



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:17 PM GMT

PDB ID : 4REB
Title : Structural Insights into 5' Flap DNA Unwinding and Incision by the Human FAN1 Dimer
Authors : Zhao, Q.; Xue, X.; Longerich, S.; Sung, P.; Xiong, Y.
Deposited on : 2014-09-22
Resolution : 4.20 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

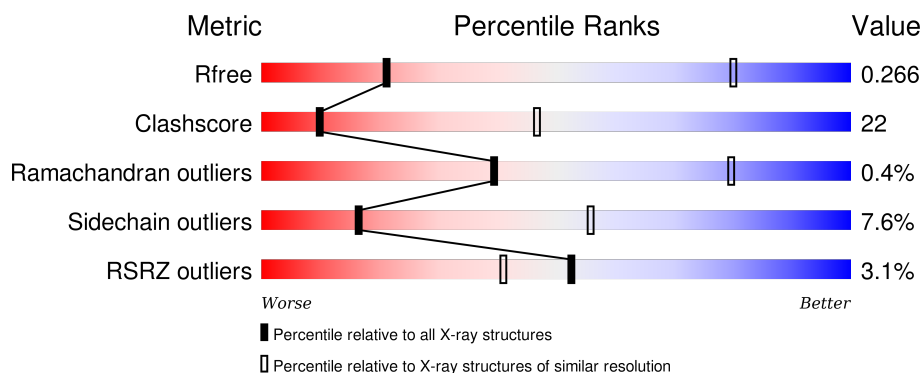
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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}	91344	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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	D	9	<div> <div>33%</div> <div>67%</div> </div>
2	E	20	<div> <div>45%</div> <div>55%</div> </div>
3	F	10	<div> <div>50%</div> <div>50%</div> </div>
4	A	647	<div> <div>3%</div> <div>56%</div> <div>27%</div> <div>13%</div> </div>
4	H	647	<div> <div>3%</div> <div>55%</div> <div>32%</div> <div>10%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10114 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 DNA chain called DNA (5'-D(P*GP*TP*GP*GP*CP*GP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	9	Total	C	N	O	P	0	0	0
			189	88	38	54	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	20	Total	C	N	O	P	0	0	0
			410	192	78	120	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	10	Total	C	N	O	P	0	0	0
			202	95	37	60	10			

- Molecule 4 is a protein called Fanconi-associated nuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	566	Total	C	N	O	S	0	1	0
			4590	2931	815	821	23			
4	H	584	Total	C	N	O	S	0	1	0
			4721	3014	841	843	23			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	371	GLU	-	EXPRESSION TAG	UNP Q9Y2M0
A	372	PHE	-	EXPRESSION TAG	UNP Q9Y2M0
A	960	ALA	ASP	ENGINEERED MUTATION	UNP Q9Y2M0
H	371	GLU	-	EXPRESSION TAG	UNP Q9Y2M0

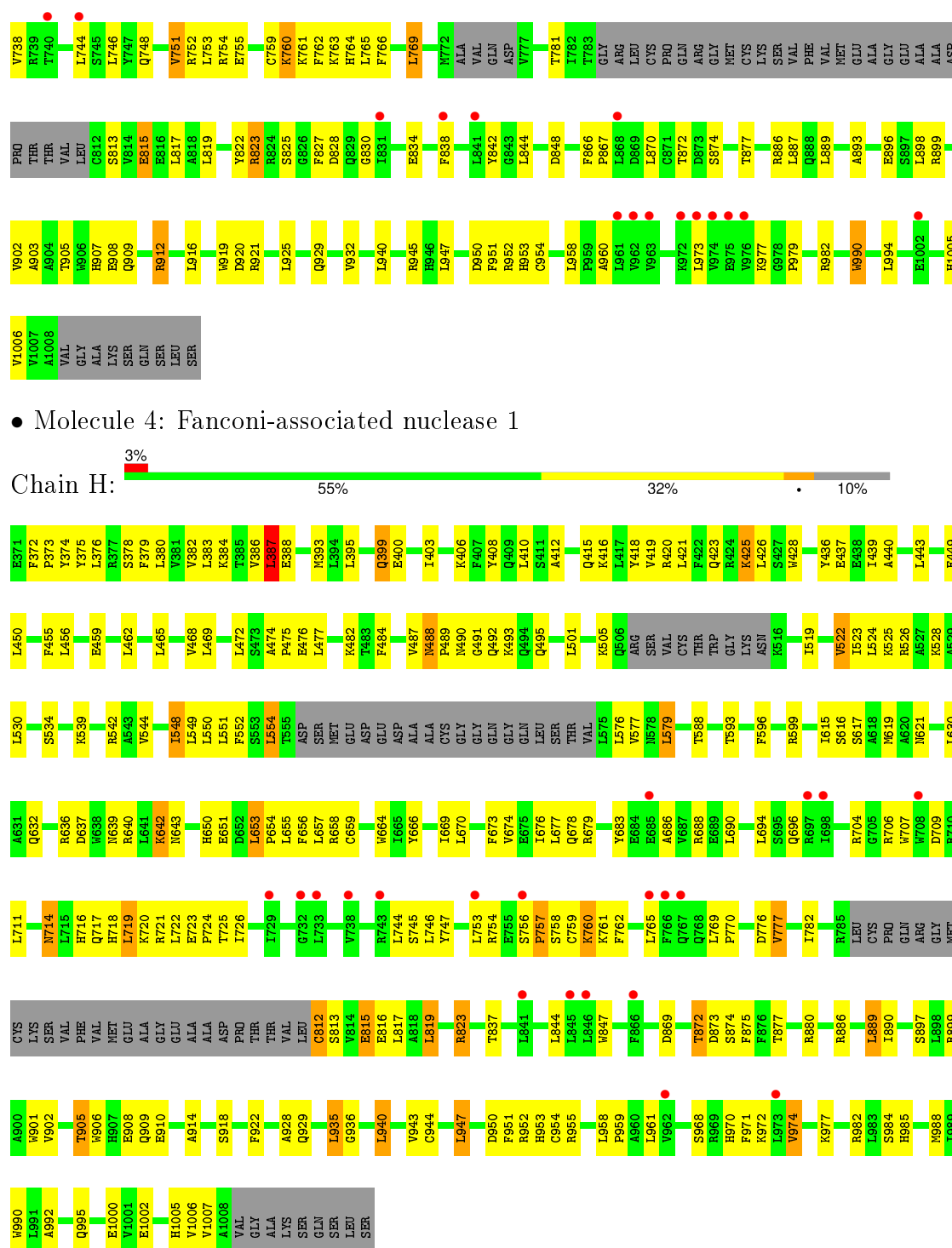
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Chain	Residue	Modelled	Actual	Comment	Reference
H	372	PHE	-	EXPRESSION TAG	UNP Q9Y2M0
H	960	ALA	ASP	ENGINEERED MUTATION	UNP Q9Y2M0

- Molecule 5 is SAMARIUM (III) ION (three-letter code: SM) (formula: Sm).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total 1	Sm 1	0	0
5	A	1	Total 1	Sm 1	0	0



• Molecule 4: Fanconi-associated nuclease 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	104.77Å 104.77Å 127.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	90.70 – 4.20 90.73 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (90.70-4.20) 99.3 (90.73-4.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 4.15Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.230 , 0.262 0.240 , 0.266	Depositor DCC
R_{free} test set	566 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	247.1	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 248.3	EDS
Estimated twinning fraction	0.495 for H, K, L 0.505 for K, H, -L 0.196 for -h,-k,l 0.359 for h,-h-k,-l 0.198 for -k,-h,-l	Xtriage
Reported twinning fraction	0.495 for H, K, L 0.505 for K, H, -L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 11360 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10114	wwPDB-VP
Average B, all atoms (Å ²)	297.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: SM

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	D	0.49	0/212	0.84	1/326 (0.3%)
2	E	0.44	0/459	0.75	0/706
3	F	0.48	0/225	0.75	0/344
4	A	0.57	0/4689	0.79	6/6339 (0.1%)
4	H	0.57	0/4822	0.80	3/6518 (0.0%)
All	All	0.56	0/10407	0.79	10/14233 (0.1%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	H	421	LEU	CB-CG-CD2	-6.66	99.68	111.00
4	A	471	LEU	CA-CB-CG	6.04	129.18	115.30
4	H	889	LEU	CA-CB-CG	5.80	128.63	115.30
4	A	630	LEU	CB-CG-CD2	5.79	120.85	111.00
4	H	387	LEU	CA-CB-CG	5.79	128.61	115.30

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	D	189	0	101	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	410	0	223	13	1
3	F	202	0	112	3	0
4	A	4590	0	4602	205	1
4	H	4721	0	4752	214	2
5	A	1	0	0	0	0
5	H	1	0	0	0	0
All	All	10114	0	9790	431	2

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 22.

The worst 5 of 431 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)
4:A:579:LEU:HB2	4:A:582:MET:CE	1.39	1.47
4:A:579:LEU:HA	4:A:582:MET:CG	1.43	1.47
4:H:374:TYR:CE2	4:H:577:VAL:HG13	1.52	1.42
4:A:579:LEU:CA	4:A:582:MET:HG2	1.50	1.36
4:A:579:LEU:CB	4:A:582:MET:CE	2.12	1.26

All (2) 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:A:580:GLY:O	4:H:688:ARG:NH2[3_664]	1.97	0.23
2:E:19:DC:OP2	4:H:436:TYR:OH[2_545]	2.07	0.13

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	
4	A	557/647 (86%)	539 (97%)	17 (3%)	1 (0%)	52	86
4	H	577/647 (89%)	552 (96%)	22 (4%)	3 (0%)	34	77
All	All	1134/1294 (88%)	1091 (96%)	39 (3%)	4 (0%)	39	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	642	LYS
4	H	490	ASN
4	H	757	PRO
4	H	777	VAL

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	
4	A	498/562 (89%)	459 (92%)	39 (8%)	16	54
4	H	511/562 (91%)	473 (93%)	38 (7%)	17	56
All	All	1009/1124 (90%)	932 (92%)	77 (8%)	16	56

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	872	THR
4	H	522	VAL
4	H	935	LEU
4	A	907	HIS
4	H	387	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	678	GLN
4	A	714	ASN

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Mol	Chain	Res	Type
4	H	678	GLN
4	H	714	ASN
4	H	718	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

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	D	9/9 (100%)	-0.44	0 100 100	292, 298, 305, 312	0
2	E	20/20 (100%)	-0.31	0 100 100	268, 286, 307, 312	0
3	F	10/10 (100%)	-0.08	0 100 100	248, 263, 328, 352	0
4	A	566/647 (87%)	-0.14	17 (3%) 54 42	243, 294, 353, 396	0
4	H	584/647 (90%)	-0.13	20 (3%) 49 38	218, 299, 364, 449	0
All	All	1189/1333 (89%)	-0.14	37 (3%) 52 41	218, 295, 358, 449	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	962	VAL	4.8
4	H	753	LEU	3.9
4	A	963	VAL	3.8
4	A	1002	GLU	3.7
4	H	685	GLU	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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
5	SM	A	1101	1/1	0.91	0.30	-	340,340,340,340	0
5	SM	H	1101	1/1	0.93	0.26	-	386,386,386,386	0

6.5 Other polymers [i](#)

There are no such residues in this entry.