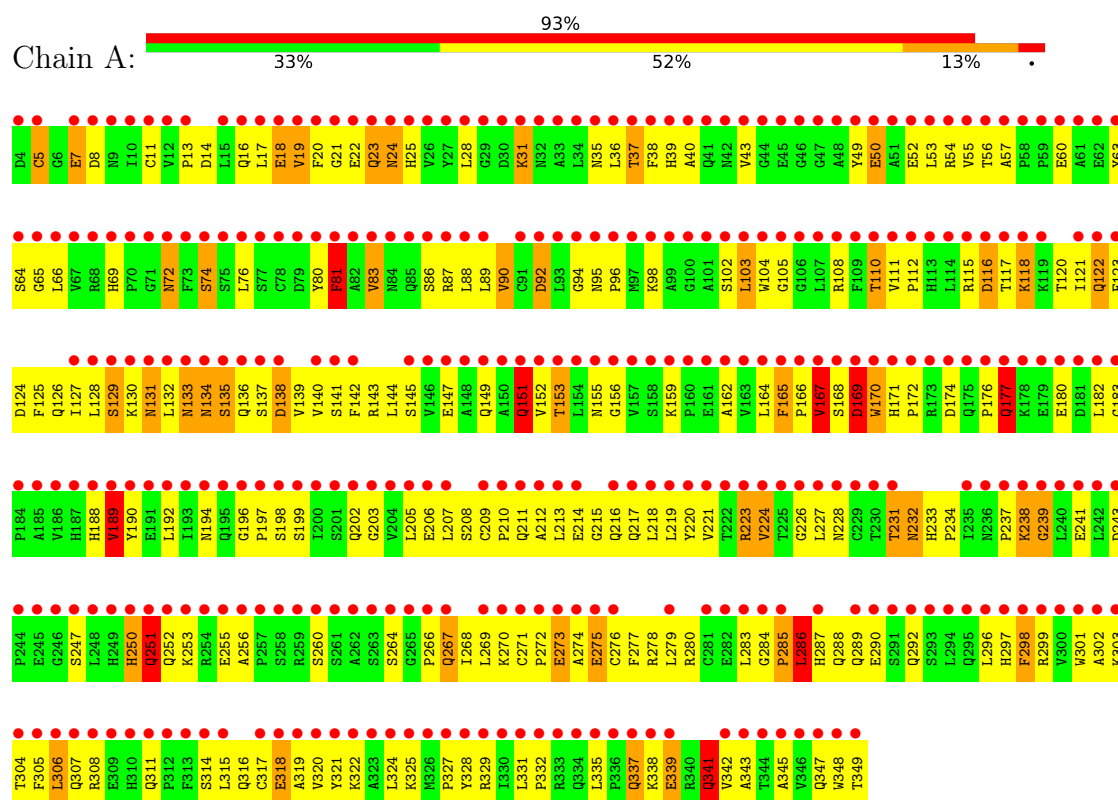
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	104	Total	O	0	0
			104	104		
3	P	4	Total	O	0	0
			4	4		

3 Residue-property plots

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
Space group	P 21 21 21
Cell constants a, b, c, α , β , γ	49.98Å 69.23Å 137.83Å 90.00° 90.00° 90.00°
Resolution (Å)	50.34 – 2.87 50.34 – 2.87
% Data completeness (in resolution range)	98.1 (50.34-2.87) 99.9 (50.34-2.87)
R_{merge}	0.20
R_{sym}	(Not available)
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.77Å)
Refinement program	REFMAC 5.8.0431 (refmacat 0.4.128), REFMAC 5.8.0431 (refmacat 0.4.128)
R, R_{free}	0.233 , 0.281 0.566 , 0.600
R_{free} test set	610 reflections (4.97%)
Wilson B-factor (Å ²)	90.2
Anisotropy	0.365
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.54 , 999.0
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$
Estimated twinning fraction	No twinning to report.
F_o, F_c correlation	0.55
Total number of atoms	2903
Average B, all atoms (Å ²)	100.0

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.61% 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	0.59	0/2786	1.47	41/3786 (1.1%)
2	P	3.20	5/74 (6.8%)	15.24	24/99 (24.2%)
All	All	0.78	5/2860 (0.2%)	2.83	65/3885 (1.7%)

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	1
2	P	4	8
All	All	4	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	361	SER	CA-C	15.89	1.75	1.52
2	P	367	GLN	CG-CD	14.14	1.87	1.52
2	P	367	GLN	CB-CG	-12.10	1.16	1.52
2	P	364	THR	C-N	7.30	1.39	1.33
2	P	363	LEU	N-CA	6.45	1.54	1.46

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	365	ASN	O-C-N	-94.48	50.61	121.47
2	P	363	LEU	O-C-N	-57.38	46.27	122.59
2	P	367	GLN	OE1-CD-NE2	-40.40	82.20	122.60
2	P	363	LEU	N-CA-CB	38.88	176.19	110.49
2	P	359	PHE	N-CA-CB	32.69	163.69	110.40

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	P	359	PHE	CA
2	P	363	LEU	CA
2	P	364	THR	CA
2	P	365	ASN	CA

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	ARG	Sidechain
2	P	358	GLU	Peptide,Mainchain
2	P	361	SER	Peptide,Mainchain
2	P	363	LEU	Mainchain
2	P	365	ASN	Mainchain

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	2721	0	2646	221	744
2	P	74	0	62	85	65
3	A	104	0	0	79	3
3	P	4	0	0	8	0
All	All	2903	0	2708	260	745

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 47.

The worst 5 of 260 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:P:361:SER:C	2:P:361:SER:CA	1.74	1.55
2:P:367:GLN:CD	2:P:367:GLN:CG	1.87	1.48
1:A:308:ARG:HB3	3:A:413:HOH:O	1.22	1.35
1:A:54:ARG:HD3	2:P:367:GLN:O	1.27	1.34
2:P:358:GLU:HG3	3:P:402:HOH:O	1.26	1.26

The worst 5 of 745 symmetry-related close contacts are listed below. The label for Atom-2 includes

the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:PHE:CZ	1:A:273:GLU:OE2[3_444]	0.19	2.01
1:A:38:PHE:CA	1:A:214:GLU:N[3_444]	0.21	1.99
1:A:168:SER:OG	1:A:283:LEU:CG[3_554]	0.22	1.98
1:A:120:THR:CB	1:A:341:GLN:OE1[3_444]	0.28	1.92
1:A:37:THR:CG2	1:A:214:GLU:OE1[3_444]	0.31	1.89

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	344/346 (99%)	299 (87%)	32 (9%)	13 (4%)	2	9
2	P	7/9 (78%)	3 (43%)	2 (29%)	2 (29%)	0	0
All	All	351/355 (99%)	302 (86%)	34 (10%)	15 (4%)	2	7

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	TRP
1	A	251	GLN
1	A	267	GLN
2	P	363	LEU
1	A	72	ASN

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	302/302 (100%)	272 (90%)	30 (10%)	7	22
2	P	9/9 (100%)	6 (67%)	3 (33%)	0	0
All	All	311/311 (100%)	278 (89%)	33 (11%)	6	19

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	GLU
1	A	341	GLN
2	P	367	GLN
1	A	133	ASN
1	A	129	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	HIS
1	A	295	GLN
1	A	341	GLN
1	A	316	GLN
1	A	177	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	346/346 (100%)	6.44	322 (93%) 0 0	53, 86, 197, 278	0
2	P	9/9 (100%)	5.95	8 (88%) 0 0	91, 114, 149, 158	0
All	All	355/355 (100%)	6.43	330 (92%) 0 0	53, 87, 197, 278	0

The worst 5 of 330 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	ASN	33.6
1	A	220	TYR	32.4
1	A	230	THR	23.9
1	A	203	GLY	22.7
1	A	149	GLN	21.6

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.