



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 30, 2025 – 04:53 pm BST

PDB ID : 8S5A / pdb_00008s5a
Title : The crystal structure of FAN1 Nuclease bound to 5' phosphorylated p(dG)/3'(dT-dT-dT-dT) double flap DNA
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Deposited on : 2024-02-23
Resolution : 2.65 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 Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

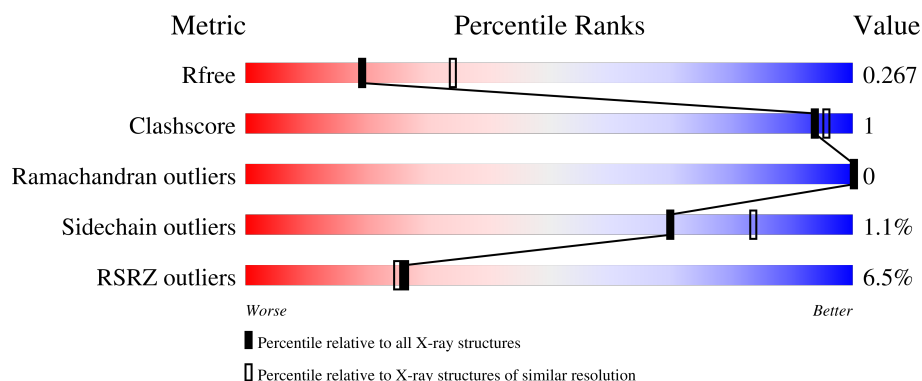
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	164625	1851 (2.66-2.62)
Clashscore	180529	1953 (2.66-2.62)
Ramachandran outliers	177936	1929 (2.66-2.62)
Sidechain outliers	177891	1929 (2.66-2.62)
RSRZ outliers	164620	1850 (2.66-2.62)

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	654	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>5%</div> <div>9%</div> </div> </div>
2	B	19	<div> <div>100%</div> </div>
3	C	8	<div> <div>100%</div> </div>
4	D	16	<div> <div>62%</div> <div>19%</div> <div>19%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5620 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 Fanconi-associated nuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	592	Total	C	N	O	S	169	0	0
			4785	3053	851	857	24			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	GLY	-	expression tag	UNP Q9Y2M0
A	356	PRO	-	expression tag	UNP Q9Y2M0
A	357	MET	-	expression tag	UNP Q9Y2M0
A	358	GLY	-	expression tag	UNP Q9Y2M0
A	359	ALA	-	expression tag	UNP Q9Y2M0
A	360	HIS	-	expression tag	UNP Q9Y2M0
A	361	MET	-	expression tag	UNP Q9Y2M0
A	362	THR	-	expression tag	UNP Q9Y2M0
A	363	ARG	-	expression tag	UNP Q9Y2M0
A	507	HIS	ARG	conflict	UNP Q9Y2M0
A	?	-	CYS	deletion	UNP Q9Y2M0
A	?	-	THR	deletion	UNP Q9Y2M0
A	?	-	TRP	deletion	UNP Q9Y2M0
A	?	-	GLY	deletion	UNP Q9Y2M0
A	?	-	LYS	deletion	UNP Q9Y2M0
A	?	-	ASN	deletion	UNP Q9Y2M0
A	?	-	LYS	deletion	UNP Q9Y2M0
A	?	-	PRO	deletion	UNP Q9Y2M0
A	?	-	GLY	deletion	UNP Q9Y2M0
A	794	ALA	LYS	conflict	UNP Q9Y2M0

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*AP*CP*AP*CP*GP*CP*CP*TP*AP*GP*AP*CP*TP*CP*CP*TP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	19	Total	C	N	O	P	0	0	0
			379	182	70	109	18			

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*AP*GP*GP*CP*GP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	P	0	0	0
			171	79	35	49	8			

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*TP*TP*GP*AP*GP*GP*AP*GP*TP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	13	Total	C	N	O	P	0	0	0
			266	129	45	80	12			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Cl	0	0
			1	1		

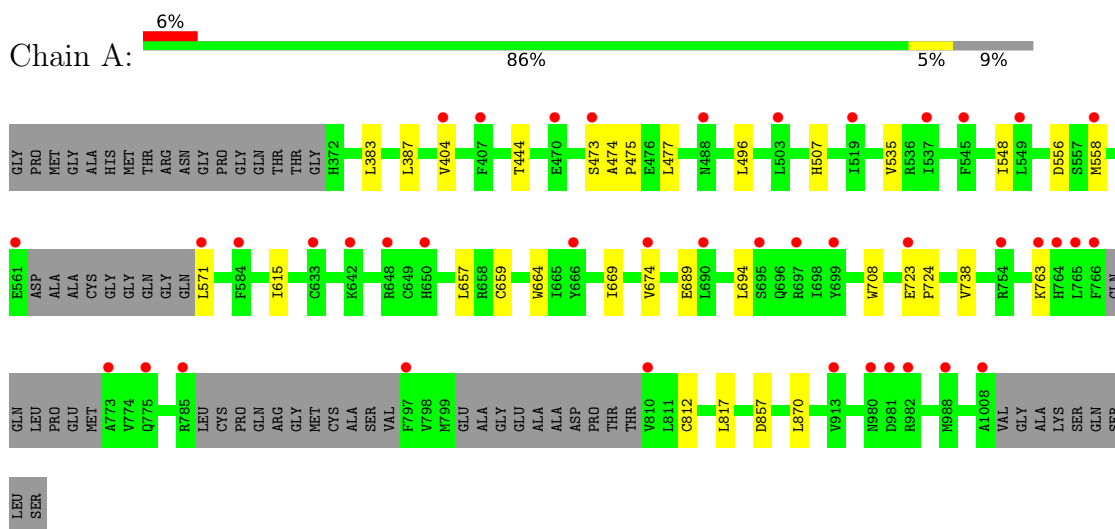
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	15	Total	O	0	0
			15	15		
7	B	1	Total	O	0	0
			1	1		

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: Fanconi-associated nuclease 1



- Molecule 2: DNA (5'-D(*AP*AP*CP*AP*CP*GP*CP*CP*TP*AP*GP*AP*CP*TP*CP*CP*TP*CP*A)-3')



There are no outlier residues recorded for this chain.

- Molecule 3: DNA (5'-D(P*GP*AP*GP*GP*CP*GP*TP*G)-3')



There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(*TP*TP*TP*GP*AP*GP*GP*AP*GP*TP*CP*TP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.63Å 100.55Å 112.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.40 – 2.65 43.40 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.40-2.65) 99.8 (43.40-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.234 , 0.273 0.236 , 0.267	Depositor DCC
R_{free} test set	826 reflections (2.65%)	wwPDB-VP
Wilson B-factor (Å ²)	85.5	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5620	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: CA, CL

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	1.04	0/4885	1.56	4/6602 (0.1%)
2	B	0.32	0/424	0.74	0/650
3	C	0.28	0/192	0.63	0/294
4	D	0.33	0/297	0.80	0/458
All	All	0.96	0/5798	1.45	4/8004 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	507	HIS	CA-C-N	5.13	127.42	120.38
1	A	507	HIS	C-N-CA	5.13	127.42	120.38
1	A	763	LYS	CA-C-N	5.04	128.39	120.82
1	A	763	LYS	C-N-CA	5.04	128.39	120.82

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	4785	0	4819	12	0
2	B	379	0	214	0	0
3	C	171	0	90	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	266	0	151	2	0
5	A	2	0	0	0	0
6	C	1	0	0	0	0
7	A	15	0	0	0	0
7	B	1	0	0	0	0
All	All	5620	0	5274	14	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 1.

The worst 5 of 14 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:387:LEU:HD11	1:A:404:VAL:HG11	1.86	0.57
4:D:1:DT:O2	4:D:1:DT:H2'	2.04	0.56
1:A:659:CYS:HA	1:A:664:TRP:CD2	2.46	0.51
1:A:694:LEU:HD22	1:A:708:TRP:CE2	2.49	0.47
1:A:474:ALA:N	1:A:475:PRO:HD2	2.32	0.45

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	582/654 (89%)	562 (97%)	20 (3%)	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	522/565 (92%)	516 (99%)	6 (1%)	70 83

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	556	ASP
1	A	571	LEU
1	A	738	VAL
1	A	473	SER
1	A	444	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	492	GLN
1	A	610	HIS
1	A	995	GLN

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

Of 3 ligands modelled in this entry, 3 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

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 [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	592/654 (90%)	0.53	41 (6%) 24 23	52, 90, 118, 141	56 (9%)
2	B	19/19 (100%)	-0.36	0 100 100	82, 90, 107, 113	0
3	C	8/8 (100%)	-0.35	0 100 100	98, 102, 107, 109	0
4	D	13/16 (81%)	-0.12	0 100 100	81, 96, 124, 164	0
All	All	632/697 (90%)	0.48	41 (6%) 26 25	52, 90, 118, 164	56 (8%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	561	GLU	8.0
1	A	571	LEU	4.2
1	A	699	TYR	4.0
1	A	775	GLN	3.9
1	A	797	PHE	3.7

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	CA	A	1102	1/1	0.84	0.20	109,109,109,109	0
5	CA	A	1101	1/1	0.90	0.11	100,100,100,100	0
6	CL	C	101	1/1	0.91	0.18	116,116,116,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.