Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 09:32 AM EDT

PDB ID	:	1KYF
Title	:	AP-2 CLATHRIN ADAPTOR ALPHA-APPENDAGE IN COMPLEX WITH EPS15 DPF PEPTIDE
Authors	:	Brett, T.J.; Traub, L.M.; Fremont, D.H.
Deposited on	:	2002-02-04
Resolution	:	1.22 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 (1)) were used in the production of this report:

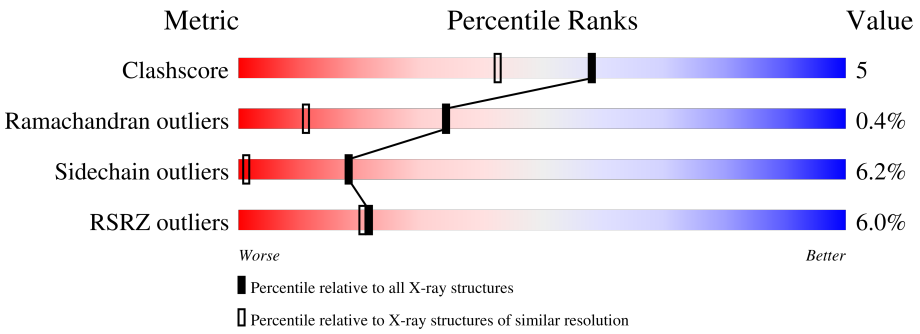
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.22 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))
Clashscore	141614	1294 (1.24-1.20)
Ramachandran outliers	138981	1251 (1.24-1.20)
Sidechain outliers	138945	1250 (1.24-1.20)
RSRZ outliers	127900	1209 (1.24-1.20)

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	247	5% 87% 10% • •
2	P	6	50% 33% 33% 17% 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4239 atoms, of which 1897 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 ALPHA-ADAPTIN C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	247	3854	1242	1897	336	370	9	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	692	GLY	-	cloning artifact	UNP P17427
A	693	SER	-	cloning artifact	UNP P17427
A	694	PRO	-	cloning artifact	UNP P17427
A	695	GLY	-	cloning artifact	UNP P17427
A	696	ILE	-	cloning artifact	UNP P17427
A	697	ARG	-	cloning artifact	UNP P17427
A	698	LEU	-	cloning artifact	UNP P17427
A	699	GLY	-	cloning artifact	UNP P17427
A	700	SER	-	cloning artifact	UNP P17427

- Molecule 2 is a protein called Epidermal growth factor receptor substrate 15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	P	5	42	27	6	9	0	0	0

- Molecule 3 is water.

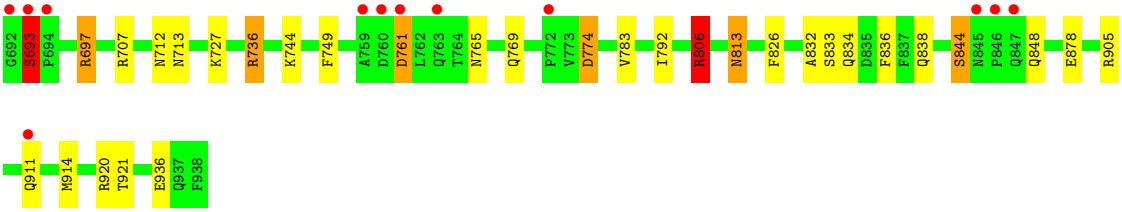
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	338	338	338	0	0
3	P	5	5	5	0	0

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.

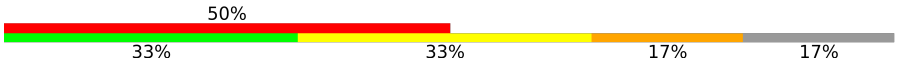
• Molecule 1: ALPHA-ADAPTIN C

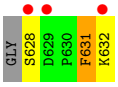
Chain A:



• Molecule 2: Epidermal growth factor receptor substrate 15

Chain P:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	40.62Å 72.82Å 41.86Å 90.00° 99.95° 90.00°	Depositor
Resolution (Å)	20.00 – 1.22 18.20 – 1.22	Depositor EDS
% Data completeness (in resolution range)	94.4 (20.00-1.22) 87.2 (18.20-1.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 1.22Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.153 , 0.211 0.152 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	12.9	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.51 , 89.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	4239	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 6.29% 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	0.64	0/1994	1.49	15/2697 (0.6%)
2	P	0.69	0/43	1.74	1/55 (1.8%)
All	All	0.64	0/2037	1.50	16/2752 (0.6%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	707	ARG	CD-NE-CZ	37.52	176.12	123.60
1	A	806	ARG	CD-NE-CZ	16.89	147.25	123.60
1	A	806	ARG	NE-CZ-NH1	11.41	126.00	120.30
1	A	806	ARG	NE-CZ-NH2	-9.63	115.49	120.30
1	A	707	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	A	920	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	A	920	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	A	749	PHE	CB-CG-CD1	6.17	125.12	120.80
1	A	736	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	A	836	PHE	CB-CG-CD2	6.12	125.08	120.80
1	A	774	ASP	CB-CG-OD1	5.89	123.60	118.30
2	P	631	PHE	CB-CG-CD1	5.80	124.86	120.80
1	A	749	PHE	CB-CG-CD2	-5.45	116.98	120.80
1	A	905	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	844	SER	O-C-N	5.25	131.10	122.70
1	A	736	ARG	NE-CZ-NH1	5.14	122.87	120.30

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	1957	1897	1953	16	0
2	P	42	0	37	3	0
3	A	338	0	0	9	0
3	P	5	0	0	1	0
All	All	2342	1897	1990	19	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 5.

All (19) 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:936:GLU:HG3	3:A:252:HOH:O	1.90	0.71
1:A:744:LYS:HE2	3:A:275:HOH:O	1.95	0.67
1:A:736:ARG:HD2	3:A:172:HOH:O	1.97	0.63
2:P:631:PHE:O	2:P:632:LYS:HB3	2.06	0.56
1:A:774:ASP:HB3	3:A:81:HOH:O	2.10	0.51
1:A:783:VAL:HG23	3:A:72:HOH:O	2.13	0.49
1:A:712:ASN:C	1:A:713:ASN:HD22	2.18	0.46
1:A:848:GLN:HB3	1:A:921:THR:O	2.16	0.46
2:P:632:LYS:HB3	2:P:632:LYS:HE2	1.37	0.46
1:A:834:GLN:NE2	1:A:838:GLN:OE1	2.49	0.45
1:A:806:ARG:NE	3:A:287:HOH:O	2.50	0.45
1:A:834:GLN:O	1:A:838:GLN:HG3	2.16	0.45
1:A:813:ASN:ND2	3:A:194:HOH:O	2.50	0.45
2:P:632:LYS:NZ	3:P:340:HOH:O	2.49	0.44
1:A:761:ASP:OD1	1:A:765:ASN:ND2	2.52	0.43
1:A:832:ALA:HA	3:A:276:HOH:O	2.20	0.41
1:A:693:SER:O	1:A:693:SER:OG	2.30	0.41
1:A:697:ARG:HG3	3:A:347:HOH:O	2.21	0.41
1:A:713:ASN:ND2	1:A:727:LYS:HA	2.35	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	245/247 (99%)	241 (98%)	3 (1%)	1 (0%)	34 11
2	P	3/6 (50%)	3 (100%)	0	0	100 100
All	All	248/253 (98%)	244 (98%)	3 (1%)	1 (0%)	34 11

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	693	SER

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	220/220 (100%)	207 (94%)	13 (6%)	19 1
2	P	5/5 (100%)	4 (80%)	1 (20%)	1 0
All	All	225/225 (100%)	211 (94%)	14 (6%)	18 1

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	693	SER
1	A	697	ARG
1	A	761	ASP
1	A	769	GLN
1	A	792	ILE

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Mol	Chain	Res	Type
1	A	806	ARG
1	A	813	ASN
1	A	826	PHE
1	A	833	SER
1	A	844	SER
1	A	878	GLU
1	A	911	GLN
1	A	914	MET
2	P	628	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	713	ASN
1	A	834	GLN
1	A	851	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	247/247 (100%)	0.22	12 (4%)	29	28	13, 19, 41, 70	0
2	P	5/6 (83%)	3.73	3 (60%)	0	0	29, 31, 53, 62	0
All	All	252/253 (99%)	0.28	15 (5%)	21	20	13, 20, 41, 70	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	692	GLY	10.3
2	P	628	SER	8.5
1	A	693	SER	7.2
1	A	694	PRO	4.4
1	A	845	ASN	4.2
1	A	760	ASP	4.2
1	A	772	PRO	4.1
2	P	632	LYS	4.0
1	A	847	GLN	3.5
1	A	911	GLN	3.2
1	A	846	PRO	3.1
1	A	761	ASP	3.1
1	A	759	ALA	2.8
2	P	629	ASP	2.5
1	A	763	GLN	2.1

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.