



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2025 – 05:31 PM EDT

PDB ID : 1L5S  
Title : Human liver glycogen phosphorylase complexed with uric acid, 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 : 2002-03-07  
Resolution : 2.10 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	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	<b>NOT EXECUTED</b>
EDS	:	<b>NOT EXECUTED</b>
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

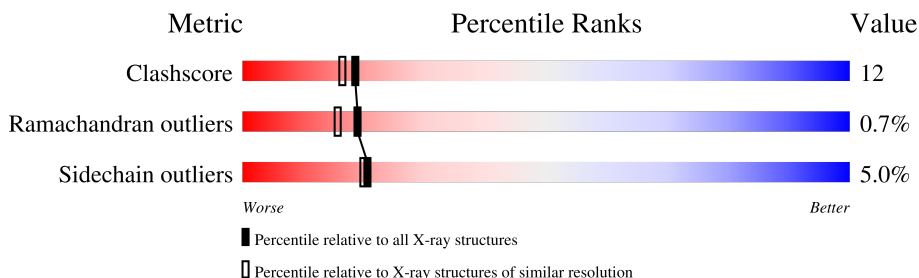
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)

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
6	MRD	B	903	-	-	X	-

## 2 Entry composition [i](#)

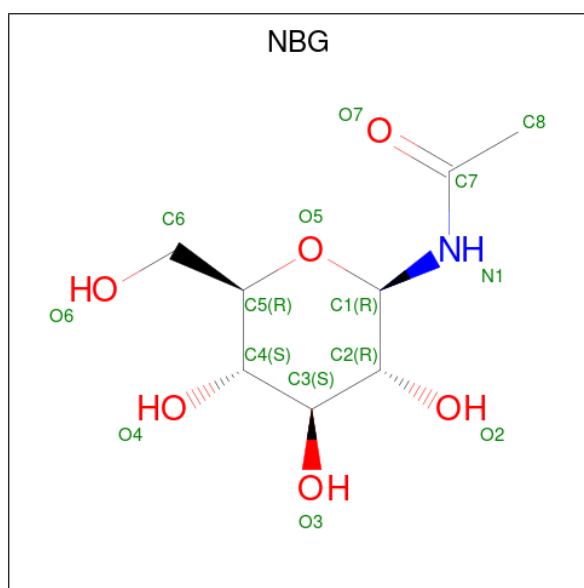
There are 7 unique types of molecules in this entry. The entry contains 13826 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			6437	4134	1092	1182	29			
1	B	791	Total	C	N	O	S	0	0	0
			6420	4125	1090	1176	29			

- Molecule 2 is N-acetyl-beta-D-glucopyranosylamine (three-letter code: NBG) (formula:  $C_8H_{15}NO_6$ ).



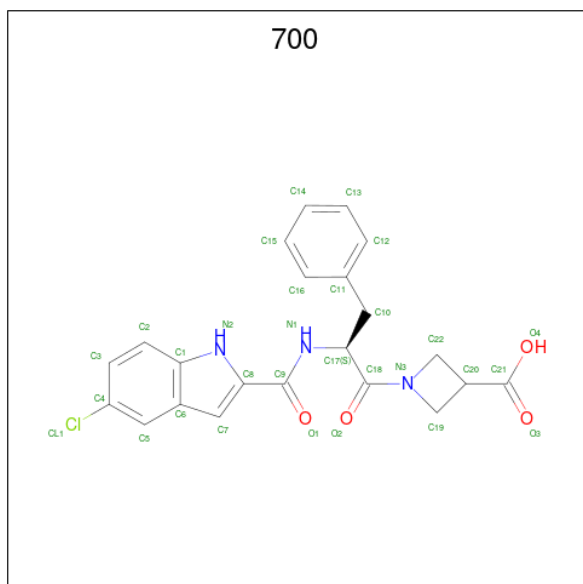
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- 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 [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>).



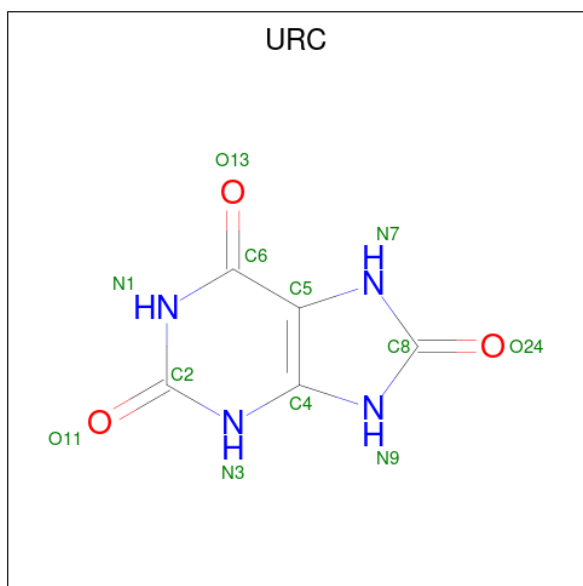
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

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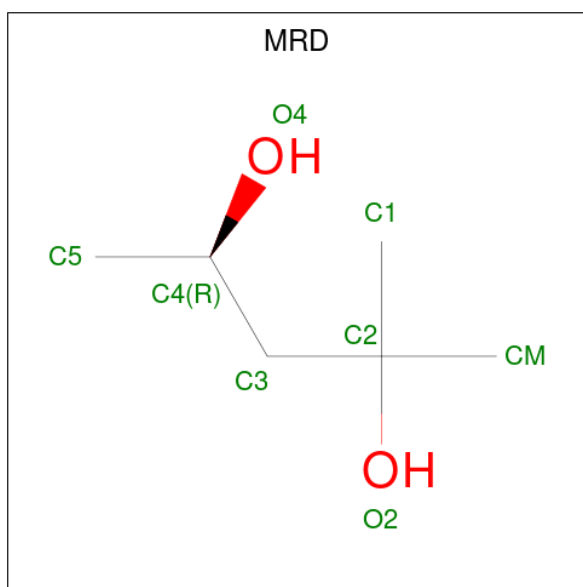
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	B	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

- Molecule 5 is URIC ACID (three-letter code: URC) (formula:  $C_5H_4N_4O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			12	5	4	3		
5	B	1	Total	C	N	O	0	0
			12	5	4	3		

- 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	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	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.

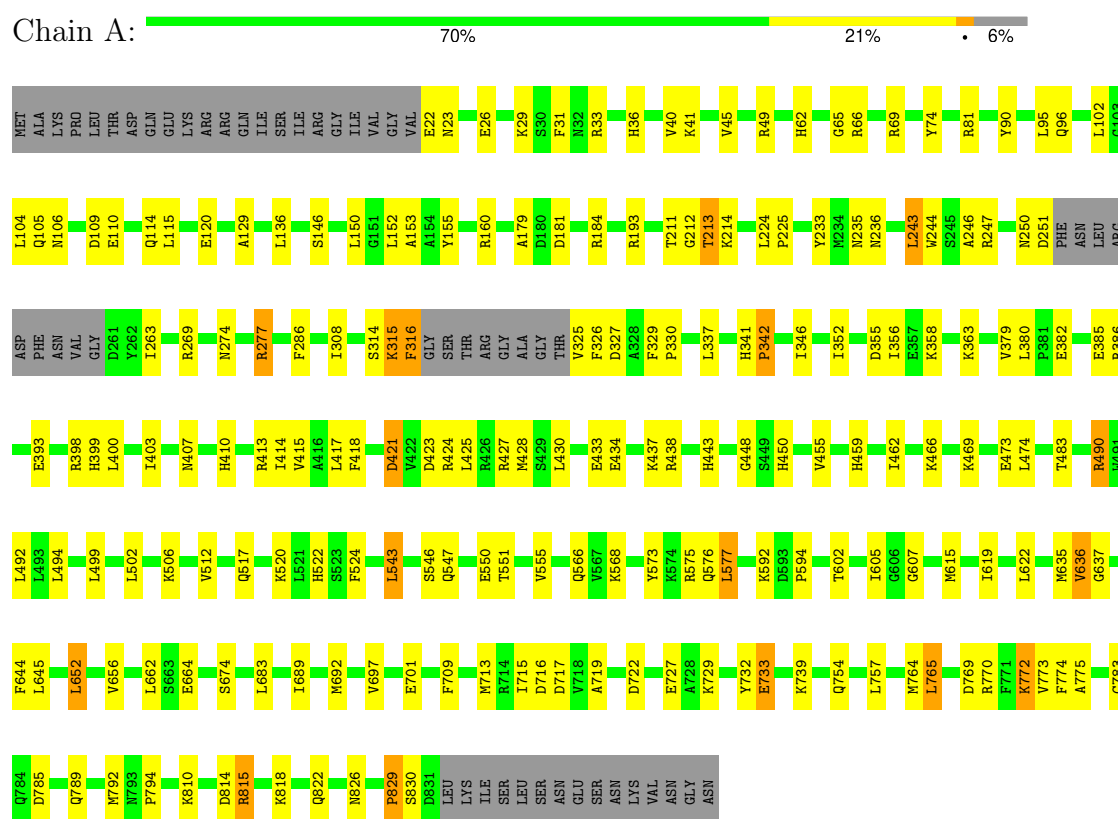
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	433	Total	O	0	0
			433	433		
7	B	352	Total	O	0	0
			352	352		

### 3 Residue-property plots

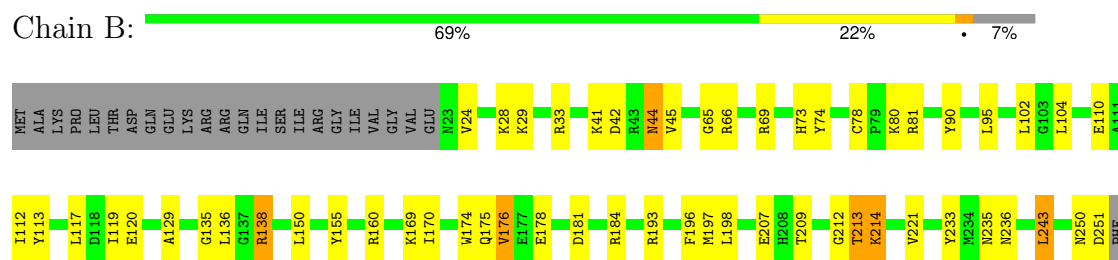
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Glycogen phosphorylase, liver form



- Molecule 1: Glycogen phosphorylase, liver form



ASN	LEU	ARG	ASP	PHE	ASN	ASN	VAL	GLY	D261	A272	E273	N274	I275	S276	R277	F286	Q295	L304	I308	R309	K315	F316	GLY	SER	THR	ARG	GLY	ALA	GLY	THR	V325	F326	F329	P330	A334	L337	I346	L349	I352	W361	S362	K363	A364	W365	E366	Q369
V379	L380	P381	E382	E385	R386	V392	E393	L400	E405	K409	R413	I414	V415	K420	D421	V422	D423	R424	L425	E432	E433	E434	G435	S436	K437	R438	I439	G448	S449	H450	V455	H459	V463	K466	W467	F468	L474	R490	W491	L492	L493	L494				
L499	L502	I503	I507	V512	D527	D528	V529	F530	K536	E540	F545	S546	Q547	F548	T551	F552	Y553	R554	V555	N558	P559	S560	Y573	R574	R575	Q576	L577	Y587	K591	K592	D593	P594	R595	K596	L597	F598	I605	Y613	H614	M615	L622	D628	V629			
V630	M631	N632	D633	V636	G637	S638	K639	F644	L645	E646	L652	L662	I666	S674	N678	M679	K680	F681	M682	L683	I689	M692	M699	I715	D716	A719	A728	K729	Y732	E733	K739	D743	P755	K759	D760	I761	M764	L765	F766							
R770	F771	K772	A775	D785	K786	V787	S788	Q789	M792	H793	P794	L802	S808	G809	K810	R815	K818	V827	E828	P829	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN									



## 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, $\alpha$ , $\beta$ , $\gamma$	124.03Å 124.03Å 123.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.60 – 2.10	Depositor
% Data completeness (in resolution range)	87.8 (40.60-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.194 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13826	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	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, MRD, URC

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	0.48	0/6581	0.70	3/8900 (0.0%)
1	B	0.47	0/6564	0.69	2/8877 (0.0%)
All	All	0.47	0/13145	0.69	5/17777 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	490	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	490	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	129	ALA	N-CA-C	-5.32	96.62	111.00
1	A	129	ALA	N-CA-C	-5.21	96.94	111.00
1	A	602	THR	N-CA-C	-5.08	97.28	111.00

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	6437	0	6418	149	0
1	B	6420	0	6408	153	0
2	A	15	0	15	0	0
2	B	15	0	15	1	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	1	0
4	A	30	0	18	0	0
4	B	30	0	18	0	0
5	A	12	0	4	0	0
5	B	12	0	4	0	0
6	A	24	0	42	3	0
6	B	16	0	28	9	0
7	A	433	0	0	16	0
7	B	352	0	0	21	0
All	All	13826	0	12984	307	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 307 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:109:ASP:HB3	7:A:2741:HOH:O	1.53	1.05
1:A:49:ARG:HH22	6:A:905:MRD:H1C2	1.26	1.01
1:A:754:GLN:HG2	1:A:757:LEU:HB2	1.43	1.00
1:B:818:LYS:NZ	1:B:818:LYS:HB3	1.81	0.95
1:A:547:GLN:O	1:A:551:THR:HG23	1.72	0.90

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%)	743 (94%)	38 (5%)	6 (1%)	16	13
1	B	785/847 (93%)	747 (95%)	33 (4%)	5 (1%)	22	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1572/1694 (93%)	1490 (95%)	71 (4%)	11 (1%)	19	16

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	ASP
1	A	555	VAL
1	B	421	ASP
1	B	435	GLY
1	A	829	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	694/740 (94%)	662 (95%)	32 (5%)	23	23
1	B	692/740 (94%)	655 (95%)	37 (5%)	19	18
All	All	1386/1480 (94%)	1317 (95%)	69 (5%)	20	20

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	615	MET
1	B	628	ASP
1	B	755	PRO
1	A	652	LEU
1	A	645	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	822	GLN
1	B	826	ASN
1	B	44	ASN

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Mol	Chain	Res	Type
1	B	96	GLN
1	B	105	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

13 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$
2	NBG	A	861	-	15,15,15	1.39	4 (26%)	21,21,21	1.21	3 (14%)
4	700	A	862	-	29,33,33	1.85	12 (41%)	39,47,47	1.77	10 (25%)
6	MRD	A	905	-	7,7,7	0.72	0	9,10,10	0.95	0
6	MRD	A	1902	-	7,7,7	0.50	0	9,10,10	0.75	0
5	URC	B	1863	-	7,13,13	2.24	2 (28%)	7,19,19	7.49	6 (85%)
6	MRD	A	904	-	7,7,7	0.88	0	9,10,10	0.91	0
6	MRD	B	903	-	7,7,7	1.35	1 (14%)	9,10,10	1.05	1 (11%)
3	PLP	B	1860	1	15,15,16	2.04	4 (26%)	21,22,23	1.12	1 (4%)
2	NBG	B	1861	-	15,15,15	1.60	4 (26%)	21,21,21	1.37	3 (14%)
6	MRD	B	902	-	7,7,7	0.64	0	9,10,10	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	URC	A	863	-	7,13,13	2.14	2 (28%)	7,19,19	7.52	4 (57%)
3	PLP	A	860	1	15,15,16	2.36	9 (60%)	21,22,23	1.21	2 (9%)
4	700	B	1862	-	29,33,33	1.81	10 (34%)	39,47,47	1.70	9 (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
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1
4	700	A	862	-	-	0/19/32/32	0/4/4/4
6	MRD	A	905	-	-	2/5/5/5	-
6	MRD	A	1902	-	-	4/5/5/5	-
5	URC	B	1863	-	-	-	0/2/2/2
6	MRD	A	904	-	-	4/5/5/5	-
6	MRD	B	903	-	-	1/5/5/5	-
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
6	MRD	B	902	-	-	2/5/5/5	-
5	URC	A	863	-	-	-	0/2/2/2
3	PLP	A	860	1	-	0/6/6/8	0/1/1/1
4	700	B	1862	-	-	2/19/32/32	0/4/4/4

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1860	PLP	C4A-C4	-5.97	1.39	1.51
5	B	1863	URC	C5-C6	4.99	1.50	1.41
5	A	863	URC	C5-C6	4.49	1.49	1.41
3	A	860	PLP	C4A-C4	-4.39	1.42	1.51
4	B	1862	700	C5-C4	4.02	1.43	1.36

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	863	URC	C4-N9-C8	16.62	111.21	101.12
5	B	1863	URC	C4-N9-C8	16.41	111.08	101.12
5	B	1863	URC	C2-N1-C6	8.98	122.67	115.09
5	A	863	URC	C2-N1-C6	8.74	122.47	115.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	863	URC	C5-C6-N1	-5.55	116.00	123.42

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	904	MRD	O2-C2-C3-C4
6	A	904	MRD	CM-C2-C3-C4
6	A	904	MRD	C2-C3-C4-C5
6	B	902	MRD	C2-C3-C4-O4
3	B	1860	PLP	C6-C5-C5A-O4P

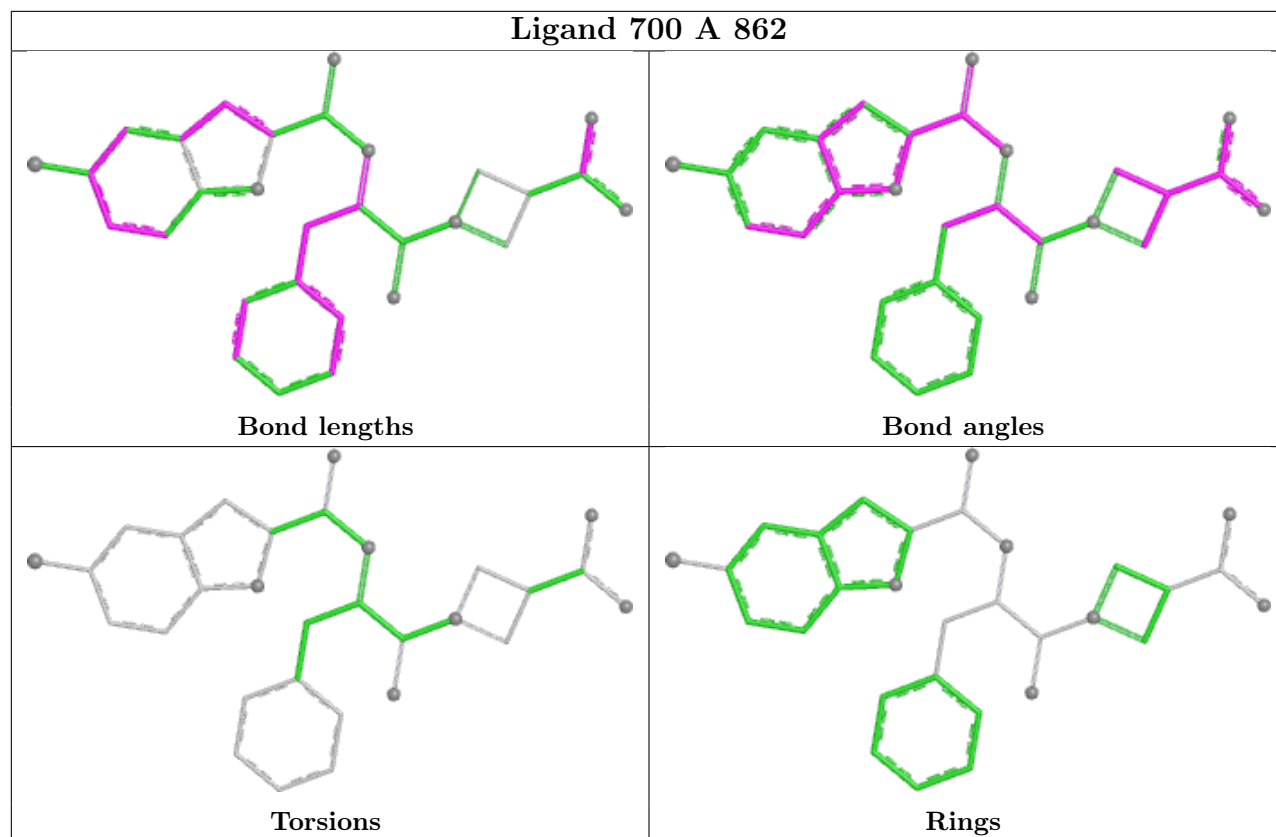
There are no ring outliers.

6 monomers are involved in 14 short contacts:

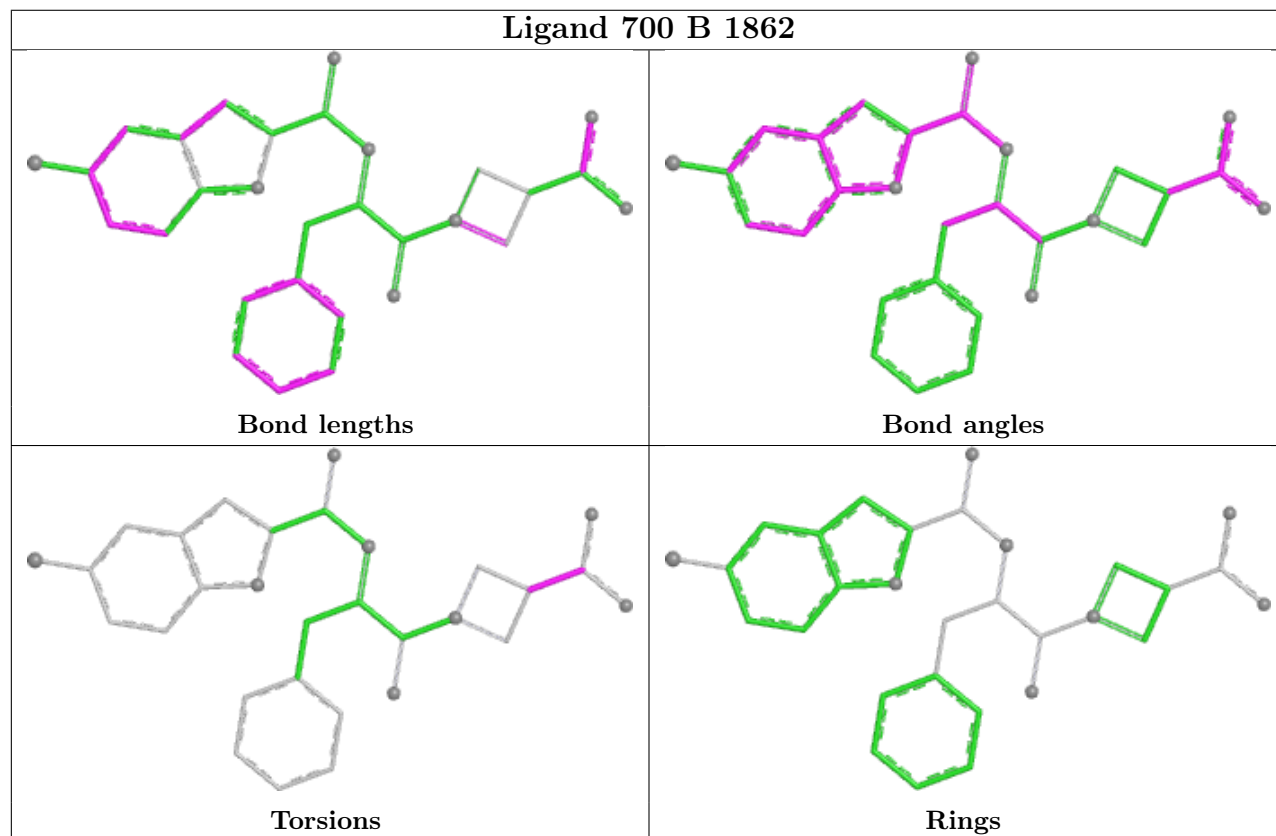
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	905	MRD	2	0
6	A	904	MRD	1	0
6	B	903	MRD	8	0
3	B	1860	PLP	1	0
2	B	1861	NBG	1	0
6	B	902	MRD	3	0

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.

## Ligand 700 A 862



## Ligand 700 B 1862





## 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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.