



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 02:14 PM JST

PDB ID : 7XM0  
Title : Crystal structure of Sau3AI-C and DNA substrate complex  
Authors : Liu, Y.; Yu, F.; He, J.  
Deposited on : 2022-04-23  
Resolution : 2.60 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](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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

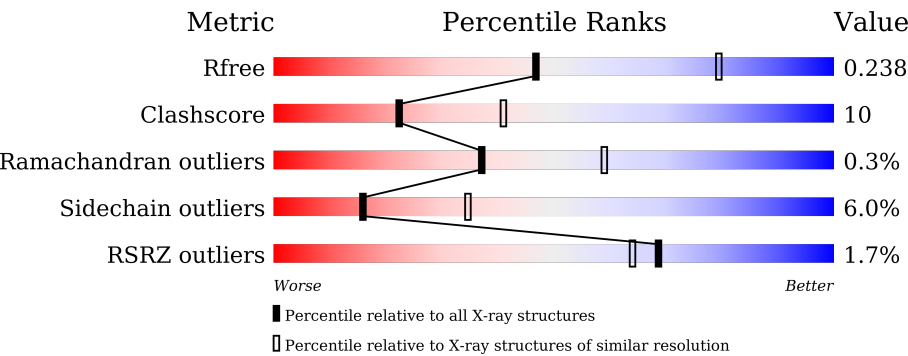
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	288	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>72%17%•10%</div></div>
1	B	288	<div><div>3%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>63%23%•12%</div></div>
1	C	288	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>58%27%•14%</div></div>
2	D	10	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>40%50%10%</div></div>
2	E	10	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>80%20%</div></div>
2	F	10	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>30%70%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	10	 10%90%
2	H	10	 60%40%
2	I	10	 30%70%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7578 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 Type II restriction enzyme Sau3AI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2143	1371	357	408	7			
1	B	254	Total	C	N	O	S	0	0	0
			2108	1349	351	402	6			
1	C	249	Total	C	N	O	S	0	0	0
			2069	1326	346	391	6			

There are 93 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	212	MET	-	initiating methionine	UNP P16667
A	213	GLY	-	expression tag	UNP P16667
A	214	SER	-	expression tag	UNP P16667
A	215	SER	-	expression tag	UNP P16667
A	216	HIS	-	expression tag	UNP P16667
A	217	HIS	-	expression tag	UNP P16667
A	218	HIS	-	expression tag	UNP P16667
A	219	HIS	-	expression tag	UNP P16667
A	220	HIS	-	expression tag	UNP P16667
A	221	HIS	-	expression tag	UNP P16667
A	222	SER	-	expression tag	UNP P16667
A	223	SER	-	expression tag	UNP P16667
A	224	GLY	-	expression tag	UNP P16667
A	225	LEU	-	expression tag	UNP P16667
A	226	VAL	-	expression tag	UNP P16667
A	227	PRO	-	expression tag	UNP P16667
A	228	ARG	-	expression tag	UNP P16667
A	229	GLY	-	expression tag	UNP P16667
A	230	SER	-	expression tag	UNP P16667
A	231	HIS	-	expression tag	UNP P16667
A	232	MET	-	expression tag	UNP P16667
A	490	CYS	-	expression tag	UNP P16667
A	491	ALA	-	expression tag	UNP P16667

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Chain	Residue	Modelled	Actual	Comment	Reference
A	492	THR	-	expression tag	UNP P16667
A	493	GLY	-	expression tag	UNP P16667
A	494	ALA	-	expression tag	UNP P16667
A	495	THR	-	expression tag	UNP P16667
A	496	CYS	-	expression tag	UNP P16667
A	497	ALA	-	expression tag	UNP P16667
A	498	THR	-	expression tag	UNP P16667
A	499	GLY	-	expression tag	UNP P16667
B	212	MET	-	initiating methionine	UNP P16667
B	213	GLY	-	expression tag	UNP P16667
B	214	SER	-	expression tag	UNP P16667
B	215	SER	-	expression tag	UNP P16667
B	216	HIS	-	expression tag	UNP P16667
B	217	HIS	-	expression tag	UNP P16667
B	218	HIS	-	expression tag	UNP P16667
B	219	HIS	-	expression tag	UNP P16667
B	220	HIS	-	expression tag	UNP P16667
B	221	HIS	-	expression tag	UNP P16667
B	222	SER	-	expression tag	UNP P16667
B	223	SER	-	expression tag	UNP P16667
B	224	GLY	-	expression tag	UNP P16667
B	225	LEU	-	expression tag	UNP P16667
B	226	VAL	-	expression tag	UNP P16667
B	227	PRO	-	expression tag	UNP P16667
B	228	ARG	-	expression tag	UNP P16667
B	229	GLY	-	expression tag	UNP P16667
B	230	SER	-	expression tag	UNP P16667
B	231	HIS	-	expression tag	UNP P16667
B	232	MET	-	expression tag	UNP P16667
B	490	CYS	-	expression tag	UNP P16667
B	491	ALA	-	expression tag	UNP P16667
B	492	THR	-	expression tag	UNP P16667
B	493	GLY	-	expression tag	UNP P16667
B	494	ALA	-	expression tag	UNP P16667
B	495	THR	-	expression tag	UNP P16667
B	496	CYS	-	expression tag	UNP P16667
B	497	ALA	-	expression tag	UNP P16667
B	498	THR	-	expression tag	UNP P16667
B	499	GLY	-	expression tag	UNP P16667
C	212	MET	-	initiating methionine	UNP P16667
C	213	GLY	-	expression tag	UNP P16667
C	214	SER	-	expression tag	UNP P16667

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Chain	Residue	Modelled	Actual	Comment	Reference
C	215	SER	-	expression tag	UNP P16667
C	216	HIS	-	expression tag	UNP P16667
C	217	HIS	-	expression tag	UNP P16667
C	218	HIS	-	expression tag	UNP P16667
C	219	HIS	-	expression tag	UNP P16667
C	220	HIS	-	expression tag	UNP P16667
C	221	HIS	-	expression tag	UNP P16667
C	222	SER	-	expression tag	UNP P16667
C	223	SER	-	expression tag	UNP P16667
C	224	GLY	-	expression tag	UNP P16667
C	225	LEU	-	expression tag	UNP P16667
C	226	VAL	-	expression tag	UNP P16667
C	227	PRO	-	expression tag	UNP P16667
C	228	ARG	-	expression tag	UNP P16667
C	229	GLY	-	expression tag	UNP P16667
C	230	SER	-	expression tag	UNP P16667
C	231	HIS	-	expression tag	UNP P16667
C	232	MET	-	expression tag	UNP P16667
C	490	CYS	-	expression tag	UNP P16667
C	491	ALA	-	expression tag	UNP P16667
C	492	THR	-	expression tag	UNP P16667
C	493	GLY	-	expression tag	UNP P16667
C	494	ALA	-	expression tag	UNP P16667
C	495	THR	-	expression tag	UNP P16667
C	496	CYS	-	expression tag	UNP P16667
C	497	ALA	-	expression tag	UNP P16667
C	498	THR	-	expression tag	UNP P16667
C	499	GLY	-	expression tag	UNP P16667

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	10	Total	C	N	O	P	0	0	0
			202	98	37	58	9			
2	E	10	Total	C	N	O	P	0	0	0
			202	98	37	58	9			
2	F	10	Total	C	N	O	P	0	0	0
			202	98	37	58	9			
2	G	10	Total	C	N	O	P	0	0	0
			202	98	37	58	9			
2	H	10	Total	C	N	O	P	0	0	0
			202	98	37	58	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	10	Total	C	N	O	P	0	0	0
			202	98	37	58	9			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

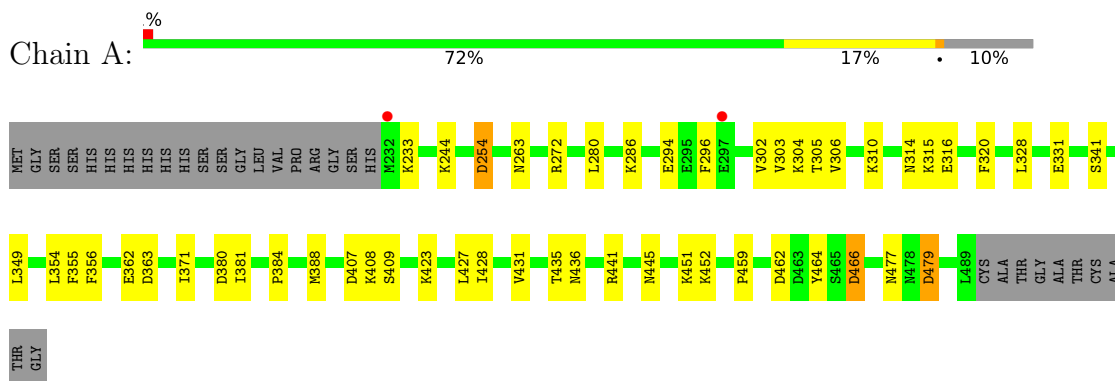
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	6	Total	O	0	0
			6	6		
4	C	6	Total	O	0	0
			6	6		
4	D	1	Total	O	0	0
			1	1		
4	E	2	Total	O	0	0
			2	2		
4	F	4	Total	O	0	0
			4	4		
4	G	3	Total	O	0	0
			3	3		
4	I	6	Total	O	0	0
			6	6		

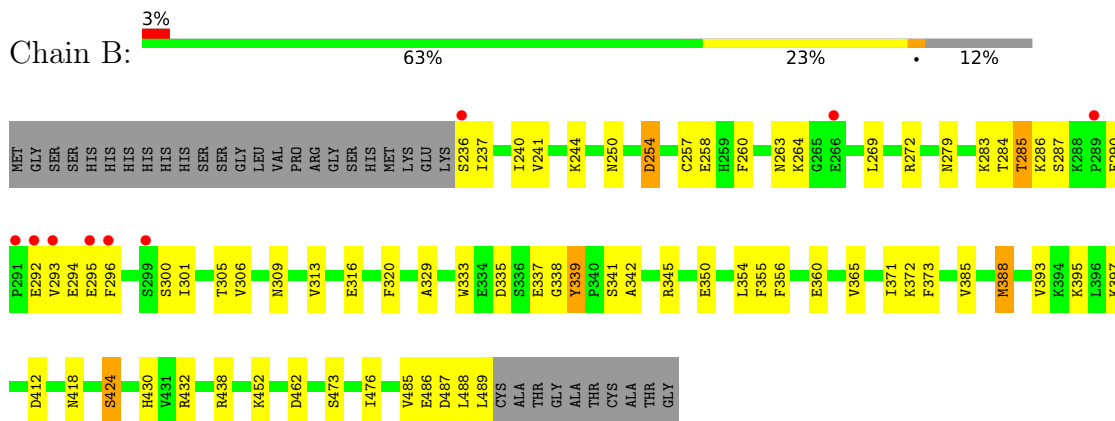
### 3 Residue-property plots [i](#)

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.

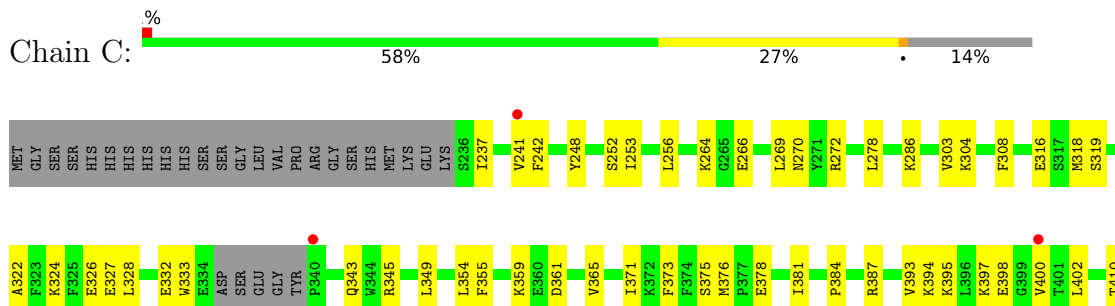
#### • Molecule 1: Type II restriction enzyme Sau3AI

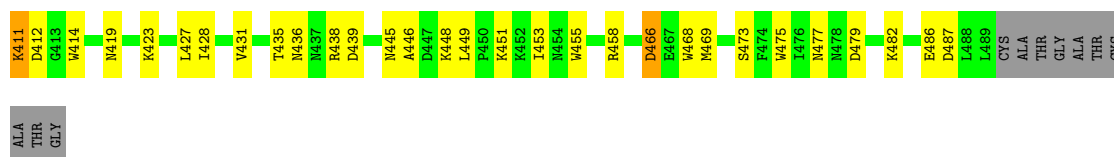


#### • Molecule 1: Type II restriction enzyme Sau3AI



#### • Molecule 1: Type II restriction enzyme Sau3AI





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

Chain D: 40% 50% 10%



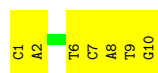
- Molecule 2: DNA (5'-D(\*CP\*AP\*TP\*GP\*AP\*TP\*CP\*AP\*TP\*G)-3')

Chain E: 80% 20%



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

Chain F: 30% 70%



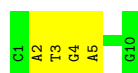
- Molecule 2: DNA (5'-D(\*CP\*AP\*TP\*GP\*AP\*TP\*CP\*AP\*TP\*G)-3')

Chain G: 10% 90%



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

Chain H: 60% 40%



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

Chain I: 30% 70%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.94Å 98.39Å 209.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.23 – 2.60 42.23 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (42.23-2.60) 98.5 (42.23-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.20 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.193 , 0.240 0.193 , 0.238	Depositor DCC
$R_{free}$ test set	2059 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.6	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7578	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.27	0/2196	0.46	0/2955
1	B	0.27	0/2161	0.50	0/2911
1	C	0.26	0/2120	0.47	0/2853
2	D	0.50	0/226	0.97	1/347 (0.3%)
2	E	0.56	0/226	0.92	0/347
2	F	0.50	0/226	0.94	0/347
2	G	0.56	0/226	0.91	0/347
2	H	0.54	0/226	0.93	0/347
2	I	0.51	0/226	0.97	0/347
All	All	0.33	0/7833	0.59	1/10801 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	DA	O4'-C4'-C3'	-5.56	102.28	104.50

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	2143	0	2087	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2108	0	2046	57	0
1	C	2069	0	2019	46	0
2	D	202	0	115	5	0
2	E	202	0	115	1	0
2	F	202	0	115	6	0
2	G	202	0	115	8	0
2	H	202	0	115	3	0
2	I	202	0	115	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	15	0	0	0	0
4	B	6	0	0	4	0
4	C	6	0	0	1	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
4	F	4	0	0	1	0
4	G	3	0	0	0	0
4	I	6	0	0	1	0
All	All	7578	0	6842	150	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 (150) 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:B:341:SER:OG	4:B:601:HOH:O	1.88	0.91
1:B:316:GLU:OE2	4:B:602:HOH:O	1.96	0.82
2:I:7:DC:OP2	4:I:101:HOH:O	2.01	0.78
1:A:305:THR:HG22	1:A:356:PHE:HB3	1.69	0.73
1:B:284:THR:HG23	1:B:285:THR:H	1.54	0.72
1:B:244:LYS:HD3	1:B:290:PHE:HD1	1.54	0.72
1:B:285:THR:HG23	1:B:286:LYS:HD3	1.71	0.71
1:B:335:ASP:OD1	1:B:339:TYR:N	2.19	0.70
1:B:260:PHE:HE1	1:B:287:SER:HB2	1.57	0.68
1:C:354:LEU:HD11	1:C:371:ILE:HG23	1.76	0.68
1:C:410:THR:OG1	1:C:438:ARG:NH2	2.31	0.63
1:B:309:ASN:HA	1:B:360:GLU:HG2	1.80	0.63
2:F:6:DT:OP2	4:F:101:HOH:O	2.15	0.63
2:G:1:DC:H2''	2:G:2:DA:H5'	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:LYS:NZ	1:C:419:ASN:O	2.23	0.63
1:B:283:LYS:N	1:B:283:LYS:HD2	2.14	0.62
1:A:303:VAL:HG22	1:A:354:LEU:HD23	1.81	0.62
1:C:378:GLU:HA	1:C:381:ILE:HD12	1.82	0.62
1:A:408:LYS:O	1:A:408:LYS:HD3	1.98	0.62
1:B:284:THR:OG1	1:B:287:SER:N	2.33	0.61
1:A:407:ASP:OD1	1:A:409:SER:OG	2.14	0.61
1:C:327:GLU:N	1:C:327:GLU:OE2	2.32	0.61
1:B:412:ASP:OD2	1:B:438:ARG:NH2	2.33	0.61
1:C:303:VAL:HG22	1:C:354:LEU:HD23	1.83	0.60
2:H:4:DG:H2''	2:H:5:DA:H5''	1.83	0.60
1:C:264:LYS:HA	1:C:269:LEU:HD12	1.84	0.59
2:D:2:DA:C8	2:D:2:DA:H5'	2.39	0.57
1:B:486:GLU:HA	1:B:489:LEU:HD22	1.85	0.57
1:B:372:LYS:HB2	1:B:488:LEU:HD11	1.87	0.57
1:B:237:ILE:O	1:B:241:VAL:HG23	2.06	0.56
2:I:2:DA:H5'	2:I:2:DA:C8	2.40	0.56
1:B:487:ASP:OD2	1:B:487:ASP:N	2.34	0.55
1:C:384:PRO:HB2	1:C:428:ILE:HG12	1.88	0.55
2:E:1:DC:H2''	2:E:2:DA:H5'	1.87	0.55
1:C:308:PHE:HB2	1:C:359:LYS:HG3	1.89	0.54
1:B:305:THR:HG22	1:B:356:PHE:HB3	1.90	0.53
1:C:237:ILE:O	1:C:241:VAL:HG23	2.09	0.53
1:C:400:VAL:HG21	1:C:449:LEU:HD22	1.90	0.53
1:C:333:TRP:CZ2	1:C:345:ARG:HD3	2.43	0.53
1:C:455:TRP:CD1	1:C:458:ARG:HD2	2.44	0.53
1:C:482:LYS:O	1:C:486:GLU:HG2	2.09	0.53
1:B:452:LYS:HG2	4:B:604:HOH:O	2.07	0.53
1:B:284:THR:HG1	1:B:287:SER:H	1.55	0.53
1:B:284:THR:O	1:B:285:THR:HG22	2.10	0.52
1:C:349:LEU:HD12	1:C:381:ILE:HD13	1.91	0.52
1:C:448:LYS:HG3	1:C:468:TRP:CE2	2.45	0.52
1:A:423:LYS:NZ	1:A:479:ASP:OD2	2.42	0.52
1:B:263:ASN:OD1	1:B:264:LYS:N	2.43	0.52
1:B:337:GLU:N	1:B:337:GLU:OE2	2.40	0.52
2:F:1:DC:H2''	2:F:2:DA:C8	2.45	0.52
1:A:380:ASP:HB3	1:A:428:ILE:HD13	1.91	0.51
1:A:314:ASN:OD1	1:A:314:ASN:N	2.39	0.51
1:B:393:VAL:HG12	1:B:397:LYS:HE2	1.92	0.51
1:B:418:ASN:ND2	4:B:603:HOH:O	2.44	0.51
1:B:264:LYS:HA	1:B:269:LEU:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:7:DC:H2''	2:I:8:DA:H5'	1.93	0.50
1:C:394:LYS:O	1:C:397:LYS:HG2	2.12	0.50
1:B:329:ALA:HA	1:B:393:VAL:HG13	1.94	0.50
1:B:257:CYS:SG	1:B:269:LEU:HD21	2.52	0.49
1:B:272:ARG:NH2	2:G:9:DT:O3'	2.44	0.49
1:C:410:THR:HG21	1:C:414:TRP:O	2.13	0.49
1:B:320:PHE:HE2	1:B:476:ILE:HG13	1.77	0.49
2:F:7:DC:H2''	2:F:8:DA:H5'	1.95	0.49
2:H:3:DT:H2''	2:H:4:DG:H5''	1.95	0.49
1:A:349:LEU:HD23	1:A:381:ILE:HD13	1.94	0.49
1:B:335:ASP:OD2	1:B:339:TYR:HB2	2.12	0.49
1:C:439:ASP:HB3	1:C:446:ALA:HB2	1.93	0.49
1:A:427:LEU:O	1:A:477:ASN:ND2	2.46	0.48
1:C:328:LEU:HG	1:C:393:VAL:HG12	1.95	0.48
1:B:438:ARG:HG2	2:G:6:DT:OP2	2.13	0.48
1:B:284:THR:C	1:B:286:LYS:H	2.15	0.48
1:B:300:SER:HB3	1:B:350:GLU:O	2.12	0.48
1:A:435:THR:OG1	1:A:436:ASN:N	2.47	0.47
1:A:286:LYS:N	1:A:286:LYS:HD2	2.29	0.47
2:D:7:DC:H2''	2:D:8:DA:H5'	1.97	0.47
2:F:9:DT:H2''	2:F:10:DG:C8	2.49	0.47
1:B:285:THR:HG23	1:B:286:LYS:CD	2.44	0.47
1:C:278:LEU:HD23	1:C:278:LEU:HA	1.77	0.47
1:A:354:LEU:HD11	1:A:371:ILE:HB	1.97	0.47
1:C:411:LYS:HD2	1:C:412:ASP:H	1.78	0.46
1:C:427:LEU:O	1:C:477:ASN:ND2	2.48	0.46
1:A:435:THR:OG1	1:A:445:ASN:OD1	2.34	0.46
1:C:345:ARG:HE	1:C:349:LEU:HD11	1.79	0.46
1:B:272:ARG:HG2	1:B:272:ARG:HH11	1.81	0.46
1:A:354:LEU:HD11	1:A:371:ILE:HD12	1.98	0.46
1:A:409:SER:HB3	2:D:9:DT:H5''	1.98	0.46
1:C:411:LYS:HD2	1:C:412:ASP:N	2.30	0.46
1:A:355:PHE:O	1:A:371:ILE:HA	2.16	0.45
1:C:479:ASP:OD1	1:C:479:ASP:N	2.49	0.45
2:I:3:DT:H2''	2:I:4:DG:C8	2.52	0.45
1:B:285:THR:O	1:B:286:LYS:HD2	2.16	0.45
1:B:316:GLU:OE1	2:F:7:DC:H5	2.00	0.45
1:B:254:ASP:OD2	1:B:254:ASP:N	2.49	0.45
1:B:432:ARG:NH2	2:G:4:DG:O6	2.47	0.45
1:A:304:LYS:HE2	1:A:320:PHE:CE1	2.52	0.45
1:C:455:TRP:HB3	1:C:458:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:SER:HB3	1:C:475:TRP:CZ3	2.51	0.45
2:D:9:DT:H2"	2:D:10:DG:C8	2.52	0.44
1:B:279:ASN:ND2	1:B:284:THR:HB	2.32	0.44
1:B:385:VAL:O	1:B:388:MET:HG3	2.16	0.44
1:C:411:LYS:H	1:C:411:LYS:HG3	1.59	0.44
1:B:272:ARG:HE	2:G:9:DT:H4'	1.83	0.44
1:B:335:ASP:OD1	1:B:338:GLY:N	2.50	0.44
1:A:459:PRO:HG2	1:A:464:TYR:CE2	2.53	0.44
1:C:316:GLU:HB3	2:I:6:DT:H72	1.99	0.43
1:A:384:PRO:HB2	1:A:428:ILE:HD12	2.00	0.43
1:B:294:GLU:H	1:B:294:GLU:HG3	1.59	0.43
1:A:280:LEU:HD21	1:A:296:PHE:CE2	2.53	0.43
1:C:248:TYR:HB3	1:C:256:LEU:HD21	2.00	0.43
1:B:240:ILE:HG22	1:B:290:PHE:CE1	2.53	0.43
1:B:333:TRP:CE2	1:B:345:ARG:HD2	2.53	0.43
2:G:7:DC:H2"	2:G:8:DA:N7	2.33	0.43
2:G:9:DT:H2"	2:G:10:DG:C8	2.53	0.43
1:C:270:ASN:ND2	4:C:601:HOH:O	2.31	0.43
1:C:354:LEU:HD13	1:C:373:PHE:CZ	2.54	0.42
1:A:254:ASP:OD1	1:A:254:ASP:N	2.51	0.42
1:B:424:SER:HB3	2:G:3:DT:OP1	2.19	0.42
1:B:309:ASN:ND2	1:B:313:VAL:HB	2.34	0.42
1:B:485:VAL:O	1:B:489:LEU:HD13	2.20	0.42
1:C:423:LYS:HE3	2:H:2:DA:OP2	2.20	0.42
1:C:435:THR:OG1	1:C:436:ASN:N	2.52	0.42
1:C:264:LYS:HA	1:C:269:LEU:CD1	2.48	0.42
1:B:279:ASN:CG	1:B:284:THR:HB	2.39	0.42
1:B:355:PHE:O	1:B:371:ILE:HA	2.19	0.42
1:C:266:GLU:HG3	1:C:269:LEU:HB2	2.02	0.42
1:B:342:ALA:HB3	1:B:345:ARG:HB3	2.00	0.42
1:A:315:LYS:HG3	1:A:316:GLU:HG2	2.01	0.42
1:A:316:GLU:HB3	2:D:6:DT:H72	2.02	0.42
1:A:452:LYS:HD2	1:A:466:ASP:HB2	2.02	0.42
1:A:304:LYS:HA	1:A:304:LYS:HD2	1.75	0.42
1:C:304:LYS:HB3	1:C:318:MET:SD	2.59	0.42
1:B:295:GLU:HG3	1:B:301:ILE:HD12	2.01	0.41
1:B:292:GLU:HG2	1:B:296:PHE:HB2	2.03	0.41
1:C:322:ALA:HA	1:C:473:SER:HB2	2.01	0.41
1:C:354:LEU:HD13	1:C:373:PHE:CE1	2.55	0.41
1:C:402:LEU:HD11	1:C:469:MET:HE3	2.02	0.41
1:C:361:ASP:CG	1:C:365:VAL:HG22	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:LEU:HD12	1:B:373:PHE:CZ	2.56	0.41
1:A:451:LYS:HD2	1:A:451:LYS:HA	1.87	0.41
2:F:1:DC:O5'	2:I:1:DC:O5'	2.23	0.41
1:A:310:LYS:HD3	1:A:362:GLU:HA	2.02	0.41
1:A:328:LEU:O	1:A:331:GLU:HB2	2.21	0.41
1:B:260:PHE:CE1	1:B:287:SER:HB2	2.47	0.41
1:B:430:HIS:NE2	1:B:432:ARG:HD3	2.36	0.41
1:C:318:MET:HE1	1:C:355:PHE:CE1	2.56	0.41
1:C:253:ILE:HD13	1:C:253:ILE:HA	1.91	0.41
1:C:439:ASP:HB2	1:C:445:ASN:HB2	2.03	0.41
1:B:360:GLU:HA	1:B:365:VAL:O	2.21	0.40
1:A:441:ARG:HD3	1:A:462:ASP:O	2.22	0.40
1:C:453:ILE:HD12	1:C:466:ASP:O	2.21	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	256/288 (89%)	252 (98%)	4 (2%)	0	100	100
1	B	252/288 (88%)	237 (94%)	13 (5%)	2 (1%)	16	34
1	C	245/288 (85%)	237 (97%)	8 (3%)	0	100	100
All	All	753/864 (87%)	726 (96%)	25 (3%)	2 (0%)	37	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	293	VAL
1	B	285	THR

### 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	239/261 (92%)	225 (94%)	14 (6%)	16	35
1	B	235/261 (90%)	224 (95%)	11 (5%)	22	45
1	C	231/261 (88%)	214 (93%)	17 (7%)	11	24
All	All	705/783 (90%)	663 (94%)	42 (6%)	16	35

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	LYS
1	A	244	LYS
1	A	254	ASP
1	A	263	ASN
1	A	272	ARG
1	A	294	GLU
1	A	302	VAL
1	A	306	VAL
1	A	341	SER
1	A	363	ASP
1	A	388	MET
1	A	431	VAL
1	A	466	ASP
1	A	479	ASP
1	B	236	SER
1	B	250	ASN
1	B	254	ASP
1	B	258	GLU
1	B	306	VAL
1	B	339	TYR
1	B	388	MET
1	B	395	LYS
1	B	424	SER
1	B	462	ASP
1	B	473	SER
1	C	242	PHE

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Mol	Chain	Res	Type
1	C	252	SER
1	C	272	ARG
1	C	286	LYS
1	C	324	LYS
1	C	326	GLU
1	C	332	GLU
1	C	343	GLN
1	C	375	SER
1	C	376	MET
1	C	387	ARG
1	C	398	GLU
1	C	411	LYS
1	C	431	VAL
1	C	451	LYS
1	C	466	ASP
1	C	487	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	343	GLN
1	B	343	GLN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are 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, 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	258/288 (89%)	-0.13	2 (0%) 82 79	34, 60, 86, 104	0
1	B	254/288 (88%)	0.14	9 (3%) 47 41	42, 70, 112, 144	0
1	C	249/288 (86%)	0.21	3 (1%) 76 72	50, 80, 107, 127	0
2	D	10/10 (100%)	-0.78	0 100 100	36, 44, 69, 77	0
2	E	10/10 (100%)	-0.80	0 100 100	44, 48, 58, 62	0
2	F	10/10 (100%)	-0.44	0 100 100	51, 66, 80, 80	0
2	G	10/10 (100%)	-0.67	0 100 100	48, 58, 73, 80	0
2	H	10/10 (100%)	-0.49	0 100 100	55, 58, 90, 92	0
2	I	10/10 (100%)	-0.29	0 100 100	53, 65, 84, 92	0
All	All	821/924 (88%)	0.03	14 (1%) 69 64	34, 69, 105, 144	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	400	VAL	4.1
1	C	340	PRO	4.1
1	B	293	VAL	3.9
1	B	299	SER	3.6
1	B	291	PRO	3.3
1	A	232	MET	3.3
1	B	296	PHE	3.0
1	B	266	GLU	2.7
1	A	297	GLU	2.6
1	B	292	GLU	2.4
1	B	236	SER	2.2
1	B	289	PRO	2.2
1	C	241	VAL	2.0
1	B	295	GLU	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	MG	A	501	1/1	0.96	0.09	42,42,42,42	0
3	MG	C	501	1/1	0.96	0.05	49,49,49,49	0
3	MG	B	501	1/1	0.97	0.12	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.