Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2022 – 01:12 am BST

PDB ID	:	8AES
Title	:	Crystal structure of a thermophilic O6-alkylguanine-DNA alkyltransferase-derived self-labeling protein-tag
Authors	:	Genta, M.; Perugino, G.; Miggiano, R.
Deposited on	:	2022-07-13
Resolution	:	2.80 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

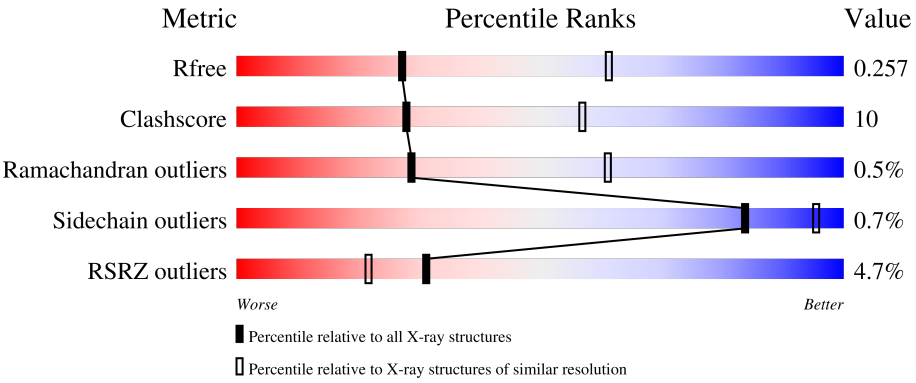
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	168	2% 73% 18% 9%
1	B	168	2% 70% 20% • 10%
1	C	168	7% 73% 17% • 10%
1	D	168	% 73% 17% • 10%
1	E	168	2% 69% 21% • 10%

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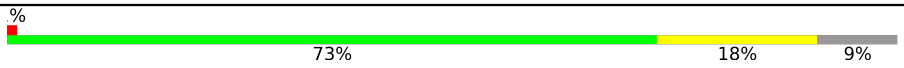
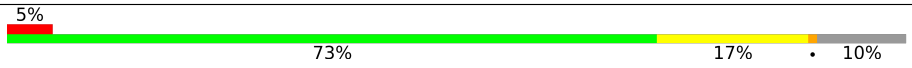
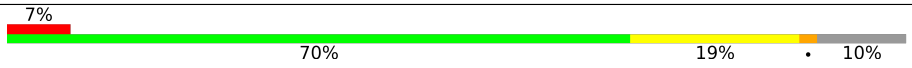
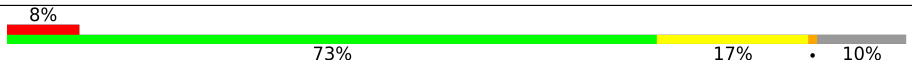
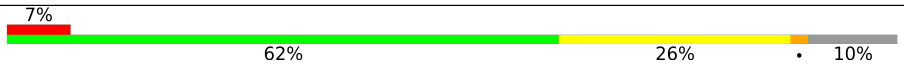
Mol	Chain	Length	Quality of chain
1	F	168	
1	G	168	
1	H	168	
1	I	168	
1	J	168	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12137 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 Methylated-DNA--protein-cysteine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1215	795	196	217	7			
1	B	152	Total	C	N	O	S	0	0	0
			1207	789	195	216	7			
1	C	152	Total	C	N	O	S	0	0	0
			1207	789	195	216	7			
1	D	152	Total	C	N	O	S	0	0	0
			1207	789	195	216	7			
1	E	152	Total	C	N	O	S	0	0	0
			1207	789	195	216	7			
1	F	153	Total	C	N	O	S	0	0	0
			1215	795	196	217	7			
1	G	152	Total	C	N	O	S	0	0	0
			1207	789	195	216	7			
1	H	152	Total	C	N	O	S	0	0	0
			1207	789	195	216	7			
1	I	152	Total	C	N	O	S	0	0	0
			1207	789	195	216	7			
1	J	152	Total	C	N	O	S	0	0	0
			1207	789	195	216	7			

There are 250 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP Q97VW7
A	-9	ALA	-	expression tag	UNP Q97VW7
A	-8	HIS	-	expression tag	UNP Q97VW7
A	-7	HIS	-	expression tag	UNP Q97VW7
A	-6	HIS	-	expression tag	UNP Q97VW7
A	-5	HIS	-	expression tag	UNP Q97VW7
A	-4	HIS	-	expression tag	UNP Q97VW7
A	-3	HIS	-	expression tag	UNP Q97VW7
A	-2	THR	-	expression tag	UNP Q97VW7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	expression tag	UNP Q97VW7
A	0	PRO	-	expression tag	UNP Q97VW7
A	100	ALA	SER	engineered mutation	UNP Q97VW7
A	102	ALA	ARG	engineered mutation	UNP Q97VW7
A	105	ASN	GLY	engineered mutation	UNP Q97VW7
A	106	THR	MET	engineered mutation	UNP Q97VW7
A	109	ASP	SER	engineered mutation	UNP Q97VW7
A	110	GLU	LYS	engineered mutation	UNP Q97VW7
A	130	PRO	GLY	engineered mutation	UNP Q97VW7
A	132	LEU	SER	engineered mutation	UNP Q97VW7
A	152	LEU	-	expression tag	UNP Q97VW7
A	153	GLN	-	expression tag	UNP Q97VW7
A	154	VAL	-	expression tag	UNP Q97VW7
A	155	PRO	-	expression tag	UNP Q97VW7
A	156	SER	-	expression tag	UNP Q97VW7
A	157	THR	-	expression tag	UNP Q97VW7
B	-10	MET	-	initiating methionine	UNP Q97VW7
B	-9	ALA	-	expression tag	UNP Q97VW7
B	-8	HIS	-	expression tag	UNP Q97VW7
B	-7	HIS	-	expression tag	UNP Q97VW7
B	-6	HIS	-	expression tag	UNP Q97VW7
B	-5	HIS	-	expression tag	UNP Q97VW7
B	-4	HIS	-	expression tag	UNP Q97VW7
B	-3	HIS	-	expression tag	UNP Q97VW7
B	-2	THR	-	expression tag	UNP Q97VW7
B	-1	ASP	-	expression tag	UNP Q97VW7
B	0	PRO	-	expression tag	UNP Q97VW7
B	100	ALA	SER	engineered mutation	UNP Q97VW7
B	102	ALA	ARG	engineered mutation	UNP Q97VW7
B	105	ASN	GLY	engineered mutation	UNP Q97VW7
B	106	THR	MET	engineered mutation	UNP Q97VW7
B	109	ASP	SER	engineered mutation	UNP Q97VW7
B	110	GLU	LYS	engineered mutation	UNP Q97VW7
B	130	PRO	GLY	engineered mutation	UNP Q97VW7
B	132	LEU	SER	engineered mutation	UNP Q97VW7
B	152	LEU	-	expression tag	UNP Q97VW7
B	153	GLN	-	expression tag	UNP Q97VW7
B	154	VAL	-	expression tag	UNP Q97VW7
B	155	PRO	-	expression tag	UNP Q97VW7
B	156	SER	-	expression tag	UNP Q97VW7
B	157	THR	-	expression tag	UNP Q97VW7
C	-10	MET	-	initiating methionine	UNP Q97VW7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	ALA	-	expression tag	UNP Q97VW7
C	-8	HIS	-	expression tag	UNP Q97VW7
C	-7	HIS	-	expression tag	UNP Q97VW7
C	-6	HIS	-	expression tag	UNP Q97VW7
C	-5	HIS	-	expression tag	UNP Q97VW7
C	-4	HIS	-	expression tag	UNP Q97VW7
C	-3	HIS	-	expression tag	UNP Q97VW7
C	-2	THR	-	expression tag	UNP Q97VW7
C	-1	ASP	-	expression tag	UNP Q97VW7
C	0	PRO	-	expression tag	UNP Q97VW7
C	100	ALA	SER	engineered mutation	UNP Q97VW7
C	102	ALA	ARG	engineered mutation	UNP Q97VW7
C	105	ASN	GLY	engineered mutation	UNP Q97VW7
C	106	THR	MET	engineered mutation	UNP Q97VW7
C	109	ASP	SER	engineered mutation	UNP Q97VW7
C	110	GLU	LYS	engineered mutation	UNP Q97VW7
C	130	PRO	GLY	engineered mutation	UNP Q97VW7
C	132	LEU	SER	engineered mutation	UNP Q97VW7
C	152	LEU	-	expression tag	UNP Q97VW7
C	153	GLN	-	expression tag	UNP Q97VW7
C	154	VAL	-	expression tag	UNP Q97VW7
C	155	PRO	-	expression tag	UNP Q97VW7
C	156	SER	-	expression tag	UNP Q97VW7
C	157	THR	-	expression tag	UNP Q97VW7
D	-10	MET	-	initiating methionine	UNP Q97VW7
D	-9	ALA	-	expression tag	UNP Q97VW7
D	-8	HIS	-	expression tag	UNP Q97VW7
D	-7	HIS	-	expression tag	UNP Q97VW7
D	-6	HIS	-	expression tag	UNP Q97VW7
D	-5	HIS	-	expression tag	UNP Q97VW7
D	-4	HIS	-	expression tag	UNP Q97VW7
D	-3	HIS	-	expression tag	UNP Q97VW7
D	-2	THR	-	expression tag	UNP Q97VW7
D	-1	ASP	-	expression tag	UNP Q97VW7
D	0	PRO	-	expression tag	UNP Q97VW7
D	100	ALA	SER	engineered mutation	UNP Q97VW7
D	102	ALA	ARG	engineered mutation	UNP Q97VW7
D	105	ASN	GLY	engineered mutation	UNP Q97VW7
D	106	THR	MET	engineered mutation	UNP Q97VW7
D	109	ASP	SER	engineered mutation	UNP Q97VW7
D	110	GLU	LYS	engineered mutation	UNP Q97VW7
D	130	PRO	GLY	engineered mutation	UNP Q97VW7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	132	LEU	SER	engineered mutation	UNP Q97VW7
D	152	LEU	-	expression tag	UNP Q97VW7
D	153	GLN	-	expression tag	UNP Q97VW7
D	154	VAL	-	expression tag	UNP Q97VW7
D	155	PRO	-	expression tag	UNP Q97VW7
D	156	SER	-	expression tag	UNP Q97VW7
D	157	THR	-	expression tag	UNP Q97VW7
E	-10	MET	-	initiating methionine	UNP Q97VW7
E	-9	ALA	-	expression tag	UNP Q97VW7
E	-8	HIS	-	expression tag	UNP Q97VW7
E	-7	HIS	-	expression tag	UNP Q97VW7
E	-6	HIS	-	expression tag	UNP Q97VW7
E	-5	HIS	-	expression tag	UNP Q97VW7
E	-4	HIS	-	expression tag	UNP Q97VW7
E	-3	HIS	-	expression tag	UNP Q97VW7
E	-2	THR	-	expression tag	UNP Q97VW7
E	-1	ASP	-	expression tag	UNP Q97VW7
E	0	PRO	-	expression tag	UNP Q97VW7
E	100	ALA	SER	engineered mutation	UNP Q97VW7
E	102	ALA	ARG	engineered mutation	UNP Q97VW7
E	105	ASN	GLY	engineered mutation	UNP Q97VW7
E	106	THR	MET	engineered mutation	UNP Q97VW7
E	109	ASP	SER	engineered mutation	UNP Q97VW7
E	110	GLU	LYS	engineered mutation	UNP Q97VW7
E	130	PRO	GLY	engineered mutation	UNP Q97VW7
E	132	LEU	SER	engineered mutation	UNP Q97VW7
E	152	LEU	-	expression tag	UNP Q97VW7
E	153	GLN	-	expression tag	UNP Q97VW7
E	154	VAL	-	expression tag	UNP Q97VW7
E	155	PRO	-	expression tag	UNP Q97VW7
E	156	SER	-	expression tag	UNP Q97VW7
E	157	THR	-	expression tag	UNP Q97VW7
F	-10	MET	-	initiating methionine	UNP Q97VW7
F	-9	ALA	-	expression tag	UNP Q97VW7
F	-8	HIS	-	expression tag	UNP Q97VW7
F	-7	HIS	-	expression tag	UNP Q97VW7
F	-6	HIS	-	expression tag	UNP Q97VW7
F	-5	HIS	-	expression tag	UNP Q97VW7
F	-4	HIS	-	expression tag	UNP Q97VW7
F	-3	HIS	-	expression tag	UNP Q97VW7
F	-2	THR	-	expression tag	UNP Q97VW7
F	-1	ASP	-	expression tag	UNP Q97VW7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	PRO	-	expression tag	UNP Q97VW7
F	100	ALA	SER	engineered mutation	UNP Q97VW7
F	102	ALA	ARG	engineered mutation	UNP Q97VW7
F	105	ASN	GLY	engineered mutation	UNP Q97VW7
F	106	THR	MET	engineered mutation	UNP Q97VW7
F	109	ASP	SER	engineered mutation	UNP Q97VW7
F	110	GLU	LYS	engineered mutation	UNP Q97VW7
F	130	PRO	GLY	engineered mutation	UNP Q97VW7
F	132	LEU	SER	engineered mutation	UNP Q97VW7
F	152	LEU	-	expression tag	UNP Q97VW7
F	153	GLN	-	expression tag	UNP Q97VW7
F	154	VAL	-	expression tag	UNP Q97VW7
F	155	PRO	-	expression tag	UNP Q97VW7
F	156	SER	-	expression tag	UNP Q97VW7
F	157	THR	-	expression tag	UNP Q97VW7
G	-10	MET	-	initiating methionine	UNP Q97VW7
G	-9	ALA	-	expression tag	UNP Q97VW7
G	-8	HIS	-	expression tag	UNP Q97VW7
G	-7	HIS	-	expression tag	UNP Q97VW7
G	-6	HIS	-	expression tag	UNP Q97VW7
G	-5	HIS	-	expression tag	UNP Q97VW7
G	-4	HIS	-	expression tag	UNP Q97VW7
G	-3	HIS	-	expression tag	UNP Q97VW7
G	-2	THR	-	expression tag	UNP Q97VW7
G	-1	ASP	-	expression tag	UNP Q97VW7
G	0	PRO	-	expression tag	UNP Q97VW7
G	100	ALA	SER	engineered mutation	UNP Q97VW7
G	102	ALA	ARG	engineered mutation	UNP Q97VW7
G	105	ASN	GLY	engineered mutation	UNP Q97VW7
G	106	THR	MET	engineered mutation	UNP Q97VW7
G	109	ASP	SER	engineered mutation	UNP Q97VW7
G	110	GLU	LYS	engineered mutation	UNP Q97VW7
G	130	PRO	GLY	engineered mutation	UNP Q97VW7
G	132	LEU	SER	engineered mutation	UNP Q97VW7
G	152	LEU	-	expression tag	UNP Q97VW7
G	153	GLN	-	expression tag	UNP Q97VW7
G	154	VAL	-	expression tag	UNP Q97VW7
G	155	PRO	-	expression tag	UNP Q97VW7
G	156	SER	-	expression tag	UNP Q97VW7
G	157	THR	-	expression tag	UNP Q97VW7
H	-10	MET	-	initiating methionine	UNP Q97VW7
H	-9	ALA	-	expression tag	UNP Q97VW7

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-8	HIS	-	expression tag	UNP Q97VW7
H	-7	HIS	-	expression tag	UNP Q97VW7
H	-6	HIS	-	expression tag	UNP Q97VW7
H	-5	HIS	-	expression tag	UNP Q97VW7
H	-4	HIS	-	expression tag	UNP Q97VW7
H	-3	HIS	-	expression tag	UNP Q97VW7
H	-2	THR	-	expression tag	UNP Q97VW7
H	-1	ASP	-	expression tag	UNP Q97VW7
H	0	PRO	-	expression tag	UNP Q97VW7
H	100	ALA	SER	engineered mutation	UNP Q97VW7
H	102	ALA	ARG	engineered mutation	UNP Q97VW7
H	105	ASN	GLY	engineered mutation	UNP Q97VW7
H	106	THR	MET	engineered mutation	UNP Q97VW7
H	109	ASP	SER	engineered mutation	UNP Q97VW7
H	110	GLU	LYS	engineered mutation	UNP Q97VW7
H	130	PRO	GLY	engineered mutation	UNP Q97VW7
H	132	LEU	SER	engineered mutation	UNP Q97VW7
H	152	LEU	-	expression tag	UNP Q97VW7
H	153	GLN	-	expression tag	UNP Q97VW7
H	154	VAL	-	expression tag	UNP Q97VW7
H	155	PRO	-	expression tag	UNP Q97VW7
H	156	SER	-	expression tag	UNP Q97VW7
H	157	THR	-	expression tag	UNP Q97VW7
I	-10	MET	-	initiating methionine	UNP Q97VW7
I	-9	ALA	-	expression tag	UNP Q97VW7
I	-8	HIS	-	expression tag	UNP Q97VW7
I	-7	HIS	-	expression tag	UNP Q97VW7
I	-6	HIS	-	expression tag	UNP Q97VW7
I	-5	HIS	-	expression tag	UNP Q97VW7
I	-4	HIS	-	expression tag	UNP Q97VW7
I	-3	HIS	-	expression tag	UNP Q97VW7
I	-2	THR	-	expression tag	UNP Q97VW7
I	-1	ASP	-	expression tag	UNP Q97VW7
I	0	PRO	-	expression tag	UNP Q97VW7
I	100	ALA	SER	engineered mutation	UNP Q97VW7
I	102	ALA	ARG	engineered mutation	UNP Q97VW7
I	105	ASN	GLY	engineered mutation	UNP Q97VW7
I	106	THR	MET	engineered mutation	UNP Q97VW7
I	109	ASP	SER	engineered mutation	UNP Q97VW7
I	110	GLU	LYS	engineered mutation	UNP Q97VW7
I	130	PRO	GLY	engineered mutation	UNP Q97VW7
I	132	LEU	SER	engineered mutation	UNP Q97VW7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	152	LEU	-	expression tag	UNP Q97VW7
I	153	GLN	-	expression tag	UNP Q97VW7
I	154	VAL	-	expression tag	UNP Q97VW7
I	155	PRO	-	expression tag	UNP Q97VW7
I	156	SER	-	expression tag	UNP Q97VW7
I	157	THR	-	expression tag	UNP Q97VW7
J	-10	MET	-	initiating methionine	UNP Q97VW7
J	-9	ALA	-	expression tag	UNP Q97VW7
J	-8	HIS	-	expression tag	UNP Q97VW7
J	-7	HIS	-	expression tag	UNP Q97VW7
J	-6	HIS	-	expression tag	UNP Q97VW7
J	-5	HIS	-	expression tag	UNP Q97VW7
J	-4	HIS	-	expression tag	UNP Q97VW7
J	-3	HIS	-	expression tag	UNP Q97VW7
J	-2	THR	-	expression tag	UNP Q97VW7
J	-1	ASP	-	expression tag	UNP Q97VW7
J	0	PRO	-	expression tag	UNP Q97VW7
J	100	ALA	SER	engineered mutation	UNP Q97VW7
J	102	ALA	ARG	engineered mutation	UNP Q97VW7
J	105	ASN	GLY	engineered mutation	UNP Q97VW7
J	106	THR	MET	engineered mutation	UNP Q97VW7
J	109	ASP	SER	engineered mutation	UNP Q97VW7
J	110	GLU	LYS	engineered mutation	UNP Q97VW7
J	130	PRO	GLY	engineered mutation	UNP Q97VW7
J	132	LEU	SER	engineered mutation	UNP Q97VW7
J	152	LEU	-	expression tag	UNP Q97VW7
J	153	GLN	-	expression tag	UNP Q97VW7
J	154	VAL	-	expression tag	UNP Q97VW7
J	155	PRO	-	expression tag	UNP Q97VW7
J	156	SER	-	expression tag	UNP Q97VW7
J	157	THR	-	expression tag	UNP Q97VW7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	10	Total O 10 10	0	0
2	B	8	Total O 8 8	0	0
2	C	6	Total O 6 6	0	0
2	D	5	Total O 5 5	0	0

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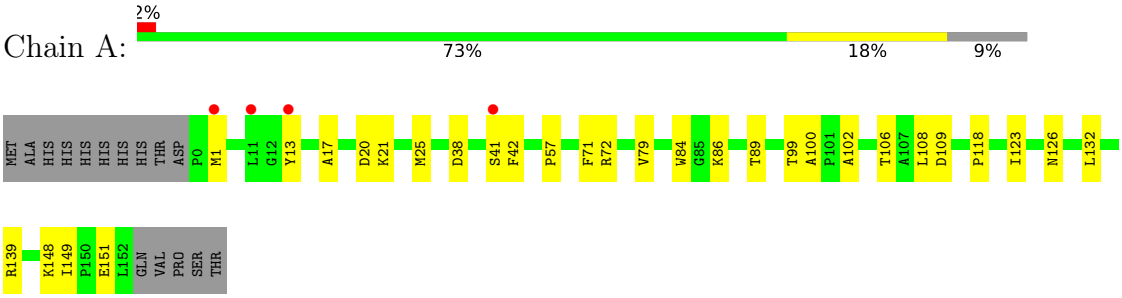
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	6	Total O 6 6	0	0
2	F	9	Total O 9 9	0	0
2	G	3	Total O 3 3	0	0
2	H	3	Total O 3 3	0	0
2	J	1	Total O 1 1	0	0

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.

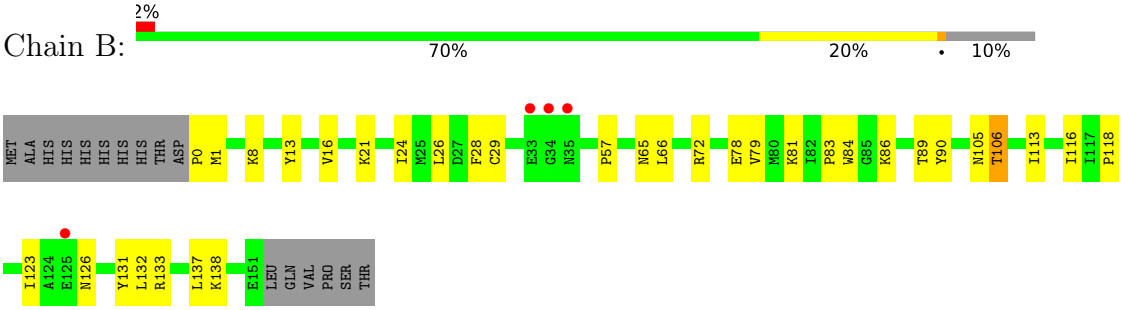
• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

Chain A:



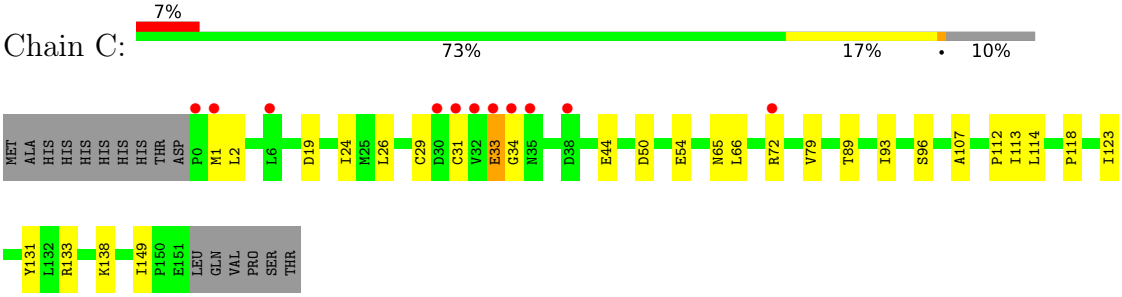
• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

Chain B:



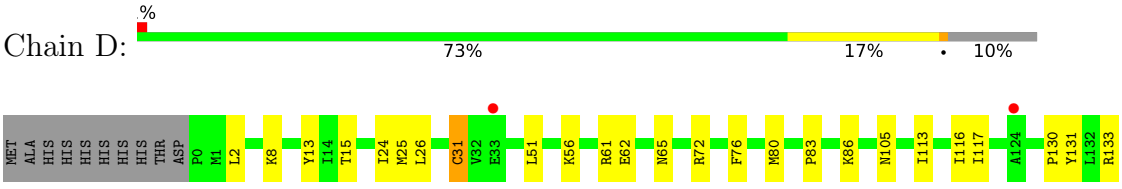
• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

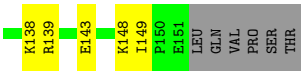
Chain C:



• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

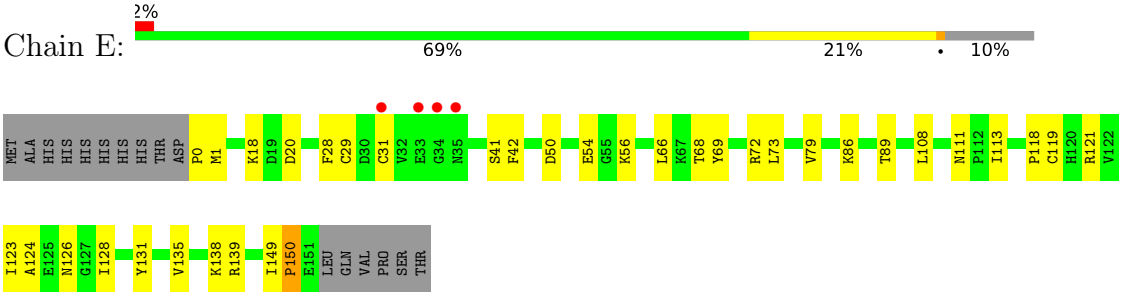
Chain D:





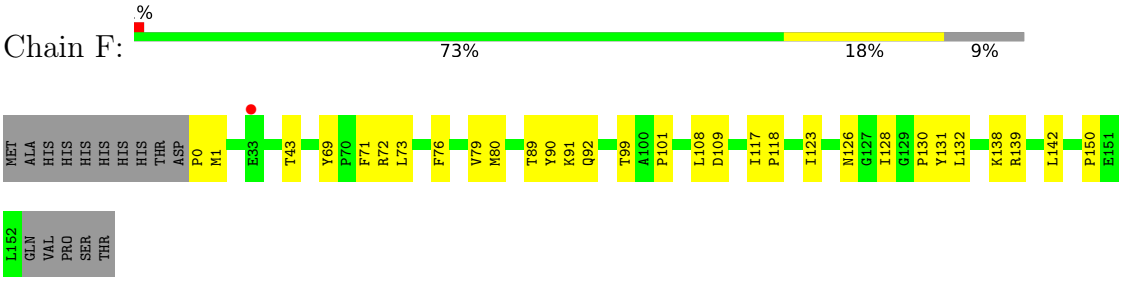
• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

Chain E:



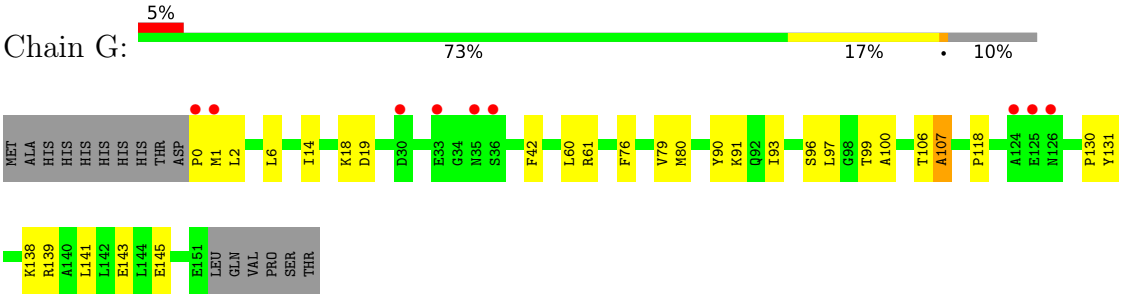
• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

Chain F:



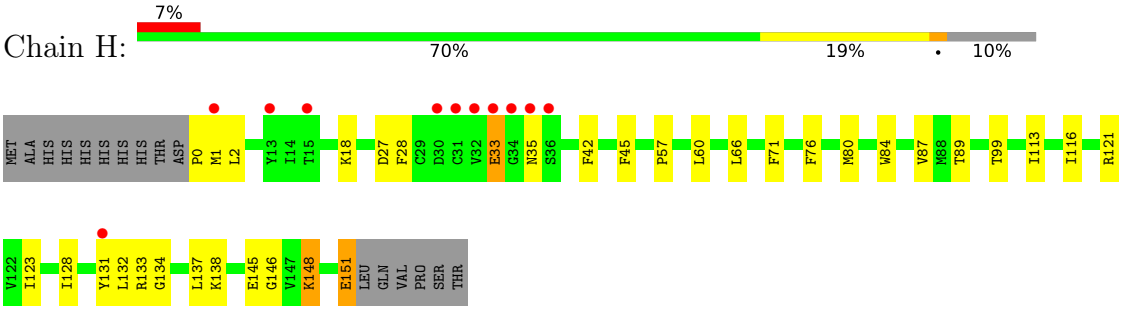
• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

Chain G:



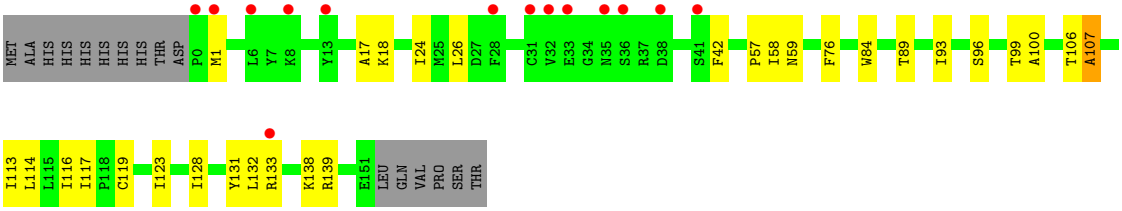
• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

Chain H:

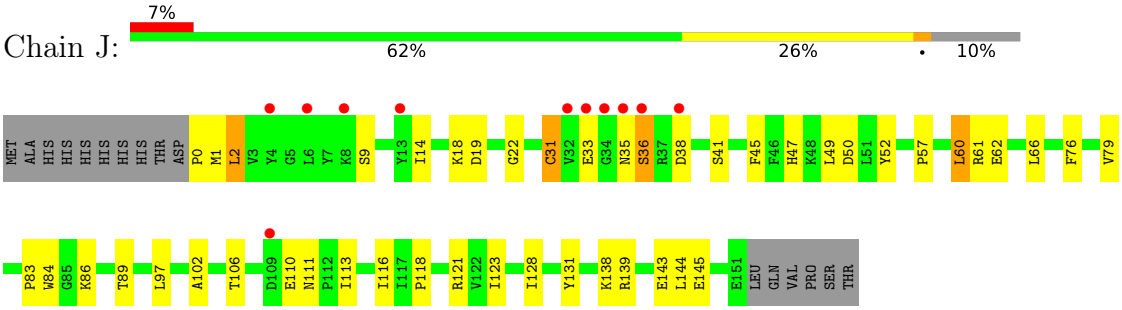


• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

Chain I:



• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.83Å 119.44Å 180.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.38 – 2.80 47.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.38-2.80) 98.0 (47.38-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.196 , 0.253 0.211 , 0.257	Depositor DCC
R_{free} test set	2643 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	56.6	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12137	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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

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	0.51	0/1244	0.69	0/1683
1	B	0.51	0/1236	0.66	0/1672
1	C	0.46	0/1236	0.67	0/1672
1	D	0.47	0/1236	0.66	0/1672
1	E	0.47	0/1236	0.61	0/1672
1	F	0.47	0/1244	0.65	0/1683
1	G	0.45	0/1236	0.65	0/1672
1	H	0.45	0/1236	0.65	0/1672
1	I	0.47	0/1236	0.68	0/1672
1	J	0.48	0/1236	0.68	3/1672 (0.2%)
All	All	0.47	0/12376	0.66	3/16742 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	31	CYS	CB-CA-C	7.10	124.61	110.40
1	J	111	ASN	N-CA-C	-5.25	96.81	111.00
1	J	2	LEU	CA-CB-CG	5.21	127.29	115.30

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	1215	0	1250	29	0
1	B	1207	0	1239	23	0
1	C	1207	0	1239	22	0
1	D	1207	0	1239	20	0
1	E	1207	0	1239	22	0
1	F	1215	0	1250	22	0
1	G	1207	0	1239	20	0
1	H	1207	0	1239	41	0
1	I	1207	0	1239	23	0
1	J	1207	0	1239	35	0
2	A	10	0	0	0	0
2	B	8	0	0	1	0
2	C	6	0	0	2	0
2	D	5	0	0	0	0
2	E	6	0	0	0	0
2	F	9	0	0	1	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	J	1	0	0	0	0
All	All	12137	0	12412	243	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 10.

All (243) 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:J:31:CYS:O	1:J:33:GLU:HG2	1.40	1.19
1:I:99:THR:HG22	1:I:100:ALA:H	1.06	1.18
1:A:99:THR:CG2	1:A:100:ALA:H	1.58	1.16
1:A:99:THR:HG22	1:A:100:ALA:N	1.55	1.14
1:A:99:THR:HG22	1:A:100:ALA:H	1.05	1.12
1:H:131:TYR:CE2	1:H:133:ARG:HB2	1.84	1.11
1:H:131:TYR:CE2	1:H:133:ARG:CB	2.36	1.07
1:I:99:THR:HG22	1:I:100:ALA:N	1.69	1.04
1:I:99:THR:CG2	1:I:100:ALA:H	1.72	1.01
1:G:1:MET:HG3	1:G:19:ASP:HB2	1.43	1.00
1:H:132:LEU:HD21	1:H:133:ARG:HH11	1.26	0.97
1:H:87:VAL:CG1	1:H:123:ILE:HG12	1.98	0.94
1:H:131:TYR:OH	1:H:137:LEU:HD23	1.69	0.92
1:H:131:TYR:CZ	1:H:133:ARG:HB2	2.07	0.90
1:J:31:CYS:O	1:J:33:GLU:CG	2.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:76:PHE:HZ	1:J:110:GLU:O	1.62	0.82
1:H:71:PHE:CE1	1:H:99:THR:HG21	2.15	0.81
1:H:131:TYR:CE2	1:H:133:ARG:HB3	2.16	0.80
1:H:131:TYR:HE2	1:H:133:ARG:HB3	1.47	0.79
1:B:105:ASN:O	1:B:106:THR:OG1	2.02	0.78
1:D:61:ARG:HD2	1:G:61:ARG:HG2	1.64	0.78
1:C:72:ARG:HH22	1:H:148:LYS:HZ3	1.33	0.77
1:H:131:TYR:CZ	1:H:137:LEU:HD23	2.21	0.76
1:I:132:LEU:HD23	1:I:133:ARG:NH1	2.03	0.73
1:A:79:VAL:HG12	1:A:118:PRO:HD2	1.69	0.73
1:F:43:THR:N	2:F:201:HOH:O	2.22	0.73
1:H:131:TYR:HD2	1:H:134:GLY:O	1.73	0.72
1:H:131:TYR:CD2	1:H:134:GLY:O	2.42	0.72
1:J:52:TYR:CZ	1:J:144:LEU:HD23	2.25	0.71
1:H:131:TYR:OH	1:H:137:LEU:CD2	2.41	0.69
1:I:18:LYS:HG2	1:I:42:PHE:HE1	1.57	0.69
1:G:79:VAL:HG12	1:G:118:PRO:HD2	1.74	0.69
1:B:131:TYR:HB2	1:B:138:LYS:HD2	1.75	0.69
1:D:139:ARG:O	1:D:143:GLU:HG3	1.93	0.68
1:H:71:PHE:HE1	1:H:99:THR:HG21	1.58	0.68
1:J:52:TYR:CE2	1:J:144:LEU:CD2	2.75	0.68
1:E:139:ARG:NH1	1:E:149:ILE:O	2.28	0.67
1:B:132:LEU:HD21	1:B:133:ARG:HH11	1.60	0.67
1:A:1:MET:O	1:A:1:MET:HG3	1.92	0.67
1:F:71:PHE:HE1	1:F:99:THR:HG21	1.59	0.67
1:B:83:PRO:HD2	1:B:86:LYS:HD3	1.77	0.67
1:J:128:ILE:HD13	1:J:139:ARG:HG2	1.77	0.67
1:F:89:THR:OG1	1:F:92:GLN:HG3	1.96	0.66
1:D:133:ARG:HG2	1:D:133:ARG:HH11	1.60	0.66
1:B:0:PRO:O	1:B:1:MET:HG3	1.97	0.64
1:E:18:LYS:HD3	1:E:42:PHE:CE1	2.33	0.63
1:J:52:TYR:CE2	1:J:144:LEU:HD23	2.33	0.63
1:D:61:ARG:NH2	1:D:80:MET:O	2.32	0.62
1:F:71:PHE:CE1	1:F:99:THR:HG21	2.33	0.62
1:H:87:VAL:HG11	1:H:123:ILE:HG12	1.78	0.62
1:A:106:THR:HG21	1:F:150:PRO:HD3	1.82	0.61
1:A:151:GLU:OE2	1:D:139:ARG:NH2	2.33	0.61
1:B:24:ILE:O	1:B:24:ILE:HG22	1.99	0.61
1:A:79:VAL:HG21	1:A:108:LEU:HD21	1.83	0.61
1:E:79:VAL:HG21	1:E:108:LEU:HD21	1.83	0.61
1:A:139:ARG:NH1	1:A:149:ILE:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:132:LEU:HD21	1:H:133:ARG:NH1	2.08	0.60
1:D:105:ASN:HD21	1:D:130:PRO:HG2	1.67	0.60
1:I:18:LYS:HG2	1:I:42:PHE:CE1	2.35	0.59
1:H:131:TYR:CE2	1:H:137:LEU:HD23	2.37	0.59
1:B:79:VAL:HG12	1:B:118:PRO:HD2	1.84	0.59
1:A:17:ALA:HB3	1:A:25:MET:HG2	1.85	0.58
1:E:50:ASP:O	1:E:54:GLU:HG3	2.02	0.58
1:F:79:VAL:HG12	1:F:118:PRO:HD2	1.86	0.58
1:E:123:ILE:HG13	1:E:124:ALA:O	2.03	0.58
1:I:128:ILE:HD12	1:I:139:ARG:HG2	1.85	0.58
1:H:27:ASP:CG	1:H:28:PHE:H	2.07	0.58
1:H:1:MET:O	1:H:1:MET:HG3	2.03	0.58
1:C:50:ASP:O	1:C:54:GLU:HG3	2.04	0.57
1:C:72:ARG:NH2	1:H:146:GLY:O	2.38	0.57
1:D:113:ILE:HB	1:D:117:ILE:HD12	1.85	0.57
1:F:89:THR:HA	1:F:123:ILE:O	2.05	0.57
1:E:118:PRO:HB2	1:E:121:ARG:HG3	1.88	0.56
1:D:139:ARG:NH1	1:D:149:ILE:O	2.39	0.55
1:J:76:PHE:CZ	1:J:110:GLU:O	2.53	0.55
1:A:41:SER:OG	1:A:42:PHE:CE1	2.58	0.55
1:E:69:TYR:HB2	1:E:72:ARG:HD3	1.88	0.55
1:B:132:LEU:HD21	1:B:133:ARG:NH1	2.22	0.55
1:J:66:LEU:HD21	1:J:113:ILE:HD11	1.88	0.55
1:A:71:PHE:O	1:A:72:ARG:C	2.43	0.55
1:A:109:ASP:O	1:A:132:LEU:CD2	2.54	0.55
1:A:41:SER:OG	1:A:42:PHE:CD1	2.61	0.54
1:A:109:ASP:O	1:A:132:LEU:HD22	2.07	0.54
1:E:28:PHE:O	1:E:29:CYS:HB3	2.08	0.54
1:E:86:LYS:NZ	1:J:97:LEU:O	2.42	0.53
1:A:148:LYS:O	1:I:106:THR:HG21	2.09	0.53
1:F:90:TYR:OH	1:F:130:PRO:HD2	2.07	0.53
1:J:35:ASN:O	1:J:36:SER:C	2.46	0.53
1:D:15:THR:HB	1:D:31:CYS:SG	2.49	0.53
1:B:8:LYS:HB2	1:B:13:TYR:CE1	2.44	0.53
1:A:38:ASP:O	1:A:41:SER:OG	2.27	0.53
1:B:24:ILE:O	1:B:24:ILE:CG2	2.57	0.53
1:I:89:THR:HA	1:I:123:ILE:O	2.08	0.52
1:H:87:VAL:HG12	1:H:123:ILE:HG12	1.83	0.52
1:H:87:VAL:HG11	1:H:123:ILE:CD1	2.39	0.52
1:D:72:ARG:HG2	1:D:76:PHE:CZ	2.45	0.52
1:G:106:THR:O	1:G:106:THR:OG1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ASN:N	1:A:126:ASN:OD1	2.42	0.52
1:B:113:ILE:HG22	1:B:116:ILE:HB	1.93	0.51
1:B:57:PRO:HA	1:B:84:TRP:CE2	2.45	0.51
1:C:2:LEU:HD12	1:C:19:ASP:HB3	1.93	0.51
1:I:117:ILE:O	1:I:119:CYS:N	2.43	0.51
1:C:79:VAL:HG12	1:C:118:PRO:HD2	1.93	0.51
1:I:106:THR:O	1:I:107:ALA:HB3	2.11	0.51
1:H:66:LEU:HD21	1:H:113:ILE:HD11	1.93	0.51
1:A:106:THR:HA	1:A:109:ASP:HB2	1.92	0.51
1:E:111:ASN:ND2	1:E:119:CYS:SG	2.82	0.50
1:C:133:ARG:NH1	2:C:201:HOH:O	2.31	0.50
1:J:61:ARG:O	1:J:62:GLU:HG2	2.12	0.50
1:E:68:THR:OG1	1:E:69:TYR:N	2.44	0.50
1:J:128:ILE:HG13	1:J:138:LYS:HD3	1.94	0.50
1:G:99:THR:OG1	1:G:100:ALA:N	2.44	0.50
1:I:58:ILE:HD12	1:I:59:ASN:H	1.77	0.50
1:E:128:ILE:HD13	1:E:135:VAL:HG13	1.94	0.50
1:C:112:PRO:HG2	1:C:113:ILE:HG13	1.93	0.49
1:H:87:VAL:HG11	1:H:123:ILE:CG1	2.42	0.49
1:E:150:PRO:HD3	1:J:106:THR:HG21	1.94	0.49
1:A:102:ALA:HB2	1:F:126:ASN:HA	1.93	0.49
1:H:0:PRO:HG2	1:H:2:LEU:HD23	1.94	0.49
1:B:21:LYS:HB2	1:B:65:ASN:ND2	2.28	0.49
1:J:139:ARG:O	1:J:143:GLU:HG3	2.12	0.49
1:G:131:TYR:HB2	1:G:138:LYS:HD2	1.95	0.49
1:D:62:GLU:HB2	1:D:116:ILE:HD13	1.94	0.48
1:I:131:TYR:HB2	1:I:138:LYS:HD2	1.95	0.48
1:F:91:LYS:NZ	1:F:101:PRO:HG2	2.28	0.48
1:H:27:ASP:CG	1:H:28:PHE:N	2.67	0.48
1:I:1:MET:O	1:I:1:MET:HG3	2.13	0.48
1:E:54:GLU:OE1	1:E:56:LYS:NZ	2.46	0.48
1:F:128:ILE:HD11	1:F:142:LEU:HD12	1.95	0.48
1:C:89:THR:HA	1:C:123:ILE:O	2.13	0.48
1:I:106:THR:O	1:I:107:ALA:CB	2.62	0.48
1:C:133:ARG:NH2	2:C:201:HOH:O	2.36	0.47
1:J:131:TYR:HB2	1:J:138:LYS:HD2	1.96	0.47
1:A:20:ASP:OD2	1:A:21:LYS:HE3	2.13	0.47
1:C:131:TYR:CD2	1:C:138:LYS:HB2	2.49	0.47
1:F:76:PHE:HB3	1:F:117:ILE:HD13	1.95	0.47
1:C:93:ILE:O	1:C:96:SER:HB3	2.14	0.47
1:B:78:GLU:HA	1:B:81:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:THR:HA	1:B:123:ILE:O	2.15	0.47
1:A:86:LYS:HE2	1:I:99:THR:OG1	2.14	0.47
1:H:60:LEU:HD23	1:H:60:LEU:HA	1.74	0.47
1:B:133:ARG:HB3	1:B:137:LEU:HD23	1.97	0.47
1:C:72:ARG:HG2	1:C:107:ALA:CB	2.44	0.47
1:I:57:PRO:HB3	1:I:84:TRP:CZ3	2.50	0.47
1:G:0:PRO:HG2	1:G:2:LEU:HD13	1.96	0.46
1:J:45:PHE:CZ	1:J:116:ILE:HD11	2.51	0.46
1:G:1:MET:HG3	1:G:19:ASP:CB	2.30	0.46
1:G:91:LYS:HB2	1:G:91:LYS:HE2	1.67	0.46
1:J:52:TYR:CD1	1:J:60:LEU:HD21	2.51	0.46
1:E:128:ILE:HD13	1:E:135:VAL:CG1	2.45	0.46
1:E:89:THR:HA	1:E:123:ILE:O	2.15	0.46
1:F:91:LYS:HD3	1:F:101:PRO:CG	2.46	0.45
1:A:99:THR:HG23	1:A:100:ALA:H	1.62	0.45
1:F:131:TYR:CG	1:F:138:LYS:HD2	2.51	0.45
1:H:151:GLU:OE2	1:H:151:GLU:HA	2.17	0.45
1:I:76:PHE:HB3	1:I:117:ILE:HD13	1.98	0.45
1:B:57:PRO:HB3	1:B:84:TRP:CE3	2.51	0.45
1:G:139:ARG:O	1:G:143:GLU:HB2	2.17	0.45
1:A:99:THR:HG22	1:A:100:ALA:CA	2.40	0.45
1:H:76:PHE:O	1:H:80:MET:HG3	2.17	0.45
1:G:97:LEU:HB2	1:G:99:THR:HG22	2.00	0.44
1:I:93:ILE:O	1:I:96:SER:HB3	2.17	0.44
1:J:52:TYR:CE2	1:J:144:LEU:HD21	2.52	0.44
1:D:131:TYR:HB2	1:D:138:LYS:HD2	2.00	0.44
1:H:87:VAL:CG1	1:H:123:ILE:CG1	2.84	0.44
1:B:66:LEU:HD21	1:B:113:ILE:HD11	2.00	0.44
1:H:0:PRO:HB2	1:H:1:MET:H	1.61	0.44
1:D:61:ARG:HD2	1:G:61:ARG:CG	2.44	0.44
1:J:57:PRO:HA	1:J:84:TRP:CE2	2.53	0.44
1:B:28:PHE:O	1:B:29:CYS:HB3	2.18	0.44
1:J:79:VAL:HG12	1:J:118:PRO:HD2	2.00	0.44
1:H:121:ARG:HH21	1:H:145:GLU:CD	2.20	0.44
1:C:33:GLU:O	1:C:34:GLY:C	2.56	0.43
1:C:44:GLU:OE1	1:C:44:GLU:N	2.38	0.43
1:F:131:TYR:CD1	1:F:138:LYS:HD2	2.53	0.43
1:C:1:MET:CE	1:C:1:MET:HA	2.48	0.43
1:E:73:LEU:HA	1:E:73:LEU:HD12	1.51	0.43
1:F:76:PHE:O	1:F:80:MET:HG3	2.18	0.43
1:F:109:ASP:OD1	1:F:132:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:45:PHE:CZ	1:H:116:ILE:HD11	2.52	0.43
1:J:47:HIS:O	1:J:50:ASP:HB2	2.18	0.43
1:B:90:TYR:CE2	1:B:105:ASN:HB2	2.54	0.43
1:D:148:LYS:O	1:D:149:ILE:HD13	2.18	0.43
1:I:17:ALA:O	1:I:24:ILE:HG13	2.19	0.43
1:D:25:MET:HG2	1:D:26:LEU:N	2.33	0.43
1:F:69:TYR:CD2	1:F:72:ARG:CZ	3.02	0.43
1:I:57:PRO:HA	1:I:84:TRP:CE2	2.54	0.43
1:I:113:ILE:HG22	1:I:116:ILE:HB	2.00	0.43
1:E:66:LEU:HD21	1:E:113:ILE:HD11	2.01	0.43
1:G:60:LEU:HD23	1:G:60:LEU:HA	1.79	0.42
1:G:76:PHE:O	1:G:80:MET:HG3	2.19	0.42
1:J:0:PRO:HD2	1:J:2:LEU:HD13	2.00	0.42
1:A:89:THR:HA	1:A:123:ILE:O	2.19	0.42
1:C:123:ILE:HD13	1:C:149:ILE:HG13	2.01	0.42
1:J:83:PRO:HD2	1:J:86:LYS:HB3	2.01	0.42
1:C:72:ARG:HH22	1:H:148:LYS:NZ	2.11	0.42
1:D:51:LEU:HD22	1:D:56:LYS:HD3	2.00	0.42
1:F:108:LEU:HA	1:F:108:LEU:HD23	1.68	0.42
1:F:0:PRO:HB2	1:F:1:MET:H	1.47	0.42
1:G:6:LEU:HD12	1:G:14:ILE:O	2.19	0.42
1:G:90:TYR:OH	1:G:130:PRO:HD2	2.20	0.42
1:G:141:LEU:O	1:G:145:GLU:HG3	2.19	0.42
1:H:18:LYS:HG2	1:H:42:PHE:CE1	2.55	0.42
1:H:128:ILE:HG13	1:H:138:LYS:HD3	2.02	0.42
1:H:33:GLU:O	1:H:35:ASN:N	2.49	0.42
1:J:89:THR:HA	1:J:123:ILE:O	2.19	0.42
1:C:24:ILE:HG22	1:C:65:ASN:O	2.19	0.41
1:D:83:PRO:HD2	1:D:86:LYS:HB3	2.02	0.41
1:E:126:ASN:HA	1:J:102:ALA:HB2	2.02	0.41
1:G:106:THR:O	1:G:107:ALA:HB2	2.20	0.41
1:D:8:LYS:HG3	1:D:13:TYR:CE1	2.56	0.41
1:J:9:SER:HB3	1:J:14:ILE:HD12	2.01	0.41
1:C:72:ARG:CZ	1:H:146:GLY:O	2.69	0.41
1:J:19:ASP:OD1	1:J:22:GLY:N	2.52	0.41
1:A:20:ASP:OD1	1:A:20:ASP:N	2.52	0.41
1:B:133:ARG:NH1	2:B:203:HOH:O	2.53	0.41
1:F:73:LEU:HD23	1:F:73:LEU:HA	1.85	0.41
1:G:18:LYS:HG2	1:G:42:PHE:CZ	2.56	0.41
1:J:31:CYS:O	1:J:33:GLU:OE2	2.38	0.41
1:C:26:LEU:HD22	1:C:114:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:TYR:CD2	1:E:138:LYS:HB2	2.55	0.41
1:I:26:LEU:HD22	1:I:114:LEU:O	2.21	0.41
1:J:0:PRO:HB2	1:J:1:MET:H	1.65	0.41
1:C:66:LEU:HD21	1:C:113:ILE:HD11	2.03	0.41
1:A:99:THR:CG2	1:A:100:ALA:N	2.23	0.41
1:A:106:THR:O	1:A:109:ASP:HB2	2.21	0.41
1:C:29:CYS:HB2	1:C:31:CYS:HB3	1.93	0.41
1:D:2:LEU:HD12	1:D:2:LEU:HA	1.82	0.41
1:A:57:PRO:HA	1:A:84:TRP:CE2	2.55	0.41
1:B:16:VAL:HG12	1:B:26:LEU:HG	2.03	0.41
1:B:126:ASN:OD1	1:B:126:ASN:C	2.59	0.40
1:E:20:ASP:OD1	1:E:20:ASP:N	2.54	0.40
1:H:89:THR:HA	1:H:123:ILE:O	2.22	0.40
1:J:49:LEU:HD23	1:J:49:LEU:HA	1.86	0.40
1:E:0:PRO:HB2	1:E:1:MET:H	1.51	0.40
1:F:91:LYS:HD3	1:F:101:PRO:HG3	2.03	0.40
1:H:57:PRO:HA	1:H:84:TRP:CE2	2.56	0.40
1:J:121:ARG:HH21	1:J:145:GLU:CD	2.25	0.40
1:J:33:GLU:C	1:J:35:ASN:H	2.24	0.40
1:J:38:ASP:OD2	1:J:41:SER:N	2.55	0.40
1:D:24:ILE:HG22	1:D:65:ASN:O	2.21	0.40
1:G:93:ILE:O	1:G:96:SER:HB3	2.21	0.40
1:J:57:PRO:HA	1:J:84:TRP:CD2	2.56	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	151/168 (90%)	140 (93%)	11 (7%)	0	100	100
1	B	150/168 (89%)	140 (93%)	9 (6%)	1 (1%)	22	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	150/168 (89%)	137 (91%)	12 (8%)	1 (1%)	22 53
1	D	150/168 (89%)	137 (91%)	13 (9%)	0	100 100
1	E	150/168 (89%)	134 (89%)	14 (9%)	2 (1%)	12 36
1	F	151/168 (90%)	144 (95%)	7 (5%)	0	100 100
1	G	150/168 (89%)	140 (93%)	9 (6%)	1 (1%)	22 53
1	H	150/168 (89%)	141 (94%)	8 (5%)	1 (1%)	22 53
1	I	150/168 (89%)	133 (89%)	16 (11%)	1 (1%)	22 53
1	J	150/168 (89%)	136 (91%)	13 (9%)	1 (1%)	22 53
All	All	1502/1680 (89%)	1382 (92%)	112 (8%)	8 (0%)	29 61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	106	THR
1	G	107	ALA
1	I	107	ALA
1	J	36	SER
1	C	33	GLU
1	H	33	GLU
1	E	31	CYS
1	E	150	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	134/148 (90%)	133 (99%)	1 (1%)	84 95
1	B	133/148 (90%)	132 (99%)	1 (1%)	81 94
1	C	133/148 (90%)	133 (100%)	0	100 100
1	D	133/148 (90%)	132 (99%)	1 (1%)	81 94
1	E	133/148 (90%)	132 (99%)	1 (1%)	81 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	134/148 (90%)	133 (99%)	1 (1%)	84 95
1	G	133/148 (90%)	133 (100%)	0	100 100
1	H	133/148 (90%)	131 (98%)	2 (2%)	65 89
1	I	133/148 (90%)	133 (100%)	0	100 100
1	J	133/148 (90%)	131 (98%)	2 (2%)	65 89
All	All	1332/1480 (90%)	1323 (99%)	9 (1%)	84 95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	TYR
1	B	72	ARG
1	D	31	CYS
1	E	41	SER
1	F	139	ARG
1	H	148	LYS
1	H	151	GLU
1	J	18	LYS
1	J	60	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	105	ASN
1	E	111	ASN
1	I	126	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 monosaccharides 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^{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	153/168 (91%)	0.21	4 (2%) 56 46	40, 50, 70, 90	0
1	B	152/168 (90%)	0.16	4 (2%) 56 46	37, 49, 70, 95	0
1	C	152/168 (90%)	0.30	11 (7%) 15 8	42, 51, 72, 97	0
1	D	152/168 (90%)	0.07	2 (1%) 77 72	41, 48, 71, 95	0
1	E	152/168 (90%)	0.16	4 (2%) 56 46	43, 51, 75, 97	0
1	F	153/168 (91%)	0.10	1 (0%) 87 84	38, 48, 67, 83	0
1	G	152/168 (90%)	0.25	9 (5%) 22 14	40, 51, 75, 98	0
1	H	152/168 (90%)	0.38	11 (7%) 15 8	47, 59, 83, 104	0
1	I	152/168 (90%)	0.43	14 (9%) 9 5	46, 57, 84, 99	0
1	J	152/168 (90%)	0.44	11 (7%) 15 8	46, 58, 83, 101	0
All	All	1522/1680 (90%)	0.25	71 (4%) 31 22	37, 52, 76, 104	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	35	ASN	5.3
1	H	34	GLY	5.1
1	H	30	ASP	4.3
1	C	34	GLY	4.2
1	J	36	SER	4.2
1	H	33	GLU	4.1
1	G	35	ASN	4.0
1	G	1	MET	4.0
1	J	38	ASP	3.9
1	C	35	ASN	3.9
1	C	33	GLU	3.9
1	H	32	VAL	3.8
1	I	8	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	32	VAL	3.7
1	C	31	CYS	3.6
1	E	33	GLU	3.6
1	I	35	ASN	3.6
1	G	126	ASN	3.6
1	H	31	CYS	3.5
1	E	35	ASN	3.4
1	H	131	TYR	3.4
1	A	1	MET	3.3
1	I	38	ASP	3.3
1	G	30	ASP	3.2
1	J	13	TYR	3.2
1	D	33	GLU	3.2
1	D	124	ALA	3.2
1	J	32	VAL	3.2
1	G	0	PRO	3.1
1	H	36	SER	3.1
1	J	6	LEU	3.0
1	B	35	ASN	3.0
1	J	33	GLU	3.0
1	C	6	LEU	2.9
1	I	31	CYS	2.9
1	I	6	LEU	2.9
1	J	34	GLY	2.8
1	C	30	ASP	2.8
1	G	33	GLU	2.7
1	G	125	GLU	2.7
1	C	72	ARG	2.7
1	I	0	PRO	2.6
1	I	33	GLU	2.6
1	G	36	SER	2.6
1	H	1	MET	2.6
1	A	11	LEU	2.5
1	I	1	MET	2.5
1	A	13	TYR	2.5
1	I	13	TYR	2.4
1	B	33	GLU	2.4
1	I	36	SER	2.4
1	B	34	GLY	2.3
1	J	8	LYS	2.3
1	C	1	MET	2.3
1	J	4	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	32	VAL	2.3
1	E	31	CYS	2.2
1	A	41	SER	2.2
1	F	33	GLU	2.2
1	H	13	TYR	2.2
1	C	38	ASP	2.2
1	J	109	ASP	2.2
1	J	35	ASN	2.1
1	I	133	ARG	2.1
1	I	41	SER	2.1
1	I	28	PHE	2.1
1	E	34	GLY	2.1
1	C	0	PRO	2.1
1	B	125	GLU	2.1
1	H	15	THR	2.1
1	G	124	ALA	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.