



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:17 PM GMT

PDB ID : 1EXV  
Title : HUMAN LIVER GLYCOGEN PHOSPHORYLASE A COMPLEXED WITH GLCNAC AND CP-403,700  
Authors : Rath, V.L.; Ammirati, M.; Danley, D.E.; Ekstrom, J.L.; Hynes, T.R.; Olson, T.V.; Hoover, D.J.  
Deposited on : 2000-05-04  
Resolution : 2.40 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 (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

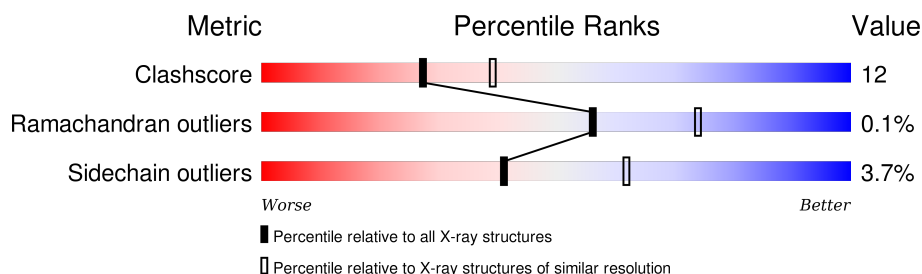
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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  $\geq 3$ , 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	847	
1	B	847	

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
5	MPD	A	1901	X	-	-	-
5	MPD	B	1902	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13223 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.

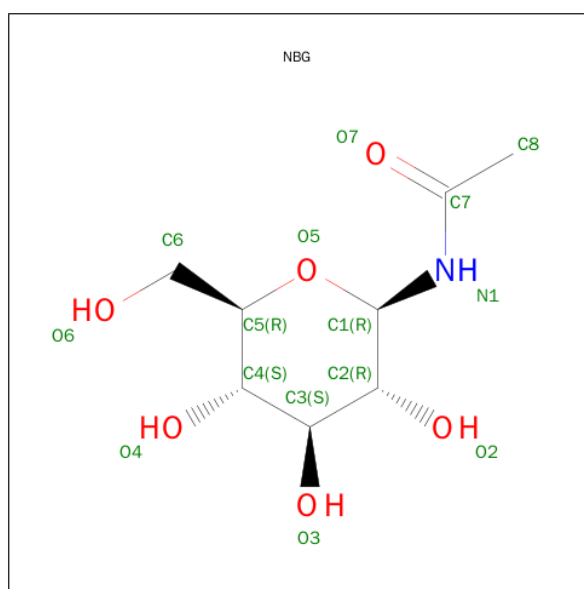
- Molecule 1 is a protein called LIVER GLYCOGEN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	786	Total	C	N	O	S	0	0	0
			6377	4098	1083	1167	29			
1	B	786	Total	C	N	O	S	0	0	0
			6377	4098	1083	1167	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	569	ARG	SER	SEE REMARK 999	UNP P06737
B	569	ARG	SER	SEE REMARK 999	UNP P06737

- Molecule 2 is SUGAR (1-N-ACETYL-BETA-D-GLUCOSAMINE) (three-letter code: NBG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



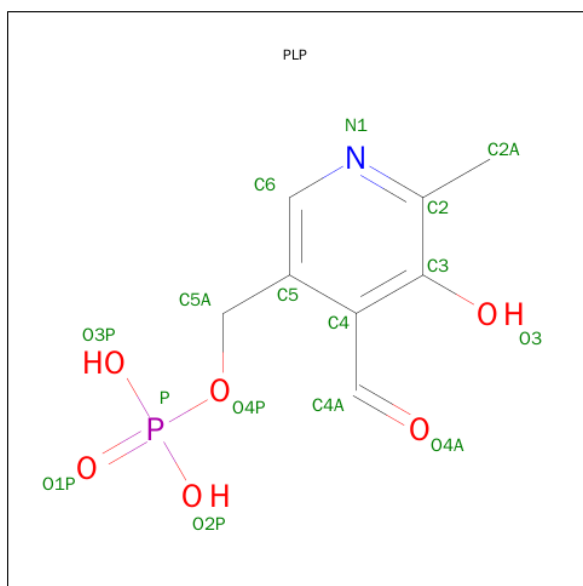
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

*Continued on next page...*

*Continued from previous page...*

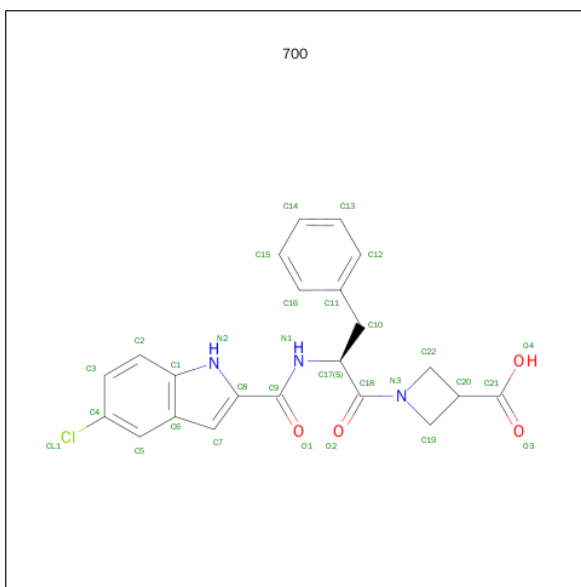
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

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



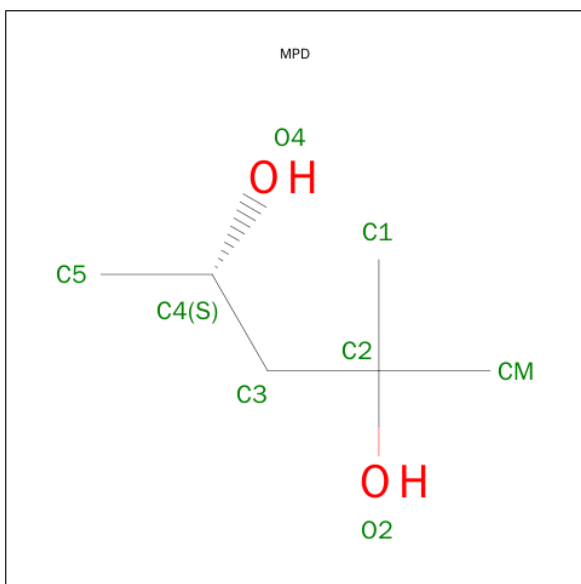
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- 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	
			30	22	1	3	4	0
4	B	1	Total	C	Cl	N	O	
			30	22	1	3	4	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O		
			8	6	2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

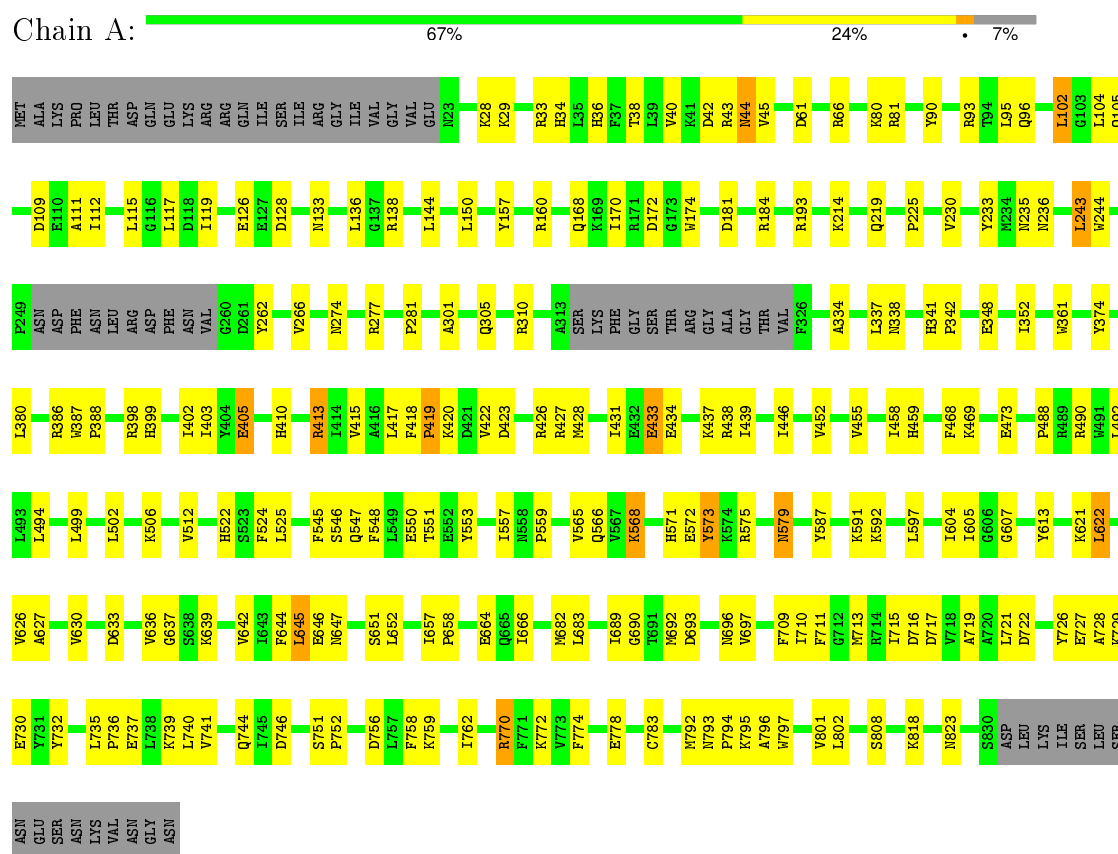
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	174	Total	O	0	0
			174	174		
6	B	159	Total	O	0	0
			159	159		

### 3 Residue-property plots

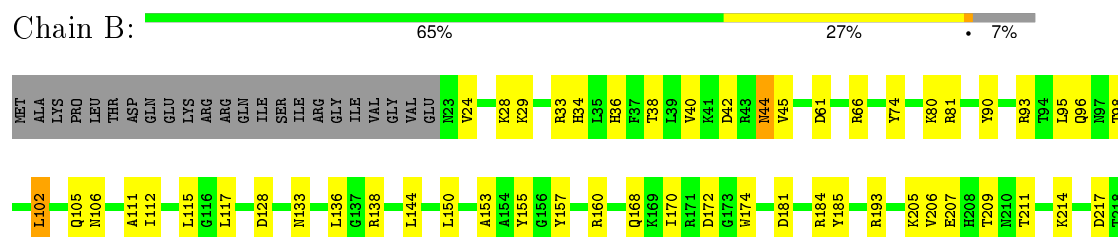
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: LIVER GLYCOGEN PHOSPHORYLASE



#### • Molecule 1: LIVER GLYCOGEN PHOSPHORYLASE



K759	Q219	GLY	R438	I557	B664	K759
I762	P225	THR	I439	N598	Q665	I762
R770	V230	VAL	I446	P559	I666	I762
F774	Y233	F326	V447	V565	M682	R770
E778	I234	A334	G448	Q566	L683	F774
C783	N235	L337	S448	V567	I689	E778
M792	N236	N338	H450	K568	G690	M792
N793	L243	H341	V452	H571	M691	N793
P794	N244	P342	V455	E572	D693	P794
A796	R247	A345	I458	Y573	M696	A796
W797	A248	I346	H459	K574	V697	W797
V801	P249	W361	F468	R575	B698	V801
L802	ASN	Y374	K469	N579	E702	L802
S808	ASP	E473	E473	Y587	L708	S808
K818	PHE	L380	P488	K591	F709	K818
S830	ASN	P381	R489	K592	I710	S830
ASP	LEU	L384	V490	L597	F711	ASP
LEU	ARG	P385	V491	I604	G712	LEU
LYS	ASP	R386	L492	I605	M713	LYS
ILE	PHE	R398	L494	Y613	R714	ILE
SER	ASN	H399	L499	K617	D716	SER
LEU	VAL	D261	L502	K621	D717	LEU
SER	GLU	Y262	K506	L622	A719	SER
ASN	GLY	V266	V512	V626	D722	ASN
GLY	ASN	I274	S516	A627	Y726	GLY
ASN	LEU	R277	T519	V630	E727	ASN
ASN	ASN	P281	R520	D633	A728	ASN
ASN	ASN	R292	L521	V636	E730	ASN
ASN	ASN	E296	H522	G637	Y731	ASN
ASN	ASN	V300	S523	S638	L735	ASN
ASN	ASN	A301	F524	K639	P736	ASN
ASN	ASN	Q305	L525	V642	E737	ASN
ASN	ASN	R310	D528	I643	L738	ASN
ASN	ASN	A313	R532	F644	V741	ASN
ASN	ASN	SER	F545	L645	Q744	ASN
ASN	ASN	LYS	S546	N647	I745	ASN
ASN	ASN	PHE	Q547	S651	D746	ASN
ASN	ASN	GLY	F548	L652	S751	ASN
ASN	ASN	SER	E549	L652	P752	ASN
ASN	ASN	THR	E550	T551	D756	ASN
ASN	ASN	ARG	T551	P558	L757	ASN
ASN	ASN	GLY	E552	Y553	F758	ASN
ASN	ASN	ALA	Y553			ASN



## 4 Data and refinement statistics

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, $\alpha$ , $\beta$ , $\gamma$	124.63Å 124.63Å 124.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.00 – 2.40	Depositor
% Data completeness (in resolution range)	99.8 (99.00-2.40)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.236 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13223	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	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: 700, MPD, 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	0.36	0/6520	0.58	0/8818
1	B	0.35	0/6520	0.58	0/8818
All	All	0.36	0/13040	0.58	0/17636

There are no bond length outliers.

There are no bond angle outliers.

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	6377	0	6372	149	0
1	B	6377	0	6372	159	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0
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	8	0	14	1	0
5	B	8	0	14	0	0
6	A	174	0	0	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	159	0	0	12	0
All	All	13223	0	12852	306	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 12.

The worst 5 of 306 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:A:96:GLN:HE21	1:A:105:GLN:HE22	1.11	0.98
1:B:96:GLN:HE21	1:B:105:GLN:HE22	1.09	0.98
1:A:168:GLN:HE21	1:A:647:ASN:H	1.21	0.87
1:B:168:GLN:HE21	1:B:647:ASN:H	1.22	0.87
1:B:81:ARG:NH1	1:B:310:ARG:HD3	1.94	0.81

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	780/847 (92%)	731 (94%)	48 (6%)	1 (0%)	56	74
1	B	780/847 (92%)	730 (94%)	50 (6%)	0	100	100
All	All	1560/1694 (92%)	1461 (94%)	98 (6%)	1 (0%)	56	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	419	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	687/740 (93%)	661 (96%)	26 (4%)	40	60
1	B	687/740 (93%)	662 (96%)	25 (4%)	42	63
All	All	1374/1480 (93%)	1323 (96%)	51 (4%)	41	62

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	683	LEU
1	B	95	LEU
1	B	652	LEU
1	A	770	ARG
1	B	102	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	579	ASN
1	B	44	ASN
1	B	566	GLN
1	A	823	ASN
1	B	32	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 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$
5	MPD	A	1901	-	6,7,7	0.49	0	7,10,10	0.73	0
3	PLP	A	860	1	15,15,16	1.53	1 (6%)	21,22,23	1.44	5 (23%)
2	NBG	A	861	-	15,15,15	1.44	3 (20%)	21,21,21	1.16	1 (4%)
4	700	A	862	-	26,33,33	2.33	8 (30%)	33,47,47	1.57	6 (18%)
3	PLP	B	1860	1	15,15,16	1.88	2 (13%)	21,22,23	1.43	2 (9%)
2	NBG	B	1861	-	15,15,15	1.69	3 (20%)	21,21,21	1.33	2 (9%)
4	700	B	1862	-	26,33,33	2.41	12 (46%)	33,47,47	1.52	6 (18%)
5	MPD	B	1902	-	6,7,7	0.74	0	7,10,10	0.62	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
5	MPD	A	1901	-	1/1/2/2	0/5/5/5	0/0/0/0
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
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	MPD	B	1902	-	1/1/2/2	0/5/5/5	0/0/0/0

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1860	PLP	C4A-C4	-5.66	1.40	1.51
4	B	1862	700	C17-C18	-4.70	1.43	1.53
3	A	860	PLP	C4A-C4	-4.62	1.42	1.51
4	A	862	700	C17-C18	-4.23	1.44	1.53
3	B	1860	PLP	C3-C2	-2.99	1.38	1.40

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	862	700	C7-C6-C1	-3.37	103.33	106.27
4	B	1862	700	C7-C6-C1	-3.01	103.65	106.27
4	B	1862	700	C3-C2-C1	-2.94	117.69	120.88
3	B	1860	PLP	O4P-P-O1P	-2.84	99.92	107.14
3	A	860	PLP	O3P-P-O4P	-2.80	98.51	106.56

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1901	MPD	C4
5	B	1902	MPD	C4

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1901	MPD	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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