



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 12:50 PM UTC

PDB ID : 1EXV / pdb_00001exv
Title : HUMAN LIVER GLYCOGEN PHOSPHORYLASE A COMPLEXED WITH
GLCNAC AND CP-403,700
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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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

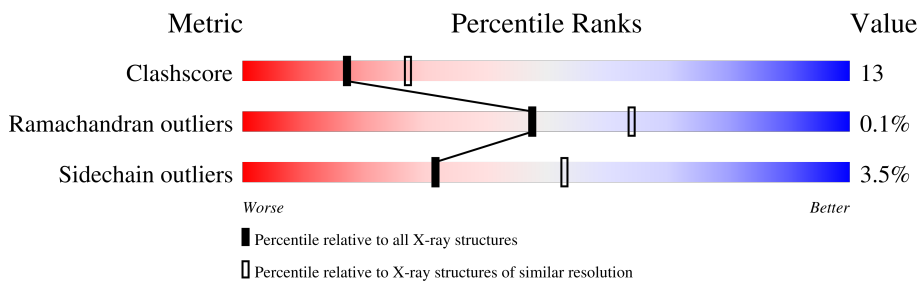
1 Overall quality at a glance

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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 ≥ 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.

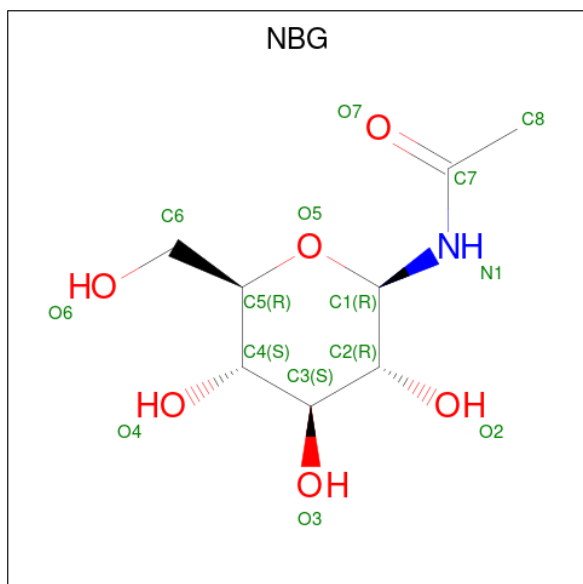
- Molecule 1 is a protein called LIVER GLYCOGEN PHOSPHORYLASE.

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

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 (CCD ID: NBG) (formula: C₈H₁₅NO₆).



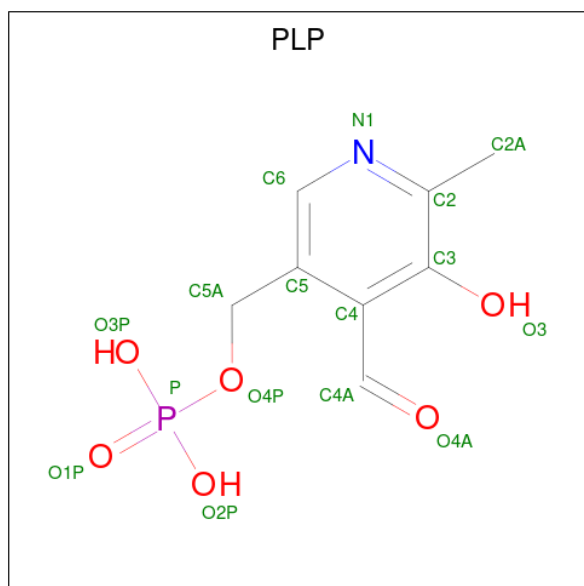
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	15	8	1	6	0	0

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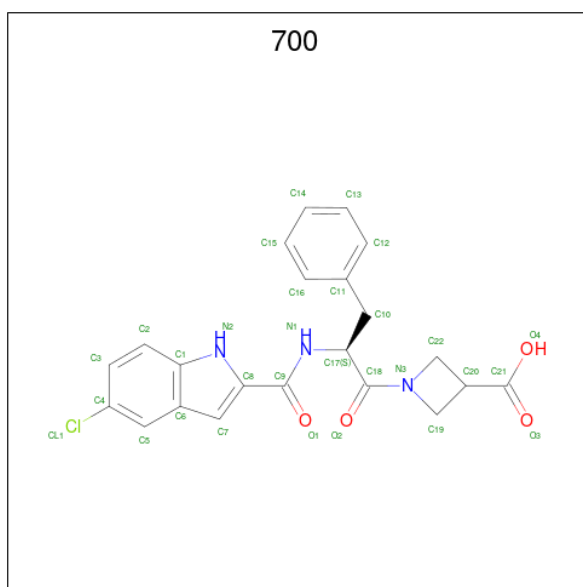
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	15	8	1	6	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



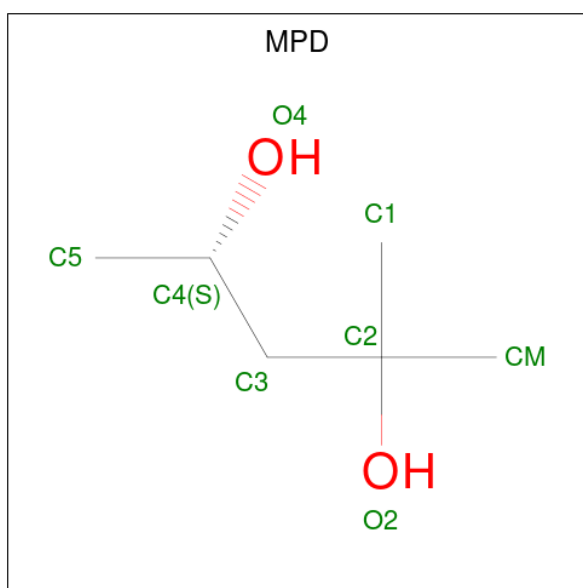
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	15	8	1	5	1	0	0
3	B	1	15	8	1	5	1	0	0

- Molecule 4 is [5-CHLORO-1H-INDOL-2-CARBONYL-PHENYLALANINYL]-AZETIDINE-3-CARBOXYLIC ACID (CCD ID: 700) (formula: C₂₂H₂₀ClN₃O₄).



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

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



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

- Molecule 6 is water.

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

SER	E730	V636	H522	L417	R208
LEU	Y731	G637	S523	F418	T209
SER	Y732	S638	F524	P419	N210
ASN	L735	K639	L525	K420	T211
GLU	P736	V642	D528	D421	K214
SER	E737	I643	R532	V422	Y215
ASN	L738	F644	F545	D423	Y216
LYS	K739	L645	S546	R424	I216
VAL	L740	E646	R426	L425	D217
ASN	V741	M647	R427	R426	T218
GLY	Q744	V650	Q547	M428	Q219
ASN	F745	L549	F548	I431	L224
	D746	E550	L549	E432	P225
	S751	T551	E550	E433	V230
	P752	F552	F552	E434	P231
	K753	Y553	Y553	F326	G232
	Q754	I557	I557	V333	Y233
	F758	M558	P559	A334	K234
	K759	P559	M562	A338	N235
	I762	E664	M562	I439	N236
	H763	Q665	V665	I446	L243
	N764	L682	Q566	G448	W244
	L765	L683	V565	S449	L247
	R770	I689	H571	H450	R249
	F774	G690	E572	A451	A248
	E778	T691	Y573	I346	P249
	C783	M692	K574	A345	ASN
	V787	D693	R575	V354	ASP
	N792	G694	Q576	W361	PHE
	N793	A695	I458	F372	ASN
	P794	M696	H459	Y374	ASN
	K795	V697	N579	L380	LEU
	A796	E698	Y587	P381	ARG
	W797	E702	K591	L384	ASP
	V801	L708	K592	E385	PHE
	L802	F709	L597	R386	ASN
	S808	I710	I604	R398	VAL
	R815	F711	I605	H399	G260
	K818	G712	M615	L400	D261
	S830	M713	M615	L400	Y262
ASP		F714	A616	E401	V266
LEU		D716	K617	I402	N274
LYS		D717	K621	I403	R277
ILE		V718	L622	Y404	P281
		A719	V626	E405	R292
		D722	A627	H410	E296
		Y726	V630	R413	V300
		A728	V633	I414	A301
		K729		V415	Q305
				A416	D306

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	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.	Xtrriage
Total number of atoms	13223	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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: 700, PLP, NBG, MPD

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	0.42	0/6520	0.93	29/8818 (0.3%)
1	B	0.41	0/6520	0.92	26/8818 (0.3%)
All	All	0.41	0/13040	0.93	55/17636 (0.3%)

There are no bond length outliers.

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	VAL	N-CA-C	8.25	119.66	108.11
1	B	565	VAL	N-CA-C	8.04	119.37	108.11
1	A	91	MET	N-CA-C	7.98	121.08	111.82
1	B	91	MET	N-CA-C	7.98	121.08	111.82
1	B	354	VAL	N-CA-C	7.63	117.68	110.74

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	6377	0	6372	157	0
1	B	6377	0	6372	170	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
6	B	159	0	0	12	0
All	All	13223	0	12852	325	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 325 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%)	48	64
1	B	780/847 (92%)	730 (94%)	50 (6%)	0	100	100
All	All	1560/1694 (92%)	1461 (94%)	98 (6%)	1 (0%)	48	64

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	240/740 (32%)	233 (97%)	7 (3%)	37	60
1	B	466/740 (63%)	448 (96%)	18 (4%)	28	48
All	All	706/1480 (48%)	681 (96%)	25 (4%)	32	53

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	405	GLU
1	B	592	LYS
1	B	770	ARG
1	B	433	GLU
1	B	622	LEU

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

Mol	Chain	Res	Type
1	B	410	HIS
1	B	459	HIS
1	B	793	ASN
1	B	789	GLN
1	B	44	ASN

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 oligosaccharides 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	-	31,33,33	2.80	15 (48%)	44,47,47	1.98	11 (25%)
2	NBG	A	861	-	15,15,15	1.39	3 (20%)	21,21,21	1.18	1 (4%)
5	MPD	B	1902	-	7,7,7	0.77	0	9,10,10	0.77	0
4	700	B	1862	-	31,33,33	2.84	17 (54%)	44,47,47	1.86	11 (25%)
3	PLP	B	1860	1	15,15,16	1.88	2 (13%)	21,22,23	1.40	4 (19%)
2	NBG	B	1861	-	15,15,15	1.62	3 (20%)	21,21,21	1.34	2 (9%)
5	MPD	A	1901	-	7,7,7	0.51	0	9,10,10	0.79	0
3	PLP	A	860	1	15,15,16	1.54	1 (6%)	21,22,23	1.46	5 (23%)

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	-	-	0/22/32/32	0/4/4/4
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1
5	MPD	B	1902	-	1/1/2/2	1/5/5/5	-
4	700	B	1862	-	-	1/22/32/32	0/4/4/4
3	PLP	B	1860	1	-	2/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NBG	B	1861	-	-	0/6/26/26	0/1/1/1
5	MPD	A	1901	-	1/1/2/2	3/5/5/5	-
3	PLP	A	860	1	-	1/6/6/8	0/1/1/1

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	862	700	C7-C8	9.72	1.52	1.37
4	B	1862	700	C7-C8	9.50	1.52	1.37
3	B	1860	PLP	C4A-C4	-5.77	1.40	1.51
4	A	862	700	C8-N2	-5.70	1.30	1.38
4	B	1862	700	C8-N2	-5.15	1.31	1.38

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	862	700	C8-C9-N1	4.75	123.20	116.86
4	A	862	700	O1-C9-C8	-4.42	115.39	121.09
2	B	1861	NBG	C5-O5-C1	4.30	118.44	112.47
4	B	1862	700	C8-C9-N1	4.27	122.56	116.86
4	A	862	700	C1-C6-C7	-4.23	103.33	106.80

All (2) chirality outliers are listed below:

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

5 of 8 torsion outliers are listed below:

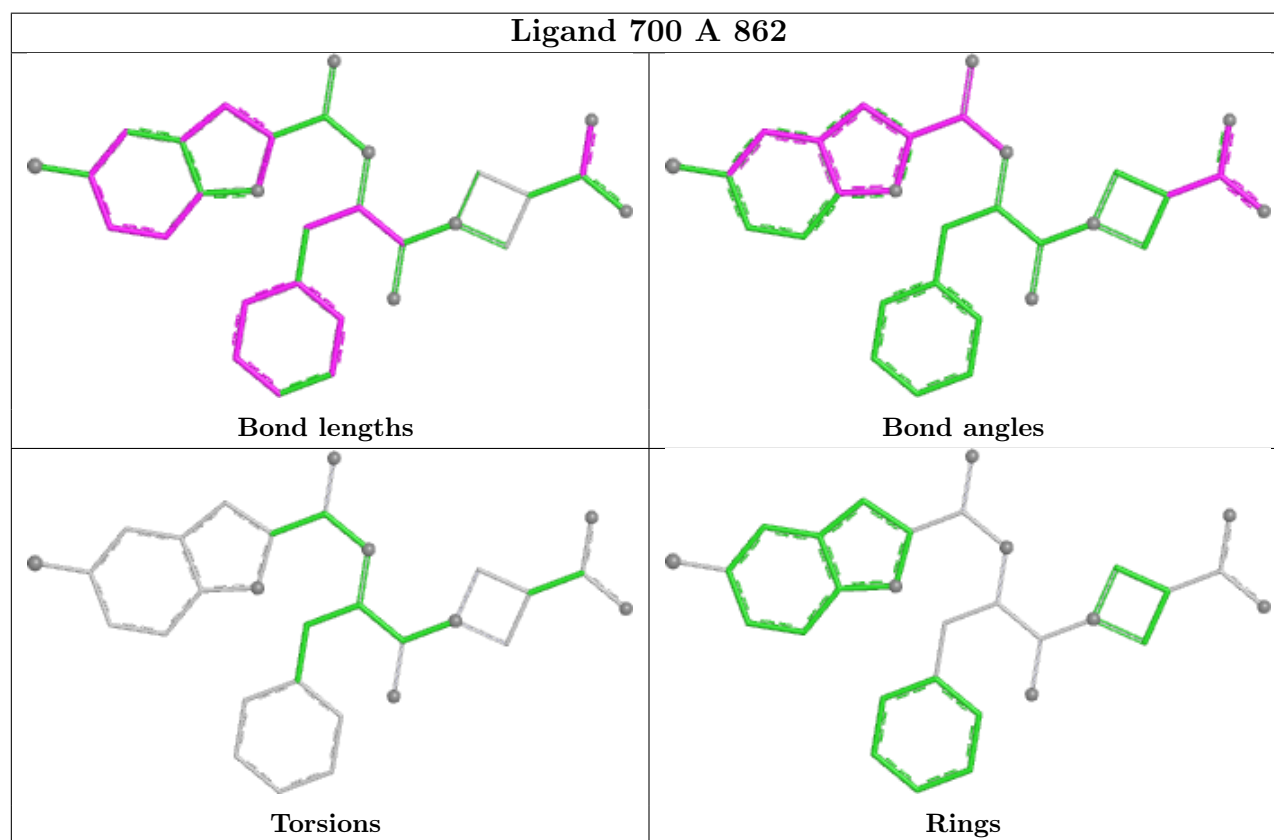
Mol	Chain	Res	Type	Atoms
3	A	860	PLP	C4-C5-C5A-O4P
3	B	1860	PLP	C5A-O4P-P-O1P
5	A	1901	MPD	C2-C3-C4-O4
5	A	1901	MPD	C2-C3-C4-C5
5	B	1902	MPD	C2-C3-C4-C5

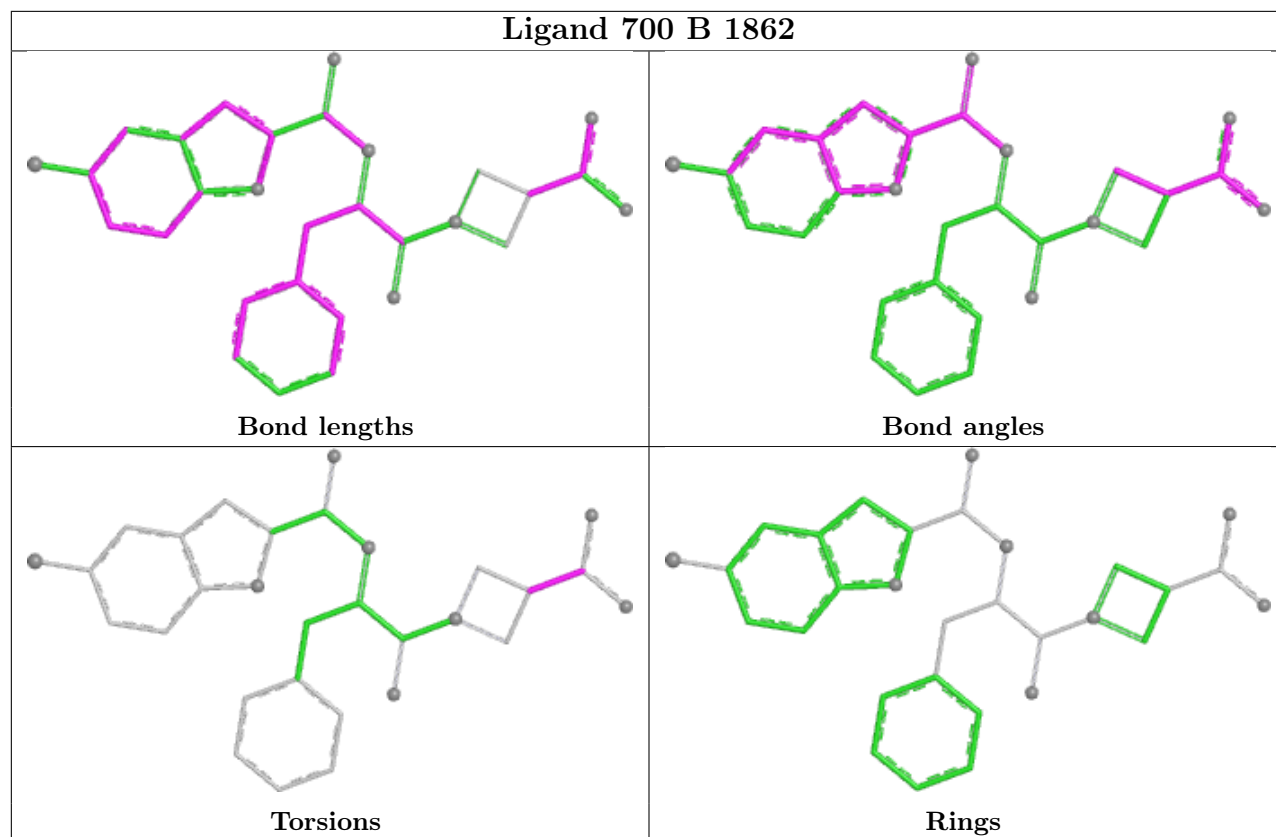
There are no ring outliers.

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.