



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 08:31 PM EDT

PDB ID : 1EXV  
Title : HUMAN LIVER GLYCOGEN PHOSPHORYLASE A COMPLEXED WITH GLCNAC AND CP-403,700  
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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

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

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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

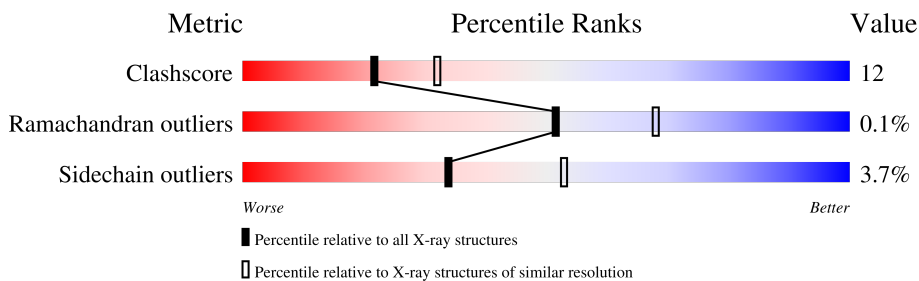
# 1 Overall quality at a glance

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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (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 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	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.

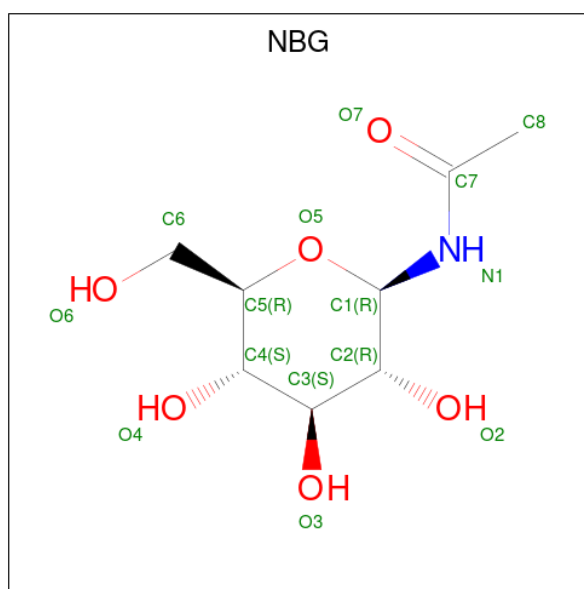
- Molecule 1 is a protein called LIVER GLYCOGEN PHOSPHORYLASE.

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 N-acetyl-beta-D-glucopyranosylamine (three-letter code: NBG) (formula:  $C_8H_{15}NO_6$ ).



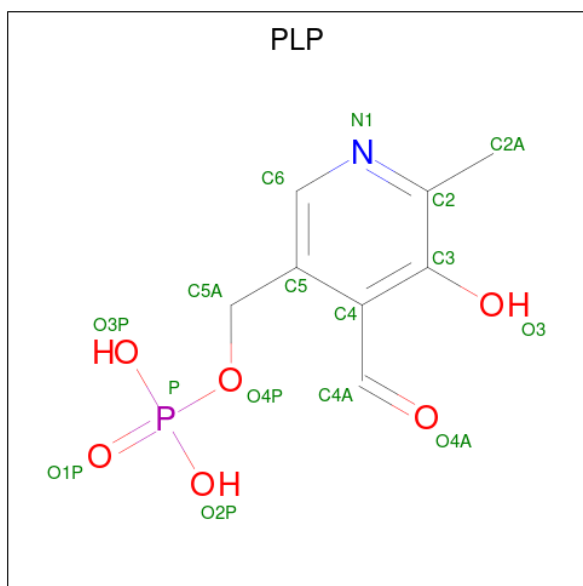
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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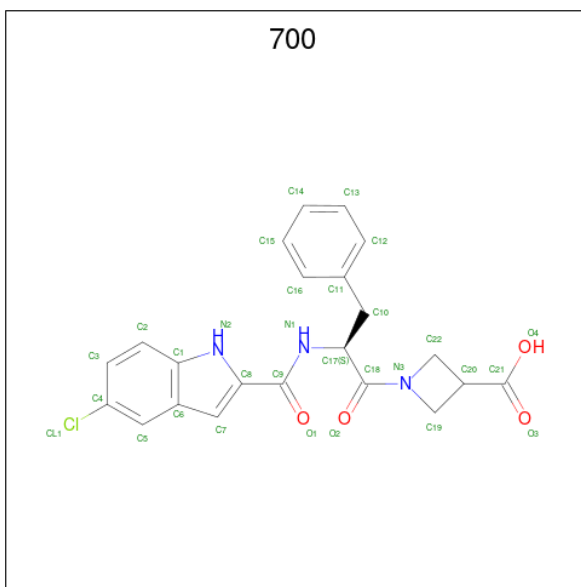
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

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



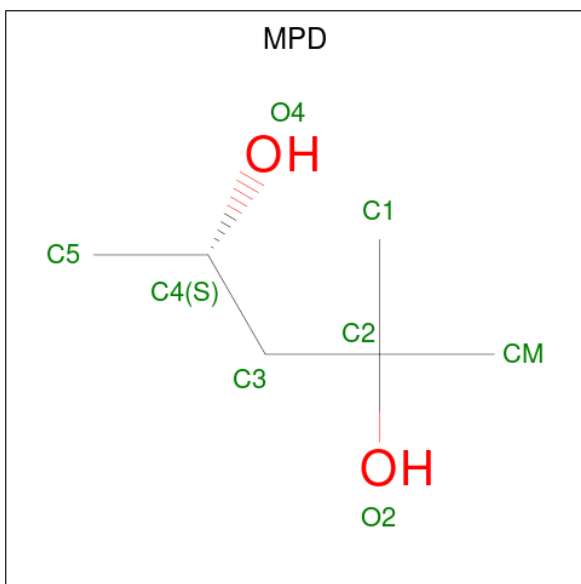
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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

- 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	0	0
			8	6	2		

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

- Molecule 6 is water.

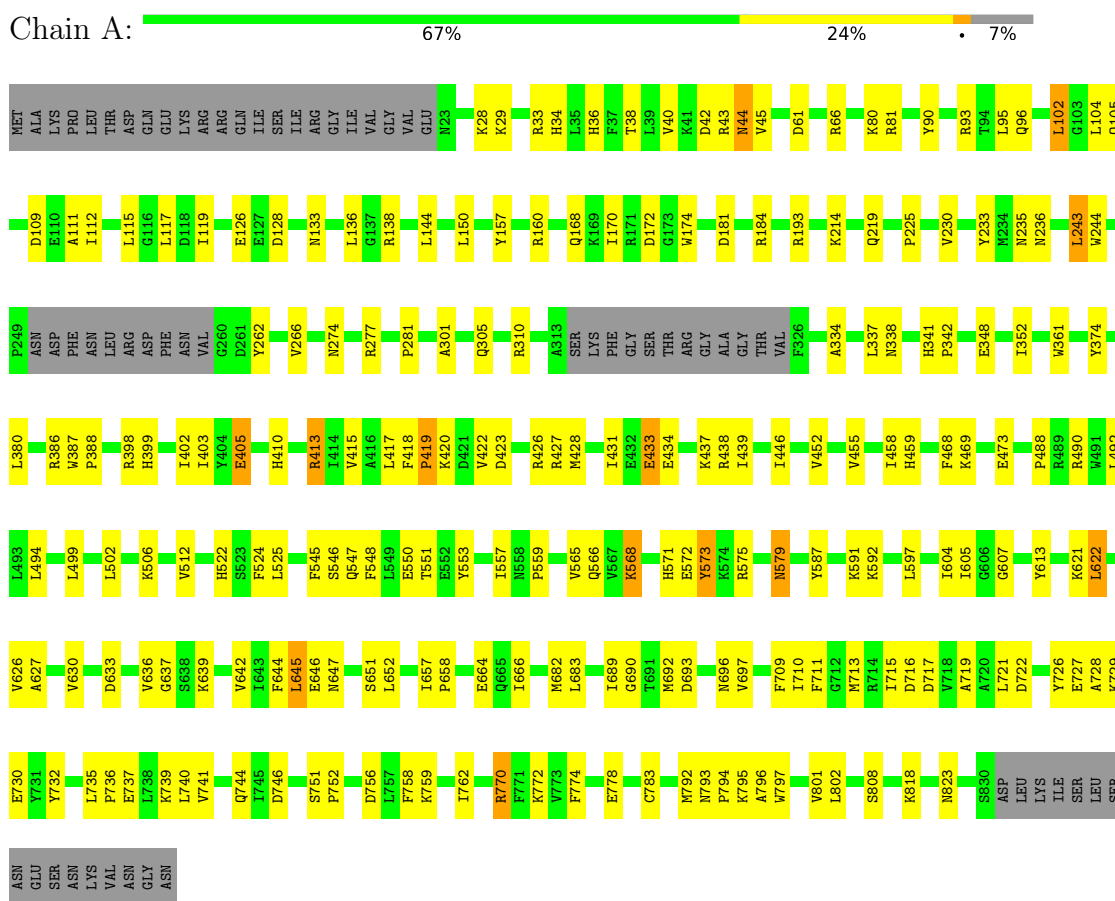
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	174	Total	O	0	0
			174	174		
6	B	159	Total	O	0	0
			159	159		

### 3 Residue-property plots

These plots are drawn for all protein, RNA, 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. 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. 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.

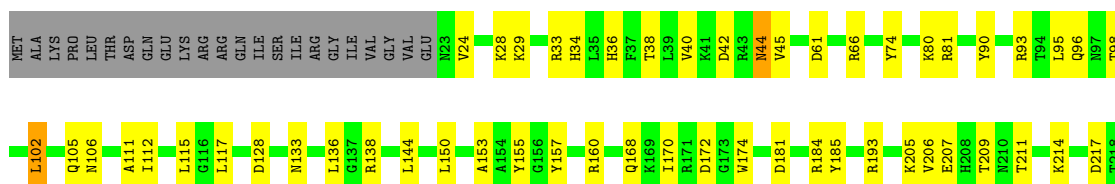
Note EDS was not executed.

#### • Molecule 1: LIVER GLYCOGEN PHOSPHORYLASE



#### • Molecule 1: LIVER GLYCOGEN PHOSPHORYLASE

Chain B: 



K759	E664	I557	R438	Q219
I762	G665	N558	I439	THR
R770	I666	P559	I446	VAL
F774	M682	V565	V447	F326
E778	L683	Q566	G448	A334
C783	I689	V567	S449	Y233
N792	G690	K568	H450	Y234
N793	T691	H571	A451	N235
P794	M692	E572	V452	N236
K795	D693	Y573	V455	
A796	N696	K574	I458	L243
W797	V697	R575	H459	W244
V801	E698	N579	F468	R247
L802	E702	Y587	K469	A248
S808	L708	K591	E473	P249
K818	F709	K592	P488	ASN
	I710	L597	R489	ASP
	G712	I604	R490	PHE
	M713	I605	W491	ASN
	R714	Y613	L492	ASN
S830	I715	K617	L493	VAL
ASP	D716	K621	L494	G260
LEU	D717	L622	K506	D261
LYS	W718	V626	V512	Y262
ILE	A719	A627	S516	V266
SER	D722	V630	T519	N274
LEU		D633	R520	R277
SER	Y726	V636	L521	P281
ASN	E727	G637	H522	R292
ASN	A728	S638	S523	E296
LYS	K729	K639	F524	V300
VAL	E730	V642	L525	A301
ASN	Y731	I643	D528	Q305
GLY	Y732	F644	R532	R310
ASN		L645	F545	A313
ASN	L745	E646	S546	SER
	D746	N647	Q547	LYS
		S651	F548	PHE
	S751	L652	E549	GLY
	P752	I657	E550	SER
		P658	T551	THR
	D756		Y552	ARG
	L757		E553	GLY
	F758		K437	ALA



## 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, $\alpha$ , $\beta$ , $\gamma$	124.63Å 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: PLP, MPD, 700, 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	0.36	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

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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%)	51	68
1	B	780/847 (92%)	730 (94%)	50 (6%)	0	100	100
All	All	1560/1694 (92%)	1461 (94%)	98 (6%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	419	PRO

### 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	687/740 (93%)	661 (96%)	26 (4%)	33	51
1	B	687/740 (93%)	662 (96%)	25 (4%)	35	54
All	All	1374/1480 (93%)	1323 (96%)	51 (4%)	34	53

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

Mol	Chain	Res	Type
1	B	95	LEU
1	B	413	ARG
1	B	756	ASP
1	B	102	LEU
1	B	243	LEU

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

Mol	Chain	Res	Type
1	B	96	GLN
1	B	274	ASN
1	B	114	GLN
1	B	236	ASN
1	B	305	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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
4	700	A	862	-	29,33,33	2.33	7 (24%)	37,47,47	1.74	9 (24%)
4	700	B	1862	-	29,33,33	2.42	14 (48%)	37,47,47	1.64	8 (21%)
5	MPD	B	1902	-	7,7,7	0.74	0	9,10,10	0.72	0
3	PLP	A	860	1	15,15,16	1.49	1 (6%)	20,22,23	1.47	5 (25%)
2	NBG	A	861	-	15,15,15	1.44	3 (20%)	21,21,21	1.20	1 (4%)
5	MPD	A	1901	-	7,7,7	0.50	0	9,10,10	0.75	0
2	NBG	B	1861	-	15,15,15	1.68	3 (20%)	21,21,21	1.36	2 (9%)
3	PLP	B	1860	1	15,15,16	1.81	2 (13%)	20,22,23	1.40	4 (20%)

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
4	700	A	862	-	-	0/19/32/32	0/4/4/4
4	700	B	1862	-	-	1/19/32/32	0/4/4/4
5	MPD	B	1902	-	1/1/2/2	1/5/5/5	-
3	PLP	A	860	1	-	1/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1
3	PLP	B	1860	1	-	2/6/6/8	0/1/1/1
2	NBG	B	1861	-	-	0/6/26/26	0/1/1/1
5	MPD	A	1901	-	1/1/2/2	1/5/5/5	-

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	862	700	C7-C8	7.15	1.52	1.39
4	B	1862	700	C7-C8	6.96	1.52	1.39
3	B	1860	PLP	C4A-C4	-5.55	1.40	1.51
4	B	1862	700	C17-C18	-5.05	1.43	1.53
4	A	862	700	C17-C18	-4.55	1.44	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1861	NBG	C5-O5-C1	4.37	118.44	112.52
4	A	862	700	C8-N2-C1	4.33	113.47	104.45
4	A	862	700	C8-C9-N1	4.31	123.20	115.20
4	B	1862	700	C8-N2-C1	4.11	113.02	104.45
4	B	1862	700	C8-C9-N1	3.96	122.56	115.20

All (2) chirality outliers are listed below:

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

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	860	PLP	C4-C5-C5A-O4P
3	B	1860	PLP	C5A-O4P-P-O1P
5	A	1901	MPD	C2-C3-C4-O4
5	B	1902	MPD	C2-C3-C4-C5
4	B	1862	700	C22-C20-C21-O3

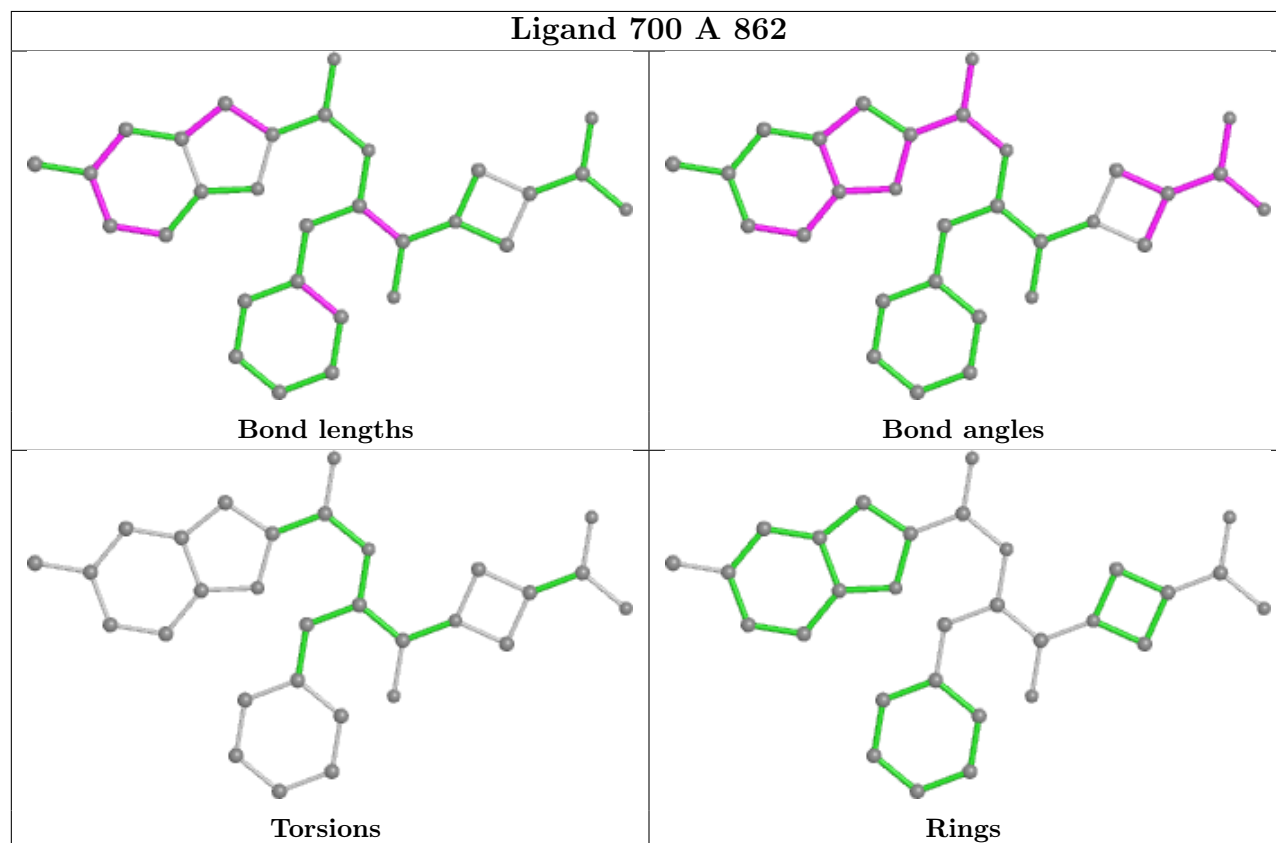
There are no ring outliers.

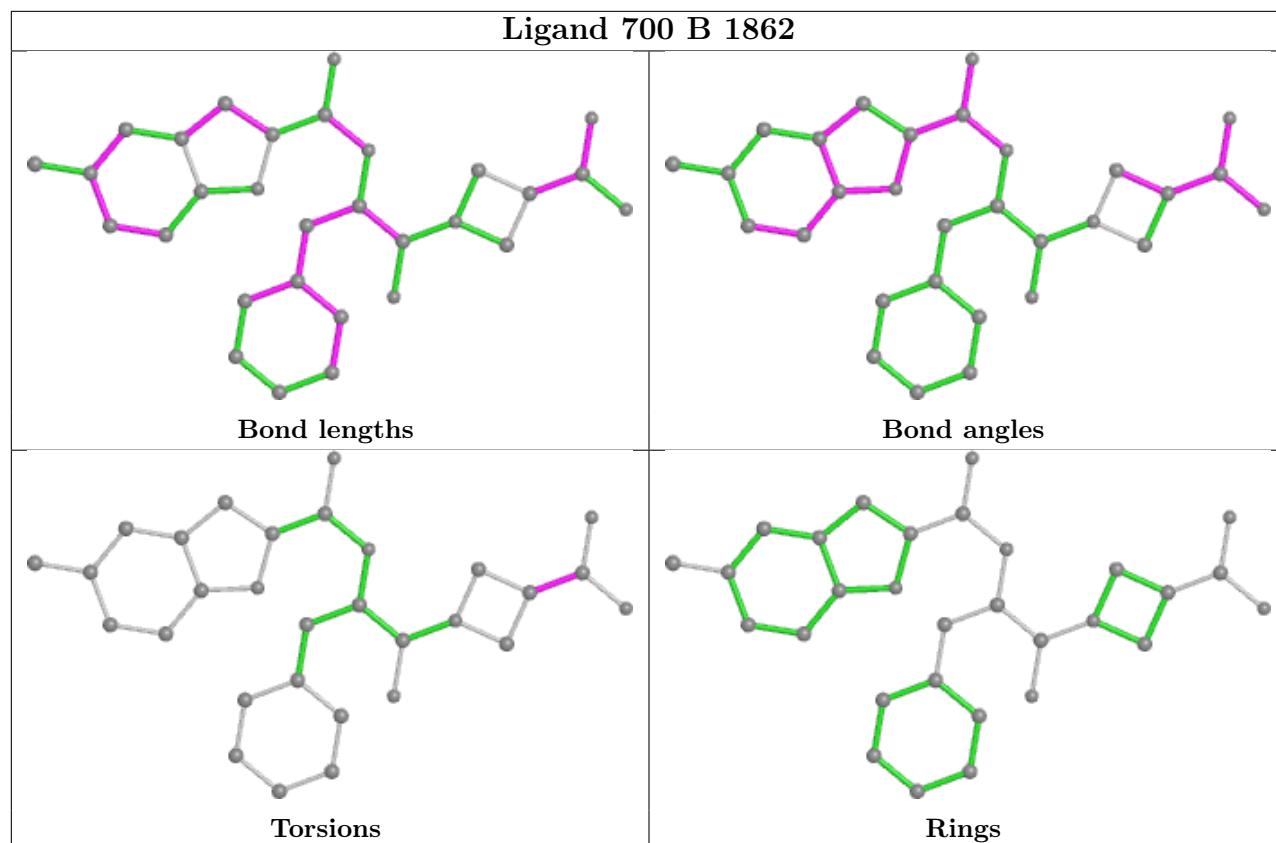
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1901	MPD	1	0

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.