



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:19 AM UTC

PDB ID : 1XOI / pdb_00001xoi
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 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)
Xtriage (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

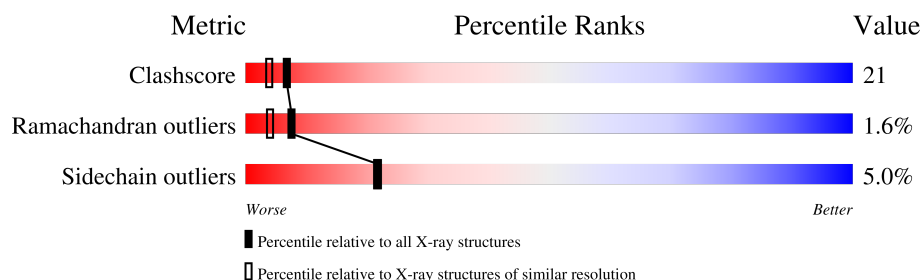
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 ≥ 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.

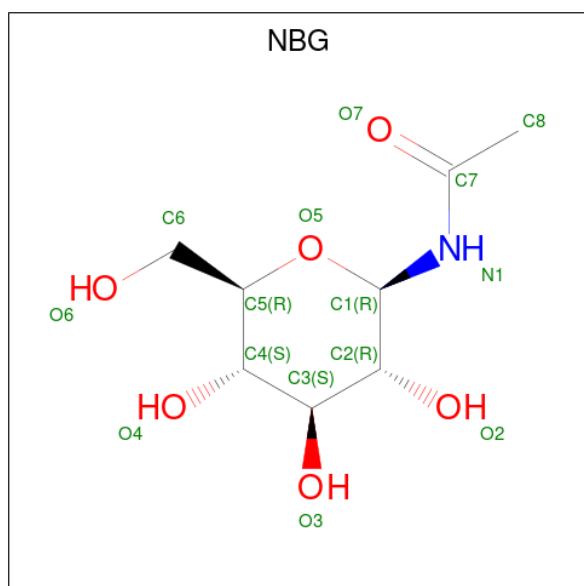
- Molecule 1 is a protein called Glycogen phosphorylase, liver form.

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 (CCD ID: NBG) (formula: C₈H₁₅NO₆).



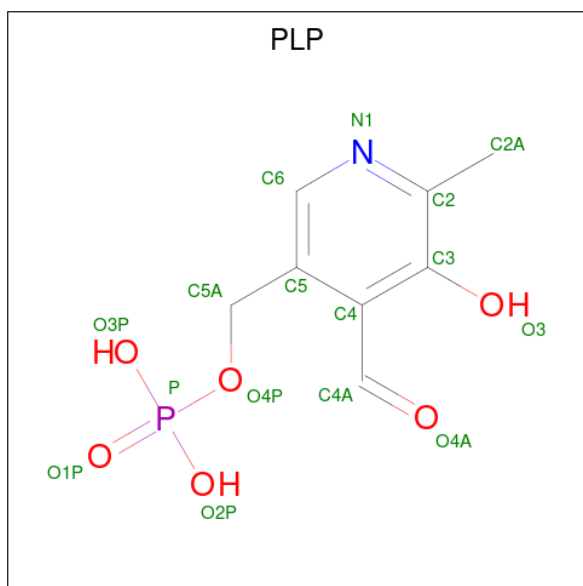
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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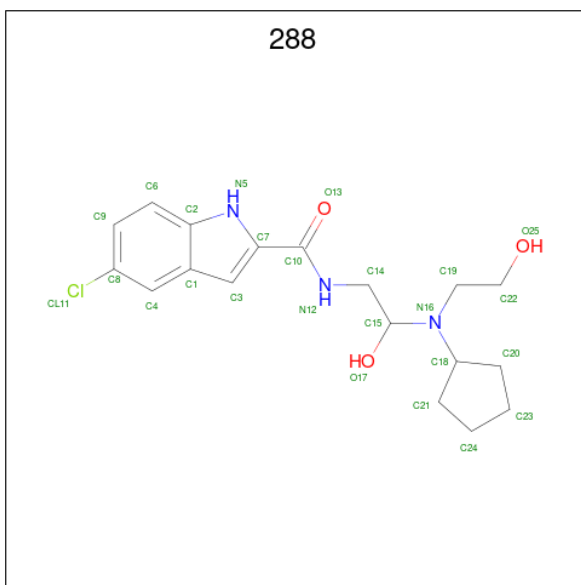
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $\text{C}_8\text{H}_{10}\text{NO}_6\text{P}$).



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

- Molecule 4 is 5-CHLORO-1H-INDOLE-2-CARBOXYLIC ACID{[CYCLOPENTYL-(2-HYDROXY-ETHYL)-CARBAMOYL]-METHYL}-AMIDE (CCD ID: 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.

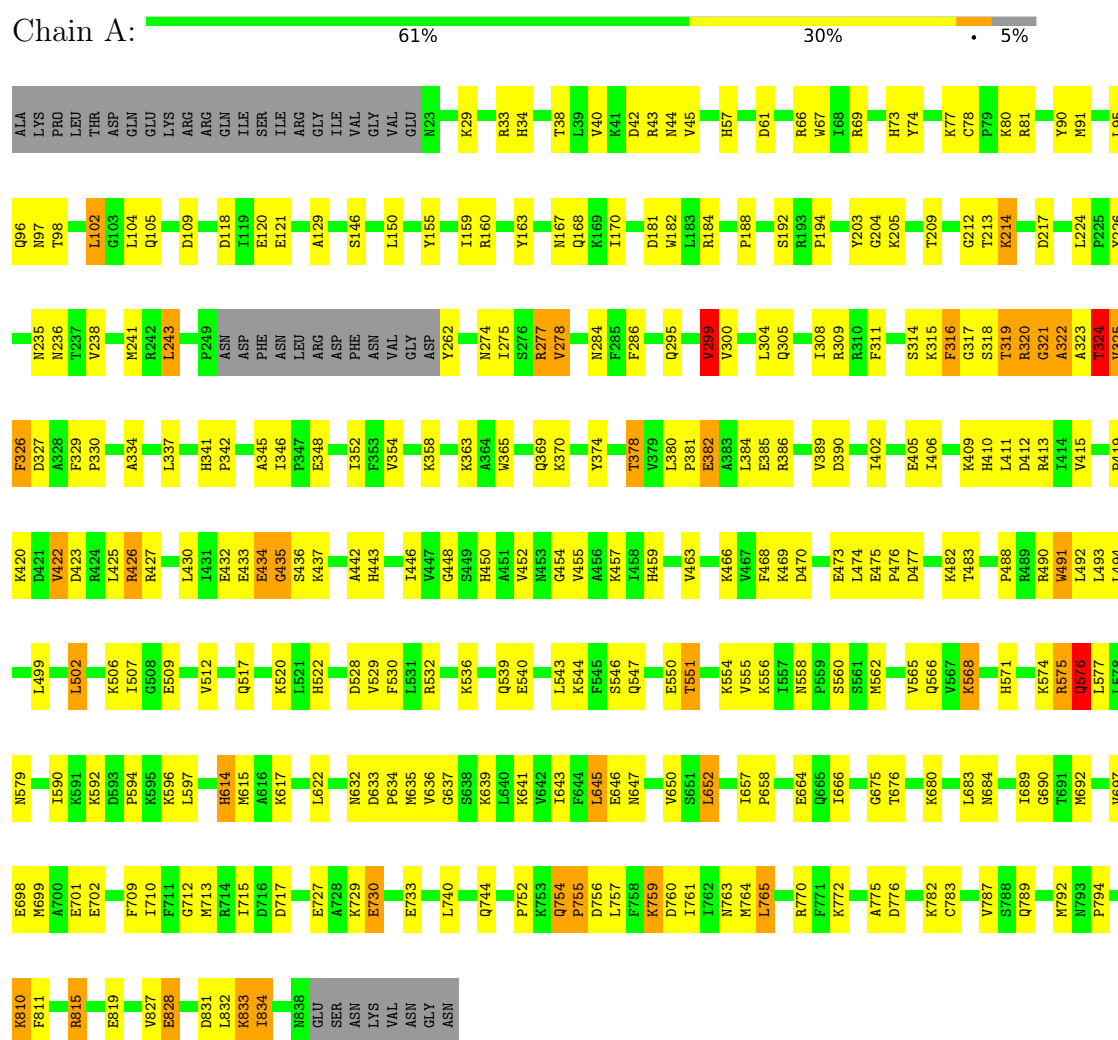
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	323	Total	O	0	0
			323	323		
5	B	313	Total	O	0	0
			313	313		

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



E1828	F1711	G1607	K1506	P1419	A1323	I1216	L1095	ALA
P1829	G1712	K1608	I1507	K1420	T1324	L1224	Q1096	LYS
D1830	I1715	K1614	G1508	D1421	F1325	P1225	N1097	PRO
L1832	E1727	M1615	E1509	D1423	F1326	D1327	T1098	THR
K1833	A1728	M1615	V1512	R1424	A1328	Y1226	L1102	ASP
I1834	K1729	K1621	D1528	L1425	F1329	M1234	L1105	GLN
S1835	E1730	L1622	V1529	R1426	P1330	N1235	Q1105	GLU
L1836	E1733	M1632	F1530	L1430	A1334	N1236	L1112	ARG
S1837	A1734	D1633	L1531	I1431	L1337	V1238	A1111	ARG
N1838	P1735	P1634	R1532	E1432	H1341	L1243	I1113	GLN
GLU	P1736	M1635	K1536	E1433	P1342	W1244	Y1112	TLE
SER	V1636	V1636	K1536	E1434	A1345	P1249	Q1114	SER
ASN	K1639	K1639	Q1539	G1435	I1346	ASN	G1116	ILE
LYS	L1640	L1640	E1540	S1436	P1347	ASP	L1117	ARG
VAL	K1641	V1642	L1543	K1437	E1348	PHE	E1120	VAL
ASN	P1752	I1643	S1546	A1442	I1352	ASN	E1121	GLY
GLY	K1753	I1643	Q1547	H1443	F1353	LEU	E1126	VAL
ASN	Q1754	F1644	Q1547	T1446	V1354	ASP	D1128	GLY
ASN	P1755	L1645	E1550	V1447	W1365	GLY	L1150	ASN
GLY	D1756	E1646	T1551	G1448	Q1369	ASP	Y1155	ASP
ASN	L1757	M1647	K1551	S1449	K1370	Y1262	E1159	R1033
F1758	F1758	V1650	V1555	H1450	T1371	R1269	R1160	H1034
K1759	K1759	S1651	K1556	H1451	A1373	N1274	Y1163	T1038
D1760	I1761	L1652	I1557	N1452	I1374	I1275	F1166	L1039
I1762	I1762	V1656	N1558	N1453	A1375	S1276	N1167	V1040
M1763	M1763	I1657	P1559	G1454	I1377	R1277	Q1168	K1041
M1764	L1765	P1658	S1560	V1455	E1378	V1278	K1169	D1042
L1765	R1770	I1666	S1561	K1457	P1381	F1286	I1170	R1043
F1771	F1771	Y1674	M1562	I1458	E1382	Q1295	W1174	N1044
K1772	K1772	G1675	V1565	H1459	E1385	V1299	R1049	V1045
A1775	A1775	T1676	Q1566	I1462	R1386	V1300	D1061	D1061
D1776	D1776	G1677	V1567	V1463	V1389	L1304	Y1064	Y1064
C1783	C1783	K1680	K1568	F1468	D1390	L1308	G1065	G1065
K1786	K1786	L1683	H1571	D1470	P1397	K1312	R1066	R1066
V1787	V1787	M1684	K1574	E1473	I1402	A1313	W1067	W1067
Q1789	Q1789	I1689	R1575	L1474	E1405	S1314	H1073	H1073
M1792	M1792	G1690	Q1576	E1475	I1406	K1315	Y1074	Y1074
N1793	N1793	T1691	L1577	P1476	K1409	F1316	K1077	K1077
P1794	P1794	M1692	L1578	D1477	L1493	G1317	P1078	P1078
L1802	L1802	V1697	N1579	P1488	R1413	T1319	E1207	E1207
K1810	K1810	E1698	K1592	V1491	I1415	R1320	H1208	H1208
D1814	D1814	A1700	P1594	L1492	G1321	A1322	R1081	R1081
R1815	R1815	E1701	K1595	L1493	V1415		M1091	M1091
K1818	K1818	E1702	F1596	L1494				
		F1709	F1598	L1499				
		I1710	V1599	L1502				
			R1601					

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

5.1 Standard geometry

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	0.43	0/6653	0.93	24/8998 (0.3%)
1	B	0.42	0/6653	0.95	36/8998 (0.4%)
All	All	0.42	0/13306	0.94	60/17996 (0.3%)

There are no bond length outliers.

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1565	VAL	N-CA-C	7.83	119.76	108.48
1	B	1754	GLN	CA-C-N	7.64	128.34	119.47
1	B	1754	GLN	C-N-CA	7.64	128.34	119.47
1	A	565	VAL	N-CA-C	7.62	119.46	108.48
1	A	754	GLN	CA-C-N	7.47	127.84	119.32

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	6508	0	6518	293	0
1	B	6508	0	6518	274	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	1	0
3	B	15	0	7	0	0
4	A	25	0	22	0	0
4	B	25	0	22	3	0
5	A	323	0	0	52	0
5	B	313	0	0	33	0
All	All	13762	0	13124	561	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 21.

The worst 5 of 561 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:CD	1:B:1434:GLU:H	1.62	1.03
1:A:434:GLU:H	1:A:434:GLU:CD	1.65	1.01
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: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%)	7 4
1	B	800/846 (95%)	749 (94%)	38 (5%)	13 (2%)	7 4
All	All	1600/1692 (95%)	1497 (94%)	77 (5%)	26 (2%)	7 4

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	PHE
1	A	318	SER
1	B	1317	GLY
1	B	1320	ARG
1	B	1322	ALA

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	702/739 (95%)	665 (95%)	37 (5%)	20	19
1	B	702/739 (95%)	669 (95%)	33 (5%)	23	24
All	All	1404/1478 (95%)	1334 (95%)	70 (5%)	22	22

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1622	LEU
1	B	1652	LEU
1	B	1810	LYS
1	A	576	GLN
1	A	568	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1062	HIS
1	B	1210	ASN
1	B	1763	ASN
1	B	1073	HIS
1	B	1114	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 oligosaccharides 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
2	NBG	B	1861	-	15,15,15	1.67	3 (20%)	21,21,21	1.31	2 (9%)
4	288	A	862	-	27,27,27	2.35	4 (14%)	32,37,37	1.63	8 (25%)
4	288	B	1862	-	27,27,27	2.42	3 (11%)	32,37,37	1.51	7 (21%)
3	PLP	B	1860	-	15,15,16	2.49	4 (26%)	21,22,23	1.28	1 (4%)
3	PLP	A	860	-	15,15,16	2.57	6 (40%)	21,22,23	1.30	2 (9%)
2	NBG	A	861	-	15,15,15	1.43	3 (20%)	21,21,21	1.34	2 (9%)

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	B	1861	-	-	0/6/26/26	0/1/1/1
4	288	A	862	-	1/1/4/5	4/18/27/27	0/3/3/3
4	288	B	1862	-	1/1/4/5	3/18/27/27	0/3/3/3
3	PLP	B	1860	-	-	0/6/6/8	0/1/1/1
3	PLP	A	860	-	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1862	288	O17-C15	-11.10	1.21	1.41
4	A	862	288	O17-C15	-10.50	1.22	1.41
3	B	1860	PLP	C4A-C4	-7.50	1.36	1.51
3	A	860	PLP	C4A-C4	-7.32	1.37	1.51
2	B	1861	NBG	C2-C1	4.15	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	861	NBG	C5-O5-C1	4.58	118.83	112.47
2	B	1861	NBG	C5-O5-C1	4.49	118.71	112.47
4	A	862	288	C7-C10-N12	4.34	122.77	116.80
4	B	1862	288	C7-C10-N12	3.97	122.26	116.80
4	B	1862	288	O17-C15-C14	3.94	119.34	108.69

All (2) chirality outliers are listed below:

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

5 of 7 torsion outliers are listed below:

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

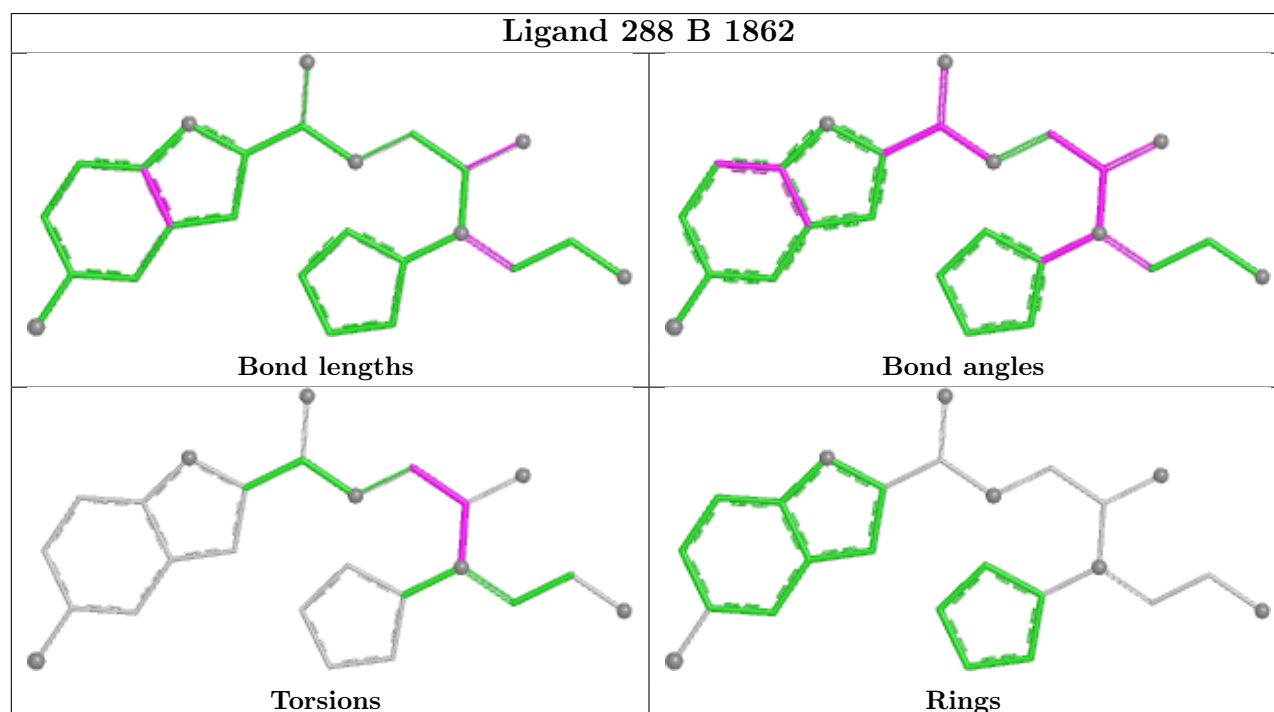
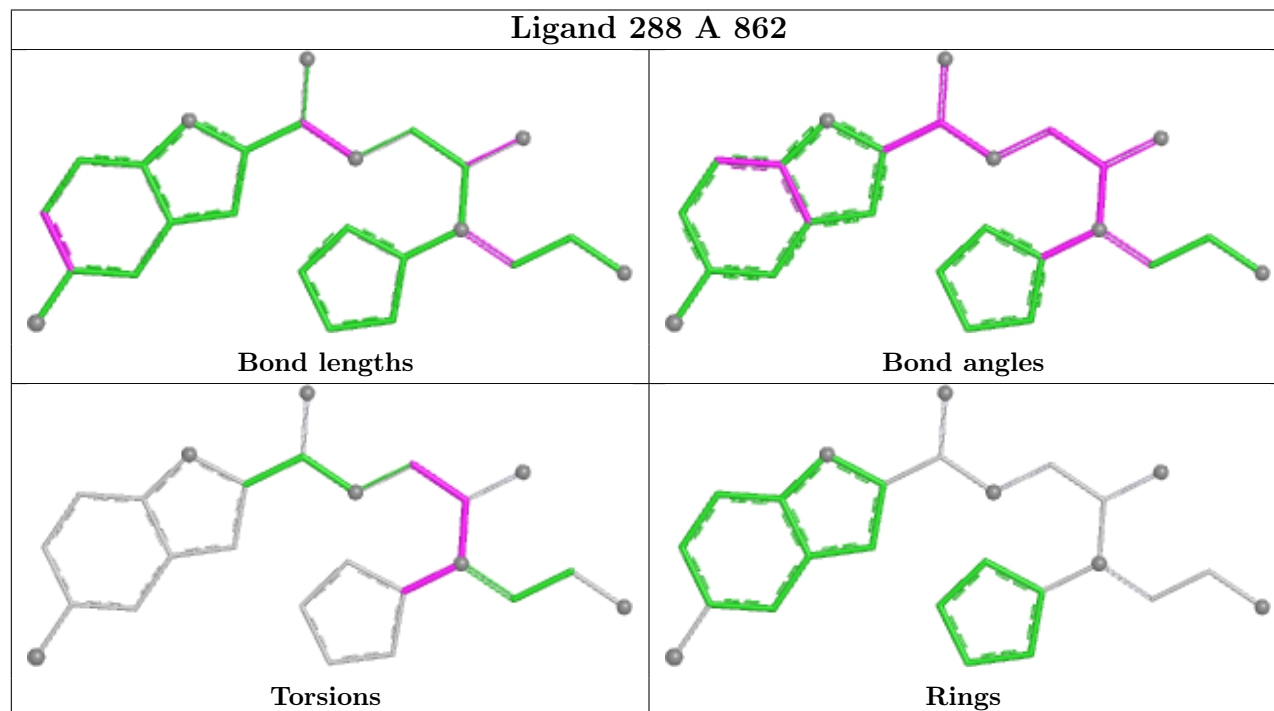
There are no ring outliers.

2 monomers are involved in 4 short contacts:

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