wwPDB X-ray Structure Validation Summary Report (i)

Feb 5, 2024 – 02:10 AM EST

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 (i) 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 (1)) were used in the production of this report:

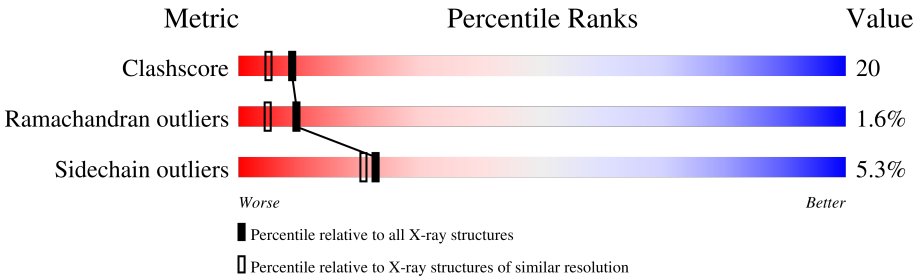
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	846	64% 28% • 5%
1	B	846	63% 28% • 5%

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

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.

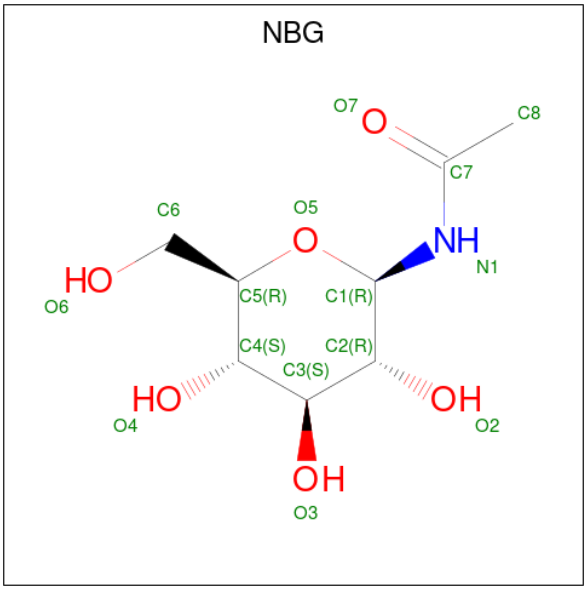
- Molecule 1 is a protein called Glycogen phosphorylase, liver form.

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: $C_8H_{15}NO_6$).



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

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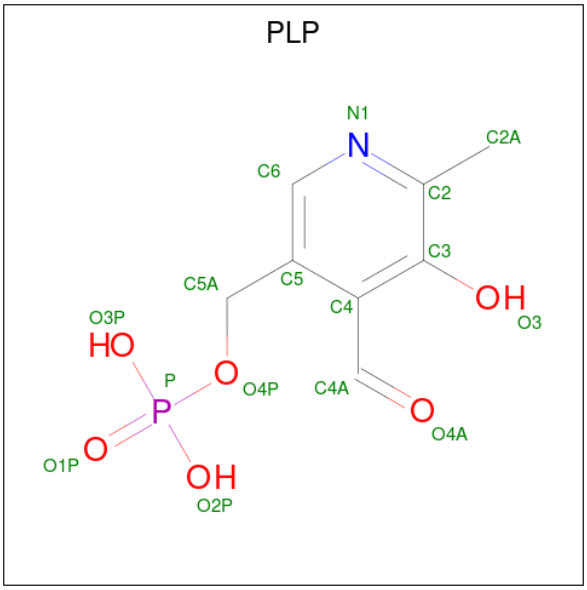
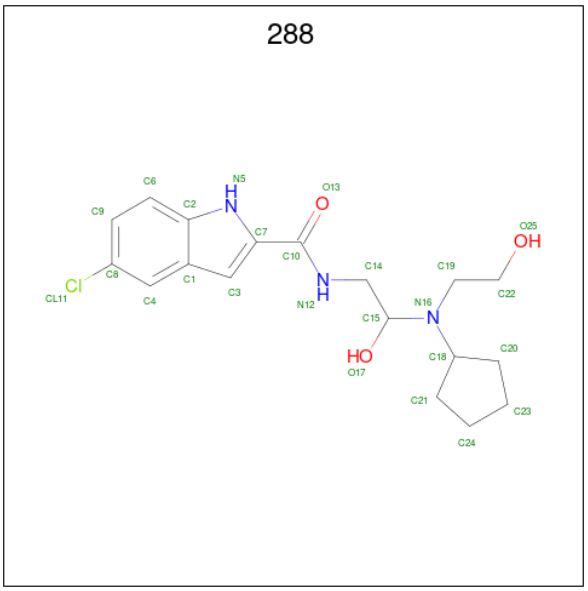
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- 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		

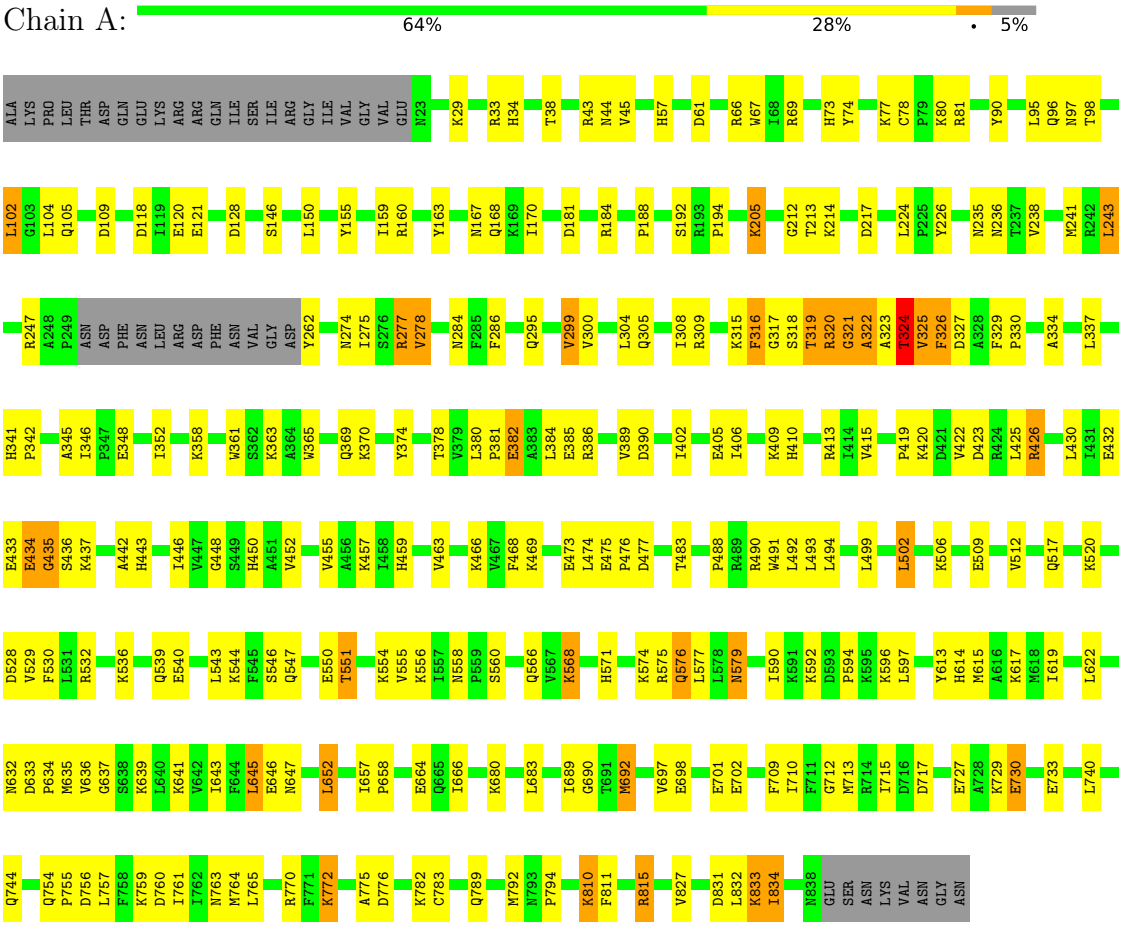
3 Residue-property plots (i)

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.

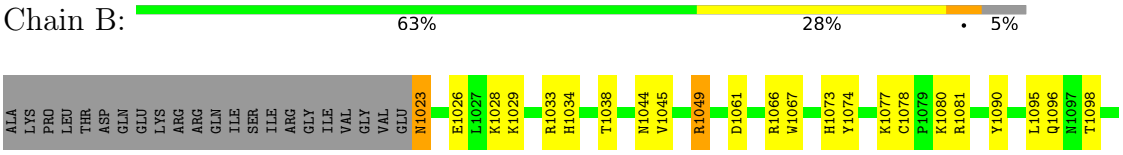
• Molecule 1: Glycogen phosphorylase, liver form

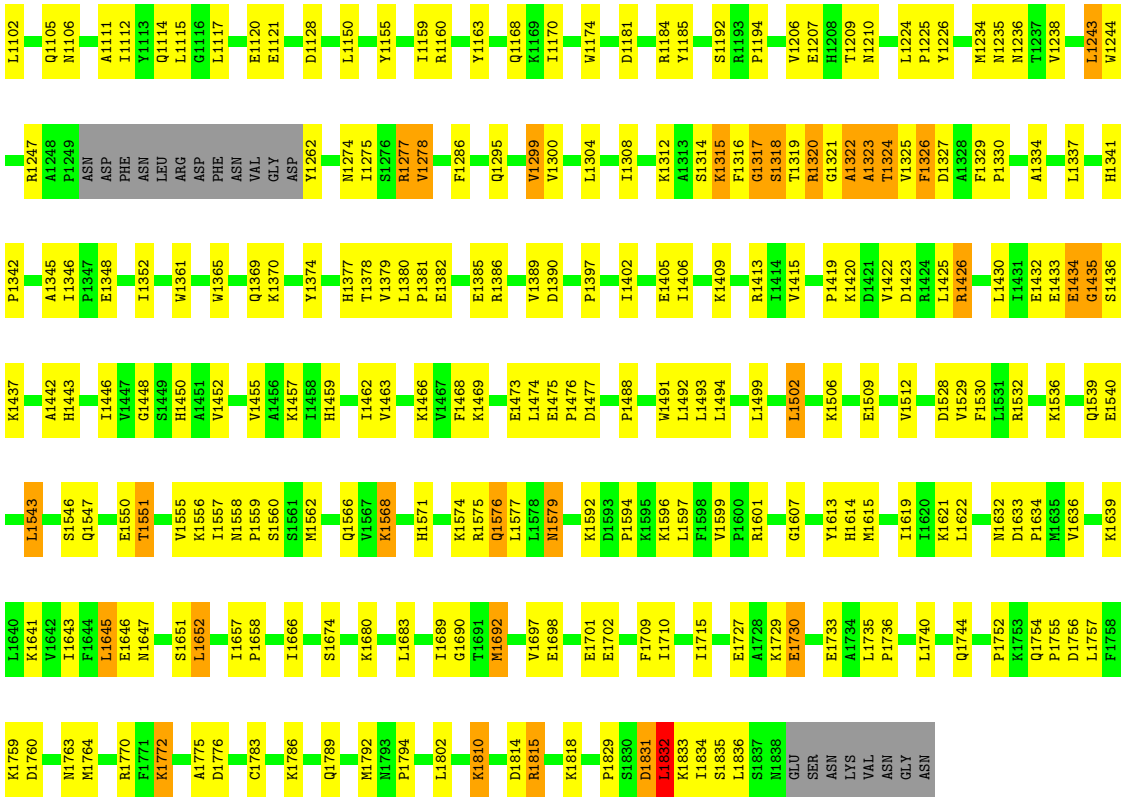
Chain A:



• Molecule 1: Glycogen phosphorylase, liver form

Chain B:




L1102 Q1105 N1106 A1111 I1112 Y1113 Q1114 L1115 G1116 L1117 E1120 E1121 D1128 L1150 Y1155 I1159 R1160 Y1163 Q1168 K1169 I1170 W1174 D1181 R1184 Y1185 S1192 R1193 P1194 V1206 E1207 H1208 T1209 N1210 L1224 P1225 Y1226 M1234 N1235 N1236 T1237 V1238 L1243 W1244
R1247 A1248 P1249 ASN ASP PHE ASN LEU ARG ASP PHE ASN VAL GLY ASP Y1262 N1274 I1275 S1276 R1277 V1278 F1286 Q1295 V1299 V1300 L1304 I1308 K1312 A1313 S1314 K1315 F1316 G1317 S1318 T1319 R1320 G1321 A1322 A1323 T1324 V1325 F1326 D1327 A1328 F1329 P1330 A1334 L1337 H1341
P1342 A1345 I1346 P1347 E1348 I1352 W1361 W1365 Q1369 K1370 Y1374 H1377 T1378 V1379 L1380 P1381 E1382 E1385 R1386 V1389 D1390 P1397 I1402 E1405 I1406 K1409 R1413 I1414 V1415 P1419 K1420 D1421 V1422 D1423 R1424 L1425 R1426 L1430 I1431 E1432 E1433 E1434 G1435 S1436
K1437 A1442 H1443 I1446 V1447 G1448 S1449 H1450 A1451 V1452 V1455 A1456 K1457 I1458 H1459 I1462 V1463 K1466 V1467 F1468 K1469 E1473 L1474 E1475 P1476 D1477 P1488 W1491 L1492 L1493 L1494 L1499 L1502 K1506 E1509 V1512 D1528 V1529 F1530 L1531 R1532 K1536 Q1539 E1540
L1543 S1546 Q1547 E1550 T1551 V1555 K1556 I1557 N1558 P1559 S1560 S1561 M1562 Q1566 V1567 K1568 H1571 K1574 R1575 Q1576 L1577 L1578 N1579 K1592 D1593 P1594 K1595 K1596 L1597 F1598 V1599 P1600 R1601 G1607 Y1613 H1614 M1615 I1619 I1620 K1621 L1622 N1632 D1633 P1634 M1635 V1636 K1639
L1640 K1641 V1642 I1643 F1644 L1645 E1646 N1647 S1651 L1652 I1657 P1658 I1666 S1674 K1680 L1683 I1689 G1690 T1691 M1692 V1697 E1698 E1701 E1702 F1709 I1710 I1715 E1727 A1728 K1729 E1730 E1733 A1734 L1735 P1736 L1740 Q1744 P1752 K1753 Q1754 P1755 D1756 L1757 F1758
K1759 D1760 N1763 M1764 R1770 F1771 K1772 A1775 D1776 C1783 K1786 Q1789 M1792 N1793 P1794 L1802 K1810 D1814 R1815 K1818 P1829 S1830 D1831 L1832 K1833 I1834 S1835 L1836 S1837 N1838 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	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: PLP, 288, NBG

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(^{o})	Ideal(^{o})
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

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:CD	1:B:1434:GLU:H	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:H	1:A:434:GLU:CD	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	B	1543	LEU
1	B	1810	LYS
1	B	1568	LYS
1	B	1645	LEU
1	A	568	LYS

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

Mol	Chain	Res	Type
1	B	1023	ASN
1	B	1614	HIS
1	B	1106	ASN
1	B	1579	ASN
1	B	1481	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	$\#\|Z\| > 2$
3	PLP	B	1860	-	15,15,16	2.42	3 (20%)	20,22,23	1.30	1 (5%)
3	PLP	A	860	-	15,15,16	2.49	6 (40%)	20,22,23	1.31	2 (10%)
2	NBG	A	861	-	15,15,15	1.48	3 (20%)	21,21,21	1.37	2 (9%)
2	NBG	B	1861	-	15,15,15	1.74	3 (20%)	21,21,21	1.32	2 (9%)
4	288	B	1862	-	24,27,27	2.44	3 (12%)	29,37,37	1.60	5 (17%)
4	288	A	862	-	24,27,27	2.40	4 (16%)	29,37,37	1.70	6 (20%)

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	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
2	NBG	B	1861	-	-	0/6/26/26	0/1/1/1
4	288	B	1862	-	1/1/4/5	3/15/27/27	0/3/3/3
4	288	A	862	-	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(^{o})	Ideal(^{o})
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.

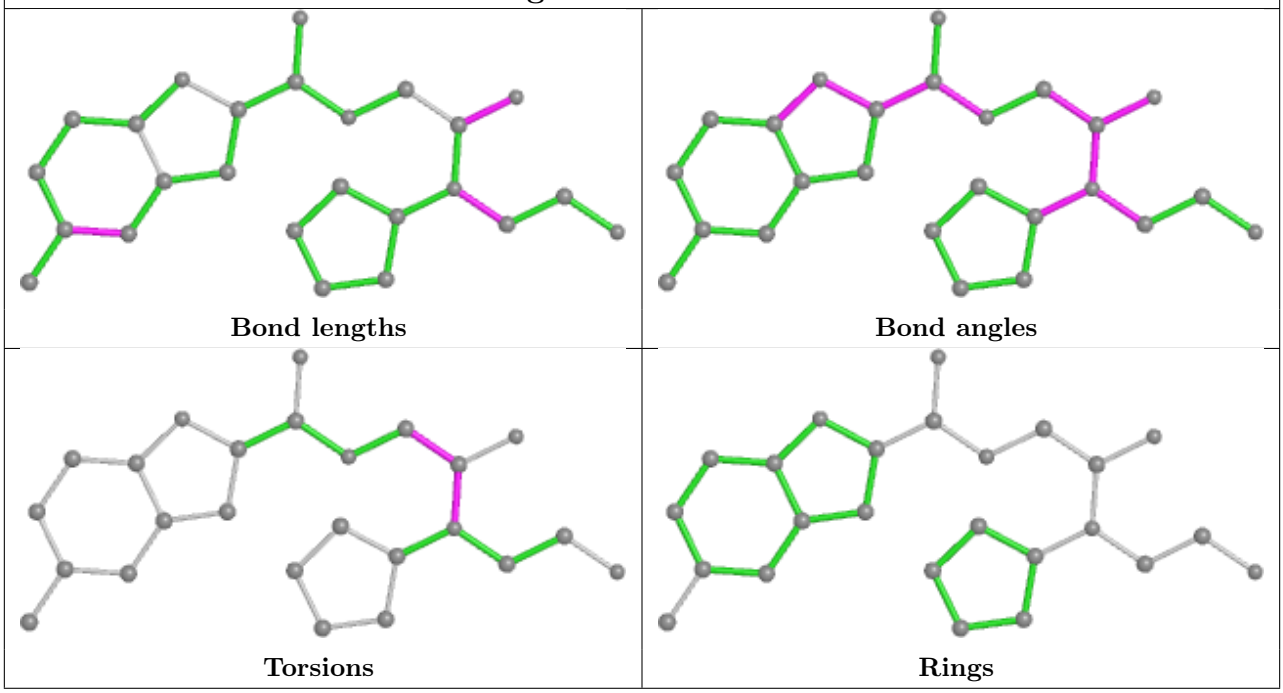
2 monomers are involved in 4 short contacts:

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

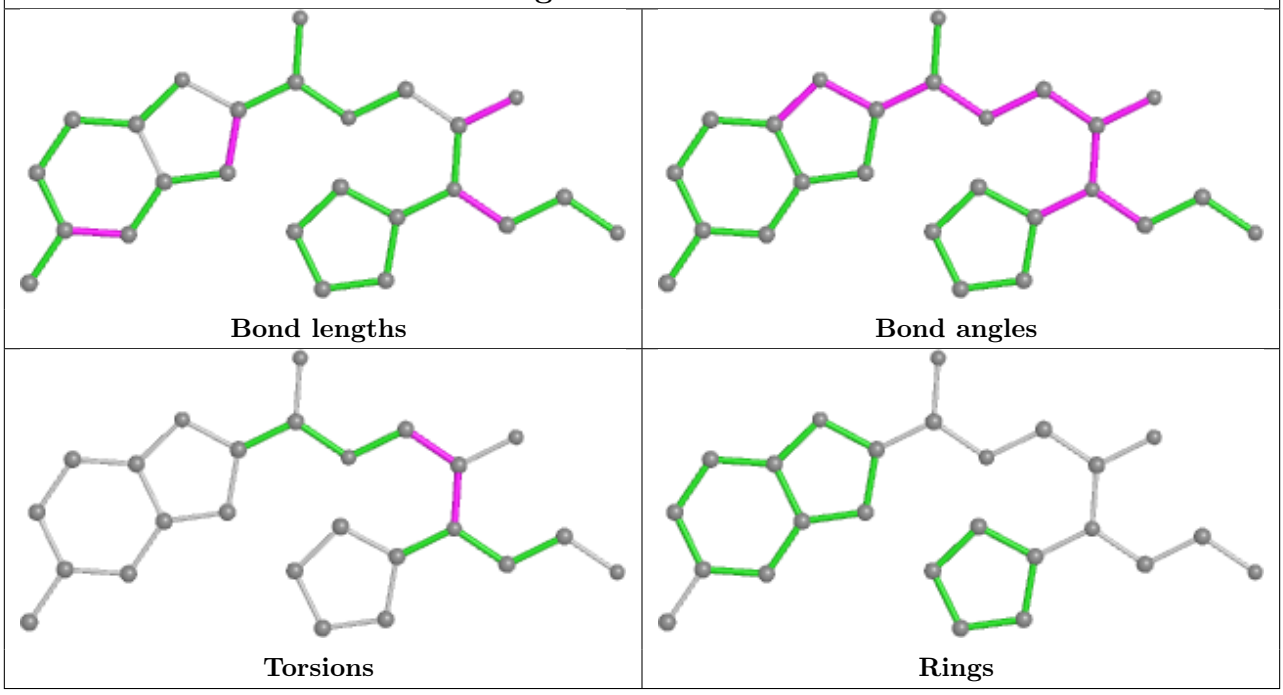
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 288 B 1862



Ligand 288 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

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.