



wwPDB EM Validation Summary Report ⓘ

Mar 31, 2024 – 12:49 AM JST

PDB ID : 8J9G
EMDB ID : EMD-36095
Title : CrtSPARTA hetero-dimer bound with guide-target, state 1
Authors : Li, Z.X.; Guo, L.J.; Huang, P.P.; Xiao, Y.B.; Chen, M.R.
Deposited on : 2023-05-03
Resolution : 3.50 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:

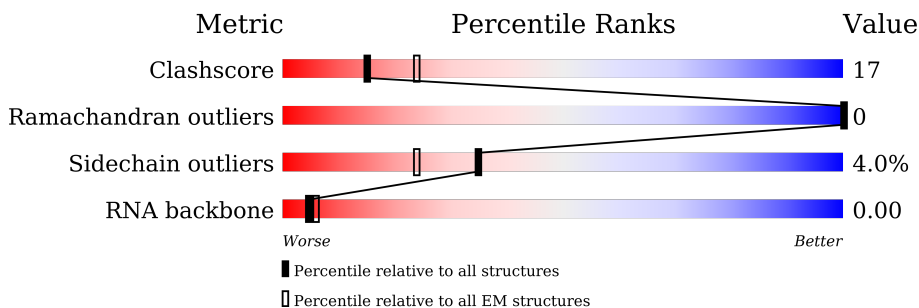
EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	541	47% 34% 17%
2	B	484	60% 32% 7%
3	E	21	52% 5% 43%
4	F	25	12% 36% 52%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7868 atoms, of which 0 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 Piwi domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	448	3618	2348	603	656	11	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	initiating methionine	UNP A0A1I7NFD7
A	-32	GLY	-	expression tag	UNP A0A1I7NFD7
A	-31	SER	-	expression tag	UNP A0A1I7NFD7
A	-30	SER	-	expression tag	UNP A0A1I7NFD7
A	-29	HIS	-	expression tag	UNP A0A1I7NFD7
A	-28	HIS	-	expression tag	UNP A0A1I7NFD7
A	-27	HIS	-	expression tag	UNP A0A1I7NFD7
A	-26	HIS	-	expression tag	UNP A0A1I7NFD7
A	-25	HIS	-	expression tag	UNP A0A1I7NFD7
A	-24	HIS	-	expression tag	UNP A0A1I7NFD7
A	-23	SER	-	expression tag	UNP A0A1I7NFD7
A	-22	SER	-	expression tag	UNP A0A1I7NFD7
A	-21	GLY	-	expression tag	UNP A0A1I7NFD7
A	-20	LEU	-	expression tag	UNP A0A1I7NFD7
A	-19	VAL	-	expression tag	UNP A0A1I7NFD7
A	-18	PRO	-	expression tag	UNP A0A1I7NFD7
A	-17	ARG	-	expression tag	UNP A0A1I7NFD7
A	-16	GLY	-	expression tag	UNP A0A1I7NFD7
A	-15	SER	-	expression tag	UNP A0A1I7NFD7
A	-14	HIS	-	expression tag	UNP A0A1I7NFD7
A	-13	MET	-	expression tag	UNP A0A1I7NFD7
A	-12	ALA	-	expression tag	UNP A0A1I7NFD7
A	-11	SER	-	expression tag	UNP A0A1I7NFD7
A	-10	MET	-	expression tag	UNP A0A1I7NFD7
A	-9	THR	-	expression tag	UNP A0A1I7NFD7
A	-8	GLY	-	expression tag	UNP A0A1I7NFD7
A	-7	GLY	-	expression tag	UNP A0A1I7NFD7
A	-6	GLN	-	expression tag	UNP A0A1I7NFD7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLN	-	expression tag	UNP A0A1I7NFD7
A	-4	MET	-	expression tag	UNP A0A1I7NFD7
A	-3	GLY	-	expression tag	UNP A0A1I7NFD7
A	-2	ARG	-	expression tag	UNP A0A1I7NFD7
A	-1	GLY	-	expression tag	UNP A0A1I7NFD7
A	0	SER	-	expression tag	UNP A0A1I7NFD7

- Molecule 2 is a protein called TIR domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	450	3759	2427	625	696	11	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-33	MET	-	initiating methionine	UNP A0A1I7NFG5
B	-32	GLY	-	expression tag	UNP A0A1I7NFG5
B	-31	SER	-	expression tag	UNP A0A1I7NFG5
B	-30	SER	-	expression tag	UNP A0A1I7NFG5
B	-29	HIS	-	expression tag	UNP A0A1I7NFG5
B	-28	HIS	-	expression tag	UNP A0A1I7NFG5
B	-27	HIS	-	expression tag	UNP A0A1I7NFG5
B	-26	HIS	-	expression tag	UNP A0A1I7NFG5
B	-25	HIS	-	expression tag	UNP A0A1I7NFG5
B	-24	HIS	-	expression tag	UNP A0A1I7NFG5
B	-23	SER	-	expression tag	UNP A0A1I7NFG5
B	-22	SER	-	expression tag	UNP A0A1I7NFG5
B	-21	GLY	-	expression tag	UNP A0A1I7NFG5
B	-20	LEU	-	expression tag	UNP A0A1I7NFG5
B	-19	VAL	-	expression tag	UNP A0A1I7NFG5
B	-18	PRO	-	expression tag	UNP A0A1I7NFG5
B	-17	ARG	-	expression tag	UNP A0A1I7NFG5
B	-16	GLY	-	expression tag	UNP A0A1I7NFG5
B	-15	SER	-	expression tag	UNP A0A1I7NFG5
B	-14	HIS	-	expression tag	UNP A0A1I7NFG5
B	-13	MET	-	expression tag	UNP A0A1I7NFG5
B	-12	ALA	-	expression tag	UNP A0A1I7NFG5
B	-11	SER	-	expression tag	UNP A0A1I7NFG5
B	-10	MET	-	expression tag	UNP A0A1I7NFG5
B	-9	THR	-	expression tag	UNP A0A1I7NFG5
B	-8	GLY	-	expression tag	UNP A0A1I7NFG5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLY	-	expression tag	UNP A0A1I7NFG5
B	-6	GLN	-	expression tag	UNP A0A1I7NFG5
B	-5	GLN	-	expression tag	UNP A0A1I7NFG5
B	-4	MET	-	expression tag	UNP A0A1I7NFG5
B	-3	GLY	-	expression tag	UNP A0A1I7NFG5
B	-2	ARG	-	expression tag	UNP A0A1I7NFG5
B	-1	GLY	-	expression tag	UNP A0A1I7NFG5
B	0	SER	-	expression tag	UNP A0A1I7NFG5

- Molecule 3 is a RNA chain called RNA (5'-R(P*UP*GP*AP*CP*GP*GP*CP*UP*CP*UP*AP*AP*UP*CP*UP*AP*UP*UP*AP*GP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	E	12	244	114	45	73	12	0	0

- Molecule 4 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	F	12	246	117	45	72	12	2	0

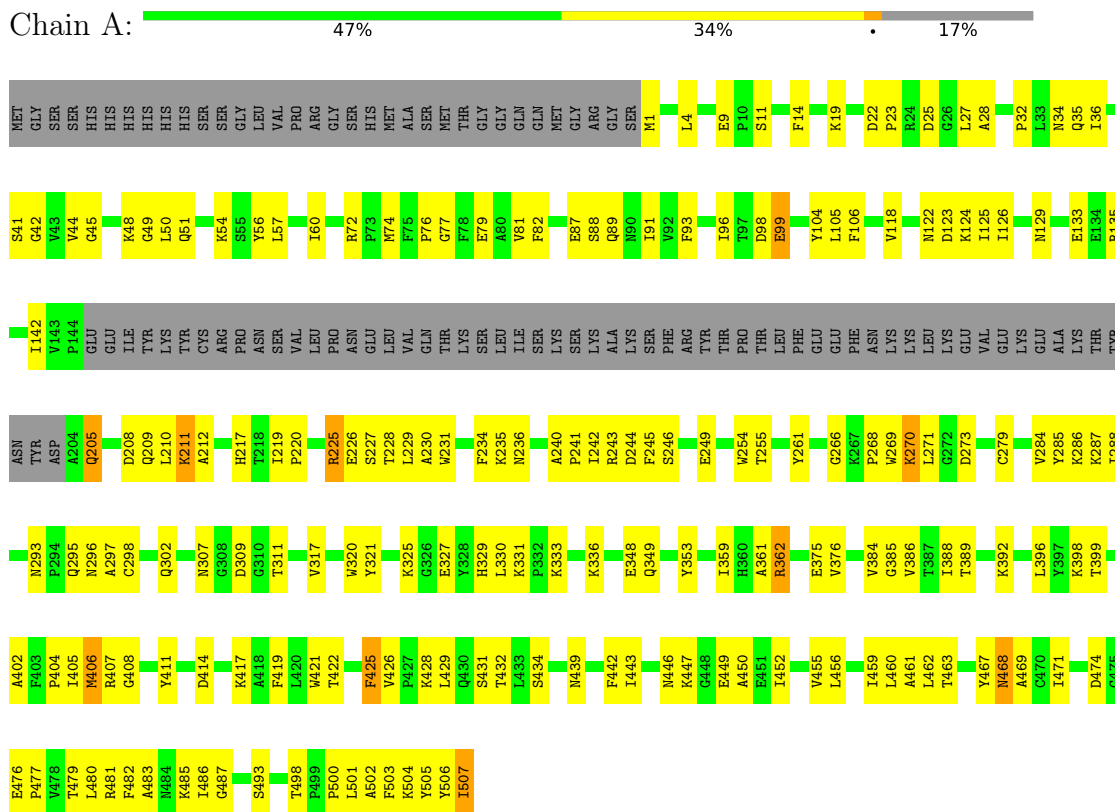
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	A	1	1	1	0

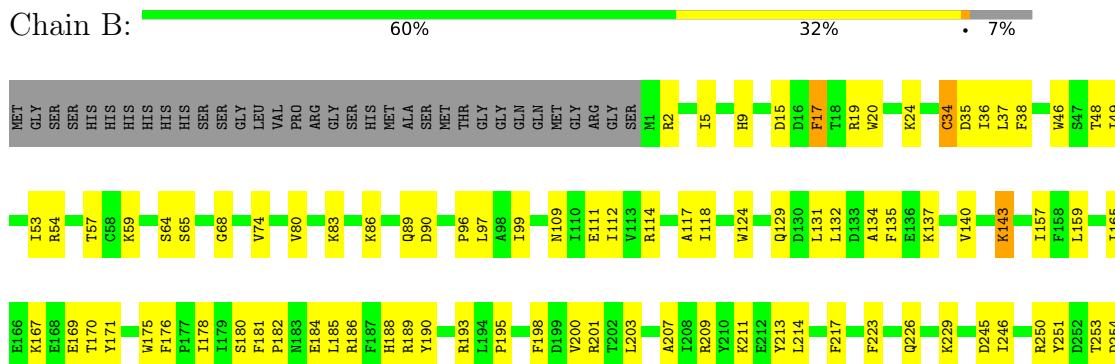
3 Residue-property plots

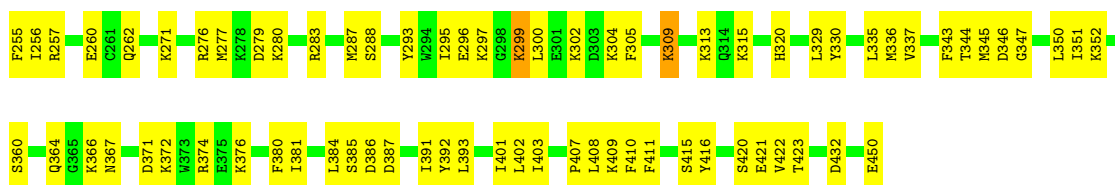
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Piwi domain-containing protein



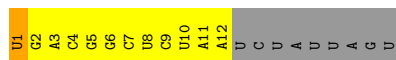
- Molecule 2: TIR domain-containing protein





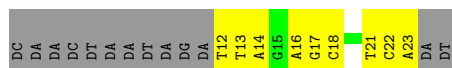
- Molecule 3: RNA (5'-R(P*UP*GP*AP*CP*GP*GP*CP*UP*CP*UP*AP*AP*UP*CP*UP*A P*UP*UP*AP*GP*U)-3')

Chain E: 52% 5% 43%



- Molecule 4: DNA (25-MER)

Chain F: 12% 36% 52%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	156464	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k 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: MG

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	0.26	0/3710	0.47	0/5023
2	B	0.25	0/3849	0.46	0/5191
3	E	0.74	1/273 (0.4%)	0.77	1/416 (0.2%)
4	F	0.50	0/275	0.91	0/422
All	All	0.29	1/8107 (0.0%)	0.50	1/11052 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	U	OP3-P	-10.72	1.48	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	U	O4'-C1'-N1	6.02	113.01	108.20

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	3618	0	3642	143	0
2	B	3759	0	3738	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	244	0	130	13	0
4	F	246	0	126	11	0
5	A	1	0	0	0	0
All	All	7868	0	7636	254	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 17.

The worst 5 of 254 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:54:LYS:HA	1:A:57:LEU:HD12	1.66	0.78
1:A:91:ILE:HG22	1:A:93:PHE:H	1.49	0.76
1:A:426:VAL:HB	1:A:429:LEU:HB2	1.70	0.74
4:F:12[A]:DT:H2''	4:F:13[A]:DT:H5''	1.68	0.74
1:A:1:MET:N	2:B:409:LYS:O	2.21	0.72

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	444/541 (82%)	418 (94%)	26 (6%)	0	100	100
2	B	448/484 (93%)	423 (94%)	25 (6%)	0	100	100
All	All	892/1025 (87%)	841 (94%)	51 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	389/472 (82%)	373 (96%)	16 (4%)	30	63
2	B	415/441 (94%)	399 (96%)	16 (4%)	32	64
All	All	804/913 (88%)	772 (96%)	32 (4%)	35	64

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	320	HIS
2	B	329	LEU
1	A	425	PHE
1	A	406	MET
2	B	416	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	GLN
1	A	329	HIS
2	B	56	ASN
2	B	151	ASN
2	B	364	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	0/21	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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](#)

Of 1 ligands modelled in this entry, 1 is 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.