



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:18 AM GMT

PDB ID : 3E1K  
Title : Crystal structure of Kluyveromyces lactis Gal80p in complex with the acidic activation domain of Gal4p  
Authors : Thoden, J.B.; Holden, H.M.  
Deposited on : 2008-08-04  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

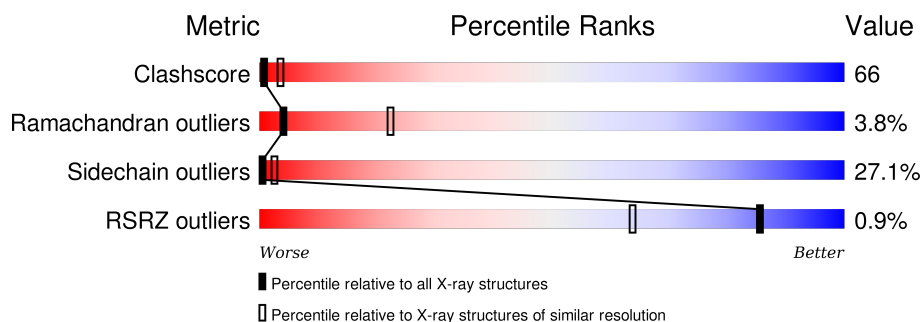
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	465	<div> <div>13%</div> <div>45%</div> <div>24%</div> <div>•</div> <div>15%</div> </div>
1	C	465	<div> <div>14%</div> <div>46%</div> <div>22%</div> <div>•</div> <div>15%</div> </div>
1	E	465	<div> <div>14%</div> <div>47%</div> <div>21%</div> <div>•</div> <div>15%</div> </div>
1	G	465	<div> <div>12%</div> <div>49%</div> <div>20%</div> <div>•</div> <div>15%</div> </div>
1	I	465	<div> <div>15%</div> <div>46%</div> <div>19%</div> <div>•</div> <div>15%</div> </div>
1	K	465	<div> <div>19%</div> <div>41%</div> <div>22%</div> <div>•</div> <div>15%</div> </div>
1	M	465	<div> <div>17%</div> <div>44%</div> <div>22%</div> <div>•</div> <div>15%</div> </div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	O	465	
2	B	22	
2	D	22	
2	F	22	
2	H	22	
2	J	22	
2	L	22	
2	N	22	
2	P	22	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26057 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 Galactose/lactose metabolism regulatory protein GAL80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3153	2024	527	593	9			
1	C	393	Total	C	N	O	S	0	0	0
			3136	2013	525	589	9			
1	E	393	Total	C	N	O	S	0	0	0
			3136	2013	525	589	9			
1	G	393	Total	C	N	O	S	0	0	0
			3136	2013	525	589	9			
1	I	393	Total	C	N	O	S	0	0	0
			3136	2013	525	589	9			
1	K	393	Total	C	N	O	S	0	0	0
			3136	2013	525	589	9			
1	M	393	Total	C	N	O	S	0	0	0
			3136	2013	525	589	9			
1	O	393	Total	C	N	O	S	0	0	0
			3136	2013	525	589	9			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	458	LEU	-	EXPRESSION TAG	UNP Q06433
A	459	GLU	-	EXPRESSION TAG	UNP Q06433
A	460	HIS	-	EXPRESSION TAG	UNP Q06433
A	461	HIS	-	EXPRESSION TAG	UNP Q06433
A	462	HIS	-	EXPRESSION TAG	UNP Q06433
A	463	HIS	-	EXPRESSION TAG	UNP Q06433
A	464	HIS	-	EXPRESSION TAG	UNP Q06433
A	465	HIS	-	EXPRESSION TAG	UNP Q06433
C	458	LEU	-	EXPRESSION TAG	UNP Q06433
C	459	GLU	-	EXPRESSION TAG	UNP Q06433
C	460	HIS	-	EXPRESSION TAG	UNP Q06433
C	461	HIS	-	EXPRESSION TAG	UNP Q06433
C	462	HIS	-	EXPRESSION TAG	UNP Q06433

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	463	HIS	-	EXPRESSION TAG	UNP Q06433
C	464	HIS	-	EXPRESSION TAG	UNP Q06433
C	465	HIS	-	EXPRESSION TAG	UNP Q06433
E	458	LEU	-	EXPRESSION TAG	UNP Q06433
E	459	GLU	-	EXPRESSION TAG	UNP Q06433
E	460	HIS	-	EXPRESSION TAG	UNP Q06433
E	461	HIS	-	EXPRESSION TAG	UNP Q06433
E	462	HIS	-	EXPRESSION TAG	UNP Q06433
E	463	HIS	-	EXPRESSION TAG	UNP Q06433
E	464	HIS	-	EXPRESSION TAG	UNP Q06433
E	465	HIS	-	EXPRESSION TAG	UNP Q06433
G	458	LEU	-	EXPRESSION TAG	UNP Q06433
G	459	GLU	-	EXPRESSION TAG	UNP Q06433
G	460	HIS	-	EXPRESSION TAG	UNP Q06433
G	461	HIS	-	EXPRESSION TAG	UNP Q06433
G	462	HIS	-	EXPRESSION TAG	UNP Q06433
G	463	HIS	-	EXPRESSION TAG	UNP Q06433
G	464	HIS	-	EXPRESSION TAG	UNP Q06433
G	465	HIS	-	EXPRESSION TAG	UNP Q06433
I	458	LEU	-	EXPRESSION TAG	UNP Q06433
I	459	GLU	-	EXPRESSION TAG	UNP Q06433
I	460	HIS	-	EXPRESSION TAG	UNP Q06433
I	461	HIS	-	EXPRESSION TAG	UNP Q06433
I	462	HIS	-	EXPRESSION TAG	UNP Q06433
I	463	HIS	-	EXPRESSION TAG	UNP Q06433
I	464	HIS	-	EXPRESSION TAG	UNP Q06433
I	465	HIS	-	EXPRESSION TAG	UNP Q06433
K	458	LEU	-	EXPRESSION TAG	UNP Q06433
K	459	GLU	-	EXPRESSION TAG	UNP Q06433
K	460	HIS	-	EXPRESSION TAG	UNP Q06433
K	461	HIS	-	EXPRESSION TAG	UNP Q06433
K	462	HIS	-	EXPRESSION TAG	UNP Q06433
K	463	HIS	-	EXPRESSION TAG	UNP Q06433
K	464	HIS	-	EXPRESSION TAG	UNP Q06433
K	465	HIS	-	EXPRESSION TAG	UNP Q06433
M	458	LEU	-	EXPRESSION TAG	UNP Q06433
M	459	GLU	-	EXPRESSION TAG	UNP Q06433
M	460	HIS	-	EXPRESSION TAG	UNP Q06433
M	461	HIS	-	EXPRESSION TAG	UNP Q06433
M	462	HIS	-	EXPRESSION TAG	UNP Q06433
M	463	HIS	-	EXPRESSION TAG	UNP Q06433
M	464	HIS	-	EXPRESSION TAG	UNP Q06433

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
M	465	HIS	-	EXPRESSION TAG	UNP Q06433
O	458	LEU	-	EXPRESSION TAG	UNP Q06433
O	459	GLU	-	EXPRESSION TAG	UNP Q06433
O	460	HIS	-	EXPRESSION TAG	UNP Q06433
O	461	HIS	-	EXPRESSION TAG	UNP Q06433
O	462	HIS	-	EXPRESSION TAG	UNP Q06433
O	463	HIS	-	EXPRESSION TAG	UNP Q06433
O	464	HIS	-	EXPRESSION TAG	UNP Q06433
O	465	HIS	-	EXPRESSION TAG	UNP Q06433

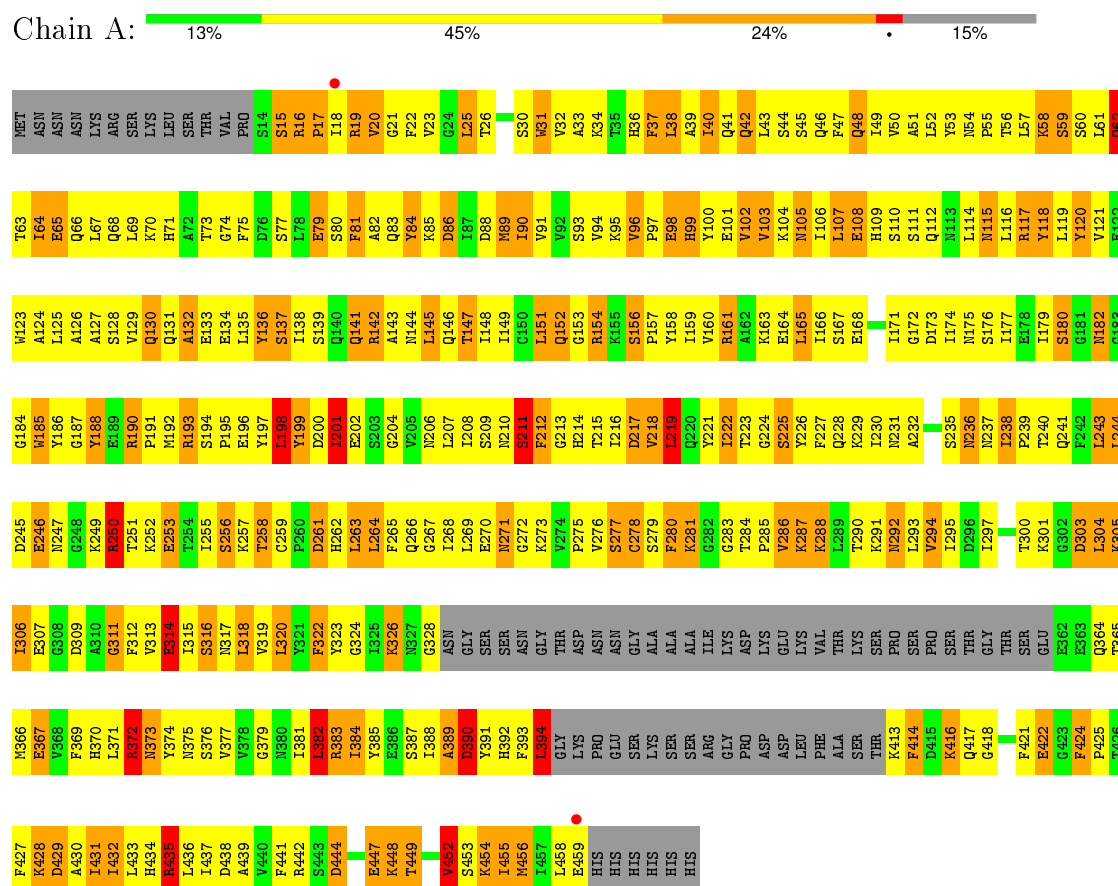
- Molecule 2 is a protein called Lactose regulatory protein LAC9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	S	0	0	0
			119	77	16	25	1			
2	D	14	Total	C	N	O	S	0	0	0
			119	77	16	25	1			
2	F	14	Total	C	N	O	S	0	0	0
			119	77	16	25	1			
2	H	14	Total	C	N	O	S	0	0	0
			119	77	16	25	1			
2	J	14	Total	C	N	O	S	0	0	0
			119	77	16	25	1			
2	L	14	Total	C	N	O	S	0	0	0
			119	77	16	25	1			
2	N	14	Total	C	N	O	S	0	0	0
			119	77	16	25	1			
2	P	14	Total	C	N	O	S	0	0	0
			119	77	16	25	1			

### 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.

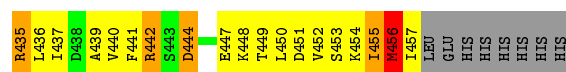
- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80



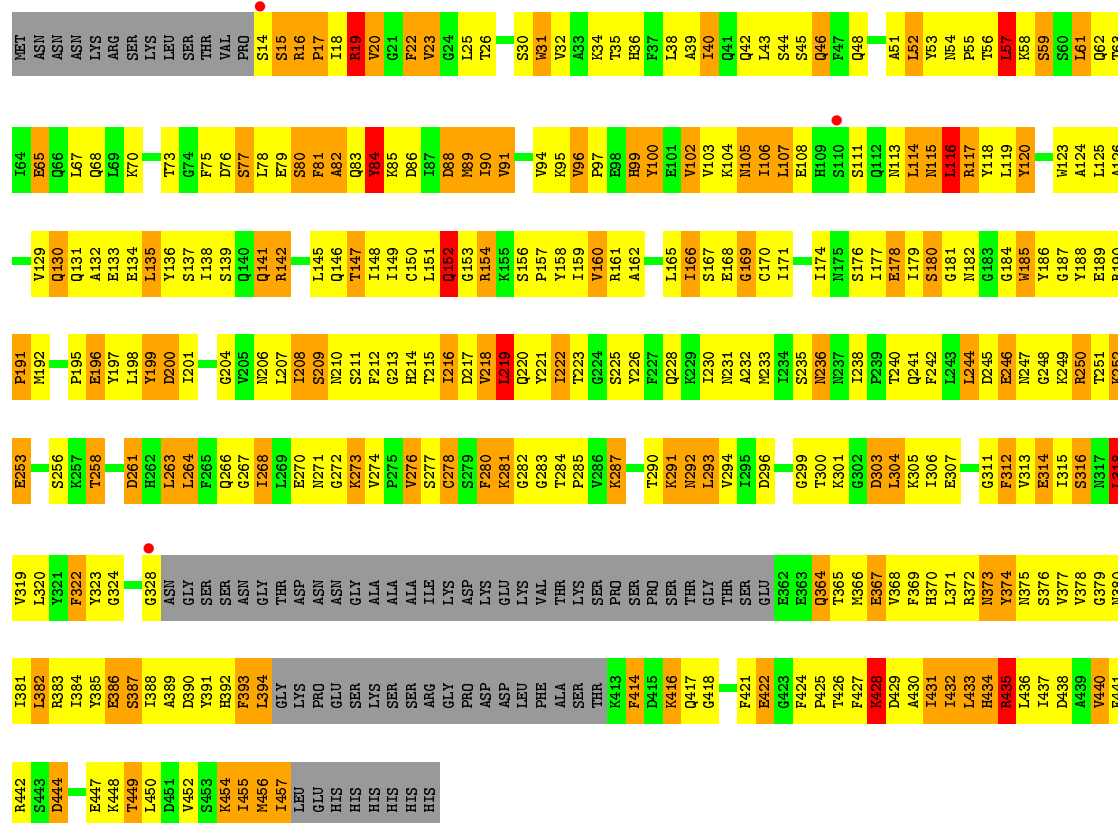
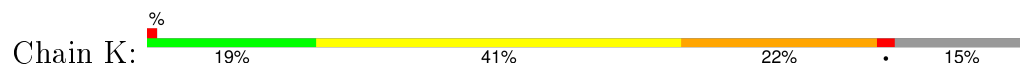




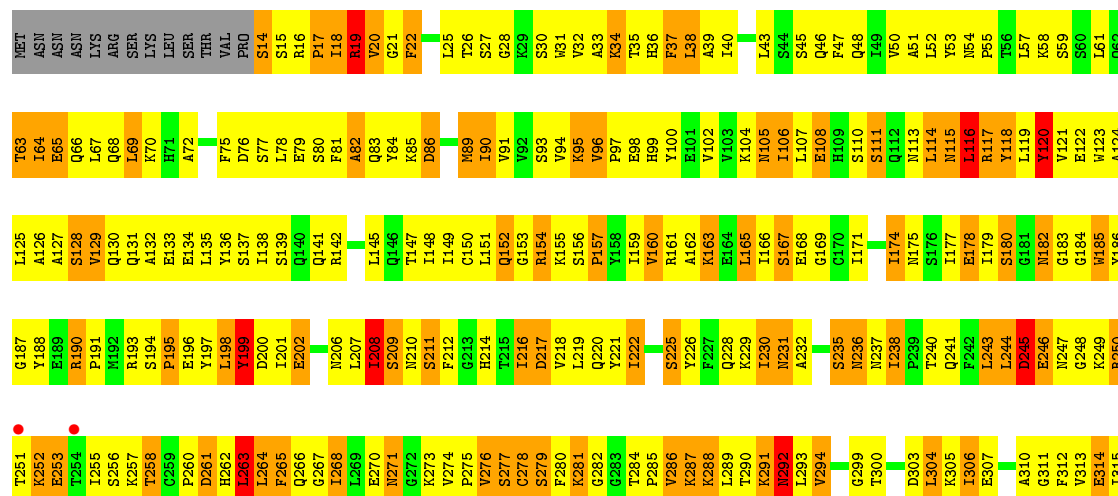
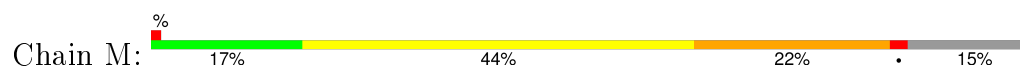


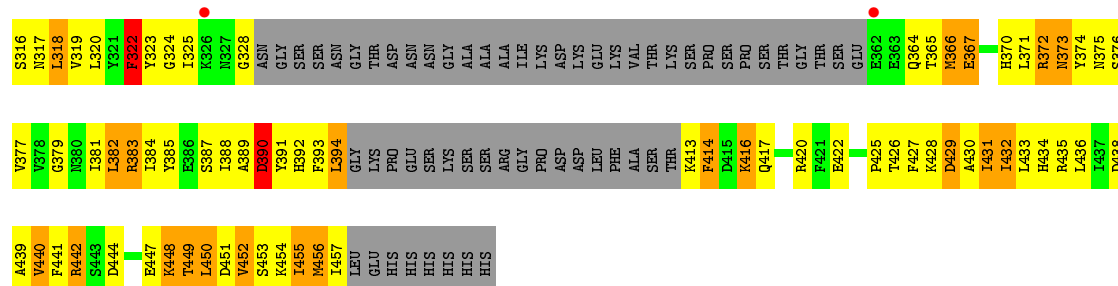


• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

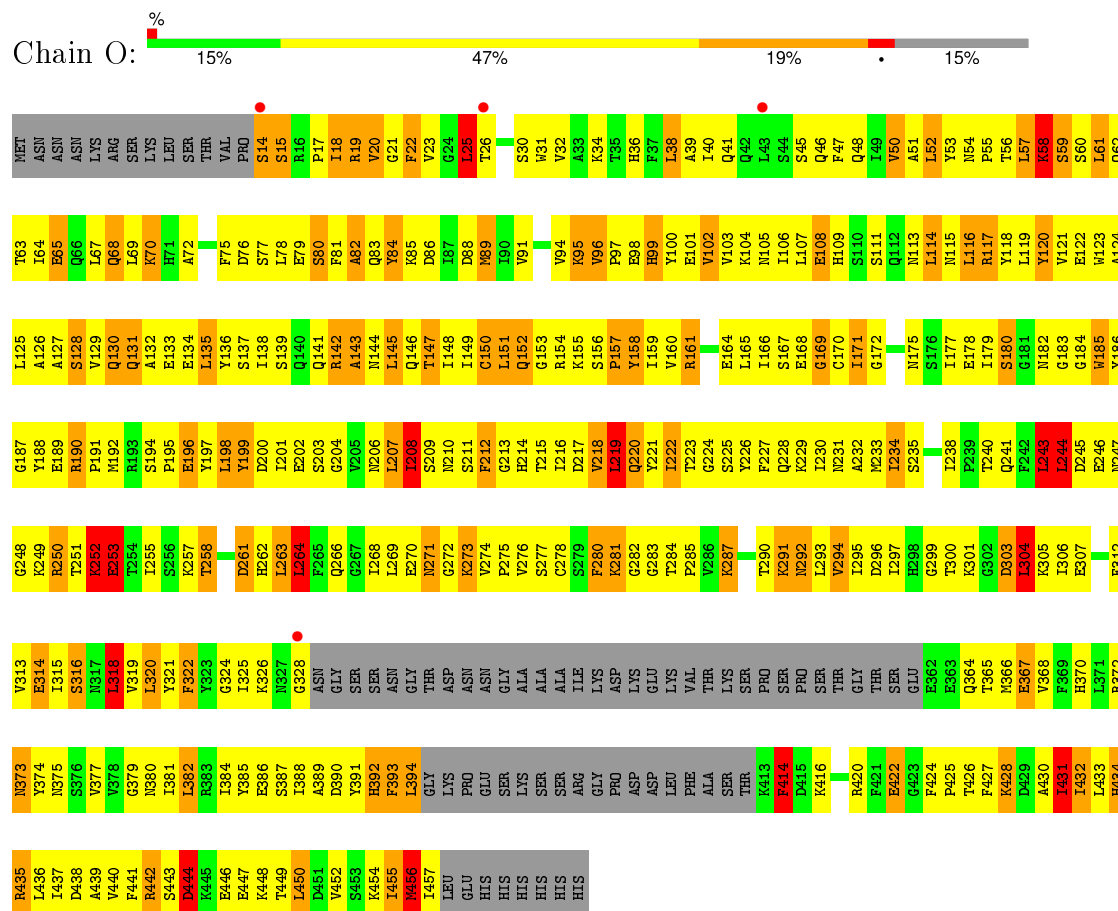


• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

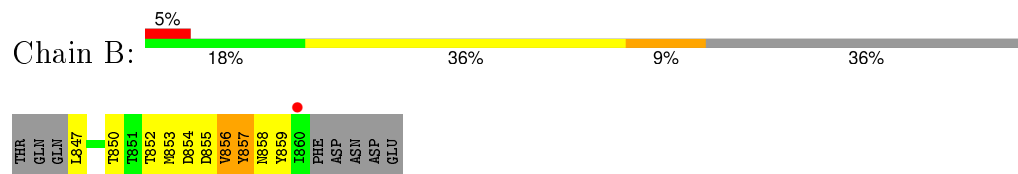




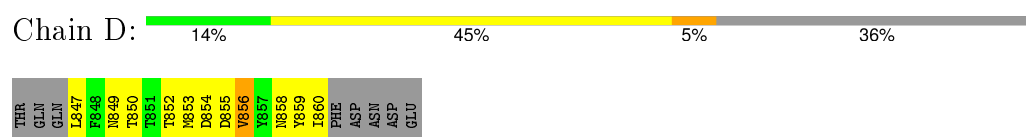
• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80



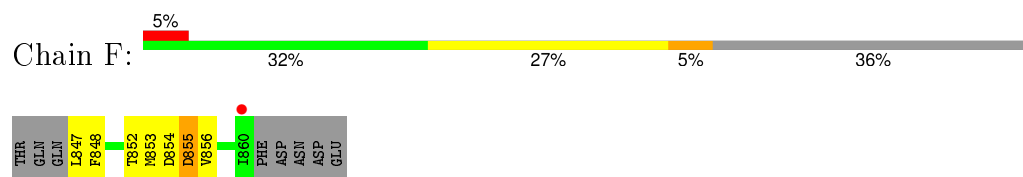
• Molecule 2: Lactose regulatory protein LAC9



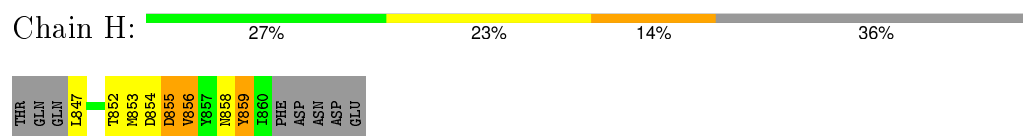
• Molecule 2: Lactose regulatory protein LAC9



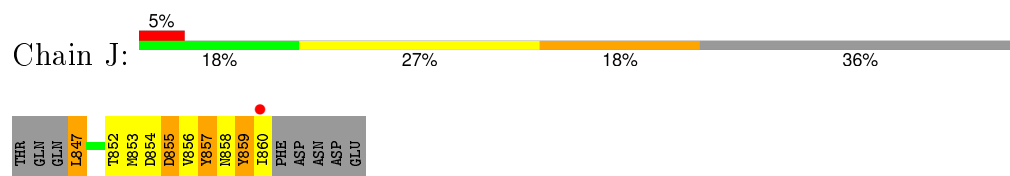
- Molecule 2: Lactose regulatory protein LAC9



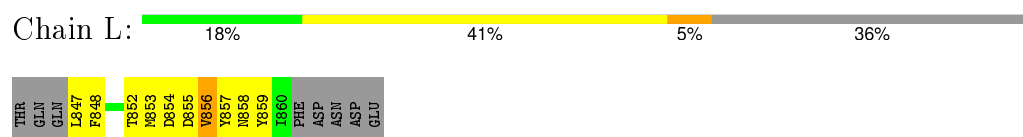
- Molecule 2: Lactose regulatory protein LAC9



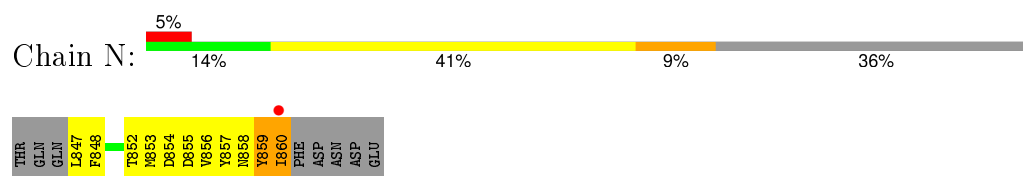
- Molecule 2: Lactose regulatory protein LAC9



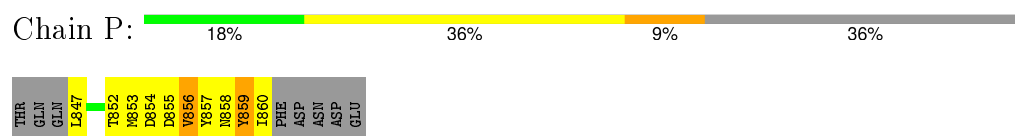
- Molecule 2: Lactose regulatory protein LAC9



- Molecule 2: Lactose regulatory protein LAC9



- Molecule 2: Lactose regulatory protein LAC9



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.10Å 160.50Å 132.60Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 48.41 – 2.99	Depositor EDS
% Data completeness (in resolution range)	88.8 (30.00-3.00) 88.3 (48.41-2.99)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.68 (at 3.01Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.228 , 0.289 0.221 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 123.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	4 of 74981 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	26057	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.86 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.8688e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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	A	1.11	7/3215 (0.2%)	1.66	65/4340 (1.5%)
1	C	0.98	7/3198 (0.2%)	1.59	46/4317 (1.1%)
1	E	1.12	5/3198 (0.2%)	1.62	45/4317 (1.0%)
1	G	1.09	11/3198 (0.3%)	1.56	37/4317 (0.9%)
1	I	1.14	8/3198 (0.3%)	1.61	57/4317 (1.3%)
1	K	1.06	4/3198 (0.1%)	1.58	50/4317 (1.2%)
1	M	1.05	4/3198 (0.1%)	1.62	53/4317 (1.2%)
1	O	0.96	1/3198 (0.0%)	1.60	48/4317 (1.1%)
2	B	0.95	0/121	1.63	0/165
2	D	1.07	0/121	1.23	0/165
2	F	0.97	0/121	1.30	1/165 (0.6%)
2	H	0.88	0/121	1.41	0/165
2	J	1.09	0/121	1.32	0/165
2	L	1.01	0/121	1.29	0/165
2	N	0.79	0/121	1.33	0/165
2	P	0.72	0/121	1.39	0/165
All	All	1.06	47/26569 (0.2%)	1.60	402/35879 (1.1%)

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	O	0	1

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	158	TYR	CD2-CE2	-6.72	1.29	1.39
1	G	158	TYR	CD2-CE2	-6.69	1.29	1.39
1	C	158	TYR	CE2-CZ	-6.55	1.30	1.38
1	A	326	LYS	CE-NZ	6.50	1.65	1.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	84	TYR	CD2-CE2	-6.30	1.29	1.39

The worst 5 of 402 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	119	LEU	CB-CG-CD2	-14.83	85.79	111.00
1	A	165	LEU	CB-CG-CD2	-12.70	89.41	111.00
1	G	38	LEU	CA-CB-CG	-12.12	87.41	115.30
1	O	38	LEU	CA-CB-CG	-10.97	90.07	115.30
1	M	165	LEU	CB-CG-CD2	-10.97	92.36	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	321	TYR	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	A	3153	0	3158	482	0
1	C	3136	0	3141	458	0
1	E	3136	0	3139	465	0
1	G	3136	0	3141	463	0
1	I	3136	0	3141	420	0
1	K	3136	0	3141	391	0
1	M	3136	0	3141	373	0
1	O	3136	0	3141	435	0
2	B	119	0	107	22	0
2	D	119	0	107	9	0
2	F	119	0	107	6	0
2	H	119	0	107	9	0
2	J	119	0	107	12	0
2	L	119	0	107	12	0
2	N	119	0	107	11	0
2	P	119	0	107	10	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	26057	0	25999	3442	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 66.

The worst 5 of 3442 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:C:452:VAL:HG13	1:C:455:ILE:CD1	1.46	1.43
1:C:452:VAL:CG1	1:C:455:ILE:HD12	1.47	1.43
1:E:198:LEU:HD13	1:E:199:TYR:CE1	1.57	1.38
1:E:194:SER:HB3	1:E:199:TYR:OH	1.20	1.27
1:I:281:LYS:HD2	1:I:282:GLY:N	1.51	1.23

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	389/465 (84%)	301 (77%)	73 (19%)	15 (4%)	4	21
1	C	387/465 (83%)	299 (77%)	71 (18%)	17 (4%)	3	18
1	E	387/465 (83%)	300 (78%)	67 (17%)	20 (5%)	2	15
1	G	387/465 (83%)	301 (78%)	75 (19%)	11 (3%)	6	30
1	I	387/465 (83%)	303 (78%)	70 (18%)	14 (4%)	4	24
1	K	387/465 (83%)	305 (79%)	66 (17%)	16 (4%)	3	20
1	M	387/465 (83%)	308 (80%)	68 (18%)	11 (3%)	6	30
1	O	387/465 (83%)	309 (80%)	67 (17%)	11 (3%)	6	30
2	B	12/22 (54%)	9 (75%)	2 (17%)	1 (8%)	1	5

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	12/22 (54%)	10 (83%)	1 (8%)	1 (8%)	1	5
2	F	12/22 (54%)	10 (83%)	2 (17%)	0	100	100
2	H	12/22 (54%)	10 (83%)	1 (8%)	1 (8%)	1	5
2	J	12/22 (54%)	11 (92%)	1 (8%)	0	100	100
2	L	12/22 (54%)	10 (83%)	1 (8%)	1 (8%)	1	5
2	N	12/22 (54%)	11 (92%)	1 (8%)	0	100	100
2	P	12/22 (54%)	9 (75%)	2 (17%)	1 (8%)	1	5
All	All	3194/3896 (82%)	2506 (78%)	568 (18%)	120 (4%)	4	22

5 of 120 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	PRO
1	A	37	PHE
1	A	42	GLN
1	A	82	ALA
1	A	201	ILE

### 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	
1	A	350/411 (85%)	251 (72%)	99 (28%)	0	2
1	C	348/411 (85%)	259 (74%)	89 (26%)	0	3
1	E	348/411 (85%)	251 (72%)	97 (28%)	0	2
1	G	348/411 (85%)	247 (71%)	101 (29%)	0	2
1	I	348/411 (85%)	254 (73%)	94 (27%)	0	3
1	K	348/411 (85%)	258 (74%)	90 (26%)	0	3
1	M	348/411 (85%)	248 (71%)	100 (29%)	0	2
1	O	348/411 (85%)	254 (73%)	94 (27%)	0	3
2	B	14/22 (64%)	13 (93%)	1 (7%)	18	54

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	14/22 (64%)	11 (79%)	3 (21%)	1	6
2	F	14/22 (64%)	13 (93%)	1 (7%)	18	54
2	H	14/22 (64%)	11 (79%)	3 (21%)	1	6
2	J	14/22 (64%)	9 (64%)	5 (36%)	0	1
2	L	14/22 (64%)	12 (86%)	2 (14%)	4	19
2	N	14/22 (64%)	11 (79%)	3 (21%)	1	6
2	P	14/22 (64%)	12 (86%)	2 (14%)	4	19
All	All	2898/3464 (84%)	2114 (73%)	784 (27%)	0	2

5 of 784 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	276	VAL
1	I	214	HIS
1	O	185	TRP
1	G	314	GLU
1	I	22	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	41	GLN
1	I	105	ASN
1	O	152	GLN
1	G	105	ASN
1	G	220	GLN

### 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 [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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	395/465 (84%)	-0.18	2 (0%) 91 76	5, 40, 76, 100	0
1	C	393/465 (84%)	-0.37	3 (0%) 87 67	2, 34, 76, 100	0
1	E	393/465 (84%)	-0.10	6 (1%) 76 49	2, 42, 78, 100	0
1	G	393/465 (84%)	-0.41	1 (0%) 94 84	4, 35, 72, 100	0
1	I	393/465 (84%)	-0.15	3 (0%) 87 67	4, 41, 76, 100	0
1	K	393/465 (84%)	-0.30	3 (0%) 87 67	1, 39, 74, 100	0
1	M	393/465 (84%)	-0.22	4 (1%) 84 60	5, 41, 76, 100	0
1	O	393/465 (84%)	-0.28	4 (1%) 84 60	4, 39, 78, 93	0
2	B	14/22 (63%)	0.15	1 (7%) 19 7	42, 59, 84, 85	0
2	D	14/22 (63%)	-0.12	0 100 100	21, 55, 77, 80	0
2	F	14/22 (63%)	0.11	1 (7%) 19 7	29, 59, 77, 91	0
2	H	14/22 (63%)	-0.46	0 100 100	25, 42, 75, 78	0
2	J	14/22 (63%)	0.12	1 (7%) 19 7	13, 54, 74, 90	0
2	L	14/22 (63%)	-0.09	0 100 100	23, 59, 88, 100	0
2	N	14/22 (63%)	0.11	1 (7%) 19 7	15, 53, 71, 81	0
2	P	14/22 (63%)	-0.20	0 100 100	19, 50, 86, 98	0
All	All	3258/3896 (83%)	-0.24	30 (0%) 85 64	1, 39, 77, 100	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	328	GLY	5.3
1	C	328	GLY	5.0
1	K	328	GLY	4.4
1	O	328	GLY	3.4
1	I	251	THR	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 carbohydrates 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.