W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report ⓘ

May 25, 2025 – 12:16 AM JST

PDB ID	:	9L43 / pdb_00009l43
EMDB ID	:	EMD-62804
Title	:	ATR Spiral -ATRIP bound with VE-822
Authors	:	Wang, G.
Deposited on	:	2024-12-19
Resolution	:	3.83 Å(reported)

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

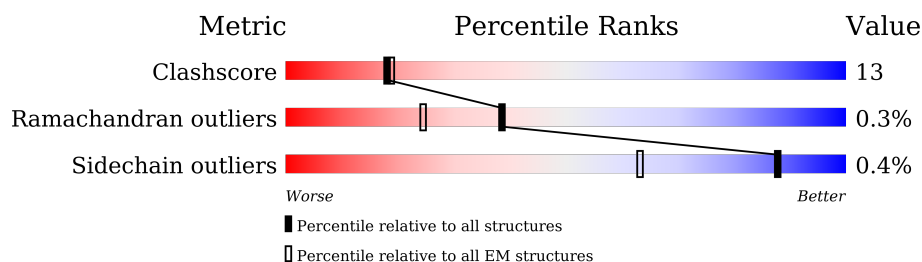|		
EMDB validation analysis	:	FAILED
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 3.83 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	Percentile Ranks	Value
Clashscore		13
Ramachandran outliers		0.3%
Sidechain outliers		0.4%

Worse — *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	2644	23% 8% 69%
1	B	2644	24% 8% 68%
2	C	791	37% 9% ·· 53%
2	D	791	36% 10% 54%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	C	801	-	-	X	-

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PROTEIN DATA BANK

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 33261 atoms, of which 15995 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
1	A	827	Total	C	H	N	O	S	0	0
			11843	3902	5783	1011	1107	40		
1	B	853	Total	C	H	N	O	S	0	0
			11860	3970	5696	1023	1129	42		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	366	Total	C	H	N	O	S	0	0
			4754	1582	2252	439	464	17		
2	C	369	Total	C	H	N	O	S	0	0
			4802	1604	2264	442	470	22		

- 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	

3   Residue-property plots ⓘ

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. 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. 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: Serine/threonine-protein kinase ATR

MET MET THR THR LEU ARG THR GLY LEU ARG ARG PHE LYS ASP ASP PHE PRO GLU LEU LEU CYS CYS ARG ALA ALA ASP CYS SER VAL ARG CYS LEU ASP HIS ALA CYS LEU GLY SER LEU LEU SER HIS VAL ILE VAL ALA LEU LEU PRO LEU ILE HIS ILE GLN LYS GLU THR ALA ALA ILE

PHE HIS TYR LEU ILE ILE GLU ASN ARG ASP ALA VAL GLN ASP PHE LEU HIS GLU ILE ILE TYR PHE LEU PRO ASP HIS PRO GLU LEU LYS LYS ILE ALA VAL LEU GLN GLU TYR ARG LYS GLU THR SER GLU SER THR ASP LEU THR THR LEU GLN GLN SER MET ALA ILE GLN

HIS GLU ASN ASP VAL ILE HIS LEU ALA LEU THR SER LEU LYS GLU THR LEU TYR LYS ASN GLN GLU LYS ILE LYS TYR ALA THR ASP SER GLU VAL THR GLU PRO ILE ILE SER GLU LEU VAL THR VAL LEU LEU LYS GLY CYS ASP ALA ALA ASN SER GLN ALA ARG LEU LEU

CYS GLY GLU CYS LEU GLY LEU GLY ILE ASP GLY ARG ASP PHE THR SER THR GLN GLN GLY LYS LEU ASP SER ARG PRO GLY ARG LEU ASP CYS ARG GLU GLY MET GLU THR GLN ASN GLY VAL VAL GLU ASP SER PHE ALA TYR GLY LEU LEU MET GLU LEU THR ARG ALA TYR LEU ALA ALA TYR ALA ASP ASN SER ARG ALA

GLN ASP SER ALA ALA TYR ALA ILE GLN GLU LEU LEU ILE TYR ASP CYS ARG GLU GLY MET GLU THR ASN GLY PRO GLY HIS LEU GLN GLY LEU HIS LEU ARG GLU ARG PHE GLU PRO GLY HIS VAL ARG GLU ILE LEU GLU LEU THR VAL LEU LEU ARG ALA SER TYR LYS SER SER GLN LYS SER THR TRP SER GLY

VAL LYS LYS PRO ILE TYR LEU SER LYS LEU GLY SER ASN PHE ALA GLU TRP SER ALA SER TRP ALA GLY TYR LEU ILE THR LYS VAL ARG HIS ASP LEU SER ILE PHE THR CYS CYS SER ILE MET MET LYS HIS ASP PHE LYS VAL THR ILE LEU LEU LEU THR PRO HIS ILE LEU

VAL TYR VAL LEU LEU GLY ASN GLN GLU ASP GLN GLN GLU VAL TYR ALA GLU ILE MET ALA VAL LEU LYS ASP ASP HIS THR ILE ASN THR GLN ASP ILE ALA SER ILE PHE THR CYS CYS SER ILE MET MET GLN THR VAL PHE SER MET LEU ASP HIS THR GLN TRP ALA ARG

HIS LYS PHE ALA LEU ALA GLU CYS PRO SER LYS SER ASN ARG ASN LYS VAL SER MET VAL SER THR VAL ARG PHE LEU ASP ILE PRO GLN ASP THR LEU ALA VAL ALA GLY SER PHE ARG SER LYS ALA TYR THR ARG

ALA VAL MET HIS GLU PHE SER PHE ILE THR GLU GLY LYS GLN ASN ILE GLN GLU HIS LEU GLY PHE LEU GLN LEU LYS TYR ALA ALA MET GLU PRO ASP GLY VAL ALA GLY VAL SER ALA ILE ARG LYS ALA GLU PRO SER LEU LYS GLN ILE GLU GLU HIS GLU SER LEU GLY

LEU LEU ARG ASP ALA THR ALA CYS TYR ASP ARG ALA ILE LEU GLU GLU PRO ASP GLN ILE ILE HIS TYR HIS GLY VAL LYS VAL LYS SER MET LEU GLY LEU GLN LEU SER THR ILE THR GLN VAL ASN GLY VAL HIS ALA ASN ARG SER GLU TRP THR ASP GLU LEU GLU ASN THR TYR

ARG VAL GLU ALA ALA TRP LYS LEU SER GLN TRP ASP LEU VAL GLU ASN TYR LEU ALA ASP GLY LYS SER THR TRP SER VAL ARG LEU GLN LEU LEU SER ALA LYS LYS ARG ASP ILE THR ALA PHE TYR ASP SER LEU LYS LEU VAL ARG ALA GLU ALA GLN GLN ILE VAL PRO

LEU SER ALA ALA SER PHE GLU ARG GLY SER TYR GLN SER ARG GLY ARG LEU LEU SER MET LEU GLU LEU HIS LYS PRO LEU PHE GLN HIS GLY SER PRO GLY ASP SER GLN GLU ASP SER SER GLN ASP ASP SER LEU ASN ASP TRP VAL ALA ARG ALA LEU GLU MET THR GLN GLN ASN SER

TYR ARG ALA LYS GLU PRO GLU ILE LEU ALA LEU ARG ARG ALA LEU LEU LEU SER LEU ASN LYS ARG PRO ASP ASP VAL GLU MET VAL GLY GLU CYS TRP LEU GLN GLU SER ALA ARG VAL ALA ARG LYS ALA GLY HIS HIS GLN THR ALA TYR ASN ALA LEU ASN ALA GLY GLU GLU SER ARG LEU ALA

GLU LEU TYR VAL GLU ARG GLU ALA LYS TRP LEU TYR SER LEU THR ARG SER LYS GLY ASP HIS GLN ALA LEU ILE LEU GLY VAL VAL GLU GLU CYS PHE PRO GLU GLN ASN GLU THR PRO GLU GLY GLY ILE LYS ASN MET LEU HIS GLY ARG ALA MET LEU LEU VAL ARG PHE MET GLU GLU THR

ALA ASN PHE GLU SER ASN ALA ILE MET LYS LYS TYR ASP LYS VAL THR ALA CYS LEU PRO GLU TRP GLU ASP GLY VAL HIS PHE TYR LEU ALA LYS TYR ASP ASP LYS MET PRO MET VAL THR ASP ASN LYS MET GLU LYS GLN ASP GLY LYS ARG PHE MET GLU GLU VAL ARG ILE VAL LEU ALA ARG ILE VAL LEU HIS PHE GLY

ARG SER LEU GLN TYR GLY ASN GLN PHE ILE TYR GLN SER MET VAL PRO ARG MET LEU THR LEU ASP TRP LEU ASP VAL PHE GLY LEU ALA TYR TYR LYS ALA GLY LYS SER VAL ALA MET ASN ARG ASP LEU GLY LYS ILE ILE ASN VAL ILE ARG GLU THR GLY HIS ASN ASP TYR LEU

ALA PRO TYR PHE LEU THR ALA PHE SER GLN LEU ILE SER ARG ILE CYS HIS SER HIS ASP GLU VAL PHE VAL VAL LEU MET GLU ILE LEU ALA LYS TYR ASP ASP LYS PRO VAL PHE LEU ALA TYR ILE ALA GLY PHE ASP MET GLU MET THR MET SER THR VAL SER SER PRO MET ARG ALA VAL ASN ARG

CYS LYS GLU ILE LEU ASN LYS ALA ILE HIS MET LYS SER LEU GLU LYS PHE VAL GLY ASP ALA THR ARG LEU THR ASP LYS LEU LEU GLU LEU CYS ASN LYS PRO VAL ASP GLY SER SER SER THR LEU SER MET SER MET SER THR HIS HIS PHE LYS MET LEU LEU LYS LEU VAL GLU GLU ALA

THR PHE SER GLU ILE LEU ILE PRO LEU GLN SER VAL ILE PRO THR LEU PRO SER ILE LEU GLY ASP ALA THR ARG HIS ALA ASN HIS ALA SER HIS GLU PRO PHE GLY PRO GLY PHE GLY TRP ALA TYR ILE ALA GLY PHE ASP MET VAL VAL GLU ILE LEU ALA SER LEU GLN LYS PRO LYS ILE SER

LEU LYS GLY SER ASP GLY LYS PHE TYR ILE MET MET CYS LYS PRO ASP ASP ARG LYS ASP MET GLU LEU HIS ILE ARG THR TYR ALA VAL ILE PRO LEU ASN ASP GLU GLU LYS GLY SER ASP ILE SER LEU ILE LEU LYS LEU VAL GLU LEU LYS VAL GLU GLU ALA

CYS GLY ILE ILE GLU TRP VAL ASN ASN THR ALA GLY ARG PRO ILE LEU THR LYS LEU TYR LYS GLY VAL TYR MET THR GLY LYS GLU LEU ARG GLN CYS MET LEU PRO LYS SER ALA ALA LEU SER GLU LEU LYS VAL PHE ARG GLU PHE LEU LEU PRO ARG HIS PRO

PRO ILE PHE HIS GLU TRP PHE PHE GLU ARG THR PHE PRO ASP PRO THR TRP TYR SER ARG ALA SER ALA VAL MET SER MET VAL GLY TYR ILE LEU GLY LEU GLY ASP ARG HIS GLY GLU ASN ILE LEU PHE ASP SER LEU THR GLY GLU CYS VAL HIS VAL

ASP PHE ASN LEU PHE LYS GLY GLU GLU THR PHE GLU VAL PRO GLU ILE VAL PHE ARG LEU THR HIS ASN MET VAL ASN GLY MET GLY PRO MET GLY THR GLU GLY LEU PHE ARG ARG ALA CYS GLU VAL THR MET ARG MET ASP GLN GLY ARG PRO LEU MET SER VAL

LEU LYS THR LEU HIS PRO LEU GLU TRP LYS PRO LYS GLY VAL HIS SER LYS ALA PRO LEU ASN GLU THR GLY GLU VAL VAL ASN GLU LYS ALA LYS THR HIS VAL LEU ASP ILE GLU GLN ARG LEU GLN GLY VAL ILE LYS THR ARG ASN ARG VAL THR GLY LEU PRO

LEU SER ILE GLY HIS HIS TYR ILE GLN ALA THR GLU ASN LEU LEU CYS MET TYR GLY TRP PRO TYR MET

• Molecule 1: Serine/threonine-protein kinase ATR

Chain B:　24%　8%　68%

MET GLY GLU HIS GLY LEU GLU LEU ALA S10 M11 I12 L15 A21 T22 E25 Y26 K32 P33 C38 Q39 F40 I41 D42 R43 I44 V48 N49 L55 VAL LYS LYS THR ASP SER GLN PRO T64 F71 I75 S79 V84 N85 VAL SER GLY SER HIS GLU

ALA K93 I97 E98 F99 S100 N101 W102 I103 I104 L108 R109 I110 A111 L118 C128 S129 L130 L131 F132 S138 I141 F142 T146 L152 F153 L156 W171 S176 R177 E178 L179 D183 GLU HIS MET GLY TYR LEU GLN SER A192 P193 L194 Q195 L196 M197 S198

M199 Q200 N201 L202 E203 F204 I205 E206 V207 T208 L209 L210 L213 I219 W230 Q231 I232 S241 P242 L247 F251 L252 L255 L261 A266 S267 F303 P304 F305 P315 V316 Y317 L318 L321 C326 V333 L334 M335 R336 L341 A344 H348 L349

L350 Q351 Y352 F353 L354 K355 F356 V357 Y371 I375 L379 L380 D381 V382 L383 G384 I385 I407 I411 Q414 THR GLN GLU GLU ASN LEU SER SER ASN ASP GLY ILE SER PRO LYS ARG ARG ARG LEU SER SER SER LEU ASN PRO SER LYS ARG ALA GLU VAL LYS GLN THR

GLU GLU I451 V454 D455 I475 S476 L477 E478 L482 K483 I487 E488 M489 G492 I493 A494 V495 V496 T500 T504 V505 S508 M512 ASN CYS ARG THR PHE LYS ASP CYS GLN HIS LYS SER LYS LYS LYS PRO S529 M535 S536 L537 D538 F539 Y540 V543

R548 L551 E552 S553 V554 Q555 K556 L559 E560 A561 T562 K565 I569 I574 N579 D584 L587 M593 L596 D604 L608 T619 L620 D626 S629 Q633 S634 R635 C636 V637 F638 L639 L640 R652 H664 E665 V666 I667 S673 F676

L679 Q682 L692 V696 S700 V703 E706 I710 V715 C716 M721 F722 Y723 L724 T725 S726 S727 L728 T729 H737 L740 K746 A747 T748 S749 G750 Q757 L758 V762 C763 F766 L767 L770 L789 L793 D794 D801 V802 V805

L806 L809 L812 H856 A857 R861 I876 A880 L884 F887 A888 L889 K899 S900 A906 A907 Y908 T909 E910 A913 LEU VAL ALA ALA LYS SER VAL K921 F925 F926 K930 S944 GLN MET THR ALA LEU PRO ASN PRO CYS LEU ASN ALA ASP

VAL ARG LYS GLN ASP VAL ASN VAL ALA HIS GLN GLU ARG GLU MET LEU LEU ASN PHE LYS THR ILE TYR ILE PHE SER GLU GLY ILE ALA ASN VAL CYS PHE ASP PRO ASP PRO ASP LEU GLU ILE ARG PHE LEU THR ARG THR ILE THR ILE SER PRO GLU MET ALA LYS SER PRO ALA SER ALA SER LEU ILE ARG THR LEU GLY

LYS GLN LEU ASN VAL ASN VAL ALA ARG ARG GLU GLU ILE LEU LEU ILE ASN ASN PHE LYS TYR ILE PHE SER HIS VAL LEU CYS SER CYS SER LYS ASP GLU LEU GLU LEU GLU ARG ALA LEU HIS TYR LEU LYS ASN GLU THR GLU ILE GLU LEU GLY GLY SER LEU LEU ARG ASP ASP PHE GLU GLY GLY LEU ALA PHE PHE ASN MET GLN LEU

LEU LEU LEU ARG ILE GLY HIS TYR ARG GLN GLN VAL PHE ASN ASN GLY SER LEU SER LEU ALA SER PHE ALA SER ASP ASP SER PRO TYR GLN VAL PRO ARG ASP ILE ILE SER PRO GLU LEU MET ALA ASP TYR LEU GLN PRO LYS LEU LEU GLY ILE LEU ALA PHE PHE ASN MET GLN LEU

LEU SER SER VAL GLY ILE ASP LYS MET ALA LEU ASN SER LEU MET SER LEU ALA SER ALA SER ASP ASP SER GLY PRO TYR GLN ASP ILE ILE SER PRO GLU MET THR LEU ARG GLY LEU PRO LYS ASP PHE PRO GLU LEU CYS ARG ALA TRP ASP CYS

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PHE VAL ARG CYS LEU ASP HIS ALA CYS LEU GLY SER LEU LEU SER HIS VAL ILE VAL ALA LEU LEU LEU PRO LEU ILE HIS ILE GLN PRO LYS GLU THR ALA ALA ILE PHE HIS TYR LEU ILE ILE GLU ASN ARG ALA VAL GLN ASP PHE LEU HIS GLU ILE ILE TYR PHE LEU PRO ASP HIS

PRO GLU LEU LYS LYS ILE LYS ALA VAL LEU GLU GLN GLU TYR ARG LYS GLU THR SER GLU SER THR ASP LEU GLN THR LEU GLN LEU LEU SER MET LYS ALA ILE GLN HIS GLU ASN VAL ASP VAL ARG ILE HIS ALA LEU THR SER LEU GLU THR LEU TYR LYS ASN GLU LYS LEU

ILE LYS TYR ALA THR ASP GLU SER THR GLU VAL GLU ASP PRO ILE ILE SER GLN LEU VAL THR VAL LEU LYS GLY CYS GLN ASP ALA ASN SER GLN ALA ARG LEU CYS GLU CYS GLY GLU GLY ALA ASP ILE ASP PRO GLY ARG LEU ASP PHE SER THR GLU THR GLN GLY

LYS ASP PHE THR PHE VAL THR GLY VAL ASP SER SER PHE ALA TYR GLY LEU LEU LEU MET GLU LEU THR ARG ALA TYR LEU ALA LEU ALA ASP ASN ASP ARG ALA LEU LEU CYS GLY GLU CYS LEU GLY LEU GLU LEU ALA ILE ASP PRO GLY ALA LEU ASP MET GLU THR ASN GLY PRO

GLY HIS GLN TRP ARG PHE PRO GLU GLU HIS VAL ARG GLU ILE GLU PRO HIS LEU ASN ARG TYR SER SER GLN LYS SER THR ASP TRP GLY VAL LYS PRO ILE TYR LEU LEU SER LEU GLU SER ASN PHE ALA GLU TRP SER ALA SER TRP ALA GLY TYR LEU

ILE THR LYS ARG HIS ASP LEU ALA LYS ILE PHE THR CYS SER SER ILE MET MET LYS HIS ASP PHE LYS VAL THR ILE TYR LEU LEU LEU PRO HIS ILE LEU VAL TYR VAL LEU GLY ASN GLN ASP GLN GLU GLU VAL TYR GLU ILE ALA VAL MET GLU ALA VAL LEU LYS HIS

ASP ASP GLN GLN HIS THR ILE ASN THR GLN ASP ILE ALA ASP LEU CYS GLN LEU SER THR GLN THR VAL PHE SER MET LEU ASP HIS LEU GLN TRP ALA ARG HIS LYS PHE GLN ALA LEU LEU LYS ALA GLU LYS CYS PRO HIS LYS SER LYS GLN ASN ARG ASN LYS VAL ASP SER MET VAL

SER THR VAL ASP TYR GLU ASP TYR GLN SER VAL THR ARG PHE LEU ASP LEU ILE PRO GLN ASP THR LEU ALA VAL ALA SER PHE ARG SER LYS ALA TYR THR ARG ALA VAL MET HIS PHE GLU PHE ILE THR GLU GLY GLN LYS LEU GLN ASN ILE GLU GLN GLY HIS LEU GLY PHE LEU GLN LYS LYS

LEU TYR ALA ALA MET HIS GLU PRO ASP GLY VAL VAL ALA GLY VAL SER ALA ILE ARG LYS GLU ALA GLU SER LEU LYS LEU GLU LEU ARG ASP ALA THR ALA CYS TYR ASP ARG ALA ILE GLN LEU GLN PRO ASP GLN ILE ILE HIS TYR HIS GLY

VAL VAL LYS SER MET LEU GLY LEU GLY LEU GLN LEU SER THR VAL ILE THR GLN VAL ASN GLY VAL HIS ALA ASN ARG GLU SER TRP THR ASP GLU LEU ASN THR ARG VAL GLU ALA ALA SER PHE GLU THR ALA CYS TYR ASP ARG ALA ILE GLN LEU GLU PRO ASP GLY ILE ILE HIS TYR HIS GLY THR

THR TRP SER VAL ARG LEU GLY GLN LEU LEU LEU SER ALA LYS LYS ARG ASP ILE THR ALA PHE TYR ASP SER LEU LYS LEU ARG ALA GLY GLN ILE ILE VAL PRO LEU SER ALA ALA SER PHE GLU ARG GLY SER TYR ARG GLN ARG GLY TYR GLU LEU HIS MET LEU CYS

GLU LEU GLU HIS ILE PRO LEU PHE GLN HIS SER PRO GLY ASP SER SER GLN GLU ASP SER LEU ASN TRP VAL ALA ARG LEU GLU MET THR GLN ASN SER TYR ARG ALA LYS GLU GLU ILE ALA ARG ALA LEU SER ASN LYS ARG PRO ASP TYR ASN GLU

MET VAL GLY GLU CYS TRP LEU GLN SER ALA ARG VAL ALA ARG LYS ALA GLY HIS HIS GLN THR ALA ASN ALA LEU LEU GLY ARG MET GLU GLU THR ALA ASN PHE GLU ASN ALA LYS GLU LEU TRP LEU SER GLY ASP VAL HIS GLN ALA LEU ILE VAL LEU GLN LYS

GLY VAL GLU LEU CYS PHE PRO GLU ASN GLU THR PRO GLU GLY GLY LYS ASN MET LEU ILE HIS GLY ARG ALA MET GLU GLU THR ALA ASN PHE GLU SER ASN ALA ILE MET LYS TYR LYS ASP VAL HIS ALA CYS LEU PRO GLU GLU TRP GLU ASP GLY

HIS PHE TYR LEU ALA LYS TYR TYR ASP LYS MET PRO MET VAL THR ASP ASN LYS MET GLU LYS GLN GLY ARG ALA MET LEU LEU ILE ARG TYR ILE VAL LEU HIS PHE GLY ARG SER LEU GLN TYR GLY ARG ALA LYS MET PRO ARG MET LEU LEU TRP ASP TYR GLY

THR LYS ALA TYR GLU TRP GLU LYS ALA GLY ARG SER ASP ARG VAL GLN MET ARG ASN ASP LEU GLY LYS ILE ASN LYS VAL ILE THR GLU HIS THR ASN TYR LEU PRO TYR GLN PHE LEU GLN THR ALA PHE SER GLN LEU ILE SER ARG ILE CYS HIS HIS ASP VAL PHE VAL

VAL LEU MET GLU ILE LYS ALA VAL PHE LEU ALA TYR PRO GLN GLN ALA MET TRP MET THR ALA VAL SER LYS GLU SER SER TYR PRO MET ARG VAL VAL ASN ARG CYS LYS GLU ILE LEU ASN ALA ILE HIS MET LYS SER LEU PHE VAL GLY ASP ALA THR ARG LEU

THR ASP LYS LEU GLU GLU LEU CYS ASN LYS PRO VAL ASP GLY SER SER THR LEU SER MET SER THR HIS PHE LYS ASN LYS MET ALA THR PHE SER GLU ILE LEU LEU PRO LEU GLN SER VAL MET ILE PRO THR LEU PRO SER ILE LEU GLY THR HIS ALA

ASN HIS ALA SER GLU HIS PRO PHE PRO GLY HIS TRP ALA TYR ILE ALA GLY PHE ASP MET VAL THR HIS PHE LYS ASN ARG ALA SER LEU GLY SER ALA GLY PHE TYR ILE MET MET CYS LYS PRO ASP ASP LEU ARG LYS ASP CYS ARG LEU

MET GLU PHE ASN SER GLU LEU ILE ASN LYS CYS LEU ARG ASP ALA LYS ALA GLU SER ARG ARG GLU HIS ILE ARG THR TYR ALA VAL ILE PRO LEU ASN ASP GLU CYS GLY ILE ILE GLU TRP VAL ASN THR ALA GLY LEU ARG PRO ILE LEU THR LYS LEU TYR LYS GLU LYS GLY
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VAL TYR MET THR GLY LYS GLU LEU ARG GLN CYS MET LEU PRO LYS SER ALA ALA LEU SER GLU LYS LEU LYS VAL PHE ARG GLU PHE LEU LEU PRO ARG HIS PRO ILE PHE HIS GLU TRP PHE LEU ARG THR PHE PRO ASP PRO THR SER TRP TYR SER SER ARG ALA TYR CYS

ARG SER THR ALA VAL MET SER MET VAL GLY TYR ILE LEU LEU GLY LEU ASP ARG HIS GLY GLU ASN ILE LEU PHE ASP SER LEU THR GLY GLU CYS VAL HIS VAL ASP PHE ASN CYS LEU PHE ASN LYS GLY GLU THR PHE GLU VAL PRO GLU ILE VAL PRO PHE ARG LEU THR HIS ASN

MET VAL ASN GLY MET GLY MET GLY PRO MET GLY THR GLU GLY LEU LEU PHE ARG ALA ARG ALA HIS GLU VAL THR MET ARG LEU MET ARG ASP GLN ARG GLU LEU MET SER VAL LEU LYS THR PHE LEU HIS ASP PRO LEU VAL GLU TRP SER LYS PRO VAL LYS GLY HIS SER LYS ALA PRO LEU ASN

GLU THR GLY GLU VAL VAL GLU LYS LYS THR VAL LEU ASP ILE GLU GLN ARG LEU GLY VAL ILE LYS THR ARG ASN THR LEU PRO SER ILE GLY HIS HIS TYR ILE GLN ALA THR GLU ASN LEU CYS GLN MET TYR LEU

GLY TRP THR TYR MET

• Molecule 2: ATR-interacting protein

Chain D:　　36%　　10%　　54%

MET ALA GLY THR SER ALA PRO GLY SER LYS ARG ARG GLU PRO ALA PRO ARG PRO GLY PRO PRO PRO GLY THR GLY HIS PRO PRO SER LYS ARG ALA ARG GLY PHE SER ALA ALA ALA PRO ASP PRO ASP ASP PHE GLY ALA HIS GLY ASP PHE THR ALA ASP ASP LEU

GLU GLU LEU ASP ALA THR LEU ALA SER GLN GLN ALA LEU SER GLN CYS PRO ALA ALA ARG ASP VAL SER SER ASP HIS LYS VAL HIS PRO SER ARG LEU ASP ALA GLY MET SER LYS ASN PRO SER GLY LYS ASN ARG GLU VAL THR VAL PRO LEU LYS ASP ASN PHE GLU LEU GLU VAL LEU GLN ALA GLN

TYR LYS GLU LEU LYS GLU LYS MET LYS VAL MET GLU GLU GLU VAL LEU ILE LYS ASN GLY ILE LYS LEU ARG ASP SER LEU HIS GLN THR GLU SER VAL LEU GLU GLN GLN ARG ASP SER HIS PHE LEU LEU GLU GLN LYS THR GLN ALA LEU ASP SER ASP LYS GLU LYS GLU

PHE SER LYS LYS LEU GLN LEU GLN SER LEU GLN SER GLU LEU GLN LEU PHE LYS ASP ALA GLU MET ASN GLU LEU ARG THR LYS LEU GLN THR SER GLU ARG ALA ASN LYS LEU ALA ALA PRO VAL SER HIS VAL SER PRO ARG LYS ASN PRO SER VAL VAL ILE LYS PRO GLU ALA CYS SER PRO

GLN PHE GLY LYS THR SER PHE PRO THR LYS GLU SER PHE SER ALA ASN MET SER GLU LEU PRO HIS PRO CYS GLN GLN THR GLY SER GLY TYR LYS PRO LEU VAL GLY ARG GLU ASP SER LYS PRO HIS SER LEU ARG ARG LYS ASN PRO SER VAL VAL ILE LYS SER ASP PHE VAL ASP SER

TRP ARG GLN ARG SER ASN THR GLN **G309** **S310** **I311** **L312** **I313** **N314** **L315** **L316** **L317** **L332** **S337** GLU SER PRO ALA GLY THR PRO LEU GLN LEU PRO GLY PHE GLY SER THR LEU ALA GLY MET SER GLY LEU ARG THR GLY SER ASP **S369** **Q379** **T384** **G385** **L386** **N387**

L388 **R406** **A407** **L420** **P421** **L422** **V423** **Q424** **F425** **F426** **I427** **G428** **L429** **H430** **C431** **Q432** **A433** **L434** **L437** ALA ALA LYS ARG SER GLY ALA PRO GLY ASP SER PRO THR HIS SER SER CYS VAL SER SER GLY VAL GLU THR ASN PRO GLU ASP **S467** **L482** **L485** **V486** **L495**

G499 VAL GLY ALA ASP SER ALA ALA GLY GLU GLY ASN ARG SER LEU VAL HIS ARG LEU SER ASP GLY ASP MET THR SER ALA LEU ARG GLY VAL ALA ASP **Q533** **L545** **S549** **V569** **K570** **D578** **F579** **L580** **F583** **Q584** **P601** **L605** **S611** **P621** **S625**

E628 **G629** **C630** **L631** **L632** **L633** **L634** **L635** **Y636** **V646** **A647** **L648** **Q651** **W652** **L653** **Q654** **L655** **V659** **L662** **L663** **S670** PRO LEU PRO PRO VAL THR GLY SER ASN **C680** **Q681** **C682** **N683** **V684** **E685** **V686** **V687** **L694** **Q713** **R714** **R715** **T716** **V717** **R718** **C719** **L720** **T723** **V724** **L725** **L726** **L727**

L730 **K733** **D734** **K735** **L736** **M739** **H740** **V751** **M752** **L758** **G761** **C768** **L776** CYS ALA ALA GLU THR ASP VAL GLU ASP PRO GLU VAL GLU CYS GLY

• Molecule 2: ATR-interacting protein

Chain C:　　37%　　9%　　··　　53%

MET ALA GLY THR SER ALA PRO GLY SER LYS ARG ARG GLU PRO ALA PRO ARG PRO GLY PRO PRO PRO GLY THR GLY HIS PRO PRO SER LYS ARG ALA ARG GLY PHE SER ALA ALA ALA PRO ASP PRO ASP ASP PHE GLY ALA HIS GLY ASP PHE THR ALA ASP ASP LEU

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66141	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 $(e^-/\text{Å}^2)$	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 ⓘ

5.1 Standard geometry ⓘ

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	0.32	5/6156 (0.1%)	0.58	14/8371 (0.2%)
1	B	0.24	2/6271 (0.0%)	0.40	2/8533 (0.0%)
2	C	0.51	7/2574 (0.3%)	0.90	19/3510 (0.5%)
2	D	0.29	1/2539 (0.0%)	0.54	4/3473 (0.1%)
All	All	0.32	15/17540 (0.1%)	0.58	39/23887 (0.2%)

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
2	C	0	3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	623	LEU	CA-C	12.36	1.69	1.52
2	C	624	CYS	C-N	-5.84	1.25	1.33
2	C	624	CYS	CA-C	-5.66	1.45	1.52
2	C	631	LEU	N-CA	5.25	1.52	1.46
2	C	488	HIS	ND1-CE1	5.24	1.37	1.32

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	622	GLN	O-C-N	-24.42	90.11	122.59
1	A	822	VAL	N-CA-CB	-22.01	83.74	112.36
2	C	624	CYS	CB-CA-C	-14.47	86.61	110.77
2	C	624	CYS	N-CA-CB	13.88	132.15	109.94

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WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	681	GLN	N-CA-C	-11.41	98.58	111.71

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	622	GLN	Mainchain,Peptide
2	C	624	CYS	Mainchain

5.2 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	6060	5783	5794	153	0
1	B	6164	5696	5700	150	0
2	C	2538	2264	2271	74	0
2	D	2502	2252	2257	55	0
3	C	1	0	0	3	0
3	D	1	0	0	0	0
All	All	17266	15995	16022	430	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 430 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:C:630:CYS:CB	2:C:680:CYS:SG	2.38	1.12
2:C:680:CYS:SG	3:C:801:ZN:ZN	1.39	1.08
1:A:822:VAL:HB	1:A:868:THR:HB	1.33	1.05
2:C:430:HIS:HA	2:C:433:ALA:HB3	1.36	1.04
2:C:308:GLN:N	2:C:394:CYS:SG	2.40	0.94

There are no symmetry-related clashes.

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 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	813/2644 (31%)	756 (93%)	54 (7%)	3 (0%)	30	65
1	B	839/2644 (32%)	769 (92%)	70 (8%)	0	100	100
2	C	355/791 (45%)	324 (91%)	28 (8%)	3 (1%)	16	51
2	D	356/791 (45%)	312 (88%)	43 (12%)	1 (0%)	37	70
All	All	2363/6870 (34%)	2161 (92%)	195 (8%)	7 (0%)	38	70

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	586	ILE
2	C	622	GLN
2	C	623	LEU
1	A	825	SER
2	C	632	LEU

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 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	599/2363 (25%)	596 (100%)	3 (0%)	86	90
1	B	585/2363 (25%)	585 (100%)	0	100	100
2	C	231/678 (34%)	229 (99%)	2 (1%)	75	83
2	D	228/678 (34%)	227 (100%)	1 (0%)	89	91
All	All	1643/6082 (27%)	1637 (100%)	6 (0%)	88	91

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	630	CYS
2	C	631	LEU
2	C	680	CYS
1	A	642	LEU
1	A	531	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	633	GLN
1	A	683	ASN
2	C	683	ASN
1	A	830	HIS
1	A	85	ASN

5.3.3   RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6   Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.