



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:35 PM UTC

PDB ID : 4QTS / pdb_00004qts
Title : Crystal structure of Csm3-Csm4 subcomplex in the type III-A CRISPR-Cas interference complex
Authors : Numata, T.; Inanaga, H.; Osawa, T.
Deposited on : 2014-07-09
Resolution : 3.10 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 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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

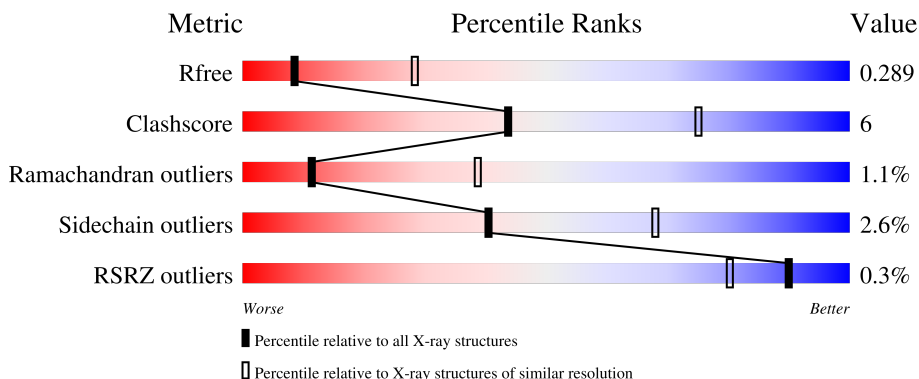
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 $\leq 5\%$. 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	376	 67% 15% 17%
1	B	376	 65% 16% 18%
2	C	268	 57% 12% 31%
2	D	268	 48% 16% 35%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8022 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 type III-associated RAMP protein Csm4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2580	1693	412	471	4			
1	B	308	Total	C	N	O	S	0	0	0
			2558	1680	410	464	4			

- Molecule 2 is a protein called CRISPR type III-associated RAMP protein Csm3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	186	Total	C	N	O	S	0	0	0
			1482	946	250	280	6			
2	D	174	Total	C	N	O	S	0	0	0
			1400	900	233	261	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	expression tag	UNP Q59063
C	-18	GLY	-	expression tag	UNP Q59063
C	-17	SER	-	expression tag	UNP Q59063
C	-16	SER	-	expression tag	UNP Q59063
C	-15	HIS	-	expression tag	UNP Q59063
C	-14	HIS	-	expression tag	UNP Q59063
C	-13	HIS	-	expression tag	UNP Q59063
C	-12	HIS	-	expression tag	UNP Q59063
C	-11	HIS	-	expression tag	UNP Q59063
C	-10	HIS	-	expression tag	UNP Q59063
C	-9	SER	-	expression tag	UNP Q59063
C	-8	SER	-	expression tag	UNP Q59063
C	-7	GLY	-	expression tag	UNP Q59063
C	-6	LEU	-	expression tag	UNP Q59063
C	-5	VAL	-	expression tag	UNP Q59063
C	-4	PRO	-	expression tag	UNP Q59063

Continued on next page...

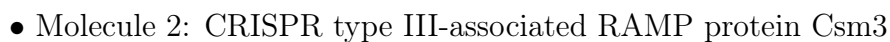
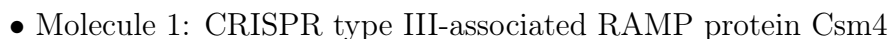
Continued from previous page...

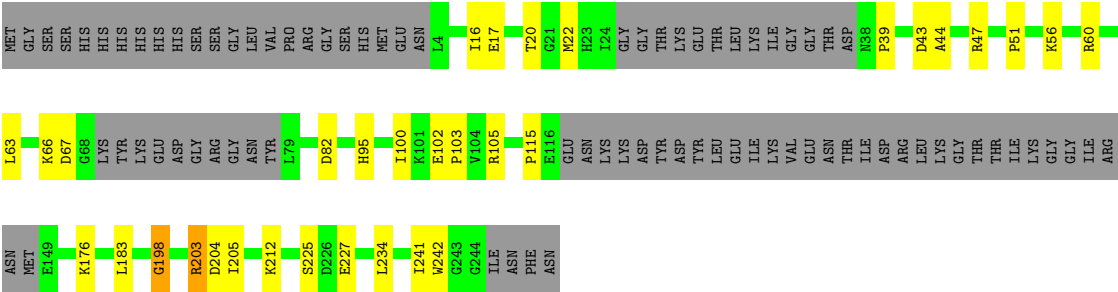
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ARG	-	expression tag	UNP Q59063
C	-2	GLY	-	expression tag	UNP Q59063
C	-1	SER	-	expression tag	UNP Q59063
C	0	HIS	-	expression tag	UNP Q59063
D	-19	MET	-	expression tag	UNP Q59063
D	-18	GLY	-	expression tag	UNP Q59063
D	-17	SER	-	expression tag	UNP Q59063
D	-16	SER	-	expression tag	UNP Q59063
D	-15	HIS	-	expression tag	UNP Q59063
D	-14	HIS	-	expression tag	UNP Q59063
D	-13	HIS	-	expression tag	UNP Q59063
D	-12	HIS	-	expression tag	UNP Q59063
D	-11	HIS	-	expression tag	UNP Q59063
D	-10	HIS	-	expression tag	UNP Q59063
D	-9	SER	-	expression tag	UNP Q59063
D	-8	SER	-	expression tag	UNP Q59063
D	-7	GLY	-	expression tag	UNP Q59063
D	-6	LEU	-	expression tag	UNP Q59063
D	-5	VAL	-	expression tag	UNP Q59063
D	-4	PRO	-	expression tag	UNP Q59063
D	-3	ARG	-	expression tag	UNP Q59063
D	-2	GLY	-	expression tag	UNP Q59063
D	-1	SER	-	expression tag	UNP Q59063
D	0	HIS	-	expression tag	UNP Q59063

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0

- Molecule 1: CRISPR type III-associated RAMP protein Csm4





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.65Å 96.32Å 194.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.46 – 3.10 43.46 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.46-3.10) 99.3 (43.46-3.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.225 , 0.288 0.232 , 0.289	Depositor DCC
R_{free} test set	1296 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	106.7	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8022	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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	0.27	0/2628	0.70	0/3520
1	B	0.26	0/2604	0.69	0/3484
2	C	0.28	0/1503	0.73	0/2004
2	D	0.27	0/1419	0.69	0/1888
All	All	0.27	0/8154	0.70	0/10896

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	2580	0	2668	34	0
1	B	2558	0	2657	33	0
2	C	1482	0	1514	17	0
2	D	1400	0	1438	21	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	8022	0	8277	100	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 6.

The worst 5 of 100 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:D:63:LEU:HD21	2:D:176:LYS:HG2	1.75	0.68
1:A:109:LYS:HB2	1:A:259:ILE:HD11	1.78	0.66
1:B:265:LYS:O	1:B:268:ASN:ND2	2.30	0.64
2:C:102:GLU:OE1	2:C:105:ARG:NH2	2.31	0.64
1:B:95:LYS:HB3	1:B:98:LYS:HE3	1.80	0.63

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	299/376 (80%)	284 (95%)	14 (5%)	1 (0%)	36	67
1	B	294/376 (78%)	281 (96%)	12 (4%)	1 (0%)	36	67
2	C	178/268 (66%)	164 (92%)	10 (6%)	4 (2%)	5	24
2	D	162/268 (60%)	150 (93%)	8 (5%)	4 (2%)	4	21
All	All	933/1288 (72%)	879 (94%)	44 (5%)	10 (1%)	11	39

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	67	ASP
2	D	115	PRO
1	A	324	ASN
1	B	324	ASN
2	C	67	ASP

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/348 (83%)	281 (97%)	8 (3%)	38	66
1	B	287/348 (82%)	284 (99%)	3 (1%)	68	79
2	C	163/233 (70%)	159 (98%)	4 (2%)	42	69
2	D	155/233 (66%)	147 (95%)	8 (5%)	21	51
All	All	894/1162 (77%)	871 (97%)	23 (3%)	40	68

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	242	TRP
2	D	152	VAL
2	D	98	LYS
2	D	168	GLU
1	A	305	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	11	ASN
1	B	170	GLN
1	B	268	ASN
1	B	267	ASN
1	A	201	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are 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.

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	311/376 (82%)	-0.22	2 (0%) 85 70	63, 98, 145, 200	0
1	B	308/376 (81%)	-0.13	1 (0%) 90 80	71, 108, 152, 176	0
2	C	186/268 (69%)	-0.18	0 100 100	69, 105, 168, 183	0
2	D	174/268 (64%)	0.03	0 100 100	97, 142, 178, 197	0
All	All	979/1288 (76%)	-0.14	3 (0%) 90 80	63, 109, 164, 200	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	295	GLU	2.6
1	A	332	ASP	2.4
1	A	94	PRO	2.1

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	ZN	D	301	1/1	0.91	0.07	221,221,221,221	0
3	ZN	C	301	1/1	0.96	0.05	182,182,182,182	0

6.5 Other polymers [i](#)

There are no such residues in this entry.