



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:41 PM GMT

PDB ID : 2J2J
Title : CANINE ADENOVIRUS FIBRE HEAD AT 1.5 A RESOLUTION
Authors : Seiradake, E.; Lortat-Jacob, H.; Billet, O.; Kremer, E.J.; Cusack, S.
Deposited on : 2006-08-16
Resolution : 1.50 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>

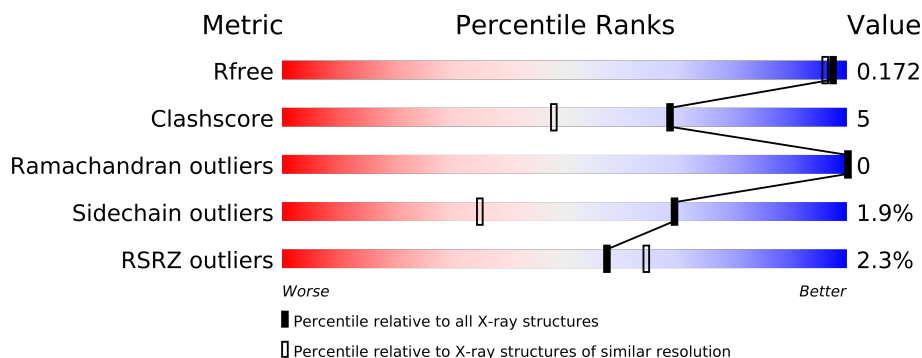
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.50 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	1513 (1.50-1.50)
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)
RSRZ outliers	66119	1514 (1.50-1.50)

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	197	
1	B	197	
1	C	197	
1	D	197	
1	E	197	
1	F	197	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10007 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 FIBER PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
1	B	182	Total	C	N	O	S	0	1	0
			1409	894	239	267	9			
1	C	182	Total	C	N	O	S	0	2	0
			1417	901	240	267	9			
1	D	182	Total	C	N	O	S	0	2	0
			1416	902	239	266	9			
1	E	182	Total	C	N	O	S	0	0	0
			1406	892	239	266	9			
1	F	182	Total	C	N	O	S	0	2	0
			1414	899	239	267	9			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	244	Total	O	0	0
			244	244		
2	B	253	Total	O	0	0
			253	253		
2	C	241	Total	O	0	0
			241	241		
2	D	276	Total	O	0	0
			276	276		
2	E	264	Total	O	0	0
			264	264		
2	F	261	Total	O	0	0
			261	261		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

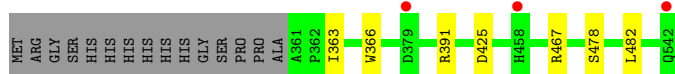
• Molecule 1: FIBER PROTEIN

Chain A: 



• Molecule 1: FIBER PROTEIN

Chain B: 



• Molecule 1: FIBER PROTEIN

Chain C: 



• Molecule 1: FIBER PROTEIN

Chain D: 



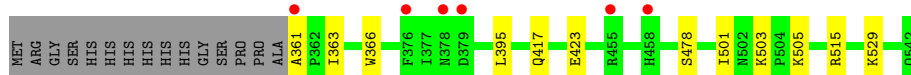
• Molecule 1: FIBER PROTEIN

Chain E: 



• Molecule 1: FIBER PROTEIN

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.83Å 88.55Å 106.91Å 90.00° 96.40° 90.00°	Depositor
Resolution (Å)	106.00 – 1.50 28.44 – 1.50	Depositor EDS
% Data completeness (in resolution range)	94.8 (106.00-1.50) 94.9 (28.44-1.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.54 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.165 , 0.206 0.173 , 0.172	Depositor DCC
R_{free} test set	3133 reflections (2.04%)	DCC
Wilson B-factor (Å ²)	6.2	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 43.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 156532 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10007	wwPDB-VP
Average B, all atoms (Å ²)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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	0.57	0/1441	0.72	0/1964
1	B	0.54	0/1447	0.73	1/1972 (0.1%)
1	C	0.57	0/1458	0.72	0/1987
1	D	0.57	0/1457	0.74	0/1986
1	E	0.54	0/1441	0.73	0/1964
1	F	0.56	0/1455	0.69	0/1983
All	All	0.56	0/8699	0.72	1/11856 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	425	ASP	CB-CG-OD1	5.28	123.05	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1406	0	0	6	0
1	B	1409	0	0	3	0
1	C	1417	0	0	7	0
1	D	1416	0	0	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1406	0	0	10	0
1	F	1414	0	0	10	0
2	A	244	0	0	4	0
2	B	253	0	0	3	0
2	C	241	0	0	6	0
2	D	276	0	0	7	1
2	E	264	0	0	10	0
2	F	261	0	0	7	0
All	All	10007	0	0	41	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 5.

All (41) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:364:THR:CG2	2:D:2041:HOH:O	2.17	0.91
1:C:442:TRP:CE3	2:C:2011:HOH:O	2.26	0.89
1:C:488:ASP:OD2	1:F:417:GLN:NE2	2.05	0.89
1:B:478[B]:SER:OG	2:B:2149:HOH:O	1.93	0.86
1:A:436:ILE:CD1	2:A:2078:HOH:O	2.32	0.77
1:A:442:TRP:CE3	2:A:2106:HOH:O	2.35	0.77
1:A:388:CYS:SG	2:D:2041:HOH:O	2.45	0.74
1:A:367:THR:CA	2:A:2106:HOH:O	2.35	0.74
1:D:501:ILE:CD1	2:D:2147:HOH:O	2.38	0.71
1:E:386:PHE:CD1	2:E:2036:HOH:O	2.44	0.70
1:B:391:ARG:CG	2:B:2004:HOH:O	2.39	0.70
1:C:367:THR:CA	2:C:2011:HOH:O	2.38	0.70
1:E:387:ILE:N	2:E:2036:HOH:O	2.24	0.69
1:D:394:ASN:ND2	2:D:2041:HOH:O	2.33	0.61
1:F:478[B]:SER:OG	2:F:2144:HOH:O	2.16	0.61
1:E:361:ALA:N	2:E:2001:HOH:O	2.35	0.60
1:C:399:ASN:CG	2:C:2046:HOH:O	2.41	0.59
1:E:420:LEU:CD2	2:E:2025:HOH:O	2.52	0.58
1:F:529:LYS:NZ	2:F:2228:HOH:O	2.36	0.57
1:E:482:LEU:CD1	2:E:2233:HOH:O	2.53	0.57
1:F:515:ARG:NH2	2:F:2201:HOH:O	2.39	0.54
1:A:417:GLN:NE2	2:A:2076:HOH:O	2.40	0.53
1:C:442:TRP:CA	2:C:2011:HOH:O	2.56	0.53
1:D:399:ASN:ND2	2:D:2254:HOH:O	2.44	0.51
1:F:361:ALA:N	2:F:2002:HOH:O	2.45	0.50
1:E:455:ARG:NH1	2:E:2126:HOH:O	2.45	0.49
1:E:386:PHE:CG	2:E:2036:HOH:O	2.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:529:LYS:NZ	2:F:2229:HOH:O	2.46	0.47
1:B:482:LEU:CD1	2:B:2223:HOH:O	2.62	0.47
1:E:386:PHE:CE1	2:E:2036:HOH:O	2.67	0.47
1:E:437:ASN:ND2	2:E:2100:HOH:O	2.48	0.47
1:F:503:LYS:NZ	2:F:2201:HOH:O	2.48	0.46
1:F:423:GLU:OE2	1:F:505:LYS:NZ	2.48	0.46
2:C:2046:HOH:O	1:F:395:LEU:CD2	2.63	0.46
1:C:521:ARG:NH1	2:C:2204:HOH:O	2.49	0.46
1:C:423:GLU:OE2	1:C:505:LYS:NZ	2.49	0.44
1:D:423:GLU:OE2	1:D:505:LYS:NZ	2.50	0.44
1:F:501:ILE:CD1	2:F:2143:HOH:O	2.68	0.42
1:D:536:THR:N	2:D:2260:HOH:O	2.53	0.41
1:E:409:ARG:CG	2:E:2054:HOH:O	2.68	0.41
1:D:378:ASN:ND2	2:D:2028:HOH:O	2.54	0.40

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)
2:D:2143:HOH:O	2:D:2237:HOH:O[2_545]	2.12	0.08

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	180/197 (91%)	171 (95%)	9 (5%)	0	100	100
1	B	181/197 (92%)	173 (96%)	8 (4%)	0	100	100
1	C	182/197 (92%)	175 (96%)	7 (4%)	0	100	100
1	D	182/197 (92%)	176 (97%)	6 (3%)	0	100	100
1	E	180/197 (91%)	171 (95%)	9 (5%)	0	100	100
1	F	182/197 (92%)	174 (96%)	8 (4%)	0	100	100
All	All	1087/1182 (92%)	1040 (96%)	47 (4%)	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	159/171 (93%)	155 (98%)	4 (2%)	60	23
1	B	160/171 (94%)	157 (98%)	3 (2%)	69	35
1	C	161/171 (94%)	157 (98%)	4 (2%)	60	23
1	D	161/171 (94%)	157 (98%)	4 (2%)	60	23
1	E	159/171 (93%)	158 (99%)	1 (1%)	92	80
1	F	161/171 (94%)	159 (99%)	2 (1%)	82	57
All	All	961/1026 (94%)	943 (98%)	18 (2%)	69	35

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	363	ILE
1	A	366	TRP
1	A	412	SER
1	A	453	GLN
1	B	363	ILE
1	B	366	TRP
1	B	467	ARG
1	C	363	ILE
1	C	366	TRP
1	C	412	SER
1	C	453	GLN
1	D	363	ILE
1	D	366	TRP
1	D	455	ARG
1	D	517	LEU
1	E	366	TRP
1	F	363	ILE
1	F	366	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	182/197 (92%)	0.08	4 (2%) 59 66	3, 6, 12, 18	0
1	B	182/197 (92%)	0.11	3 (1%) 68 75	3, 6, 12, 17	0
1	C	182/197 (92%)	0.01	2 (1%) 77 84	3, 5, 10, 15	0
1	D	182/197 (92%)	0.23	7 (3%) 38 42	3, 7, 14, 21	0
1	E	182/197 (92%)	0.07	3 (1%) 68 75	3, 6, 12, 17	0
1	F	182/197 (92%)	0.15	6 (3%) 44 47	3, 6, 12, 20	0
All	All	1092/1182 (92%)	0.11	25 (2%) 57 64	3, 6, 13, 21	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	458	HIS	5.6
1	F	458	HIS	5.1
1	F	378	ASN	4.1
1	E	458	HIS	4.0
1	D	378	ASN	3.8
1	F	455	ARG	3.7
1	D	455	ARG	3.1
1	D	379	ASP	3.1
1	A	458	HIS	3.0
1	B	542	GLN	3.0
1	D	361	ALA	2.8
1	C	467	ARG	2.8
1	A	467	ARG	2.7
1	C	507	VAL	2.7
1	F	379	ASP	2.6
1	E	379	ASP	2.6
1	D	427	PHE	2.6
1	A	507	VAL	2.5
1	F	376	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	458	HIS	2.4
1	A	361	ALA	2.2
1	E	467	ARG	2.1
1	D	380	THR	2.1
1	F	361	ALA	2.1
1	B	379	ASP	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.