wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2020 – 11:33 AM BST

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

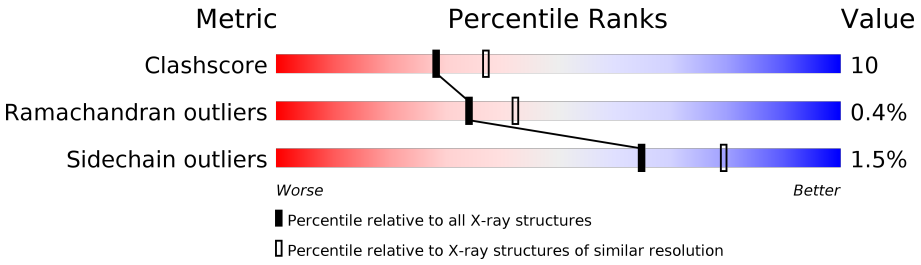
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	847	74% 19% 6%
1	B	847	72% 21% • 6%

2 Entry composition

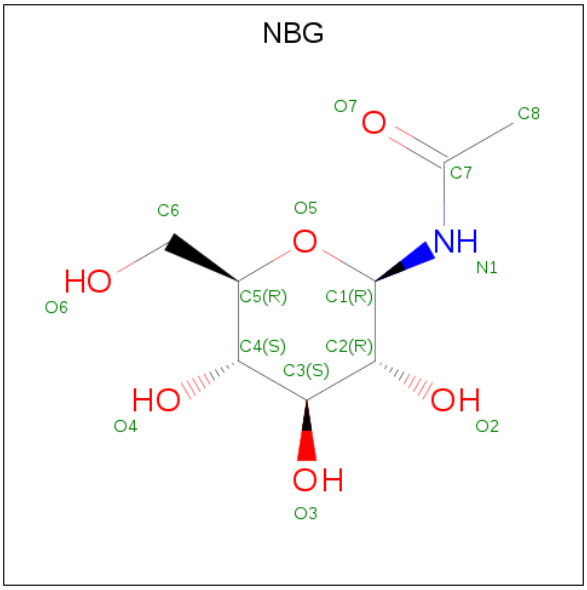
There are 7 unique types of molecules in this entry. The entry contains 13542 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

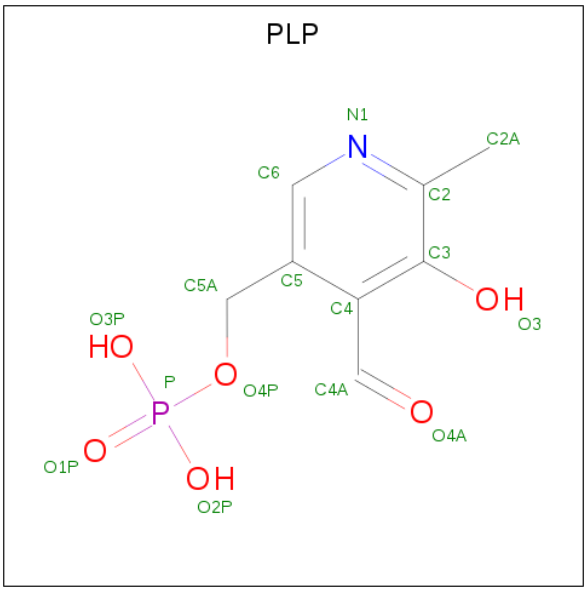
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	793	Total	C	N	O	S	0	0	0
			6436	4135	1092	1180	29			
1	B	795	Total	C	N	O	S	0	0	0
			6446	4141	1094	1182	29			

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



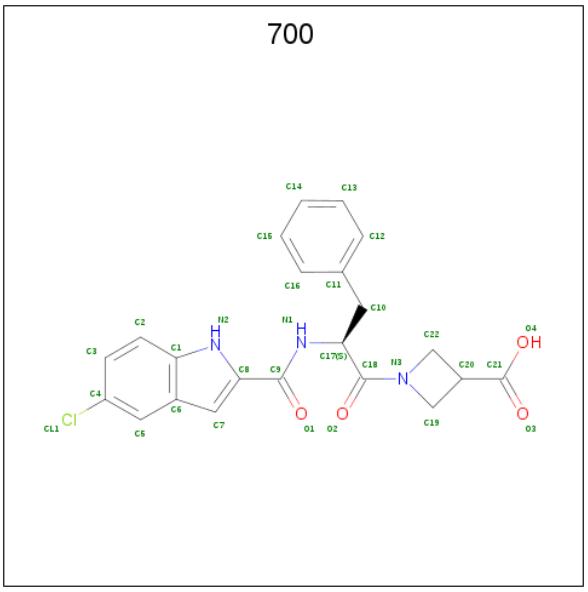
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- 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: $C_{22}H_{20}ClN_3O_4$).



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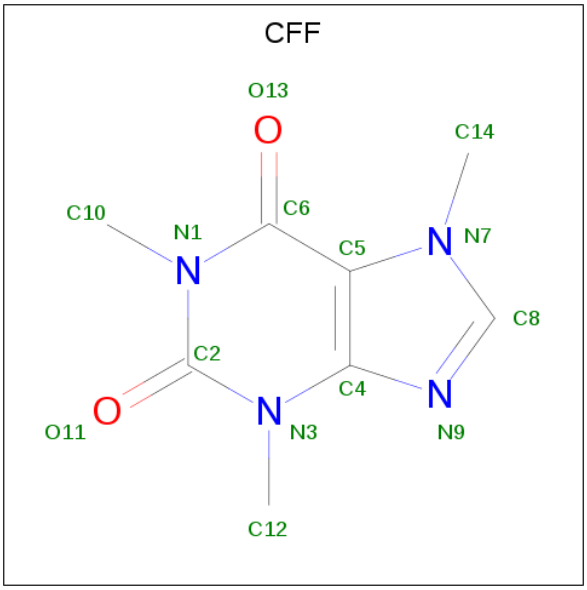
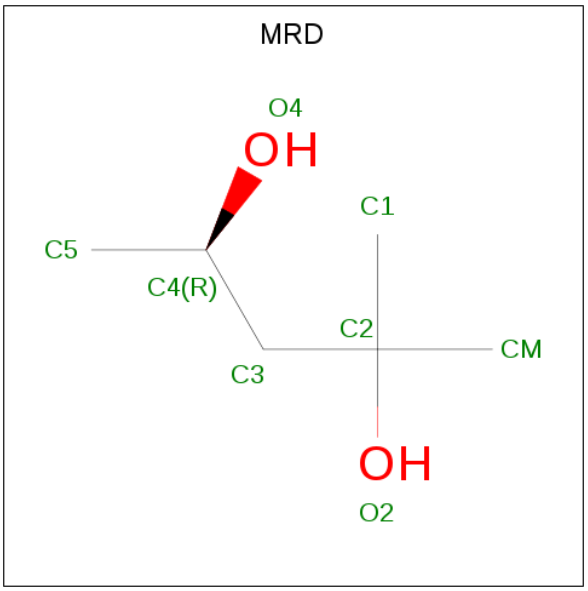
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

- 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	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			

- 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 8 6 2	0	0
6	B	1	Total C O 8 6 2	0	0
6	B	1	Total C O 8 6 2	0	0

- Molecule 7 is water.

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

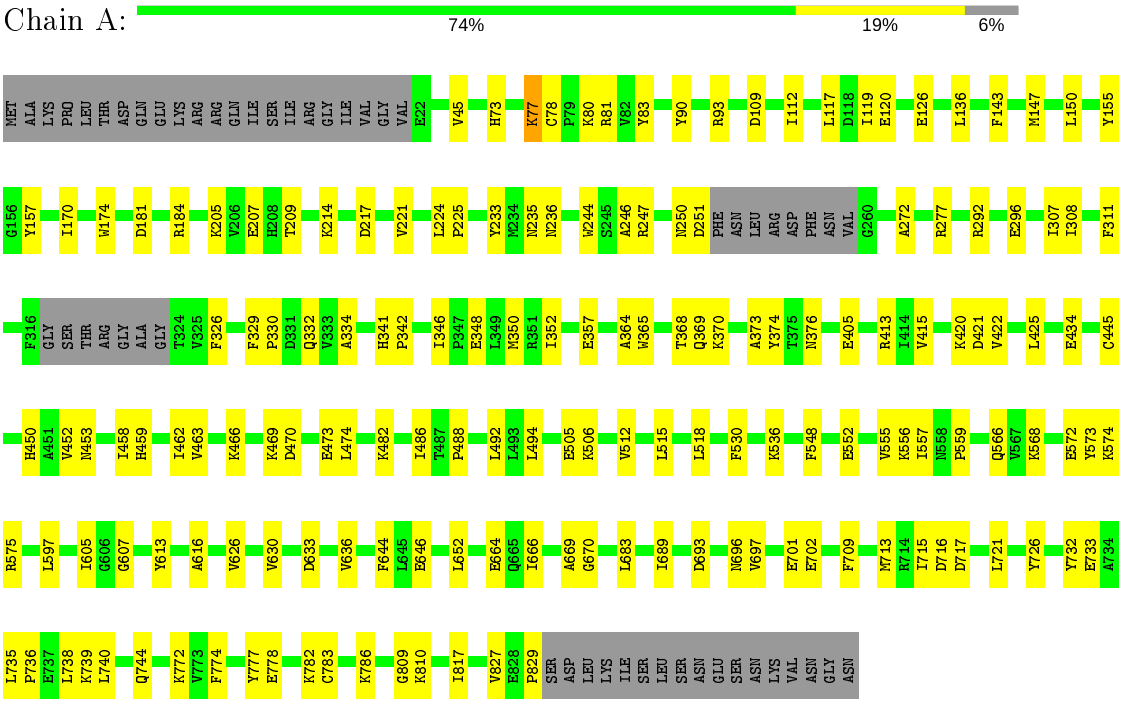
3 Residue-property plots (i)

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.

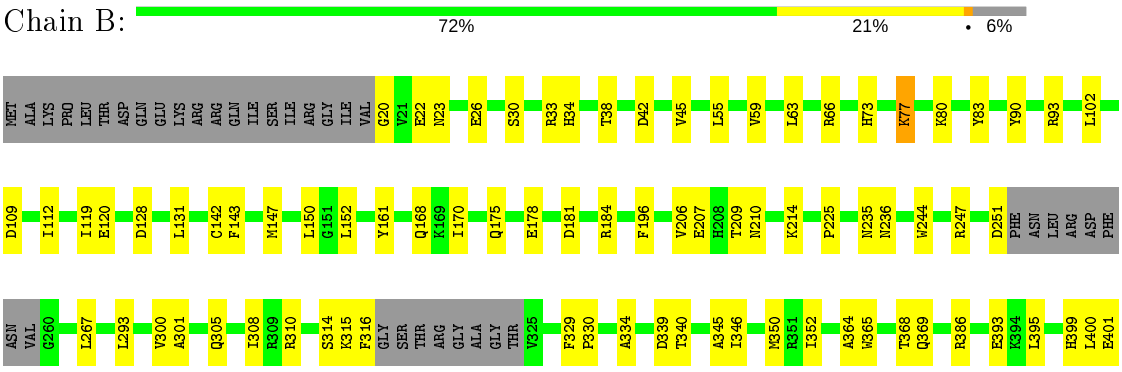
- Molecule 1: Glycogen phosphorylase, liver form

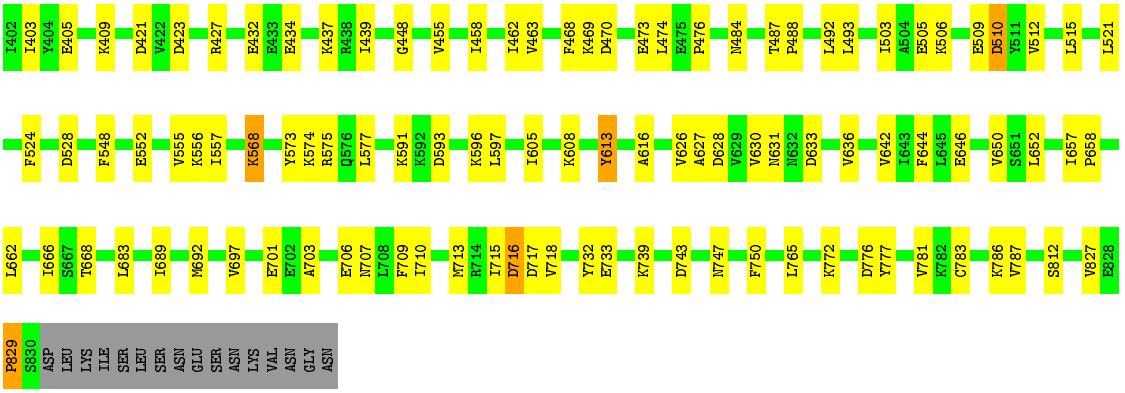
Chain A:



- Molecule 1: Glycogen phosphorylase, liver form

Chain B:




I402 I403 Y404 E405 K409 D421 V422 D423 R427 E432 E433 E434 K437 R438 I439 G448 V455 I458 I462 V463 F468 K469 D470 E473 L474 E475 P476 N484 T487 P488 L492 L493 I503 A504 E505 K506 E509 D510 Y511 V512 L515 L521
F524 D528 F548 E552 V555 K556 I557 K568 Y573 K574 R575 Q576 L577 K591 K592 D593 K596 L597 I605 K608 Y613 A616 V626 A627 D628 V629 V630 N631 N632 D633 V636 V642 I643 F644 L645 E646 V650 S651 L652 I657 P658
L662 I666 S667 T668 L683 I689 M692 V697 E701 E702 A703 E706 N707 L708 F709 I710 M713 R714 I715 D716 D717 V718 Y732 E733 K739 D743 N747 F750 L765 K772 D776 Y777 V781 K782 C783 K786 V787 S812 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 (i)

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, α, β, γ	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^2)	36.0	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: 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

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

5.3.1 Protein backbone

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%)	34	42
1	B	789/847 (93%)	743 (94%)	43 (5%)	3 (0%)	34	42
All	All	1576/1694 (93%)	1495 (95%)	75 (5%)	6 (0%)	34	42

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%)	78 89
1	B	695/740 (94%)	680 (98%)	15 (2%)	52 69
All	All	1389/1480 (94%)	1368 (98%)	21 (2%)	65 79

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 monosaccharides 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	$\#\|Z\| > 2$
6	MRD	B	903	-	7,7,7	0.71	0	9,10,10	0.90	0
5	CFF	B	1863	-	8,15,15	1.35	1 (12%)	8,23,23	1.14	1 (12%)
2	NBG	B	1861	-	15,15,15	1.65	2 (13%)	21,21,21	1.34	2 (9%)
5	CFF	A	864	-	8,15,15	1.47	1 (12%)	8,23,23	1.18	2 (25%)
2	NBG	A	861	-	15,15,15	1.47	3 (20%)	21,21,21	1.20	1 (4%)
5	CFF	A	863	-	8,15,15	1.39	1 (12%)	8,23,23	1.15	2 (25%)
6	MRD	B	1902	-	7,7,7	0.56	0	9,10,10	0.69	0
6	MRD	B	902	-	7,7,7	0.60	0	9,10,10	0.66	0
3	PLP	B	1860	1	15,15,16	1.72	2 (13%)	20,22,23	1.42	4 (20%)
4	700	A	862	-	28,33,33	1.94	10 (35%)	32,47,47	1.65	5 (15%)
3	PLP	A	860	1	15,15,16	2.00	4 (26%)	20,22,23	1.11	1 (5%)
4	700	B	1862	-	28,33,33	2.12	8 (28%)	32,47,47	1.62	6 (18%)

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	CFF	A	863	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MRD	B	1902	-	-	2/5/5/5	-
5	CFF	B	1863	-	-	-	0/2/2/2
2	NBG	B	1861	-	-	0/6/26/26	0/1/1/1
5	CFF	A	864	-	-	-	0/2/2/2
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1
6	MRD	B	903	-	-	0/5/5/5	-
3	PLP	B	1860	1	-	3/6/6/8	0/1/1/1
6	MRD	B	902	-	-	2/5/5/5	-
3	PLP	A	860	1	-	1/6/6/8	0/1/1/1
4	700	A	862	-	-	0/15/32/32	0/4/4/4
4	700	B	1862	-	-	0/15/32/32	0/4/4/4

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1862	700	C22-C20	5.59	1.60	1.55
3	B	1860	PLP	C4A-C4	-5.05	1.41	1.51
3	A	860	PLP	C4A-C4	-5.02	1.41	1.51
4	A	862	700	C22-C20	4.60	1.59	1.55
2	B	1861	NBG	C2-C1	4.40	1.57	1.52

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	862	700	C7-C6-C1	-4.49	102.36	106.27
2	B	1861	NBG	C5-O5-C1	4.46	118.57	112.52
4	A	862	700	C8-C9-N1	4.43	123.43	115.20
4	B	1862	700	C7-C6-C1	-4.41	102.43	106.27
4	B	1862	700	C8-C9-N1	4.01	122.64	115.20

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1860	PLP	C5A-O4P-P-O1P
3	B	1860	PLP	C5A-O4P-P-O2P
3	B	1860	PLP	C5A-O4P-P-O3P
6	B	1902	MRD	C2-C3-C4-O4
6	B	902	MRD	C2-C3-C4-O4

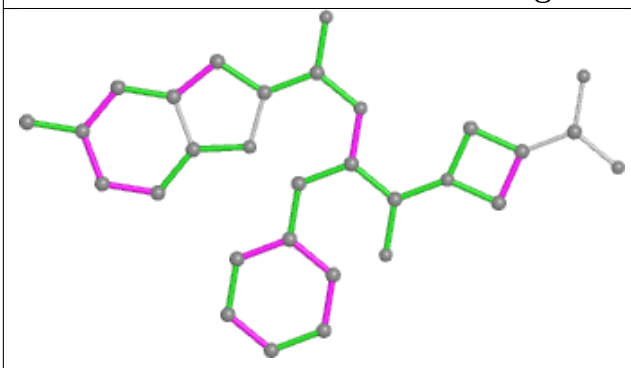
There are no ring outliers.

1 monomer is involved in 1 short contact:

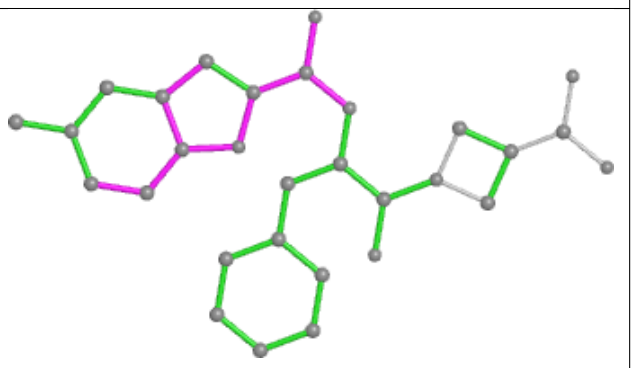
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	903	MRD	1	0

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 then 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.

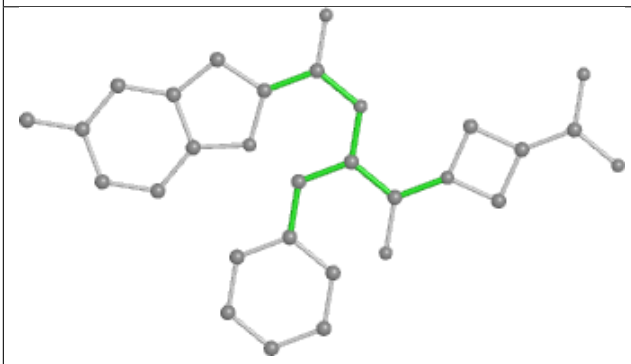
Ligand 700 A 862



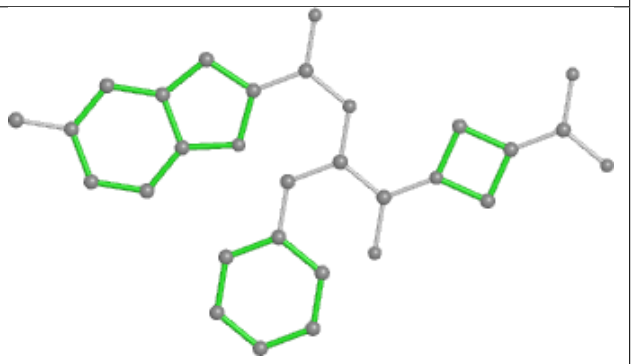
Bond lengths



Bond angles

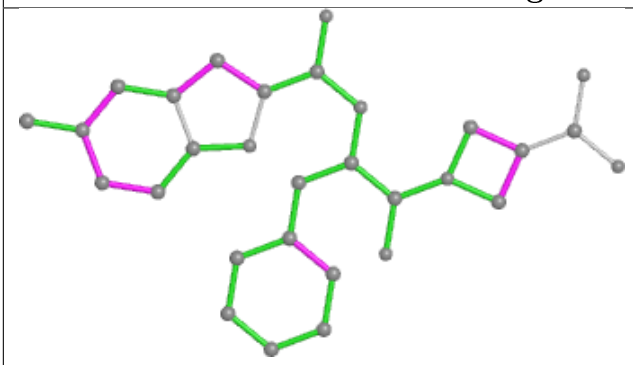


Torsions

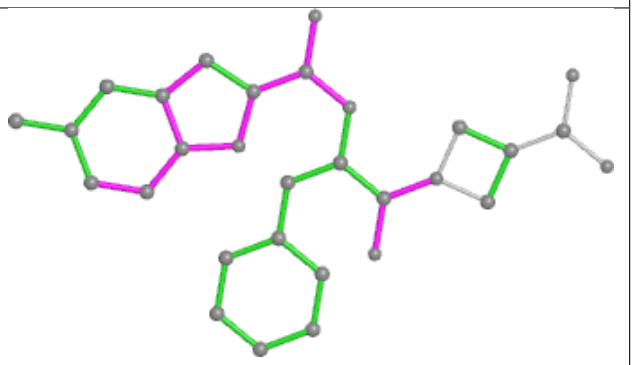


Rings

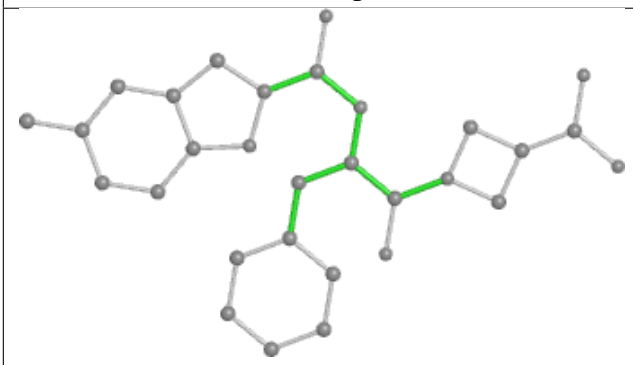
Ligand 700 B 1862



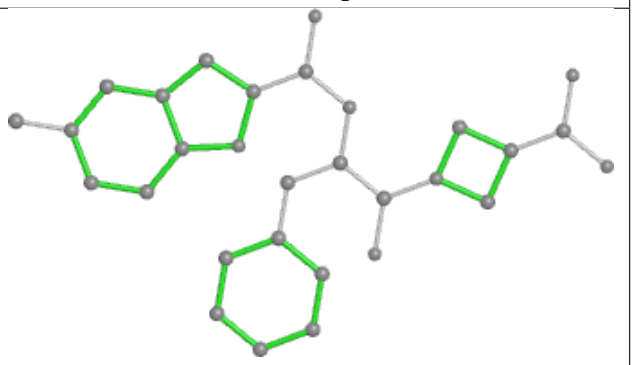
Bond lengths



Bond angles



Torsions



Rings

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.