Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 11:22 AM EDT

PDB ID	:	3H1Z
Title	:	Molecular basis for the association of PIPKIgamma -p90 with the clathrin adaptor AP-2
Authors	:	Vahedi-Faridi, A.; Kahlfeldt, N.; Schaefer, J.G.; Krainer, G.; Keller, S.; Saenger, W.; Krauss, M.; Haucke, V.
Deposited on	:	2009-04-14
Resolution	:	1.83 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 (i) 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 (i)) were used in the production of this report:

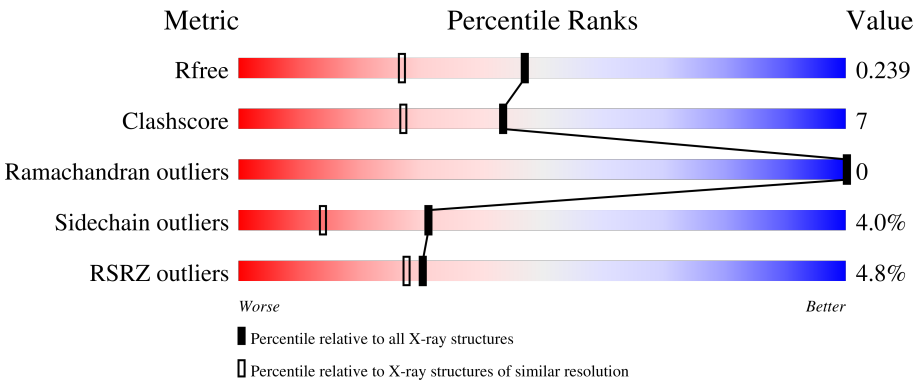
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	260	5% 77% 11% • 10%
2	P	15	93% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2270 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 beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	233	1881	1211	313	346	11	0	5	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	678	MET	-	expression tag	UNP P62944
A	679	GLY	-	expression tag	UNP P62944
A	680	SER	-	expression tag	UNP P62944
A	681	SER	-	expression tag	UNP P62944
A	682	HIS	-	expression tag	UNP P62944
A	683	HIS	-	expression tag	UNP P62944
A	684	HIS	-	expression tag	UNP P62944
A	685	HIS	-	expression tag	UNP P62944
A	686	HIS	-	expression tag	UNP P62944
A	687	HIS	-	expression tag	UNP P62944
A	688	SER	-	expression tag	UNP P62944
A	689	SER	-	expression tag	UNP P62944
A	690	GLY	-	expression tag	UNP P62944
A	691	LEU	-	expression tag	UNP P62944
A	692	VAL	-	expression tag	UNP P62944
A	693	PRO	-	expression tag	UNP P62944
A	694	ARG	-	expression tag	UNP P62944
A	695	GLY	-	expression tag	UNP P62944
A	696	SER	-	expression tag	UNP P62944
A	697	HIS	-	expression tag	UNP P62944
A	698	MET	-	expression tag	UNP P62944
A	699	ALA	-	expression tag	UNP P62944
A	700	SER	-	expression tag	UNP P62944

- Molecule 2 is a protein called Phosphatidylinositol-4-phosphate 5-kinase type-1 gamma.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	P	15	136	90	21	25	0	0	0

- Molecule 3 is water.

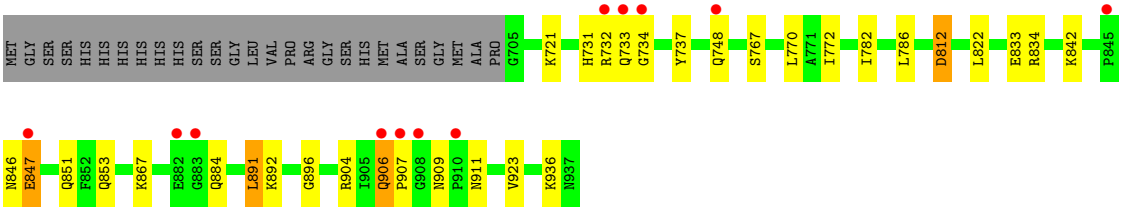
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	235	235	235	0	0
			Total	O		
3	P	18	18	18	0	0

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.

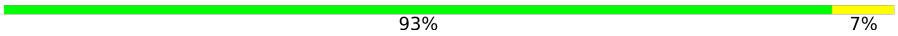
• Molecule 1: AP-2 complex subunit beta-1

Chain A:



• Molecule 2: Phosphatidylinositol-4-phosphate 5-kinase type-1 gamma

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	37.56Å 83.47Å 91.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.25 – 1.83 34.25 – 1.83	Depositor EDS
% Data completeness (in resolution range)	94.5 (34.25-1.83) 94.5 (34.25-1.83)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 1.83Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.236 0.197 , 0.239	Depositor DCC
R_{free} test set	1258 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	20.4	Xtriage
Anisotropy	0.751	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2270	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (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	0.78	0/1939	0.74	2/2634 (0.1%)
2	P	0.84	0/143	0.73	0/195
All	All	0.78	0/2082	0.74	2/2829 (0.1%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	891	LEU	CA-CB-CG	5.69	128.39	115.30
1	A	834	ARG	NE-CZ-NH2	-5.67	117.47	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	734	GLY	Peptide

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	1881	0	1903	27	0
2	P	136	0	120	0	0
3	A	235	0	0	9	0
3	P	18	0	0	0	0
All	All	2270	0	2023	27	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 7.

All (27) 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:906:GLN:HG2	1:A:909:ASN:HB3	1.53	0.90
1:A:884:GLN:OE1	1:A:904:ARG:HD3	1.73	0.88
1:A:906:GLN:HB2	3:A:195:HOH:O	1.75	0.85
1:A:731:HIS:HD2	3:A:161:HOH:O	1.64	0.81
1:A:906:GLN:HG2	1:A:909:ASN:CB	2.10	0.80
1:A:772:ILE:HG12	1:A:782[A]:ILE:CD1	2.25	0.66
1:A:721:LYS:NZ	1:A:812:ASP:OD2	2.28	0.60
1:A:906:GLN:NE2	1:A:906:GLN:H	2.01	0.58
1:A:732:ARG:C	1:A:733:GLN:HG2	2.25	0.57
1:A:846:ASN:HB3	3:A:146:HOH:O	2.04	0.57
1:A:884:GLN:HG2	1:A:907:PRO:HD2	1.91	0.53
1:A:892:LYS:HE2	1:A:896:GLY:HA2	1.91	0.52
1:A:833:GLU:HG3	3:A:40:HOH:O	2.09	0.51
1:A:731:HIS:CD2	3:A:161:HOH:O	2.50	0.50
1:A:842:LYS:HE3	3:A:249:HOH:O	2.12	0.49
1:A:936:LYS:HD2	3:A:109:HOH:O	2.13	0.48
1:A:906:GLN:H	1:A:906:GLN:CD	2.18	0.47
1:A:732:ARG:NH2	1:A:737:TYR:CZ	2.68	0.47
1:A:847:GLU:H	1:A:847:GLU:HG3	1.50	0.46
1:A:732:ARG:O	1:A:733:GLN:HG2	2.16	0.45
1:A:770:LEU:HD23	1:A:786:LEU:HD13	1.97	0.45
1:A:853:GLN:HE21	1:A:911:ASN:HB3	1.83	0.43
1:A:833:GLU:HB3	3:A:104:HOH:O	2.19	0.43
1:A:732:ARG:O	1:A:733:GLN:CG	2.68	0.42
1:A:923:VAL:O	1:A:923:VAL:HG12	2.19	0.42
1:A:867:LYS:HE3	3:A:131:HOH:O	2.21	0.40
1:A:732:ARG:C	1:A:733:GLN:CG	2.89	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	236/260 (91%)	233 (99%)	3 (1%)	0	100	100
2	P	13/15 (87%)	13 (100%)	0	0	100	100
All	All	249/275 (90%)	246 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	214/230 (93%)	205 (96%)	9 (4%)	30	12
2	P	15/15 (100%)	14 (93%)	1 (7%)	16	4
All	All	229/245 (94%)	219 (96%)	10 (4%)	31	11

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	748	GLN
1	A	767[A]	SER
1	A	767[B]	SER
1	A	812	ASP
1	A	822	LEU
1	A	847	GLU
1	A	851	GLN
1	A	891	LEU

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Mol	Chain	Res	Type
1	A	906	GLN
2	P	7	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	731	HIS
1	A	733	GLN
1	A	749	HIS
1	A	853	GLN
1	A	880	ASN
1	A	906	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	233/260 (89%)	0.06	12 (5%) 27 24	9, 20, 40, 51	1 (0%)
2	P	15/15 (100%)	-0.19	0 100 100	15, 20, 34, 37	0
All	All	248/275 (90%)	0.05	12 (4%) 30 28	9, 20, 39, 51	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	733	GLN	6.4
1	A	908	GLY	6.1
1	A	734	GLY	5.5
1	A	732	ARG	4.9
1	A	907	PRO	4.5
1	A	906	GLN	4.5
1	A	847	GLU	3.6
1	A	882	GLU	3.1
1	A	883	GLY	2.7
1	A	910	PRO	2.7
1	A	845	PRO	2.4
1	A	748	GLN	2.2

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 monosaccharides 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.