



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:06 AM GMT

PDB ID : 2FOK
Title : STRUCTURE OF RESTRICTION ENDONUCLEASE FOKI
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Deposited on : 1998-03-30
Resolution : 2.30 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

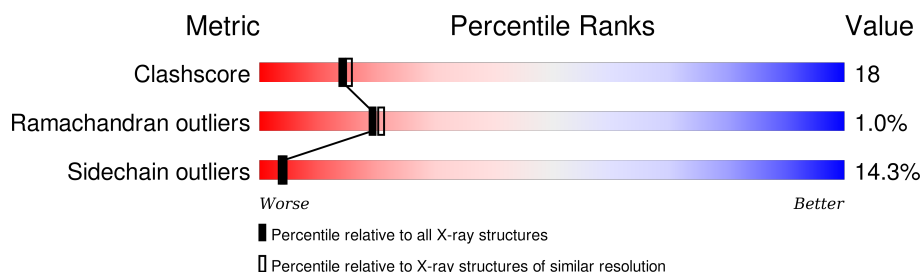
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	579	 55% 35% 7% •
1	B	579	 57% 34% 6% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9427 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 FOKI RESTRICTION ENDONUCLEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4458	2859	764	824	11			
1	B	560	Total	C	N	O	S	0	0	0
			4453	2860	759	823	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	LEU	GLY	CONFLICT	UNP P14870
A	381	GLY	VAL	CONFLICT	UNP P14870
A	382	LYS	THR	CONFLICT	UNP P14870
A	383	PRO	LYS	CONFLICT	UNP P14870
A	384	ASP	GLN	CONFLICT	UNP P14870
B	380	LEU	GLY	CONFLICT	UNP P14870
B	381	GLY	VAL	CONFLICT	UNP P14870
B	382	LYS	THR	CONFLICT	UNP P14870
B	383	PRO	LYS	CONFLICT	UNP P14870
B	384	ASP	GLN	CONFLICT	UNP P14870

- Molecule 2 is water.

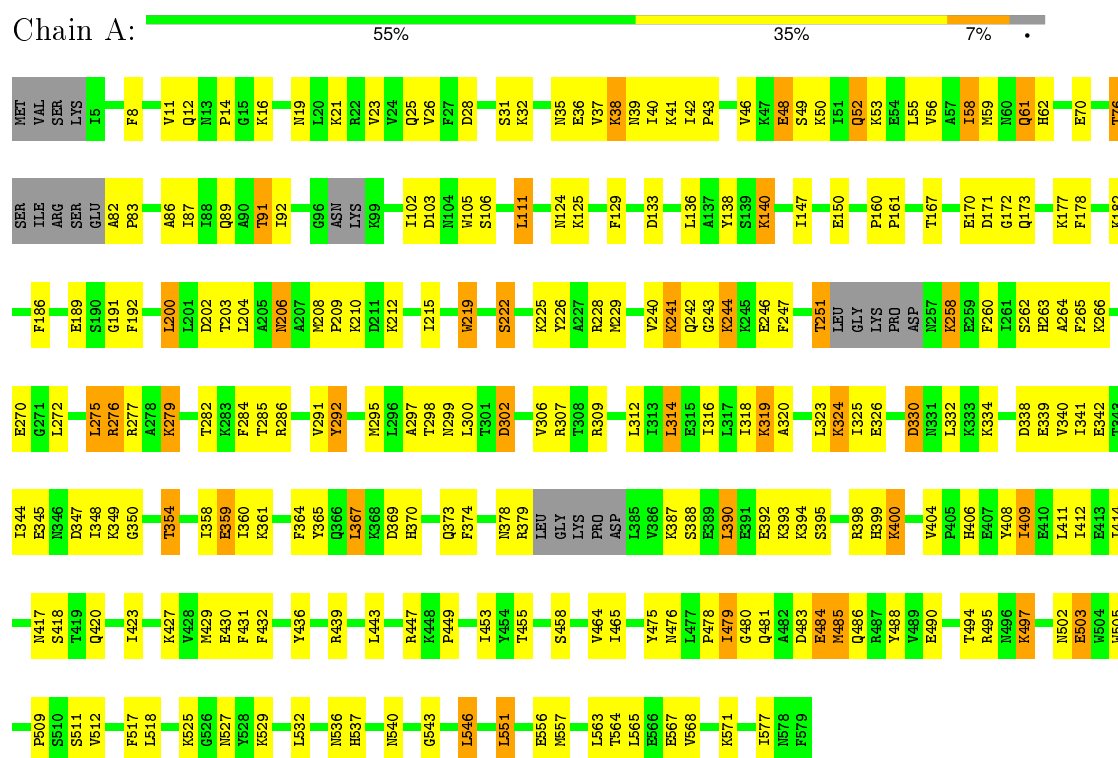
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	282	Total	O	0	0
			282	282		
2	B	234	Total	O	0	0
			234	234		

3 Residue-property plots

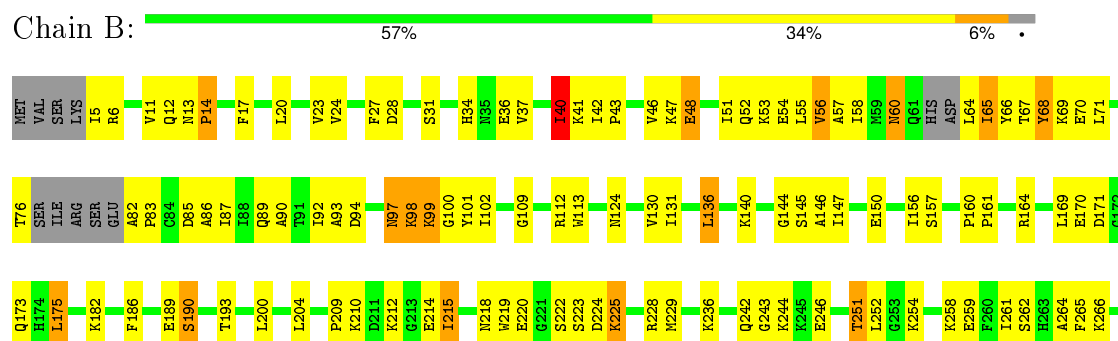
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: FOKI RESTRICTION ENDONUCLEASE



• Molecule 1: FOKI RESTRICTION ENDONUCLEASE



V545	D347	K427	E270
K559	I348	K428	I275
L565	K349	M429	R276
E566	G350	M433	R277
E567	I351	M433	A278
V568	I352	K441	K279
R569	I353		
K571	I354		T282
I577	F357	I453	K283
M578	I358	I454	F284
F579	E359	T455	T285
	I360	S458	R286
	K361	Y462	
	L367	G463	R290
	K368	V464	V291
	I371		Y292
	L296	T468	W293
	A297	K469	F294
	V375		H295
	I376	S472	L296
	P377	G473	T298
	M378	G474	W299
	ARG	Y475	I300
	LEU	M476	T301
	GLY	L477	D302
	LYS		K303
	PRO	Q481	E304
	ASP		Y305
	LEU	E484	V306
	VAL	R487	R307
	K387	Y488	T308
	S388		R309
	E389	K497	R310
	L390		A311
	E391		L312
	E392	N502	F313
	K393	E503	L314
	K394		E315
	S395	K506	I316
	R398	L518	K319
	H406	F519	S322
	E407	V520	L323
	Y408		K324
	I409	H523	I325
		F524	
		K525	I331
	I412	G526	L332
	E413	N527	K333
	I414	Y528	K334
	A415	K529	L335
	R416	A530	
	M417	G531	V340
		L532	I341
	Q420		E342
		H537	T343
	I423		I344

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.01Å 137.17Å 188.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	96.5 (6.00-2.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.211 , 0.306	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9427	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.38	0/4543	0.61	0/6118
1	B	0.38	0/4539	0.60	1/6115 (0.0%)
All	All	0.38	0/9082	0.60	1/12233 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	518	LEU	CA-CB-CG	5.64	128.28	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	A	4458	0	4494	155	0
1	B	4453	0	4486	172	0
2	A	282	0	0	14	0
2	B	234	0	0	8	0
All	All	9427	0	8980	326	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 18.

The worst 5 of 326 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:497:LYS:HD2	1:A:497:LYS:H	1.35	0.91
1:B:417:ASN:HB2	1:B:420:GLN:HG2	1.54	0.89
1:B:390:LEU:HD21	1:B:413:GLU:HG2	1.53	0.88
1:B:37:VAL:HA	1:B:41:LYS:HB2	1.55	0.88
1:B:131:ILE:HD13	1:B:136:LEU:HD13	1.53	0.88

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	548/579 (95%)	514 (94%)	31 (6%)	3 (0%)	34	41
1	B	552/579 (95%)	512 (93%)	32 (6%)	8 (1%)	14	13
All	All	1100/1158 (95%)	1026 (93%)	63 (6%)	11 (1%)	19	21

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	48	GLU
1	A	400	LYS
1	A	48	GLU
1	B	503	GLU
1	B	14	PRO

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	478/503 (95%)	406 (85%)	72 (15%)	3	3
1	B	475/503 (94%)	411 (86%)	64 (14%)	5	4
All	All	953/1006 (95%)	817 (86%)	136 (14%)	4	4

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	458	SER
1	B	68	TYR
1	B	481	GLN
1	A	481	GLN
1	A	532	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	527	ASN
1	A	578	ASN
1	B	97	ASN
1	A	406	HIS
1	B	331	ASN

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 ⓘ

There are no ligands in this entry.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.