wwPDB X-ray Structure Validation Summary Report (i)

Jun 29, 2024 – 01:16 AM EDT

PDB ID	:	9GPB
Title	:	THE ALLOSTERIC TRANSITION OF GLYCOGEN PHOSPHORYLASE
Authors	:	Barford, D.; Johnson, L.N.
Deposited on	:	1990-12-17
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

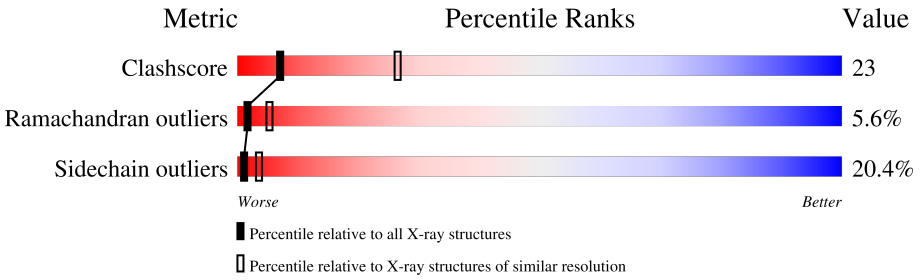
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	39% 38% 18%
1	B	842	40% 40% 14%
1	C	842	41% 40% 13%
1	D	842	32% 42% 18% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	900	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26873 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.

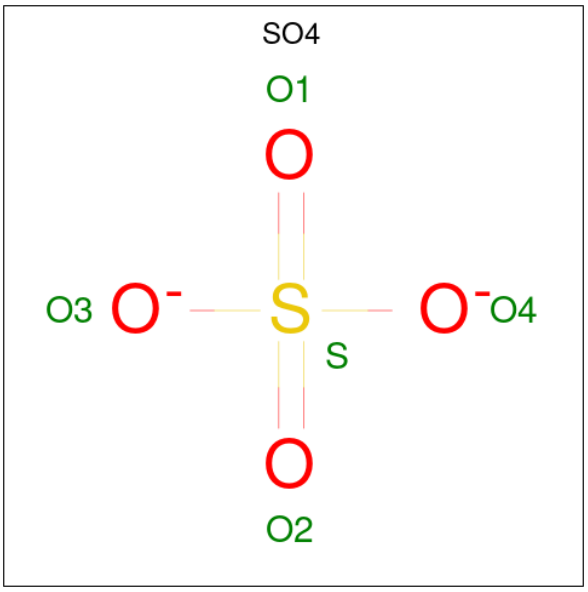
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	823	Total	C	N	O	S	0	0	0
			6688	4264	1184	1210	30			
1	B	823	Total	C	N	O	S	0	0	0
			6688	4264	1184	1210	30			
1	C	823	Total	C	N	O	S	0	0	0
			6688	4263	1184	1211	30			
1	D	823	Total	C	N	O	S	0	0	0
			6689	4264	1184	1211	30			

There are 4 discrepancies between the modelled and reference sequences:

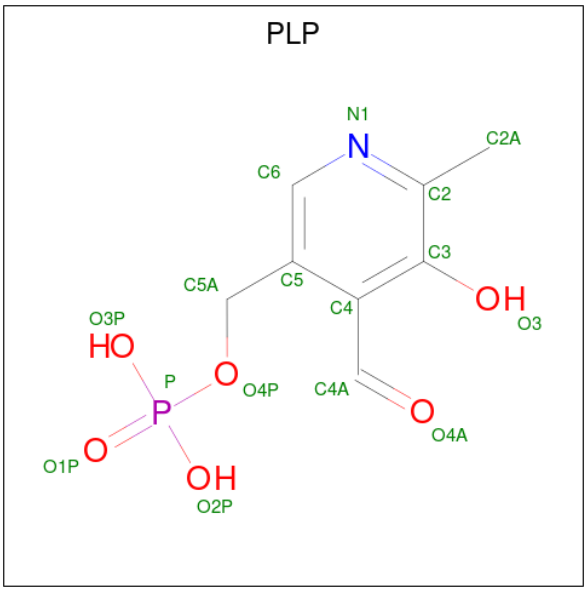
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	CONFLICT	UNP P00489
B	380	ILE	LEU	CONFLICT	UNP P00489
C	380	ILE	LEU	CONFLICT	UNP P00489
D	380	ILE	LEU	CONFLICT	UNP P00489

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

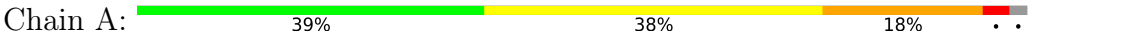
3 Residue-property plots (i)

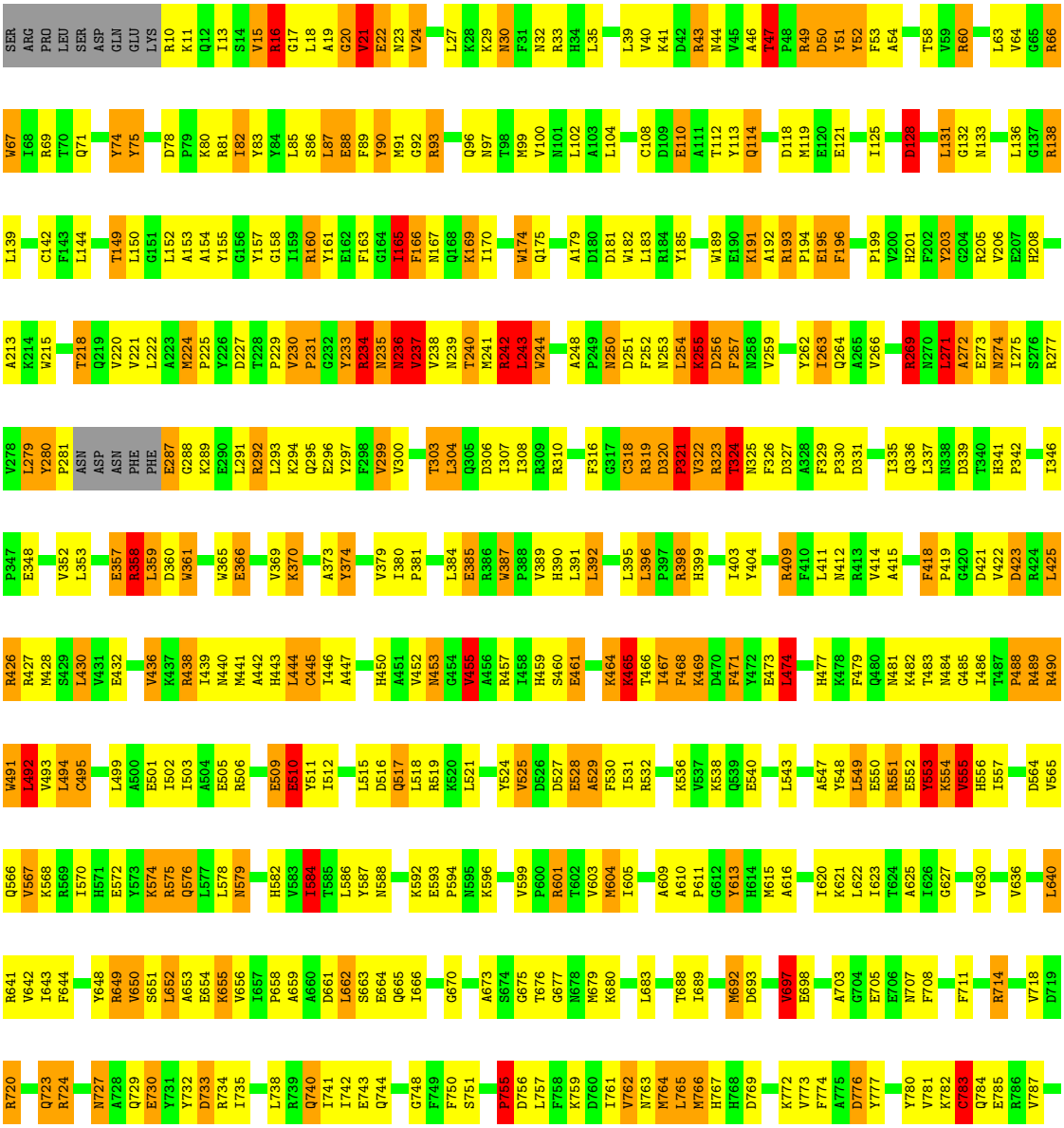
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

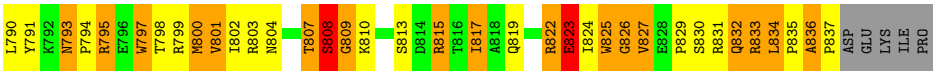
Note EDS was not executed.

• Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain A:

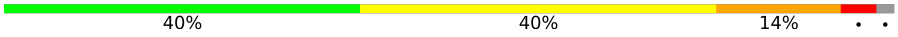


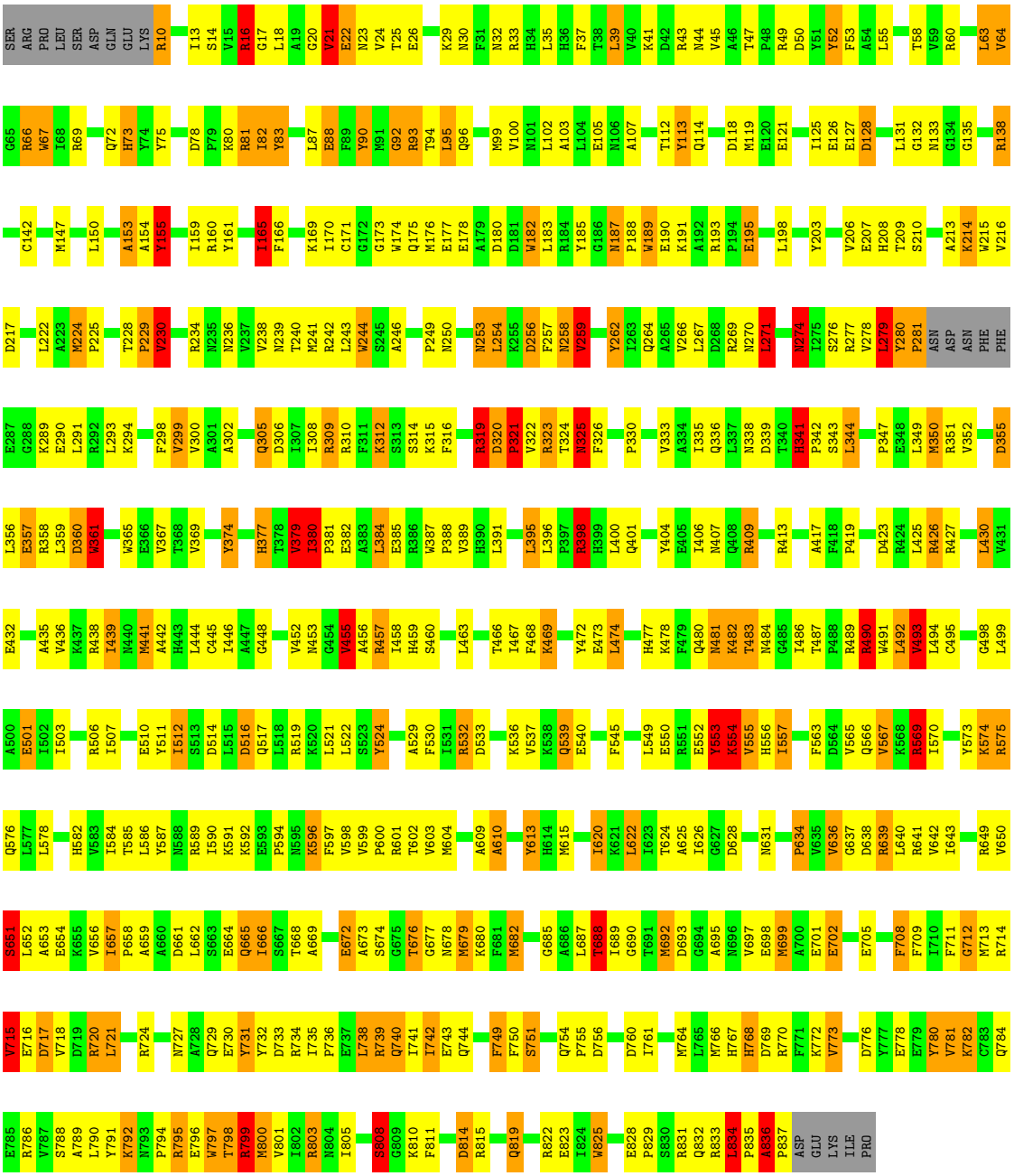




• Molecule 1: GLYCOGEN PHOSPHORYLASE B

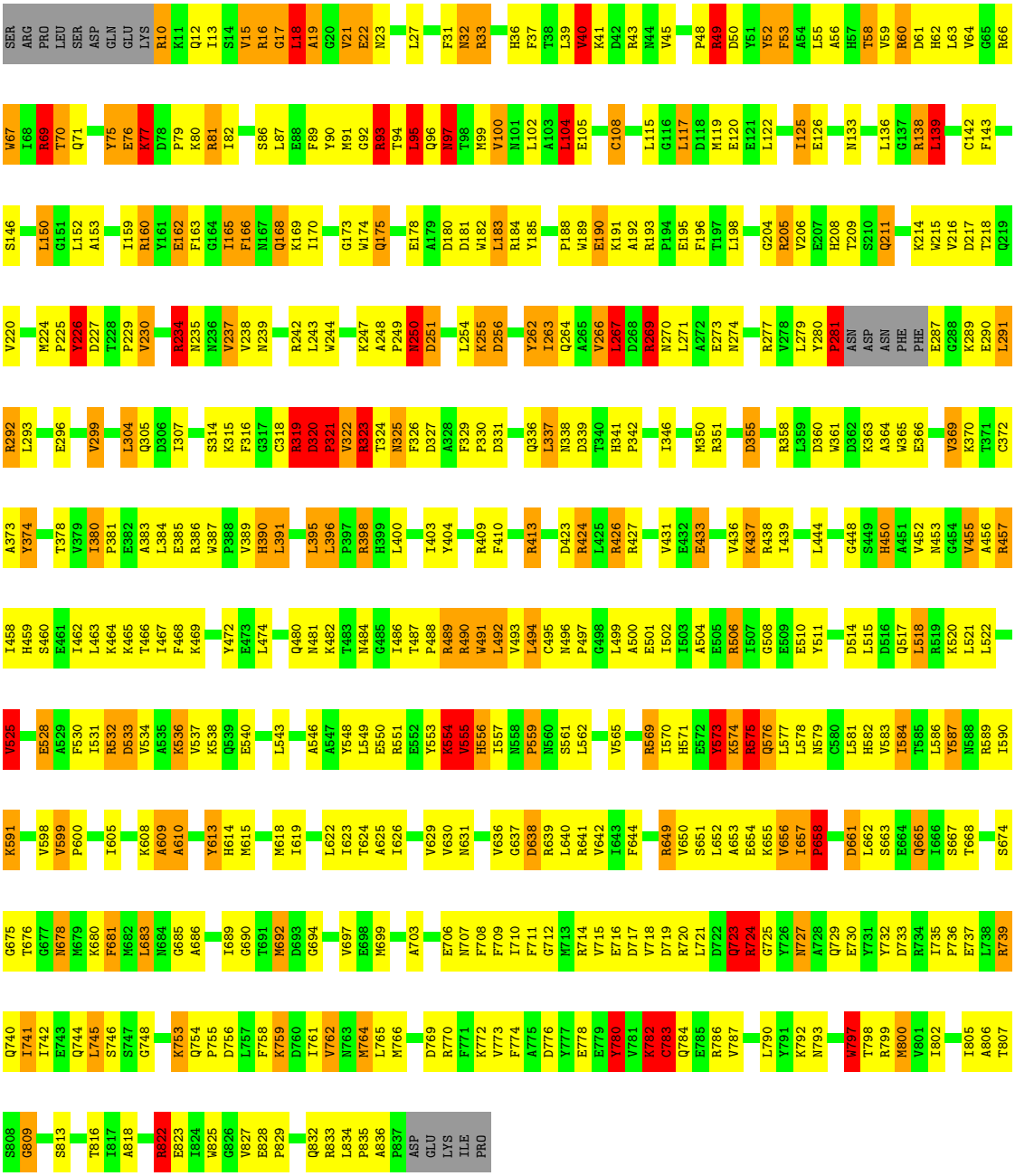
Chain B:





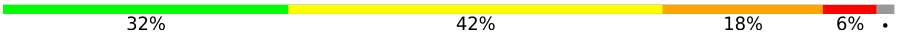
• Molecule 1: GLYCOGEN PHOSPHORYLASE B

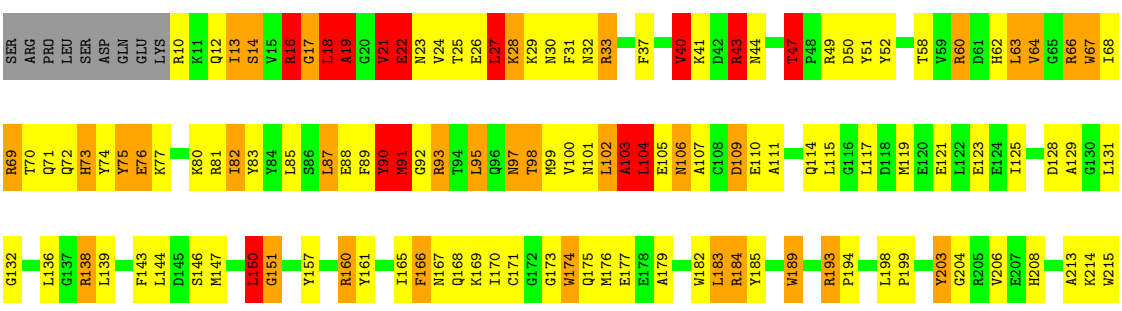
Chain C:

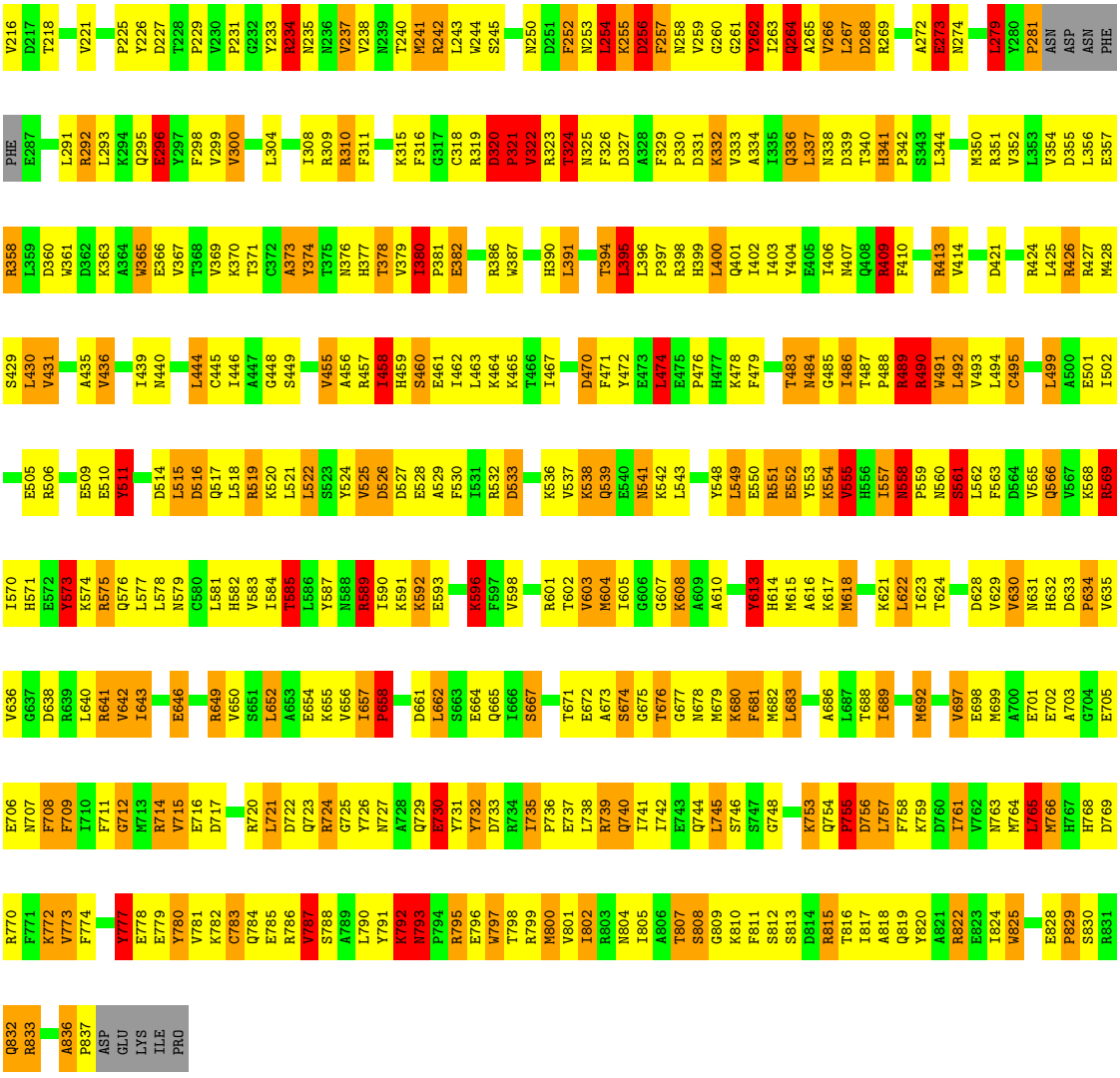


• Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain D:






V216 D217 T218 V221 P225 Y226 D227 T228 P229 V230 P231 G232 Y233 R234 M235 N236 V237 V238 N239 T240 M241 R242 L243 W244 S245 N250 D251 F252 N253 L254 K255 D256 F257 N258 V259 G260 G261 Y262 I263 Q264 A265 V266 L267 D268 R269 A272 E273 N274 L279 Y280 P281 ASN ASP ASN PHE
PHE E287 L291 R292 L293 K294 Q295 E296 Y297 F298 V299 V300 L304 I308 R309 R310 F311 K315 F316 G317 C318 R319 D320 P321 V322 R323 T324 N325 F326 D327 A328 F329 P330 D331 K332 V333 A334 I335 Q336 L337 N338 D339 T340 H341 P342 S343 L344 M350 R351 V352 L353 V354 D355 L356 E357
R358 L359 D360 W361 D362 K363 A364 W365 E366 V367 T368 V369 K370 T371 C372 A373 Y374 T375 N376 H377 T378 V379 I380 P381 E382 R386 W387 H390 L391 T394 L395 L396 P397 R398 H399 L400 Q401 I402 I403 Y404 E405 I406 N407 Q408 R409 F410 R413 V414 D421 R424 L425 R426 R427 M428
S429 L430 V431 A435 V436 I439 N440 L444 C445 I446 A447 G448 S449 V455 A456 R457 I458 H459 S460 E461 I462 L463 K464 K465 T466 I467 D470 F471 Y472 E473 L474 E475 P476 H477 K478 F479 T483 N484 G485 I486 T487 P488 R489 R490 W491 L492 V493 L494 C495 L499 A500 E501 I502
E505 R506 E509 E510 Y511 D514 L515 D516 Q517 L518 R519 K520 L521 L522 S523 Y524 V525 D526 D527 E528 A529 F530 I531 R532 D533 K536 V537 K538 Q539 E540 N541 K542 L543 Y548 L549 E550 R551 E552 Y553 K554 V555 H556 I557 N558 P559 N560 S561 L562 F563 D564 V565 Q566 V567 K568 R569
I570 H571 E572 Y573 K574 R575 Q576 L577 L578 N579 C580 L581 H582 V583 I584 T585 L586 Y587 N588 R589 I590 K591 K592 E593 K596 F597 V598 R601 T602 V603 M604 I605 G606 G607 K608 A609 A610 Y613 H614 M615 A616 K617 M618 K621 L622 I623 T624 D628 V629 V630 N631 H632 D633 P634 V635
V636 G637 D638 R639 L640 R641 V642 I643 E646 R649 V650 S651 L652 A653 E654 K655 V656 I657 P658 D661 L662 S663 E664 Q665 I666 S667 T671 E672 A673 S674 G675 T676 G677 N678 M679 K680 F681 M682 L683 A686 L687 T688 I689 M692 V697 E698 M699 A700 E701 E702 A703 G704 E705
E706 N707 F708 F709 I710 F711 G712 M713 R714 V715 E716 D717 R720 L721 D722 Q723 R724 G725 Y726 N727 A728 Q729 E730 Y731 Y732 D733 R734 I735 P736 E737 L738 R739 Q740 I741 I742 E743 Q744 L745 S746 S747 G748 K753 Q754 P755 D756 L757 F758 K759 D760 T761 V762 N763 M764 L765 M766 H767 H768 D769
R770 F771 K772 V773 F774 Y777 E778 E779 Y780 V781 K782 C783 Q784 E785 R786 V787 S788 A789 L790 Y791 K792 N793 P794 R795 E796 W797 T798 R799 M800 V801 I802 R803 N804 I805 A806 T807 S808 G809 K810 F811 S812 S813 D814 R815 T816 I817 A818 Q819 Y820 A821 R822 E823 I824 W825 E828 P829 S830 R831
Q832 R833 A836 P837 ASP GLU LYS ILE PRO

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	119.00Å 190.00Å 88.20Å 90.00° 109.35° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26873	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PLP

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	0.98	1/6837 (0.0%)	1.95	202/9250 (2.2%)
1	B	0.98	3/6837 (0.0%)	1.92	190/9250 (2.1%)
1	C	1.00	4/6837 (0.1%)	1.96	208/9251 (2.2%)
1	D	0.99	4/6839 (0.1%)	1.97	231/9254 (2.5%)
All	All	0.99	12/27350 (0.0%)	1.95	831/37005 (2.2%)

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	A	0	9
1	B	0	8
1	C	0	10
1	D	0	6
All	All	0	33

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	18	LEU	N-CA	-6.78	1.32	1.46
1	B	230	VAL	CA-CB	6.26	1.67	1.54
1	A	565	VAL	CA-CB	6.06	1.67	1.54
1	D	17	GLY	N-CA	-5.95	1.37	1.46
1	B	244	TRP	CG-CD2	-5.53	1.34	1.43

The worst 5 of 831 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	17	GLY	O-C-N	19.05	153.18	122.70
1	C	17	GLY	CA-C-N	-14.07	86.25	117.20
1	C	780	TYR	CB-CG-CD2	-13.43	112.94	121.00
1	B	780	TYR	CB-CG-CD2	-13.31	113.02	121.00
1	C	319	ARG	NE-CZ-NH2	-12.42	114.09	120.30

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	A	233	TYR	Sidechain
1	A	242	ARG	Sidechain
1	A	256	ASP	Mainchain
1	A	51	TYR	Sidechain

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	6688	0	6652	304	0
1	B	6688	0	6652	285	0
1	C	6688	0	6646	290	0
1	D	6689	0	6653	389	0
2	A	15	0	0	0	0
2	B	15	0	0	1	0
2	C	15	0	0	3	0
2	D	15	0	0	2	0
3	A	15	0	6	1	0
3	B	15	0	7	0	0
3	C	15	0	7	0	0
3	D	15	0	6	2	0
All	All	26873	0	26629	1221	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 23.

The worst 5 of 1221 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:37:PHE:CE2	1:D:18:LEU:HB3	1.46	1.51
1:C:37:PHE:HE2	1:D:18:LEU:CB	1.32	1.42
1:C:37:PHE:CE2	1:D:18:LEU:CB	2.06	1.32
1:C:15:VAL:O	1:C:17:GLY:N	1.79	1.14
1:D:16:ARG:HG3	1:D:17:GLY:N	1.64	1.07

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	817/842 (97%)	652 (80%)	112 (14%)	53 (6%)	1	3
1	B	817/842 (97%)	670 (82%)	107 (13%)	40 (5%)	2	8
1	C	819/842 (97%)	679 (83%)	102 (12%)	38 (5%)	2	9
1	D	819/842 (97%)	644 (79%)	124 (15%)	51 (6%)	1	4
All	All	3272/3368 (97%)	2645 (81%)	445 (14%)	182 (6%)	2	5

5 of 182 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	21	VAL
1	A	152	LEU
1	A	166	PHE
1	A	236	ASN

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	712/731 (97%)	580 (82%)	132 (18%)	1	5
1	B	712/731 (97%)	569 (80%)	143 (20%)	1	4
1	C	711/731 (97%)	580 (82%)	131 (18%)	1	5
1	D	712/731 (97%)	537 (75%)	175 (25%)	0	2
All	All	2847/2924 (97%)	2266 (80%)	581 (20%)	1	3

5 of 581 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	300	VAL
1	D	793	ASN
1	D	374	TYR
1	D	296	GLU
1	D	573	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	727	ASN
1	D	401	GLN
1	D	72	GLN
1	D	187	ASN
1	D	481	ASN

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)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	902	-	4,4,4	0.44	0	6,6,6	0.35	0
2	SO4	C	901	-	4,4,4	0.30	0	6,6,6	0.31	0
2	SO4	B	900	-	4,4,4	0.24	0	6,6,6	0.61	0
2	SO4	C	902	-	4,4,4	0.18	0	6,6,6	0.67	0
2	SO4	D	902	-	4,4,4	0.36	0	6,6,6	0.31	0
3	PLP	A	999	1	15,15,16	1.69	3 (20%)	20,22,23	1.27	4 (20%)
3	PLP	C	999	1	15,15,16	1.41	1 (6%)	20,22,23	2.23	2 (10%)
2	SO4	B	902	-	4,4,4	0.20	0	6,6,6	0.51	0
2	SO4	D	900	-	4,4,4	0.46	0	6,6,6	0.42	0
3	PLP	B	999	1	15,15,16	1.45	4 (26%)	20,22,23	1.64	4 (20%)
2	SO4	B	901	1	4,4,4	0.62	0	6,6,6	0.26	0
3	PLP	D	999	1	15,15,16	1.86	3 (20%)	20,22,23	1.32	1 (5%)
2	SO4	D	901	-	4,4,4	0.54	0	6,6,6	0.51	0
2	SO4	A	901	-	4,4,4	0.49	0	6,6,6	0.37	0
2	SO4	A	900	-	4,4,4	0.19	0	6,6,6	0.49	0
2	SO4	C	900	1	4,4,4	0.55	0	6,6,6	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	D	999	1	-	5/6/6/8	0/1/1/1
3	PLP	A	999	1	-	1/6/6/8	0/1/1/1
3	PLP	C	999	1	-	0/6/6/8	0/1/1/1
3	PLP	B	999	1	-	2/6/6/8	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	999	PLP	C3-C2	-5.76	1.35	1.40
3	A	999	PLP	C3-C2	-4.79	1.36	1.40
3	C	999	PLP	C3-C2	-3.35	1.37	1.40
3	A	999	PLP	C5-C4	-2.97	1.37	1.40
3	B	999	PLP	C3-C2	-2.80	1.38	1.40

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	999	PLP	O4P-C5A-C5	8.75	126.03	109.35
3	B	999	PLP	O4P-C5A-C5	5.05	118.98	109.35
3	D	999	PLP	O4P-C5A-C5	4.61	118.14	109.35
3	B	999	PLP	C6-C5-C4	2.91	120.45	118.16
3	A	999	PLP	C6-C5-C4	2.67	120.26	118.16

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	999	PLP	C5A-O4P-P-O3P
3	D	999	PLP	C4-C5-C5A-O4P
3	D	999	PLP	C5A-O4P-P-O1P
3	D	999	PLP	C5A-O4P-P-O2P
3	D	999	PLP	C5A-O4P-P-O3P

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	902	SO4	1	0
3	A	999	PLP	1	0
2	B	902	SO4	1	0
2	D	900	SO4	1	0
3	D	999	PLP	2	0
2	C	900	SO4	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	18:LEU	C	19:ALA	N	22.68
1	B	18:LEU	C	19:ALA	N	19.70

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.