



wwPDB EM Validation Summary Report ⓘ

May 25, 2025 – 12:10 AM JST

PDB ID : 9L4C / pdb_0000914c
EMDB ID : EMD-62809
Title : ATR Spiral -ATRIP bound with RP-3500
Authors : Wang, G.
Deposited on : 2024-12-20
Resolution : 4.06 Å (reported)

This is a wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

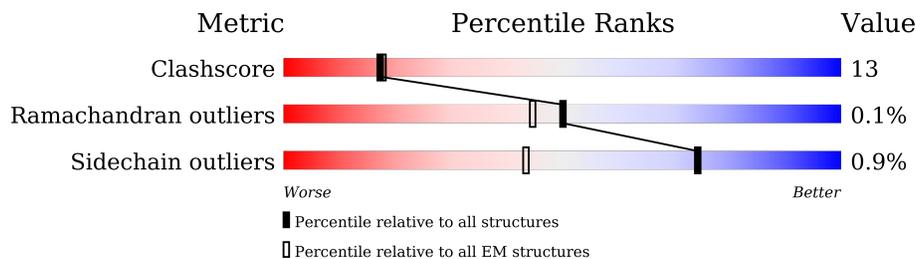
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.06 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	2644	
1	B	2644	
2	C	791	
2	D	791	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21507 atoms, of which 7891 are hydrogens and 0 are deuteriums.

In the tables below, 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 Serine/threonine-protein kinase ATR.

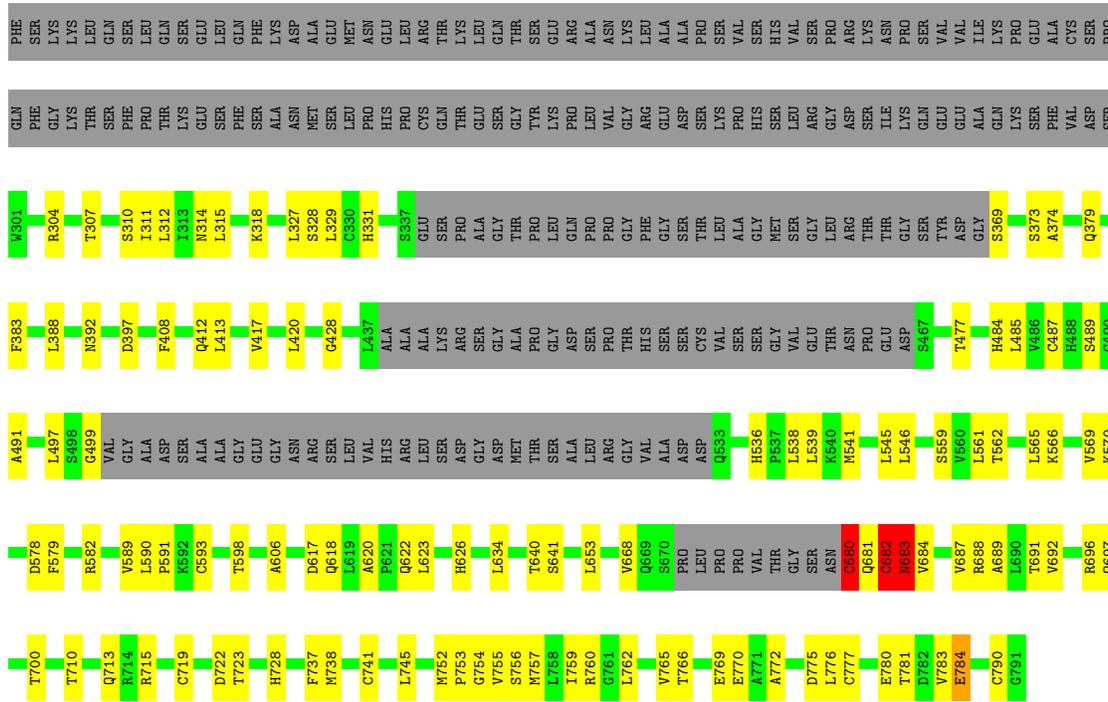
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	832	6713	2679	2307	853	870	4	0	0
1	B	854	6000	2534	1758	854	854		0	0

- Molecule 2 is a protein called ATR-interacting protein.

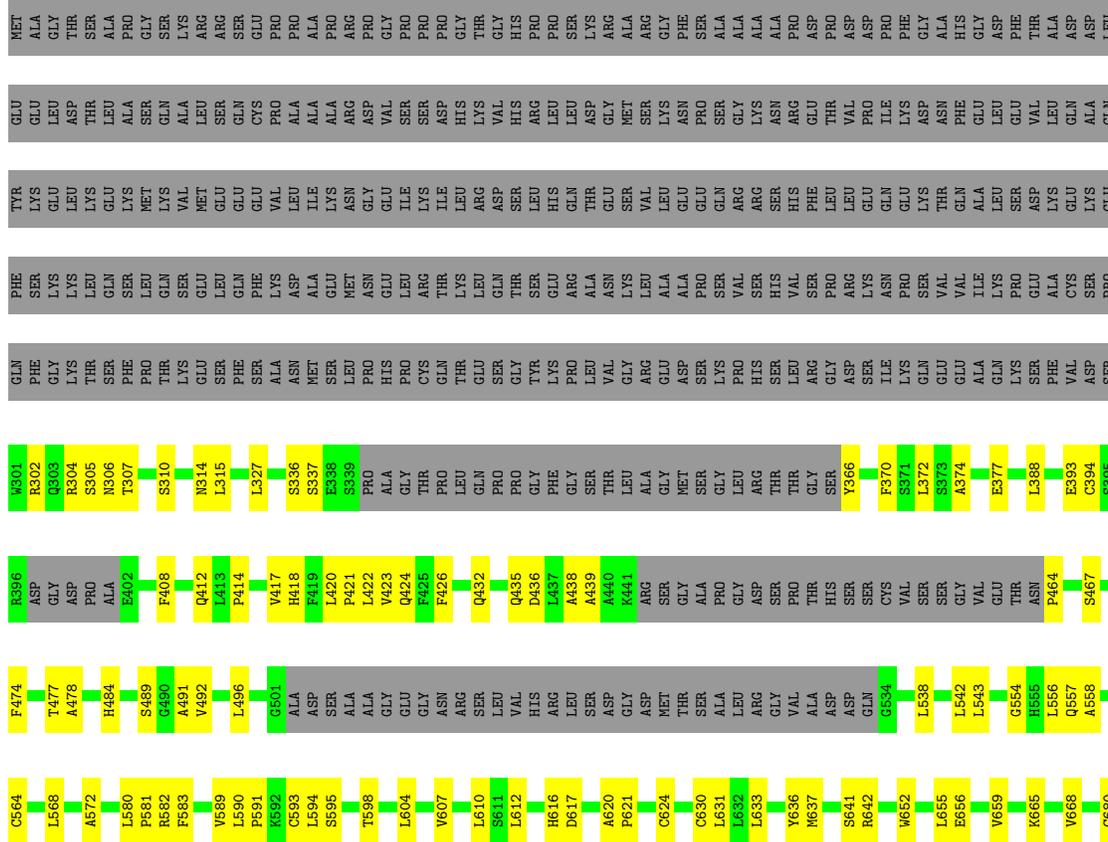
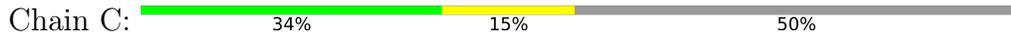
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	D	389	4382	1494	1900	462	507	19	0	0
2	C	393	4410	1525	1926	452	490	17	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	D	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	



• Molecule 2: ATR-interacting protein





VAL
GLU
CYS
GLY

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77631	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	0.29	0/4418	0.43	0/6131
1	B	0.21	0/4235	0.36	0/5901
2	C	0.39	0/2518	0.51	0/3458
2	D	0.44	1/2505 (0.0%)	0.64	7/3419 (0.2%)
All	All	0.32	1/13676 (0.0%)	0.47	7/18909 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	680	CYS	CA-CB	6.35	1.66	1.53

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	681	GLN	N-CA-C	-11.56	98.42	111.71
2	D	680	CYS	CA-CB-SG	8.93	134.95	114.40
2	D	682	CYS	CA-C-O	-6.20	113.98	120.55
2	D	682	CYS	CB-CA-C	5.90	120.58	110.79
2	D	683	ASN	CA-C-N	5.24	127.91	120.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	171	TRP	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	4406	2307	2373	78	0
1	B	4242	1758	1851	43	0
2	C	2484	1926	1926	98	0
2	D	2482	1900	1902	81	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	13616	7891	8052	290	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 13.

The worst 5 of 290 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)
2:D:307:THR:O	2:D:310:SER:OG	1.86	0.93
2:C:595:SER:O	2:C:598:THR:OG1	1.89	0.89
2:C:750:GLN:NE2	2:C:751:VAL:HG23	1.91	0.85
2:C:680:CYS:SG	2:C:682:CYS:N	2.50	0.85
2:D:754:GLY:HA2	2:D:757:MET:HE2	1.59	0.83

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 PDB entries followed by that with respect to all EM entries.

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	820/2644 (31%)	796 (97%)	22 (3%)	2 (0%)	44	76
1	B	841/2644 (32%)	831 (99%)	10 (1%)	0	100	100
2	C	383/791 (48%)	369 (96%)	14 (4%)	0	100	100
2	D	379/791 (48%)	367 (97%)	11 (3%)	1 (0%)	37	71
All	All	2423/6870 (35%)	2363 (98%)	57 (2%)	3 (0%)	50	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	821	ARG
2	D	784	GLU
1	A	820	VAL

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 PDB entries followed by that with respect to all EM entries.

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	83/2363 (4%)	83 (100%)	0	100	100
2	C	183/678 (27%)	183 (100%)	0	100	100
2	D	183/678 (27%)	179 (98%)	4 (2%)	47	66
All	All	449/3719 (12%)	445 (99%)	4 (1%)	74	84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	626	HIS
2	D	680	CYS
2	D	682	CYS
2	D	683	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	746	HIS
2	C	536	HIS
2	C	303	GLN
2	C	681	GLN
2	C	432	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.