



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:41 am GMT

PDB ID : 1L7X  
Title : Human liver glycogen phosphorylase b complexed with caffeine, N-acetyl-beta-D-glucopyranosylamine, and CP-403,700  
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 : 2002-03-18  
Resolution : 2.30 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.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

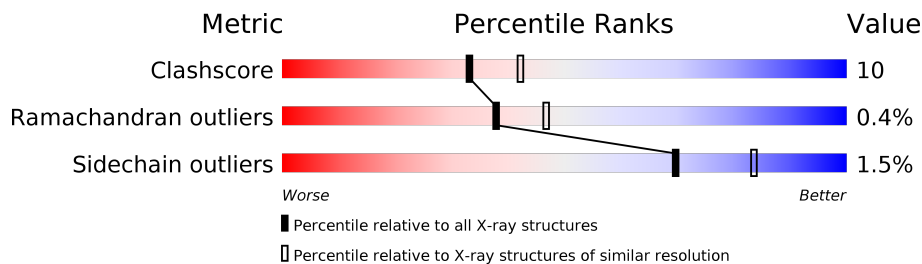
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)

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	

## 2 Entry composition [i](#)

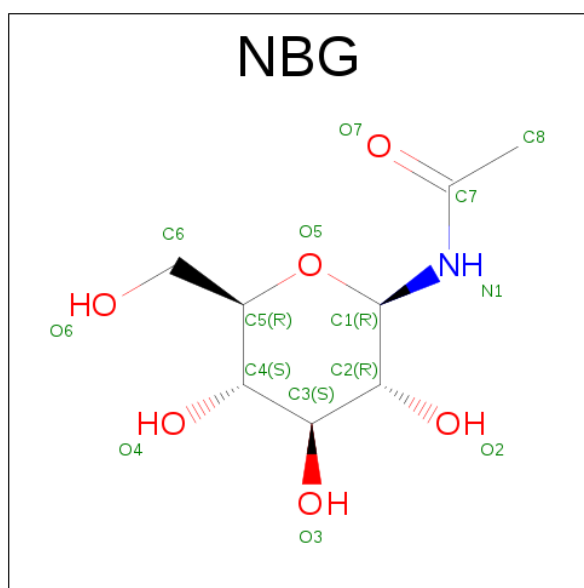
There are 7 unique types of molecules in this entry. The entry contains 13542 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	793	Total	C	N	O	S	0	0	0
			6436	4135	1092	1180	29			
1	B	795	Total	C	N	O	S	0	0	0
			6446	4141	1094	1182	29			

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



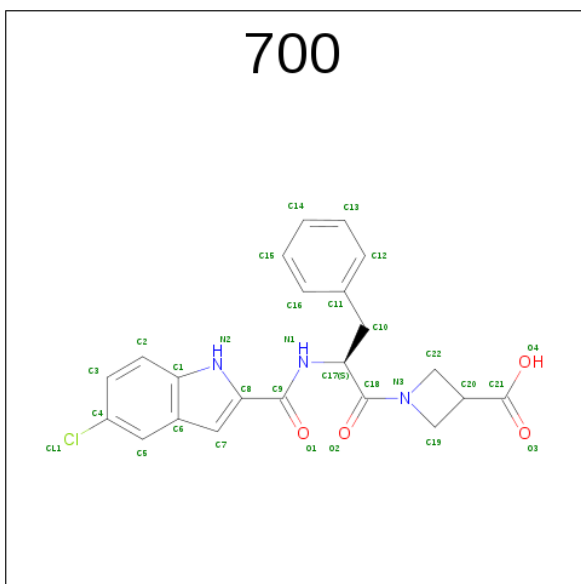
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- 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<sub>22</sub>H<sub>20</sub>ClN<sub>3</sub>O<sub>4</sub>).



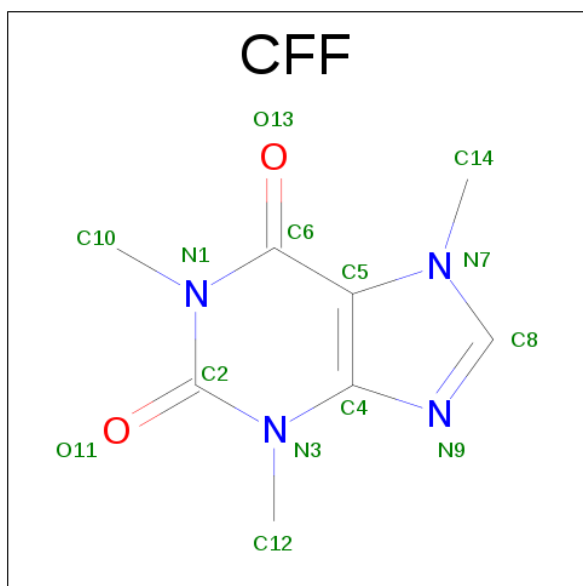
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

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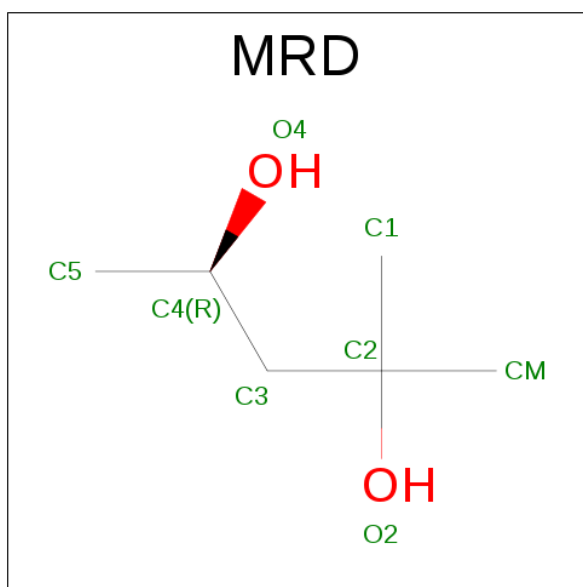
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

- 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		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



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

- Molecule 7 is water.

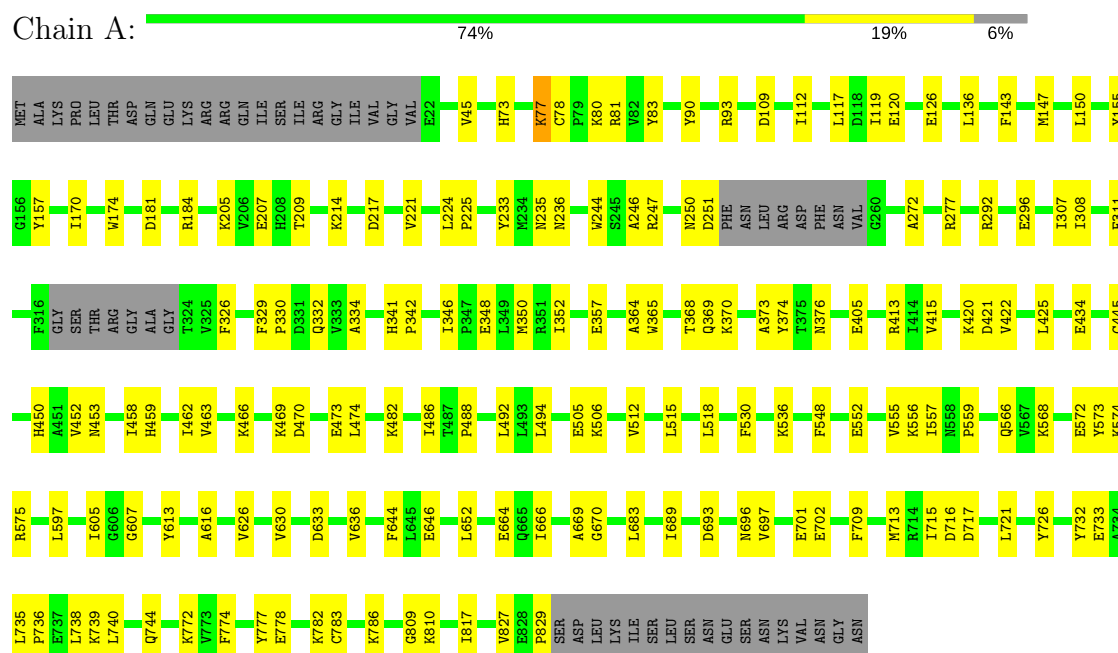
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	252	Total	O	0	0
			252	252		
7	B	222	Total	O	0	0
			222	222		

### 3 Residue-property plots [i](#)

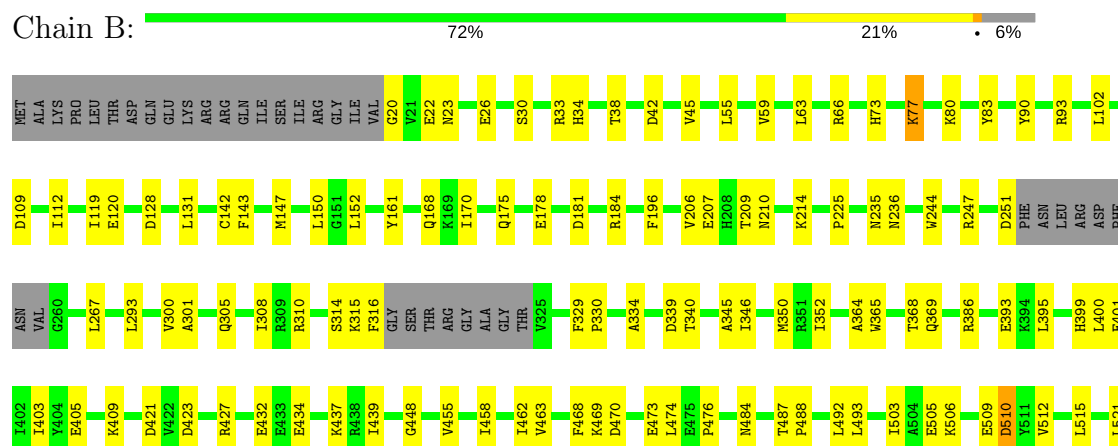
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

- Molecule 1: Glycogen phosphorylase, liver form



- Molecule 1: Glycogen phosphorylase, liver form



P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	L662	F524
																		F666	D528
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	S667	F548
																		T668	E552
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	L683	V555
																		L689	K556
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	R692	I557
																		V697	F573
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	E701	K568
																		A703	Y573
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	E706	K574
																		N707	R575
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	L708	Q576
																		F709	L577
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	I710	K591
																		M713	D592
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	R714	K596
																		I715	L597
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	D716	T605
																		V718	K608
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	Y732	Y613
																		E733	A616
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	K739	V626
																		D743	A627
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	N747	D628
																		F750	V629
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	V630	V630
																		L765	N631
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	K772	N632
																		C783	D633
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	D776	V636
																		Y777	V642
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	V781	T643
																		K782	F644
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	C783	L645
																		C783	E646
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	K786	V650
																		V787	S651
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	S812	L652
																		S812	
P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	V827	I657
																		E828	P658



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.07Å 124.07Å 122.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.39 – 2.30	Depositor
% Data completeness (in resolution range)	96.6 (34.39-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.206 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13542	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	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: CFF, MRD, 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	0.36	0/6580	0.59	0/8899
1	B	0.35	0/6590	0.59	0/8912
All	All	0.35	0/13170	0.59	0/17811

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 [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	6436	0	6426	126	0
1	B	6446	0	6436	133	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	19	0	0
4	B	30	0	19	0	0
5	A	28	0	20	0	0
5	B	14	0	10	0	0
6	B	24	0	42	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	252	0	0	7	0
7	B	222	0	0	4	0
All	All	13542	0	13016	256	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 256 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:350:MET:HE1	1:A:364:ALA:HB1	1.56	0.86
1:B:77:LYS:HA	1:B:77:LYS:HE3	1.59	0.84
1:A:80:LYS:HB3	1:A:827:VAL:HG12	1.60	0.83
1:A:721:LEU:HD23	1:A:772:LYS:HD3	1.60	0.83
1:B:80:LYS:HB3	1:B:827:VAL:HG12	1.62	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	787/847 (93%)	752 (96%)	32 (4%)	3 (0%)	38	47
1	B	789/847 (93%)	743 (94%)	43 (5%)	3 (0%)	38	47
All	All	1576/1694 (93%)	1495 (95%)	75 (5%)	6 (0%)	38	47

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	ASP
1	A	555	VAL

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Mol	Chain	Res	Type
1	B	421	ASP
1	A	434	GLU
1	B	434	GLU

### 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	694/740 (94%)	688 (99%)	6 (1%)	82	91
1	B	695/740 (94%)	680 (98%)	15 (2%)	57	74
All	All	1389/1480 (94%)	1368 (98%)	21 (2%)	70	83

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	210	ASN
1	B	510	ASP
1	B	652	LEU
1	B	120	GLU
1	B	706	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	822	GLN
1	B	23	ASN
1	B	484	ASN
1	A	484	ASN
1	A	517	GLN

### 5.3.3 RNA ⓘ

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$
3	PLP	A	860	1	15,15,16	2.11	3 (20%)	20,22,23	1.08	1 (5%)
2	NBG	A	861	-	15,15,15	1.47	3 (20%)	21,21,21	1.19	1 (4%)
4	700	A	862	-	24,33,33	1.86	9 (37%)	33,47,47	1.64	6 (18%)
5	CFF	A	863	-	7,15,15	1.22	0	8,23,23	1.17	2 (25%)
5	CFF	A	864	-	7,15,15	1.39	1 (14%)	8,23,23	1.20	2 (25%)
3	PLP	B	1860	1	15,15,16	1.75	2 (13%)	20,22,23	1.38	4 (20%)
2	NBG	B	1861	-	15,15,15	1.65	2 (13%)	21,21,21	1.33	2 (9%)
4	700	B	1862	-	24,33,33	1.88	7 (29%)	33,47,47	1.62	6 (18%)
5	CFF	B	1863	-	7,15,15	1.16	0	8,23,23	1.16	2 (25%)
6	MRD	B	1902	-	7,7,7	0.53	0	9,10,10	0.64	0
6	MRD	B	902	-	7,7,7	0.56	0	9,10,10	0.60	0
6	MRD	B	903	-	7,7,7	0.67	0	9,10,10	0.83	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
3	PLP	A	860	1	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NBG	A	861	-	-	0/5/26/26	0/1/1/1
4	700	A	862	-	-	0/15/32/32	0/4/4/4
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
6	MRD	B	1902	-	-	0/5/5/5	0/0/0/0
6	MRD	B	902	-	-	0/5/5/5	0/0/0/0
6	MRD	B	903	-	-	0/5/5/5	0/0/0/0

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1860	PLP	C4A-C4	-5.18	1.41	1.51
3	A	860	PLP	C4A-C4	-5.15	1.41	1.51
3	A	860	PLP	C3-C2	-4.11	1.37	1.40
4	B	1862	700	C7-C8	-2.27	1.35	1.39
3	B	1860	PLP	C3-C2	-2.13	1.39	1.40

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	862	700	C7-C6-C1	-4.49	102.36	106.27
4	B	1862	700	C7-C6-C1	-4.41	102.43	106.27
4	B	1862	700	C4-C5-C6	-2.89	117.21	119.18
4	B	1862	700	C3-C2-C1	-2.86	117.33	120.84
3	B	1860	PLP	O4P-P-O1P	-2.85	98.48	106.47

There are no chirality outliers.

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
6	B	903	MRD	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.