



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:20 PM UTC

PDB ID : 1PVR / pdb_00001pvr
Title : BASIS FOR A SWITCH IN SUBSTRATE SPECIFICITY: CRYSTAL STRUCTURE OF SELECTED VARIANT OF CRE SITE-SPECIFIC RECOMBINASE, LNSGG BOUND TO THE LOXP (WILDTYPE) RECOGNITION SITE
Authors : Baldwin, E.P.; Martin, S.S.; Abel, J.; Gelato, K.A.; Kim, H.; Schultz, P.G.; Santoro, S.W.
Deposited on : 2003-06-28
Resolution : 2.65 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engl & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

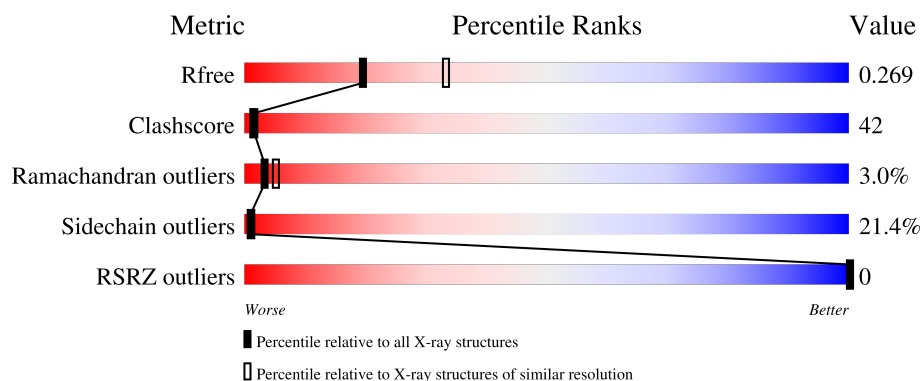
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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 of 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 $\leq 5\%$. 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	34	
2	D	34	
3	A	349	
3	B	349	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6622 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 34-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	33	Total	C	N	O	P	0	1	1
			677	326	121	198	32			

- Molecule 2 is a DNA chain called 34-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	34	Total	C	N	O	P	0	4	0
			774	374	139	224	37			

- Molecule 3 is a protein called Recombinase CRE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	324	Total	C	N	O	S	52	0	0
			2548	1582	486	465	15			
3	B	320	Total	C	N	O	S	6	0	0
			2520	1567	482	456	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP P06956
A	-4	HIS	-	expression tag	UNP P06956
A	-3	HIS	-	expression tag	UNP P06956
A	-2	HIS	-	expression tag	UNP P06956
A	-1	HIS	-	expression tag	UNP P06956
A	0	HIS	-	expression tag	UNP P06956
A	1	HIS	-	expression tag	UNP P06956
A	174	LEU	ILE	engineered mutation	UNP P06956
A	258	ASN	THR	engineered mutation	UNP P06956
A	259	SER	ARG	engineered mutation	UNP P06956
A	262	GLY	GLU	engineered mutation	UNP P06956
A	266	GLY	GLU	engineered mutation	UNP P06956

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	MET	-	initiating methionine	UNP P06956
B	-4	HIS	-	expression tag	UNP P06956
B	-3	HIS	-	expression tag	UNP P06956
B	-2	HIS	-	expression tag	UNP P06956
B	-1	HIS	-	expression tag	UNP P06956
B	0	HIS	-	expression tag	UNP P06956
B	1	HIS	-	expression tag	UNP P06956
B	174	LEU	ILE	engineered mutation	UNP P06956
B	258	ASN	THR	engineered mutation	UNP P06956
B	259	SER	ARG	engineered mutation	UNP P06956
B	262	GLY	GLU	engineered mutation	UNP P06956
B	266	GLY	GLU	engineered mutation	UNP P06956

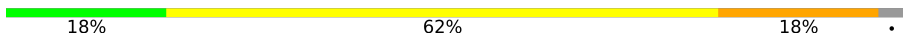
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	11	Total O 11 11	0	0
4	D	17	Total O 17 17	0	0
4	A	28	Total O 28 28	0	0
4	B	47	Total O 47 47	0	0

3 Residue-property plots

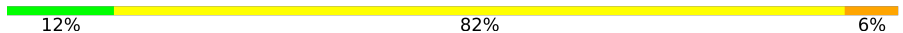
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

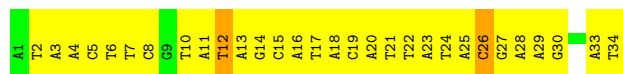
• Molecule 1: 34-MER

Chain C: 

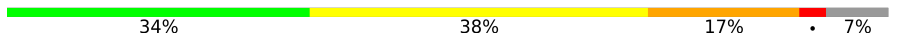


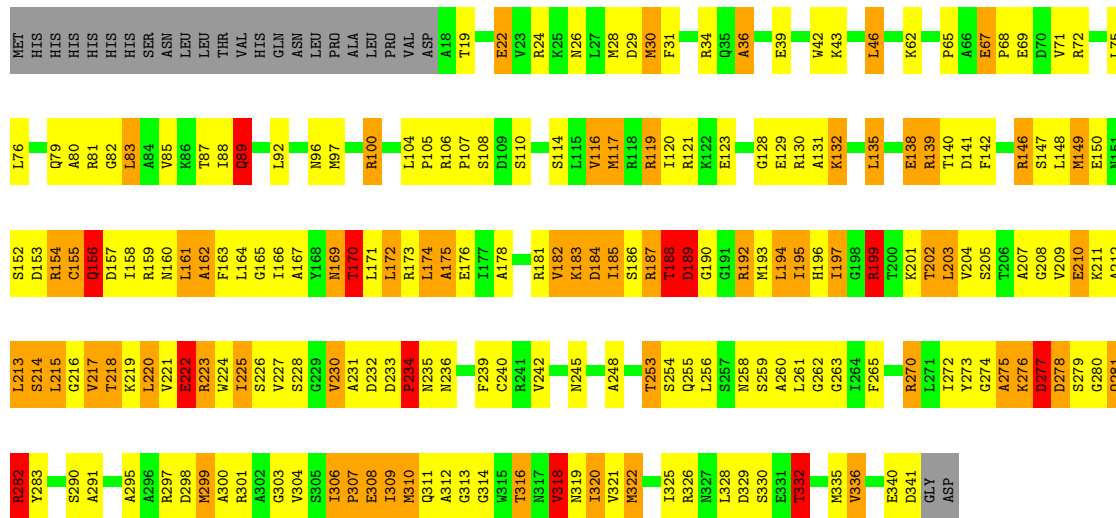
• Molecule 2: 34-MER

Chain D: 

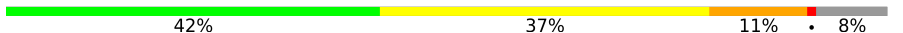


• Molecule 3: Recombinase CRE

Chain A: 



• Molecule 3: Recombinase CRE

Chain B: 





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	107.39Å 121.57Å 179.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.65 5.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.0 (5.00-2.65) 82.5 (5.00-2.65)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.65Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.212 , 0.287 0.217 , 0.269	Depositor DCC
R_{free} test set	1691 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 109.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6622	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [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	0.37	0/757	1.30	10/1164 (0.9%)
2	D	0.37	0/868	1.29	4/1337 (0.3%)
3	A	0.63	3/2589 (0.1%)	1.25	33/3491 (0.9%)
3	B	0.56	0/2560	1.13	18/3450 (0.5%)
All	All	0.55	3/6774 (0.0%)	1.22	65/9442 (0.7%)

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	A	1	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	196	HIS	CA-CB	8.09	1.63	1.53
3	A	195	ILE	CA-C	6.21	1.60	1.52
3	A	196	HIS	N-CA	5.86	1.53	1.46

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	12	DT	P-O5'-C5'	-13.38	99.92	120.00
3	B	325	ILE	N-CA-C	12.56	123.13	111.45
3	B	335	MET	N-CA-C	12.42	127.26	111.24
3	A	318	VAL	N-CA-C	12.40	124.76	110.62
3	A	326	ARG	N-CA-C	9.47	121.60	111.28

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	318	VAL	CA

There are no planarity outliers.

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	677	0	379	49	0
2	D	774	0	434	96	0
3	A	2548	0	2568	243	0
3	B	2520	0	2547	200	0
4	A	28	0	0	4	0
4	B	47	0	0	1	0
4	C	11	0	0	2	0
4	D	17	0	0	2	0
All	All	6622	0	5928	516	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 42.

The worst 5 of 516 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:D:19[B]:DC:O3'	2:D:20:DA:P	0.81	1.21
2:D:21:DT:H2''	2:D:22:DT:H5'	1.27	1.12
2:D:15:DC:C2'	2:D:16[B]:DA:C8	2.36	1.09
2:D:19[B]:DC:HO3'	2:D:20:DA:P	0.81	1.09
3:A:139:ARG:HH22	3:B:339:LEU:HD23	1.19	1.06

There are no symmetry-related clashes.

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	322/349 (92%)	268 (83%)	39 (12%)	15 (5%)	2	2
3	B	316/349 (90%)	288 (91%)	24 (8%)	4 (1%)	9	16
All	All	638/698 (91%)	556 (87%)	63 (10%)	19 (3%)	3	5

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	189	ASP
3	A	234	PRO
3	A	275	ALA
3	A	307	PRO
3	B	129	GLU

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	268/291 (92%)	196 (73%)	72 (27%)	0	0
3	B	265/291 (91%)	223 (84%)	42 (16%)	2	3
All	All	533/582 (92%)	419 (79%)	114 (21%)	1	1

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	276	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	328	LEU
3	A	336	VAL
3	B	327	ASN
3	B	211	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	89	GLN
3	B	133	GLN
3	B	124	ASN
3	B	255	GLN
3	A	235	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 oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	15:DC	O3'	16[B]:DA	P	1.78
1	D	19[B]:DC	O3'	20:DA	P	0.81

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, 95th 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 ²)	Q<0.9
1	C	33/34 (97%)	-1.17	0 100 100	27, 46, 66, 100	1 (3%)
2	D	34/34 (100%)	-1.09	0 100 100	26, 44, 60, 79	4 (11%)
3	A	324/349 (92%)	-0.63	0 100 100	23, 60, 93, 99	17 (5%)
3	B	320/349 (91%)	-1.04	0 100 100	20, 39, 80, 99	3 (0%)
All	All	711/766 (92%)	-0.86	0 100 100	20, 48, 91, 100	25 (3%)

There are no RSRZ outliers to report.

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 oligosaccharides 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.