



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 01:04 am BST

PDB ID : 2CRX
Title : STRUCTURE OF THE HOLLIDAY JUNCTION INTERMEDIATE IN CRE-
LOXP SITE-SPECIFIC RECOMBINATION
Authors : Gopaul, D.N.; Guo, F.; Vanduyne, G.D.
Deposited on : 1998-06-19
Resolution : 2.50 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

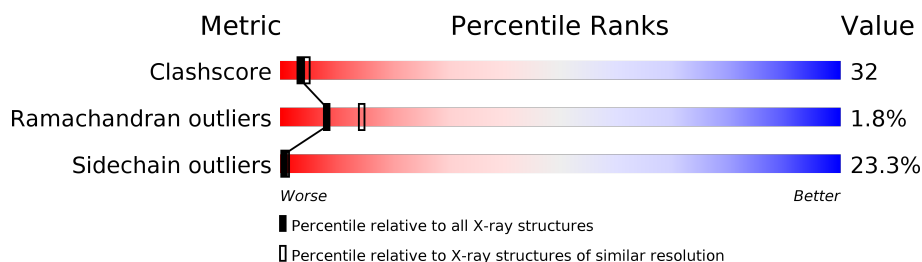
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	35	
1	D	35	
2	A	343	
2	B	343	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6639 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 DNA 35-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	35	Total	C	N	O	P	0	0	0
			711	345	126	207	33			
1	D	34	Total	C	N	O	P	0	0	0
			694	335	124	202	33			

- Molecule 2 is a protein called PROTEIN (CRE RECOMBINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	305	Total	C	N	O	S	0	0	0
			2424	1510	460	439	15			
2	B	309	Total	C	N	O	S	0	0	0
			2449	1524	468	442	15			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	31	Total	O	0	0
			31	31		
3	D	54	Total	O	0	0
			54	54		
3	A	126	Total	O	0	0
			126	126		
3	B	150	Total	O	0	0
			150	150		

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. 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. 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: 



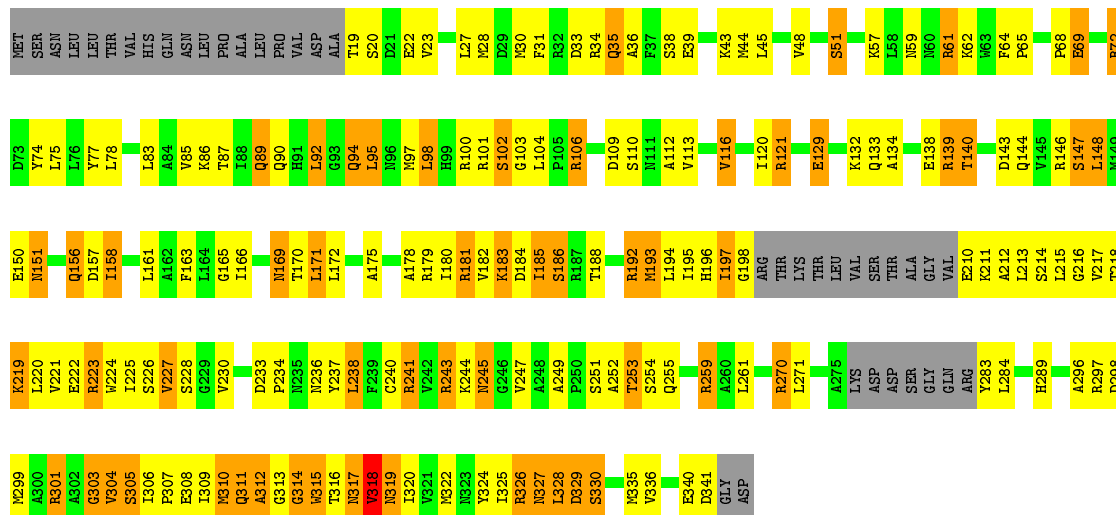
• Molecule 1: DNA 35-MER

Chain D: 



• Molecule 2: PROTEIN (CRE RECOMBINASE)

Chain A: 



• Molecule 2: PROTEIN (CRE RECOMBINASE)

Chain B: 

T316	M317	V318	M319	I320	V321	M322									T325	R326	ASN	LEU	ASP	SER	GLU	THR	G333	A334	M335	V336	R337	L338	L339	E340	D341	GLY	ASP																										
D233	P234	N235	N236	Y237	L238		R241	V242	R243	R244	N245	G246	V247	A248	A249		A252	T253	S254	Q255	L256	S257	T258	R259	A260	L261		E266		L271		D277	D278	S279	G280	Q281	R282	Y283	L284	A291	R292	V293		D298	M299	A300		V304	S305	I306	P307	E308	I309	M310		G313	G314	W315	
D157	I158	R159	N160	L161		I166	A167	Y168	N169	T170	L171	L172	R173		I177		I180	R181	Y182	K183	D184	I185	S186	R187	T188		R192	M193	L194		I197	G198	ARG	THR	LYS	THR	LEU	VAL	SER	THR	A207	G208	V209	E210	R211	L212	S214		T218	R219		E222	R223	W224	E225	S226	V227		
K86	T87	I88	Q89	Q90	H91	L92		L95	M96	M97		R100	R101	S102	G103	L104	P105	R106	P107	S108	D109	S110		V113	S114	L115	V116	M117	R118	R119	I120	R121	K122	E123	N124		E129	R130		Q133	A134		R139	T140		D143	Q144	V145	R146	S147	L148	M149	E150	M151	S152	D153	R154	C155	Q156
MET	SER	ASN	LEU	LEU	THR	VAL	HIS	GLN	ASN	LEU	PRO	ALA	LEU	PRO	VAL	ASP	ALA		T19	V23	R24	K25	N26	L27	M28	D29	M30		R34	Q35		S38	E39		W42		L45	L46		S51		K57		M60	R61		F64	P65	A66	E67	P68		R72		L78	Q79		L83	

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	106.90Å 122.50Å 180.00Å 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}	0.05	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	6639	wwPDB-VP
Average B, all atoms (Å ²)	58.0	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	0.48	0/796	0.80	0/1225
1	D	0.58	0/777	0.84	1/1195 (0.1%)
2	A	0.38	0/2463	0.64	1/3319 (0.0%)
2	B	0.43	0/2488	0.64	1/3350 (0.0%)
All	All	0.44	0/6524	0.69	3/9089 (0.0%)

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
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	17	DA	C5'-C4'-C3'	-7.04	101.42	114.10
2	B	207	ALA	N-CA-C	-5.78	95.38	111.00
2	A	102	SER	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	24	DA	Sidechain
1	D	24	DA	Sidechain

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	711	0	402	23	0
1	D	694	0	389	28	0
2	A	2424	0	2437	219	0
2	B	2449	0	2465	126	0
3	A	126	0	0	18	0
3	B	150	0	0	9	0
3	C	31	0	0	1	0
3	D	54	0	0	5	0
All	All	6639	0	5693	380	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 32.

The worst 5 of 380 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)
2:A:19:THR:HA	2:A:22:GLU:HG3	1.31	1.10
1:D:19:DA:H2''	1:D:20:DT:H5''	1.32	1.10
2:B:333:GLY:HA2	2:B:336:VAL:HB	1.27	1.05
2:A:132:LYS:HB3	2:A:283:TYR:CE2	1.96	1.00
2:B:333:GLY:O	2:B:334:ALA:C	2.02	0.94

There are no symmetry-related clashes.

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	
2	A	299/343 (87%)	262 (88%)	29 (10%)	8 (3%)	5	7
2	B	303/343 (88%)	286 (94%)	14 (5%)	3 (1%)	15	28
All	All	602/686 (88%)	548 (91%)	43 (7%)	11 (2%)	8	14

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	334	ALA
2	A	103	GLY
2	A	303	GLY
2	A	312	ALA
2	A	318	VAL

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	
2	A	255/287 (89%)	189 (74%)	66 (26%)	0	1
2	B	256/287 (89%)	203 (79%)	53 (21%)	1	2
All	All	511/574 (89%)	392 (77%)	119 (23%)	1	1

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	305	SER
2	B	19	THR
2	B	305	SER
2	A	311	GLN
2	A	320	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	245	ASN

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Mol	Chain	Res	Type
2	A	311	GLN
2	B	281	GLN
2	A	156	GLN
2	B	89	GLN

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.