



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:30 AM UTC

PDB ID : 3E1K / pdb_00003e1k
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

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

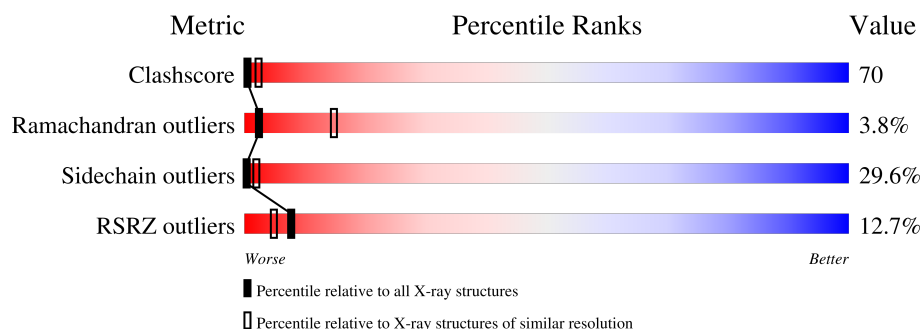
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



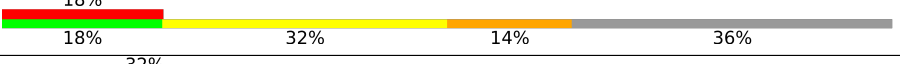
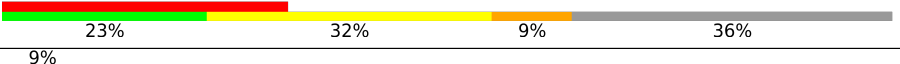
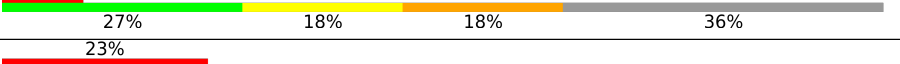
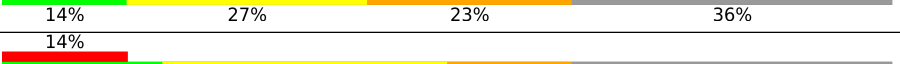
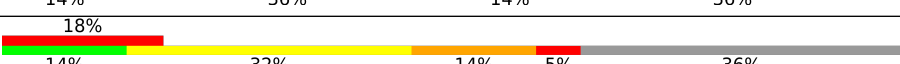
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 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	465	14% 9% 41% 29% 6% 15%
1	C	465	7% 8% 41% 30% 5% 15%
1	E	465	16% 9% 40% 28% 7% 15%
1	G	465	5% 8% 42% 27% 8% 15%
1	I	465	13% 11% 41% 27% 6% 15%
1	K	465	8% 12% 36% 31% 5% 15%
1	M	465	12% 14% 39% 28% • 15%

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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

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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

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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

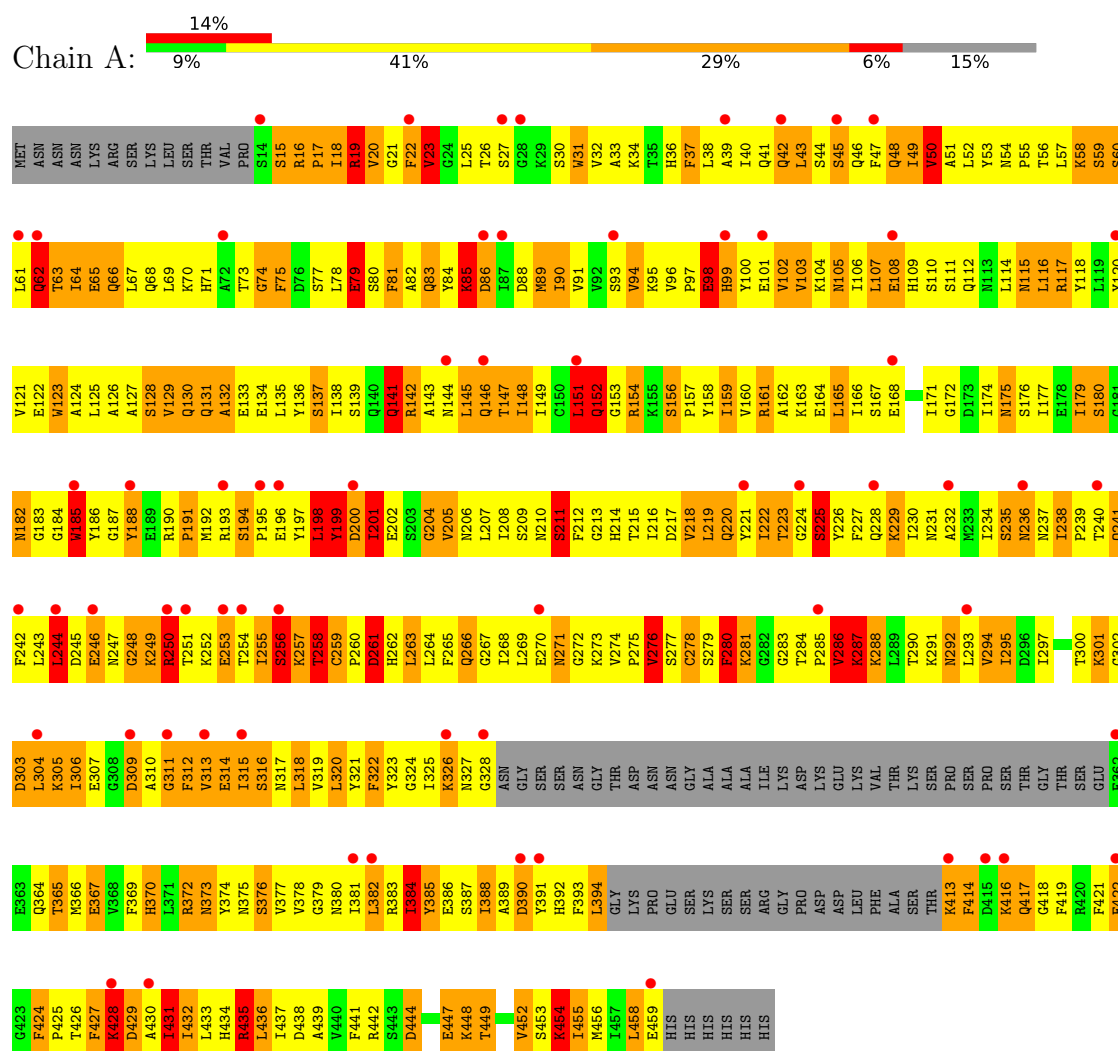
- Molecule 2 is a protein called Lactose regulatory protein LAC9.

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			

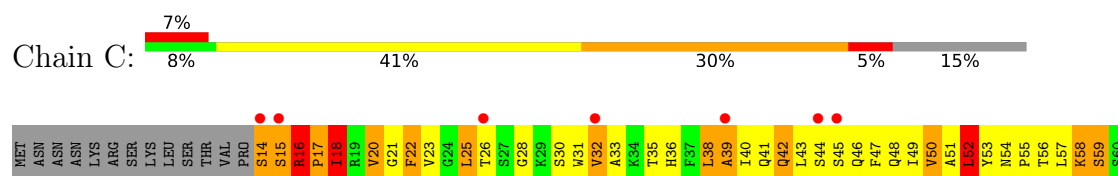
3 Residue-property plots

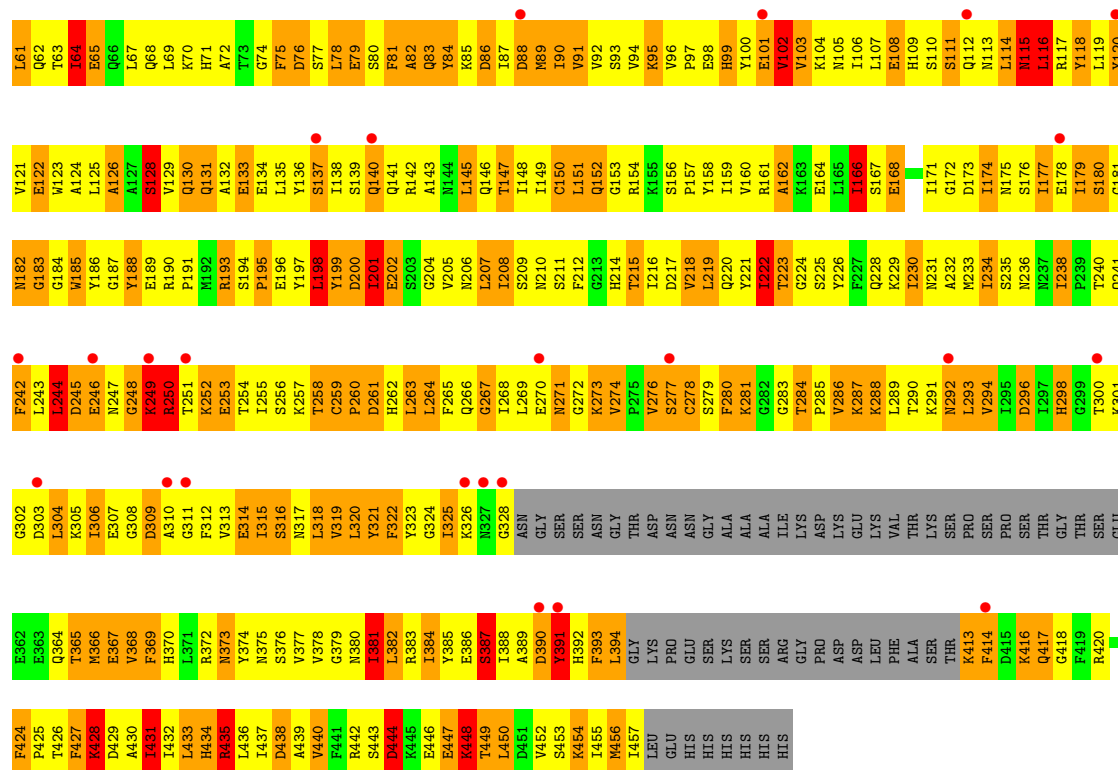
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Galactose/lactose metabolism regulatory protein GAL80

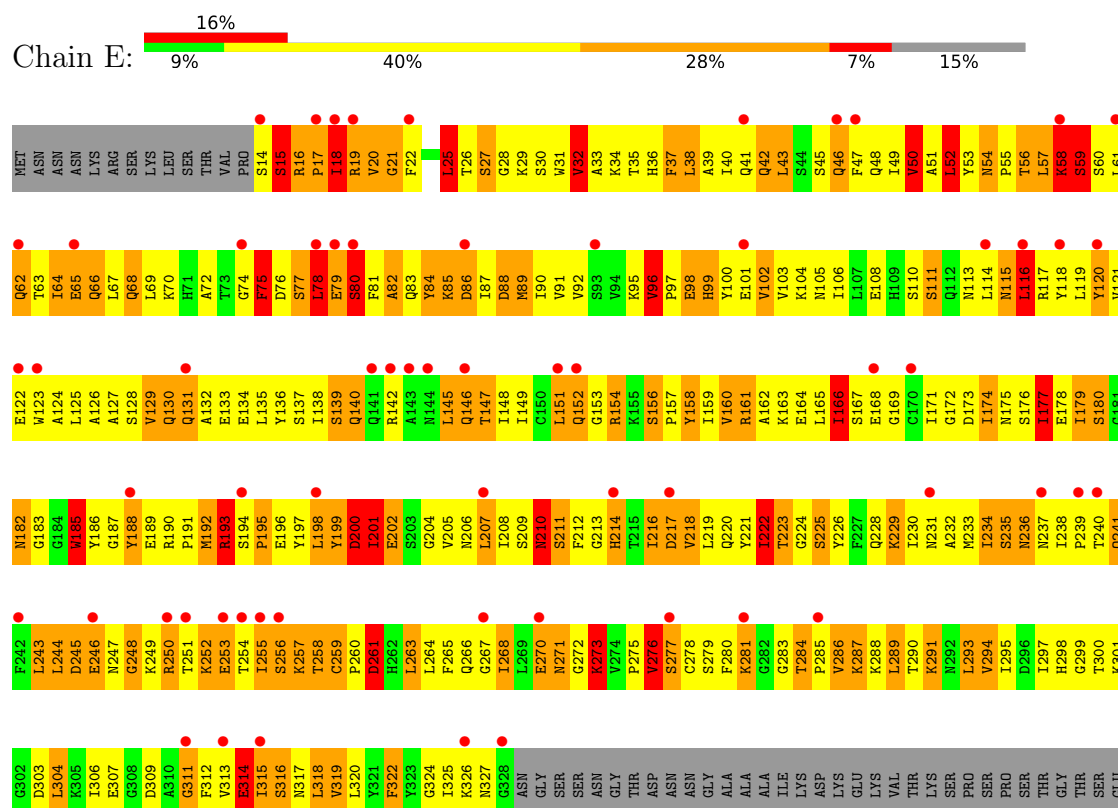


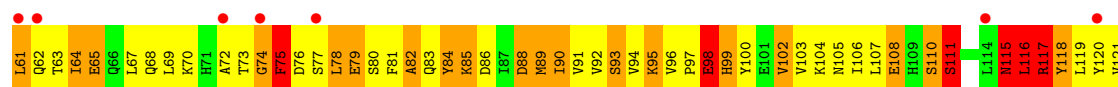
- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

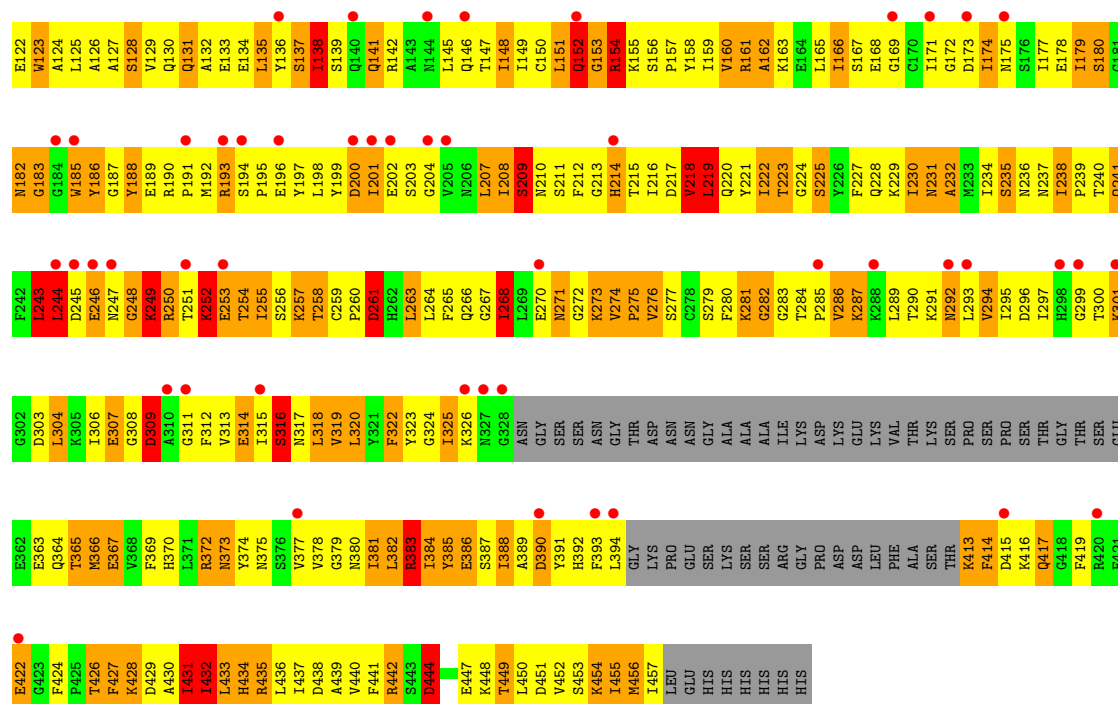




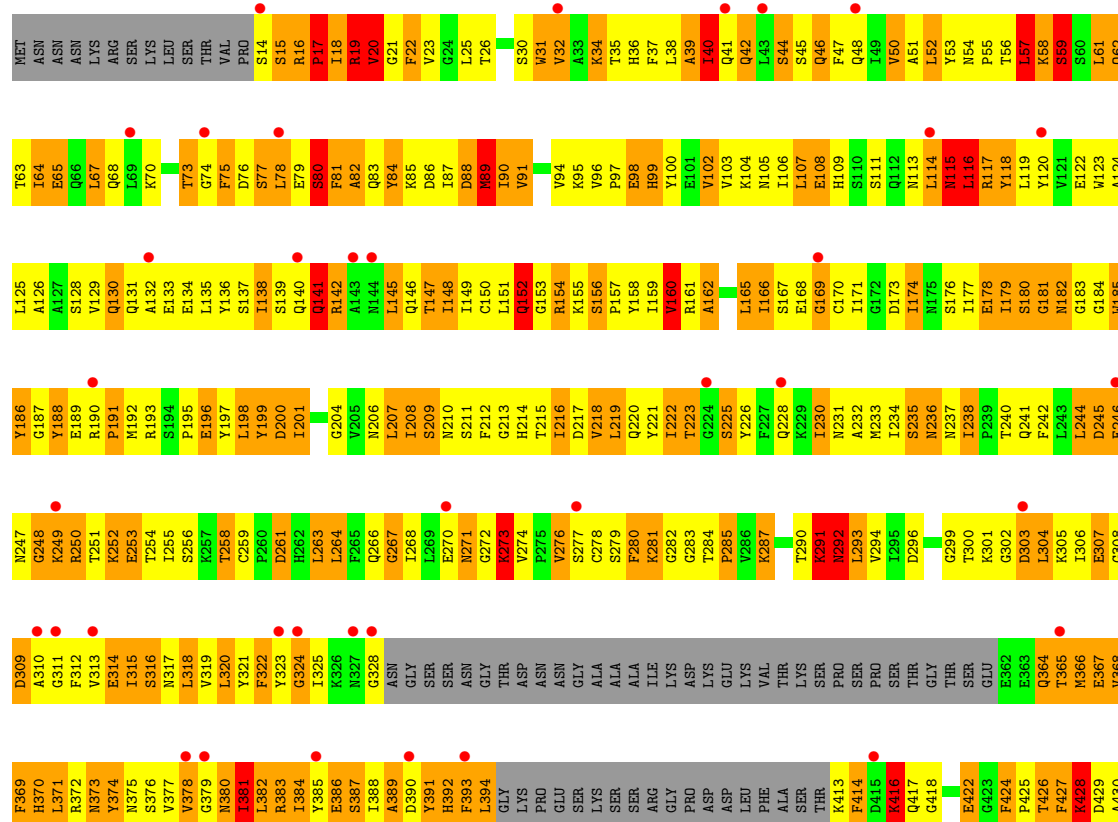
● Molecule 1: Galactose/lactose metabolism regulatory protein GAL80





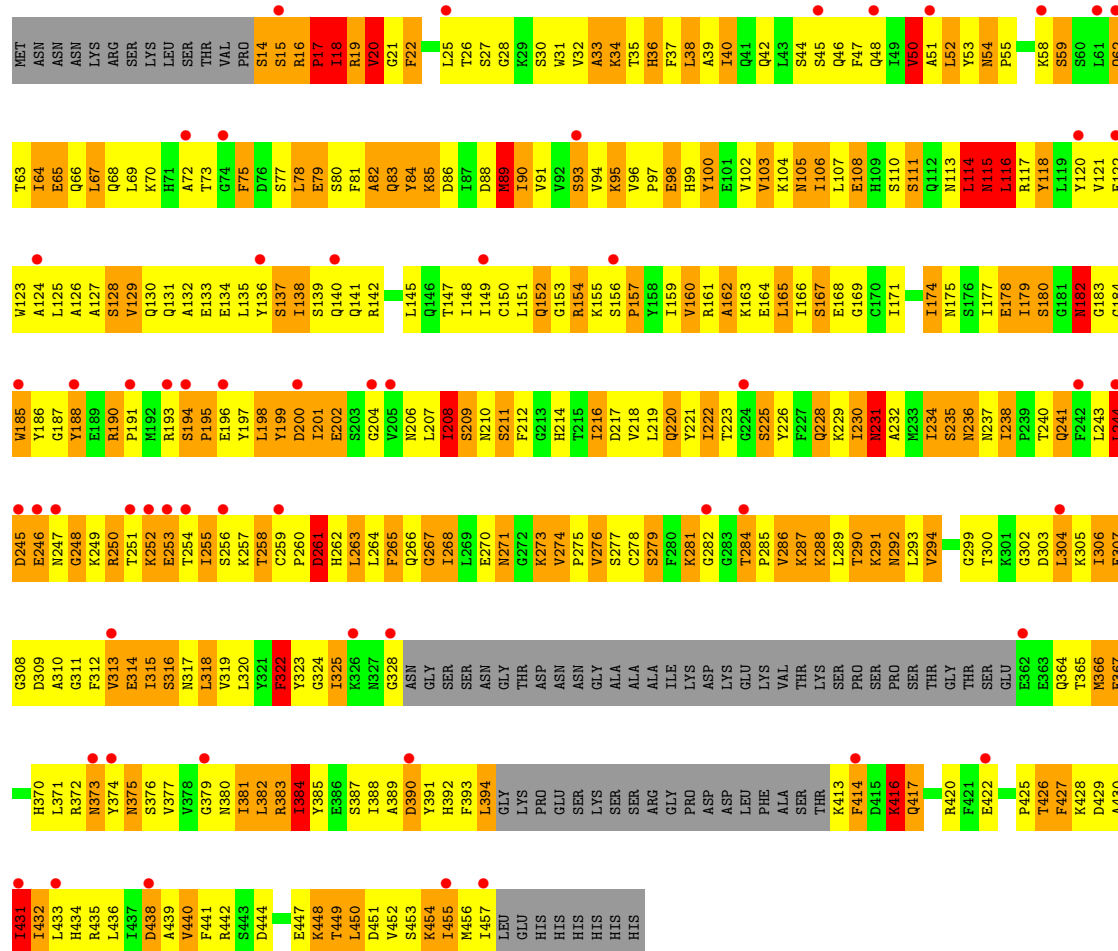


● Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

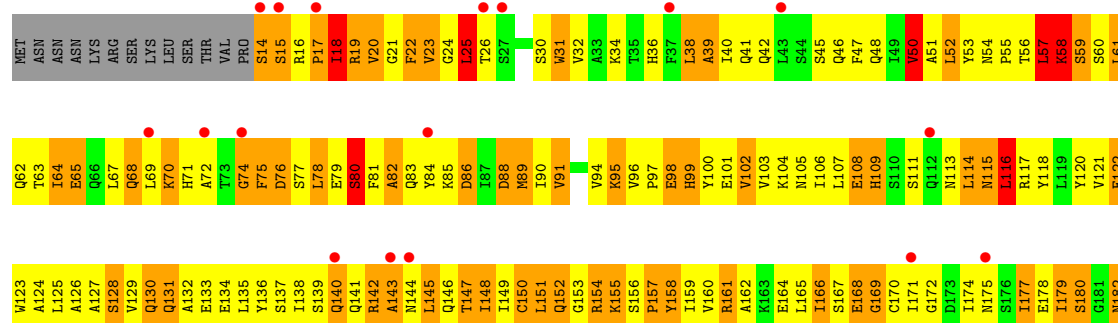


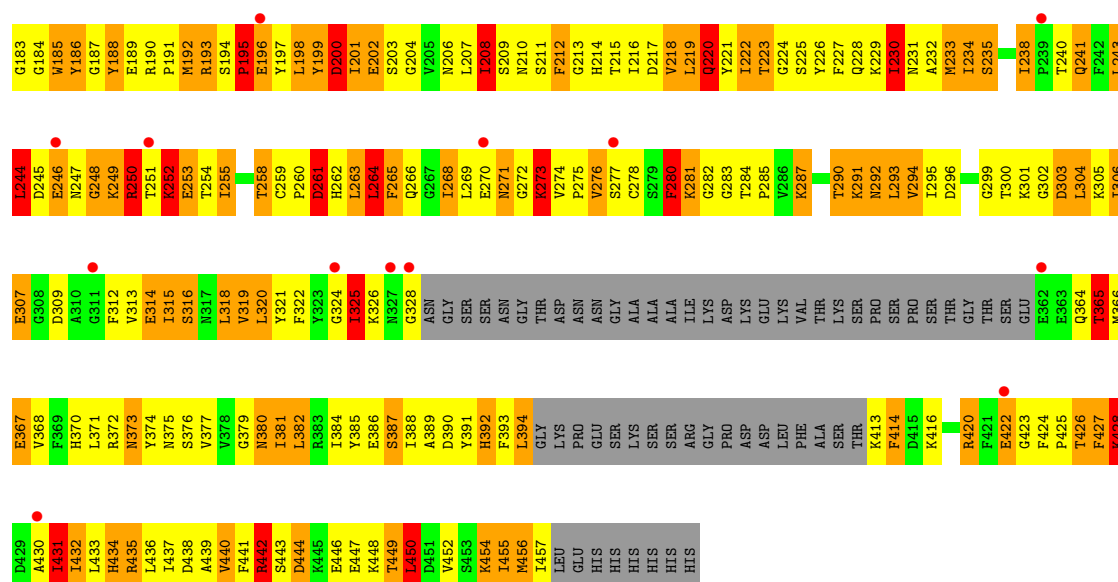


• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80



• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80





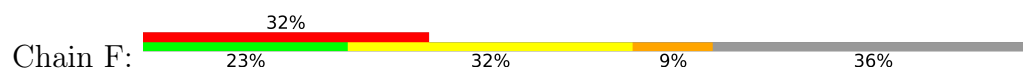
• Molecule 2: Lactose regulatory protein LAC9



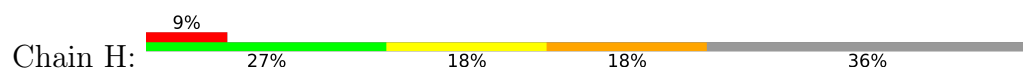
• Molecule 2: Lactose regulatory protein LAC9



• Molecule 2: Lactose regulatory protein LAC9



• Molecule 2: Lactose regulatory protein LAC9



• Molecule 2: Lactose regulatory protein LAC9

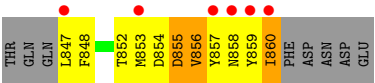




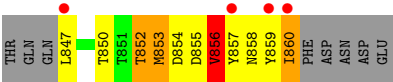
● Molecule 2: Lactose regulatory protein LAC9



● 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, α , β , γ	101.10Å 160.50Å 132.60Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.8 (30.00-3.00) 88.6 (30.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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.	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 113.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	26057	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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 ⓘ

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	1.32	11/3215 (0.3%)	2.08	140/4340 (3.2%)
1	C	1.18	5/3198 (0.2%)	2.11	144/4317 (3.3%)
1	E	1.36	17/3198 (0.5%)	2.07	141/4317 (3.3%)
1	G	1.30	13/3198 (0.4%)	2.09	140/4317 (3.2%)
1	I	1.33	9/3198 (0.3%)	2.13	142/4317 (3.3%)
1	K	1.30	15/3198 (0.5%)	2.10	150/4317 (3.5%)
1	M	1.29	6/3198 (0.2%)	2.06	116/4317 (2.7%)
1	O	1.18	9/3198 (0.3%)	2.09	131/4317 (3.0%)
2	B	0.93	0/121	1.81	0/165
2	D	1.05	0/121	1.54	3/165 (1.8%)
2	F	0.97	0/121	1.67	4/165 (2.4%)
2	H	0.94	0/121	1.60	1/165 (0.6%)
2	J	1.04	0/121	1.66	1/165 (0.6%)
2	L	1.16	1/121 (0.8%)	1.57	1/165 (0.6%)
2	N	1.00	0/121	1.60	1/165 (0.6%)
2	P	0.90	0/121	1.78	4/165 (2.4%)
All	All	1.28	86/26569 (0.3%)	2.08	1119/35879 (3.1%)

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 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	216	ILE	CA-CB	-11.77	1.41	1.54
1	K	40	ILE	CA-CB	-8.27	1.44	1.54
1	A	132	ALA	CA-CB	-8.25	1.40	1.53
1	E	200	ASP	CA-C	-8.05	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	151	LEU	CA-C	-7.49	1.45	1.53

The worst 5 of 1119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	220	GLN	N-CA-C	-18.09	91.60	111.14
1	C	220	GLN	N-CA-C	-17.27	92.48	111.14
1	O	102	VAL	N-CA-C	16.79	129.76	110.62
1	K	220	GLN	N-CA-C	-15.31	94.69	111.07
1	K	18	ILE	N-CA-C	-15.25	92.98	110.21

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	502	0
1	C	3136	0	3141	483	0
1	E	3136	0	3139	488	0
1	G	3136	0	3141	496	0
1	I	3136	0	3141	443	0
1	K	3136	0	3141	411	0
1	M	3136	0	3141	388	0
1	O	3136	0	3141	454	0
2	B	119	0	107	19	0
2	D	119	0	107	9	0
2	F	119	0	107	8	0
2	H	119	0	107	10	0
2	J	119	0	107	13	0
2	L	119	0	107	12	0
2	N	119	0	107	11	0
2	P	119	0	107	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	26057	0	25999	3622	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 70.

The worst 5 of 3622 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%)	2	14
1	C	387/465 (83%)	299 (77%)	71 (18%)	17 (4%)	2	12
1	E	387/465 (83%)	300 (78%)	67 (17%)	20 (5%)	1	9
1	G	387/465 (83%)	301 (78%)	75 (19%)	11 (3%)	4	21
1	I	387/465 (83%)	303 (78%)	70 (18%)	14 (4%)	2	16
1	K	387/465 (83%)	305 (79%)	66 (17%)	16 (4%)	2	13
1	M	387/465 (83%)	308 (80%)	68 (18%)	11 (3%)	4	21
1	O	387/465 (83%)	309 (80%)	67 (17%)	11 (3%)	4	21
2	B	12/22 (54%)	9 (75%)	2 (17%)	1 (8%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	12/22 (54%)	10 (83%)	1 (8%)	1 (8%)	0	3
2	F	12/22 (54%)	10 (83%)	2 (17%)	0	100	100
2	H	12/22 (54%)	10 (83%)	1 (8%)	1 (8%)	0	3
2	J	12/22 (54%)	11 (92%)	1 (8%)	0	100	100
2	L	12/22 (54%)	10 (83%)	1 (8%)	1 (8%)	0	3
2	N	12/22 (54%)	11 (92%)	1 (8%)	0	100	100
2	P	12/22 (54%)	9 (75%)	2 (17%)	1 (8%)	0	3
All	All	3194/3896 (82%)	2506 (78%)	568 (18%)	120 (4%)	2	15

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%)	240 (69%)	110 (31%)	0	1
1	C	348/411 (85%)	248 (71%)	100 (29%)	0	2
1	E	348/411 (85%)	243 (70%)	105 (30%)	0	1
1	G	348/411 (85%)	238 (68%)	110 (32%)	0	1
1	I	348/411 (85%)	243 (70%)	105 (30%)	0	1
1	K	348/411 (85%)	248 (71%)	100 (29%)	0	2
1	M	348/411 (85%)	248 (71%)	100 (29%)	0	2
1	O	348/411 (85%)	244 (70%)	104 (30%)	0	2
2	B	14/22 (64%)	11 (79%)	3 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	14/22 (64%)	12 (86%)	2 (14%)	3	16
2	F	14/22 (64%)	12 (86%)	2 (14%)	3	16
2	H	14/22 (64%)	11 (79%)	3 (21%)	1	6
2	J	14/22 (64%)	8 (57%)	6 (43%)	0	0
2	L	14/22 (64%)	12 (86%)	2 (14%)	3	16
2	N	14/22 (64%)	11 (79%)	3 (21%)	1	6
2	P	14/22 (64%)	11 (79%)	3 (21%)	1	6
All	All	2898/3464 (84%)	2040 (70%)	858 (30%)	0	2

5 of 858 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	111	SER
1	K	114	LEU
1	O	202	GLU
1	I	174	ILE
1	I	108	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	228	GLN
1	M	62	GLN
1	I	236	ASN
1	K	115	ASN
1	M	241	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 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

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, 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	395/465 (84%)	1.05	64 (16%) 4 3	5, 40, 76, 100	0
1	C	393/465 (84%)	0.78	31 (7%) 18 10	2, 34, 76, 100	0
1	E	393/465 (84%)	1.19	75 (19%) 3 2	2, 42, 78, 100	0
1	G	393/465 (84%)	0.58	23 (5%) 28 14	4, 35, 72, 100	0
1	I	393/465 (84%)	1.02	61 (15%) 5 3	4, 41, 76, 100	0
1	K	393/465 (84%)	0.82	38 (9%) 13 7	1, 39, 74, 100	0
1	M	393/465 (84%)	1.04	57 (14%) 6 3	5, 41, 76, 100	0
1	O	393/465 (84%)	0.75	30 (7%) 20 10	4, 39, 78, 93	0
2	B	14/22 (63%)	1.91	4 (28%) 1 1	42, 59, 84, 85	0
2	D	14/22 (63%)	1.22	4 (28%) 1 1	21, 55, 77, 80	0
2	F	14/22 (63%)	2.03	7 (50%) 0 0	29, 59, 77, 91	0
2	H	14/22 (63%)	0.86	2 (14%) 6 3	25, 42, 75, 78	0
2	J	14/22 (63%)	1.90	5 (35%) 1 1	13, 54, 74, 90	0
2	L	14/22 (63%)	1.40	3 (21%) 2 1	23, 59, 88, 100	0
2	N	14/22 (63%)	1.82	6 (42%) 0 1	15, 53, 70, 81	0
2	P	14/22 (63%)	1.43	4 (28%) 1 1	19, 50, 86, 98	0
All	All	3258/3896 (83%)	0.93	414 (12%) 8 5	1, 39, 77, 100	0

The worst 5 of 414 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	328	GLY	7.5
1	K	328	GLY	6.9
1	M	251	THR	6.7
2	F	860	ILE	6.6
1	C	328	GLY	6.5

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 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.