wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:37 PM GMT

PDB ID	:	1L5Q
Title	:	Human liver glycogen phosphorylase a complexed with caffeine, N-Acetyl-bet a-D-glucopyranosylamine, and CP-403700
Authors	:	Ekstrom, J.L.; Pauly, T.A.; Carty, M.D.; Soeller, W.C.; Culp, J.; Danley, D.E.; Hoover, D.J.; Treadway, J.L.; Gibbs, E.M.; Fletterick, R.J.; Day, Y.S.N.; Myszka, D.G.; Rath, V.L.
Deposited on	:	2002-03-07
Resolution	:	2.25 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

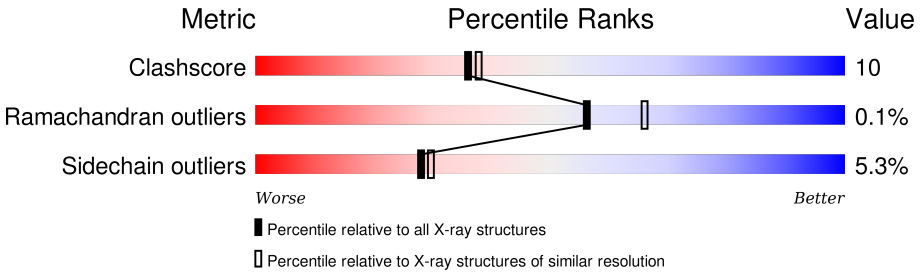
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.25 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	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)

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 <=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	847	73% 19% • 7%
1	B	847	74% 18% • 7%

2 Entry composition

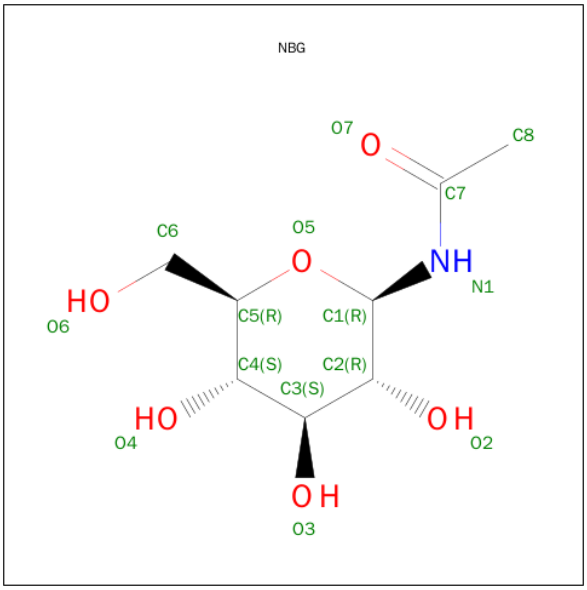
There are 6 unique types of molecules in this entry. The entry contains 13620 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, liver form.

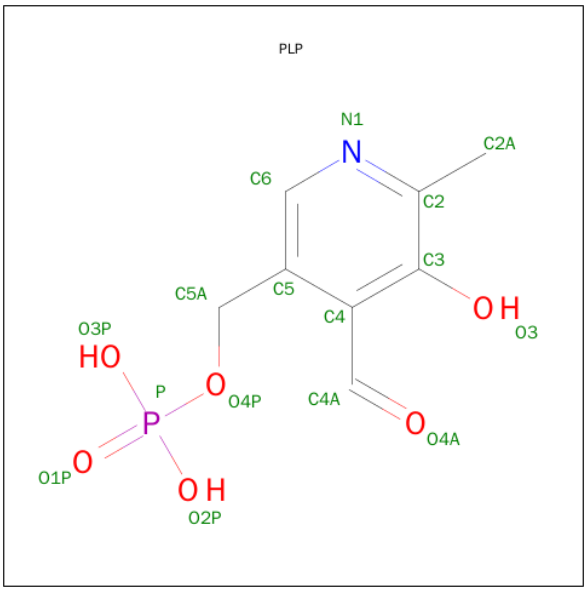
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	791	Total	C	N	O	S	0	0	0
			6423	4128	1090	1176	29			
1	B	790	Total	C	N	O	S	0	0	0
			6414	4123	1089	1173	29			

- Molecule 2 is SUGAR (1-N-ACETYL-BETA-D-GLUCOSAMINE) (three-letter code: NBG) (formula: $C_8H_{15}NO_6$).



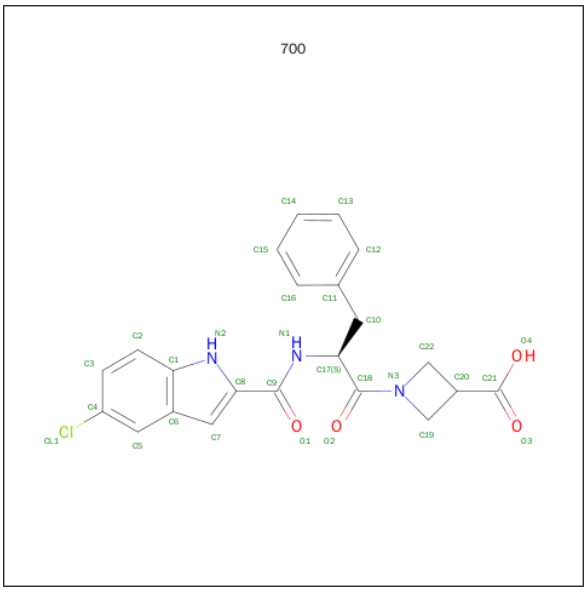
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- 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		

- Molecule 4 is [5-CHLORO-1H-INDOL-2-CARBONYL-PHENYLALANINYL]-AZETIDINE -3-CARBOXYLIC ACID (three-letter code: 700) (formula: $C_{22}H_{20}ClN_3O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

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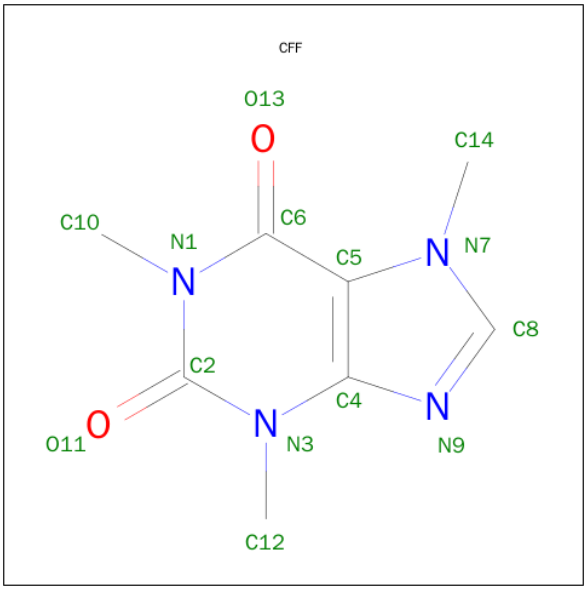
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

- Molecule 5 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	4	2		
5	B	1	Total	C	N	O	0	0
			14	8	4	2		
5	A	1	Total	C	N	O	0	0
			14	8	4	2		
5	B	1	Total	C	N	O	0	0
			14	8	4	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	324	Total	O	0	0
			324	324		
6	B	283	Total	O	0	0
			283	283		

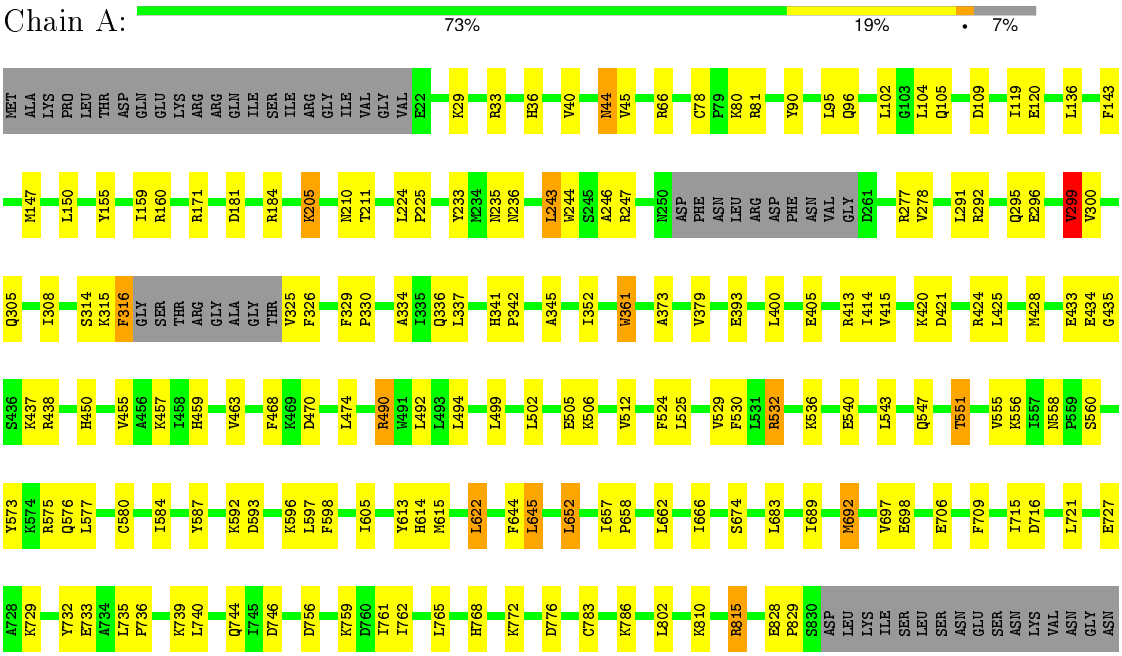
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

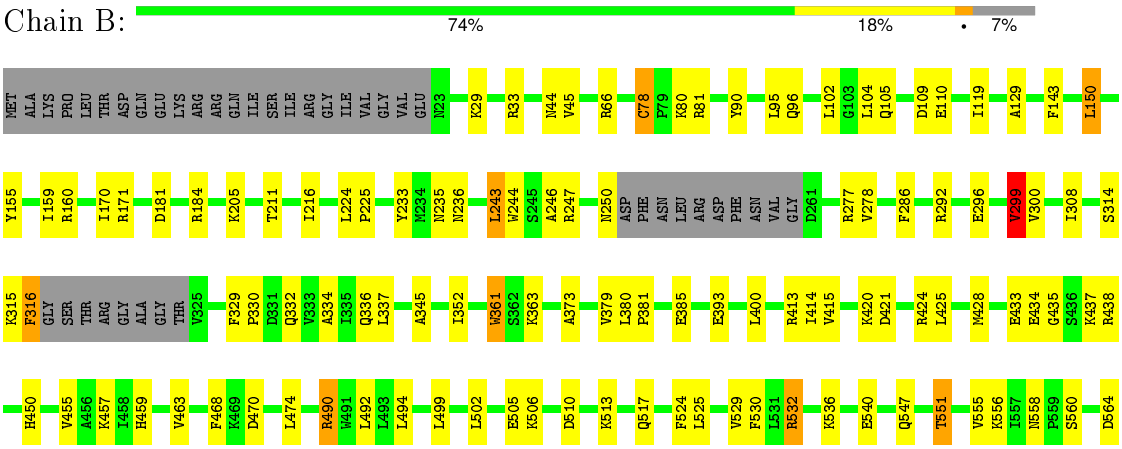
- Molecule 1: Glycogen phosphorylase, liver form

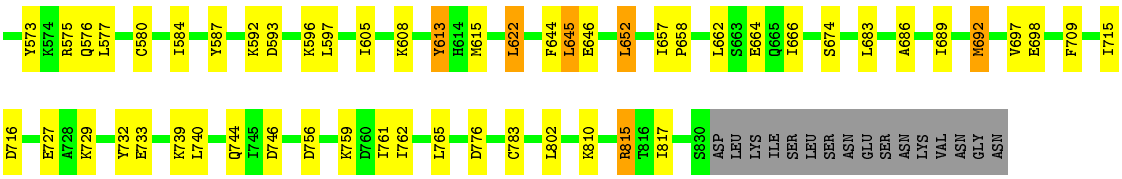
Chain A:



- Molecule 1: Glycogen phosphorylase, liver form

Chain B:




V573 K574 R575 Q576 L577 C580 I584 Y587 K592 D593 K596 L597 I605 K608 Y613 H614 M615 L622 F644 L645 E646 L652 I657 P658 L662 S663 E664 Q665 I666 S674 L683 A686 I689 M692 V697 E698 F709 I715
D716 E727 A728 K729 Y732 E733 K739 L740 Q744 I745 D746 D756 K759 D760 I761 I762 L765 D776 C783 L802 K810 R815 T816 I817 S830 ASP LEU LYS ILE SER LEU SER ASN GLU SER ASN LYS VAL ASN GLY ASN

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	124.71Å 124.71Å 124.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.82 – 2.25	Depositor
% Data completeness (in resolution range)	89.2 (40.82-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13620	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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: CFF, 700, NBG, 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	0.47	0/6567	0.69	2/8881 (0.0%)
1	B	0.46	0/6558	0.69	3/8869 (0.0%)
All	All	0.47	0/13125	0.69	5/17750 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	490	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	490	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	B	129	ALA	N-CA-C	-5.86	95.19	111.00
1	B	299	VAL	CB-CA-C	-5.06	101.79	111.40
1	A	299	VAL	CB-CA-C	-5.01	101.88	111.40

There are no chirality outliers.

There are no planarity outliers.

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	6423	0	6417	127	0
1	B	6414	0	6411	120	0
2	A	15	0	15	0	0
2	B	15	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	15	0	7	0	0
3	B	15	0	7	0	0
4	A	30	0	18	0	0
4	B	30	0	18	0	0
5	A	28	0	20	2	0
5	B	28	0	20	1	0
6	A	324	0	0	16	0
6	B	283	0	0	19	0
All	All	13620	0	12948	248	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 10.

The worst 5 of 248 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:B:170:ILE:HG12	1:B:646:GLU:HG2	1.56	0.86
1:B:615:MET:HE1	1:B:761:ILE:HG12	1.58	0.84
1:A:205:LYS:HG3	6:A:2509:HOH:O	1.76	0.84
1:A:615:MET:HE1	1:A:761:ILE:HG12	1.60	0.82
1:A:532:ARG:HB2	1:A:532:ARG:HH11	1.44	0.82

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	785/847 (93%)	754 (96%)	30 (4%)	1 (0%)	56	66
1	B	784/847 (93%)	749 (96%)	34 (4%)	1 (0%)	56	66
All	All	1569/1694 (93%)	1503 (96%)	64 (4%)	2 (0%)	56	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	GLU
1	B	434	GLU

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	693/740 (94%)	656 (95%)	37 (5%)	28	30
1	B	692/740 (94%)	656 (95%)	36 (5%)	29	31
All	All	1385/1480 (94%)	1312 (95%)	73 (5%)	28	30

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	706	GLU
1	B	95	LEU
1	B	662	LEU
1	B	44	ASN
1	B	104	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	HIS
1	B	32	ASN
1	B	369	GLN
1	A	369	GLN
1	B	450	HIS

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)

10 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	A	860	1	15,15,16	1.88	4 (26%)	21,22,23	1.48	5 (23%)
2	NBG	A	861	-	15,15,15	1.99	3 (20%)	21,21,21	1.03	1 (4%)
4	700	A	862	-	26,33,33	1.74	5 (19%)	33,47,47	1.65	8 (24%)
5	CFF	A	863	-	8,15,15	1.78	2 (25%)	8,23,23	1.41	2 (25%)
5	CFF	A	864	-	8,15,15	2.53	2 (25%)	8,23,23	1.29	1 (12%)
3	PLP	B	1860	1	15,15,16	2.67	4 (26%)	21,22,23	1.27	1 (4%)
2	NBG	B	1861	-	15,15,15	2.20	3 (20%)	21,21,21	1.14	1 (4%)
4	700	B	1862	-	26,33,33	1.89	9 (34%)	33,47,47	1.67	6 (18%)
5	CFF	B	1863	-	8,15,15	1.88	1 (12%)	8,23,23	1.31	2 (25%)
5	CFF	B	1864	-	8,15,15	2.79	2 (25%)	8,23,23	1.16	1 (12%)

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	A	860	1	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/5/26/26	0/1/1/1
4	700	A	862	-	-	0/15/32/32	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CFF	A	863	-	-	0/0/0/0	0/2/2/2
5	CFF	A	864	-	-	0/0/0/0	0/2/2/2
3	PLP	B	1860	1	-	0/6/6/8	0/1/1/1
2	NBG	B	1861	-	-	0/5/26/26	0/1/1/1
4	700	B	1862	-	-	0/15/32/32	0/4/4/4
5	CFF	B	1863	-	-	0/0/0/0	0/2/2/2
5	CFF	B	1864	-	-	0/0/0/0	0/2/2/2

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1860	PLP	C4A-C4	-6.75	1.37	1.51
3	B	1860	PLP	C3-C2	-5.86	1.36	1.40
3	A	860	PLP	C4A-C4	-4.43	1.42	1.51
3	A	860	PLP	P-O2P	-2.26	1.46	1.54
4	A	862	700	C4-CL1	-2.25	1.69	1.74

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	862	700	C7-C6-C1	-5.01	101.90	106.27
4	B	1862	700	C7-C6-C1	-4.28	102.54	106.27
4	B	1862	700	C3-C2-C1	-3.46	117.13	120.88
4	B	1862	700	C10-C17-C18	-2.75	103.88	109.88
5	A	863	CFF	C10-N1-C2	-2.75	113.61	119.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	864	CFF	2	0
2	B	1861	NBG	1	0
5	B	1863	CFF	1	0

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.