



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 7, 2019 – 02:07 PM EDT

PDB ID : 6O7B
Title : Crystal structure of Csm1-Csm4 cassette in complex with cA4
Authors : Jia, N.; Patel, D.J.
Deposited on : 2019-03-07
Resolution : 2.40 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 ⓘ 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	:	2.4
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

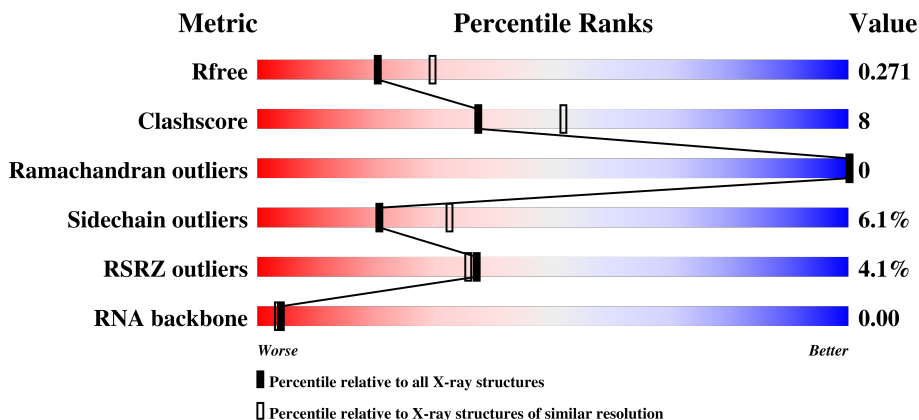
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)
RNA backbone	2636	1023 (2.80-2.00)

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. 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	791	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>•</div> <div>11%</div> </div> </div>
2	B	289	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>10%</div> <div>•</div> <div>12%</div> </div> </div>
3	C	4	<div> <div>25%</div> <div>75%</div> </div>
3	D	4	<div> <div>100%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7884 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 CRISPR system single-strand-specific deoxyribonuclease Cas10/Csm1 (subtype III-A).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	703	Total	C	N	O	S	0	0	0
			5653	3642	971	1024	16			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP B6YWB8
A	-12	GLY	-	expression tag	UNP B6YWB8
A	-11	SER	-	expression tag	UNP B6YWB8
A	-10	SER	-	expression tag	UNP B6YWB8
A	-9	HIS	-	expression tag	UNP B6YWB8
A	-8	HIS	-	expression tag	UNP B6YWB8
A	-7	HIS	-	expression tag	UNP B6YWB8
A	-6	HIS	-	expression tag	UNP B6YWB8
A	-5	HIS	-	expression tag	UNP B6YWB8
A	-4	HIS	-	expression tag	UNP B6YWB8
A	-3	SER	-	expression tag	UNP B6YWB8
A	-2	GLN	-	expression tag	UNP B6YWB8
A	-1	ASP	-	expression tag	UNP B6YWB8
A	0	PRO	-	expression tag	UNP B6YWB8
A	589	ALA	ASP	engineered mutation	UNP B6YWB8

- Molecule 2 is a protein called Csm4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	254	Total	C	N	O	S	0	0	0
			2027	1320	334	369	4			

- Molecule 3 is a RNA chain called Cyclic RNA cA4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	4	Total 88	C 40	N 20	O 24	P 4	0	0	0
3	D	4	Total 88	C 40	N 20	O 24	P 4	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total 21	O 21	0	0
4	B	7	Total 7	O 7	0	0

- Molecule 3: Cyclic RNA cA4

Chain C:  25% 75%

A1
A2
A3
A4

- Molecule 3: Cyclic RNA cA4

Chain D:  100%

A1
A2
A3
A4

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	156.58Å 156.58Å 187.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.48 – 2.40 49.43 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.48-2.40) 99.4 (49.43-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.222 , 0.271 0.226 , 0.271	Depositor DCC
R_{free} test set	5165 reflections (9.76%)	wwPDB-VP
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7884	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.64	0/5775	0.78	0/7787
2	B	0.62	0/2078	0.78	0/2811
3	C	4.81	34/99 (34.3%)	7.65	68/152 (44.7%)
3	D	5.35	32/99 (32.3%)	6.85	53/152 (34.9%)
All	All	1.01	66/8051 (0.8%)	1.44	121/10902 (1.1%)

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	A	N7-C5	-13.99	1.30	1.39
3	D	3	A	N7-C5	-13.60	1.31	1.39
3	D	1	A	N7-C5	-12.05	1.32	1.39
3	D	2	A	N7-C5	-11.54	1.32	1.39
3	C	3	A	N7-C5	-11.31	1.32	1.39

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	A	N1-C2-N3	-22.24	118.18	129.30
3	C	2	A	N1-C2-N3	-22.23	118.19	129.30
3	C	1	A	N1-C2-N3	-22.21	118.19	129.30
3	D	1	A	N1-C2-N3	-21.62	118.49	129.30
3	D	2	A	N1-C2-N3	-21.11	118.74	129.30

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	5653	0	5663	98	0
2	B	2027	0	2025	22	0
3	C	88	0	44	2	0
3	D	88	0	44	19	0
4	A	21	0	0	0	0
4	B	7	0	0	0	0
All	All	7884	0	7776	132	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 8.

The worst 5 of 132 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:B:90:TYR:HD1	2:B:94:LYS:NZ	1.45	1.13
1:A:244:GLN:HG3	3:D:1:A:N7	1.64	1.12
1:A:726:ALA:CB	1:A:748:ILE:HD11	1.98	0.93
1:A:494:ASP:OD2	1:A:500:ALA:HA	1.68	0.92
2:B:90:TYR:CD1	2:B:94:LYS:NZ	2.38	0.90

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 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	685/791 (87%)	652 (95%)	33 (5%)	0	100	100
2	B	244/289 (84%)	231 (95%)	13 (5%)	0	100	100
All	All	929/1080 (86%)	883 (95%)	46 (5%)	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	592/664 (89%)	556 (94%)	36 (6%)	20	32
2	B	215/240 (90%)	202 (94%)	13 (6%)	21	33
All	All	807/904 (89%)	758 (94%)	49 (6%)	20	32

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	429	LEU
1	A	567	ASP
2	B	194	LEU
1	A	530	SER
1	A	568	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	668	HIS
2	B	255	ASN
1	A	676	HIS
1	A	472	ASN
1	A	675	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	4/4 (100%)	3 (75%)	2 (50%)
3	D	4/4 (100%)	3 (75%)	3 (75%)
All	All	8/8 (100%)	6 (75%)	5 (62%)

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	2	A
3	C	3	A
3	C	4	A
3	D	2	A
3	D	3	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	C	1	A
3	C	3	A
3	D	1	A
3	D	2	A
3	D	3	A

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	703/791 (88%)	0.22	27 (3%) 40 39	44, 70, 116, 147	0
2	B	254/289 (87%)	0.08	13 (5%) 28 26	48, 70, 123, 164	0
3	C	4/4 (100%)	0.23	0 100 100	78, 80, 87, 109	0
3	D	4/4 (100%)	-0.06	0 100 100	77, 92, 149, 164	0
All	All	965/1088 (88%)	0.18	40 (4%) 37 36	44, 70, 117, 164	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	416	CYS	5.2
1	A	250	VAL	5.2
2	B	243	ARG	5.0
2	B	90	TYR	4.9
1	A	1	MET	4.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.