



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:09 am BST

PDB ID : 5ZOF
Title : Crystal Structure of D181A/R192F hFen1 in complex with DNA
Authors : Han, W.; Hua, Y.; Zhao, Y.
Deposited on : 2018-04-13
Resolution : 2.25 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

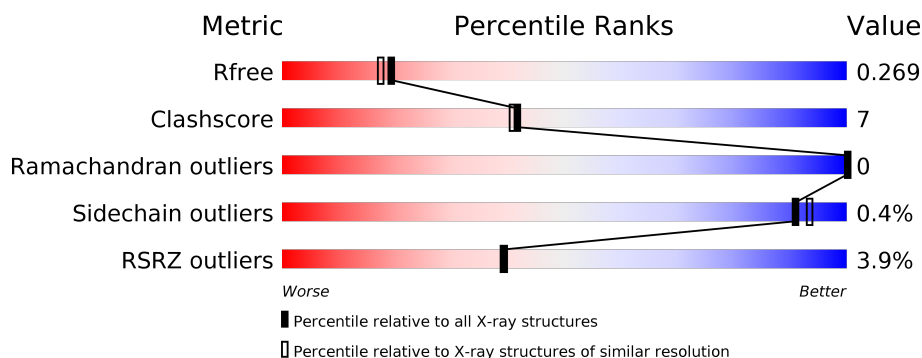
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 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	333	<div> <div>4%</div> <div>78%</div> <div>9%</div> <div>13%</div> </div>
2	B	18	<div> <div>78%</div> <div>22%</div> </div>
3	C	8	<div> <div>38%</div> <div>63%</div> </div>
4	D	14	<div> <div>7%</div> <div>64%</div> <div>36%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	K	A	401	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3107 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 Flap endonuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2290	1453	392	430	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	ALA	ASP	engineered mutation	UNP P39748
A	192	PHE	ARG	engineered mutation	UNP P39748

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	18	Total	C	N	O	P	0	0	0
			363	173	67	106	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	P	0	0	0
			155	75	27	46	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	14	Total	C	N	O	P	0	0	0
			288	138	57	80	13			

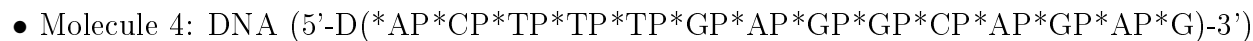
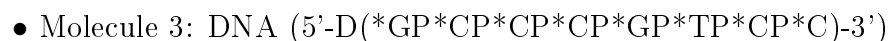
- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	9	Total O 9 9	0	0
6	D	1	Total O 1 1	0	0

- Molecule 1: Flap endonuclease 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.67Å 92.73Å 102.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.82 – 2.25 27.82 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.8 (27.82-2.25) 98.9 (27.82-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, R_{free}	0.235 , 0.269 0.235 , 0.269	Depositor DCC
R_{free} test set	1114 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3107	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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:
K

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	0.46	0/2332	0.57	0/3140
2	B	0.87	0/406	0.92	0/624
3	C	0.68	0/172	0.75	0/263
4	D	0.74	0/324	0.90	0/500
All	All	0.57	0/3234	0.68	0/4527

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 [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	2290	0	2302	21	0
2	B	363	0	203	12	0
3	C	155	0	88	7	0
4	D	288	0	156	6	0
5	A	1	0	0	0	0
6	A	9	0	0	0	0
6	D	1	0	0	0	0
All	All	3107	0	2749	40	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 7.

All (40) 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:B:3:DT:H2''	2:B:4:DC:C5'	1.87	1.04
2:B:3:DT:H2''	2:B:4:DC:H5''	1.46	0.95
2:B:3:DT:H2''	2:B:4:DC:O5'	1.69	0.91
3:C:2:DC:H2''	3:C:3:DC:H5''	1.73	0.70
1:A:242:GLY:N	2:B:3:DT:H5''	2.08	0.68
1:A:332:ARG:O	1:A:333:GLN:HB2	1.93	0.68
1:A:142:LYS:NZ	1:A:154:ASP:OD2	2.28	0.64
2:B:12:DA:C5	4:D:2:DC:C5	2.86	0.63
4:D:6:DG:H2''	4:D:7:DA:H5''	1.80	0.63
2:B:3:DT:C2'	2:B:4:DC:O5'	2.46	0.62
2:B:4:DC:H5''	2:B:4:DC:H6	1.66	0.60
3:C:4:DC:H2''	3:C:5:DG:C8	2.38	0.58
1:A:225:ASP:OD1	1:A:280:HIS:ND1	2.35	0.58
3:C:3:DC:H2''	3:C:4:DC:H5''	1.86	0.56
2:B:4:DC:H2''	2:B:5:DT:H5'	1.88	0.56
1:A:3:ILE:HD12	1:A:227:CYS:HB3	1.87	0.56
1:A:156:PRO:HB2	1:A:287:GLU:HG2	1.88	0.55
3:C:1:DG:H2''	3:C:2:DC:H5'	1.89	0.55
1:A:239:ARG:NH2	2:B:5:DT:OP1	2.38	0.54
1:A:213:LEU:HB3	1:A:218:LEU:O	2.09	0.53
1:A:278:GLU:OE2	1:A:278:GLU:N	2.37	0.53
1:A:37:MET:O	1:A:41:GLN:HG2	2.10	0.51
4:D:5:DT:H2''	4:D:6:DG:H5''	1.93	0.50
3:C:1:DG:H2'	3:C:2:DC:C6	2.47	0.49
4:D:6:DG:H8	4:D:6:DG:H5'	1.78	0.48
1:A:44:ILE:HD13	4:D:1:DA:C6	2.49	0.48
1:A:6:LEU:HD23	1:A:180:MET:HB3	1.97	0.45
2:B:3:DT:H4'	2:B:4:DC:OP1	2.16	0.45
1:A:240:GLY:N	2:B:4:DC:OP1	2.50	0.44
1:A:37:MET:HG2	1:A:41:GLN:NE2	2.32	0.44
1:A:41:GLN:H	1:A:41:GLN:HG2	1.68	0.44
3:C:3:DC:C5'	3:C:3:DC:H6	2.31	0.44
1:A:147:LEU:HA	1:A:147:LEU:HD23	1.82	0.42
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.90	0.42
1:A:245:ARG:HG3	2:B:3:DT:OP1	2.20	0.41
3:C:2:DC:C2'	3:C:3:DC:H5''	2.46	0.41
1:A:246:ALA:O	1:A:250:ILE:HG12	2.20	0.41
1:A:290:ASP:O	1:A:293:SER:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:HIS:HB3	1:A:258:GLU:HG2	2.03	0.40
4:D:2:DC:O2	4:D:2:DC:C5'	2.70	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	286/333 (86%)	279 (98%)	7 (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	250/285 (88%)	249 (100%)	1 (0%)	91	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	CYS

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

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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

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, 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	290/333 (87%)	0.44	12 (4%) 37 37	33, 49, 81, 99	0
2	B	18/18 (100%)	0.23	0 100 100	44, 64, 82, 84	0
3	C	8/8 (100%)	-0.29	0 100 100	42, 54, 67, 70	0
4	D	14/14 (100%)	0.57	1 (7%) 16 15	58, 74, 88, 90	0
All	All	330/373 (88%)	0.42	13 (3%) 39 39	33, 50, 83, 99	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	LYS	3.3
1	A	285	GLU	2.8
1	A	290	ASP	2.8
1	A	319	GLU	2.7
1	A	64	LEU	2.7
1	A	67	MET	2.5
1	A	3	ILE	2.3
1	A	33	ILE	2.3
1	A	39	ILE	2.2
1	A	295	GLU	2.1
1	A	264	ASP	2.1
1	A	230	LEU	2.1
4	D	8	DG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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. 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	K	A	401	1/1	0.47	0.46	133,133,133,133	0

6.5 Other polymers [i](#)

There are no such residues in this entry.