

wwPDB X-ray Structure Validation Summary Report (i)

Apr 21, 2024 – 10:13 am BST

PDB ID	:	4C8Y
Title	:	Cas6 (TTHA0078) substrate mimic complex
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Deposited on	:	2013-10-02
Resolution	:	1.80 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

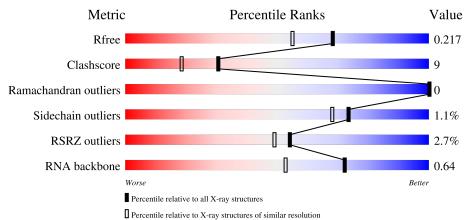
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.80 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)
RNA backbone	3102	1060 (2.40-1.20)

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 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 o	f chain	
1	А	243	3%	83%		15% •
1	В	243	2%	83%		11% • 5%
2	С	16	31%	19%	31%	6% 12%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8178 atoms, of which 3854 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Λ	238	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
	Л	230	3737	1196	1880	337	323	1	0	0	0
1	В	230	Total	С	Η	Ν	Ο	S	0	0	0
	D	230	3627	1161	1829	326	310	1	0	0	0

• Molecule 1 is a protein called CAS6A.

There are 8 discrepancies between the modelled and reference sequences:

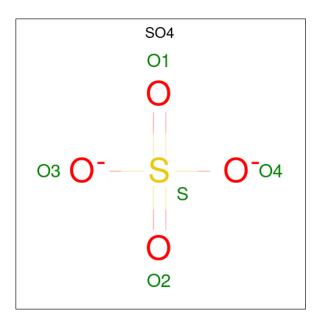
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q5SM65
А	-2	ALA	-	expression tag	UNP Q5SM65
A	-1	ALA	-	expression tag	UNP Q5SM65
A	0	SER	-	expression tag	UNP $Q5SM65$
В	-3	GLY	-	expression tag	UNP Q5SM65
В	-2	ALA	-	expression tag	UNP Q5SM65
В	-1	ALA	-	expression tag	UNP $Q5SM65$
В	0	SER	_	expression tag	UNP Q5SM65

• Molecule 2 is a RNA chain called R1 REPEAT RNA SUBSTRATE MIMIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	С	14	Total	С	Η	Ν	Ο	Р	0	0	1
	U	14	424	125	145	54	88	12	0	0	1 I

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

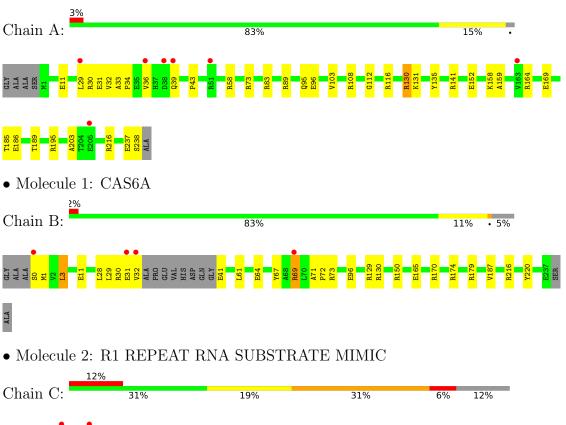
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	140	Total O 140 140	0	0
4	В	221	Total O 221 221	0	0
4	С	19	Total O 19 19	0	0



3 Residue-property plots (i)

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: CAS6A



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	43.07Å 83.30Å 73.44Å	Depositor
a, b, c, α , β , γ	90.00° 101.41° 90.00°	Depositor
Resolution (Å)	71.99 - 1.80	Depositor
Resolution (A)	71.99 - 1.80	EDS
% Data completeness	98.8 (71.99-1.80)	Depositor
(in resolution range)	98.8(71.99-1.80)	EDS
R _{merge}	0.06	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.60 (at 1.80 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.191 , 0.216	Depositor
II, II, <i>free</i>	0.192 , 0.217	DCC
R_{free} test set	2347 reflections $(5.04%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	22.3	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.41 , 52.2	EDS
L-test for twinning ²	$< L > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8178	wwPDB-VP
Average B, all atoms $(Å^2)$	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.55% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: SO4

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).

Mal	Mol Chain		lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.33	0/1906	0.57	0/2588	
1	В	0.36	0/1844	0.58	1/2501~(0.0%)	
2	С	0.68	0/311	2.00	12/483~(2.5%)	
All	All	0.38	0/4061	0.81	13/5572~(0.2%)	

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	26	G	N3-C2-N2	14.17	129.82	119.90
2	С	27	G	N3-C2-N2	13.75	129.53	119.90
2	С	25	G	N3-C2-N2	13.70	129.49	119.90
2	С	26	G	N1-C2-N2	-11.17	106.14	116.20
2	С	25	G	N1-C2-N2	-11.02	106.28	116.20

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	А	1857	1880	1876	33	1
1	В	1798	1829	1826	30	1
2	С	279	145	145	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	А	5	0	0	1	0
3	В	5	0	0	1	0
4	А	140	0	0	7	0
4	В	221	0	0	14	3
4	С	19	0	0	3	0
All	All	4324	3854	3847	72	4

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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 9.

The worst 5 of 72 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:195:ARG:NH1	1:A:237:GLU:OE1	1.98	0.96
1:B:96:GLU:OE1	4:B:2102:HOH:O	1.88	0.91
2:C:24:A:N7	4:C:2015:HOH:O	2.06	0.88
1:B:29:LEU:O	1:B:69:ARG:NH2	2.07	0.87
1:A:96:GLU:OE2	4:A:2072:HOH:O	1.92	0.87

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2025:HOH:O	4:B:2146:HOH:O[1_655]	2.08	0.12
1:A:185:THR:O	1:B:30:ARG:HH22[2_656]	1.53	0.07
4:B:2004:HOH:O	4:B:2155:HOH:O[1_655]	2.17	0.03
4:B:2048:HOH:O	4:B:2192:HOH:O[2_656]	2.17	0.03

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 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	Perce	\mathbf{ntiles}
1	А	236/243~(97%)	230~(98%)	6(2%)	0	100	100
1	В	226/243~(93%)	221 (98%)	5(2%)	0	100	100
All	All	462/486~(95%)	451 (98%)	11 (2%)	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 X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	185/186~(100%)	182~(98%)	3 (2%)	62 54		
1	В	179/186~(96%)	178 (99%)	1 (1%)	86 84		
All	All	364/372~(98%)	360~(99%)	4 (1%)	73 68		

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

Mol	Chain	Res	Type
1	А	30	ARG
1	А	58	ARG
1	А	130	ARG
1	В	3	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type	
1	А	39	GLN	

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	С	10/16~(62%)	1 (10%)	0

All (1) RNA backbone outliers are listed below:



Mol	Chain	Res	Type
2	С	25	G

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)

2 ligands are modelled in this entry.

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		B	ond leng	gths	В	ond ang	gles
INIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	SO4	А	1239	-	4,4,4	0.13	0	$6,\!6,\!6$	0.07	0
3	SO4	В	1238	-	4,4,4	0.14	0	$6,\!6,\!6$	0.09	0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	1239	SO4	1	0
3	В	1238	SO4	1	0



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.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	238/243~(97%)	0.04	7 (2%) 51 46	15, 33, 66, 101	0
1	В	230/243~(94%)	-0.22	4 (1%) 70 66	12, 23, 47, 91	0
2	С	14/16~(87%)	1.08	2 (14%) 2 1	62, 75, 106, 122	0
All	All	482/502~(96%)	-0.06	13 (2%) 54 49	12, 28, 68, 122	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	32	VAL	5.8
1	А	163	VAL	3.7
2	С	21	G	2.9
1	В	0	SER	2.6
1	А	29	LEU	2.4

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 monosaccharides 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, 95^{th} 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	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
3	SO4	В	1238	5/5	0.92	0.18	45,46,52,61	0
3	SO4	А	1239	5/5	0.97	0.12	46,47,48,53	0

6.5 Other polymers (i)

There are no such residues in this entry.

