



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:55 AM UTC

PDB ID : 3V21 / pdb\_00003v21  
Title : Crystal structure of Type IIF restriction endonuclease Bse634I with cognate DNA  
Authors : Manakova, E.N.; Grazulis, S.; Golovenko, D.; Tamulaitiene, G.  
Deposited on : 2011-12-11  
Resolution : 2.70 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](mailto: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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

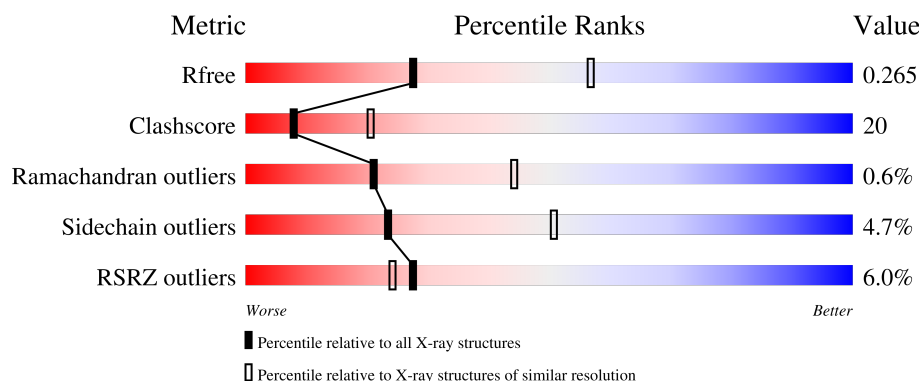
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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  $\geq 3$ , 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	293	<div> <div>3%</div> <div>61%</div> <div>35%</div> <div>...</div> </div>
1	B	293	<div> <div>2%</div> <div>57%</div> <div>40%</div> <div>..</div> </div>
1	C	293	<div> <div>5%</div> <div>62%</div> <div>34%</div> <div>..</div> </div>
1	D	293	<div> <div>8%</div> <div>55%</div> <div>40%</div> <div>..</div> </div>
1	E	293	<div> <div>5%</div> <div>55%</div> <div>39%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	293	
1	G	293	
1	H	293	
2	I	13	
2	J	13	
2	K	13	
2	L	13	
2	M	13	
2	N	13	
2	O	13	
2	P	13	
2	R	13	
2	S	13	
2	V	13	
2	X	13	
2	Y	13	
2	Z	13	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22656 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 Endonuclease Bse634IR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	7	0	0
			2344	1495	404	439	6			
1	B	289	Total	C	N	O	S	2	0	0
			2344	1495	404	439	6			
1	C	288	Total	C	N	O	S	146	0	0
			2336	1491	402	437	6			
1	D	289	Total	C	N	O	S	264	0	0
			2344	1495	404	439	6			
1	E	289	Total	C	N	O	S	267	0	0
			2344	1495	404	439	6			
1	F	287	Total	C	N	O	S	359	0	0
			2328	1485	401	436	6			
1	G	289	Total	C	N	O	S	23	0	0
			2344	1495	404	439	6			
1	H	290	Total	C	N	O	S	11	0	0
			2351	1499	405	441	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	PHE	LEU	SEE REMARK 999	UNP Q8RT53
A	111	ASP	HIS	SEE REMARK 999	UNP Q8RT53
A	130	SER	THR	SEE REMARK 999	UNP Q8RT53
A	226	ALA	ARG	engineered mutation	UNP Q8RT53
B	110	PHE	LEU	SEE REMARK 999	UNP Q8RT53
B	111	ASP	HIS	SEE REMARK 999	UNP Q8RT53
B	130	SER	THR	SEE REMARK 999	UNP Q8RT53
B	226	ALA	ARG	engineered mutation	UNP Q8RT53
C	110	PHE	LEU	SEE REMARK 999	UNP Q8RT53
C	111	ASP	HIS	SEE REMARK 999	UNP Q8RT53
C	130	SER	THR	SEE REMARK 999	UNP Q8RT53
C	226	ALA	ARG	engineered mutation	UNP Q8RT53
D	110	PHE	LEU	SEE REMARK 999	UNP Q8RT53

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Chain	Residue	Modelled	Actual	Comment	Reference
D	111	ASP	HIS	SEE REMARK 999	UNP Q8RT53
D	130	SER	THR	SEE REMARK 999	UNP Q8RT53
D	226	ALA	ARG	engineered mutation	UNP Q8RT53
E	110	PHE	LEU	SEE REMARK 999	UNP Q8RT53
E	111	ASP	HIS	SEE REMARK 999	UNP Q8RT53
E	130	SER	THR	SEE REMARK 999	UNP Q8RT53
E	226	ALA	ARG	engineered mutation	UNP Q8RT53
F	110	PHE	LEU	SEE REMARK 999	UNP Q8RT53
F	111	ASP	HIS	SEE REMARK 999	UNP Q8RT53
F	130	SER	THR	SEE REMARK 999	UNP Q8RT53
F	226	ALA	ARG	engineered mutation	UNP Q8RT53
G	110	PHE	LEU	SEE REMARK 999	UNP Q8RT53
G	111	ASP	HIS	SEE REMARK 999	UNP Q8RT53
G	130	SER	THR	SEE REMARK 999	UNP Q8RT53
G	226	ALA	ARG	engineered mutation	UNP Q8RT53
H	110	PHE	LEU	SEE REMARK 999	UNP Q8RT53
H	111	ASP	HIS	SEE REMARK 999	UNP Q8RT53
H	130	SER	THR	SEE REMARK 999	UNP Q8RT53
H	226	ALA	ARG	engineered mutation	UNP Q8RT53

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	13	Total 263	C 126	N 48	O 77	P 12	0	0	0
2	J	13	Total 263	C 126	N 48	O 77	P 12	9	0	0
2	K	13	Total 263	C 126	N 48	O 77	P 12	21	0	0
2	L	12	Total 243	C 116	N 46	O 70	P 11	0	0	0
2	M	12	Total 243	C 116	N 46	O 70	P 11	82	0	0
2	N	12	Total 243	C 116	N 46	O 70	P 11	17	0	0
2	O	13	Total 263	C 126	N 48	O 77	P 12	0	0	0
2	P	12	Total 243	C 116	N 46	O 70	P 11	0	0	0
2	R	12	Total 243	C 116	N 46	O 70	P 11	81	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	13	Total 263	C 126	N 48	O 77	P 12	62	0	0
2	V	13	Total 263	C 126	N 48	O 77	P 12	0	0	0
2	X	13	Total 263	C 126	N 48	O 77	P 12	0	0	0
2	Y	13	Total 263	C 126	N 48	O 77	P 12	0	0	0
2	Z	12	Total 243	C 116	N 46	O 70	P 11	36	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total 55	O 55	0	0
3	B	44	Total 44	O 44	0	0
3	C	35	Total 35	O 35	0	0
3	D	22	Total 22	O 22	0	0
3	E	36	Total 36	O 36	0	0
3	F	25	Total 25	O 25	0	0
3	G	37	Total 37	O 37	0	0
3	H	50	Total 50	O 50	0	0
3	I	9	Total 9	O 9	0	0
3	J	12	Total 12	O 12	0	0
3	K	1	Total 1	O 1	0	0
3	L	2	Total 2	O 2	0	0
3	M	3	Total 3	O 3	0	0
3	N	1	Total 1	O 1	0	0

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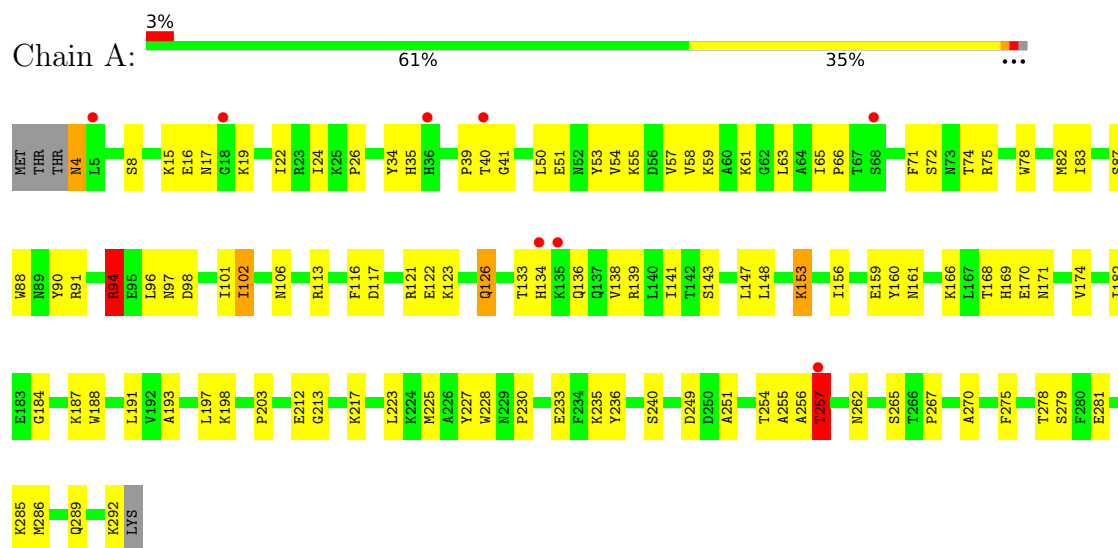
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	6	Total 6	O 6	0	0
3	P	3	Total 3	O 3	0	0
3	R	2	Total 2	O 2	0	0
3	S	5	Total 5	O 5	0	0
3	V	2	Total 2	O 2	0	0
3	X	4	Total 4	O 4	0	0
3	Y	3	Total 3	O 3	0	0
3	Z	2	Total 2	O 2	0	0

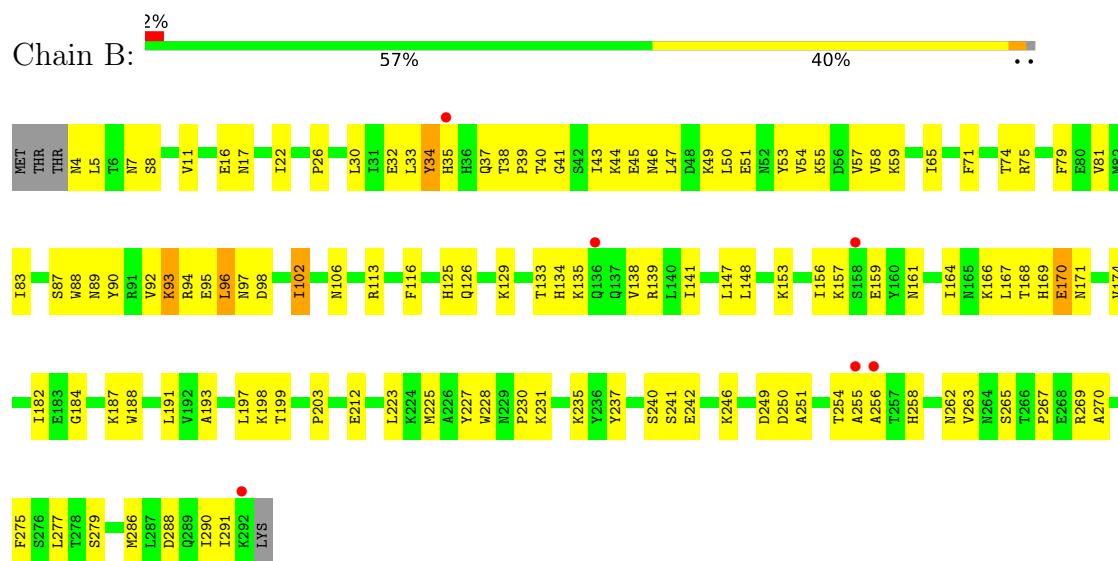
### 3 Residue-property plots [i](#)

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: Endonuclease Bse634IR



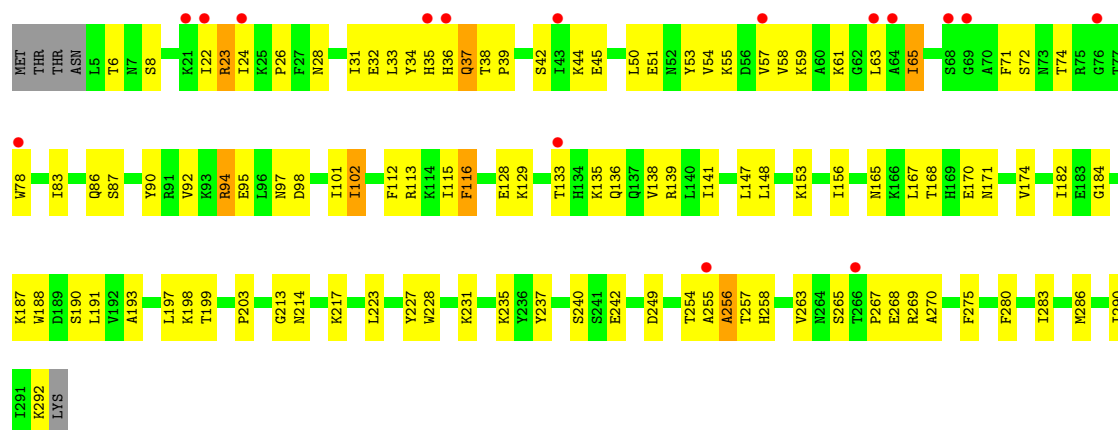
#### • Molecule 1: Endonuclease Bse634IR



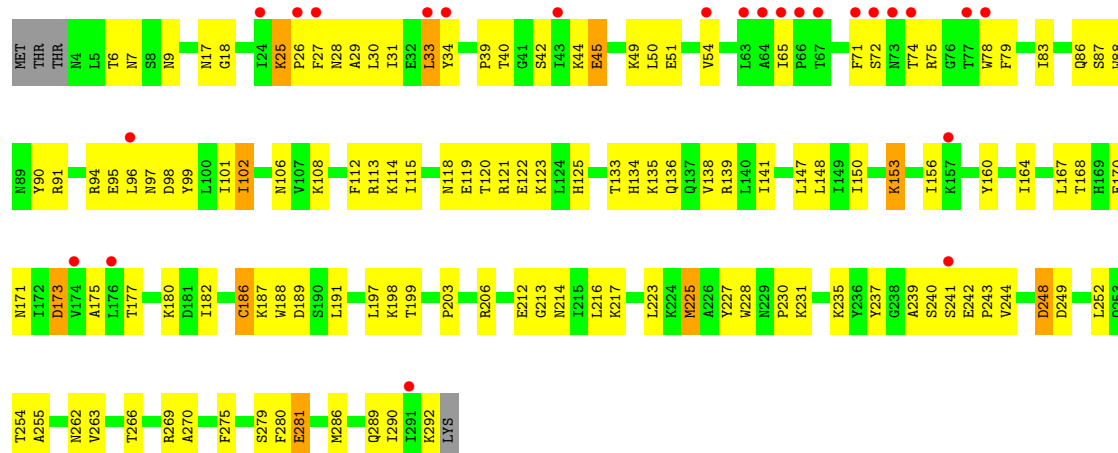
#### • Molecule 1: Endonuclease Bse634IR



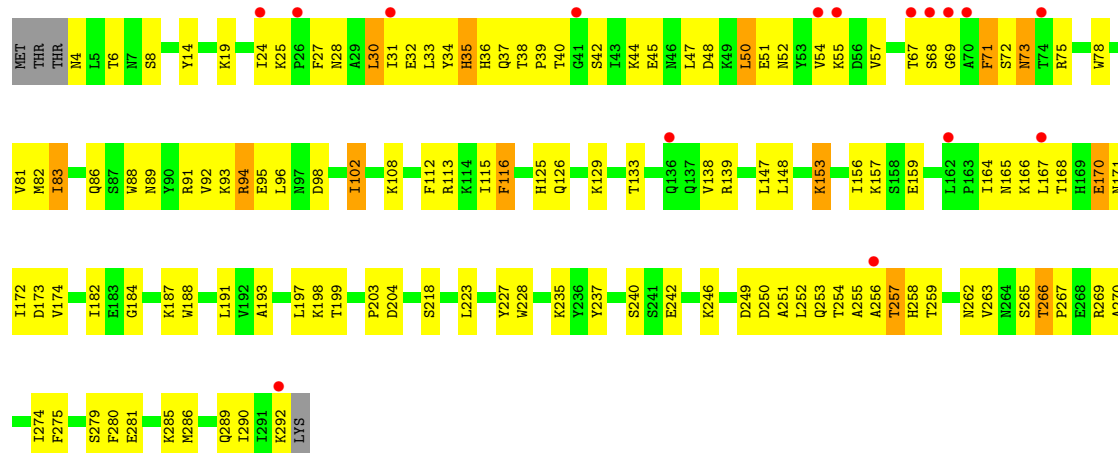




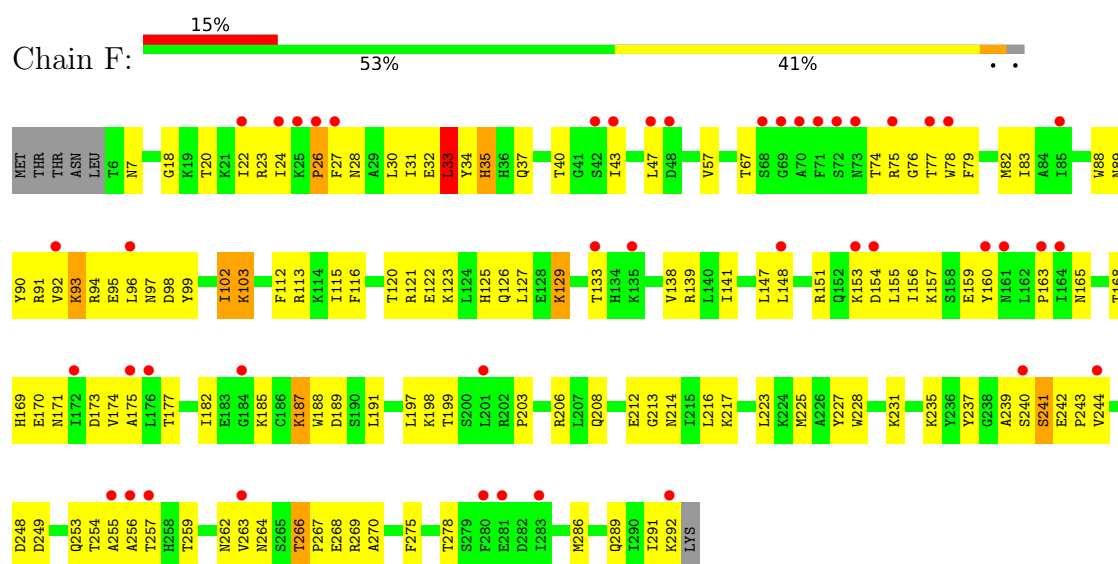
• Molecule 1: Endonuclease Bse634IR



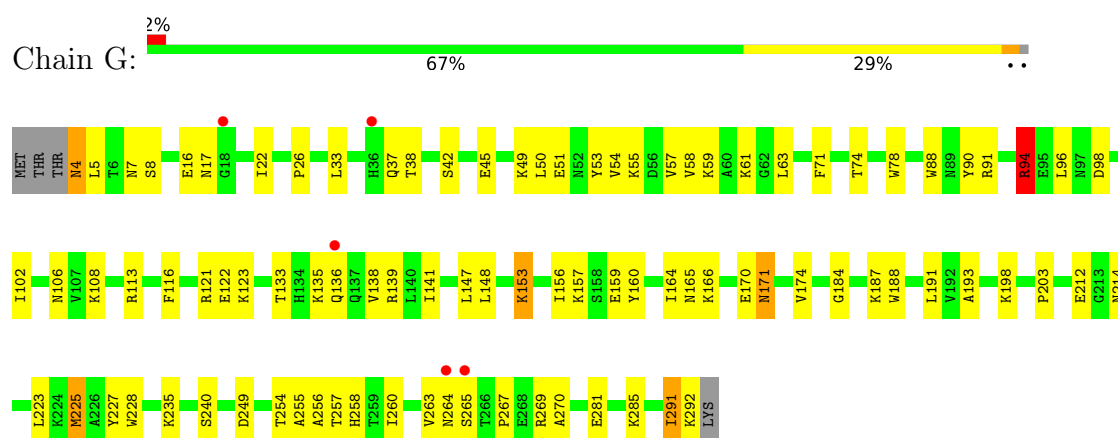
• Molecule 1: Endonuclease Bse634IR



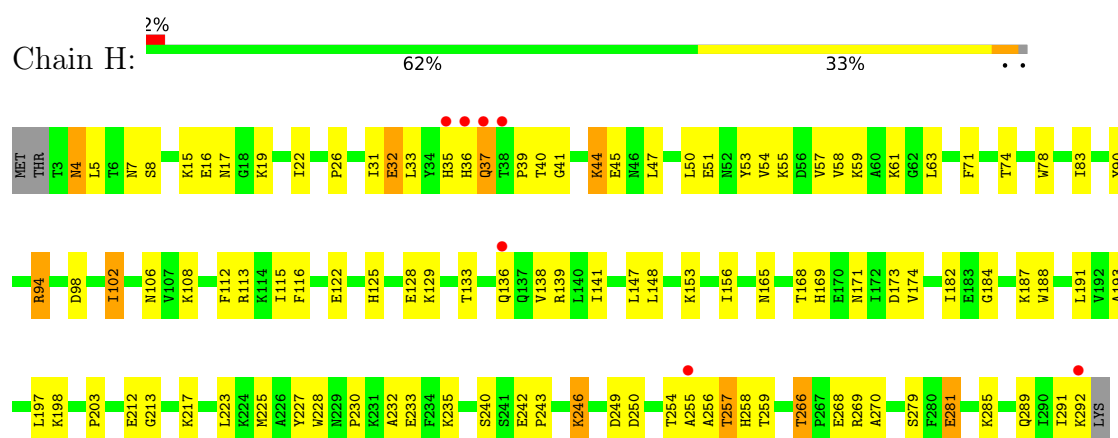
• Molecule 1: Endonuclease Bse634IR



• Molecule 1: Endonuclease Bse634IR



• Molecule 1: Endonuclease Bse634IR



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





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



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



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



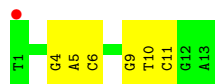
- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')



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



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

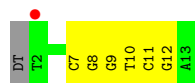


- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

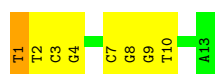
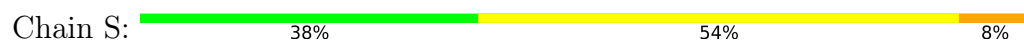




- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')



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



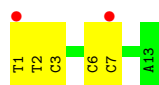
- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')



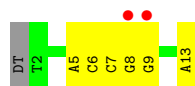
- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.88Å 115.31Å 130.24Å 90.00° 112.50° 90.00°	Depositor
Resolution (Å)	65.09 – 2.70 65.09 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.09-2.70) 100.0 (65.09-2.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.230 , 0.267 0.227 , 0.265	Depositor DCC
$R_{free}$ test set	7973 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.8	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 63.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	22656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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	0.52	0/2389	0.94	8/3228 (0.2%)
1	B	0.52	0/2389	0.96	9/3228 (0.3%)
1	C	0.49	0/2381	0.96	9/3217 (0.3%)
1	D	0.52	0/2389	0.99	13/3228 (0.4%)
1	E	0.46	0/2389	0.97	13/3228 (0.4%)
1	F	0.45	0/2373	0.96	11/3206 (0.3%)
1	G	0.53	0/2389	0.93	7/3228 (0.2%)
1	H	0.54	0/2396	0.95	10/3238 (0.3%)
2	I	0.36	0/294	0.78	0/452
2	J	0.35	0/294	0.78	0/452
2	K	0.35	0/294	0.77	0/452
2	L	0.31	0/272	0.73	0/418
2	M	0.34	0/272	0.80	1/418 (0.2%)
2	N	0.33	0/272	0.75	0/418
2	O	0.37	0/294	0.76	0/452
2	P	0.37	0/272	0.84	1/418 (0.2%)
2	R	0.34	0/272	0.68	0/418
2	S	0.37	0/294	0.82	0/452
2	V	0.33	0/294	0.67	0/452
2	X	0.34	0/294	0.73	0/452
2	Y	0.33	0/294	0.75	0/452
2	Z	0.31	0/272	0.62	0/418
All	All	0.48	0/23079	0.92	82/31925 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	J	0	1
2	M	0	1
2	S	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	3

There are no bond length outliers.

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	THR	N-CA-C	-9.46	100.98	114.12
1	D	18	GLY	N-CA-C	-8.24	103.14	115.00
1	B	291	ILE	N-CA-C	8.16	118.17	110.74
1	D	9	ASN	N-CA-C	-7.29	104.36	113.18
2	P	2	DT	O5'-C5'-C4'	7.29	121.73	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	J	6	DC	Sidechain
2	M	6	DC	Sidechain
2	S	1	DT	Sidechain

## 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	2344	0	2385	95	0
1	B	2344	0	2385	111	0
1	C	2336	0	2379	88	0
1	D	2344	0	2385	112	0
1	E	2344	0	2385	113	0
1	F	2328	0	2368	147	0
1	G	2344	0	2385	83	0
1	H	2351	0	2392	93	0
2	I	263	0	148	7	0
2	J	263	0	148	6	0
2	K	263	0	148	5	0
2	L	243	0	136	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	243	0	136	3	0
2	N	243	0	136	8	0
2	O	263	0	148	6	0
2	P	243	0	136	6	0
2	R	243	0	136	8	0
2	S	263	0	148	9	0
2	V	263	0	148	16	0
2	X	263	0	148	4	0
2	Y	263	0	148	8	0
2	Z	243	0	136	7	0
3	A	55	0	0	3	0
3	B	44	0	0	1	0
3	C	35	0	0	0	0
3	D	22	0	0	0	0
3	E	36	0	0	1	0
3	F	25	0	0	0	0
3	G	37	0	0	2	0
3	H	50	0	0	0	0
3	I	9	0	0	0	0
3	J	12	0	0	0	0
3	K	1	0	0	0	0
3	L	2	0	0	0	0
3	M	3	0	0	0	0
3	N	1	0	0	0	0
3	O	6	0	0	0	0
3	P	3	0	0	0	0
3	R	2	0	0	0	0
3	S	5	0	0	0	0
3	V	2	0	0	0	0
3	X	4	0	0	0	0
3	Y	3	0	0	0	0
3	Z	2	0	0	1	0
All	All	22656	0	21064	798	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 20.

The worst 5 of 798 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:G:138:VAL:CG1	1:H:255:ALA:HB2	1.30	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:ALA:HB2	1:F:138:VAL:CG1	1.56	1.33
1:A:138:VAL:CG1	1:B:255:ALA:HB2	1.60	1.31
1:E:138:VAL:CG1	1:F:255:ALA:HB2	1.66	1.25
1:A:255:ALA:HB2	1:B:138:VAL:CG1	1.72	1.20

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	287/293 (98%)	278 (97%)	8 (3%)	1 (0%)	36	60
1	B	287/293 (98%)	268 (93%)	18 (6%)	1 (0%)	36	60
1	C	286/293 (98%)	267 (93%)	18 (6%)	1 (0%)	36	60
1	D	287/293 (98%)	267 (93%)	20 (7%)	0	100	100
1	E	287/293 (98%)	260 (91%)	24 (8%)	3 (1%)	12	32
1	F	285/293 (97%)	246 (86%)	33 (12%)	6 (2%)	5	15
1	G	287/293 (98%)	275 (96%)	12 (4%)	0	100	100
1	H	288/293 (98%)	278 (96%)	9 (3%)	1 (0%)	36	60
All	All	2294/2344 (98%)	2139 (93%)	142 (6%)	13 (1%)	21	44

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	257	THR
1	H	257	THR
1	A	257	THR
1	F	57	VAL
1	B	97	ASN

### 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	263/267 (98%)	250 (95%)	13 (5%)	22	49
1	B	263/267 (98%)	252 (96%)	11 (4%)	26	55
1	C	262/267 (98%)	256 (98%)	6 (2%)	44	73
1	D	263/267 (98%)	251 (95%)	12 (5%)	24	51
1	E	263/267 (98%)	244 (93%)	19 (7%)	13	32
1	F	261/267 (98%)	248 (95%)	13 (5%)	22	48
1	G	263/267 (98%)	253 (96%)	10 (4%)	29	58
1	H	264/267 (99%)	250 (95%)	14 (5%)	20	46
All	All	2102/2136 (98%)	2004 (95%)	98 (5%)	23	51

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	246	LYS
1	F	173	ASP
1	E	266	THR
1	F	40	THR
1	G	22	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	165	ASN
1	H	214	ASN
1	G	171	ASN
1	H	7	ASN
1	D	28	ASN

### 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 [i](#)

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 ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	289/293 (98%)	0.33	8 (2%) 55 51	23, 40, 60, 76	2 (0%)
1	B	289/293 (98%)	0.37	6 (2%) 63 61	23, 45, 63, 79	1 (0%)
1	C	272/293 (92%)	0.58	16 (5%) 28 25	19, 47, 80, 89	5 (1%)
1	D	257/293 (87%)	0.82	24 (9%) 14 12	26, 56, 87, 98	3 (1%)
1	E	258/293 (88%)	0.61	16 (6%) 26 23	27, 52, 82, 90	8 (3%)
1	F	245/293 (83%)	1.17	45 (18%) 3 3	32, 61, 90, 94	9 (3%)
1	G	289/293 (98%)	0.31	5 (1%) 69 67	20, 41, 58, 66	7 (2%)
1	H	290/293 (98%)	0.20	7 (2%) 59 56	20, 39, 58, 82	4 (1%)
2	I	13/13 (100%)	-0.03	1 (7%) 19 17	28, 37, 61, 81	0
2	J	13/13 (100%)	-0.08	0 100 100	30, 41, 54, 66	1 (7%)
2	K	12/13 (92%)	0.75	0 100 100	47, 66, 83, 87	1 (8%)
2	L	12/13 (92%)	0.76	0 100 100	52, 69, 78, 84	0
2	M	8/13 (61%)	1.30	1 (12%) 8 7	55, 61, 73, 88	0
2	N	11/13 (84%)	1.68	4 (36%) 1 0	60, 81, 88, 89	0
2	O	13/13 (100%)	0.06	1 (7%) 19 17	27, 37, 79, 99	0
2	P	12/13 (92%)	-0.11	0 100 100	26, 39, 50, 51	0
2	R	8/13 (61%)	1.04	1 (12%) 8 7	54, 58, 82, 99	0
2	S	10/13 (76%)	0.69	0 100 100	45, 53, 86, 97	0
2	V	13/13 (100%)	1.81	3 (23%) 2 2	80, 95, 100, 100	0
2	X	13/13 (100%)	0.98	0 100 100	55, 67, 86, 87	0
2	Y	13/13 (100%)	1.21	2 (15%) 5 4	41, 69, 82, 84	0
2	Z	10/13 (76%)	1.53	2 (20%) 3 2	68, 88, 98, 100	0
All	All	2350/2526 (93%)	0.55	142 (6%) 27 24	19, 47, 83, 100	41 (1%)

The worst 5 of 142 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	69	GLY	6.0
1	D	66	PRO	4.7
1	D	27	PHE	4.7
1	F	70	ALA	4.6
1	F	24	ILE	4.5

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.