



# wwPDB X-ray Structure Validation Summary Report i

Mar 1, 2014 – 12:40 AM GMT

PDB ID : 3CRX  
Title : CRE RECOMBINASE/DNA COMPLEX INTERMEDIATE I  
Authors : Gopaul, D.N.; Guo, F.; Vanduyne, G.D.  
Deposited on : 1998-06-19  
Resolution : 2.50 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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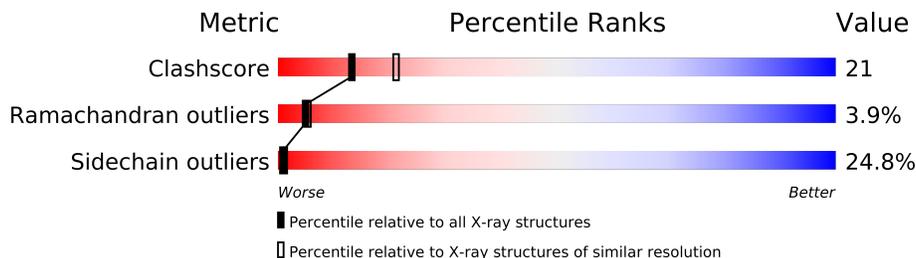
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	35	
2	D	35	
3	E	35	
4	F	35	
5	A	343	
5	B	343	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8168 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA 35-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	35	714	346	125	209	34	0	0	0

- Molecule 2 is a DNA chain called DNA 35-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	34	694	335	121	204	34	0	0	0

- Molecule 3 is a DNA chain called DNA 35-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	35	714	346	125	209	34	0	0	0

- Molecule 4 is a DNA chain called DNA 35-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	F	34	700	337	125	204	34	0	0	0

- Molecule 5 is a protein called CRE RECOMBINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	A	323	2555	1588	485	467	15	0	0	0
5	B	323	2555	1588	485	467	15	0	0	0

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 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	82	Total O 82 82	0	0
6	B	99	Total O 99 99	0	0
6	C	14	Total O 14 14	0	0
6	D	32	Total O 32 32	0	0
6	E	9	Total O 9 9	0	0

### 3 Residue-property plots

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.

Note EDS was not executed.

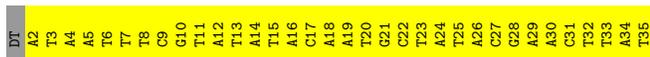
- Molecule 1: DNA 35-MER

Chain C:



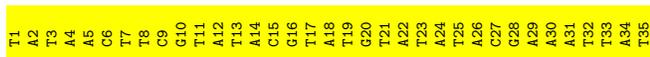
- Molecule 2: DNA 35-MER

Chain D:



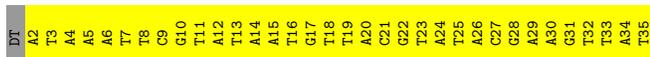
- Molecule 3: DNA 35-MER

Chain E:



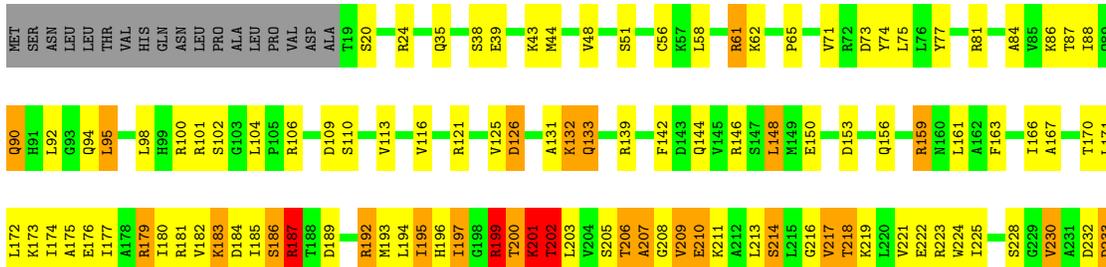
- Molecule 4: DNA 35-MER

Chain F:



- Molecule 5: CRE RECOMBINASE

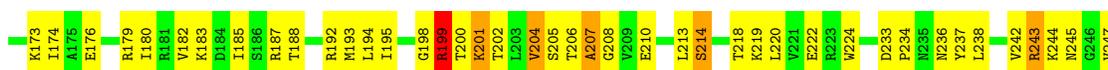
Chain A:





- Molecule 5: CRE RECOMBINASE

Chain B:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.30Å 122.70Å 179.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.30 – 2.50	Depositor
% Data completeness (in resolution range)	94.4 (27.30-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.198 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8168	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

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	0.21	0/800	0.65	0/1233
2	D	0.21	0/777	0.65	0/1196
3	E	0.22	0/800	0.65	0/1233
4	F	0.20	0/785	0.64	0/1210
5	A	0.43	1/2596 (0.0%)	0.65	7/3500 (0.2%)
5	B	0.42	0/2596	0.64	7/3500 (0.2%)
All	All	0.36	1/8354 (0.0%)	0.65	14/11872 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	283	TYR	CB-CG	7.26	1.62	1.51

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	326	ARG	NE-CZ-NH2	7.32	123.96	120.30
5	A	283	TYR	CB-CG-CD1	7.30	125.38	121.00
5	A	187	ARG	NE-CZ-NH2	7.13	123.86	120.30
5	A	282	ARG	NE-CZ-NH2	7.12	123.86	120.30
5	B	326	ARG	NE-CZ-NH2	6.74	123.67	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts i

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	714	0	401	20	2455
2	D	694	0	388	33	2398
3	E	714	0	401	14	2446
4	F	700	0	388	22	2407
5	A	2555	0	2578	146	1
5	B	2555	0	2578	98	1
6	A	82	0	0	4	0
6	B	99	0	0	11	0
6	C	14	0	0	1	1
6	D	32	0	0	2	0
6	E	9	0	0	0	1
All	All	8168	0	6734	301	4855

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

The worst 5 of 301 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:60:ASN:HB2	6:B:404:HOH:O	1.35	1.23
4:F:21:DC:H2''	4:F:22:DG:H5''	1.42	1.01
2:D:21:DG:H2''	2:D:22:DC:H5''	1.42	1.01
3:E:5:DA:H2''	3:E:6:DC:H5''	1.50	0.94
1:C:5:DA:H2''	1:C:6:DG:H5''	1.50	0.93

The worst 5 of 4855 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	Distance(Å)	Clash(Å)
1:C:6:DG:C1'	3:E:6:DC:C1'[4.566]	0.00	2.20
1:C:7:DT:N1	3:E:7:DT:N1[4.566]	0.00	2.20
1:C:7:DT:C2	3:E:7:DT:C2[4.566]	0.00	2.20
1:C:7:DT:O2	3:E:7:DT:O2[4.566]	0.00	2.20
1:C:7:DT:N3	3:E:7:DT:N3[4.566]	0.00	2.20

## 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	
5	A	321/343 (94%)	275 (86%)	31 (10%)	15 (5%)	4	3
5	B	321/343 (94%)	287 (89%)	24 (8%)	10 (3%)	7	8
All	All	642/686 (94%)	562 (88%)	55 (9%)	25 (4%)	5	5

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	200	THR
5	A	201	LYS
5	A	207	ALA
5	A	276	LYS
5	A	283	TYR

### 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	
5	A	270/287 (94%)	197 (73%)	73 (27%)	1	1
5	B	270/287 (94%)	209 (77%)	61 (23%)	1	2
All	All	540/574 (94%)	406 (75%)	134 (25%)	1	1

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	305	SER
5	B	22	GLU
5	B	311	GLN
5	A	311	GLN

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Mol	Chain	Res	Type
5	A	327	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
5	A	235	ASN
5	A	245	ASN
5	B	40	HIS
5	A	144	GLN
5	B	35	GLN

### 5.3.3 RNA [i](#)

There are no RNA chains 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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.