



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2021 – 05:17 AM EDT

PDB ID : 3BDN
Title : Crystal Structure of the Lambda Repressor
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Deposited on : 2007-11-15
Resolution : 3.91 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)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

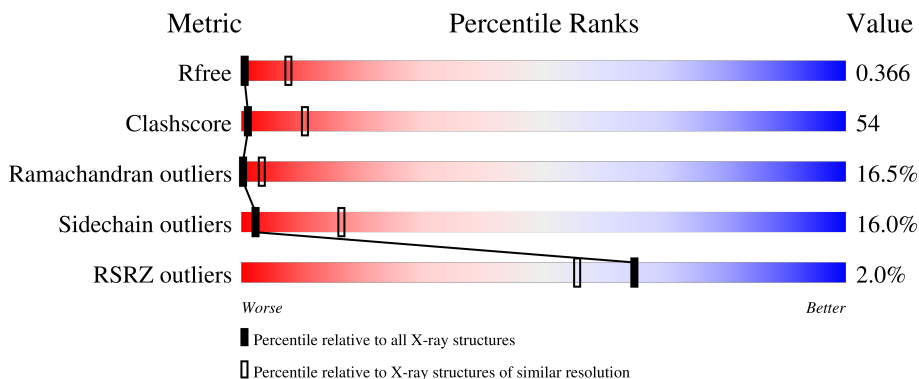
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.91 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}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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	20	<div> <div>5%</div> <div>50%</div> <div>40%</div> <div>5%</div> </div>
2	D	20	<div> <div>15%</div> <div>55%</div> <div>25%</div> <div>5%</div> </div>
3	A	236	<div> <div>3%</div> <div>24%</div> <div>55%</div> <div>17%</div> <div>...</div> </div>
3	B	236	<div> <div>%</div> <div>25%</div> <div>47%</div> <div>24%</div> <div>..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4405 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 (5'-D(*DAP*DAP*DTP*DAP*DCP*DCP*DAP*DCP*DTP*DGP*DGP*DCP*DGP*DGP*DTP*DGP*DAP*DTP*DAP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	19	Total	C	N	O	P	0	0	0
			391	186	72	114	19			

- Molecule 2 is a DNA chain called DNA (5'-D(*DTP*DAP*DTP*DAP*DTP*DCP*DAP*DCP*DCP*DGP*DCP*DCP*DAP*DGP*DTP*DGP*DGP*DTP*DAP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	19	Total	C	N	O	P	0	0	0
			388	185	70	114	19			

- Molecule 3 is a protein called Lambda Repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	234	Total	C	N	O	S	0	0	0
			1814	1154	298	352	10			
3	B	234	Total	C	N	O	S	0	0	0
			1812	1152	298	352	10			

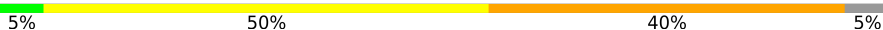
There are 2 discrepancies between the modelled and reference sequences:

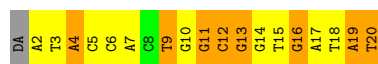
Chain	Residue	Modelled	Actual	Comment	Reference
A	197	GLY	ASP	engineered mutation	UNP P03034
B	197	GLY	ASP	engineered mutation	UNP P03034

3 Residue-property plots

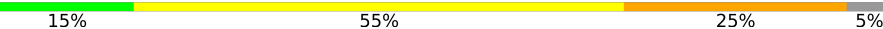
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA (5'-D(*DAP*DAP*DTP*DAP*DCP*DCP*DAP*DCP*DTP*DGP*DGP*DCP*DGP*DGP*DTP*DGP*DAP*DTP*DAP*DT)-3')

Chain C: 



- Molecule 2: DNA (5'-D(*DTP*DAP*DTP*DAP*DTP*DCP*DAP*DCP*DCP*DGP*DCP*DCP*DAP*DGP*DTP*DGP*DGP*DTP*DAP*DT)-3')

Chain D: 



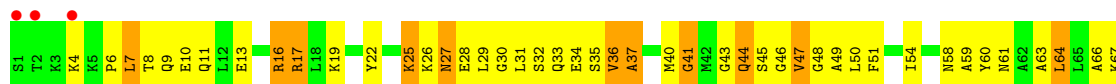
- Molecule 3: Lambda Repressor

Chain A: 



- Molecule 3: Lambda Repressor

Chain B: 



I196	G197	S198	G199	Q200	V201	Q204	P205	L206	N207	P208	Q209	Y210	P211	M212	I213	P214	CYS	ASN	E217	V221	V222	G223	K224	V225	I226	A227	S228	Q229	V230	P231	E232	E233	T234	F235	G236																					
T132	T133	K134	K135	A136	S137	D138	S139	A140	F141	W142	L143	E144	V145	E146	G147	N148	S149	M150	T151	A152	P153	T154	G155	S156	K157	P158	S159	F160	P161	M164	L165	I166	L167	V168	D169	P170	E171	Q172	A173	V174	E175	P176	G177	D178	I181	A182	R183	L184	E188	F189	T190	F191	K192	R193	L194	I195
L68	L69	K70	V71	S72	V73	E74	E75	F76	S77	P78	S79	I80	A81	R82	E83	I84	Y85	E86	M87	Y88	A90	V91	S92	M93	Q94	P95	S96	L97	R98	S99	E100	Y101	E102	Y103	P104	V105	F106	S107	H108	V109	Q110	A111	G112	M113	F114	S115	P116	E117	T122	D125	A126	E127	R128	W129	V130	S131

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	74.43Å 161.10Å 135.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.61 – 3.91 34.60 – 3.91	Depositor EDS
% Data completeness (in resolution range)	98.9 (34.61-3.91) 98.9 (34.60-3.91)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.12 (at 3.87Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.292 , 0.374 0.285 , 0.366	Depositor DCC
R_{free} test set	350 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	150.2	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 88.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4405	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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	0.95	0/438	1.88	26/674 (3.9%)
2	D	1.02	1/434 (0.2%)	1.82	15/667 (2.2%)
3	A	1.12	9/1853 (0.5%)	0.95	6/2500 (0.2%)
3	B	1.04	7/1851 (0.4%)	0.89	2/2497 (0.1%)
All	All	1.06	17/4576 (0.4%)	1.18	49/6338 (0.8%)

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	0	1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	128	ARG	CZ-NH1	23.18	1.63	1.33
3	B	25	LYS	CE-NZ	17.80	1.93	1.49
3	A	25	LYS	CE-NZ	16.20	1.89	1.49
3	A	119	ARG	CZ-NH1	10.27	1.46	1.33
3	B	157	LYS	CE-NZ	8.70	1.70	1.49

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	119	ARG	NE-CZ-NH2	-12.45	114.08	120.30
3	A	128	ARG	NE-CZ-NH1	12.11	126.36	120.30
2	D	38	DT	O4'-C1'-N1	11.37	115.96	108.00
3	A	128	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	C	5	DC	O4'-C1'-N1	9.23	114.46	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	157	LYS	Peptide

5.2 Too-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 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	391	0	215	20	0
2	D	388	0	215	15	0
3	A	1814	0	1798	207	0
3	B	1812	0	1791	235	0
All	All	4405	0	4019	447	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 54.

The worst 5 of 447 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:157:LYS:CE	3:B:157:LYS:NZ	1.70	1.53
3:A:25:LYS:CE	3:A:25:LYS:NZ	1.89	1.33
3:B:25:LYS:CE	3:B:25:LYS:NZ	1.93	1.31
3:B:73:VAL:HG12	3:B:77:SER:O	1.48	1.13
1:C:3:DT:H2''	1:C:4:DA:C8	1.88	1.08

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	230/236 (98%)	136 (59%)	61 (26%)	33 (14%)	0	4
3	B	230/236 (98%)	128 (56%)	59 (26%)	43 (19%)	0	2
All	All	460/472 (98%)	264 (57%)	120 (26%)	76 (16%)	0	3

5 of 76 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	9	GLN
3	A	11	GLN
3	A	73	VAL
3	A	103	TYR
3	A	116	PRO

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	
3	A	197/199 (99%)	167 (85%)	30 (15%)	3	17
3	B	196/199 (98%)	163 (83%)	33 (17%)	2	15
All	All	393/398 (99%)	330 (84%)	63 (16%)	2	16

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	226	ILE
3	B	174	VAL
3	B	44	GLN
3	B	172	GLN
3	B	196	ARG

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

Mol	Chain	Res	Type
3	B	94	GLN
3	B	172	GLN
3	B	229	GLN
3	B	200	GLN
3	A	229	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 monosaccharides 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 [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(Å²)	Q<0.9
1	C	19/20 (95%)	-0.37	0	100	100	178, 189, 207, 213	0
2	D	19/20 (95%)	-0.11	0	100	100	182, 207, 222, 225	0
3	A	234/236 (99%)	-0.33	7 (2%)	50	38	95, 138, 187, 195	0
3	B	234/236 (99%)	-0.46	3 (1%)	77	68	83, 118, 170, 175	0
All	All	506/512 (98%)	-0.38	10 (1%)	65	55	83, 136, 195, 225	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	1	SER	4.0
3	B	4	LYS	3.6
3	A	1	SER	3.3
3	A	97	LEU	2.6
3	B	2	THR	2.5

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 monosaccharides 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.