



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 18, 2018 – 01:24 pm GMT

PDB ID : 1PYG
Title : STRUCTURAL BASIS FOR THE ACTIVATION OF GLYCOGEN PHOSPHORYLASE B BY ADENOSINE MONOPHOSPHATE
Authors : Sprang, S.
Deposited on : 1992-07-07
Resolution : 2.87 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

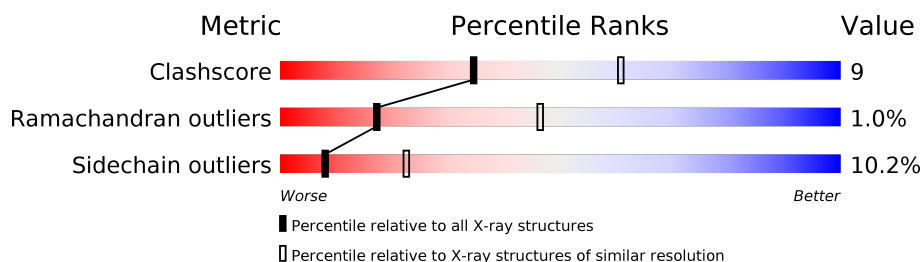
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	122078	2579 (2.90-2.86)
Ramachandran outliers	120005	2524 (2.90-2.86)
Sidechain outliers	119972	2527 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	 63% 26% 5% • 5%
1	B	842	 62% 27% 5% • 6%
1	C	842	 61% 26% 7% • 5%
1	D	842	 63% 25% 6% • 5%

2 Entry composition [i](#)

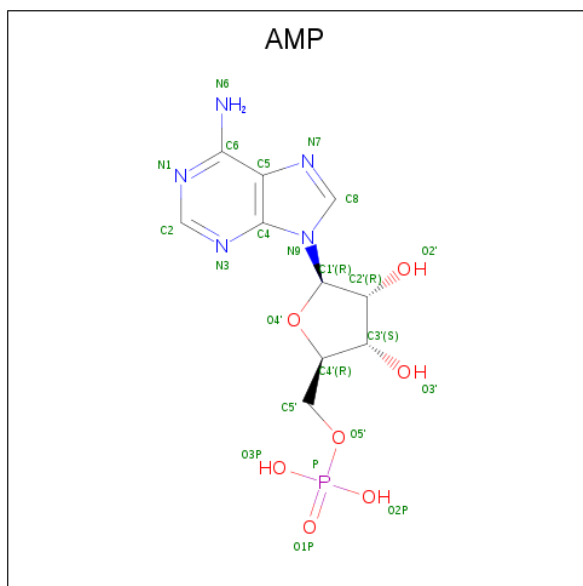
There are 3 unique types of molecules in this entry. The entry contains 26214 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	801	Total	C	N	O	S	0	0	0
			6512	4147	1155	1180	30			
1	B	791	Total	C	N	O	S	0	0	0
			6434	4099	1137	1168	30			
1	C	801	Total	C	N	O	S	0	0	0
			6512	4147	1155	1180	30			
1	D	801	Total	C	N	O	S	0	0	0
			6512	4147	1155	1180	30			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



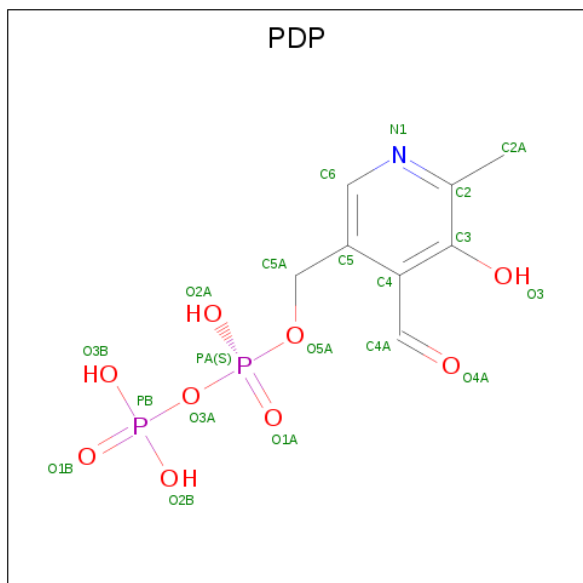
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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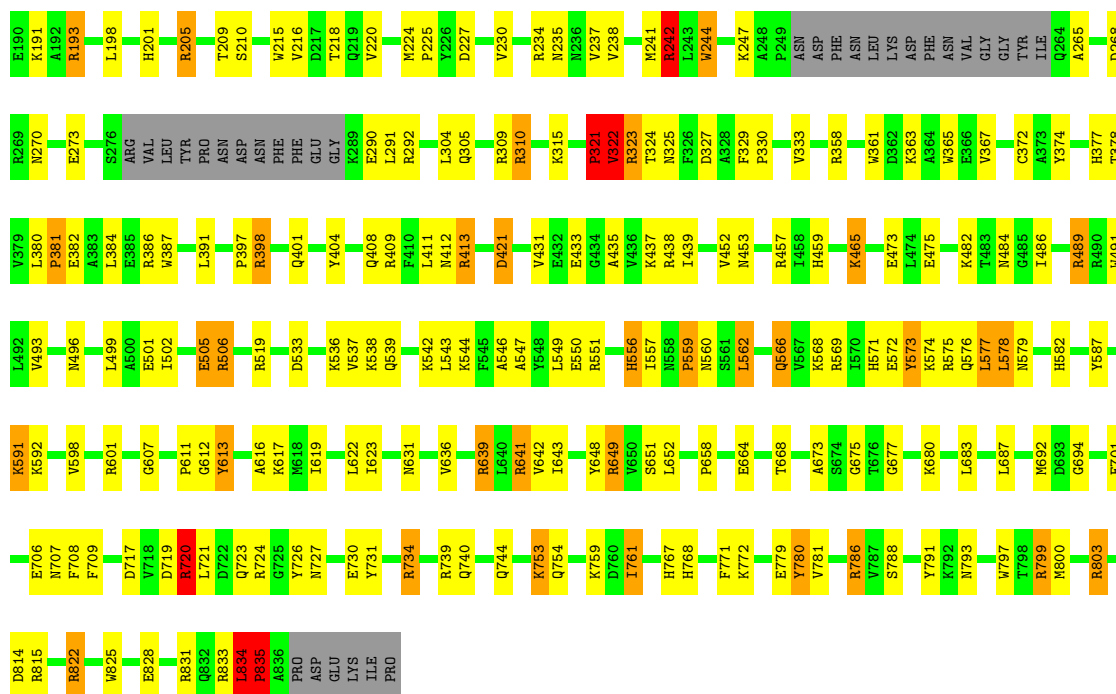
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

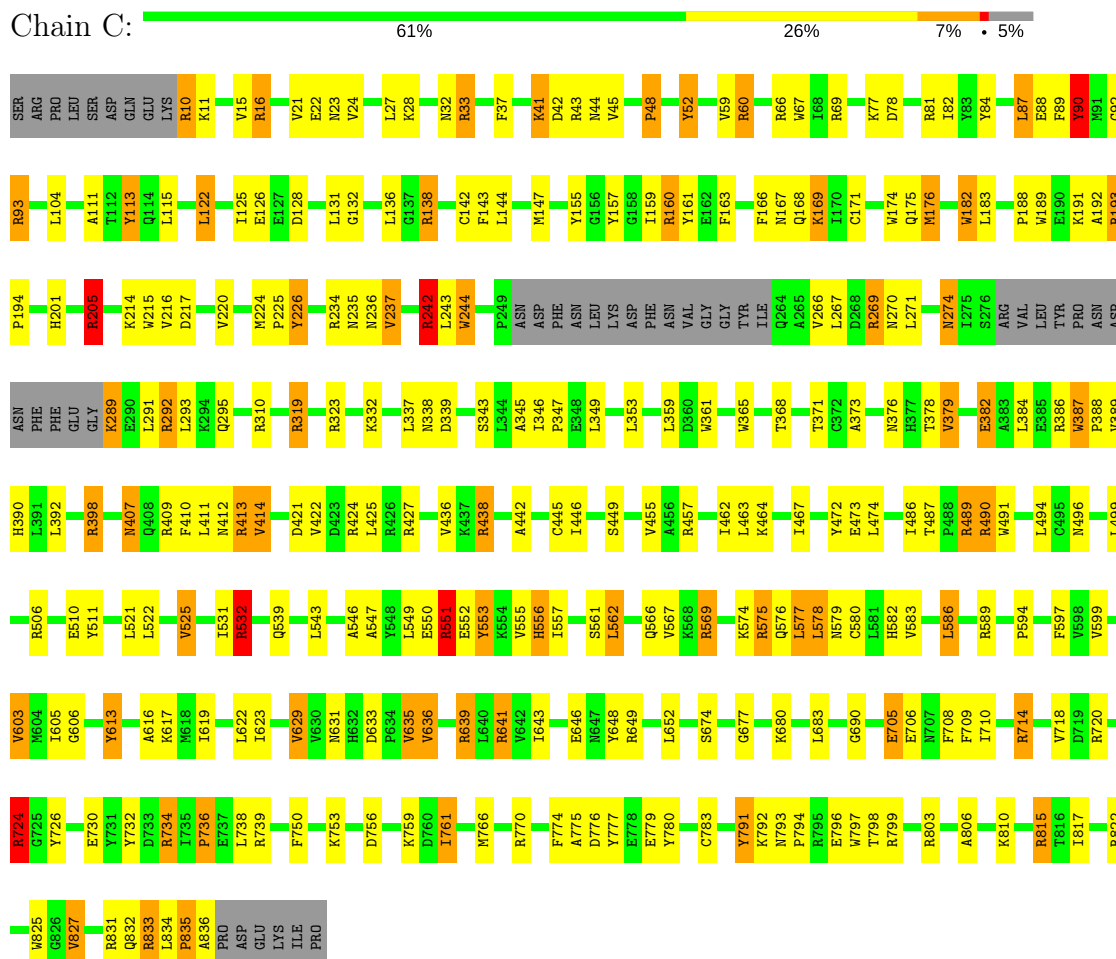
- Molecule 3 is PYRIDOXAL-5'-DIPHOSPHATE (three-letter code: PDP) (formula: $C_8H_{11}NO_9P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			38	16	2	16	4		
3	B	1	Total	C	N	O	P	0	1
			38	16	2	16	4		
3	C	1	Total	C	N	O	P	0	1
			38	16	2	16	4		
3	D	1	Total	C	N	O	P	0	1
			38	16	2	16	4		

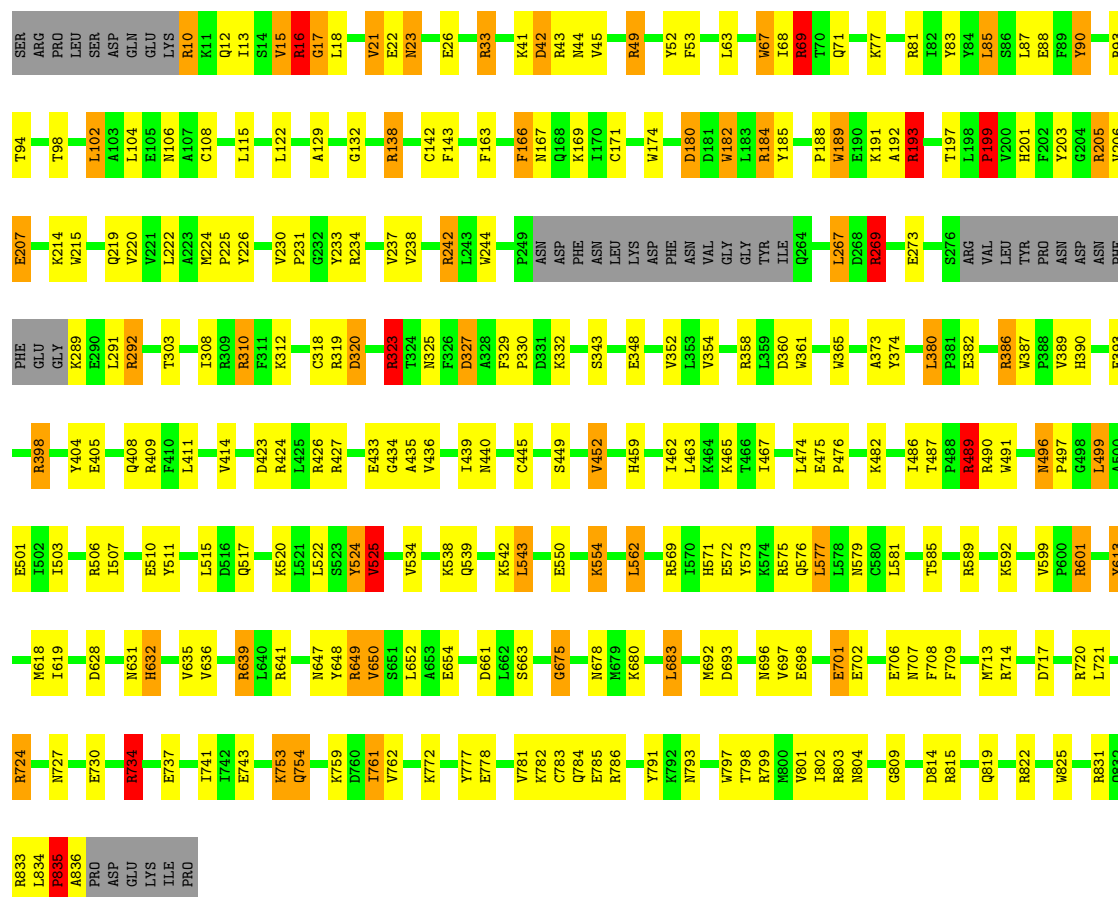


• Molecule 1: GLYCOGEN PHOSPHORYLASE B



● Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain D:  63% 25% 6% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	169.90Å 209.90Å 123.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.87	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.87)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26214	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.85	0/6655	1.66	128/9001 (1.4%)
1	B	0.86	0/6577	1.63	129/8898 (1.4%)
1	C	0.82	0/6655	1.63	124/9001 (1.4%)
1	D	0.86	0/6655	1.65	132/9001 (1.5%)
All	All	0.85	0/26542	1.64	513/35901 (1.4%)

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	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

The worst 5 of 513 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	310	ARG	NE-CZ-NH2	-14.56	113.02	120.30
1	D	601	ARG	NE-CZ-NH1	14.01	127.31	120.30
1	A	639	ARG	NE-CZ-NH2	-12.78	113.91	120.30
1	B	489	ARG	NE-CZ-NH1	12.58	126.59	120.30
1	D	138	ARG	NE-CZ-NH2	-12.42	114.09	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	TYR	Sidechain
1	A	52	TYR	Sidechain
1	B	52	TYR	Sidechain
1	B	834	LEU	Peptide
1	C	52	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	6512	0	6484	115	0
1	B	6434	0	6393	121	0
1	C	6512	0	6484	131	0
1	D	6512	0	6484	113	0
2	A	23	0	12	0	0
2	B	23	0	12	1	0
2	C	23	0	12	0	0
2	D	23	0	12	0	0
3	A	38	0	14	0	0
3	B	38	0	14	1	0
3	C	38	0	13	0	0
3	D	38	0	14	0	0
All	All	26214	0	25948	468	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 9.

The worst 5 of 468 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:193:ARG:HB2	1:D:225:PRO:HG2	1.63	0.81
1:C:225:PRO:HB2	1:C:242:ARG:HD2	1.61	0.79
1:C:549:LEU:HD12	1:C:557:ILE:HD13	1.65	0.79
1:B:325:ASN:HD21	1:B:327:ASP:HB2	1.52	0.75
1:C:88:GLU:HB2	1:C:132:GLY:HA2	1.68	0.75

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	795/842 (94%)	733 (92%)	51 (6%)	11 (1%)	12	37
1	B	785/842 (93%)	725 (92%)	52 (7%)	8 (1%)	17	46
1	C	795/842 (94%)	727 (91%)	61 (8%)	7 (1%)	19	49
1	D	795/842 (94%)	746 (94%)	42 (5%)	7 (1%)	19	49
All	All	3170/3368 (94%)	2931 (92%)	206 (6%)	33 (1%)	17	46

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	166	PHE
1	A	322	VAL
1	B	166	PHE
1	B	321	PRO

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	693/731 (95%)	631 (91%)	62 (9%)	11	29
1	B	685/731 (94%)	614 (90%)	71 (10%)	8	21
1	C	693/731 (95%)	614 (89%)	79 (11%)	6	17
1	D	693/731 (95%)	622 (90%)	71 (10%)	8	22
All	All	2764/2924 (94%)	2481 (90%)	283 (10%)	8	22

5 of 283 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	779	GLU
1	C	270	ASN
1	D	576	GLN
1	B	834	LEU
1	C	113	TYR

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

Mol	Chain	Res	Type
1	B	684	ASN
1	C	341	HIS
1	D	571	HIS
1	B	740	GLN
1	C	12	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	AMP	A	843	-	22,25,25	0.94	1 (4%)	23,38,38	1.02	1 (4%)
3	PDP	A	860[A]	1	18,19,20	2.78	6 (33%)	22,29,30	1.61	3 (13%)
3	PDP	A	860[B]	1	18,19,20	3.15	7 (38%)	22,29,30	1.62	6 (27%)
2	AMP	B	843	-	22,25,25	1.08	0	23,38,38	0.95	0
3	PDP	B	860[A]	1	18,19,20	2.93	6 (33%)	22,29,30	1.45	4 (18%)
3	PDP	B	860[B]	1	18,19,20	2.75	6 (33%)	22,29,30	2.31	5 (22%)
2	AMP	C	843	-	22,25,25	1.17	2 (9%)	23,38,38	1.30	3 (13%)
3	PDP	C	860[A]	1	18,19,20	3.30	7 (38%)	22,29,30	1.57	3 (13%)
3	PDP	C	860[B]	1	18,19,20	3.13	6 (33%)	22,29,30	1.43	5 (22%)
2	AMP	D	843	-	22,25,25	1.02	2 (9%)	23,38,38	1.59	4 (17%)
3	PDP	D	860[A]	1	18,19,20	2.96	6 (33%)	22,29,30	1.61	6 (27%)
3	PDP	D	860[B]	1	18,19,20	3.08	6 (33%)	22,29,30	1.76	5 (22%)

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
2	AMP	A	843	-	-	0/6/26/26	0/3/3/3
3	PDP	A	860[A]	1	-	0/12/12/14	0/1/1/1
3	PDP	A	860[B]	1	-	0/12/12/14	0/1/1/1
2	AMP	B	843	-	-	0/6/26/26	0/3/3/3
3	PDP	B	860[A]	1	-	0/12/12/14	0/1/1/1
3	PDP	B	860[B]	1	-	0/12/12/14	0/1/1/1
2	AMP	C	843	-	-	0/6/26/26	0/3/3/3
3	PDP	C	860[A]	1	-	0/12/12/14	0/1/1/1
3	PDP	C	860[B]	1	-	0/12/12/14	0/1/1/1
2	AMP	D	843	-	-	0/6/26/26	0/3/3/3
3	PDP	D	860[A]	1	-	0/12/12/14	0/1/1/1
3	PDP	D	860[B]	1	-	0/12/12/14	0/1/1/1

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	860[B]	PDP	PB-O3A	-8.01	1.47	1.60
3	C	860[A]	PDP	C3-C2	-7.79	1.35	1.40
3	A	860[B]	PDP	C3-C2	-7.65	1.35	1.40
3	A	860[A]	PDP	PB-O3A	-7.50	1.48	1.60
3	B	860[A]	PDP	PB-O3A	-7.33	1.48	1.60

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	860[B]	PDP	PA-O3A-PB	-5.41	114.44	132.63
3	C	860[A]	PDP	PA-O3A-PB	-4.48	117.56	132.63
3	A	860[A]	PDP	PA-O3A-PB	-4.39	117.88	132.63
3	D	860[B]	PDP	PA-O3A-PB	-4.37	117.93	132.63
3	A	860[B]	PDP	PA-O3A-PB	-4.07	118.94	132.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	843	AMP	1	0
3	B	860[B]	PDP	1	0

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.