



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:56 PM GMT

PDB ID : 1Z1G  
Title : Crystal structure of a lambda integrase tetramer bound to a Holliday junction  
Authors : Biswas, T.; Aihara, H.; Radman-Livaja, M.; Filman, D.; Landy, A.; Ellenberger, T.  
Deposited on : 2005-03-03  
Resolution : 4.40 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

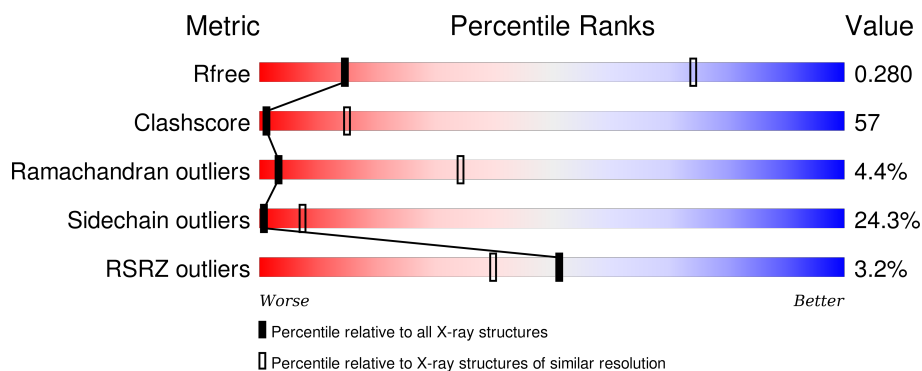
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*






The reported resolution of this entry is 4.40 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.




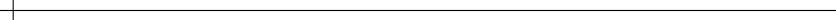





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1067 (5.20-3.60)
Clashscore	102246	1175 (5.20-3.60)
Ramachandran outliers	100387	1114 (5.20-3.60)
Sidechain outliers	100360	1096 (5.20-3.60)
RSRZ outliers	91569	1071 (5.20-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	I	29	
2	J	29	
3	K	29	
4	L	29	
5	E	25	

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Mol	Chain	Length	Quality of chain
5	G	25	 12%80%
6	F	25	 24%76%
6	H	25	 4%96%
7	A	356	 4%34%43%17%••
7	B	356	 3%30%40%21%•6%
7	C	356	 3%34%46%15%••
7	D	356	 3%37%42%15%•6%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15156 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 DNA chain called 29-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	29	Total	C	N	O	P	0	0	0
			588	284	103	173	28			

- Molecule 2 is a DNA chain called 29-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	29	Total	C	N	O	P	0	0	0
			594	286	110	170	28			

- Molecule 3 is a DNA chain called 29-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	29	Total	C	N	O	P	0	0	0
			590	285	102	175	28			

- Molecule 4 is a DNA chain called 29-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	29	Total	C	N	O	P	0	0	0
			594	285	111	170	28			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	24	Total	C	N	O	P	0	0	0
			487	234	93	137	23			
5	G	24	Total	C	N	O	P	0	0	0
			487	234	93	137	23			

- Molecule 6 is a DNA chain called 25-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	25	Total	C	N	O	P	0	0	0
			513	247	89	153	24			
6	H	25	Total	C	N	O	P	0	0	0
			513	247	89	153	24			

- Molecule 7 is a protein called Integrase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	A	349	Total	C	N	O	S	Se	0	0	0
			2763	1730	505	517	4	7			
7	B	336	Total	C	N	O	S	Se	0	0	0
			2630	1652	474	494	4	6			
7	C	349	Total	C	N	O	S	Se	0	0	0
			2767	1732	506	518	4	7			
7	D	336	Total	C	N	O	S	Se	0	0	0
			2630	1652	474	494	4	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P03700
A	101	MSE	MET	modified residue	UNP P03700
A	127	MSE	MET	modified residue	UNP P03700
A	203	MSE	MET	modified residue	UNP P03700
A	219	MSE	MET	modified residue	UNP P03700
A	255	MSE	MET	modified residue	UNP P03700
A	290	MSE	MET	modified residue	UNP P03700
A	338	MSE	MET	modified residue	UNP P03700
A	342	PHE	TYR	engineered	UNP P03700
B	1	MSE	MET	modified residue	UNP P03700
B	101	MSE	MET	modified residue	UNP P03700
B	127	MSE	MET	modified residue	UNP P03700
B	203	MSE	MET	modified residue	UNP P03700
B	219	MSE	MET	modified residue	UNP P03700
B	255	MSE	MET	modified residue	UNP P03700
B	290	MSE	MET	modified residue	UNP P03700
B	338	MSE	MET	modified residue	UNP P03700
B	342	PHE	TYR	engineered	UNP P03700
C	1	MSE	MET	modified residue	UNP P03700
C	101	MSE	MET	modified residue	UNP P03700
C	127	MSE	MET	modified residue	UNP P03700
C	203	MSE	MET	modified residue	UNP P03700
C	219	MSE	MET	modified residue	UNP P03700

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Chain	Residue	Modelled	Actual	Comment	Reference
C	255	MSE	MET	modified residue	UNP P03700
C	290	MSE	MET	modified residue	UNP P03700
C	338	MSE	MET	modified residue	UNP P03700
C	342	PHE	TYR	engineered	UNP P03700
D	1	MSE	MET	modified residue	UNP P03700
D	101	MSE	MET	modified residue	UNP P03700
D	127	MSE	MET	modified residue	UNP P03700
D	203	MSE	MET	modified residue	UNP P03700
D	219	MSE	MET	modified residue	UNP P03700
D	255	MSE	MET	modified residue	UNP P03700
D	290	MSE	MET	modified residue	UNP P03700
D	338	MSE	MET	modified residue	UNP P03700
D	342	PHE	TYR	engineered	UNP P03700

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

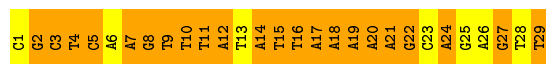
#### • Molecule 1: 29-MER

Chain I: 



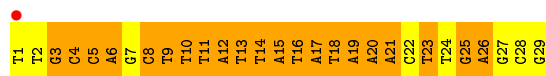
#### • Molecule 2: 29-MER

Chain J: 



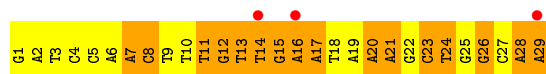
#### • Molecule 3: 29-MER

Chain K: 



#### • Molecule 4: 29-MER

Chain L: 



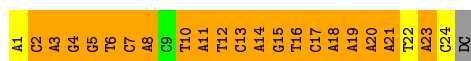
#### • Molecule 5: 5'-D(\*AP\*CP\*AP\*GP\*GP\*TP\*CP\*AP\*CP\*TP\*AP\*TP\*CP\*AP\*GP\*TP\*CP\*AP\*AP\*AP\*TP\*AP\*CP\*C)-3'

Chain E: 



#### • Molecule 5: 5'-D(\*AP\*CP\*AP\*GP\*GP\*TP\*CP\*AP\*CP\*TP\*AP\*TP\*CP\*AP\*GP\*TP\*CP\*AP\*AP\*AP\*TP\*AP\*CP\*C)-3'

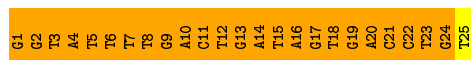
Chain G: 



- Molecule 6: 25-MER

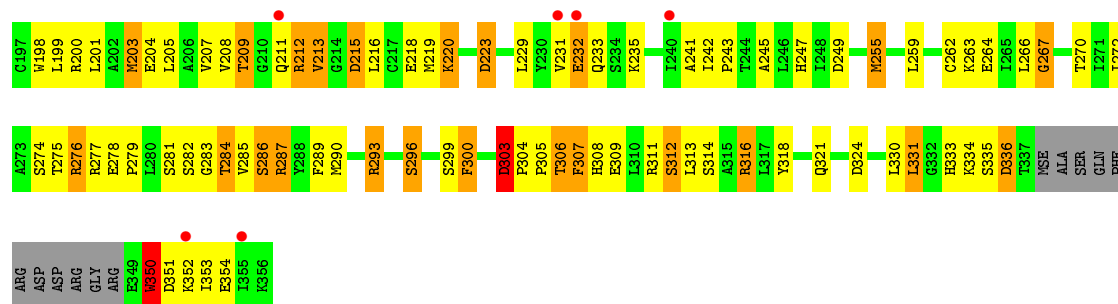


- Molecule 6: 25-MER

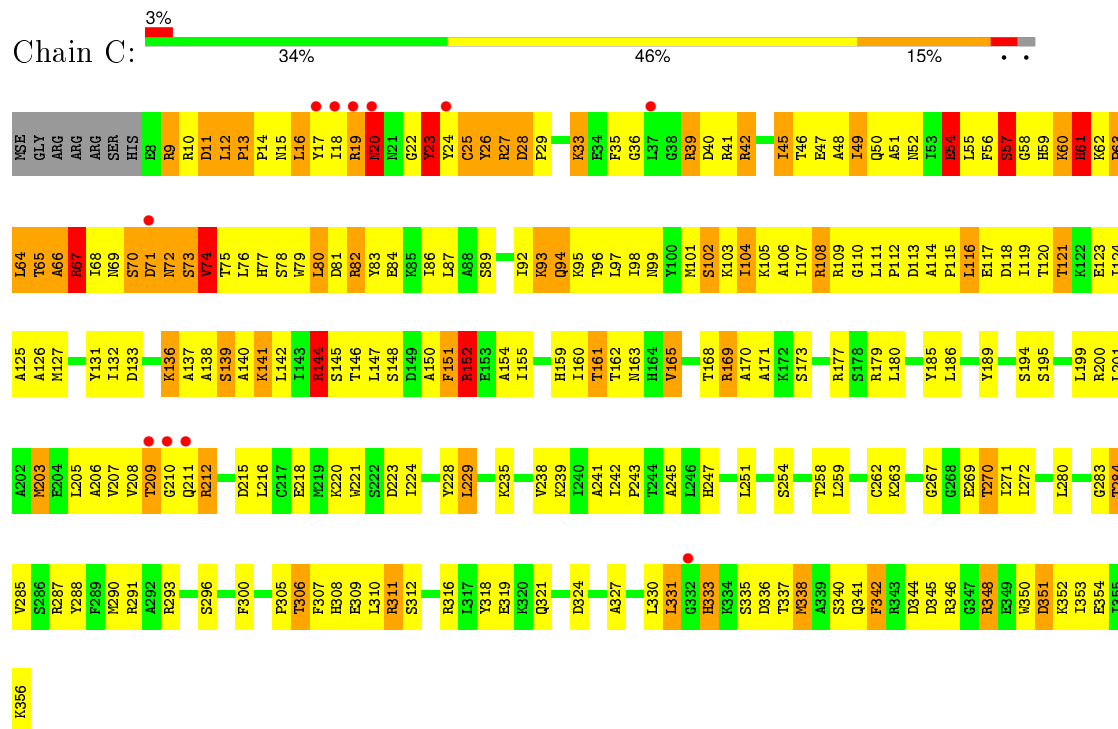


- Molecule 7: Integrase

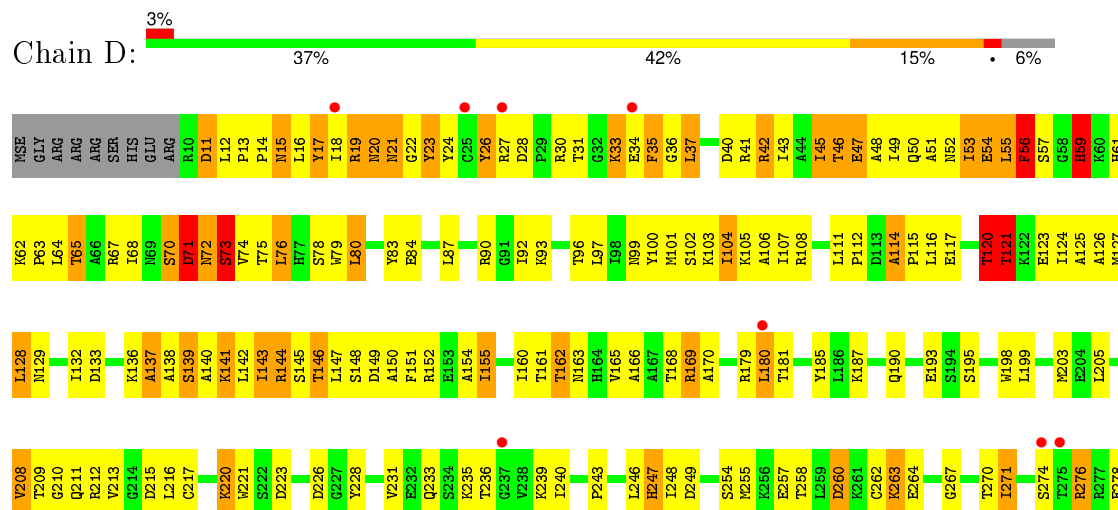


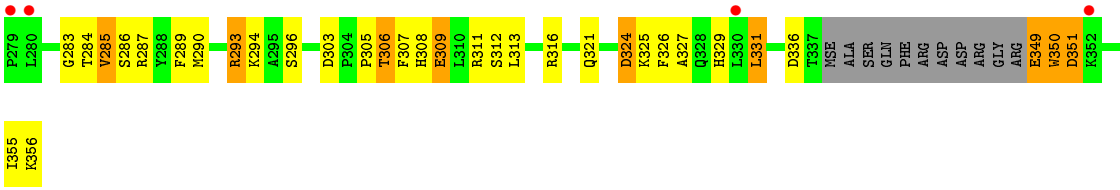


• Molecule 7: Integrase



• Molecule 7: Integrase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.76Å 109.76Å 265.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.40 44.75 – 4.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-4.40) 99.7 (44.75-4.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 4.45Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.244 , 0.292 0.235 , 0.280	Depositor DCC
$R_{free}$ test set	1146 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	241.9	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.18 , 176.3	EDS
Estimated twinning fraction	0.025 for -h,-k,l 0.066 for h,-h-k,-l 0.044 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 22650 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	I	1.74	11/658 (1.7%)	2.96	78/1013 (7.7%)
2	J	1.89	15/667 (2.2%)	2.88	93/1028 (9.0%)
3	K	2.05	19/660 (2.9%)	3.19	110/1017 (10.8%)
4	L	1.84	8/667 (1.2%)	2.80	81/1028 (7.9%)
5	E	1.75	7/547 (1.3%)	3.17	87/841 (10.3%)
5	G	2.19	17/547 (3.1%)	3.59	107/841 (12.7%)
6	F	1.96	10/574 (1.7%)	3.24	93/886 (10.5%)
6	H	2.16	20/574 (3.5%)	3.67	124/886 (14.0%)
7	A	1.18	15/2804 (0.5%)	1.35	31/3762 (0.8%)
7	B	1.35	26/2670 (1.0%)	1.37	24/3589 (0.7%)
7	C	1.11	8/2808 (0.3%)	1.25	25/3767 (0.7%)
7	D	1.09	12/2670 (0.4%)	1.27	26/3589 (0.7%)
All	All	1.47	168/15846 (1.1%)	2.14	879/22247 (4.0%)

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
7	A	0	1
7	C	0	1
All	All	0	2

The worst 5 of 168 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	15	DT	P-O5'	16.54	1.76	1.59
1	I	15	DC	C1'-N1	13.79	1.67	1.49
4	L	27	DC	C1'-N1	13.64	1.67	1.49
3	K	16	DT	C1'-N1	12.60	1.65	1.49
6	F	11	DC	C1'-N1	12.47	1.65	1.49

The worst 5 of 879 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	27	DA	O4'-C1'-N9	22.20	123.54	108.00
1	I	12	DT	O4'-C1'-N1	-21.48	92.97	108.00
5	G	5	DG	O4'-C1'-N9	19.77	121.84	108.00
6	F	11	DC	O4'-C1'-N1	19.04	121.33	108.00
6	F	6	DT	O4'-C1'-N1	18.36	120.86	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A	73	SER	Peptide
7	C	73	SER	Peptide

## 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	I	588	0	331	75	0
2	J	594	0	328	70	1
3	K	590	0	332	54	0
4	L	594	0	329	39	0
5	E	487	0	271	56	1
5	G	487	0	271	46	0
6	F	513	0	287	62	0
6	H	513	0	287	63	0
7	A	2763	0	2795	342	0
7	B	2630	0	2628	350	0
7	C	2767	0	2801	322	0
7	D	2630	0	2628	293	0
All	All	15156	0	13288	1615	1

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 57.

The worst 5 of 1615 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)
7:A:71:ASP:CB	7:A:71:ASP:CG	1.75	1.55
7:C:101:MSE:CE	7:C:101:MSE:SE	2.18	1.41
7:D:101:MSE:CE	7:D:101:MSE:SE	2.18	1.40
1:I:13:DT:N3	2:J:17:DA:N6	1.69	1.39
1:I:13:DT:H3	2:J:17:DA:N6	1.12	1.39

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:29:DT:OP2	5:E:1:DA:O5'[1_565]	1.99	0.21

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	
7	A	347/356 (98%)	286 (82%)	45 (13%)	16 (5%)	3	33
7	B	332/356 (93%)	277 (83%)	42 (13%)	13 (4%)	4	37
7	C	347/356 (98%)	286 (82%)	44 (13%)	17 (5%)	3	32
7	D	332/356 (93%)	285 (86%)	33 (10%)	14 (4%)	3	35
All	All	1358/1424 (95%)	1134 (84%)	164 (12%)	60 (4%)	3	34

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	63	PRO
7	A	67	ARG
7	A	74	VAL
7	A	335	SER
7	A	348	ARG

### 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	
7	A	292/292 (100%)	220 (75%)	72 (25%)	1	7
7	B	273/292 (94%)	201 (74%)	72 (26%)	0	5
7	C	293/292 (100%)	226 (77%)	67 (23%)	1	9
7	D	273/292 (94%)	209 (77%)	64 (23%)	1	8
All	All	1131/1168 (97%)	856 (76%)	275 (24%)	1	7

5 of 275 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	B	282	SER
7	C	42	ARG
7	D	264	GLU
7	B	293	ARG
7	B	331	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
7	B	333	HIS
7	C	20	ASN
7	D	50	GLN
7	B	21	ASN
7	B	129	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 carbohydrates 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	I	29/29 (100%)	-0.30	0 100 100	108, 108, 108, 108	0
2	J	29/29 (100%)	-0.22	0 100 100	108, 108, 108, 108	0
3	K	29/29 (100%)	-0.07	1 (3%) 49 39	108, 108, 108, 108	0
4	L	29/29 (100%)	0.24	3 (10%) 9 7	108, 108, 108, 108	0
5	E	24/25 (96%)	-0.09	0 100 100	108, 108, 108, 108	0
5	G	24/25 (96%)	-0.37	0 100 100	108, 108, 108, 108	0
6	F	25/25 (100%)	-0.02	0 100 100	108, 108, 108, 108	0
6	H	25/25 (100%)	-0.37	0 100 100	108, 108, 108, 108	0
7	A	342/356 (96%)	-0.22	13 (3%) 44 35	108, 108, 108, 200	0
7	B	330/356 (92%)	-0.23	10 (3%) 54 42	108, 108, 108, 108	0
7	C	342/356 (96%)	-0.15	11 (3%) 51 40	108, 108, 108, 200	0
7	D	330/356 (92%)	-0.13	12 (3%) 46 37	103, 108, 108, 108	0
All	All	1558/1640 (95%)	-0.18	50 (3%) 51 40	103, 108, 108, 200	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	C	210	GLY	5.4
7	C	18	ILE	5.4
7	C	209	THR	5.2
7	B	231	VAL	5.2
7	C	17	TYR	4.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.