W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 23, 2023 – 06:41 AM EDT

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)

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

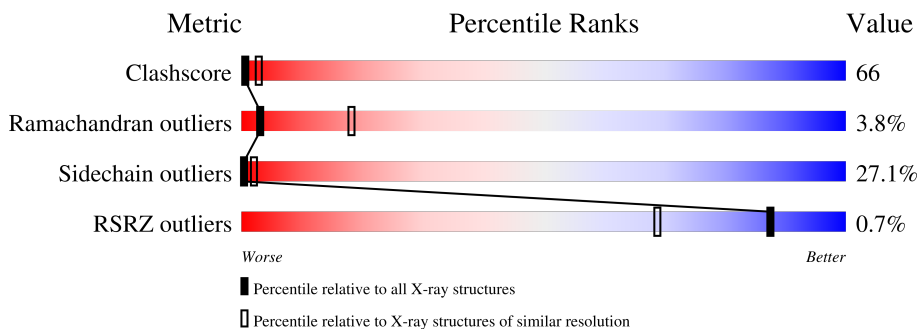|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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	Percentile Ranks	Value
Clashscore		66
Ramachandran outliers		3.8%
Sidechain outliers		27.1%
RSRZ outliers		0.7%

Worse ... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 <=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	13% 45% 24% • 15%
1	C	465	14% 46% 22% • 15%
1	E	465	% 14% 47% 21% • 15%
1	G	465	12% 49% 20% • 15%
1	I	465	15% 46% 19% • 15%
1	K	465	19% 41% 22% • 15%
1	M	465	% 17% 44% 22% • 15%

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Mol	Chain	Length	Quality of chain
1	O	465	15% 47% 19% 15%
2	B	22	5% 18% 36% 9% 36%
2	D	22	14% 45% 5% 36%
2	F	22	5% 32% 27% 5% 36%
2	H	22	27% 23% 14% 36%
2	J	22	5% 18% 27% 18% 36%
2	L	22	18% 41% 5% 36%
2	N	22	5% 14% 41% 9% 36%
2	P	22	18% 36% 9% 36%

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.

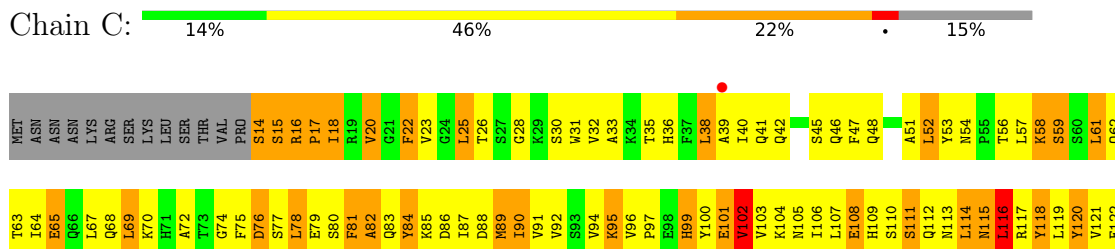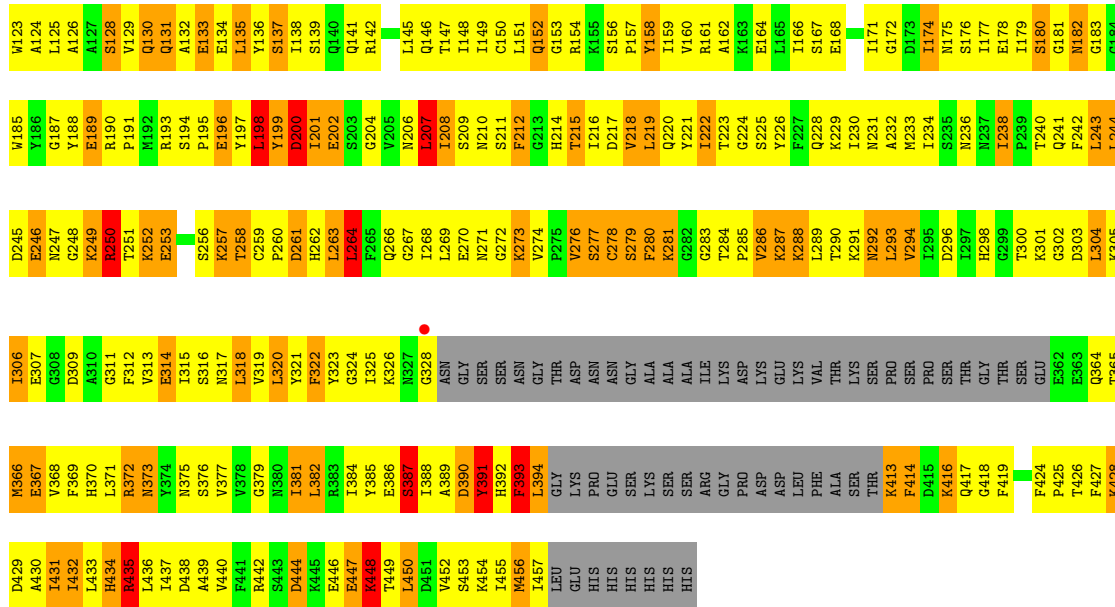| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total 119	C 77	N 16	O 25	S 1	0	0	0
2	D	14	Total 119	C 77	N 16	O 25	S 1	0	0	0
2	F	14	Total 119	C 77	N 16	O 25	S 1	0	0	0
2	H	14	Total 119	C 77	N 16	O 25	S 1	0	0	0
2	J	14	Total 119	C 77	N 16	O 25	S 1	0	0	0
2	L	14	Total 119	C 77	N 16	O 25	S 1	0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

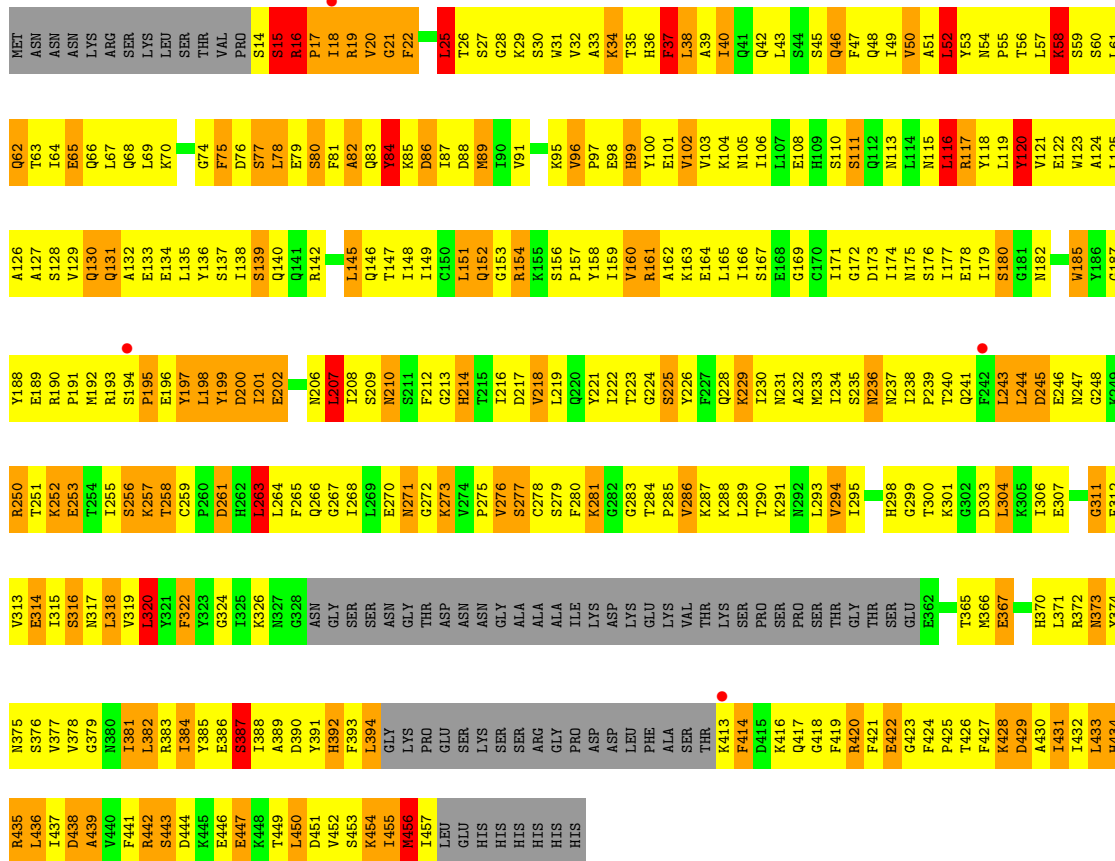- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

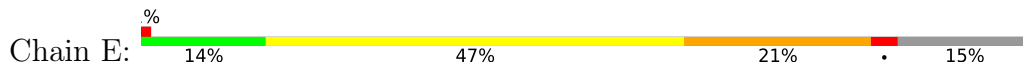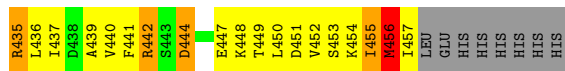• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

Chain G:

• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

Chain I:

N375 S376 V377 V378 G379 N380 I381 L382 R383 I384 Y385 E386 S387 I388 A389 D390 Y391 H392 F393 L394 GLY LYS PRO GLU SER LYS SER SER ARG GLY PRO ASP ASP LEU PHE ALA SER THR K413 F414 D415 K416 Q417 G418 F419 R420 F421 E422 G423 F424 P425 T426 F427 K428 D429 A430 I431 I432 L433 H434

R435 L436 I437 D438 A439 V440 F441 R442 S443 D444 E447 K448 T449 L450 D451 V452 S453 K454 I455 M456 I457 LEU GLU HIS HIS HIS HIS HIS HIS
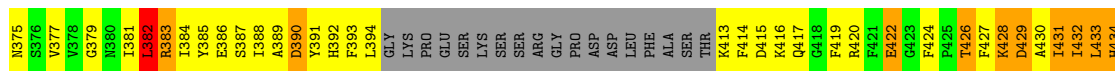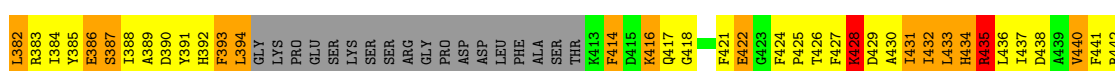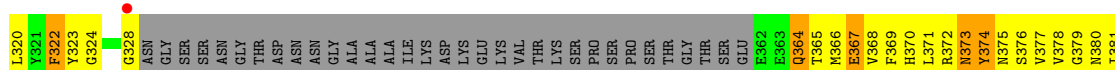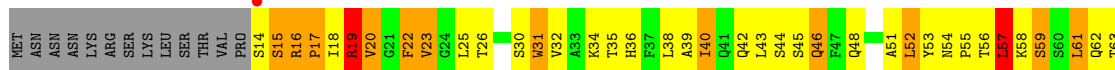
• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

Chain K: 19% 41% 22% • 15%

MET ASN ASN LYS ARG SER LYS LEU SER THR VAL PRO S14 S15 R16 P17 I18 R19 V20 G21 F22 V23 G24 L25 T26 S30 W31 V32 A33 K34 T35 H36 F37 L38 A39 I40 Q41 Q42 L43 S44 S45 Q46 F47 Q48 A51 L52 Y53 N54 P55 T56 L57 K58 S59 S60 L61 Q62 T63

I64 E65 Q66 L67 Q68 L69 K70 T73 G74 F75 D76 S77 L78 E79 S80 F81 A82 Q83 Y84 K85 D86 M89 I87 D88 I90 V91 V94 K95 V96 P97 E98 H99 Y100 E101 V102 V103 K104 N106 L107 E108 S111 Q112 N113 L114 N115 L116 R117 Y118 L119 Y120 W123 A124 L125 A126

V129 Q130 Q131 A132 E133 E134 L135 Y136 S137 I138 S139 G140 Q141 R142 L145 Q146 T147 I148 I149 C150 L151 Q152 G153 R154 K155 S156 P157 Y158 I159 V160 R161 A162 L165 I166 S167 E168 G169 C170 I171 I174 N175 S176 I177 E178 I179 S180 G181 N182 G183 G184 W185 Y186 G187 Y188 E189 R190 P191

M192 P195 E196 Y197 L198 Y199 D200 I201 G204 V205 N206 L207 I208 S209 N210 S211 F212 G213 H214 T215 I216 D217 V218 L219 Q220 Y221 I222 T223 G224 S225 Y226 F227 Q228 K229 I230 N231 A232 M233 I234 S235 N236 N237 I238 P239 T240 Q241 F242 L243 L244 D245 E246 N247 G248 R250 K249 T251 K252 E253

S256 K257 T258 D261 H262 L263 F264 F265 Q266 G267 I268 L269 E270 N271 G272 K273 V274 P275 V276 S277 C278 S279 F280 K281 G282 G283 T284 P285 V286 K287 T290 K291 N292 L293 V294 I295 D296 G299 T300 K301 G302 D303 L304 K305 I306 E307 C311 F312 V313 E314 I315 S316 N317 L318 V319

L320 Y321 F322 Y323 G324 G328 ASN GLY SER ASN GLY THR ASP ASN ASN GLY ALA ALA ALA ILE LYS ASP LYS GLU LYS VAL THR LYS SER PRO SER PRO SER THR GLY THR SER GLU E362 E363 Q364 T365 M366 E367 V368 F369 H370 L371 R372 N373 Y374 N375 S376 V377 V378 G379 N380 I381

L382 R383 I384 Y385 E386 S387 I388 A389 D390 Y391 H392 F393 L394 GLY LYS PRO GLU SER LYS SER SER ARG GLY PRO ASP ASP LEU PHE ALA SER THR K413 F414 D415 K416 Q417 G418 F421 E422 G423 F424 P425 T426 F427 K428 D429 A430 I431 I432 L433 H434 R435 L436 I437 D438 A439 V440 F441 R442

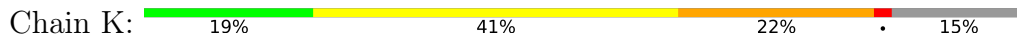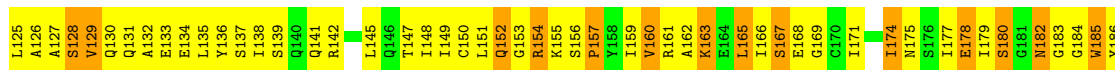S443 D444 E447 K448 T449 L450 D451 V452 S453 K454 I455 M456 I457 LEU GLU HIS HIS HIS HIS HIS HIS
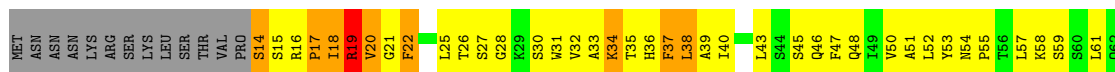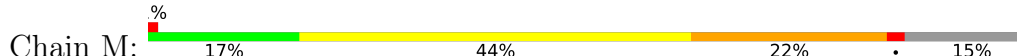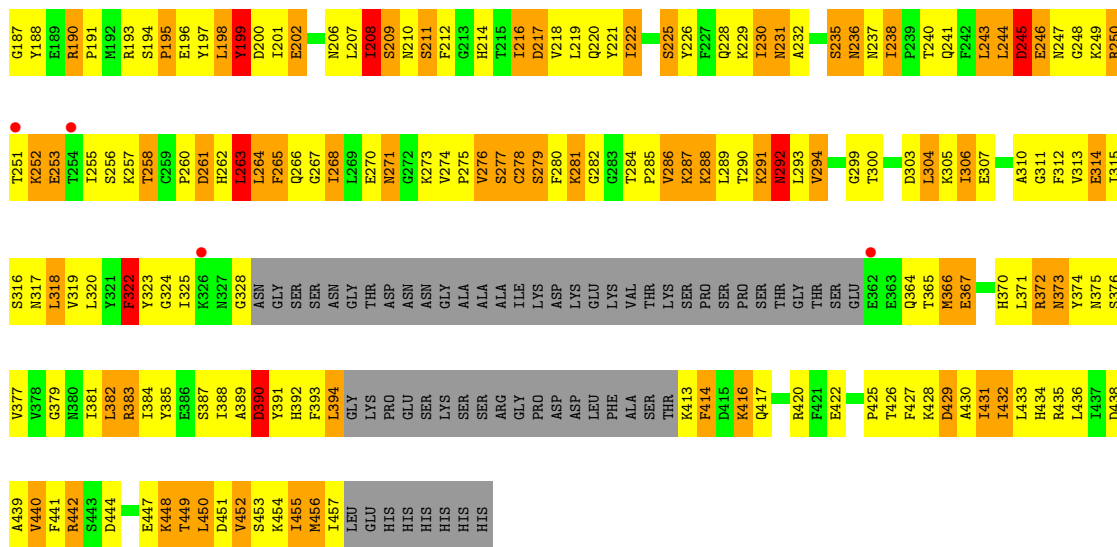
• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

Chain M: %　17% 44% 22% • 15%

MET ASN ASN LYS ARG SER LYS LEU SER THR VAL PRO S14 S15 R16 P17 I18 R19 V20 G21 F22 L25 T26 S27 G28 K29 S30 W31 V32 A33 K34 T35 H36 F37 L38 A39 I40 L43 S44 S45 Q46 F47 Q48 I49 V50 A51 L52 Y53 N54 P55 T56 L57 K58 S59 S60 L61 Q62

T63 I64 E65 Q66 L67 Q68 L69 K70 H71 A72 F75 D76 S77 L78 E79 S80 F81 A82 Q83 Y84 K85 D86 M89 I90 V91 V92 S93 V94 K95 V96 P97 E98 H99 Y100 E101 V102 V103 K104 N105 I106 L107 E108 H109 S110 S111 Q112 N113 L114 N115 L116 R117 Y118 L119 Y120 V121 E122 W123 A124

L125 A126 A127 S128 V129 Q130 Q131 A132 E133 E134 L135 Y136 I138 S137 S139 Q140 Q141 R142 L145 Q146 T147 I148 I149 C150 L151 Q152 G153 R154 K155 S156 P157 Y158 I159 V160 R161 A162 K163 E164 L165 I166 S167 E168 G169 C170 I171 I174 N175 S176 I177 E178 I179 S180 G181 N182 G183 G184 W185 Y186

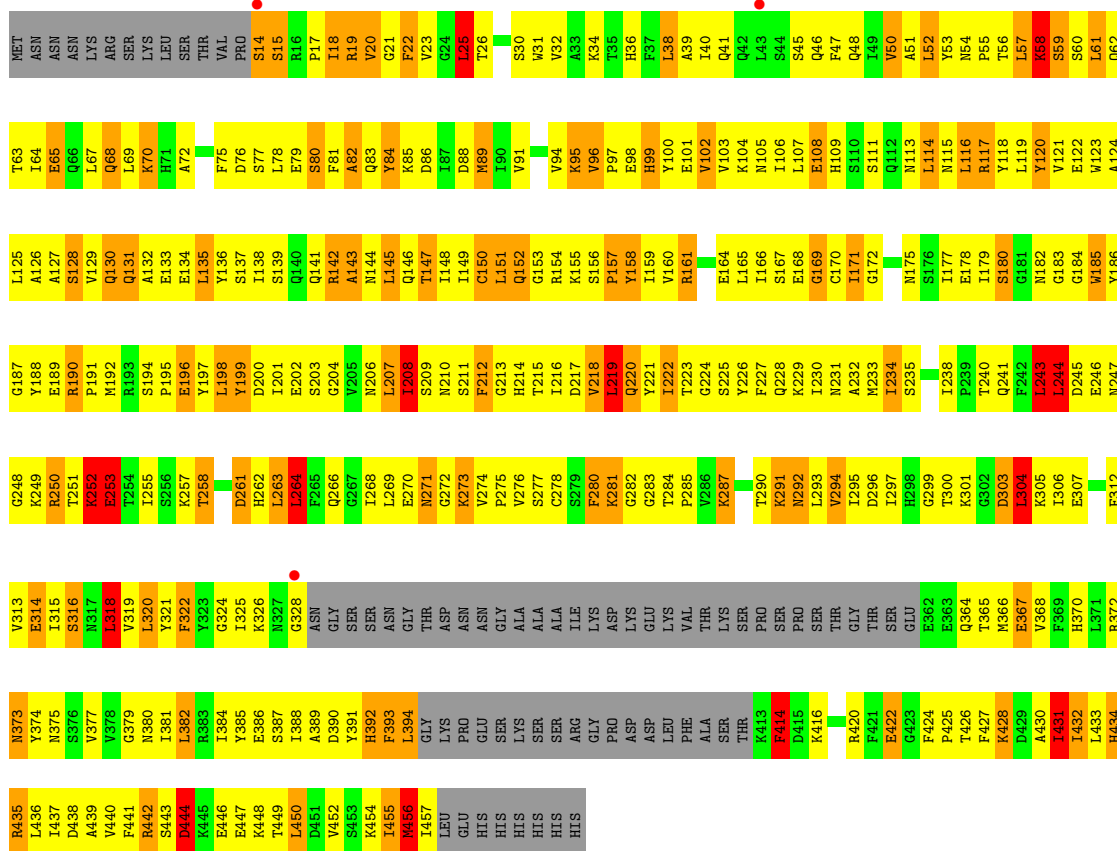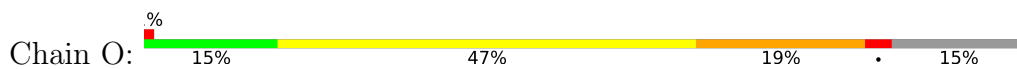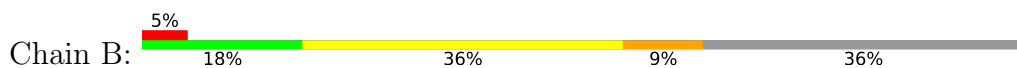• Molecule 1: Galactose/lactose metabolism regulatory protein GAL80
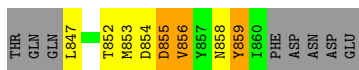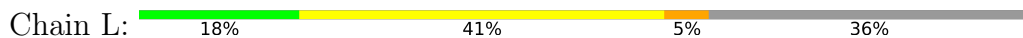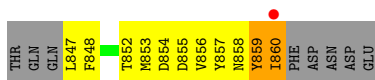
• Molecule 2: Lactose regulatory protein LAC9

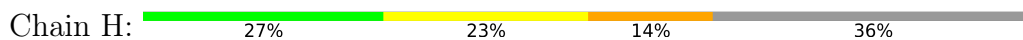THR GLN GLN L847 T850 T851 T852 M853 D854 D855 V856 Y857 N858 Y859 I860 PHE ASP ASN ASP GLU

• Molecule 2: Lactose regulatory protein LAC9

Chain D: 14% 45% 5% 36%

THR GLN GLN L847 F848 N849 T850 T851 T852 M853 D854 D855 V856 Y857 N858 Y859 I860 PHE ASP ASN ASP GLU

• Molecule 2: Lactose regulatory protein LAC9

Chain F: 5% 32% 27% 5% 36%

THR GLN GLN L847 F848 T852 M853 D854 D855 V856 I860 PHE ASP ASN ASP GLU

• Molecule 2: Lactose regulatory protein LAC9

Chain H: 27% 23% 14% 36%

THR GLN GLN L847 T852 M853 D854 D855 V856 Y857 N858 Y859 I860 PHE ASP ASN ASP GLU

• Molecule 2: Lactose regulatory protein LAC9

Chain J: 5% 18% 27% 18% 36%

THR GLN GLN L847 T852 M853 D854 D855 V856 Y857 N858 Y859 I860 PHE ASP ASN ASP GLU

• Molecule 2: Lactose regulatory protein LAC9

Chain L: 18% 41% 5% 36%

THR GLN GLN L847 F848 T852 M853 D854 D855 V856 Y857 N858 Y859 I860 PHE ASP ASN ASP GLU

• Molecule 2: Lactose regulatory protein LAC9

Chain N: 5% 14% 41% 9% 36%

THR GLN GLN L847 F848 T852 M853 D854 D855 V856 Y857 N858 Y859 I860 PHE ASP ASN ASP GLU

• Molecule 2: Lactose regulatory protein LAC9

Chain P: 18% 36% 9% 36%

THR GLN GLN L847 T852 M853 D854 D855 V856 Y857 N858 Y859 I860 PHE ASP ASN ASP GLU

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 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
$< I/\sigma(I) >$ [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)	0.32 , 123.2	EDS
L-test for twinning[2]	$< |L| > = 0.44$, $< L^2 > = 0.27$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	1.11	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

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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(^{o})	Ideal(^{o})
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

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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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	3	17
1	C	387/465 (83%)	299 (77%)	71 (18%)	17 (4%)	2	15
1	E	387/465 (83%)	300 (78%)	67 (17%)	20 (5%)	2	12
1	G	387/465 (83%)	301 (78%)	75 (19%)	11 (3%)	5	25
1	I	387/465 (83%)	303 (78%)	70 (18%)	14 (4%)	3	19
1	K	387/465 (83%)	305 (79%)	66 (17%)	16 (4%)	3	16
1	M	387/465 (83%)	308 (80%)	68 (18%)	11 (3%)	5	25
1	O	387/465 (83%)	309 (80%)	67 (17%)	11 (3%)	5	25
2	B	12/22 (54%)	9 (75%)	2 (17%)	1 (8%)	1	4

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

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	2
1	K	348/411 (85%)	258 (74%)	90 (26%)	0	2
1	M	348/411 (85%)	248 (71%)	100 (29%)	0	2
1	O	348/411 (85%)	254 (73%)	94 (27%)	0	2
2	B	14/22 (64%)	13 (93%)	1 (7%)	14	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	14/22 (64%)	11 (79%)	3 (21%)	1	5
2	F	14/22 (64%)	13 (93%)	1 (7%)	14	46
2	H	14/22 (64%)	11 (79%)	3 (21%)	1	5
2	J	14/22 (64%)	9 (64%)	5 (36%)	0	1
2	L	14/22 (64%)	12 (86%)	2 (14%)	3	15
2	N	14/22 (64%)	11 (79%)	3 (21%)	1	5
2	P	14/22 (64%)	12 (86%)	2 (14%)	3	15
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	I	320	LEU
1	K	434	HIS
1	I	422	GLU
1	I	318	LEU
1	K	141	GLN

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

Mol	Chain	Res	Type
1	K	105	ASN
1	M	373	ASN
1	K	130	GLN
1	M	105	ASN
1	O	105	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.19	1 (0%)	94	84	5, 40, 76, 100	0
1	C	393/465 (84%)	-0.38	2 (0%)	91	75	2, 34, 76, 100	0
1	E	393/465 (84%)	-0.12	4 (1%)	82	59	2, 42, 78, 100	0
1	G	393/465 (84%)	-0.43	1 (0%)	94	84	4, 35, 72, 100	0
1	I	393/465 (84%)	-0.17	2 (0%)	91	75	4, 41, 76, 100	0
1	K	393/465 (84%)	-0.31	2 (0%)	91	75	1, 39, 74, 100	0
1	M	393/465 (84%)	-0.24	4 (1%)	82	59	5, 41, 76, 100	0
1	O	393/465 (84%)	-0.29	3 (0%)	86	65	4, 39, 78, 93	0
2	B	14/22 (63%)	0.12	1 (7%)	16	5	42, 59, 84, 85	0
2	D	14/22 (63%)	-0.14	0	100	100	21, 55, 77, 80	0
2	F	14/22 (63%)	0.08	1 (7%)	16	5	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%)	0.09	1 (7%)	16	5	13, 54, 74, 90	0
2	L	14/22 (63%)	-0.12	0	100	100	23, 59, 88, 100	0
2	N	14/22 (63%)	0.09	1 (7%)	16	5	15, 53, 70, 81	0
2	P	14/22 (63%)	-0.22	0	100	100	19, 50, 86, 98	0
All	All	3258/3896 (83%)	-0.26	23 (0%)	87	69	1, 39, 77, 100	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	328	GLY	5.2
1	C	328	GLY	4.9
1	K	328	GLY	4.3
1	O	328	GLY	3.3
2	N	860	ILE	3.2

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

There are no ligands in this entry.

6.5   Other polymers ⓘ

There are no such residues in this entry.