



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:01 AM UTC

PDB ID : 2V8N / pdb_00002v8n
Title : Wild-type Structure of Lactose Permease
Authors : Guan, L.; Mirza, O.; Verner, G.; Iwata, S.; Kaback, H.R.
Deposited on : 2007-08-09
Resolution : 3.60 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)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

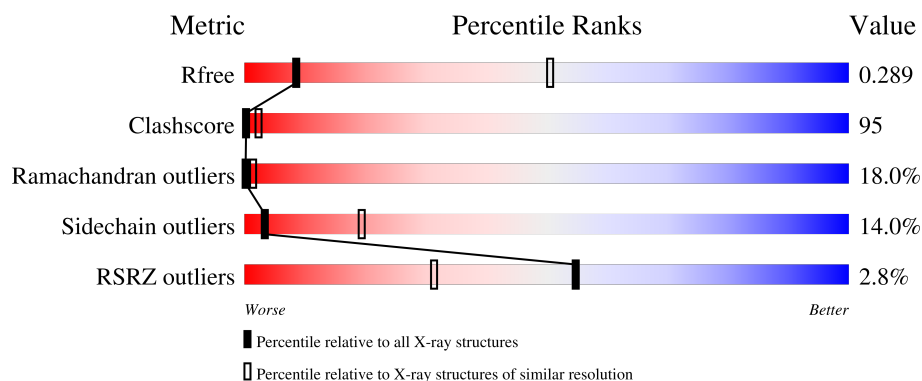
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 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	A	417	2% 17% 50% 31% .
1	B	417	4% 15% 53% 29% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6584 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.

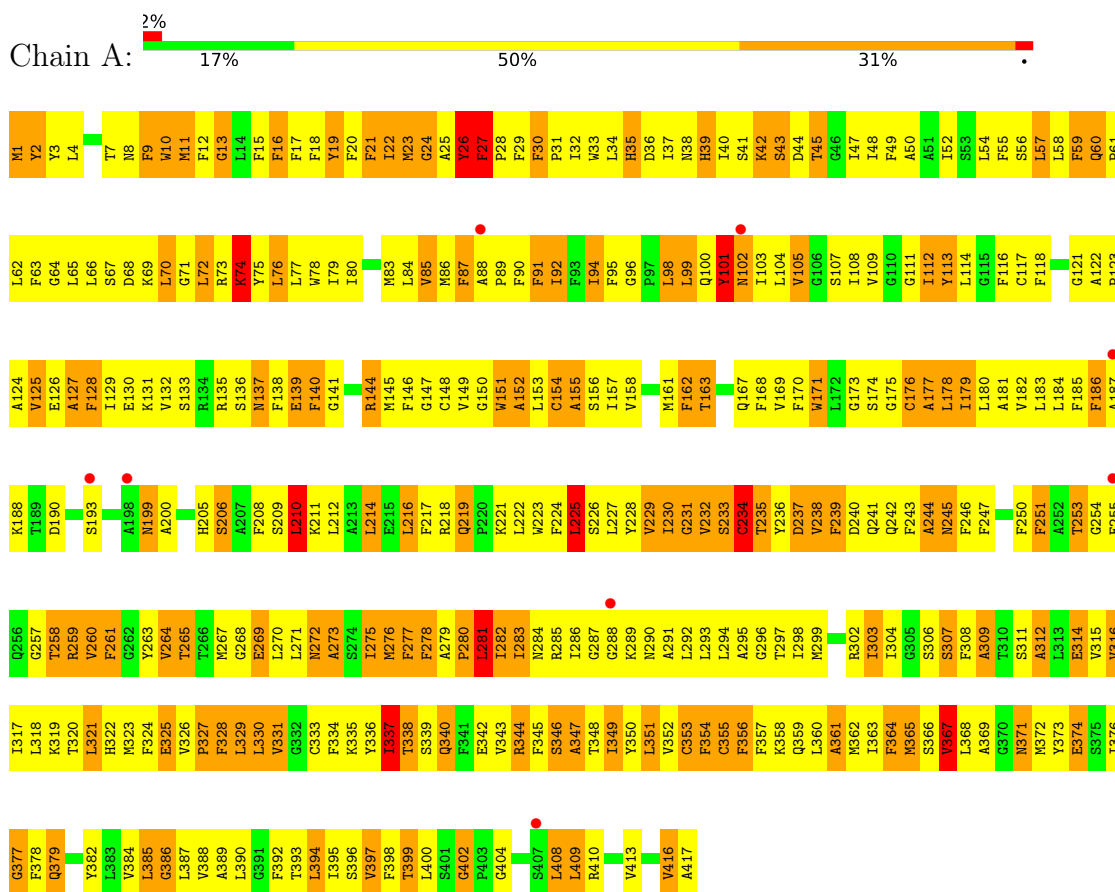
- Molecule 1 is a protein called LACTOSE PERMEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3292	2223	506	541	22			
1	B	417	Total	C	N	O	S	0	0	0
			3292	2223	506	541	22			

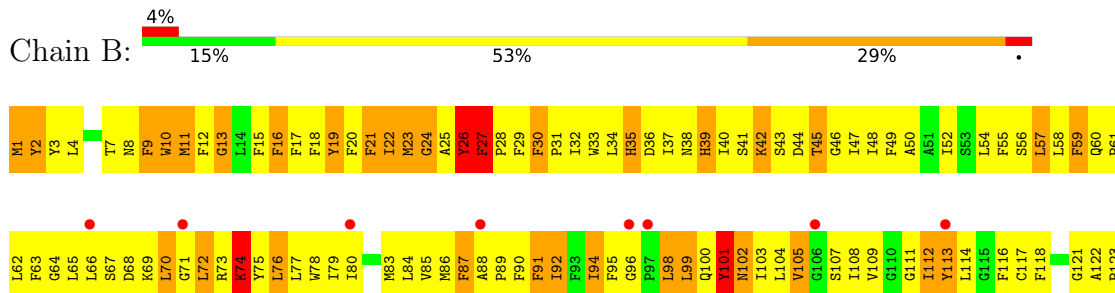
3 Residue-property plots

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: LACTOSE PERMEASE



• Molecule 1: LACTOSE PERMEASE



M372	Y373	E374	S375	I376	G377	F378	Q379		Y382	L383	V384	L385	G386		V388	A389	L390	G391	F392	T393	L394	I395	S396	V397	F398	T399	L400	S401	G402	P403	G404		S407	L408	L409	R410		V413		V416	A417																		
A124	V125	E126	A127	F128	I129	E130	K131	V132	S133	R134	R135	S136	M137	F138	E139	F140	G141		R144	M145	F146	G147	C148	V149	G150	W151	A152	L153	C154	A155	S156	I157	V158		M161	F162	T163		Q167	F168	V169	F170	W171	L172	G173	S174	G175	C176	A177	L178	I179	L180	A181	V182	L183	L184	F185	A187	
K188	T189	D190	A191	Q192	S193	S194	A195	T196	V197	A198	M199	A200		H205	S206	A207	F208	S209	L210	K211	L212	A213	L214	E215	L216	F217	R218	Q219	P220	K221	L222	W223	F224	L225	S226	L227	Y228	V229	I230	G231	V232	S233	C234	T235	Y236	D237	V238	F239	D240	Q241	Q242	F243	A244	N245	F246	F247		F250	F251
L252	T253	G254	E255	Q256	P257	T258	R259	V260	T261	G262	Y263	V264	T265	T266	M267	G268	E269	L270	L271	N272	A273	S274	I275	M276	F277	F278	A279	P280	Q281	L282	L283	N284	R285	L286	G287	G288	K289	N290	A291	L292	L293	L294	A295	G296	T297	L298	Q299	S300	V301	R302	L303	F304	G305	S306	S307	F308	A309	T310	S311
A312	L313	E314	V315	V316	I317	L318	K319	T320	L321	F322	M323	F324	E325	V326	F327	F328	L329	L330	V331	G332	C333	F334	K335	L336	R337	T338	S339	Q340	F341	G342	V343	R344	F345	S346	A347	T348	T349	Y350	L351	V352	C353	F354	C355	F356	F357	K358	Q359	L360	A361	K362	L363	F364	M365	S366	V367	L368	A369	G370	N371

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.37Å 127.40Å 188.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.60 10.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	82.7 (10.00-3.60) 81.0 (10.00-3.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.47Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.294 , 0.333 0.308 , 0.289	Depositor DCC
R_{free} test set	1308 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	87.1	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 101.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6584	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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	A	0.64	0/3389	1.26	51/4591 (1.1%)
1	B	0.64	0/3389	1.26	50/4591 (1.1%)
All	All	0.64	0/6778	1.26	101/9182 (1.1%)

There are no bond length outliers.

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	TYR	N-CA-C	-12.24	98.62	113.19
1	A	113	TYR	N-CA-C	-11.91	99.02	113.19
1	A	314	GLU	N-CA-C	-10.98	98.66	112.72
1	B	314	GLU	N-CA-C	-10.87	98.81	112.72
1	A	151	TRP	N-CA-C	-10.25	99.80	110.97

There are no chirality outliers.

There are no planarity outliers.

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	A	3292	0	3335	622	0
1	B	3292	0	3335	638	0
All	All	6584	0	6670	1259	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 95.

The worst 5 of 1259 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)
1:B:264:VAL:HG13	1:B:265:THR:H	1.09	1.10
1:B:302:ARG:HH22	1:B:319:LYS:HD2	1.10	1.09
1:A:396:SER:HA	1:A:399:THR:HB	1.34	1.09
1:B:396:SER:HA	1:B:399:THR:HB	1.33	1.09
1:A:302:ARG:HH22	1:A:319:LYS:HD2	1.09	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	
1	A	415/417 (100%)	228 (55%)	113 (27%)	74 (18%)	0	1
1	B	415/417 (100%)	229 (55%)	111 (27%)	75 (18%)	0	1
All	All	830/834 (100%)	457 (55%)	224 (27%)	149 (18%)	0	1

5 of 149 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	39	HIS
1	A	70	LEU
1	A	102	ASN
1	A	105	VAL

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	
1	A	346/346 (100%)	297 (86%)	49 (14%)	3	19
1	B	346/346 (100%)	298 (86%)	48 (14%)	3	19
All	All	692/692 (100%)	595 (86%)	97 (14%)	3	19

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	59	PHE
1	B	171	TRP
1	B	74	LYS
1	B	128	PHE
1	B	217	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	245	ASN
1	B	379	GLN
1	B	8	ASN
1	B	60	GLN
1	B	166	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 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](#)

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(Å ²)	Q<0.9
1	A	417/417 (100%)	0.13	8 (1%) 66 39	15, 81, 164, 196	0
1	B	417/417 (100%)	0.18	15 (3%) 46 26	21, 80, 164, 196	0
All	All	834/834 (100%)	0.15	23 (2%) 55 31	15, 81, 164, 196	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	404	GLY	4.7
1	B	97	PRO	3.7
1	A	198	ALA	3.4
1	B	96	GLY	3.4
1	A	407	SER	3.3

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.