Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 12:09 PM EST

PDB ID	:	5K97
Title	:	Flap endonuclease 1 (FEN1) D233N with cleaved product fragment and Sm3+
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Deposited on	:	2016-05-31
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) 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 (1)) were used in the production of this report:

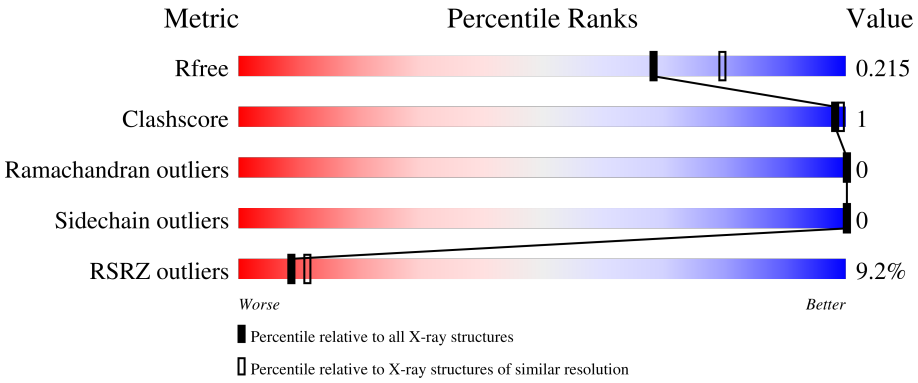
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	341	10%, 98%, .
2	D	18	100%
3	E	11	91%, 9%
4	F	7	86%, 14%
5	G	5	40%, 40%, 60%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7431 atoms, of which 3255 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 Flap endonuclease 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	341	Total	C	H	N	O	S	0	10	0
			5584	1747	2816	487	517	17			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	ASN	ASP	engineered mutation	UNP P39748
A	337	LEU	-	expression tag	UNP P39748
A	338	GLU	-	expression tag	UNP P39748
A	339	VAL	-	expression tag	UNP P39748
A	340	LEU	-	expression tag	UNP P39748
A	341	PHE	-	expression tag	UNP P39748
A	342	GLN	-	expression tag	UNP P39748

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*CP*TP*CP*TP*GP*CP*CP*TP*CP*AP*AP*GP*AP*CP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	18	Total	C	H	N	O	P	0	0	0
			567	174	204	66	106	17			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	11	Total	C	H	N	O	P	0	0	0
			357	109	124	47	66	11			

- Molecule 4 is a DNA chain called DNA (5'-D(*AP*CP*CP*GP*TP*CP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	7	Total	C	H	N	O	P	0	0	0
			216	66	80	24	40	6			

- Molecule 5 is a DNA chain called DNA (5'-D(P*TP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	G	2	Total	C	H	N	O	P	0	0	0
			65	20	25	4	14	2			

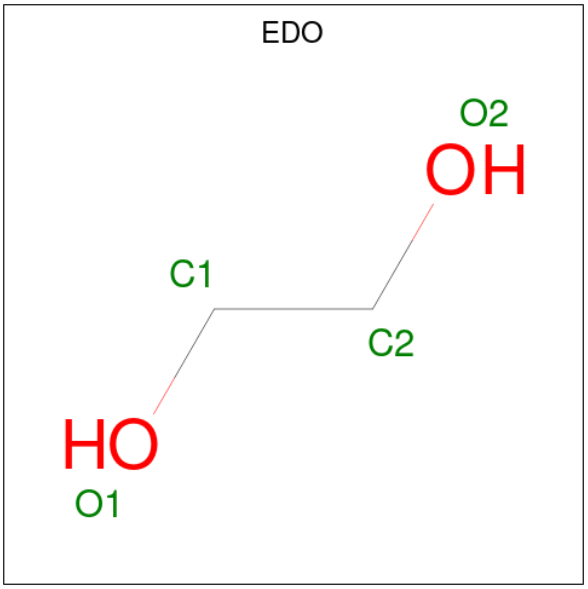
- Molecule 6 is SAMARIUM (III) ION (three-letter code: SM) (formula: Sm).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	Sm	0	0
			8	8		

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	K	0	0
			1	1		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			10	2	6	2		

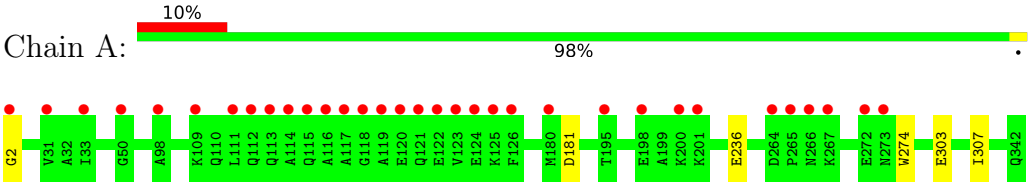
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	439	Total O 439 439	0	0
9	D	97	Total O 97 97	0	0
9	E	51	Total O 51 51	0	0
9	F	33	Total O 33 33	0	0
9	G	3	Total O 3 3	0	0

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.

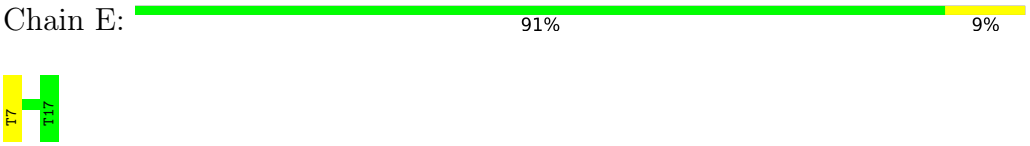
• Molecule 1: Flap endonuclease 1



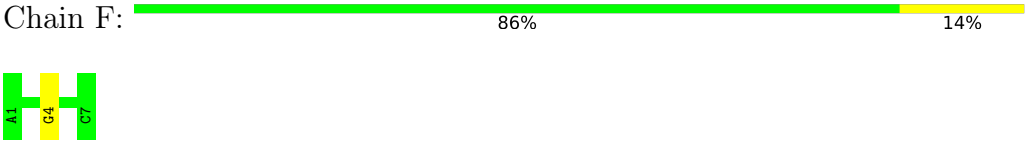
• Molecule 2: DNA (5'-D(*AP*CP*TP*CP*TP*GP*CP*CP*TP*CP*AP*AP*GP*AP*CP*GP*GP*T)-3')

There are no outlier residues recorded for this chain.

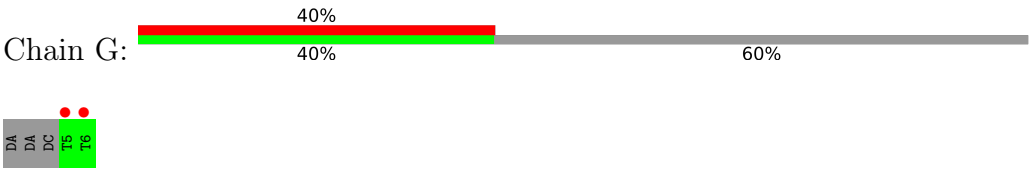
• Molecule 3: DNA (5'-D(P*TP*GP*AP*GP*GP*CP*AP*GP*AP*GP*T)-3')



• Molecule 4: DNA (5'-D(*AP*CP*CP*GP*TP*CP*C)-3')



• Molecule 5: DNA (5'-D(P*TP*T)-3')



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.24Å 105.24Å 104.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.85 – 2.10 34.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (34.85-2.10) 95.9 (34.85-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.66 (at 2.10Å)	Xtriage
Refinement program	PHENIX (dev_2383: ???)	Depositor
R, R_{free}	0.182 , 0.219 0.180 , 0.215	Depositor DCC
R_{free} test set	1985 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 66.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7431	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SM, K, EDO

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	0.26	0/2838	0.40	0/3809
2	D	0.50	0/406	0.90	0/624
3	E	0.81	1/262 (0.4%)	0.81	0/402
4	F	0.47	0/151	0.82	0/230
5	G	0.52	0/43	1.35	0/64
All	All	0.37	1/3700 (0.0%)	0.57	0/5129

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	7	DT	OP3-P	-10.68	1.48	1.61

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	2768	2816	2829	3	0
2	D	363	204	204	0	0
3	E	233	124	124	0	0
4	F	136	80	80	1	0
5	G	40	25	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	8	0	0	0	0
7	A	1	0	0	0	0
8	A	4	6	6	0	0
9	A	439	0	0	0	0
9	D	97	0	0	0	0
9	E	51	0	0	0	0
9	F	33	0	0	1	0
9	G	3	0	0	0	0
All	All	4176	3255	3268	4	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.

All (4) 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:236:GLU:O	1:A:274:TRP:NE1	2.43	0.43
4:F:4:DG:N3	9:F:101:HOH:O	2.36	0.43
1:A:303:GLU:O	1:A:307:ILE:HG12	2.21	0.41
1:A:2:GLY:N	1:A:181:ASP:OD1	2.54	0.40

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	349/341 (102%)	342 (98%)	7 (2%)	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	303/293 (103%)	303 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
8	EDO	A	410	-	3,3,3	0.46	0	2,2,2	0.27	0

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
8	EDO	A	410	-	-	0/1/1/1	-

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	341/341 (100%)	0.41	33 (9%) 7 10	31, 49, 121, 191	0
2	D	18/18 (100%)	0.01	0 100 100	52, 71, 98, 100	0
3	E	11/11 (100%)	0.74	0 100 100	73, 81, 94, 95	0
4	F	7/7 (100%)	-0.56	0 100 100	47, 58, 75, 78	0
5	G	2/5 (40%)	6.89	2 (100%) 0 0	84, 84, 84, 100	2 (100%)
All	All	379/382 (99%)	0.41	35 (9%) 9 11	31, 51, 120, 191	2 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	ALA	8.5
5	G	6	DT	8.5
1	A	111	LEU	6.6
1	A	118	GLY	5.7
1	A	116	ALA	5.4
5	G	5	DT	5.3
1	A	120	GLU	5.2
1	A	119	ALA	4.5
1	A	124	GLU	4.3
1	A	115	GLN	4.3
1	A	123	VAL	4.2
1	A	122	GLU	4.1
1	A	98	ALA	3.6
1	A	114	ALA	3.6
1	A	121	GLN	3.5
1	A	112	GLN	3.2
1	A	113	GLN	3.1
1	A	2	GLY	2.9
1	A	267	LYS	2.9
1	A	200	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	125	LYS	2.8
1	A	198	GLU	2.8
1	A	273	ASN	2.8
1	A	126	PHE	2.8
1	A	266	ASN	2.7
1	A	264	ASP	2.5
1	A	265	PRO	2.5
1	A	180	MET	2.4
1	A	272	GLU	2.3
1	A	195	THR	2.2
1	A	50	GLY	2.2
1	A	33	ILE	2.1
1	A	109	LYS	2.1
1	A	201	LYS	2.1
1	A	31	VAL	2.0

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 monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
6	SM	A	409	1/1	0.73	0.34	324,324,324,324	0
8	EDO	A	410	4/4	0.78	0.36	52,80,96,96	0
6	SM	A	401	1/1	0.92	0.05	58,58,58,58	1
6	SM	A	408	1/1	0.95	0.07	122,122,122,122	1
6	SM	A	403	1/1	0.98	0.05	45,45,45,45	1
7	K	A	405	1/1	0.98	0.07	72,72,72,72	0
6	SM	A	402	1/1	0.98	0.06	88,88,88,88	1
6	SM	A	404	1/1	0.99	0.04	41,41,41,41	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SM	A	406	1/1	1.00	0.09	37,37,37,37	0
6	SM	A	407	1/1	1.00	0.09	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.