



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2025 – 01:29 PM EDT

PDB ID : 1EM6  
Title : HUMAN LIVER GLYCOGEN PHOSPHORYLASE A COMPLEXED WITH GLCNAC AND CP-526,423  
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Deposited on : 2000-03-16  
Resolution : 2.20 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4



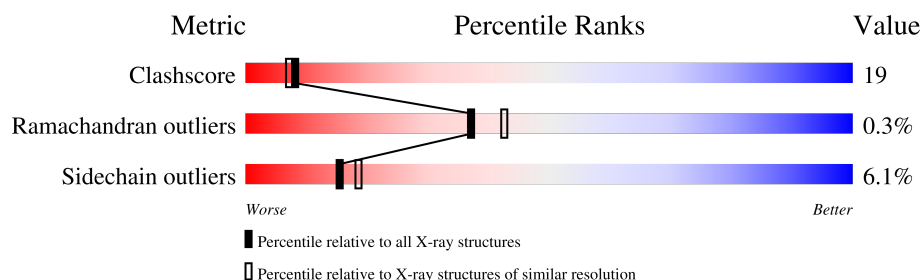
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)

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 of 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  $\leq 5\%$ .

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	B	1902	X	-	-	-



## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13599 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.

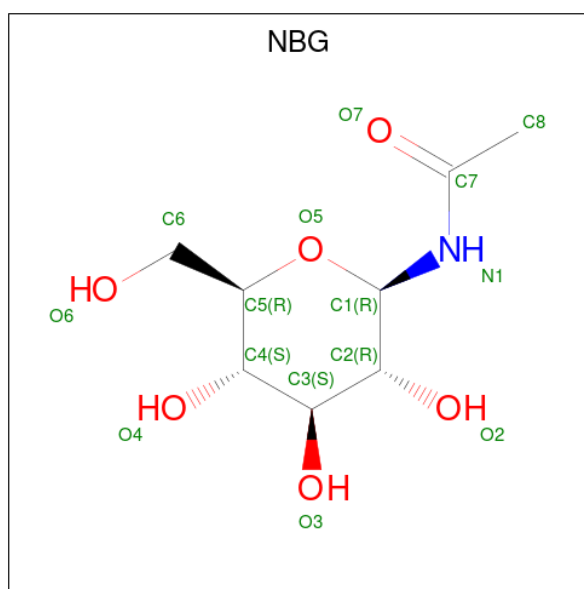
- Molecule 1 is a protein called LIVER GLYCOGEN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	787	Total	C	N	O	S	0	0	0
			6380	4097	1082	1172	29			
1	B	787	Total	C	N	O	S	0	0	0
			6380	4097	1082	1172	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 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		

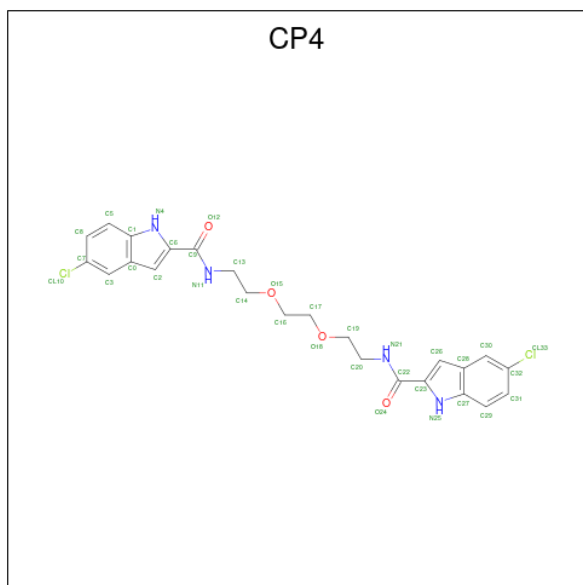
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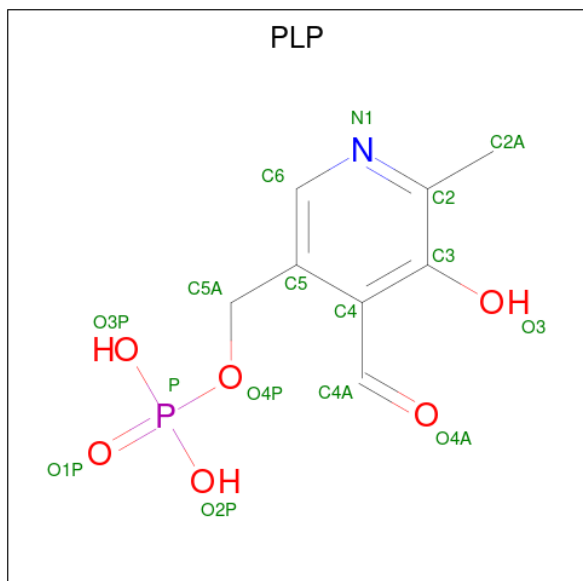
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is BIS[5-CHLORO-1H-INDOL-2-YL-CARBONYL-AMINOETHYL]-ETHYLEN E GLYCOL (three-letter code: CP4) (formula:  $C_{24}H_{24}Cl_2N_4O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	
			34	24	2	4	4	0

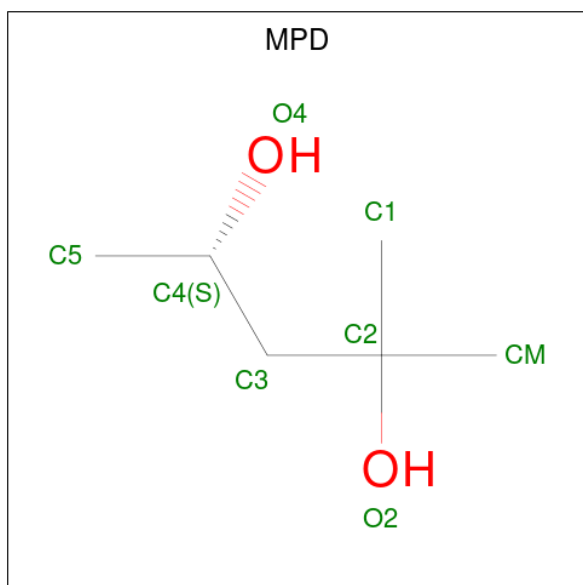
- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).





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

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



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

- Molecule 6 is water.

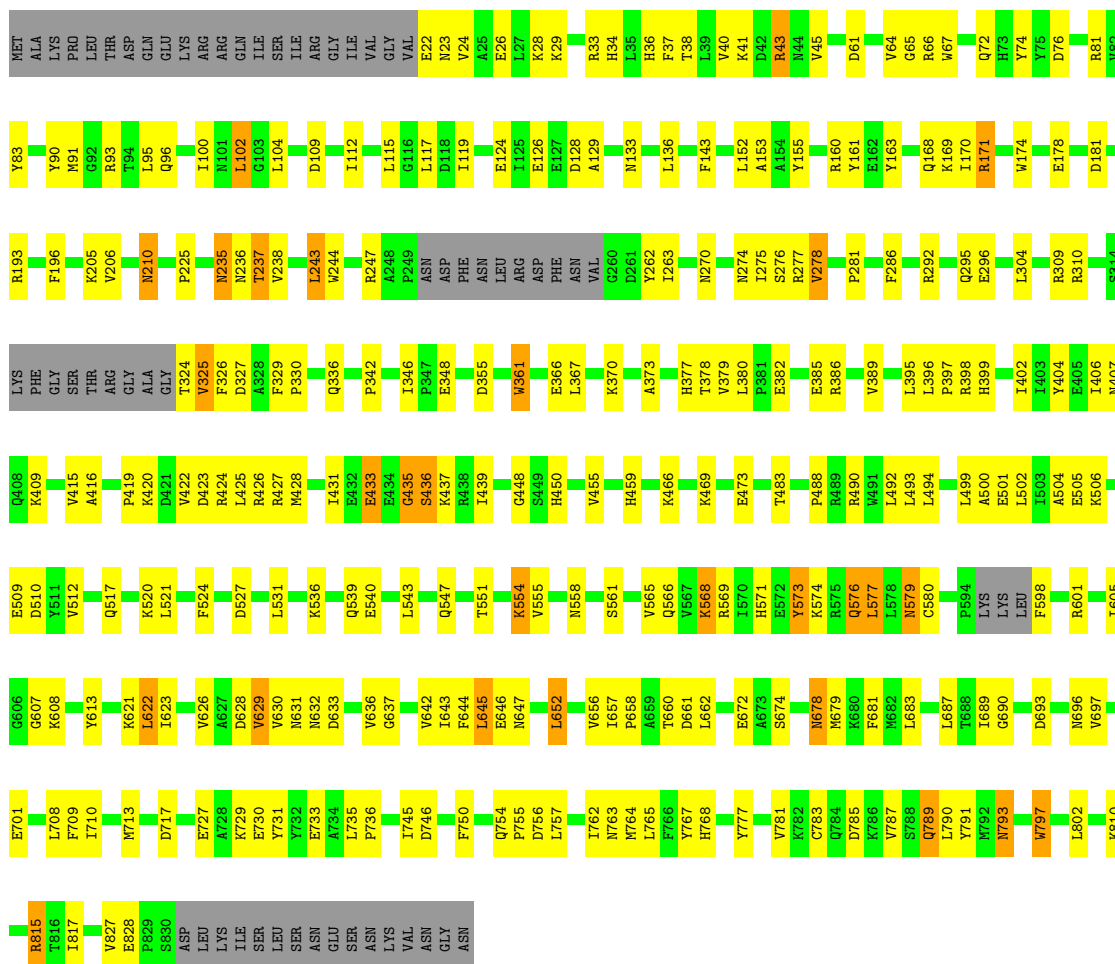
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	379	Total	O	0	0
			379	379		
6	B	358	Total	O	0	0
			358	358		





Note EDS was not executed.

Chain A:  61% 29% 7%



Chain B:  58% 32% 7%





LEU	L735	V565	E473	E382	R292	R81
SER	F736	Q566	E473	E382	R292	V82
ASN		Q567	T483	E385		Y83
GLU	V656	F567		R386	D181	
SER	I657	K568		E296	R184	
ASN	P658	R569	P488	V300	R193	Y90
LYS	A659	H571	R489		F196	G92
VAL	T660	S572	R490	L304		R93
ASN	D661	Y573	L396	I308	N210	I94
GLY	L662	K574	L492	R309	T211	Q96
ASN	G670	R575	L493	H399		
	L671	Q576	L494			
	T672	L577		F311	K214	I100
	E673	S578	L499	K312	W215	H101
	S674	C580	A500	A313	I216	L102
			L502	LYS	P225	
	N678	F594	E505	PHE		N106
	M679	LYS	K506	GLY	N235	D109
	K680	LYS	I507	SER	N236	E110
	F681	LEU	K409	THR	T237	A111
	M682	F598	H410	ARG	V238	I112
	L683			GLY		
		R601	I414	ALA	L243	L115
	L687		V415	GLY	W244	G116
	T688	I605	A416			L117
	G689	G606	P419	V325	R287	D118
	G690	G607	K420	F326	A248	I119
	D693	K608		P249	P249	
			D421	A328	ASN	E126
	N696	Y613	V422	F329	ASP	E127
	V697	H614	D423	P330	PHE	D128
	E698	M615	R424		ASN	A129
			L425	Q336	LEU	
		I619	R426		ARG	N133
	E701	I620	R427	D339	ASP	
	E702	K621	M428		PHE	L136
		L622		P342	ASN	
	L708	I623	I431		VAL	F143
	F709		E432	A345	G260	
	I710	V626	E433	I346	D261	M147
	F711	A627	E434	P347	Y262	
	G712	D628	G435	E348	I263	L152
	M713	W629	S436			A153
		V630	S437	D355	N270	A154
	D717	N631	R438		Y155	Y155
	A720	N632	I439	W361	R160	
		D633			I275	
			G448	E366	S276	Y161
	K723	V636	S449	L367	R277	E162
		G637	H450		V278	Y163
	Y726	V642	V455	K370	L279	
	E727	I643				
	A728	K554	A373	Y280	P281	Q168
	K729	F644	I458			K169
	E730	L645	H459	H377	N284	I170
	Y731	E646		T378	F285	R171
	Y732	M647	K466	V379	P286	
	E733	Y648	L380			W174
	A734	R649	K469			E178



## 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, $\alpha$ , $\beta$ , $\gamma$	123.31Å 123.31Å 122.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.00 – 2.20	Depositor
% Data completeness (in resolution range)	92.7 (99.00-2.20)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.233 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13599	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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: PLP, CP4, MPD, NBG

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	0/6522	0.60	0/8822
1	B	0.35	0/6522	0.60	0/8822
All	All	0.35	0/13044	0.60	0/17644

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	6380	0	6361	236	2
1	B	6380	0	6361	258	1
2	A	15	0	15	1	0
2	B	15	0	15	1	0
3	A	34	0	24	0	0
4	A	15	0	7	0	0
4	B	15	0	6	0	0
5	B	8	0	14	0	0
6	A	379	0	0	21	0
6	B	358	0	0	32	1
All	All	13599	0	12803	490	2



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 19.

The worst 5 of 490 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:133:ASN:HD22	1:B:569:ARG:NH2	1.56	1.02
1:B:789:GLN:HE21	1:B:789:GLN:HA	1.24	1.02
1:A:133:ASN:HD22	1:A:569:ARG:NH2	1.60	1.00
1:A:789:GLN:HE21	1:A:789:GLN:HA	1.24	0.98
1:A:133:ASN:HD21	1:A:281:PRO:HA	1.29	0.97

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:GLU:OE1	1:B:312:LYS:NZ[2_555]	2.03	0.17
1:A:210:ASN:OD1	6:B:2026:HOH:O[2_665]	2.16	0.04

## 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	779/847 (92%)	737 (95%)	39 (5%)	3 (0%)	30	34
1	B	779/847 (92%)	733 (94%)	44 (6%)	2 (0%)	37	42
All	All	1558/1694 (92%)	1470 (94%)	83 (5%)	5 (0%)	37	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	436	SER
1	B	436	SER
1	A	435	GLY

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Mol	Chain	Res	Type
1	B	435	GLY
1	A	342	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	688/740 (93%)	647 (94%)	41 (6%)	16	19
1	B	688/740 (93%)	645 (94%)	43 (6%)	15	17
All	All	1376/1480 (93%)	1292 (94%)	84 (6%)	15	18

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	466	LYS
1	B	629	VAL
1	B	494	LEU
1	B	573	TYR
1	B	683	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	579	ASN
1	B	754	GLN
1	A	579	ASN
1	A	576	GLN
1	B	789	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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	B	1902	-	7,7,7	0.74	0	9,10,10	0.71	0
3	CP4	A	862	-	33,37,37	1.87	10 (30%)	40,50,50	1.92	10 (25%)
4	PLP	B	1860	1	15,15,16	1.99	2 (13%)	21,22,23	1.39	2 (9%)
2	NBG	A	861	-	15,15,15	1.48	3 (20%)	21,21,21	1.08	1 (4%)
2	NBG	B	1861	-	15,15,15	1.54	3 (20%)	21,21,21	1.23	2 (9%)
4	PLP	A	860	1	15,15,16	1.61	2 (13%)	21,22,23	1.28	3 (14%)

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	B	1902	-	1/1/2/2	2/5/5/5	-
3	CP4	A	862	-	-	2/15/21/21	0/4/4/4
4	PLP	B	1860	1	-	0/6/6/8	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
4	PLP	A	860	1	-	1/6/6/8	0/1/1/1



The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1860	PLP	C4A-C4	-6.16	1.39	1.51
4	A	860	PLP	C4A-C4	-4.41	1.42	1.51
2	A	861	NBG	C2-C1	4.01	1.57	1.53
3	A	862	CP4	C30-C32	3.74	1.43	1.36
3	A	862	CP4	C3-C7	3.70	1.43	1.36

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	862	CP4	C23-C22-N21	4.48	121.79	115.56
3	A	862	CP4	C2-C0-C1	-4.19	102.62	106.27
3	A	862	CP4	C6-C9-N11	3.96	121.07	115.56
3	A	862	CP4	C26-C28-C27	-3.90	102.87	106.27
3	A	862	CP4	C6-N4-C1	3.72	112.20	104.45

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1902	MPD	C4

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1902	MPD	C2-C3-C4-O4
5	B	1902	MPD	C2-C3-C4-C5
4	A	860	PLP	C4-C5-C5A-O4P
3	A	862	CP4	C20-C19-O18-C17
3	A	862	CP4	C13-C14-O15-C16

There are no ring outliers.

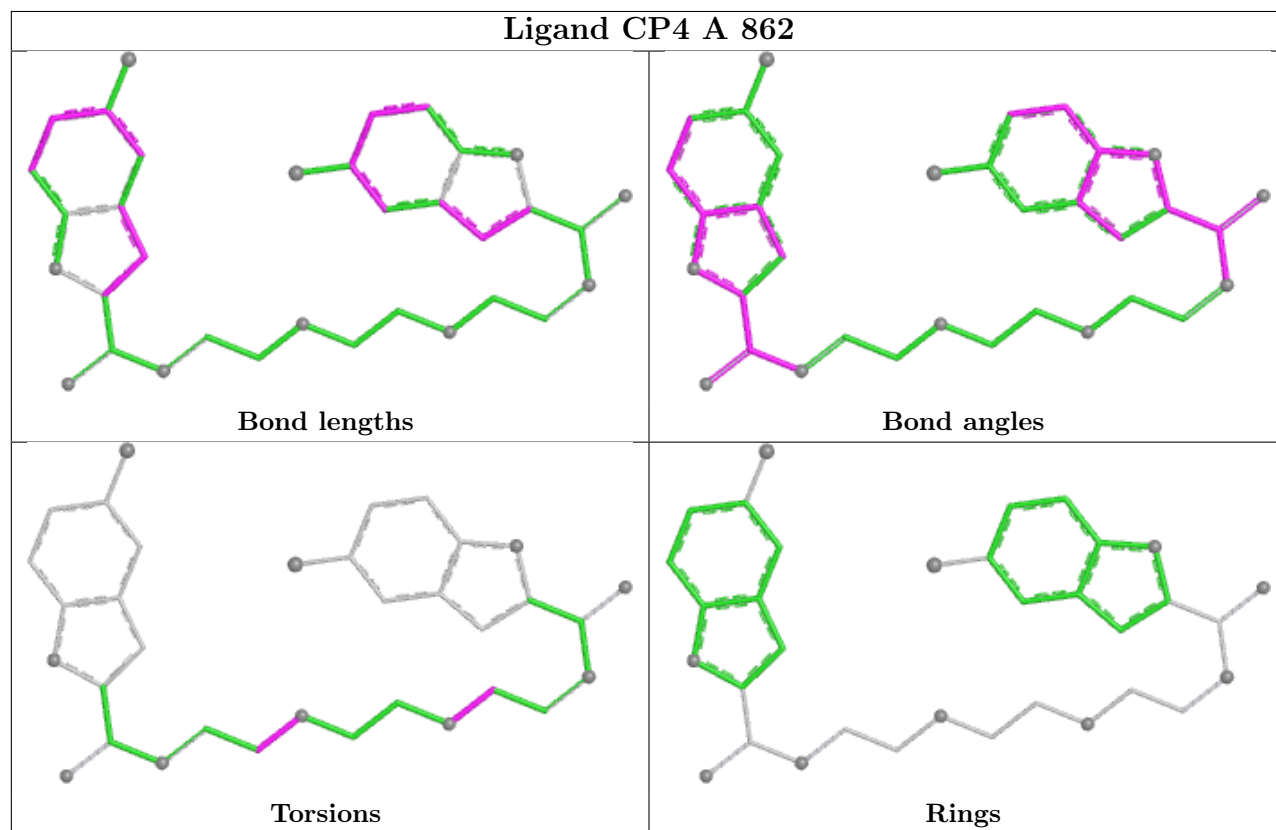
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	861	NBG	1	0
2	B	1861	NBG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.



Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.