



wwPDB X-ray Structure Validation Summary Report

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

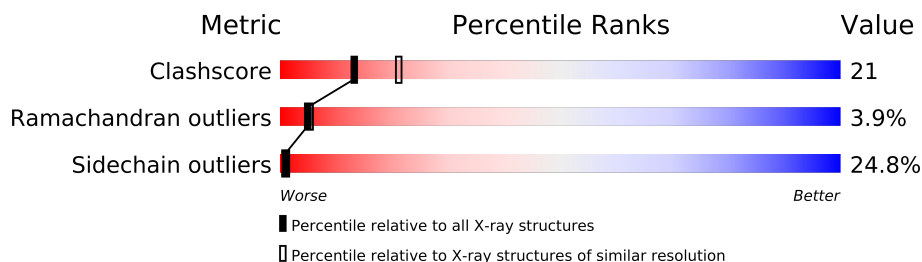
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (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 ≥ 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
1	C	35	Total	C	N	O	P	0	0	0
			714	346	125	209	34			

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

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

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

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

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

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

- Molecule 5 is a protein called CRE RECOMBINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	323	Total	C	N	O	S	0	0	0
			2555	1588	485	467	15			
5	B	323	Total	C	N	O	S	0	0	0
			2555	1588	485	467	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 6 is water.

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

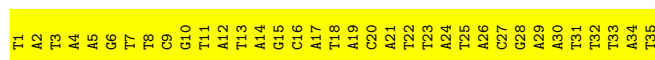
3 Residue-property plots

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.

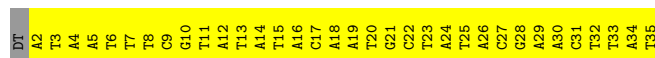
• Molecule 1: DNA 35-MER

Chain C:



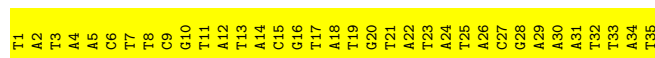
• Molecule 2: DNA 35-MER

Chain D:



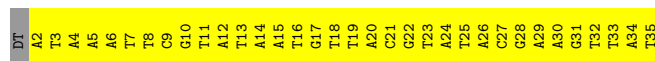
• Molecule 3: DNA 35-MER

Chain E:



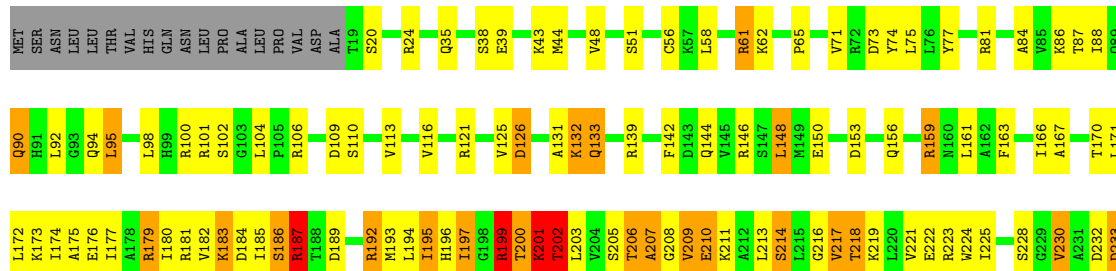
• Molecule 4: DNA 35-MER

Chain F:



• Molecule 5: CRE RECOMBINASE

Chain A:



P234	G314	R241	A252	L261	T268	R282	R301	A302	G313
N235	W315	V242	L328	L268	H269	Y283	A302	G303	
N236	T316	R243	T253	L270	L271	L284	G303	V304	
Y237	N317	N243	S254	L271	K276	A285	S305	S305	
L238	V318	N244	Q255		D277	W286	L306	L306	
	T320	Y245			D278	S287	P307	P307	
	V321	G246				G288	E308	E308	
	M322	Y247				H289	T309	T309	
	N323					S290	R310	R310	
	Y324					A291	Q311	Q311	
	Y325					R292	A312	A312	
	R326					V293	G313	G313	
	N327					G294			
	L328					A295			
	D329					A296			
	S230					R297			
	E331								
	T332								
	G333								
	V336								
	R337								
	L338								
	L339								
	E340								
	D341								
	GLY								
	ASP								

• Molecule 5: CRE RECOMBINASE

Chain B: 

E340	T258	K173	L83	MET
D341	L271	I174	A84	SER
GLY		A175	V85	ASN
ASP		E176	K86	LEU
	D277		T87	LEU
	D278	R179	I88	THR
	S279	I180	Q89	VAL
	G280	R181		GLN
	Q281	V182	L92	ASN
	Z282	K183	L95	LEU
	Y283	D184	N96	PRO
		I185	M97	ALA
	S287	S186	L98	LEU
	G288	R187	H99	PRO
	H289	T188	R100	VAL
	S290		R101	ASP
	A291	R192	S102	ALA
	R292	M193		
	V293	L194	R106	T19
		I195	S20	S20
	R297		P107	D21
			S108	E22
	R301	G198	D109	V23
		R199	S110	R24
		T200		
	V304	K201	V113	L27
	S305	T202		
	I306	L203	V116	M30
	P307	V204	M117	
		S205	R118	Q35
		T206		
	M310			
	Q311	A207	N124	S38
	A312	G208	V125	
	G313	V209	D126	W42
	G314	E210	A127	K43
	W315		G128	M44
	T316	L213	E129	L45
	N317	S214	R130	L46
	V318		A131	S47
	N319		K132	V48
	I320	T218	Q133	C49
	V321	K219	A134	R50
	N322	L220	L135	S51
	N323	V221	A136	
	Y324	E222	F137	K57
	I325	R293	E138	
		W224	R139	M60
	R326			R61
	N327	D233	Q144	K62
	L328	P234		
	D329	W235		
	S330	R236	R154	V71
	E331	Y237	C155	
	T332	L238	Q156	Y74
	G333		D157	L75
	A334	V242	I158	L76
	M335	R243	R159	Y77
	V336	K244	H160	L78
	R337	N245	L161	
	L338	G246		R81
	L339	V247	N169	G82

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, α , β , γ	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 ²)	44.0	wwPDB-VP

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	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

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 ⓘ

There are no RNA chains 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 ⓘ

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.