wwPDB X-ray Structure Validation Summary Report (i)

Aug 3, 2023 – 07:29 AM EDT

PDB ID	:	1FC0
Title	:	HUMAN LIVER GLYCOGEN PHOSPHORYLASE COMPLEXED WITH N -ACETYL-BETA-D-GLUCOPYRANOSYLAMINE
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Deposited on	:	2000-07-17
Resolution	:	2.40 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:

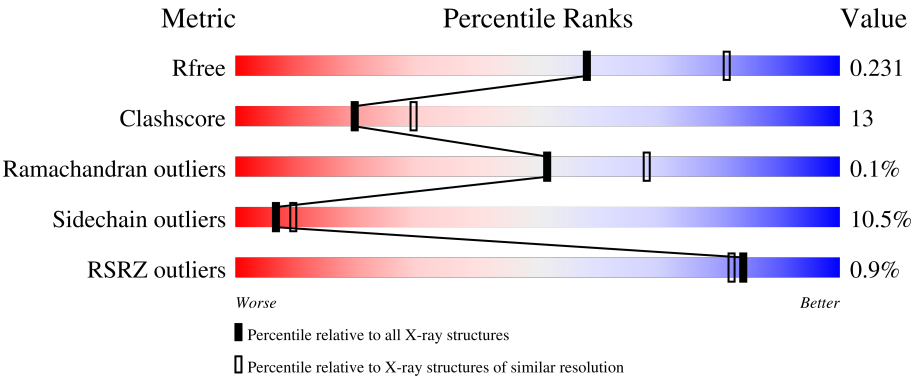
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.40 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))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	846	63% 27% 6%
1	B	846	62% 28% 6%

2 Entry composition (i)

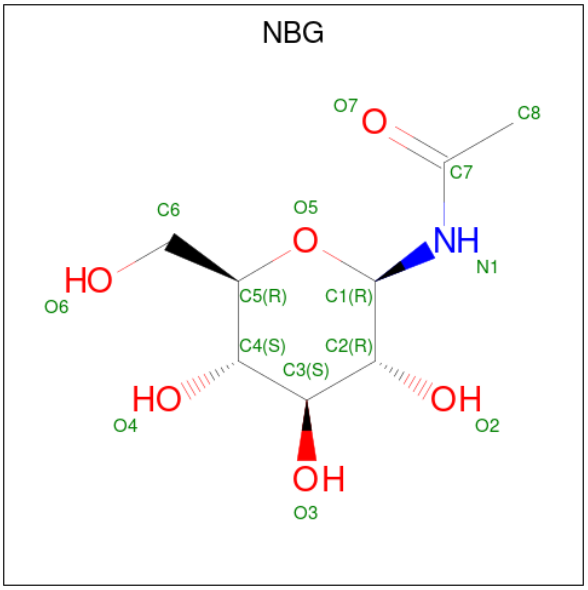
There are 4 unique types of molecules in this entry. The entry contains 13169 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

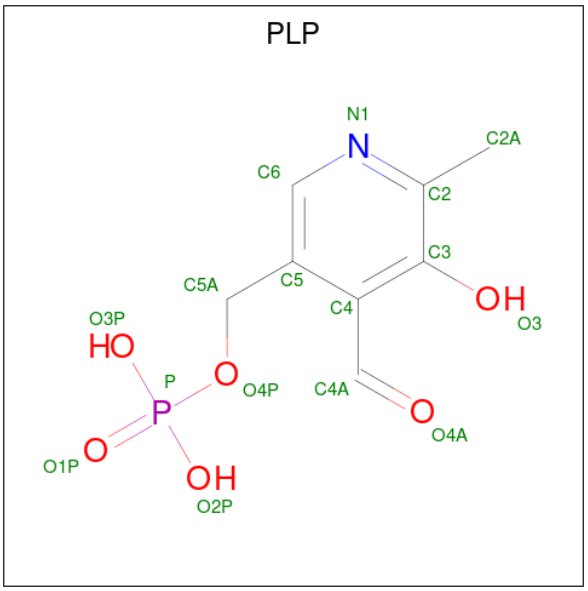
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	792	Total	C	N	O	S	0	0	0
			6425	4129	1090	1177	29			
1	B	793	Total	C	N	O	S	0	0	0
			6429	4131	1091	1178	29			

- 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 15 8 1 5 1	0	0
3	B	1	Total C N O P 15 8 1 5 1	0	0

- Molecule 4 is water.

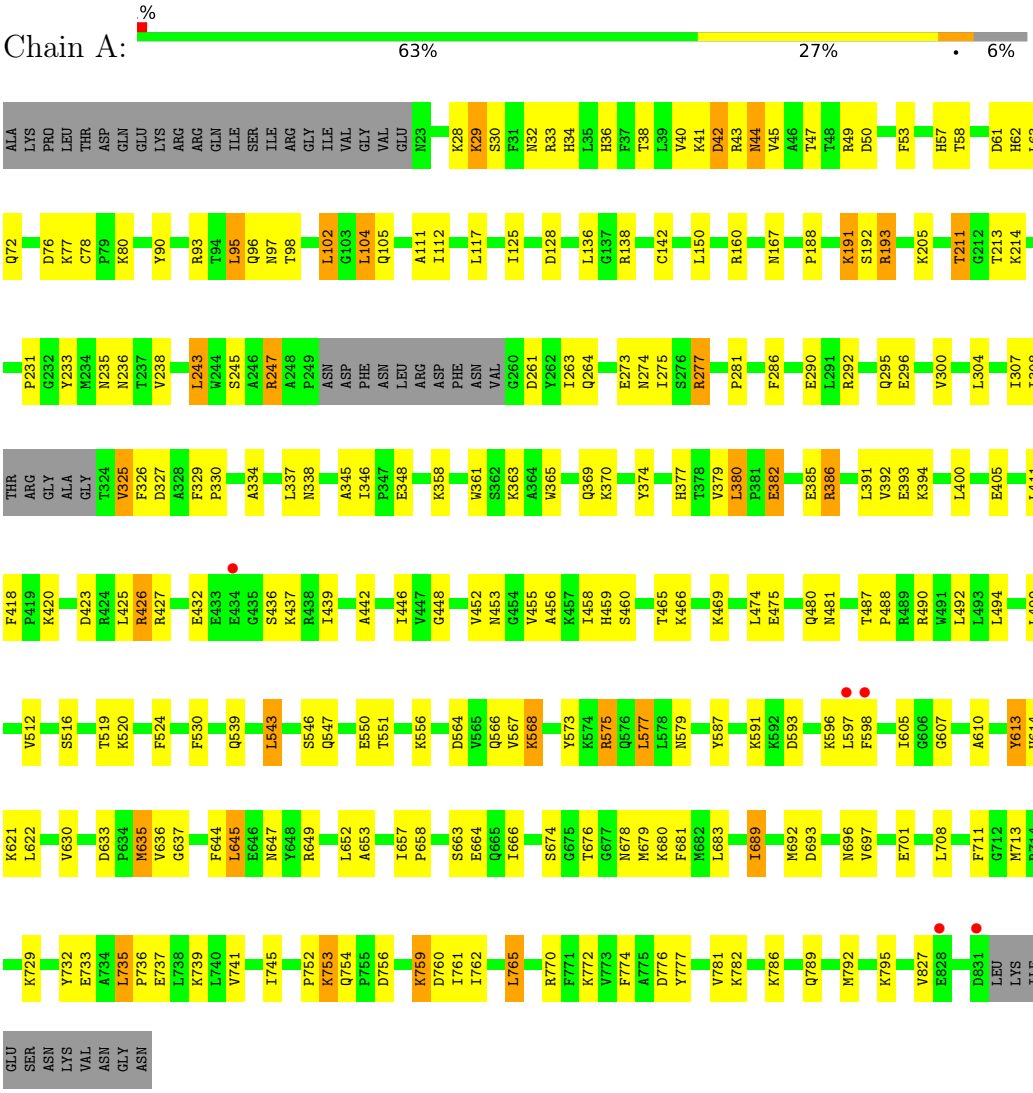
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	151	Total O 151 151	0	0
4	B	104	Total O 104 104	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

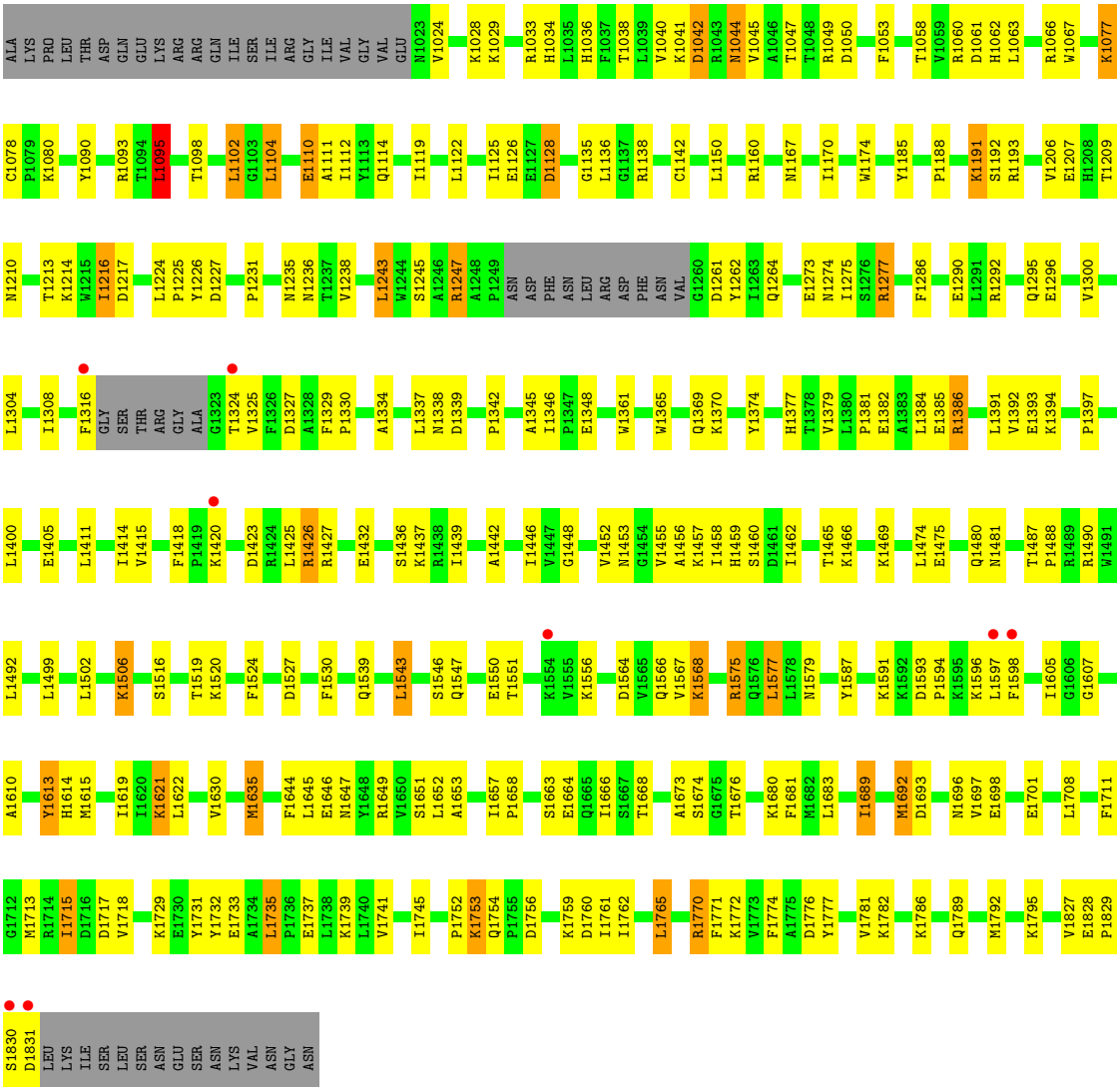
• Molecule 1: GLYCOGEN PHOSPHORYLASE, LIVER FORM

Chain A:



• Molecule 1: GLYCOGEN PHOSPHORYLASE, LIVER FORM

Chain B:


ALA LYS PRO LEU THR ASP GLN GLU LYS ARG ARG GLN ILE SER ILE ARG GLY ILE VAL GLY VAL GLU N1023 V1024 K1028 K1029 R1033 H1034 L1035 H1036 F1037 T1038 L1039 V1040 K1041 D1042 R1043 N1044 V1045 A1046 T1047 T1048 R1049 D1050 F1053 T1058 W1059 R1060 D1061 H1062 L1063 R1066 W1067 K1077
C1078 P1079 K1080 Y1090 R1093 T1094 L1095 T1098 L1102 G1103 L1104 E1110 A1111 I1112 Y1113 Q1114 I1119 L1122 I1125 E1126 E1127 D1128 G1135 L1136 G1137 R1138 C1142 L1150 R1160 N1167 I1170 W1174 Y1185 P1188 K1191 S1192 R1193 V1206 E1207 H1208 T1209
N1210 T1213 K1214 W1215 I1216 D1217 L1224 P1225 Y1226 D1227 P1231 N1235 N1236 T1237 V1238 L1243 W1244 S1245 A1246 R1247 A1248 P1249 ASN ASP PHE ASN LEU ARG ASP PHE ASN VAL G1260 D1261 Y1262 I1263 Q1264 E1273 N1274 I1275 S1276 R1277 F1286 E1290 L1291 R1292 Q1295 E1296 V1300
L1304 I1308 F1316 GLY SER THR ARG GLY ALA G1323 T1324 V1325 F1326 D1327 A1328 F1329 P1330 A1334 L1337 N1338 D1339 P1342 A1345 I1346 P1347 E1348 W1361 W1365 Q1369 K1370 Y1374 H1377 T1378 V1379 L1380 P1381 E1382 A1383 L1384 E1385 R1386 L1391 V1392 E1393 K1394 P1397
L1400 E1405 L1411 I1414 V1415 F1418 P1419 K1420 D1423 R1424 L1425 R1426 R1427 E1432 S1436 K1437 R1438 I1439 A1442 I1446 V1447 G1448 V1452 N1453 G1454 V1455 A1456 K1457 I1458 H1459 S1460 D1461 I1462 T1465 K1466 K1469 L1474 E1475 Q1480 N1481 T1487 P1488 R1489 R1490 W1491
L1492 L1499 L1502 K1506 S1516 T1519 K1520 F1524 D1527 F1530 Q1539 L1643 S1546 Q1547 E1550 T1551 K1554 V1555 K1556 D1564 V1565 Q1566 V1567 K1568 R1575 Q1576 L1577 L1578 N1579 Y1587 K1591 K1592 D1593 P1594 K1595 K1596 L1597 F1598 I1605 G1606 G1607
A1610 Y1613 H1614 M1615 I1619 I1620 K1621 L1622 V1630 M1635 F1644 L1645 E1646 N1647 Y1648 R1649 V1650 S1651 L1652 A1653 I1657 P1658 S1663 E1664 Q1665 I1666 S1667 T1668 A1673 S1674 G1675 T1676 K1680 F1681 M1682 L1683 I1689 M1692 D1693 N1696 V1697 E1698 E1701 L1708 F1711
G1712 M1713 R1714 I1715 D1716 D1717 V1718 K1729 E1730 Y1731 Y1732 E1733 A1734 L1735 P1736 E1737 L1738 K1739 L1740 V1741 I1745 P1752 K1753 Q1754 P1755 D1756 K1759 D1760 I1761 I1762 L1765 R1770 F1771 K1772 V1773 F1774 A1775 D1776 Y1777 V1781 K1782 K1786 Q1789 M1792 K1795 V1827 E1828 P1829
S1830 D1831 LEU LYS ILE SER LEU SER ASN GLU SER ASN LYS VAL ASN GLY ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	124.00Å 124.00Å 122.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.40 19.58 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.1 (30.00-2.40) 95.2 (19.58-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.76 (at 2.41Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.235 0.192 , 0.231	Depositor DCC
R_{free} test set	8191 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l 0.082 for h,-h-k,-l 0.033 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13169	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.35	0/6569	0.57	0/8884
1	B	0.34	0/6573	0.56	0/8889
All	All	0.34	0/13142	0.56	0/17773

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	6425	0	6419	154	0
1	B	6429	0	6422	175	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0
3	A	15	0	6	0	0
3	B	15	0	7	0	0
4	A	151	0	0	6	0
4	B	104	0	0	2	0
All	All	13169	0	12884	328	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 13.

The worst 5 of 328 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:1274:ASN:ND2	1:B:1277:ARG:HH11	1.61	0.97
1:B:1713:MET:HB2	1:B:1717:ASP:HB2	1.47	0.95
1:A:547:GLN:O	1:A:551:THR:HG23	1.66	0.95
1:A:713:MET:HB2	1:A:717:ASP:HB2	1.47	0.94
1:A:274:ASN:ND2	1:A:277:ARG:HH11	1.66	0.94

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	786/846 (93%)	739 (94%)	46 (6%)	1 (0%)	51 68
1	B	787/846 (93%)	738 (94%)	48 (6%)	1 (0%)	51 68
All	All	1573/1692 (93%)	1477 (94%)	94 (6%)	2 (0%)	51 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	LEU
1	B	1095	LEU

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	693/739 (94%)	618 (89%)	75 (11%)	6 9
1	B	693/739 (94%)	622 (90%)	71 (10%)	7 10
All	All	1386/1478 (94%)	1240 (90%)	146 (10%)	7 9

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1567	VAL
1	B	1795	LYS
1	B	1579	ASN
1	B	1692	MET
1	A	573	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1044	ASN
1	B	1274	ASN
1	B	1062	HIS
1	B	1167	ASN
1	B	1305	GLN

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)

4 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	1.47	2 (13%)	21,21,21	1.31	3 (14%)
3	PLP	B	1860	1	15,15,16	1.92	4 (26%)	20,22,23	0.99	2 (10%)
2	NBG	A	861	-	15,15,15	1.22	1 (6%)	21,21,21	1.58	4 (19%)
3	PLP	A	860	1	15,15,16	1.86	3 (20%)	20,22,23	1.28	2 (10%)

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
3	PLP	B	1860	1	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1
3	PLP	A	860	1	-	2/6/6/8	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1860	PLP	C4A-C4	-5.47	1.40	1.51
3	A	860	PLP	C4A-C4	-4.36	1.42	1.51
3	A	860	PLP	C3-C2	-3.91	1.37	1.40
2	B	1861	NBG	C2-C1	3.74	1.56	1.52
2	A	861	NBG	C2-C1	3.56	1.56	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	861	NBG	C5-O5-C1	4.73	118.93	112.52
2	B	1861	NBG	C5-O5-C1	3.97	117.90	112.52
2	A	861	NBG	C3-C2-C1	2.78	114.00	109.94
2	A	861	NBG	C2-C1-N1	-2.66	108.19	111.30
2	B	1861	NBG	C3-C2-C1	2.44	113.49	109.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	792/846 (93%)	-0.57	6 (0%)	86	84	15, 31, 57, 101	0
1	B	793/846 (93%)	-0.52	8 (1%)	82	80	16, 32, 60, 101	0
All	All	1585/1692 (93%)	-0.54	14 (0%)	84	82	15, 32, 59, 101	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1831	ASP	4.9
1	B	1316	PHE	4.7
1	A	831	ASP	4.7
1	B	1420	LYS	4.0
1	A	598	PHE	3.7

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NBG	B	1861	15/15	0.96	0.12	17,31,35,38	0
2	NBG	A	861	15/15	0.98	0.11	14,23,31,32	0
3	PLP	B	1860	15/16	0.98	0.09	14,19,31,34	0
3	PLP	A	860	15/16	0.99	0.09	3,13,26,31	0

6.5 Other polymers (i)

There are no such residues in this entry.