



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 10:09 AM BST

PDB ID : 1XOI
Title : Human Liver Glycogen Phosphorylase A complexed with Chloroindoloyl glycine amide
Authors : Wright, S.W.; Rath, V.L.; Gibbs, E.M.; Treadway, J.L.
Deposited on : 2004-10-06
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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) : 2.13.1

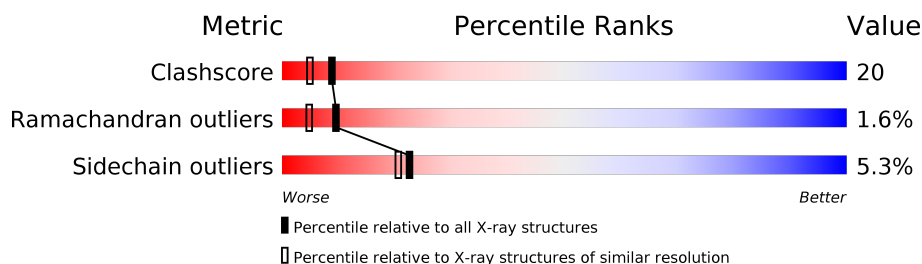
1 Overall quality at a glance

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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	846	
1	B	846	

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
4	288	A	862	X	-	-	-
4	288	B	1862	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13762 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.

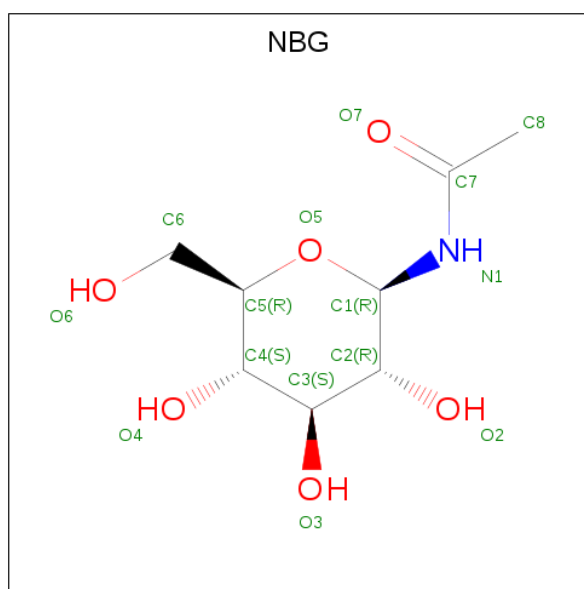
- Molecule 1 is a protein called Glycogen phosphorylase, liver form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	804	Total	C	N	O	S	0	0	0
			6508	4180	1107	1192	29			
1	B	804	Total	C	N	O	S	0	0	0
			6508	4180	1107	1192	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	ALA	GLY	conflict	UNP P06737
B	1323	ALA	GLY	conflict	UNP P06737

- Molecule 2 is N-acetyl-beta-D-glucopyranosylamine (three-letter code: NBG) (formula: C₈H₁₅NO₆).



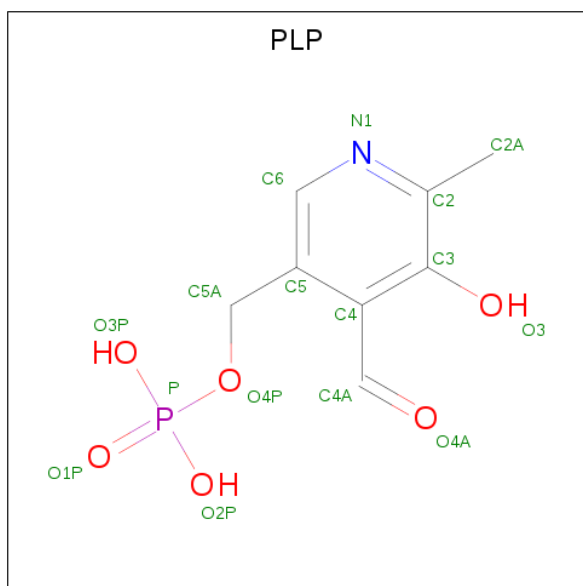
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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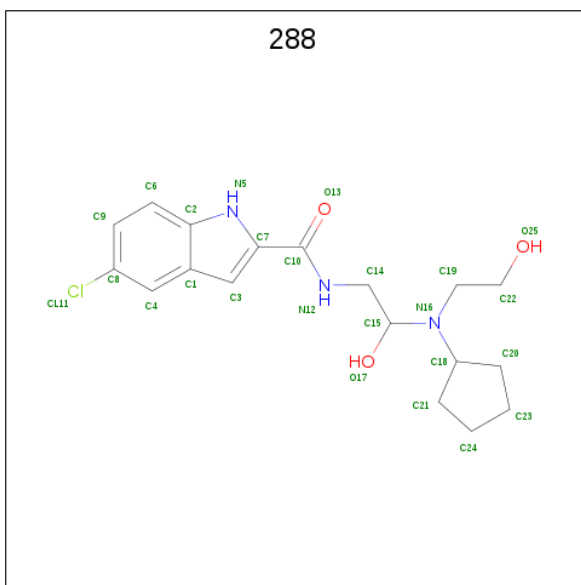
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- 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-INDOLE-2-CARBOXYLIC ACID{[CYCLOPENTYL-(2-HYDROXY-ETHYL)-CARBAMOYL]-METHYL}-AMIDE (three-letter code: 288) (formula: $C_{18}H_{24}ClN_3O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			25	18	1	3	3		
4	B	1	Total	C	Cl	N	O	0	0
			25	18	1	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	323	Total	O	0	0
			323	323		
5	B	313	Total	O	0	0
			313	313		

K1759	L1640	K1437	P1342	R1247	L1102
D1760	K1641	A1442	A1345	A1248	Q1105
M1763	V1642	H1443	I1346	P1249	M1106
M1764	F1644	I1446	P1347	ASN	A1111
B1770	L1645	V1447	E1348	ASP	I1112
F1771	E1646	G1448	I1352	PHE	Y1113
K1772	N1647	S1449	W1361	ASN	Q1114
A1775	L1651	H1450	W1365	LEU	L1115
D1776	S1652	A1451	V1452	ASP	G1116
G1783	I1657	V1455	Q1369	PHE	L1117
P1786	P1658	A1456	K1370	ASN	E1120
K1786	I1666	K1457	I1374	VAL	E1121
Q1789	S1674	I1458	Y1377	GLY	ASP
M1792	K1680	H1459	H1377	Y1262	D1128
M1793	L1683	Q1566	T1378	M1274	L1150
P1794	L1689	Y1567	V1379	I1275	Y1155
L1802	G1690	K1568	L1380	S1276	V1159
K1810	T1691	H1571	P1381	R1277	R1160
D1814	M1692	K1574	E1382	V1278	
R1815	K1697	R1575	E1385	F1286	Y1163
K1818	M1698	Q1576	R1396	Q1295	Q1168
P1829	V1697	L1577	V1389	V1299	K1169
S1830	E1698	K1579	D1390	V1300	I1170
D1831	E1701	K1582	P1397	L1304	H1174
K1832	E1702	D1593	I1402	I1308	D1181
I1833	F1709	P1594	E1405	K1312	R1184
I1834	I1710	K1595	I1406	A1313	Y1185
S1835	I1715	L1596	K1409	S1314	S1192
L1836	E1727	F1597	R1413	K1315	R1193
S1837	K1728	P1600	I1414	G1317	P1194
M1838	K1729	R1601	V1415	S1318	V1206
GLU	E1730	G1607	L1502	T1319	E1207
SER	E1733	Y1613	K1506	R1320	H1208
ASN	A1734	H1614	E1509	G1321	T1209
LYS	L1735	M1615	V1512	A1322	M1210
VAL	P1736	I1619	D1528	A1323	L1224
ASN	L1740	T1620	V1529	T1324	P1225
GLY	Q1744	K1621	F1530	D1423	Y1226
ASN	P1752	L1622	L1430	R1424	P1327
	P1753	M1632	L1431	L1425	A1328
	Q1754	D1633	E1432	R1426	M1234
	P1755	P1634	E1433	L1436	M1235
	D1756	M1635	K1536	Y1437	N1236
	L1757	V1636	Q1539	E1434	T1237
	F1758	K1639	G1435	A1334	V1238
			E1540	L1337	L1243
				S1436	W1244

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, α , β , γ	123.91Å 123.91Å 123.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.00 – 2.10	Depositor
% Data completeness (in resolution range)	92.6 (99.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13762	wwPDB-VP
Average B, all atoms (Å ²)	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: 288, 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	0/6653	0.61	0/8998
1	B	0.37	0/6653	0.62	1/8998 (0.0%)
All	All	0.36	0/13306	0.61	1/17996 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1323	ALA	N-CA-C	-5.38	96.46	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	6508	0	6518	278	0
1	B	6508	0	6518	264	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0
3	A	15	0	7	1	0
3	B	15	0	7	0	0
4	A	25	0	22	0	0
4	B	25	0	22	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	323	0	0	51	0
5	B	313	0	0	35	0
All	All	13762	0	13124	536	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 20.

The worst 5 of 536 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:1434:GLU:H	1:B:1434:GLU:CD	1.62	0.98
1:A:96:GLN:HE21	1:A:105:GLN:HE22	1.10	0.98
1:A:236:ASN:HB3	1:A:834:ILE:HB	1.46	0.97
1:A:434:GLU:CD	1:A:434:GLU:H	1.65	0.96
1:B:1168:GLN:HE21	1:B:1647:ASN:H	1.03	0.96

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	800/846 (95%)	748 (94%)	39 (5%)	13 (2%)	9 5
1	B	800/846 (95%)	749 (94%)	38 (5%)	13 (2%)	9 5
All	All	1600/1692 (95%)	1497 (94%)	77 (5%)	26 (2%)	9 5

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	PHE
1	A	318	SER

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Mol	Chain	Res	Type
1	B	1317	GLY
1	B	1320	ARG
1	B	1322	ALA

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	702/739 (95%)	663 (94%)	39 (6%)	21	18
1	B	702/739 (95%)	666 (95%)	36 (5%)	24	22
All	All	1404/1478 (95%)	1329 (95%)	75 (5%)	22	20

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	692	MET
1	B	1078	CYS
1	B	1730	GLU
1	A	730	GLU
1	A	833	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	614	HIS
1	B	1073	HIS
1	B	1576	GLN
1	A	754	GLN
1	B	1032	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	288	A	862	-	24,27,27	2.40	4 (16%)	29,37,37	1.70	6 (20%)
2	NBG	B	1861	-	15,15,15	1.74	3 (20%)	21,21,21	1.32	2 (9%)
3	PLP	B	1860	-	15,15,16	2.42	3 (20%)	20,22,23	1.30	1 (5%)
2	NBG	A	861	-	15,15,15	1.48	3 (20%)	21,21,21	1.37	2 (9%)
3	PLP	A	860	-	15,15,16	2.49	6 (40%)	20,22,23	1.31	2 (10%)
4	288	B	1862	-	24,27,27	2.44	3 (12%)	29,37,37	1.60	5 (17%)

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	288	A	862	-	1/1/4/5	3/15/27/27	0/3/3/3
2	NBG	B	1861	-	-	0/6/26/26	0/1/1/1
3	PLP	B	1860	-	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1
3	PLP	A	860	-	-	0/6/6/8	0/1/1/1
4	288	B	1862	-	1/1/4/5	3/15/27/27	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1862	288	O17-C15	-10.53	1.21	1.41
4	A	862	288	O17-C15	-9.96	1.22	1.41
3	B	1860	PLP	C4A-C4	-7.21	1.36	1.51
3	A	860	PLP	C4A-C4	-7.04	1.37	1.51
2	B	1861	NBG	C2-C1	4.27	1.57	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	862	288	C7-C10-N12	5.13	122.77	115.59
4	B	1862	288	C7-C10-N12	4.77	122.26	115.59
2	A	861	NBG	C5-O5-C1	4.65	118.83	112.52
2	B	1861	NBG	C5-O5-C1	4.56	118.71	112.52
4	B	1862	288	O17-C15-C14	4.09	119.34	108.61

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	862	288	C15
4	B	1862	288	C15

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	862	288	N12-C14-C15-O17
4	B	1862	288	N12-C14-C15-O17
4	A	862	288	C14-C15-N16-C19
4	B	1862	288	C14-C15-N16-C19
4	A	862	288	C14-C15-N16-C18

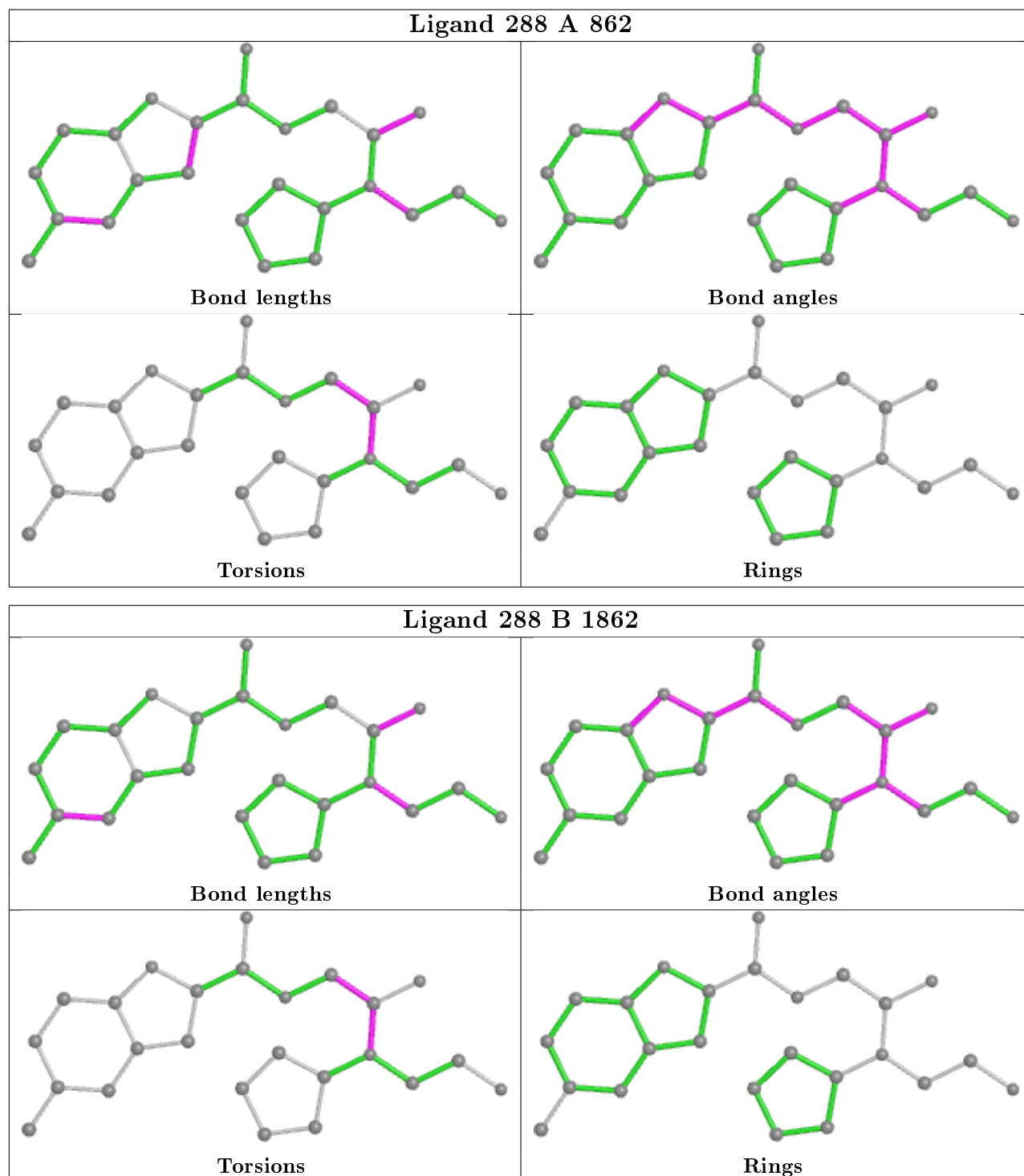
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	860	PLP	1	0
4	B	1862	288	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.



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.