wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 08:21 pm GMT

PDB ID	:	2VYP
Title	:	Rabbit-muscle G-actin in complex with myxobacterial rhizopodin
Authors	:	Hagelueken, G.; Albrecht, S.C.; Steinmetz, H.; Jansen, R.; Heinz, D.W.; Kalesse, M.; Schubert, W.-D.
Deposited on	:	2008-07-25
Resolution	:	2.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Mogul	:	NOT EXECUTED
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	NOT EXECUTED
Percentile statistics	:	NOT EXECUTED
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 2.35 Å.

There are no overall percentile quality scores available for this entry.

2 Entry composition (i)

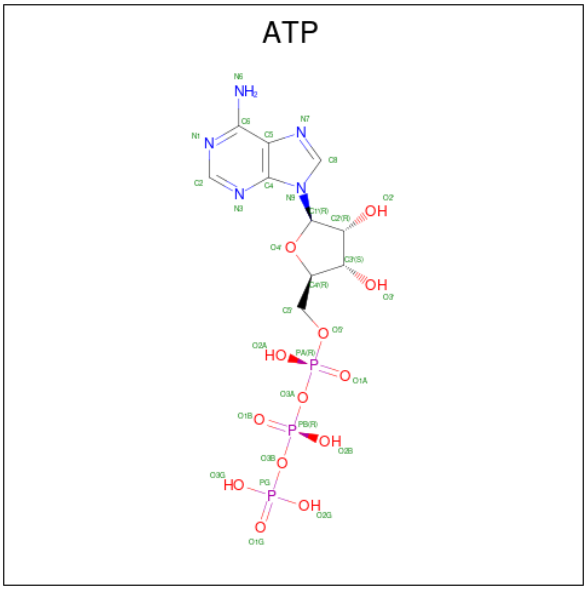
There are 6 unique types of molecules in this entry. The entry contains 5844 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	4	0
			2823	1790	472	541	20			
1	B	330	Total	C	N	O	S	0	5	1
			2613	1664	432	496	21			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

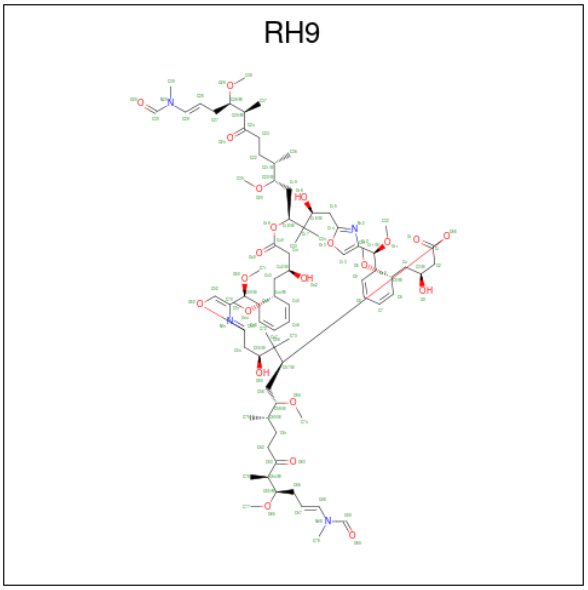


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

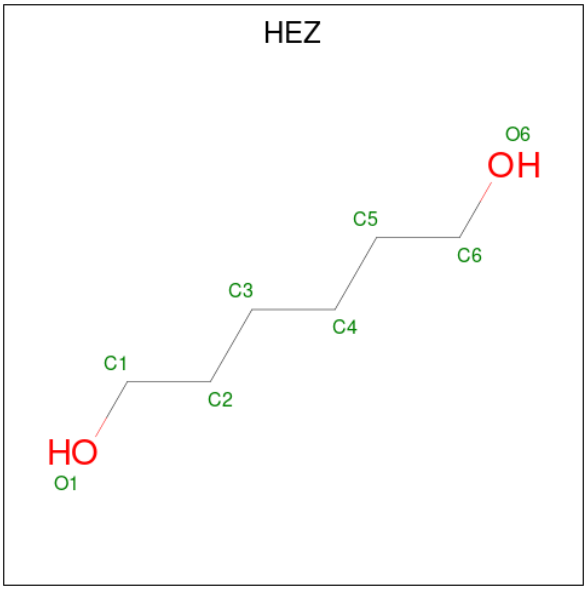
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	3	Total Ca 3 3	0	0

- Molecule 4 is RHIZOPODIN (three-letter code: RH9) (formula: $C_{78}H_{124}N_4O_{22}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 104 78 4 22	0	0

- Molecule 5 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	152	Total O 152 152	0	0
6	B	62	Total O 62 62	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	77.65Å 194.86Å 53.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.41 – 2.35 19.41 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.41-2.35) 100.0 (19.41-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.12 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.241 0.273 , 0.307	Depositor DCC
R_{free} test set	1760 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5844	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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.

4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RH9, HEZ, ATP, CA

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	0.86	0/2892	0.83	1/3920 (0.0%)
1	B	0.76	1/2685 (0.0%)	0.75	1/3637 (0.0%)
All	All	0.81	1/5577 (0.0%)	0.79	2/7557 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	ASP	C-O	13.96	1.49	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	206	ARG	CG-CD-NE	-5.62	100.00	111.80
1	B	242	LEU	N-CA-C	5.48	125.80	111.00

There are no chirality outliers.

There are no planarity outliers.

4.2 Too-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 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	2823	0	2801	34	0
1	B	2613	0	2588	63	0
2	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	12	0	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
4	A	104	0	124	2	0
5	A	24	0	42	1	0
6	A	152	0	0	1	0
6	B	62	0	0	1	0
All	All	5844	0	5579	98	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 9.

The worst 5 of 98 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:B:206:ARG:O	1:B:209:VAL:HG22	1.69	0.93
1:B:190:MET:HE2	1:B:209:VAL:HG21	1.48	0.92
1:B:242:LEU:HD21	1:B:248:ILE:CD1	2.02	0.89
1:A:107:GLU:OE1	1:A:116:ARG:HD2	1.86	0.76
1:B:200:PHE:O	1:B:202:THR:HG22	1.85	0.75

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

4.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

4.3.3 RNA (i)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

Mogul was not executed - this section is therefore empty.

4.5 Carbohydrates (i)

Mogul was not executed - this section is therefore empty.

4.6 Ligand geometry (i)

Mogul was not executed - this section is therefore empty.

4.7 Other polymers (i)

Mogul was not executed - this section is therefore empty.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

5.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

5.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

5.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.