



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:30 AM UTC

PDB ID : 7D3J / pdb_00007d3j
Title : Crystal structure of the Cas12i1 R-loop complex after target DNA cleavage
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Deposited on : 2020-09-19
Resolution : 2.45 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

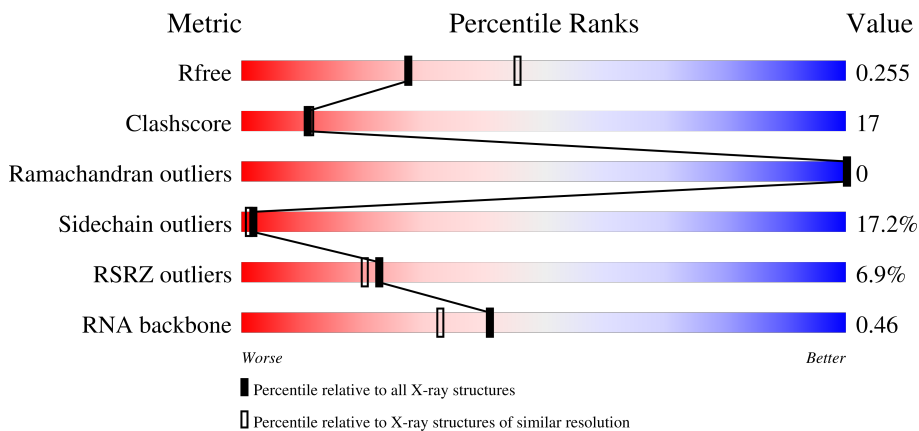
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)
RNA backbone	3983	1023 (2.72-2.20)

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 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	1101	Upper bar: 7% Lower bar: 61% (green), 28% (yellow), 8% (orange), 3% (red), 2% (grey)
2	B	43	Upper bar: 2% Lower bar: 37% (green), 47% (yellow), 16% (orange)
3	C	40	Lower bar: 45% (green), 25% (yellow), 30% (grey)
4	D	40	Upper bar: 12% Lower bar: 22% (green), 30% (yellow), 5% (orange), 42% (grey)

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10727 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 12i1-WT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1077	8717	5545	1507	1625	40	0	0	0

- Molecule 2 is a RNA chain called RNA (43-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	43	914	409	158	304	43	0	0	0

- Molecule 3 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	28	568	274	98	168	28	0	0	0

- Molecule 4 is a DNA chain called DNA (23-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	23	475	227	88	137	23	0	0	0

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 6 7	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	33	Total O 33 33	0	0
6	B	1	Total O 1 1	0	0
6	C	5	Total O 5 5	0	0
6	D	1	Total O 1 1	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	129.80Å 141.97Å 208.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.73 – 2.45 58.73 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (58.73-2.45) 99.9 (58.73-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.45Å)	Xtrriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.220 , 0.257 (Not available) , 0.255	Depositor DCC
R_{free} test set	3545 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtrriage
Anisotropy	0.008	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10727	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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](#)

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

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	1.07	3/8895 (0.0%)	1.30	17/11971 (0.1%)
2	B	1.13	12/1021 (1.2%)	0.97	4/1588 (0.3%)
3	C	0.56	0/635	1.00	0/976
4	D	0.89	1/533 (0.2%)	0.95	3/821 (0.4%)
All	All	1.05	16/11084 (0.1%)	1.23	24/15356 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	23

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	G	O3'-P	-6.59	1.51	1.61
2	B	29	A	O3'-P	-6.24	1.51	1.61
2	B	25	A	O3'-P	-5.98	1.52	1.61
2	B	26	U	O3'-P	-5.96	1.52	1.61
2	B	19	G	O3'-P	-5.94	1.52	1.61

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	14	U	C3'-C2'-O2'	-10.31	99.13	114.60
1	A	399	LYS	N-CA-C	-9.05	102.23	113.18
4	D	12	DT	C2'-C3'-O3'	8.54	124.31	111.50
1	A	541	TYR	N-CA-C	7.29	119.01	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	474	PRO	N-CA-C	6.33	121.45	111.38

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	ARG	Sidechain
1	A	22	ARG	Sidechain
1	A	225	ARG	Sidechain
1	A	228	ARG	Sidechain
1	A	233	ARG	Sidechain

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	8717	0	8774	316	0
2	B	914	0	459	13	0
3	C	568	0	319	11	0
4	D	475	0	261	21	0
5	A	13	0	5	2	0
6	A	33	0	0	0	0
6	B	1	0	0	0	0
6	C	5	0	0	0	0
6	D	1	0	0	0	0
All	All	10727	0	9818	339	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 17.

The worst 5 of 339 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:824:LYS:HE3	1:A:825:PRO:CD	1.59	1.31
1:A:575:ILE:HD11	1:A:579:ARG:NH2	1.48	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:LYS:CE	1:A:825:PRO:HD3	1.66	1.22
1:A:387:TYR:HB2	1:A:402:ARG:NH1	1.53	1.22
1:A:574:GLN:HG2	1:A:593:MET:CE	1.72	1.19

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	1073/1101 (98%)	1047 (98%)	26 (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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	960/984 (98%)	795 (83%)	165 (17%)	2 1

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	744	GLU
1	A	974	LYS
1	A	763	LEU

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Mol	Chain	Res	Type
1	A	824	LYS
1	A	1006	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	616	ASN
1	A	736	GLN
1	A	993	ASN
1	A	724	ASN
1	A	774	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	42/43 (97%)	3 (7%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	U
2	B	17	U
2	B	24	U

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CIT	A	1201	-	12,12,12	1.26	2 (16%)	17,17,17	1.64	2 (11%)

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
5	CIT	A	1201	-	-	5/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1201	CIT	C4-C3	2.04	1.56	1.54
5	A	1201	CIT	O2-C1	-2.04	1.24	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1201	CIT	O6-C6-C3	4.10	121.00	113.14
5	A	1201	CIT	O4-C5-C4	2.54	122.41	114.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1201	CIT	C2-C3-C4-C5
5	A	1201	CIT	O7-C3-C4-C5
5	A	1201	CIT	C6-C3-C4-C5
5	A	1201	CIT	C3-C4-C5-O3
5	A	1201	CIT	C3-C4-C5-O4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1201	CIT	2	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, 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	1077/1101 (97%)	0.56	75 (6%) 22 20	31, 56, 108, 162	0
2	B	43/43 (100%)	-0.25	1 (2%) 61 63	37, 49, 92, 112	2 (4%)
3	C	28/40 (70%)	-0.38	0 100 100	35, 47, 97, 128	0
4	D	23/40 (57%)	0.87	5 (21%) 2 2	40, 61, 106, 133	3 (13%)
All	All	1171/1224 (95%)	0.51	81 (6%) 23 20	31, 56, 108, 162	5 (0%)

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	64	ALA	5.7
1	A	825	PRO	5.5
1	A	834	ALA	5.2
1	A	359	VAL	4.7
1	A	691	ARG	4.4

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 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(\AA^2)	Q<0.9
5	CIT	A	1201	13/13	0.87	0.11	51,62,87,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.