Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 03:15 AM EDT

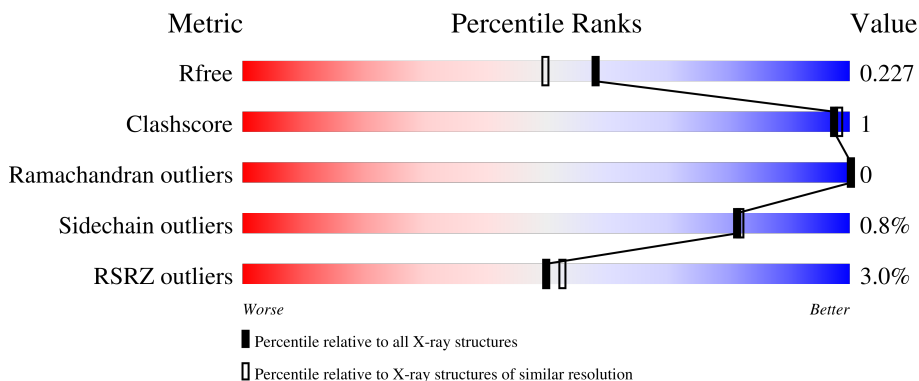|		
PDB ID	:	7S48
Title	:	PAK4cat in complex with Integrin beta5 760-770 peptide
Authors	:	Ha, B.H.; Boggon, T.J.
Deposited on	:	2021-09-08
Resolution	:	1.90 Å(reported)

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 1.90 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	Percentile Ranks	Value
Rfree		0.227
Clashscore		1
Ramachandran outliers		0
Sidechain outliers		0.8%
RSRZ outliers		3.0%

Worse ———————————————————— *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	% 80% • 16%
2	B	11	55% 64% 36%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2492 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 Serine/threonine-protein kinase PAK 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	290	2311	1474	407	415	1	14	0	2	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	MET	-	expression tag	UNP O96013
A	247	GLY	-	expression tag	UNP O96013
A	248	SER	-	expression tag	UNP O96013
A	249	SER	-	expression tag	UNP O96013
A	250	HIS	-	expression tag	UNP O96013
A	251	HIS	-	expression tag	UNP O96013
A	252	HIS	-	expression tag	UNP O96013
A	253	HIS	-	expression tag	UNP O96013
A	254	HIS	-	expression tag	UNP O96013
A	255	HIS	-	expression tag	UNP O96013
A	256	SER	-	expression tag	UNP O96013
A	257	SER	-	expression tag	UNP O96013
A	258	GLY	-	expression tag	UNP O96013
A	259	LEU	-	expression tag	UNP O96013
A	260	VAL	-	expression tag	UNP O96013
A	261	PRO	-	expression tag	UNP O96013
A	262	ARG	-	expression tag	UNP O96013
A	263	GLY	-	expression tag	UNP O96013
A	264	SER	-	expression tag	UNP O96013
A	265	HIS	-	expression tag	UNP O96013
A	266	MET	-	expression tag	UNP O96013
A	267	GLU	-	expression tag	UNP O96013
A	268	ASN	-	expression tag	UNP O96013
A	269	LEU	-	expression tag	UNP O96013
A	270	TYR	-	expression tag	UNP O96013
A	271	PHE	-	expression tag	UNP O96013
A	272	GLN	-	expression tag	UNP O96013

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Chain	Residue	Modelled	Actual	Comment	Reference
A	273	GLY	-	expression tag	UNP O96013

- Molecule 2 is a protein called Integrin beta-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	7	Total 62	C 37	N 13	O 11	S 1	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total 119	O 119	0	0

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: Serine/threonine-protein kinase PAK 4
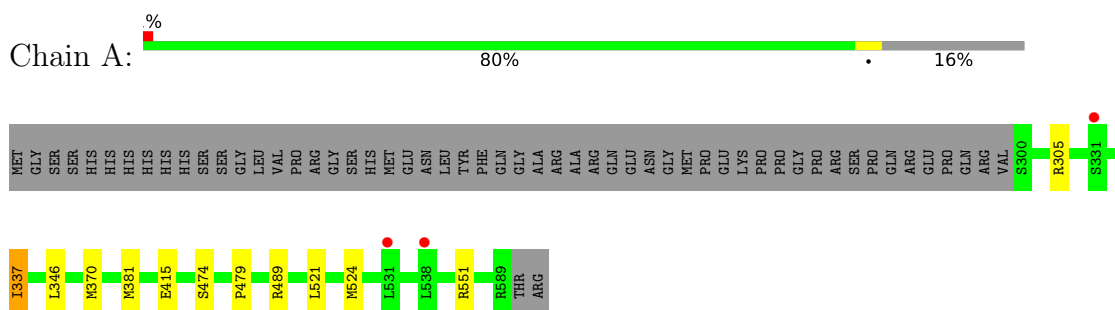
• Molecule 2: Integrin beta-5
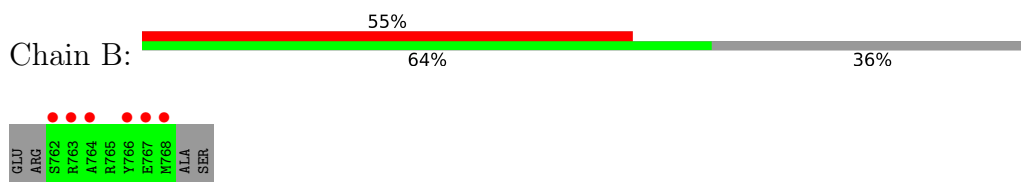
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	61.73Å 61.73Å 179.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 1.90 43.65 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.01-1.90) 99.5 (43.65-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.179 , 0.222 0.186 , 0.227	Depositor DCC
R_{free} test set	1475 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.1	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2492	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SEP

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	0.70	0/2348	0.84	4/3179 (0.1%)
2	B	0.54	0/62	0.81	0/80
All	All	0.70	0/2410	0.84	4/3259 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	305	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	305	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	551	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	551	ARG	NE-CZ-NH2	-5.51	117.54	120.30

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	A	2311	0	2371	4	1
2	B	62	0	59	0	0
3	A	119	0	0	0	0
All	All	2492	0	2430	4	1

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 1.

All (4) 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:337[A]:ILE:HD11	1:A:346:LEU:HD13	1.86	0.57
1:A:521:LEU:HD23	1:A:524:MET:HE3	1.97	0.46
1:A:521:LEU:HA	1:A:524:MET:HE3	2.00	0.44
1:A:370:MET:HE2	1:A:381:MET:HB3	1.99	0.43

All (1) 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:415:GLU:OE2	1:A:489:ARG:NH2[7_455]	2.03	0.17

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	289/346 (84%)	283 (98%)	6 (2%)	0	100	100
2	B	5/11 (46%)	5 (100%)	0	0	100	100
All	All	294/357 (82%)	288 (98%)	6 (2%)	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	254/300 (85%)	251 (99%)	3 (1%)	71	70
2	B	6/9 (67%)	6 (100%)	0	100	100
All	All	260/309 (84%)	257 (99%)	3 (1%)	81	70

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337[A]	ILE
1	A	337[B]	ILE
1	A	479	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	464	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
1	SEP	A	474	1	8,9,10	0.71	0	8,12,14	1.33	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	474	1	-	1/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	474	SEP	O2P-P-OG	-2.28	100.66	106.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	474	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	289/346 (83%)	-0.08	3 (1%)	82	84	27, 38, 57, 64	0
2	B	7/11 (63%)	2.77	6 (85%)	0	0	64, 80, 97, 102	0
All	All	296/357 (82%)	-0.01	9 (3%)	50	53	27, 38, 60, 102	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	766	TYR	5.1
2	B	763	ARG	4.0
1	A	331	SER	2.8
2	B	762	SER	2.6
2	B	767	GLU	2.4
2	B	768	MET	2.4
1	A	538	LEU	2.3
1	A	531	LEU	2.2
2	B	764	ALA	2.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
1	SEP	A	474	10/11	0.99	0.07	28,32,32,33	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.