



Full wwPDB X-ray Structure Validation Report

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PDB ID : 2G30
Title : beta appendage of AP2 complexed with ARH peptide
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Deposited on : 2006-02-17
Resolution : 1.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

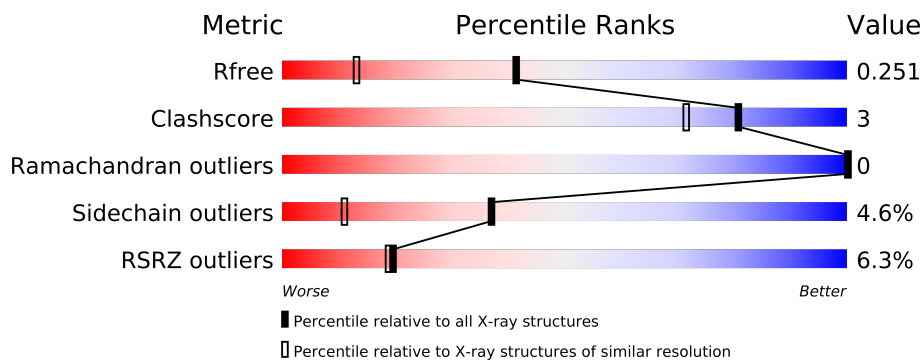
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.60 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}	66092	1872 (1.60-1.60)
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (1.60-1.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	258	
2	P	16	
3	S	3	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2134 atoms, of which 0 are hydrogen and 0 are deuterium.

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	1848	1190	309	338	11	5	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	CLONING ARTIFACT	UNP P63010
A	-20	GLY	-	CLONING ARTIFACT	UNP P63010
A	-19	SER	-	CLONING ARTIFACT	UNP P63010
A	-18	SER	-	CLONING ARTIFACT	UNP P63010
A	-17	HIS	-	CLONING ARTIFACT	UNP P63010
A	-16	HIS	-	CLONING ARTIFACT	UNP P63010
A	-15	HIS	-	CLONING ARTIFACT	UNP P63010
A	-14	HIS	-	CLONING ARTIFACT	UNP P63010
A	-13	HIS	-	CLONING ARTIFACT	UNP P63010
A	-12	HIS	-	CLONING ARTIFACT	UNP P63010
A	-11	SER	-	CLONING ARTIFACT	UNP P63010
A	-10	SER	-	CLONING ARTIFACT	UNP P63010
A	-9	GLY	-	CLONING ARTIFACT	UNP P63010
A	-8	LEU	-	CLONING ARTIFACT	UNP P63010
A	-7	VAL	-	CLONING ARTIFACT	UNP P63010
A	-6	PRO	-	CLONING ARTIFACT	UNP P63010
A	-5	ARG	-	CLONING ARTIFACT	UNP P63010
A	-4	GLY	-	CLONING ARTIFACT	UNP P63010
A	-3	SER	-	CLONING ARTIFACT	UNP P63010
A	-2	HIS	-	CLONING ARTIFACT	UNP P63010
A	-1	MET	-	CLONING ARTIFACT	UNP P63010

- Molecule 2 is a protein called 16-mer peptide from Low density lipoprotein receptor adapter protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	16	Total	C	N	O	0	0	0
			121	72	23	26			

- Molecule 3 is a protein called peptide sequence AAF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	S	3	Total	C	N	O	0	0	0
			21	15	3	3			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	132	Total	O	0	0
			132	132		
4	P	8	Total	O	0	0
			8	8		
4	S	4	Total	O	0	0
			4	4		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	37.75Å 36.31Å 98.98Å 90.00° 92.91° 90.00°	Depositor
Resolution (Å)	20.00 – 1.60 35.84 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-1.60) 99.2 (35.84-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.215 , 0.243 0.223 , 0.251	Depositor DCC
R_{free} test set	1781 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.5	EDS
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 35513 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2134	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.67	2/1891 (0.1%)	0.82	3/2570 (0.1%)
2	P	0.45	0/121	0.86	0/161
3	S	0.98	0/21	0.73	0/27
All	All	0.67	2/2033 (0.1%)	0.83	3/2758 (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
3	S	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	737	TYR	CB-CG	-5.26	1.43	1.51
1	A	931	TYR	CD1-CE1	-5.17	1.31	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	829	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	885	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	826	PHE	CB-CG-CD1	5.19	124.43	120.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	906	GLN	Peptide
3	S	6	ALA	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1848	0	1855	12	0
2	P	121	0	113	2	0
3	S	21	0	18	0	0
4	A	132	0	0	3	1
4	P	8	0	0	1	1
4	S	4	0	0	0	0
All	All	2134	0	1986	13	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (13) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:909:ASN:O	4:A:36:HOH:O	1.95	0.82
1:A:775:PRO:HB2	1:A:777:MET:CE	2.15	0.75
1:A:891:LEU:HD11	1:A:899:ILE:HD13	1.80	0.63
1:A:880:ASN:ND2	4:A:98:HOH:O	2.29	0.62
1:A:775:PRO:HB2	1:A:777:MET:HE2	1.82	0.60
1:A:739:GLU:OE1	1:A:785:SER:OG	2.23	0.54
1:A:775:PRO:HB2	1:A:777:MET:HE3	1.91	0.53
1:A:867:LYS:NZ	1:A:937:ASN:O	2.43	0.50
1:A:835:GLN:HG3	2:P:4:LEU:HD11	1.93	0.50
2:P:3:GLY:C	4:P:28:HOH:O	2.50	0.50
1:A:759:LYS:HB2	1:A:795:MET:HE3	1.95	0.49
1:A:907:PRO:HA	4:A:118:HOH:O	2.17	0.44
1:A:859:LEU:O	1:A:912:TYR:OH	2.23	0.41

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	Distance(Å)	Clash(Å)
4:A:143:HOH:O	4:P:144:HOH:O[1_455]	1.44	0.76

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	231/258 (90%)	228 (99%)	3 (1%)	0	100	100
2	P	14/16 (88%)	14 (100%)	0	0	100	100
3	S	1/3 (33%)	1 (100%)	0	0	100	100
All	All	246/277 (89%)	243 (99%)	3 (1%)	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	206/229 (90%)	197 (96%)	9 (4%)	39	12
2	P	12/13 (92%)	11 (92%)	1 (8%)	16	2
3	S	1/1 (100%)	1 (100%)	0	100	100
All	All	219/243 (90%)	209 (95%)	10 (5%)	37	11

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

Mol	Chain	Res	Type
1	A	731	HIS
1	A	749	HIS
1	A	808	LYS
1	A	822	LEU

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Mol	Chain	Res	Type
1	A	835	GLN
1	A	906	GLN
1	A	909	ASN
1	A	931	TYR
1	A	936	LYS
2	P	9	SER

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

Mol	Chain	Res	Type
1	A	880	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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(Å ²)	Q<0.9
1	A	233/258 (90%)	0.42	14 (6%)	21 20	15, 25, 41, 50	2 (0%)
2	P	16/16 (100%)	0.73	1 (6%)	19 19	22, 36, 39, 46	0
3	S	3/3 (100%)	1.37	1 (33%)	1 1	23, 23, 27, 33	0
All	All	252/277 (90%)	0.45	16 (6%)	19 19	15, 25, 41, 50	2 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	771	ALA	7.0
1	A	910	PRO	6.4
1	A	907	PRO	6.2
1	A	773	HIS	4.4
1	A	908	GLY	4.4
2	P	16	THR	4.4
1	A	858	HIS	4.1
1	A	772	ILE	3.4
1	A	909	ASN	3.3
1	A	856	GLU	3.1
1	A	843	ASP	3.1
1	A	847	GLU	2.8
1	A	906	GLN	2.7
3	S	6	ALA	2.7
1	A	731	HIS	2.6
1	A	911	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.