



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:45 PM UTC

PDB ID : 5FPI / pdb_00005fpi
Title : Mu2 adaptin subunit of the AP2 adaptor (C-terminal domain) complexed with Integrin alpha4 internalisation peptide QYKSILQE
Authors : Owen, D.J.; Evans, P.R.; Ivaska, J.
Deposited on : 2015-11-30
Resolution : 2.77 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

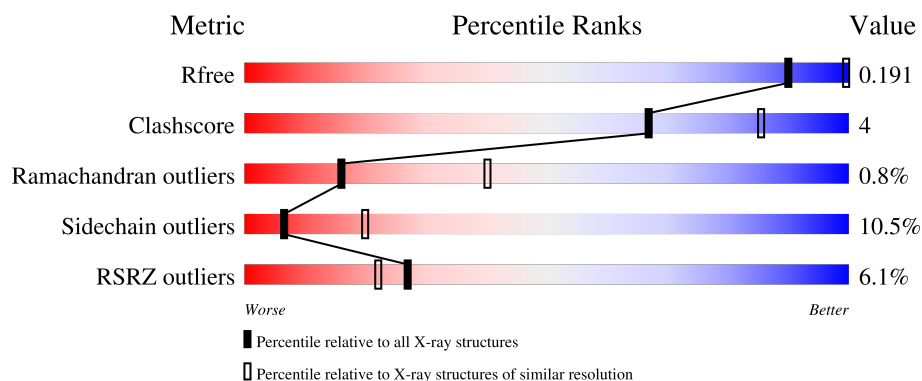
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	446	3% 46% 10% • 42%
2	B	8	25% 75% 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2175 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 AP-2 COMPLEX SUBUNIT MU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2078	1335	366	363	14			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	237	MET	-	insertion	UNP P84092
A	237A	GLU	-	insertion	UNP P84092
A	237B	GLN	-	insertion	UNP P84092
A	237C	LYS	-	insertion	UNP P84092
A	237D	LEU	-	insertion	UNP P84092
A	237E	ILE	-	insertion	UNP P84092
A	237F	SER	-	insertion	UNP P84092
A	237G	GLU	-	insertion	UNP P84092
A	237H	GLU	-	insertion	UNP P84092
A	237I	ASP	-	insertion	UNP P84092
A	237J	LEU	-	insertion	UNP P84092

- Molecule 2 is a protein called INTEGRIN ALPHA-4 SUBUNIT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	0
			52	35	8	9			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		
3	B	3	Total	O	0	0
			3	3		

4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	125.65Å 125.65Å 74.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	108.82 – 2.77 108.82 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.3 (108.82-2.77) 99.2 (108.82-2.77)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.174 , 0.224 0.201 , 0.191	Depositor DCC
R_{free} test set	864 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	86.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2175	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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	1.28	4/2119 (0.2%)	1.21	6/2848 (0.2%)
2	B	1.22	0/52	1.27	0/68
All	All	1.28	4/2171 (0.2%)	1.21	6/2916 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	PRO	CA-CB	-6.65	1.49	1.53
1	A	364	SER	CA-C	-5.53	1.45	1.52
1	A	267	PRO	C-O	-5.32	1.18	1.24
1	A	299	THR	CA-C	5.08	1.59	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	GLY	N-CA-C	5.90	127.16	113.18
1	A	241	ILE	N-CA-C	5.60	116.98	108.80
1	A	166	ILE	N-CA-C	5.38	115.99	108.89
1	A	323	ARG	CB-CA-C	5.30	118.96	110.16
1	A	430	ILE	CB-CA-C	-5.03	104.58	111.33
1	A	165	GLY	N-CA-C	5.01	123.69	115.73

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	2078	0	2170	16	0
2	B	52	0	59	0	0
3	A	42	0	0	4	0
3	B	3	0	0	0	0
All	All	2175	0	2229	16	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 4.

All (16) 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:256:LYS:O	1:A:260:GLU:N	2.16	0.78
1:A:218:ASP:OD2	1:A:261:ARG:NH1	2.32	0.62
1:A:399:LEU:HD23	1:A:400:LYS:N	2.16	0.60
1:A:323:ARG:NH2	1:A:348:GLU:OE1	2.38	0.53
1:A:380:LYS:HG2	1:A:381:TRP:N	2.25	0.52
1:A:256:LYS:C	1:A:260:GLU:N	2.68	0.52
1:A:399:LEU:HD23	1:A:399:LEU:C	2.35	0.52
1:A:420:LYS:NZ	3:A:2036:HOH:O	2.47	0.47
1:A:163:ARG:HG2	3:A:2001:HOH:O	2.15	0.47
1:A:311:PHE:O	1:A:312:LYS:C	2.58	0.47
1:A:294:ARG:HD3	3:A:2015:HOH:O	2.17	0.45
1:A:212:CYS:HA	1:A:405:LYS:O	2.17	0.45
1:A:278:ARG:HG3	1:A:278:ARG:HH11	1.84	0.43
1:A:209:MET:N	1:A:408:GLU:OE1	2.47	0.42
1:A:265:PHE:CD1	1:A:265:PHE:N	2.88	0.42
1:A:199:ARG:HD3	3:A:2009:HOH:O	2.21	0.41

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	252/446 (56%)	234 (93%)	16 (6%)	2 (1%)	16	40
2	B	4/8 (50%)	4 (100%)	0	0	100	100
All	All	256/454 (56%)	238 (93%)	16 (6%)	2 (1%)	16	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	GLY
1	A	376	ASN

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	233/398 (58%)	208 (89%)	25 (11%)	6	19
2	B	6/8 (75%)	6 (100%)	0	100	100
All	All	239/406 (59%)	214 (90%)	25 (10%)	6	20

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	ARG
1	A	180	SER
1	A	188	GLN
1	A	197	SER
1	A	204	SER
1	A	213	LYS
1	A	221	VAL
1	A	240	SER
1	A	241	ILE
1	A	253	ARG
1	A	256	LYS
1	A	279	THR
1	A	292	LEU
1	A	300	LYS

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Mol	Chain	Res	Type
1	A	304	LYS
1	A	309	SER
1	A	323	ARG
1	A	331	SER
1	A	341	LYS
1	A	345	LYS
1	A	357	ARG
1	A	376	ASN
1	A	377	ASP
1	A	380	LYS
1	A	434	ARG

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	188	GLN
1	A	239	GLN
1	A	349	ASN
1	A	376	ASN

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	258/446 (57%)	-0.03	14 (5%) 31 26	36, 57, 101, 125	0
2	B	6/8 (75%)	1.01	2 (33%) 1 1	43, 62, 82, 86	0
All	All	264/454 (58%)	-0.01	16 (6%) 27 22	36, 57, 100, 125	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	SER	5.5
1	A	221	VAL	4.5
1	A	379	LYS	4.3
1	A	256	LYS	3.7
1	A	254	LEU	3.5
1	A	238	LYS	3.3
2	B	6	LEU	3.3
1	A	220	ILE	3.0
2	B	1	GLN	2.9
1	A	380	LYS	2.6
1	A	407	PHE	2.3
1	A	409	PRO	2.2
1	A	239	GLN	2.2
1	A	260	GLU	2.2
1	A	378	LYS	2.1
1	A	377	ASP	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.