wwPDB X-ray Structure Validation Summary Report (i)

Jun 26, 2024 – 02:20 AM EDT

PDB ID	:	7GPB
Title	:	STRUCTURAL MECHANISM FOR GLYCOGEN PHOSPHORYLASE CONTROL BY PHOSPHORYLATION AND AMP
Authors	:	Barford, D.; Hu, S.-H.; Johnson, L.N.
Deposited on	:	1990-11-13
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 (1)) were used in the production of this report:

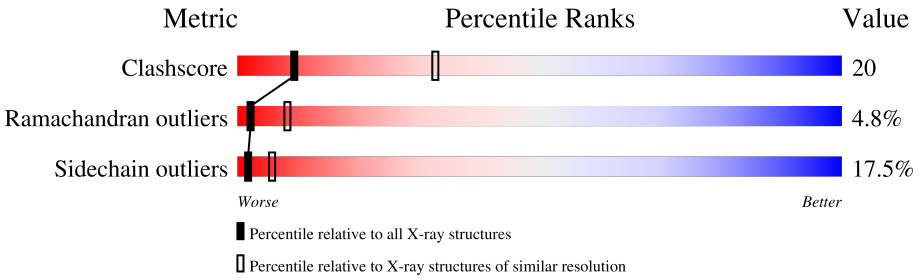
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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	41% 40% 13%
1	B	842	43% 38% 14%
1	C	842	46% 38% 11%
1	D	842	36% 42% 16%

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	A	901	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26955 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.

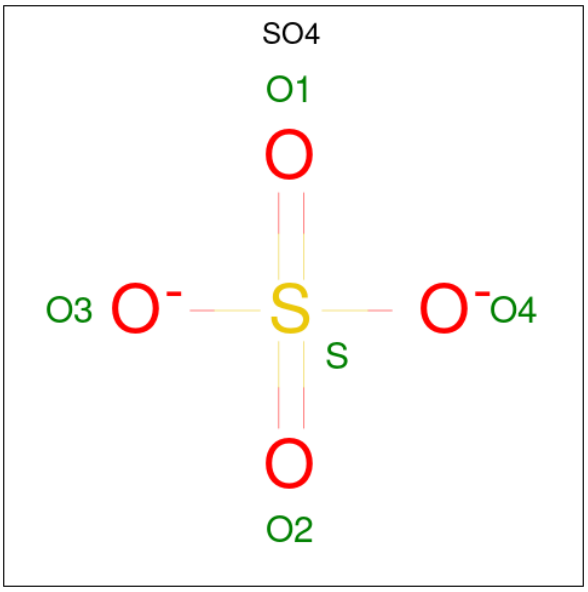
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			
1	B	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			
1	C	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			
1	D	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			

There are 4 discrepancies between the modelled and reference sequences:

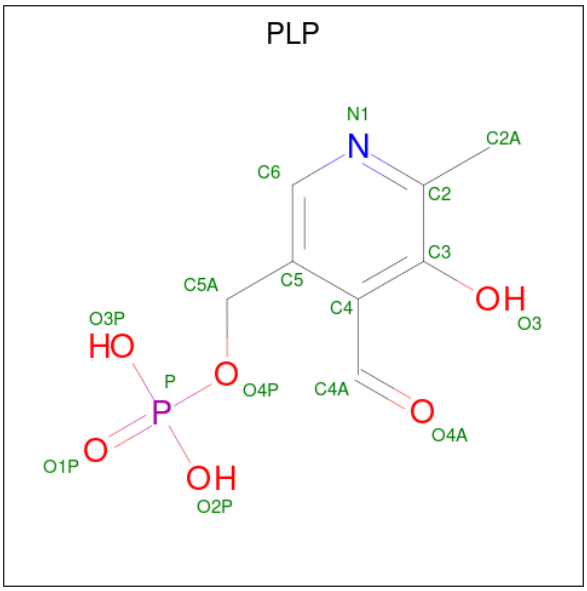
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	CONFLICT	UNP P00489
B	380	ILE	LEU	CONFLICT	UNP P00489
C	380	ILE	LEU	CONFLICT	UNP P00489
D	380	ILE	LEU	CONFLICT	UNP P00489

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



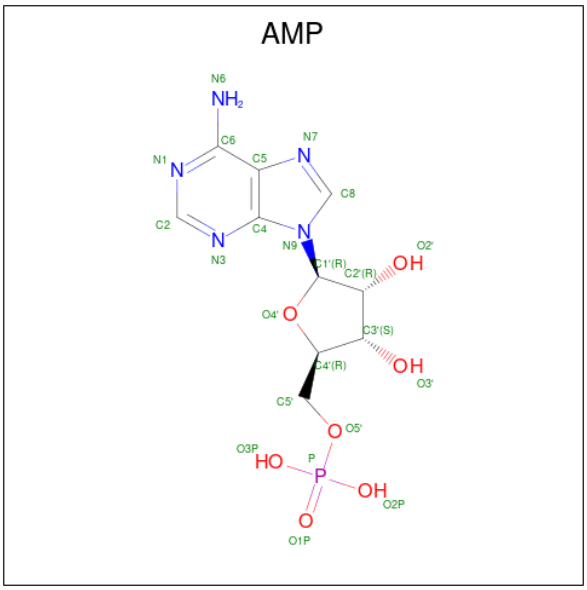
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- 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		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

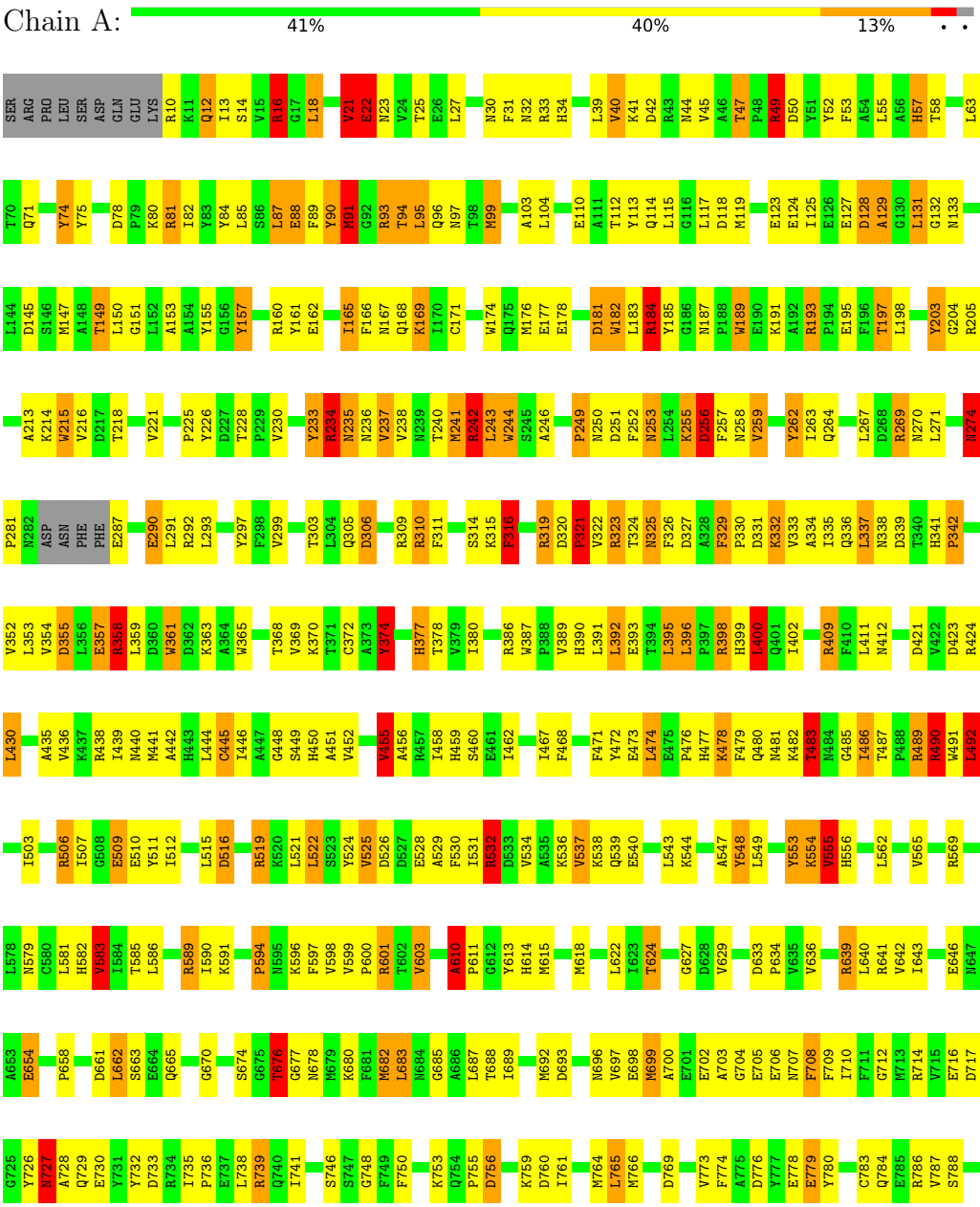
3 Residue-property plots (i)

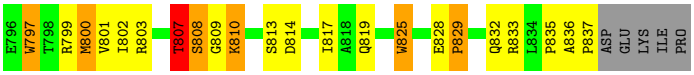
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

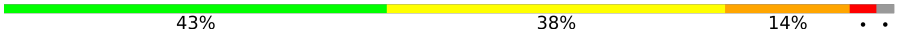
Chain A:

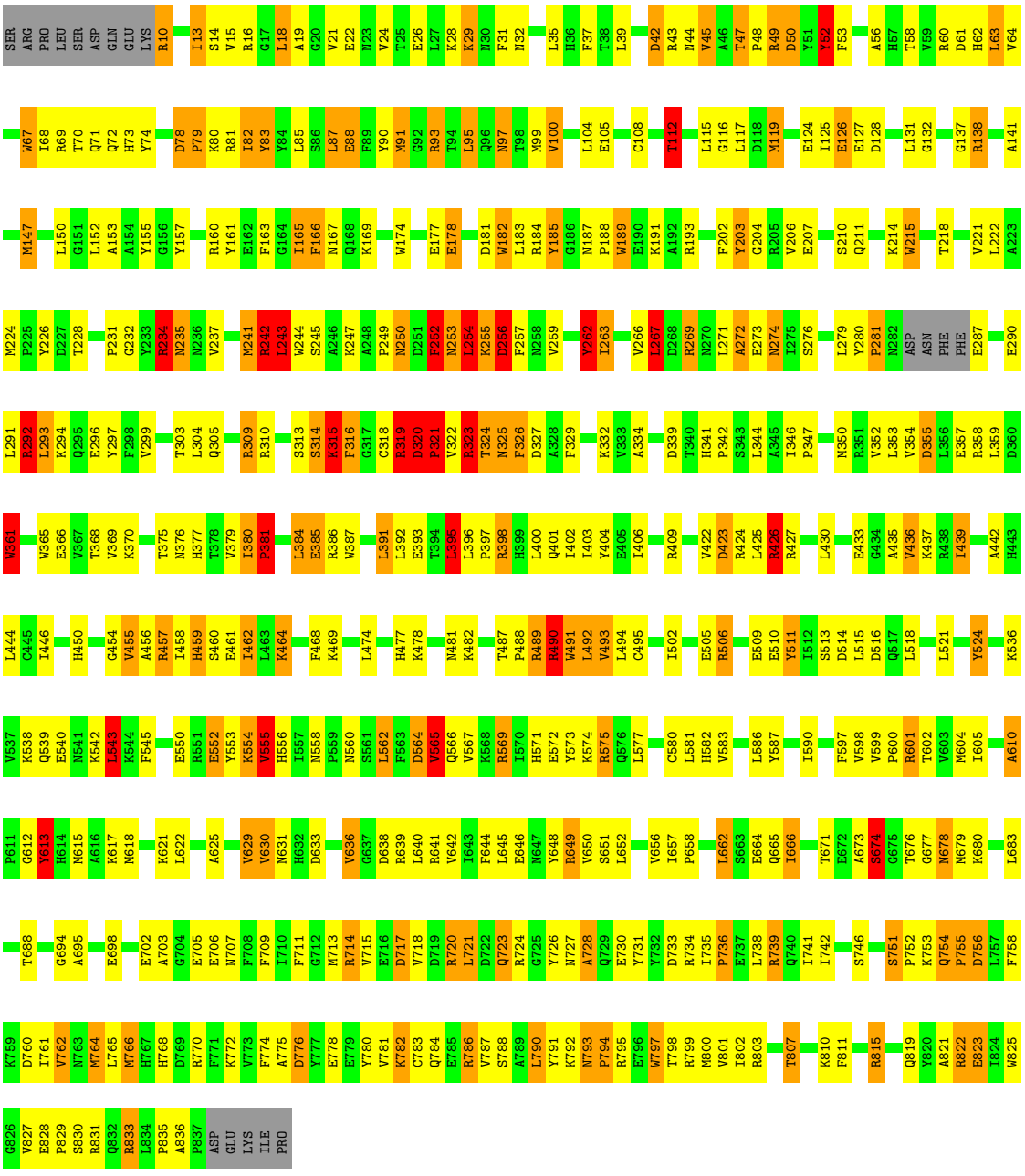




• Molecule 1: GLYCOGEN PHOSPHORYLASE B

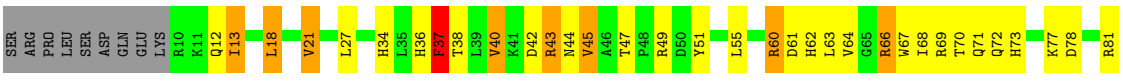
Chain B:

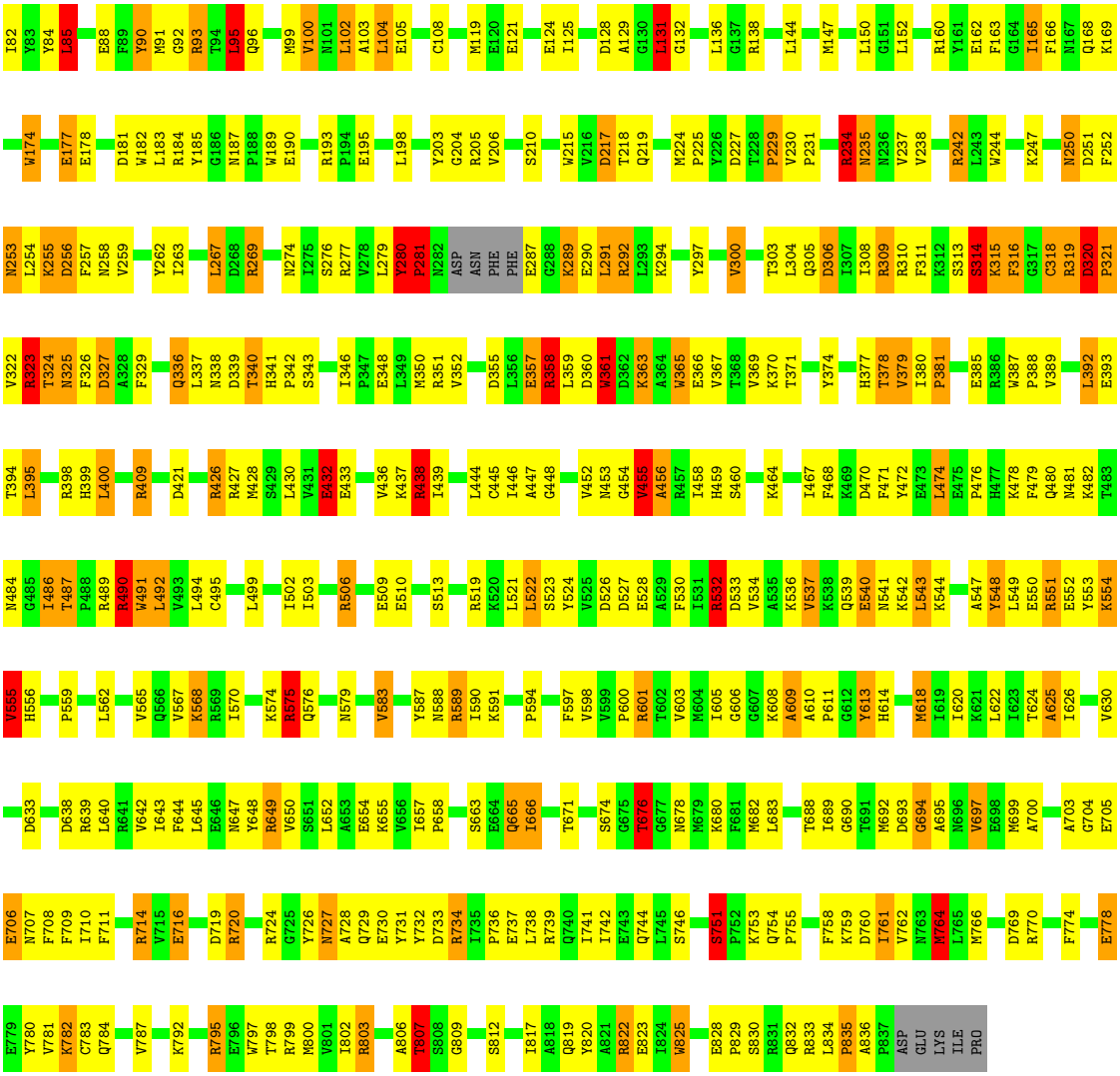




• Molecule 1: GLYCOGEN PHOSPHORYLASE B

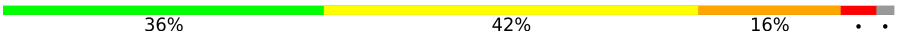
Chain C:

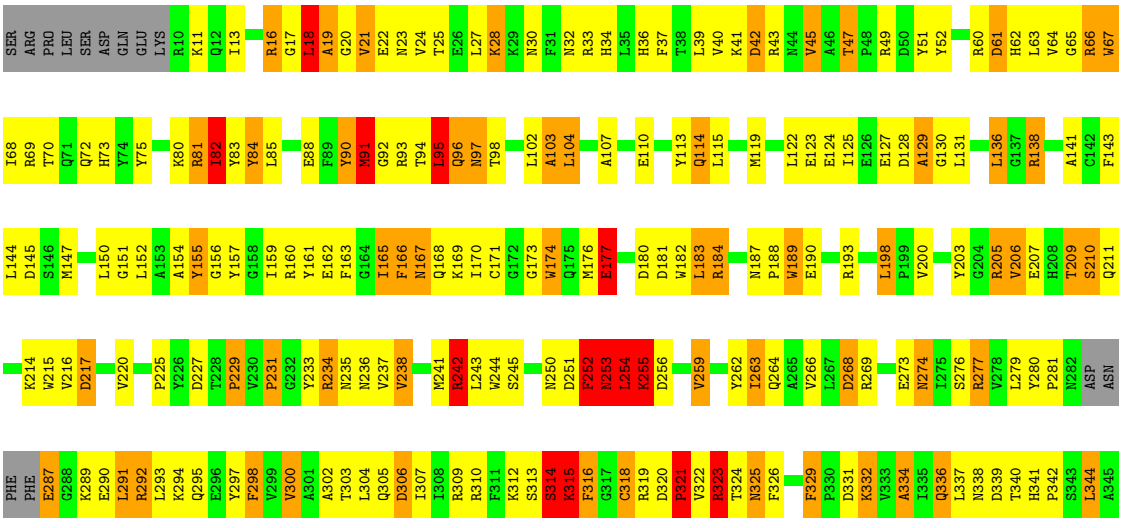


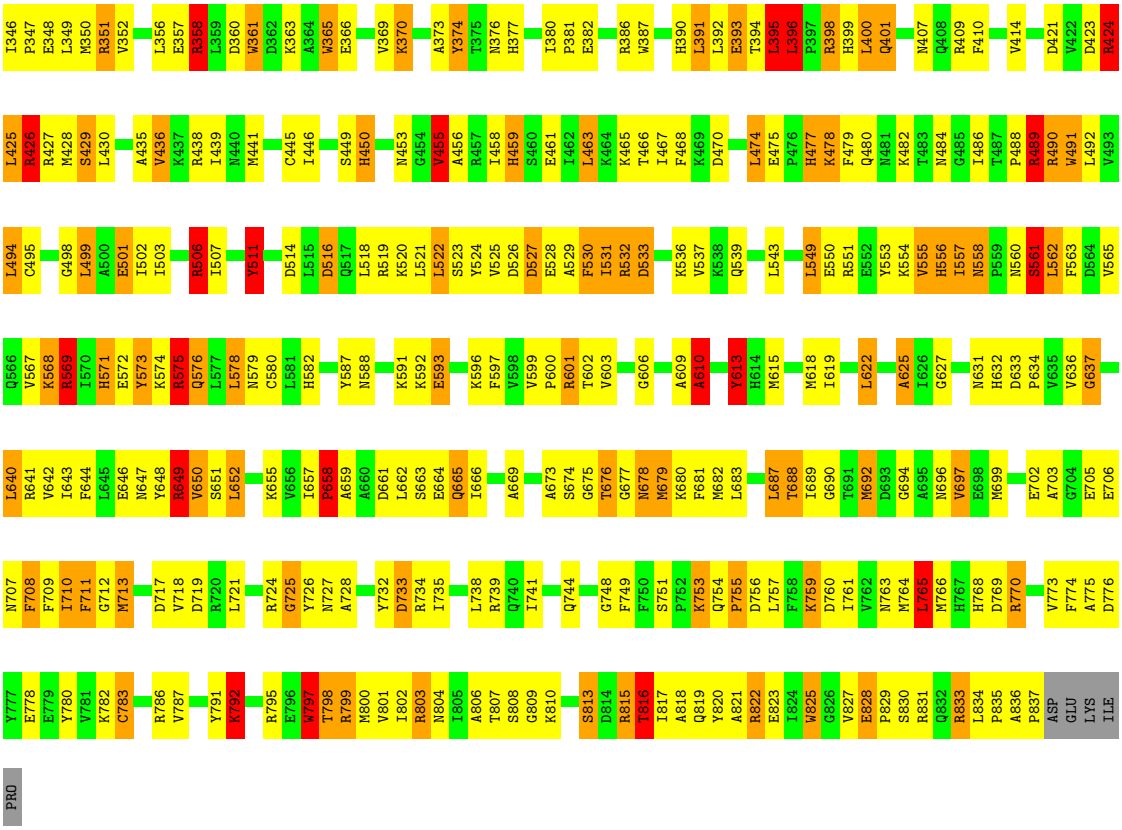


• Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain D:






I346 P347 E348 L349 M350 R351 V352 L356 E357 R358 L359 D360 W361 D362 K363 A364 W365 E366 V369 K370 A373 Y374 T375 N376 H377 I380 P381 E382 R386 W387 H390 L391 L392 E393 T394 L395 L396 P397 R398 H399 L400 Q401 N407 Q408 R409 F410 V414 D421 V422 D423 R424
L425 R426 R427 M428 S429 L430 A435 V436 K437 R438 I439 N440 M441 C445 I446 S449 H450 N453 G454 V455 A456 R457 I458 H459 S460 E461 I462 L463 K464 K465 T466 I467 F468 K469 D470 L474 E475 P476 H477 K478 F479 Q480 N481 K482 T483 N484 G485 I486 T487 P488 R489 R490 W491 L492 V493
L494 C495 G498 L499 A500 E501 I502 I503 R506 I507 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 L543 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 Y587 N588 K591 K592 E593 K596 F597 V598 V599 P600 R601 T602 V603 G606 A609 A610 Y613 H614 M615 M618 I619 L622 A625 I626 G627 N631 H632 D633 P634 V635 V636 G637
L640 R641 V642 I643 F644 L645 E646 N647 Y648 R649 V650 S651 L652 K655 V656 I657 P658 A659 A660 D661 L662 S663 E664 Q665 I666 A669 A673 S674 G675 T676 G677 M678 M679 K680 F681 M682 L683 L687 T688 I689 G690 T691 M692 D693 G694 A695 N696 V697 E698 M699 E702 A703 G704 E705 E706
N707 F708 F709 I710 F711 G712 M713 D717 V718 D719 R720 L721 R724 G725 Y726 N727 A728 Y732 D733 R734 I735 L738 R739 Q740 I741 Q744 G748 F749 F750 S751 P752 K753 Q754 P755 D756 L757 F758 K759 D760 I761 V762 N763 M764 L765 M766 H767 H768 D769 R770 V773 F774 A775 D776
Y777 E778 E779 Y780 V781 K782 C783 R786 V787 Y791 K792 R795 E796 W797 T798 R799 M800 V801 I802 R803 N804 I805 A806 T807 S808 G809 K810 S813 D814 R815 T816 I817 A818 Q819 Y820 A821 R822 E823 I824 W825 G826 V827 E828 P829 S830 R831 Q832 R833 L834 P835 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}	0.171 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26955	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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: AMP, PLP, SO4

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	1.00	6/6842 (0.1%)	2.02	223/9258 (2.4%)
1	B	1.00	5/6842 (0.1%)	1.90	186/9258 (2.0%)
1	C	1.00	2/6842 (0.0%)	1.96	190/9258 (2.1%)
1	D	0.99	2/6842 (0.0%)	2.00	203/9258 (2.2%)
All	All	1.00	15/27368 (0.1%)	1.97	802/37032 (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	6
1	B	0	6
1	C	0	5
1	D	0	8
All	All	0	25

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	323	ARG	CZ-NH1	8.57	1.44	1.33
1	B	100	VAL	CA-CB	7.53	1.70	1.54
1	B	319	ARG	CZ-NH1	7.05	1.42	1.33
1	B	323	ARG	CZ-NH2	6.47	1.41	1.33
1	A	323	ARG	NE-CZ	6.26	1.41	1.33

The worst 5 of 802 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	67	TRP	CG-CD2-CE3	-40.61	97.35	133.90
1	D	67	TRP	NE1-CE2-CZ2	-33.92	93.09	130.40
1	A	49	ARG	NE-CZ-NH2	-19.84	110.38	120.30
1	A	16	ARG	NE-CZ-NH2	14.98	127.79	120.30
1	D	490	ARG	NE-CZ-NH2	-14.37	113.11	120.30

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	A	277	ARG	Sidechain
1	A	280	TYR	Peptide
1	A	47	THR	Peptide
1	A	49	ARG	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	6692	0	6653	248	1
1	B	6692	0	6653	244	0
1	C	6692	0	6653	246	0
1	D	6692	0	6653	337	1
2	A	10	0	0	2	0
2	B	10	0	0	1	0
2	C	10	0	0	1	0
2	D	5	0	0	0	0
3	A	15	0	6	2	0
3	B	15	0	7	1	0
3	C	15	0	7	1	0
3	D	15	0	7	3	0
4	A	23	0	12	3	0
4	B	23	0	12	1	0
4	C	23	0	12	1	0
4	D	23	0	12	2	0
All	All	26955	0	26687	1056	1

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 20.

The worst 5 of 1056 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:D:85:LEU:HD21	1:D:303:THR:HG21	1.43	1.00
1:D:251:ASP:HB3	1:D:255:LYS:HB3	1.46	0.98
1:D:707:ASN:HA	1:D:800:MET:SD	2.04	0.97
1:A:45:VAL:HG21	4:B:920:AMP:H3'	1.44	0.97
1:A:682:MET:SD	1:A:699:MET:HG2	2.09	0.92

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:GLU:N	1:D:321:PRO:O[2_646]	2.18	0.02

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	820/842 (97%)	669 (82%)	116 (14%)	35 (4%)	2 10
1	B	820/842 (97%)	687 (84%)	92 (11%)	41 (5%)	2 7
1	C	820/842 (97%)	708 (86%)	82 (10%)	30 (4%)	3 13
1	D	820/842 (97%)	669 (82%)	100 (12%)	51 (6%)	1 4
All	All	3280/3368 (97%)	2733 (83%)	390 (12%)	157 (5%)	2 8

5 of 157 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	ASN

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Mol	Chain	Res	Type
1	A	321	PRO
1	A	358	ARG
1	A	553	TYR
1	A	674	SER

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%)	589 (83%)	123 (17%)	2	6
1	B	712/731 (97%)	595 (84%)	117 (16%)	2	7
1	C	712/731 (97%)	592 (83%)	120 (17%)	2	6
1	D	712/731 (97%)	573 (80%)	139 (20%)	1	4
All	All	2848/2924 (97%)	2349 (82%)	499 (18%)	2	6

5 of 499 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	764	MET
1	D	499	LEU
1	C	306	ASP
1	D	477	HIS
1	D	683	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	264	GLN
1	D	727	ASN
1	C	566	GLN
1	D	665	GLN
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)

15 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	$\#\|Z\| > 2$
3	PLP	B	999	1	15,15,16	1.58	1 (6%)	20,22,23	1.09	1 (5%)
2	SO4	B	901	-	4,4,4	0.31	0	6,6,6	0.29	0
2	SO4	C	901	-	4,4,4	0.22	0	6,6,6	0.41	0
2	SO4	A	900	-	4,4,4	0.16	0	6,6,6	0.38	0
2	SO4	C	900	-	4,4,4	0.28	0	6,6,6	0.35	0
3	PLP	D	999	1	15,15,16	1.09	1 (6%)	20,22,23	1.88	2 (10%)
3	PLP	A	999	1	15,15,16	1.83	5 (33%)	20,22,23	1.06	1 (5%)
4	AMP	B	920	-	22,25,25	0.92	1 (4%)	25,38,38	0.98	0
2	SO4	B	900	-	4,4,4	0.36	0	6,6,6	0.46	0
4	AMP	A	920	-	22,25,25	0.96	2 (9%)	25,38,38	1.08	0
4	AMP	D	920	-	22,25,25	0.93	0	25,38,38	0.97	0
2	SO4	D	900	-	4,4,4	0.12	0	6,6,6	0.32	0
2	SO4	A	901	-	4,4,4	0.24	0	6,6,6	0.40	0
4	AMP	C	920	-	22,25,25	0.97	1 (4%)	25,38,38	1.00	0
3	PLP	C	999	1	15,15,16	1.11	1 (6%)	20,22,23	0.99	1 (5%)

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	B	999	1	-	0/6/6/8	0/1/1/1
3	PLP	D	999	1	-	0/6/6/8	0/1/1/1
3	PLP	A	999	1	-	0/6/6/8	0/1/1/1
4	AMP	B	920	-	-	2/6/26/26	0/3/3/3
4	AMP	A	920	-	-	3/6/26/26	0/3/3/3
4	AMP	D	920	-	-	3/6/26/26	0/3/3/3
4	AMP	C	920	-	-	3/6/26/26	0/3/3/3
3	PLP	C	999	1	-	0/6/6/8	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	999	PLP	C3-C2	-4.06	1.36	1.40
3	A	999	PLP	C3-C2	-4.00	1.36	1.40
3	C	999	PLP	C3-C2	-2.58	1.38	1.40
3	A	999	PLP	P-O2P	-2.49	1.45	1.54
3	A	999	PLP	C5-C4	-2.41	1.37	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	999	PLP	O4P-C5A-C5	7.37	123.39	109.35
3	C	999	PLP	C6-C5-C4	2.36	120.01	118.16
3	A	999	PLP	C5-C6-N1	-2.22	120.12	123.82
3	D	999	PLP	C5-C6-N1	-2.20	120.16	123.82
3	B	999	PLP	O4P-C5A-C5	2.19	113.52	109.35

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

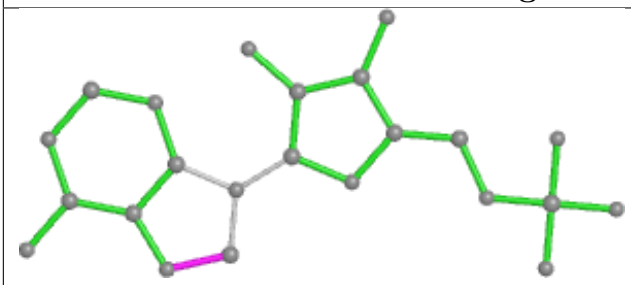
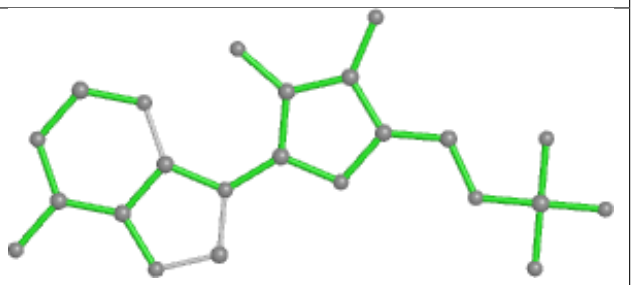
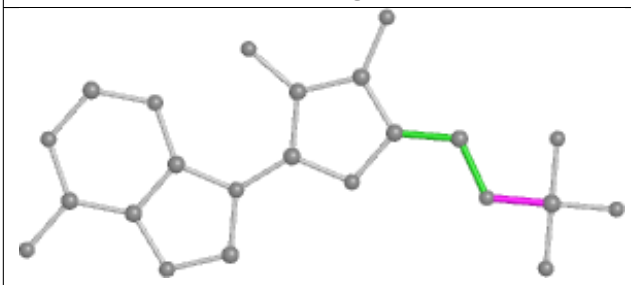
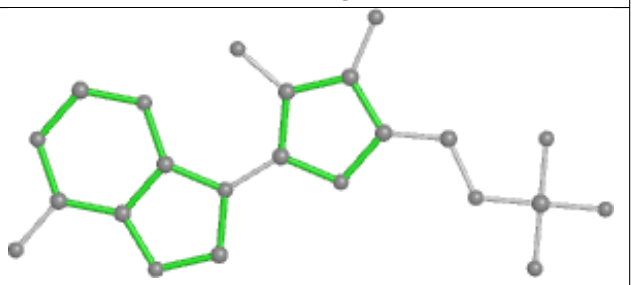
Mol	Chain	Res	Type	Atoms
4	A	920	AMP	C5'-O5'-P-O2P
4	A	920	AMP	C5'-O5'-P-O3P
4	B	920	AMP	C5'-O5'-P-O2P
4	B	920	AMP	C5'-O5'-P-O3P
4	C	920	AMP	C5'-O5'-P-O2P

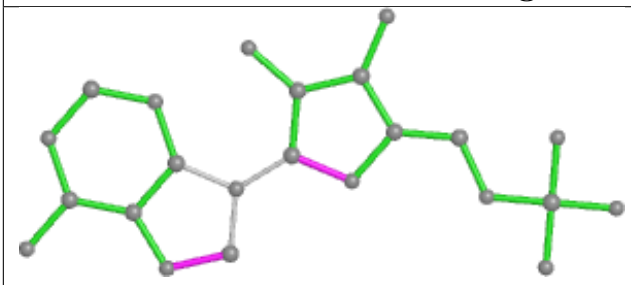
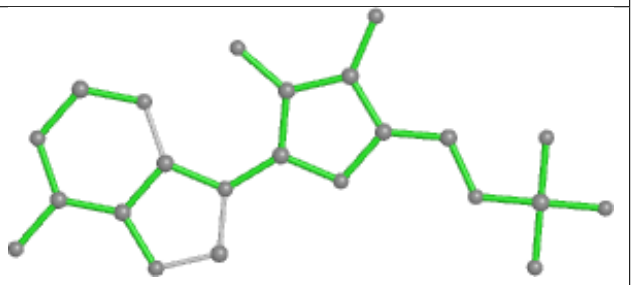
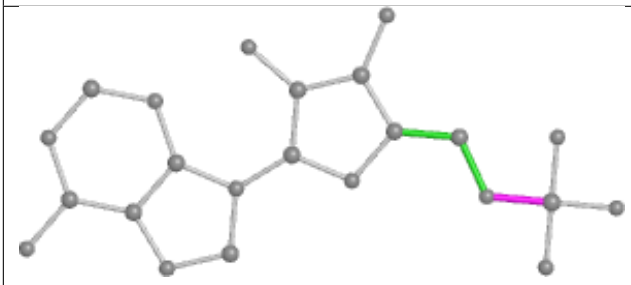
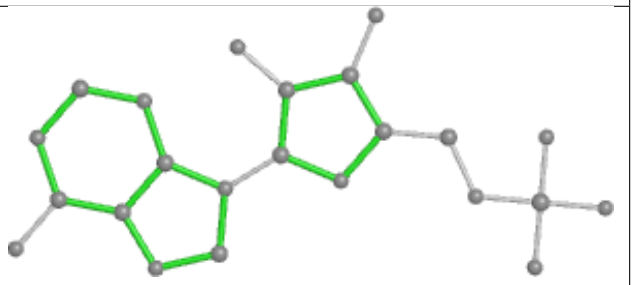
There are no ring outliers.

11 monomers are involved in 18 short contacts:

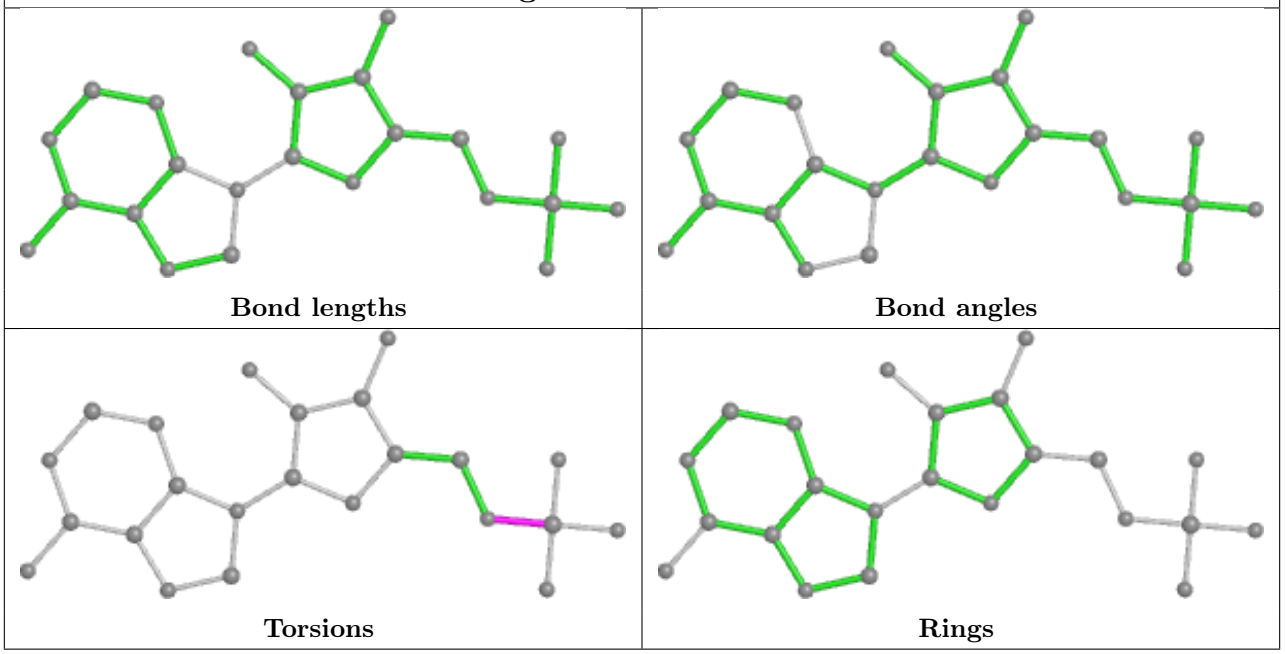
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	999	PLP	1	0
2	B	901	SO4	1	0
2	C	901	SO4	1	0
3	D	999	PLP	3	0
3	A	999	PLP	2	0
4	B	920	AMP	1	0
4	A	920	AMP	3	0
4	D	920	AMP	2	0
2	A	901	SO4	2	0
4	C	920	AMP	1	0
3	C	999	PLP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

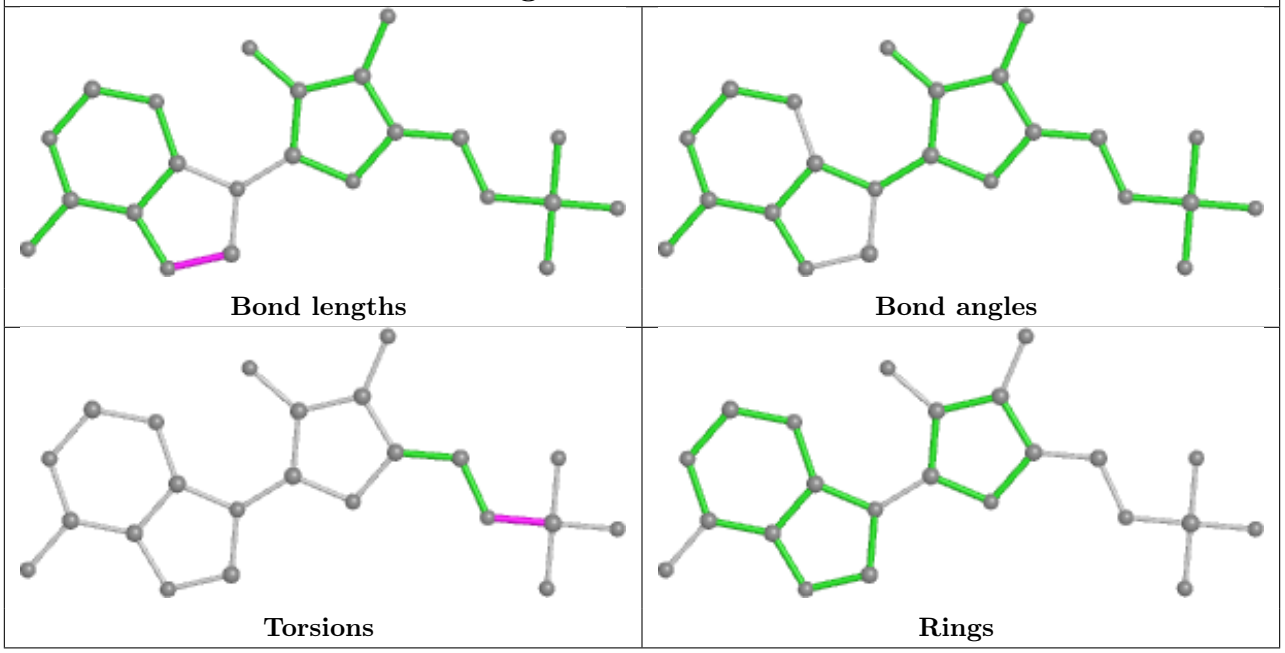
Ligand AMP B 920	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AMP A 920	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AMP D 920



Ligand AMP C 920



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

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.