



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2017 – 08:09 PM EDT

PDB ID : 1XO0  
Title : High resolution structure of the holliday junction intermediate in cre-loxp site-specific recombination  
Authors : Ghosh, K.; Lau, C.K.; Guo, F.; Segall, A.M.; Van Duyne, G.D.  
Deposited on : 2004-10-05  
Resolution : 2.00 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029077

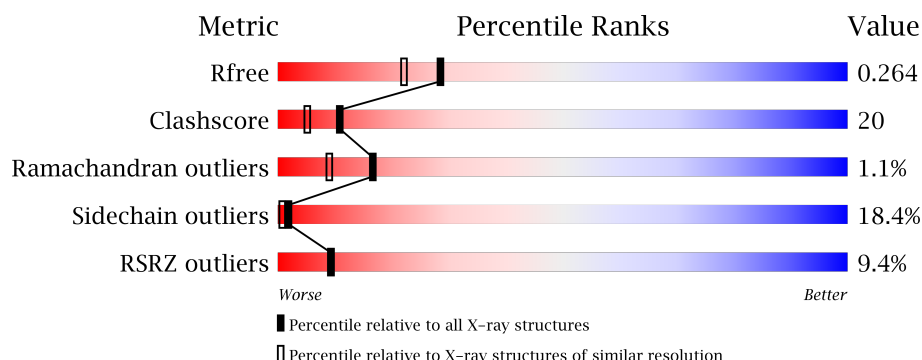
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	C	35	<div> <div>9%</div> <div>43%</div> <div>54%</div> <div>.</div> </div>
2	D	35	<div> <div>3%</div> <div>29%</div> <div>60%</div> <div>11%</div> </div>
3	A	324	<div> <div>10%</div> <div>59%</div> <div>35%</div> <div>6%</div> <div>.</div> </div>
3	B	324	<div> <div>9%</div> <div>63%</div> <div>28%</div> <div>6%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7017 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 loxP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	35	Total	C	N	O	P	0	0	0
			715	346	125	210	34			

- Molecule 2 is a DNA chain called loxP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	35	Total	C	N	O	P	0	0	0
			713	345	126	208	34			

- Molecule 3 is a protein called Recombinase CRE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	322	Total	C	N	O	S	0	0	0
			2548	1584	484	465	15			
3	B	322	Total	C	N	O	S	0	0	0
			2548	1584	484	465	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	173	LYS	ARG	ENGINEERED	UNP P06956
B	173	LYS	ARG	ENGINEERED	UNP P06956

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	154	Total	O	0	0
			154	154		
4	B	191	Total	O	0	0
			191	191		
4	C	60	Total	O	0	0
			60	60		

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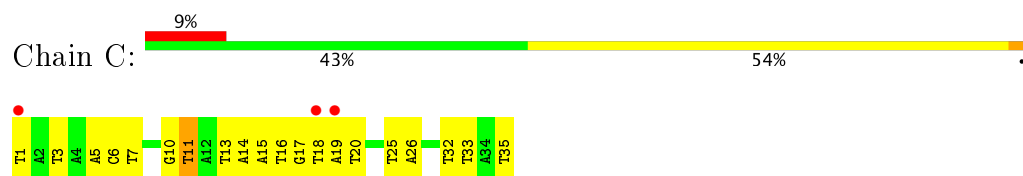
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	88	Total	O	0	0
			88	88		

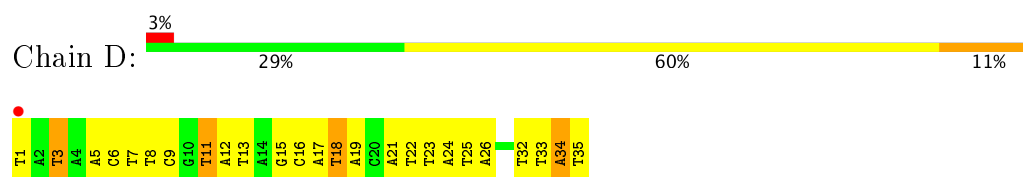
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

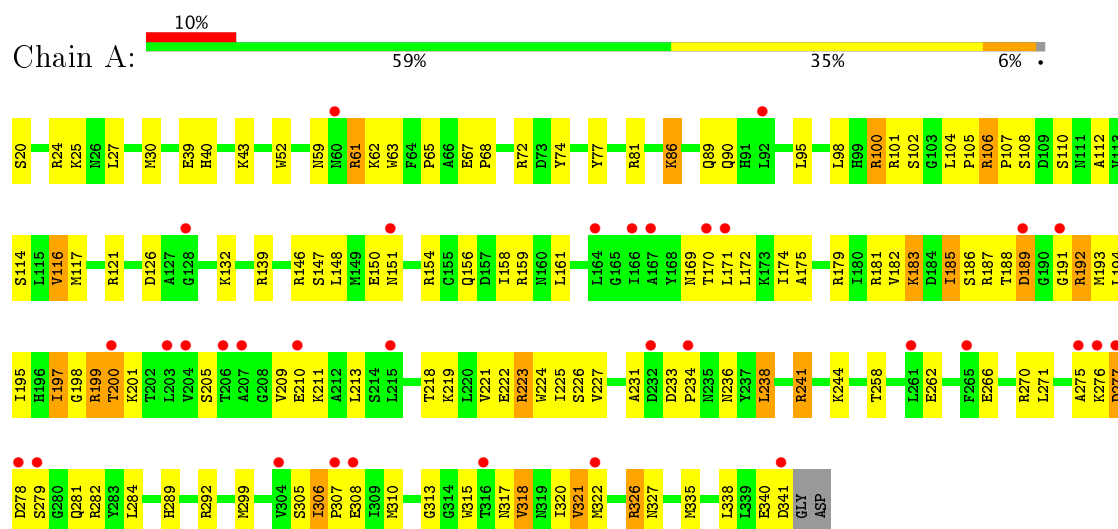
#### • Molecule 1: loxP

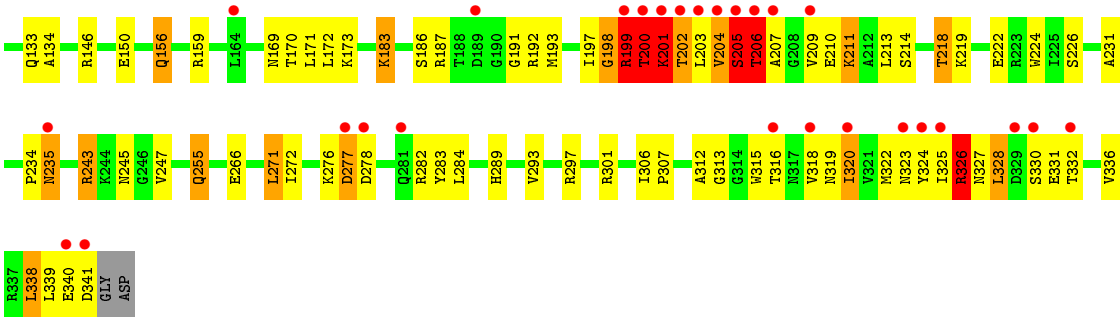


#### • Molecule 2: loxP



#### • Molecule 3: Recombinase CRE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.40 Å 123.00 Å 180.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.00 – 2.00 26.68 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (26.00-2.00) 82.9 (26.68-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 1.99 Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.219 , 0.265 0.225 , 0.264	Depositor DCC
$R_{free}$ test set	3400 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.8	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 84.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7017	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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	C	1.39	11/801 (1.4%)	1.68	15/1235 (1.2%)
2	D	1.93	11/799 (1.4%)	1.78	15/1231 (1.2%)
3	A	0.40	0/2589	0.57	0/3490
3	B	1.01	6/2589 (0.2%)	1.13	15/3490 (0.4%)
All	All	1.06	28/6778 (0.4%)	1.17	45/9446 (0.5%)

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
3	B	0	3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	DT	O3'-P	42.24	2.11	1.61
3	B	199	ARG	CD-NE	-25.77	1.02	1.46
1	C	1	DT	O3'-P	24.51	1.90	1.61
3	B	202	THR	C-N	22.71	1.86	1.34
3	B	206	THR	C-N	-17.07	0.94	1.34

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	DT	O3'-P-O5'	35.94	172.28	104.00
2	D	1	DT	OP1-P-O3'	-30.19	38.78	105.20
2	D	1	DT	P-O3'-C3'	25.10	149.82	119.70
3	B	198	GLY	O-C-N	-24.75	83.10	122.70
3	B	201	LYS	C-N-CA	-21.53	67.88	121.70

There are no chirality outliers.



All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	198	GLY	Mainchain
3	B	199	ARG	Sidechain
3	B	201	LYS	Mainchain

## 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	C	715	0	401	29	0
2	D	713	0	400	32	0
3	A	2548	0	2571	88	1
3	B	2548	0	2565	142	1
4	A	154	0	0	9	0
4	B	191	0	0	5	0
4	C	60	0	0	1	0
4	D	88	0	0	5	0
All	All	7017	0	5937	253	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 20.

The worst 5 of 253 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)
3:B:202:THR:HG1	3:B:203:LEU:N	0.96	1.43
2:D:24:DA:C5'	3:B:201:LYS:HG2	1.56	1.33
1:C:17:DG:H5''	3:B:202:THR:CB	1.62	1.30
3:B:202:THR:C	3:B:203:LEU:N	1.86	1.28
1:C:17:DG:C5'	3:B:202:THR:HB	1.66	1.26

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)
3:A:126:ASP:OD2	3:B:199:ARG:NH2[4_566]	2.17	0.03

### 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	
3	A	320/324 (99%)	301 (94%)	16 (5%)	3 (1%)	20	12
3	B	320/324 (99%)	302 (94%)	14 (4%)	4 (1%)	14	7
All	All	640/648 (99%)	603 (94%)	30 (5%)	7 (1%)	17	9

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	281	GLN
3	B	200	THR
3	B	201	LYS
3	B	277	ASP
3	A	275	ALA

#### 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	
3	A	269/270 (100%)	215 (80%)	54 (20%)	1	0
3	B	269/270 (100%)	224 (83%)	45 (17%)	2	1
All	All	538/540 (100%)	439 (82%)	99 (18%)	2	1

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	292	ARG
3	B	27	LEU
3	B	293	VAL
3	A	306	ILE
3	A	322	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	90	GLN
3	B	311	GLN
3	B	133	GLN
3	A	144	GLN
3	B	235	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	C	35/35 (100%)	0.29	3 (8%)	11 11	25, 39, 75, 90	0
2	D	35/35 (100%)	0.04	1 (2%)	52 52	24, 36, 60, 70	0
3	A	322/324 (99%)	0.64	33 (10%)	7 8	22, 47, 82, 99	0
3	B	322/324 (99%)	0.68	30 (9%)	9 9	19, 35, 83, 99	0
All	All	714/718 (99%)	0.61	67 (9%)	9 9	19, 41, 83, 99	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	203	LEU	13.4
3	B	205	SER	13.3
3	B	204	VAL	12.9
3	B	202	THR	12.7
3	B	200	THR	11.3

### 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 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.