



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:40 am BST

PDB ID : 6CRM
Title : Crystal Structure of RecQ catalytic core from *C. sakazakii* bound to an unfolded G-quadruplex
Authors : Voter, A.F.; Keck, J.L.
Deposited on : 2018-03-19
Resolution : 2.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
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)	:	2.11

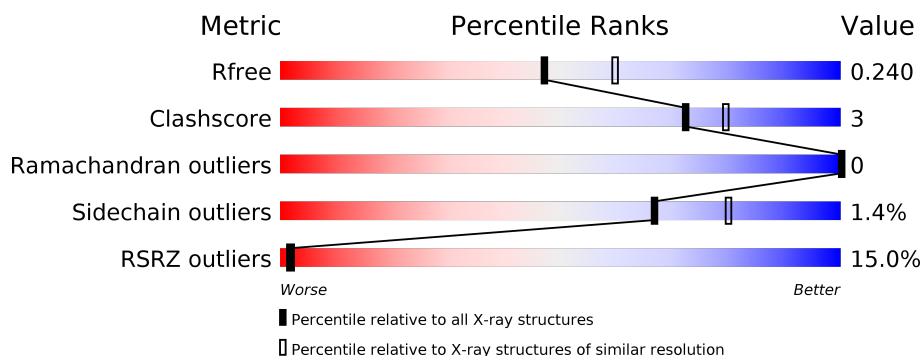
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	541	<div> <div>14%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>5%</div> </div> </div>
2	B	37	<div> <div>8%</div> <div> <div></div> <div>32%</div> <div>5%</div> <div>62%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4468 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 RecQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	2	0
			4035	2537	735	737	26			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A7MQK9
A	-18	GLY	-	expression tag	UNP A7MQK9
A	-17	SER	-	expression tag	UNP A7MQK9
A	-16	SER	-	expression tag	UNP A7MQK9
A	-15	HIS	-	expression tag	UNP A7MQK9
A	-14	HIS	-	expression tag	UNP A7MQK9
A	-13	HIS	-	expression tag	UNP A7MQK9
A	-12	HIS	-	expression tag	UNP A7MQK9
A	-11	HIS	-	expression tag	UNP A7MQK9
A	-10	HIS	-	expression tag	UNP A7MQK9
A	-9	SER	-	expression tag	UNP A7MQK9
A	-8	SER	-	expression tag	UNP A7MQK9
A	-7	GLY	-	expression tag	UNP A7MQK9
A	-6	LEU	-	expression tag	UNP A7MQK9
A	-5	VAL	-	expression tag	UNP A7MQK9
A	-4	PRO	-	expression tag	UNP A7MQK9
A	-3	ARG	-	expression tag	UNP A7MQK9
A	-2	GLY	-	expression tag	UNP A7MQK9
A	-1	SER	-	expression tag	UNP A7MQK9
A	0	HIS	-	expression tag	UNP A7MQK9

- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*GP*GP*TP*CP*GP*GP*TP*GP*C P*CP*TP*TP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	P	0	0	0
			290	137	52	87	14			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

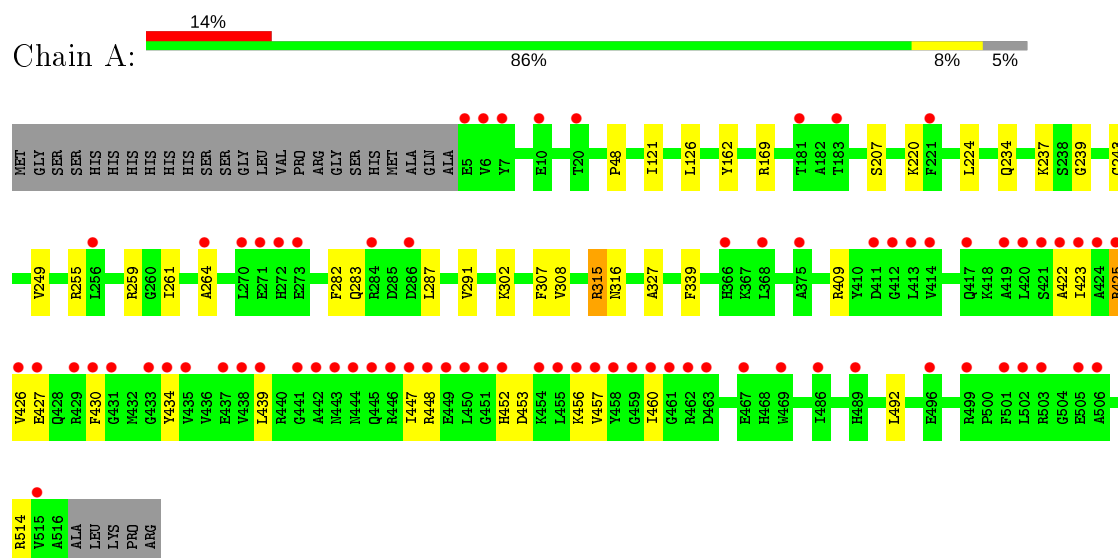
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	136	Total	O	0	0
			136	136		
4	B	6	Total	O	0	0
			6	6		

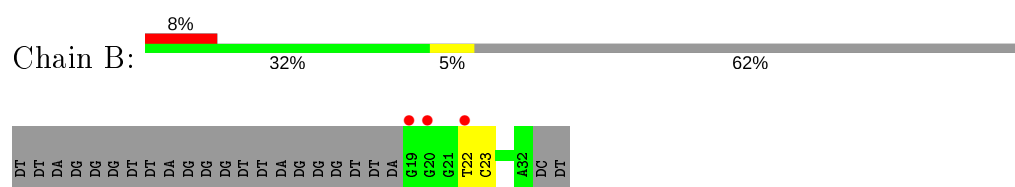
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 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: RecQ



• Molecule 2: DNA (5'-D(P*GP*GP*GP*TP*CP*GP*GP*TP*GP*CP*CP*TP*TP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	78.47Å 94.67Å 98.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.83 – 2.19 43.83 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.83-2.19) 99.1 (43.83-2.19)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.205 , 0.240 0.206 , 0.240	Depositor DCC
R_{free} test set	1994 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.001 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4468	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.28	0/4113	0.47	0/5566
2	B	0.60	0/324	0.91	0/499
All	All	0.31	0/4437	0.52	0/6065

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4035	0	4039	28	0
2	B	290	0	159	1	0
3	A	1	0	0	0	0
4	A	136	0	0	0	0
4	B	6	0	0	0	0
All	All	4468	0	4198	29	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 3.

All (29) 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:220:LYS:HG3	1:A:339:PHE:HB3	1.74	0.68
1:A:422:ALA:HB3	1:A:439:LEU:HD21	1.76	0.68
1:A:457:VAL:O	1:A:460:ILE:HG22	2.02	0.58
1:A:422:ALA:CB	1:A:439:LEU:HD21	2.35	0.57
1:A:448:ARG:HG2	1:A:453:ASP:OD2	2.06	0.56
1:A:430:PHE:HB3	1:A:434:TYR:HB2	1.88	0.56
1:A:426:VAL:HG11	1:A:430:PHE:CD2	2.41	0.55
1:A:447:ILE:O	1:A:452:HIS:N	2.41	0.52
1:A:315:ARG:HG3	1:A:316:ASN:ND2	2.28	0.49
1:A:283:GLN:HA	1:A:302:LYS:HD2	1.94	0.49
1:A:243:CYS:HB2	1:A:249:VAL:HG12	1.93	0.49
1:A:423:ILE:CD1	1:A:492:LEU:HB2	2.46	0.46
1:A:423:ILE:O	1:A:426:VAL:HG22	2.16	0.46
1:A:48:PRO:HG2	1:A:207:SER:O	2.16	0.46
1:A:264:ALA:HB3	1:A:287:LEU:HD21	1.98	0.45
1:A:224:LEU:HD21	1:A:255:ARG:HD2	1.99	0.45
1:A:423:ILE:HD11	1:A:492:LEU:O	2.16	0.45
2:B:22:DT:H3'	2:B:23:DC:C5'	2.47	0.45
1:A:308:VAL:HG23	1:A:327:ALA:HB2	1.99	0.45
1:A:425:ARG:HA	1:A:425:ARG:HD3	1.50	0.44
1:A:234:GLN:O	1:A:237:LYS:HG2	2.18	0.44
1:A:447:ILE:HA	1:A:452:HIS:HB2	1.99	0.43
1:A:121:ILE:HD13	1:A:126:LEU:HB2	2.00	0.43
1:A:239:GLY:HA3	1:A:307:PHE:CZ	2.54	0.42
1:A:249:VAL:HB	1:A:291:VAL:HG12	2.02	0.42
1:A:456:LYS:HB2	1:A:456:LYS:HE2	1.85	0.42
1:A:282:PHE:CE2	1:A:302:LYS:HD3	2.55	0.42
1:A:426:VAL:O	1:A:427:GLU:HB2	2.20	0.41
1:A:259:ARG:HB2	1:A:261:ILE:HG13	2.03	0.41

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 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	512/541 (95%)	503 (98%)	9 (2%)	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	423/444 (95%)	417 (99%)	6 (1%)	67	80

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	TYR
1	A	169	ARG
1	A	315	ARG
1	A	409	ARG
1	A	425	ARG
1	A	514	ARG

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 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 carbohydrates in this entry.

5.6 Ligand geometry

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

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	512/541 (94%)	0.96	76 (14%) 2 2	48, 73, 151, 204	0
2	B	14/37 (37%)	1.19	3 (21%) 0 0	61, 116, 201, 216	0
All	All	526/578 (91%)	0.97	79 (15%) 2 2	48, 73, 158, 216	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	434	TYR	10.3
1	A	457	VAL	10.0
1	A	450	LEU	9.7
1	A	439	LEU	8.4
2	B	19	DG	7.9
1	A	6	VAL	7.7
1	A	455	LEU	7.3
1	A	7	TYR	7.2
1	A	413	LEU	6.8
1	A	444	ASN	6.3
1	A	441	GLY	6.3
1	A	458	TYR	6.1
1	A	443	ASN	6.0
1	A	435	VAL	5.8
1	A	417	GLN	5.7
1	A	442	ALA	5.7
1	A	445	GLN	5.7
1	A	449	GLU	5.6
1	A	447	ILE	5.6
1	A	456	LYS	5.4
1	A	459	GLY	5.3
1	A	446	ARG	5.3
1	A	423	ILE	5.2
2	B	22	DT	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	420	LEU	5.1
1	A	427	GLU	5.0
1	A	451	GLY	4.9
1	A	421	SER	4.5
1	A	430	PHE	4.5
1	A	460	ILE	4.3
1	A	270	LEU	4.2
1	A	489	HIS	4.0
1	A	499	ARG	3.9
1	A	424	ALA	3.9
1	A	422	ALA	3.9
1	A	502	LEU	3.9
1	A	452	HIS	3.7
1	A	501	PHE	3.7
1	A	425	ARG	3.6
1	A	505	GLU	3.5
1	A	448	ARG	3.5
1	A	284	ARG	3.5
1	A	426	VAL	3.3
1	A	366[A]	HIS	3.2
1	A	469	TRP	3.2
1	A	461	GLY	3.2
1	A	419	ALA	3.2
1	A	414	VAL	3.2
1	A	506	ALA	3.1
1	A	438	VAL	3.1
1	A	411	ASP	3.0
1	A	463	ASP	2.9
1	A	503	ARG	2.9
1	A	431	GLY	2.9
1	A	273	GLU	2.9
1	A	437	GLU	2.8
1	A	454	LYS	2.8
1	A	515	VAL	2.6
2	B	20	DG	2.6
1	A	429	ARG	2.6
1	A	496	GLU	2.6
1	A	467	GLU	2.5
1	A	221	PHE	2.5
1	A	271	GLU	2.4
1	A	20	THR	2.4
1	A	368	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	5	GLU	2.4
1	A	10	GLU	2.3
1	A	181	THR	2.3
1	A	272	HIS	2.3
1	A	264	ALA	2.2
1	A	412	GLY	2.2
1	A	183	THR	2.2
1	A	462	ARG	2.2
1	A	256	LEU	2.1
1	A	486	ILE	2.1
1	A	433	GLY	2.1
1	A	375	ALA	2.0
1	A	286	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	A	601	1/1	0.99	0.13	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.