



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 12:16 PM BST

PDB ID : 1FC0  
Title : HUMAN LIVER GLYCOGEN PHOSPHORYLASE COMPLEXED WITH N-ACETYL-BETA-D-GLUCOPYRANOSYLAMINE  
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Deposited on : 2000-07-17  
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

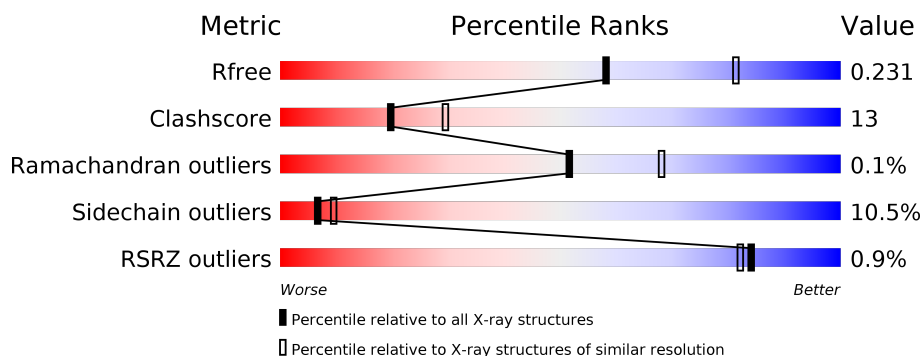
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	846	 % 63% 27% • 6%
1	B	846	 % 62% 28% • 6%

## 2 Entry composition [i](#)

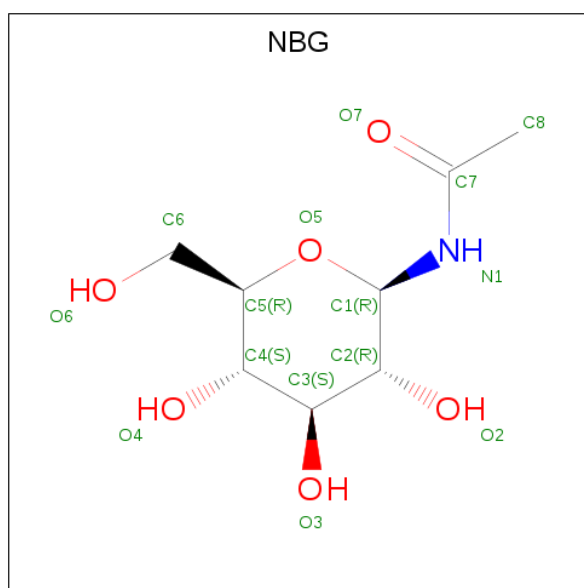
There are 4 unique types of molecules in this entry. The entry contains 13169 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

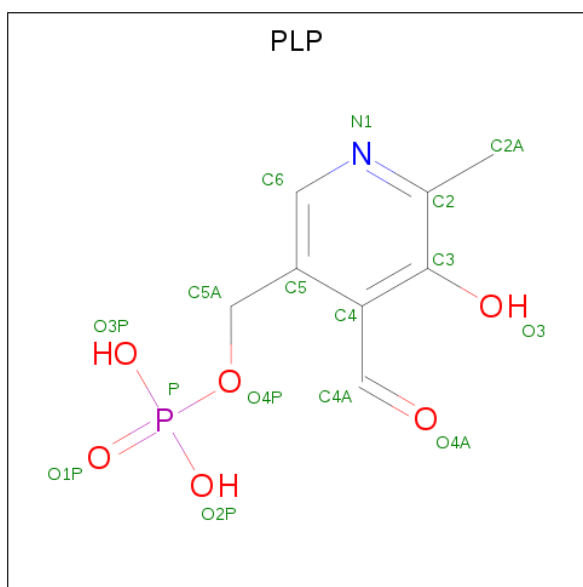
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	792	Total	C	N	O	S	0	0	0
			6425	4129	1090	1177	29			
1	B	793	Total	C	N	O	S	0	0	0
			6429	4131	1091	1178	29			

- Molecule 2 is N-acetyl-beta-D-glucopyranosylamine (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		

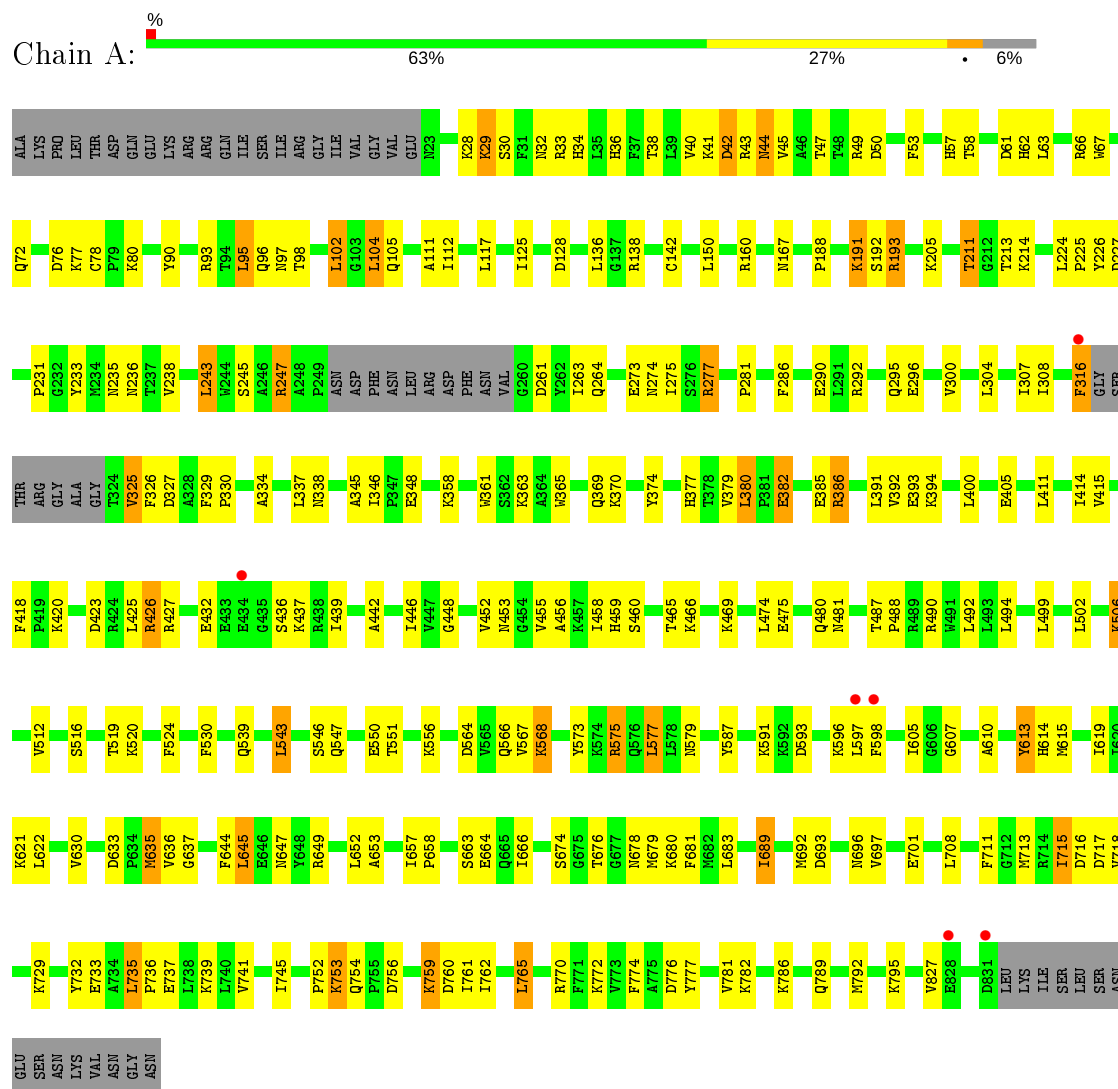
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total	O	0	0
			151	151		
4	B	104	Total	O	0	0
			104	104		

### 3 Residue-property plots

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 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.

#### • Molecule 1: GLYCOGEN PHOSPHORYLASE, LIVER FORM



#### • Molecule 1: GLYCOGEN PHOSPHORYLASE, LIVER FORM



S1830	G1712	A1610	L1492	L1400	L1304	N1210	G1078	ALA
D1831	M1713		L1499	E1405	I1308	T1213	P1079	LYS
LEU	R1714	Y1613				K1080	K1080	PRO
LYS	I1715	H1614				K1214		LEU
I1E	D1716	M1615	L1502	L1411	F1316	I1216	Y1090	THR
SER	D1717		K1506	I1414	GLY	D1217		ASP
LEU	V1718	I1619		V1415	SER		R1093	GLN
SER		I1620	S1516	F1418	THR	L1224	T1094	GLU
K1729	K1729	E1730	S1516	F1418	ARG	P1225	L1095	LYS
E1731	E1731	L1622	T1519	P1419	GLY	Y1226	T1098	ARG
GLU	Y1731	L1622	K1520	K1420	ALA	D1227		ARG
Y1732	Y1732	V1630			G1323			GLN
ASN	E1733		F1524	D1423	T1324	P1231	L1102	TLE
LYS	E1733			R1424	V1325		G1103	SER
VAL	A1734	M1635	D1527	R1424	F1326	N1235	L1104	ILE
ASN	L1735			L1425	D1327	N1236	E1110	ARG
GLY	P1736	F1644	L1543	R1426	A1328	T1237	A1111	GLY
ASN	E1737	L1645	F1530	R1427	F1329	V1238	I1112	ILE
LYS	L1738	E1646		E1432	P1330		Y1113	VAL
K1739	L1738	M1647	Q1539		A1334	L1243	Q1114	GLY
L1740	Y1648			S1436	L1337	W1244	I1119	GLU
V1741	R1649	V1650	L1543	K1437	N1338	A1246		N1023
I1745	S1651	L1652	Q1546	I1439	D1339	R1247	L1122	V1024
	A1653		Q1547			A1248		
P1752		I1657	E1550	A1442	P1342	P1249	I1125	K1028
K1753		P1658	T1551		A1345	ASN	E1126	K1029
Q1754	S1663		K1554	I1446	I1346	ASP	E1127	H1033
D1756	E1664		V1555	V1447	P1347	PHE	D1128	R1034
K1759	Q1665		K1556	G1448	E1348	ASN		L1035
D1760	I1666			V1452		LEU	G1135	H1036
I1761	S1667		D1564	N1453	W1361	ASP	L1136	F1037
I1762	T1668		V1565	G1454	W1365	PHE	G1137	L1038
			Q1566	V1455		ASN	R1138	V1040
L1765		A1673	V1567	A1456		VAL	G1142	K1041
R1770	S1674		K1568	K1457	Q1369	G1260		D1042
F1771	G1675			I1458	K1370	D1261	L1150	R1043
K1772	T1676		R1575	H1459	Y1374	Y1262		N1044
F1773		K1680	Q1576	S1460		Q1264	R1160	V1045
V1774		F1681	L1577	D1461	H1377		M1167	A1046
A1775		M1682	L1578	I1462	T1378	E1273	T1047	T1048
D1776		L1683	N1579		V1379	N1274	A1049	
Y1777			Y1587	T1465	L1380	I1275	D1050	
	V1781			K1466	P1381	S1276	W1174	
K1782	K1782	I1689		K1469	E1382	R1277		F1053
			K1591		A1383		Y1185	
K1786		M1692	K1592	L1474	L1384	F1286	P1188	T1058
		D1693	D1593	E1475	E1385			V1059
Q1789		M1696	P1594		R1386	E1290	K1191	R1060
	V1697		K1595	Q1480	L1391	L1291	S1192	H1061
M1792	E1698		K1596	N1481	V1392	R1292	H1062	L1063
			L1597		E1393			
K1795	E1701		F1598	T1487	K1394	Q1295	V1206	R1066
				P1488		E1296	H1207	W1067
V1827	L1708		I1605	R1489	P1397	V1300	E1208	
E1828			G1606	G1491			T1209	K1077
P1829	F1711		G1607					

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.00Å 124.00Å 122.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.40 19.58 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.1 (30.00-2.40) 95.2 (19.58-2.40)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.76 (at 2.41Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.198 , 0.235 0.192 , 0.231	Depositor DCC
$R_{free}$ test set	8191 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 32.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l 0.082 for h,-h-k,-l 0.033 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13169	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.35	0/6569	0.57	0/8884
1	B	0.34	0/6573	0.56	0/8889
All	All	0.34	0/13142	0.56	0/17773

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	6425	0	6419	154	0
1	B	6429	0	6422	175	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0
3	A	15	0	6	0	0
3	B	15	0	7	0	0
4	A	151	0	0	6	0
4	B	104	0	0	2	0
All	All	13169	0	12884	328	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 13.

The worst 5 of 328 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:1274:ASN:ND2	1:B:1277:ARG:HH11	1.61	0.97
1:B:1713:MET:HB2	1:B:1717:ASP:HB2	1.47	0.95
1:A:547:GLN:O	1:A:551:THR:HG23	1.66	0.95
1:A:713:MET:HB2	1:A:717:ASP:HB2	1.47	0.94
1:A:274:ASN:ND2	1:A:277:ARG:HH11	1.66	0.94

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	786/846 (93%)	739 (94%)	46 (6%)	1 (0%)	51	68
1	B	787/846 (93%)	738 (94%)	48 (6%)	1 (0%)	51	68
All	All	1573/1692 (93%)	1477 (94%)	94 (6%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	LEU
1	B	1095	LEU

### 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	693/739 (94%)	618 (89%)	75 (11%)	6	9
1	B	693/739 (94%)	622 (90%)	71 (10%)	7	10
All	All	1386/1478 (94%)	1240 (90%)	146 (10%)	7	9

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	735	LEU
1	B	1102	LEU
1	B	1733	GLU
1	A	753	LYS
1	A	795	LYS

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	541	ASN
1	B	1032	ASN
1	B	1566	GLN
1	A	566	GLN
1	A	579	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 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	1.86	3 (20%)	20,22,23	1.28	2 (10%)
2	NBG	A	861	-	15,15,15	1.22	1 (6%)	21,21,21	1.58	4 (19%)
2	NBG	B	1861	-	15,15,15	1.47	2 (13%)	21,21,21	1.31	3 (14%)
3	PLP	B	1860	1	15,15,16	1.92	4 (26%)	20,22,23	0.99	2 (10%)

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	-	2/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1
2	NBG	B	1861	-	-	0/6/26/26	0/1/1/1
3	PLP	B	1860	1	-	0/6/6/8	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1860	PLP	C4A-C4	-5.47	1.40	1.51
3	A	860	PLP	C4A-C4	-4.36	1.42	1.51
3	A	860	PLP	C3-C2	-3.91	1.37	1.40
2	B	1861	NBG	C2-C1	3.74	1.56	1.52
2	A	861	NBG	C2-C1	3.56	1.56	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	861	NBG	C5-O5-C1	4.73	118.93	112.52
2	B	1861	NBG	C5-O5-C1	3.97	117.90	112.52
2	A	861	NBG	C3-C2-C1	2.78	114.00	109.94
2	A	861	NBG	C2-C1-N1	-2.66	108.19	111.30
2	B	1861	NBG	C3-C2-C1	2.44	113.49	109.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	860	PLP	C6-C5-C5A-O4P
3	A	860	PLP	C4-C5-C5A-O4P

There are no ring outliers.

No monomer is involved in short contacts.

## 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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	792/846 (93%)	-0.57	6 (0%) 86 84	15, 31, 57, 101	0
1	B	793/846 (93%)	-0.52	8 (1%) 82 80	16, 32, 60, 101	0
All	All	1585/1692 (93%)	-0.54	14 (0%) 84 82	15, 32, 59, 101	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1831	ASP	4.9
1	B	1316	PHE	4.7
1	A	831	ASP	4.7
1	B	1420	LYS	4.0
1	A	598	PHE	3.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NBG	B	1861	15/15	0.96	0.12	17,31,35,38	0
2	NBG	A	861	15/15	0.98	0.11	14,23,31,32	0
3	PLP	B	1860	15/16	0.98	0.09	14,19,31,34	0
3	PLP	A	860	15/16	0.99	0.09	3,13,26,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.