Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2024 – 05:06 AM EST

PDB ID	:	5C2F
Title	:	K428A mutant nuclease domain of the large terminase subunit gp2 of bacterial virus Sf6 with Manganese and beta-thujaplicinol
Authors	:	Zhao, H.; Tang, L.
Deposited on	:	2015-06-15
Resolution	:	1.86 Å(reported)

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

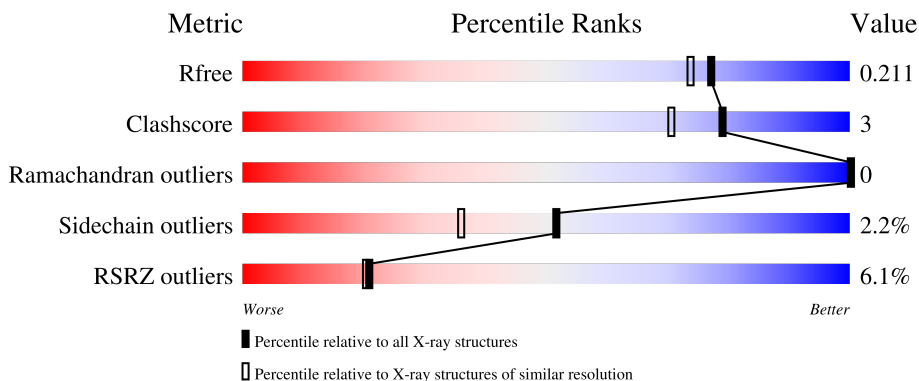|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.86 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
Rfree		0.211
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		2.2%
RSRZ outliers		6.1%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 of 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 <=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	278	5% / 76% / 7% / 17%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 1939 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 Gene 2 protein.

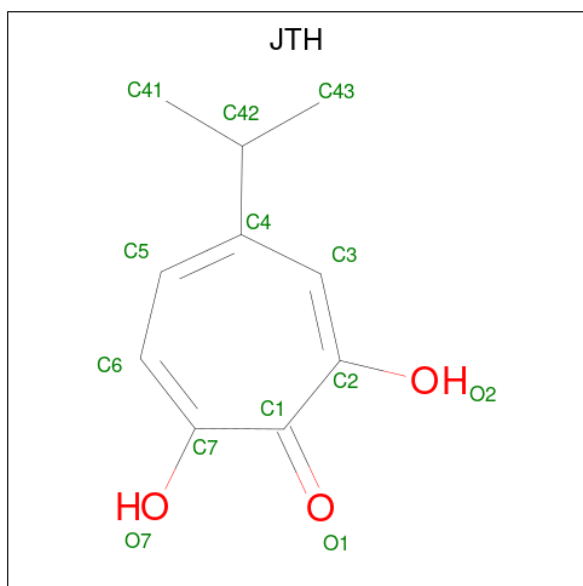| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	230	1796	1132	312	339	13	0	2	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	193	MET	-	expression tag	UNP Q716H3
A	194	GLY	-	expression tag	UNP Q716H3
A	195	SER	-	expression tag	UNP Q716H3
A	196	SER	-	expression tag	UNP Q716H3
A	197	HIS	-	expression tag	UNP Q716H3
A	198	HIS	-	expression tag	UNP Q716H3
A	199	HIS	-	expression tag	UNP Q716H3
A	200	HIS	-	expression tag	UNP Q716H3
A	201	HIS	-	expression tag	UNP Q716H3
A	202	HIS	-	expression tag	UNP Q716H3
A	203	SER	-	expression tag	UNP Q716H3
A	204	SER	-	expression tag	UNP Q716H3
A	205	GLY	-	expression tag	UNP Q716H3
A	206	LEU	-	expression tag	UNP Q716H3
A	207	VAL	-	expression tag	UNP Q716H3
A	208	PRO	-	expression tag	UNP Q716H3
A	209	ARG	-	expression tag	UNP Q716H3
A	210	GLY	-	expression tag	UNP Q716H3
A	211	SER	-	expression tag	UNP Q716H3
A	212	HIS	-	expression tag	UNP Q716H3
A	428	ALA	LYS	engineered mutation	UNP Q716H3

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total Mn 2 2		0	0

- Molecule 3 is 2,7-dihydroxy-4-(propan-2-yl)cyclohepta-2,4,6-trien-1-one (three-letter code: JTH) (formula: $C_{10}H_{12}O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total C O 13 10 3			0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	128	Total O 128 128		0	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 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: Gene 2 protein
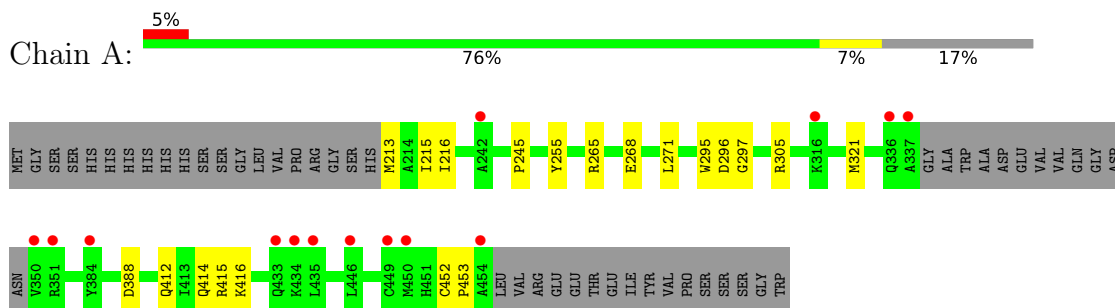
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.59Å 58.42Å 53.38Å 90.00° 96.43° 90.00°	Depositor
Resolution (Å)	19.26 – 1.86 28.79 – 1.86	Depositor EDS
% Data completeness (in resolution range)	95.4 (19.26-1.86) 91.4 (28.79-1.86)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 1.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.168 , 0.208 0.170 , 0.211	Depositor DCC
R_{free} test set	1146 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.5	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	0.96	EDS
Total number of atoms	1939	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.35	0/1838	0.52	0/2475

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	1796	0	1768	10	0
2	A	2	0	0	0	0
3	A	13	0	10	0	0
4	A	128	0	0	2	0
All	All	1939	0	1778	10	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 (10) 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:295:TRP:HH2	1:A:305[A]:ARG:HG3	1.73	0.52
1:A:213:MET:N	4:A:606:HOH:O	2.44	0.48
1:A:215:ILE:HG13	1:A:216:ILE:HG13	1.97	0.46
1:A:245:PRO:HD2	1:A:296:ASP:HB3	1.97	0.46
1:A:452:CYS:HA	1:A:453:PRO:HD2	1.77	0.44
1:A:453:PRO:HG3	4:A:621:HOH:O	2.18	0.44
1:A:416:LYS:HE3	1:A:416:LYS:HB2	1.86	0.42
1:A:297:GLY:HA3	1:A:321:MET:HG3	2.01	0.42
1:A:412:GLN:O	1:A:414:GLN:HG3	2.20	0.41
1:A:255:TYR:CE1	1:A:265:ARG:HD2	2.56	0.40

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	228/278 (82%)	228 (100%)	0	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	183/221 (83%)	179 (98%)	4 (2%)	52	36

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

Mol	Chain	Res	Type
1	A	268	GLU
1	A	271	LEU
1	A	388	ASP
1	A	415	ARG

Sometimes 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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	JTH	A	503	2	13,13,13	1.96	1 (7%)	17,18,18	1.64	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	JTH	A	503	2	-	0/4/4/4	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	JTH	O1-C1	5.86	1.36	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	503	JTH	C5-C6-C7	-4.29	127.71	130.44
3	A	503	JTH	C2-C3-C4	-3.16	128.32	132.18
3	A	503	JTH	C5-C4-C3	2.02	128.48	124.75

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	230/278 (82%)	0.16	14 (6%)	21	20	20, 31, 57, 89	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	VAL	6.8
1	A	337	ALA	5.8
1	A	336	GLN	4.0
1	A	454	ALA	3.7
1	A	449[A]	CYS	3.7
1	A	435	LEU	3.0
1	A	433	GLN	2.7
1	A	351	ARG	2.6
1	A	434	LYS	2.6
1	A	446	LEU	2.5
1	A	242	ALA	2.5
1	A	384	TYR	2.4
1	A	450	MET	2.3
1	A	316	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
3	JTH	A	503	13/13	0.95	0.10	24,34,50,51	0
2	MN	A	502	1/1	0.99	0.05	27,27,27,27	0
2	MN	A	501	1/1	1.00	0.06	25,25,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.