wwPDB X-ray Structure Validation Summary Report (i)

Aug 9, 2020 – 04:12 AM BST

PDB ID	:	1L5Q
Title	:	Human liver glycogen phosphorylase a complexed with caffeine, N-Acetyl-bet a-D-glucopyranosylamine, and CP-403700
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	:	2.25 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:

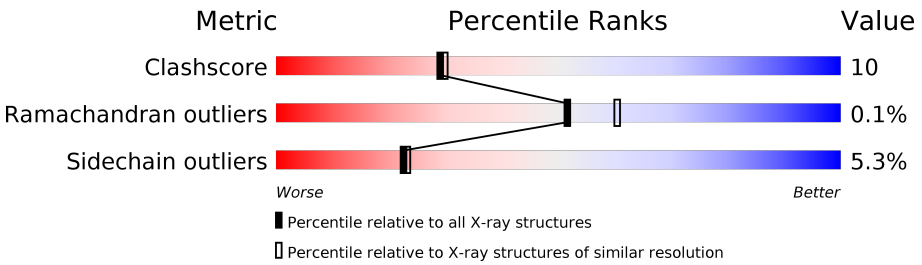
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.25 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	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)

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	73% 19% • 7%
1	B	847	74% 18% • 7%

2 Entry composition (i)

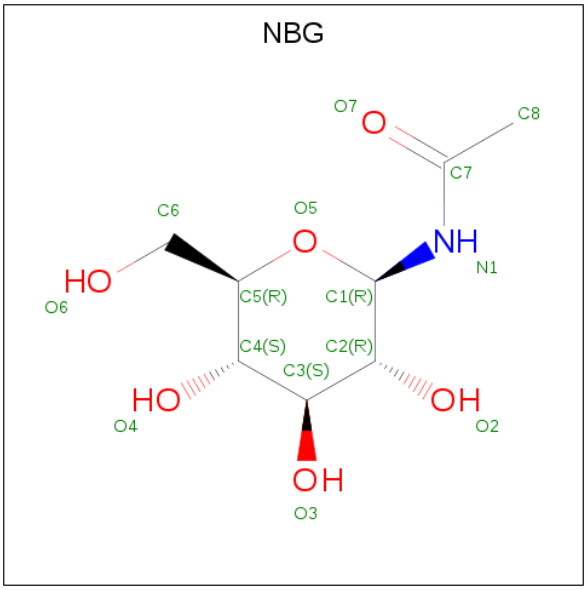
There are 6 unique types of molecules in this entry. The entry contains 13620 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

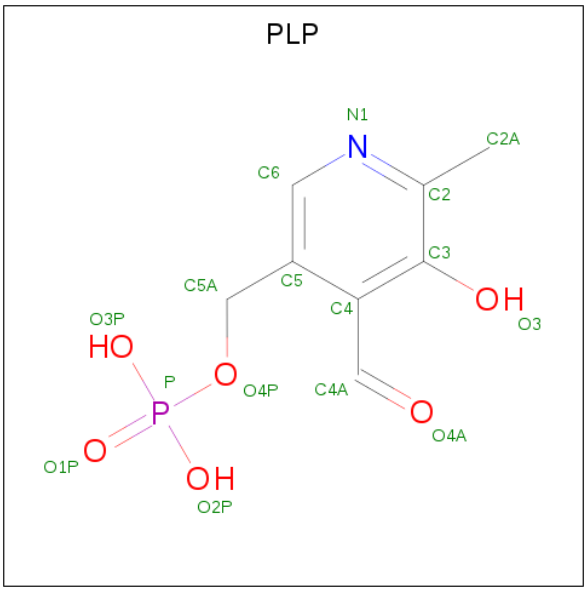
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	791	6423	4128	1090	1176	29	0	0	0
1	B	790	6414	4123	1089	1173	29	0	0	0

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



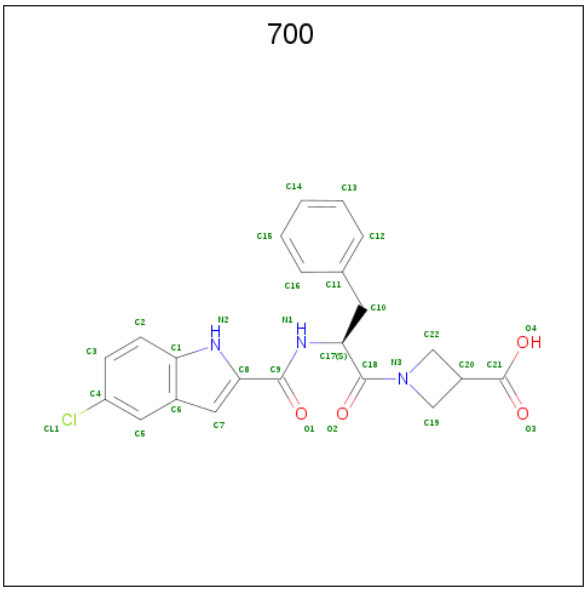
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	15	8	1	6	0	0
2	B	1	15	8	1	6	0	0

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



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

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

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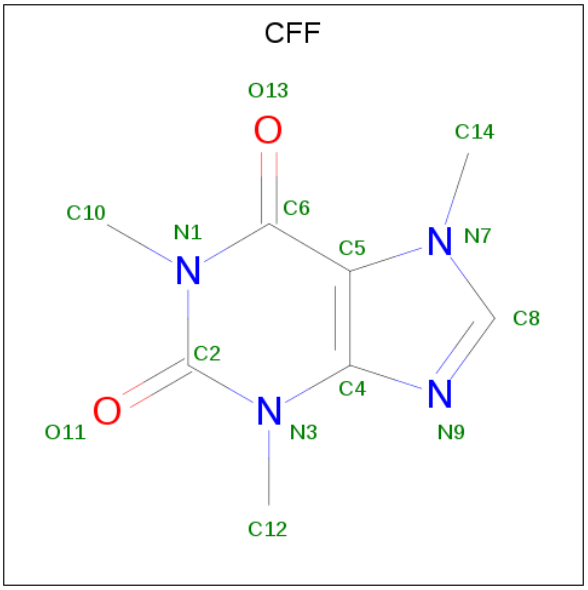
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
4	B	1	30	22	1	3	4	0	0

- Molecule 5 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	4	2	0	0
			Total	C	N	O		
5	A	1	14	8	4	2	0	0
			Total	C	N	O		
5	B	1	14	8	4	2	0	0
			Total	C	N	O		
5	B	1	14	8	4	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	324	324	324	0	0
			Total	O		
6	B	283	283	283	0	0

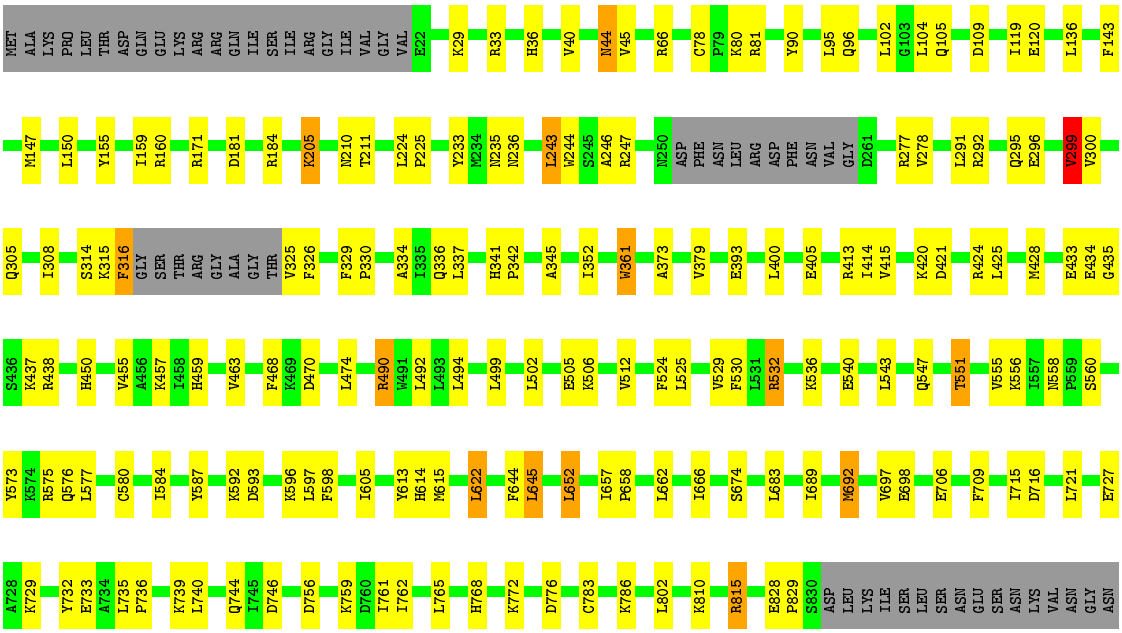
3 Residue-property plots (i)

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.

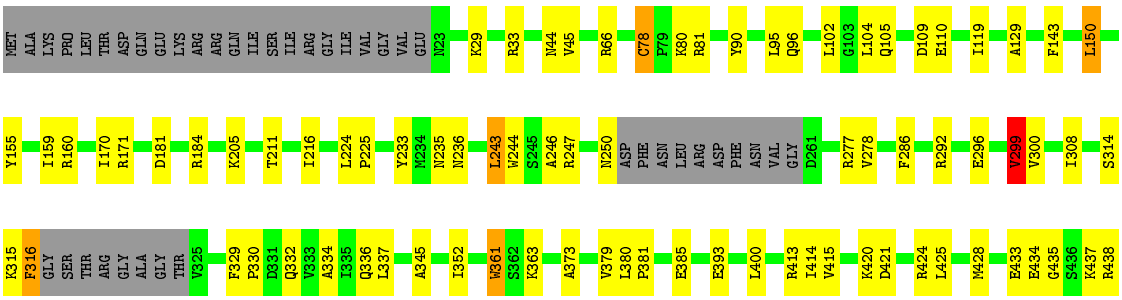
- Molecule 1: Glycogen phosphorylase, liver form

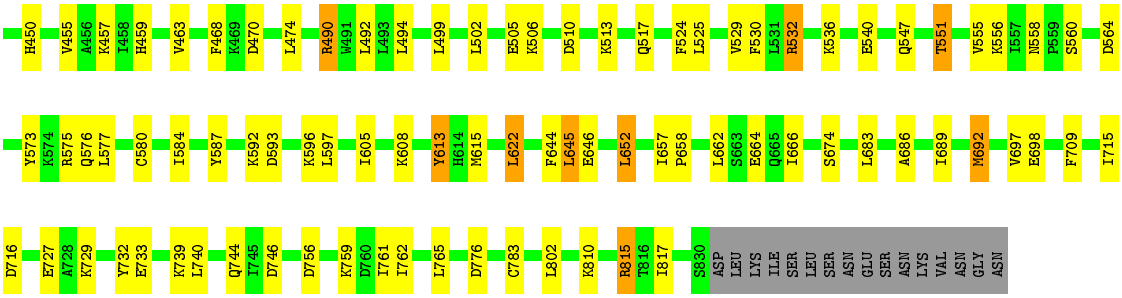
Chain A: 73% 19% • 7%



- Molecule 1: Glycogen phosphorylase, liver form

Chain B: 74% 18% • 7%




H450
V455
A456
K457
I458
H459
V463
F468
K469
D470
L474
R490
W491
L492
L493
L494
L499
L502
E505
K506
D510
K513
Q517
F524
L525
V529
F530
L531
R532
K536
E540
Q547
T551
V555
K556
I557
N558
P559
S560
D564
Y573
K574
R575
Q576
L577
C580
I584
Y587
K592
D593
K596
L597
I605
K608
Y613
H614
M615
L622
F644
L645
E646
L652
I657
P658
L662
S663
E664
Q665
I666
S674
L683
A686
I689
M692
V697
E698
F709
I715
D716
E727
A728
K729
Y732
E733
K739
L740
Q744
I745
D746
D756
K759
D760
I761
I762
L765
D776
C783
L802
K810
R815
T816
I817
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	124.71Å 124.71Å 124.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.82 – 2.25	Depositor
% Data completeness (in resolution range)	89.2 (40.82-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13620	wwPDB-VP
Average B, all atoms ($Å^2$)	30.0	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: CFF, 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	0.47	0/6567	0.69	2/8881 (0.0%)
1	B	0.46	0/6558	0.69	3/8869 (0.0%)
All	All	0.47	0/13125	0.69	5/17750 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	490	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	490	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	B	129	ALA	N-CA-C	-5.86	95.19	111.00
1	B	299	VAL	CB-CA-C	-5.06	101.79	111.40
1	A	299	VAL	CB-CA-C	-5.01	101.88	111.40

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	6423	0	6417	127	0
1	B	6414	0	6411	120	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	0	0
4	A	30	0	18	0	0
4	B	30	0	18	0	0
5	A	28	0	20	2	0
5	B	28	0	20	1	0
6	A	324	0	0	16	0
6	B	283	0	0	19	0
All	All	13620	0	12948	248	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 248 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:170:ILE:HG12	1:B:646:GLU:HG2	1.56	0.86
1:B:615:MET:HE1	1:B:761:ILE:HG12	1.58	0.84
1:A:205:LYS:HG3	6:A:2509:HOH:O	1.76	0.84
1:A:615:MET:HE1	1:A:761:ILE:HG12	1.60	0.82
1:A:532:ARG:HH11	1:A:532:ARG:HB2	1.44	0.82

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	785/847 (93%)	754 (96%)	30 (4%)	1 (0%)	51	60
1	B	784/847 (93%)	749 (96%)	34 (4%)	1 (0%)	51	60
All	All	1569/1694 (93%)	1503 (96%)	64 (4%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	GLU
1	B	434	GLU

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	693/740 (94%)	656 (95%)	37 (5%)	22	23
1	B	692/740 (94%)	656 (95%)	36 (5%)	23	24
All	All	1385/1480 (94%)	1312 (95%)	73 (5%)	22	23

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	706	GLU
1	B	95	LEU
1	B	662	LEU
1	B	44	ASN
1	B	104	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	HIS
1	B	32	ASN
1	B	369	GLN
1	A	369	GLN
1	B	450	HIS

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)

10 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	$\#\|Z\| > 2$
3	PLP	A	860	1	15,15,16	1.90	4 (26%)	20,22,23	1.47	4 (20%)
5	CFF	A	864	-	8,15,15	1.52	2 (25%)	8,23,23	1.26	2 (25%)
4	700	B	1862	-	28,33,33	2.02	12 (42%)	32,47,47	1.70	6 (18%)
5	CFF	B	1864	-	8,15,15	1.57	1 (12%)	8,23,23	1.11	1 (12%)
4	700	A	862	-	28,33,33	2.02	8 (28%)	32,47,47	1.68	7 (21%)
5	CFF	B	1863	-	8,15,15	1.33	0	8,23,23	1.30	2 (25%)
2	NBG	B	1861	-	15,15,15	2.14	3 (20%)	21,21,21	1.20	2 (9%)
5	CFF	A	863	-	8,15,15	1.49	1 (12%)	8,23,23	1.40	2 (25%)
3	PLP	B	1860	1	15,15,16	2.48	4 (26%)	20,22,23	1.28	1 (5%)
2	NBG	A	861	-	15,15,15	1.95	3 (20%)	21,21,21	1.07	1 (4%)

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
3	PLP	A	860	1	-	2/6/6/8	0/1/1/1
5	CFF	A	864	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	700	B	1862	-	-	0/15/32/32	0/4/4/4
5	CFF	B	1864	-	-	-	0/2/2/2
4	700	A	862	-	-	0/15/32/32	0/4/4/4
5	CFF	B	1863	-	-	-	0/2/2/2
2	NBG	B	1861	-	-	0/6/26/26	0/1/1/1
5	CFF	A	863	-	-	-	0/2/2/2
3	PLP	B	1860	1	-	1/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1860	PLP	C4A-C4	-6.62	1.37	1.51
2	B	1861	NBG	C1-N1	5.09	1.49	1.43
4	A	862	700	C22-C20	4.83	1.59	1.55
2	B	1861	NBG	C2-C1	4.79	1.57	1.52
4	A	862	700	C5-C4	4.73	1.45	1.36

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	862	700	C7-C6-C1	-5.01	101.90	106.27
4	B	1862	700	C7-C6-C1	-4.28	102.54	106.27
4	A	862	700	C8-C9-N1	4.24	123.07	115.20
4	B	1862	700	C8-C9-N1	4.14	122.89	115.20
2	B	1861	NBG	C5-O5-C1	3.97	117.90	112.52

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	860	PLP	C4-C5-C5A-O4P
3	A	860	PLP	C6-C5-C5A-O4P
3	B	1860	PLP	C4-C5-C5A-O4P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	864	CFF	2	0
5	B	1863	CFF	1	0

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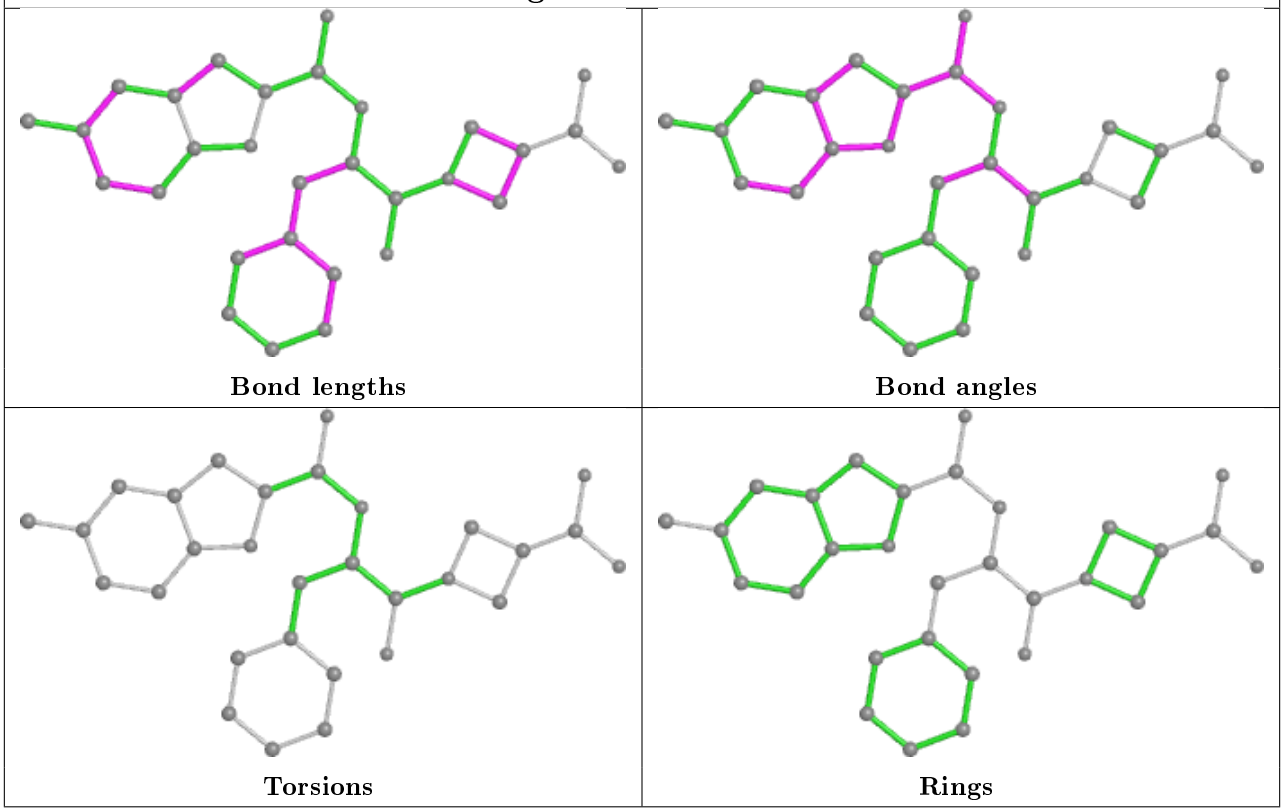
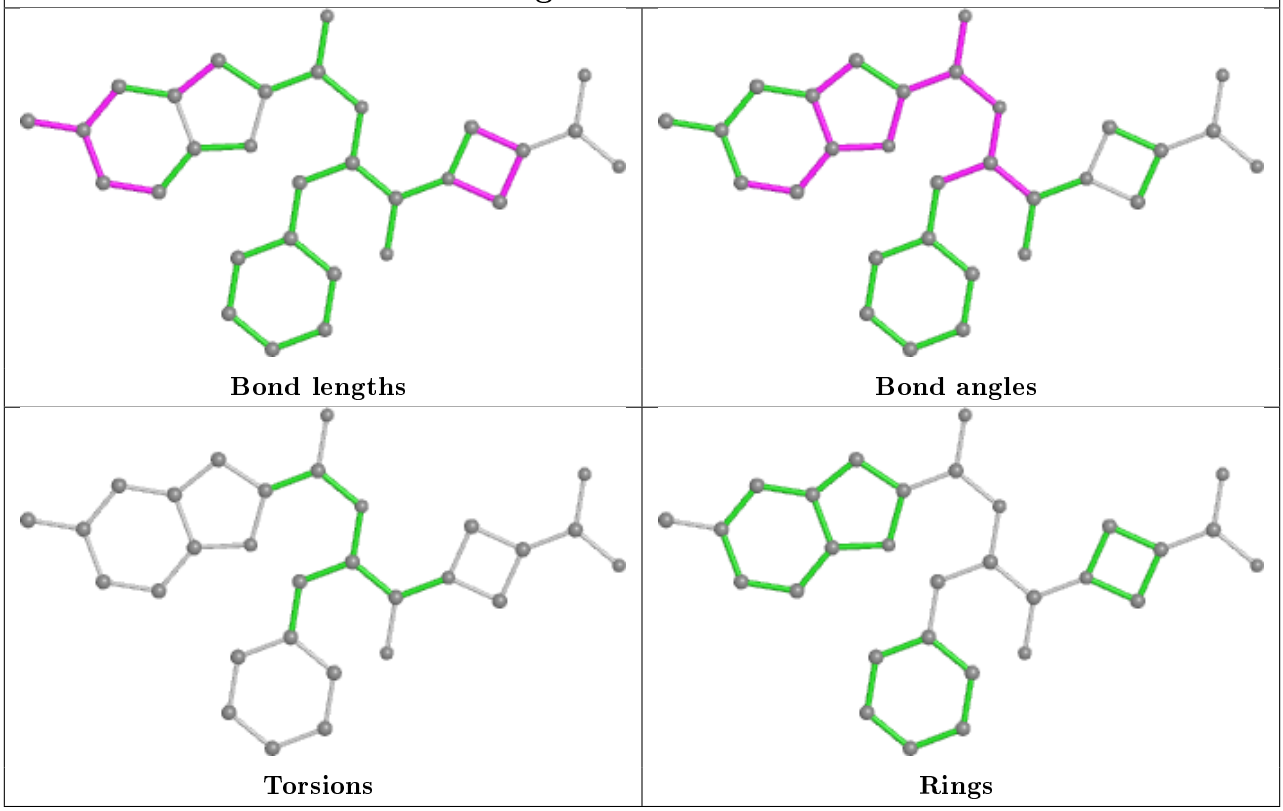
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1861	NBG	1	0

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 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 B 1862



Ligand 700 A 862



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.