Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:23 PM GMT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/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:

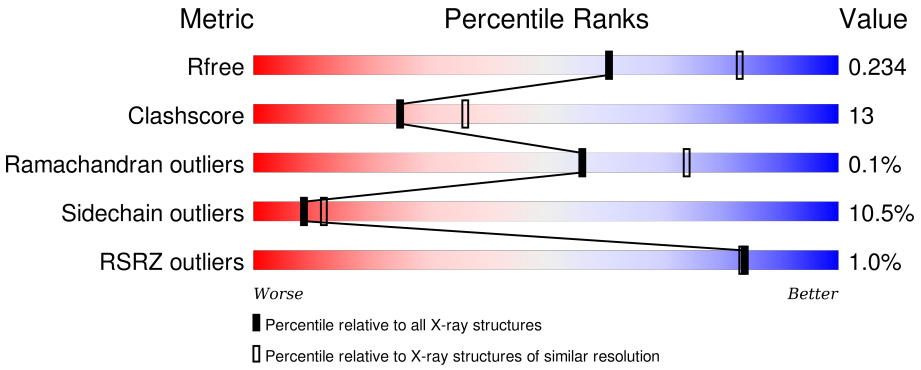
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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

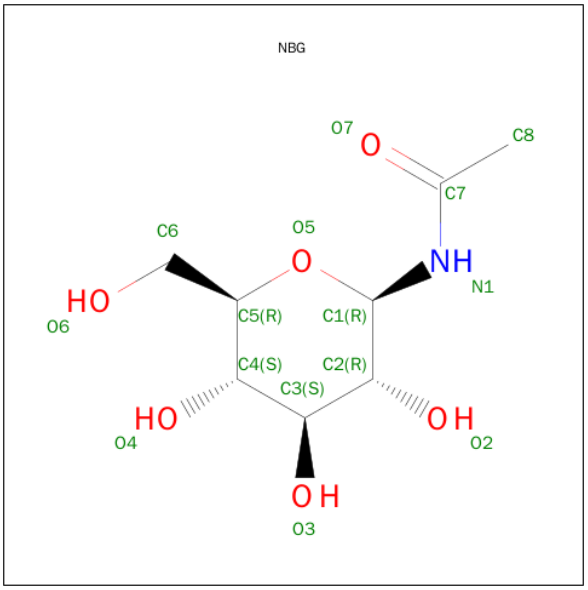
There are 4 unique types of molecules in this entry. The entry contains 13169 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

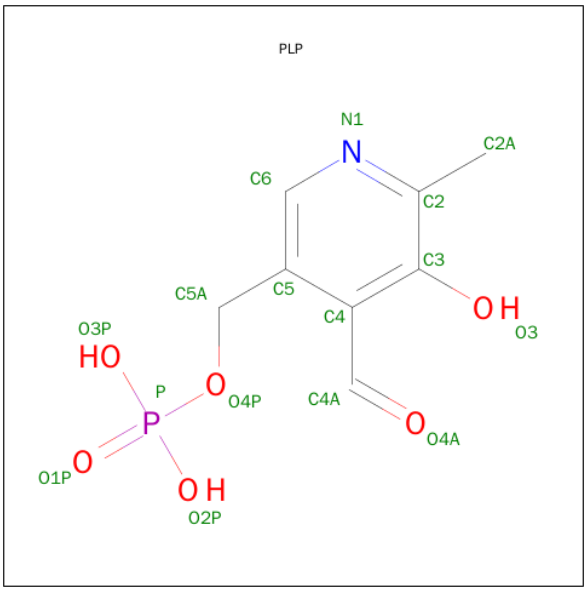
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	792	Total	C	N	O	S	0	0	0
			6425	4129	1090	1177	29			
1	B	793	Total	C	N	O	S	0	0	0
			6429	4131	1091	1178	29			

- Molecule 2 is SUGAR (1-N-ACETYL-BETA-D-GLUCOSAMINE) (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	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 water.

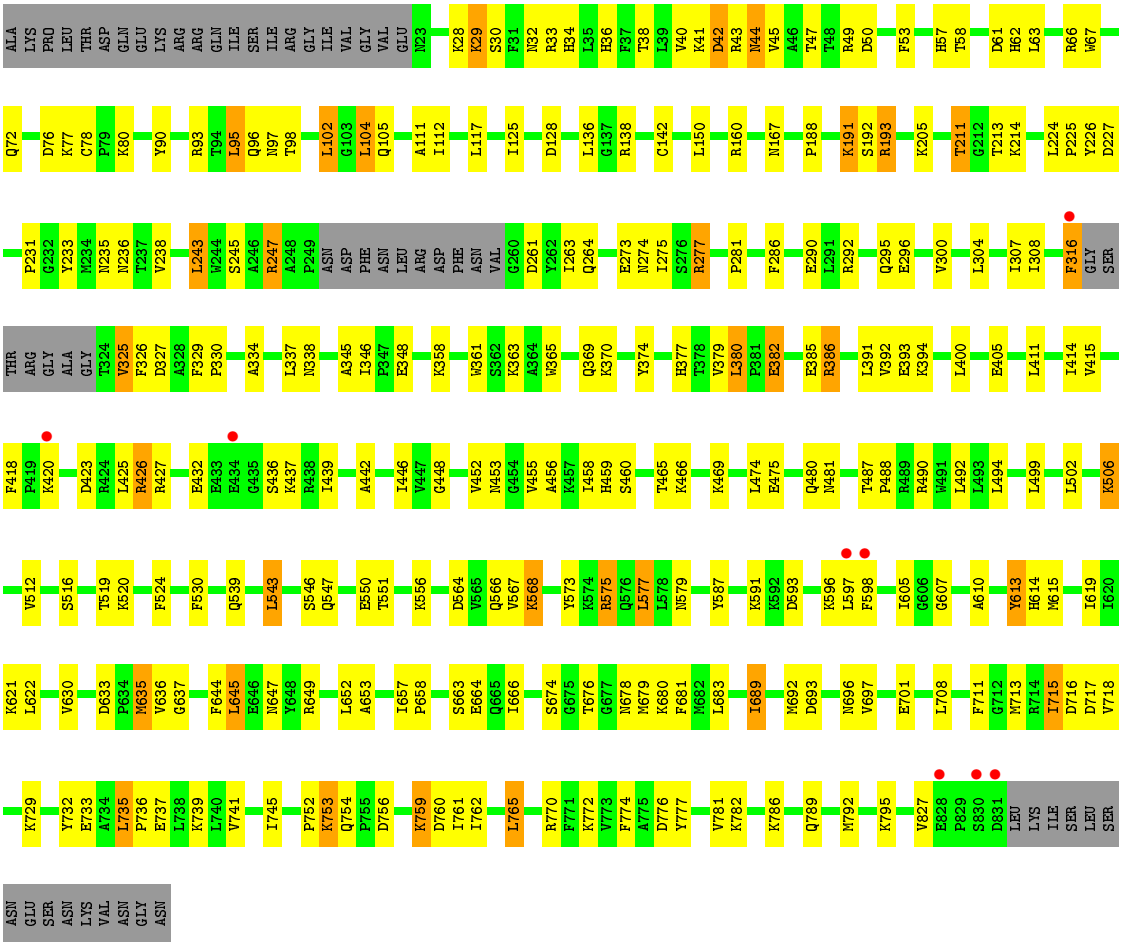
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total	O	0	0
			151	151		
4	B	104	Total	O	0	0
			104	104		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

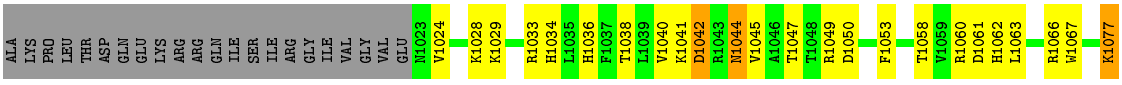
- Molecule 1: GLYCOGEN PHOSPHORYLASE, LIVER FORM

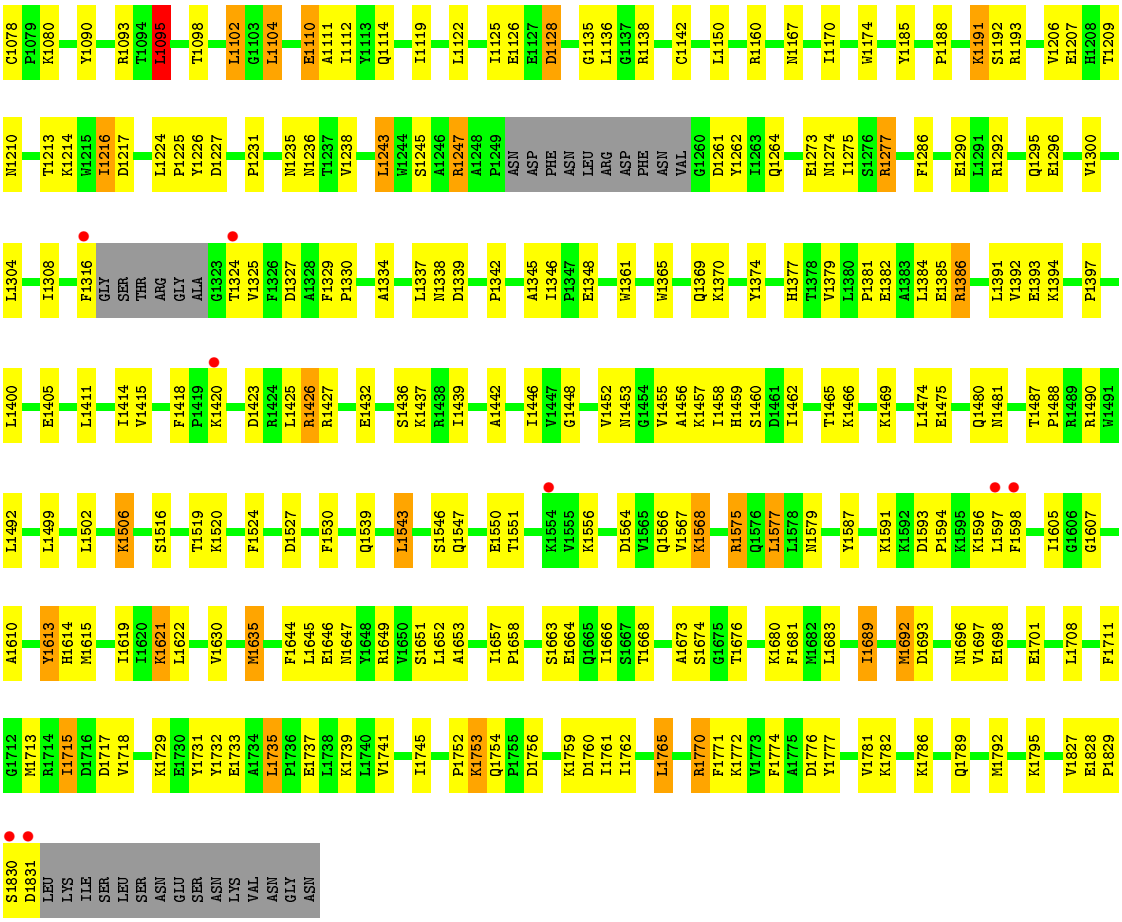
Chain A:



- Molecule 1: GLYCOGEN PHOSPHORYLASE, LIVER FORM

Chain B:




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 Y1447 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 L1543 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 0.5	Depositor
R, R_{free}	0.198 , 0.235 0.195 , 0.234	Depositor DCC
R_{free} test set	7804 reflections (10.00%)	DCC
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 , 32.9	EDS
Estimated twinning fraction	0.025 for -h,-k,l 0.082 for h,-h-k,-l 0.033 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 81694 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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.

All (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
1:B:1274:ASN:HD22	1:B:1277:ARG:HH11	1.16	0.93
1:B:1547:GLN:O	1:B:1551:THR:HG23	1.69	0.93
1:A:274:ASN:HD22	1:A:277:ARG:HH11	1.20	0.89
1:B:1411:LEU:HA	1:B:1414:ILE:HD12	1.54	0.89
1:A:411:LEU:HA	1:A:414:ILE:HD12	1.56	0.86
1:B:1615:MET:HE3	1:B:1761:ILE:HG12	1.58	0.85
1:A:615:MET:HE3	1:A:761:ILE:HG12	1.55	0.85
1:A:42:ASP:HB3	1:A:44:ASN:ND2	1.96	0.81
1:B:1042:ASP:HB3	1:B:1044:ASN:ND2	1.97	0.78
1:B:1752:PRO:HB2	1:B:1753:LYS:HE2	1.69	0.74
1:A:752:PRO:HB2	1:A:753:LYS:HE2	1.70	0.72
1:A:224:LEU:HD12	1:A:225:PRO:HD2	1.72	0.70
1:B:1224:LEU:HD12	1:B:1225:PRO:HD2	1.72	0.70
1:A:93:ARG:O	1:A:490:ARG:NH2	2.25	0.69
1:B:1207:GLU:HG2	1:B:1209:THR:HG23	1.74	0.69
1:B:1329:PHE:HB3	1:B:1330:PRO:HD3	1.74	0.69
1:A:506:LYS:HD3	1:A:524:PHE:CE2	2.28	0.68
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.75	0.68
1:B:1235:ASN:O	1:B:1236:ASN:HB2	1.91	0.68
1:B:1160:ARG:HB2	1:B:1243:LEU:HB3	1.74	0.68
1:B:1170:ILE:CG1	1:B:1646:GLU:HG3	2.24	0.68
1:B:1029:LYS:HB3	1:B:1033:ARG:NH2	2.10	0.67
1:A:653:ALA:O	1:A:657:ILE:HG13	1.95	0.67
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.75	0.67
1:B:1653:ALA:O	1:B:1657:ILE:HG13	1.95	0.67
1:B:1591:LYS:HD2	1:B:1635:MET:HG2	1.77	0.67
1:B:1128:ASP:OD2	1:B:1651:SER:HB3	1.94	0.67
1:B:1506:LYS:HD3	1:B:1524:PHE:CE2	2.30	0.67
1:A:566:GLN:HA	4:A:2108:HOH:O	1.94	0.66
1:A:235:ASN:O	1:A:236:ASN:HB2	1.94	0.66
1:B:1049:ARG:NH2	1:B:1185:TYR:HB3	2.11	0.66
1:B:1292:ARG:O	1:B:1296:GLU:HG3	1.96	0.66
1:B:1615:MET:HE1	1:B:1761:ILE:HA	1.78	0.65
1:A:591:LYS:HD2	1:A:635:MET:HG2	1.77	0.65
1:B:1206:VAL:HG23	1:B:1397:PRO:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ARG:O	1:A:296:GLU:HG3	1.96	0.65
1:A:615:MET:HE1	1:A:761:ILE:HA	1.79	0.65
1:B:1170:ILE:HG13	1:B:1646:GLU:HG3	1.79	0.65
1:B:1777:TYR:O	1:B:1781:VAL:HG23	1.98	0.63
1:A:777:TYR:O	1:A:781:VAL:HG23	1.99	0.62
1:A:29:LYS:HB3	1:A:33:ARG:NH2	2.13	0.62
1:B:1042:ASP:HB3	1:B:1044:ASN:HD21	1.65	0.62
1:A:455:VAL:H	1:A:459:HIS:HD2	1.47	0.62
1:B:1455:VAL:H	1:B:1459:HIS:HD2	1.46	0.61
1:A:290:GLU:HG3	1:A:391:LEU:HD11	1.83	0.61
1:A:96:GLN:HG2	1:A:494:LEU:HG	1.82	0.61
1:B:1275:ILE:O	1:B:1295:GLN:HG2	2.00	0.60
1:A:42:ASP:HB3	1:A:44:ASN:HD21	1.65	0.60
1:B:1566:GLN:HB2	1:B:1664:GLU:HB2	1.83	0.60
1:B:1034:HIS:HD2	1:B:1038:THR:OG1	1.83	0.60
1:A:275:ILE:O	1:A:295:GLN:HG2	2.02	0.59
1:A:488:PRO:O	1:A:492:LEU:HB3	2.02	0.59
1:B:1098:THR:HG22	1:B:1102:LEU:HD22	1.84	0.59
1:A:274:ASN:HD22	1:A:277:ARG:HD2	1.68	0.59
1:B:1539:GLN:HE21	1:B:1543:LEU:HD12	1.68	0.59
1:B:1024:VAL:HG22	1:B:1110:GLU:HB3	1.83	0.59
1:A:539:GLN:HE21	1:A:543:LEU:HD12	1.68	0.58
1:A:80:LYS:HB3	1:A:827:VAL:HG12	1.85	0.58
1:B:1290:GLU:HG3	1:B:1391:LEU:HD11	1.84	0.58
1:B:1693:ASP:O	1:B:1696:ASN:HB2	2.03	0.58
1:B:1488:PRO:O	1:B:1492:LEU:HB3	2.04	0.58
1:B:1575:ARG:HD3	1:B:1666:ILE:O	2.03	0.58
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.85	0.58
1:B:1274:ASN:HD22	1:B:1277:ARG:HD2	1.69	0.58
1:B:1346:ILE:HD13	1:B:1448:GLY:HA3	1.85	0.58
1:A:575:ARG:HD3	1:A:666:ILE:O	2.03	0.58
1:A:693:ASP:O	1:A:696:ASN:HB2	2.04	0.57
1:B:1411:LEU:HD23	1:B:1414:ILE:CD1	2.35	0.57
1:A:697:VAL:O	1:A:701:GLU:HG3	2.05	0.57
1:A:566:GLN:HB2	1:A:664:GLU:HB2	1.85	0.57
1:A:615:MET:CE	1:A:761:ILE:HA	2.36	0.56
1:B:1615:MET:CE	1:B:1761:ILE:HA	2.36	0.56
1:B:1432:GLU:O	1:B:1437:LYS:HA	2.06	0.56
1:A:393:GLU:HB2	1:A:400:LEU:CD2	2.35	0.56
1:B:1713:MET:HB2	1:B:1717:ASP:CB	2.30	0.56
1:A:96:GLN:NE2	1:A:105:GLN:HE22	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ALA:O	1:A:446:ILE:HG13	2.06	0.56
1:B:1024:VAL:CG2	1:B:1110:GLU:HB3	2.37	0.55
1:B:1575:ARG:NH2	1:B:1776:ASP:HB2	2.22	0.55
1:B:1193:ARG:NH1	1:B:1227:ASP:OD1	2.40	0.55
1:B:1697:VAL:O	1:B:1701:GLU:HG3	2.06	0.55
1:A:346:ILE:HD13	1:A:448:GLY:HA3	1.89	0.55
1:B:1080:LYS:HE2	1:B:1334:ALA:HB2	1.88	0.55
1:B:1338:ASN:OD1	1:B:1377:HIS:NE2	2.40	0.55
1:B:1122:LEU:O	1:B:1125:ILE:HB	2.07	0.55
1:B:1216:ILE:HD12	1:B:1217:ASP:OD2	2.06	0.55
1:B:1506:LYS:HD2	1:B:1530:PHE:CD1	2.41	0.55
1:B:1053:PHE:HE1	1:B:1188:PRO:HD3	1.71	0.55
1:B:1174:TRP:CZ2	1:B:1621:LYS:HG3	2.42	0.55
1:B:1261:ASP:OD1	1:B:1264:GLN:HB2	2.07	0.55
1:A:732:TYR:CE1	1:A:739:LYS:HG3	2.43	0.54
1:A:316:PHE:CZ	1:A:325:VAL:HB	2.41	0.54
1:B:1324:THR:HG22	1:B:1325:VAL:N	2.22	0.54
1:A:411:LEU:HD23	1:A:414:ILE:CD1	2.37	0.54
1:B:1029:LYS:HB3	1:B:1033:ARG:HH21	1.72	0.54
1:A:53:PHE:HE1	1:A:188:PRO:HD3	1.72	0.54
1:A:432:GLU:O	1:A:437:LYS:HA	2.06	0.54
1:B:1170:ILE:HG12	1:B:1646:GLU:HG3	1.89	0.54
1:B:1462:ILE:HD11	1:B:1715:ILE:HD13	1.90	0.54
1:A:506:LYS:HD2	1:A:530:PHE:CD1	2.43	0.53
1:A:575:ARG:NH2	1:A:776:ASP:HB2	2.22	0.53
1:B:1192:SER:HB3	1:B:1226:TYR:CE1	2.43	0.53
1:B:1093:ARG:O	1:B:1490:ARG:NH2	2.37	0.53
1:B:1393:GLU:HB2	1:B:1400:LEU:CD2	2.39	0.53
1:B:1286:PHE:CD1	1:B:1385:GLU:HG2	2.44	0.53
1:A:713:MET:HB2	1:A:717:ASP:CB	2.30	0.53
1:B:1415:VAL:HG22	1:B:1425:LEU:HD11	1.91	0.53
1:A:465:THR:O	1:A:469:LYS:HB2	2.09	0.53
1:A:415:VAL:HG22	1:A:425:LEU:HD11	1.91	0.53
1:B:1274:ASN:ND2	1:B:1277:ARG:NH1	2.45	0.52
1:B:1732:TYR:CE1	1:B:1739:LYS:HG3	2.44	0.52
1:B:1465:THR:O	1:B:1469:LYS:HB2	2.10	0.52
1:A:649:ARG:HH11	1:A:649:ARG:HG2	1.75	0.52
1:B:1274:ASN:ND2	1:B:1277:ARG:HD2	2.24	0.52
1:B:1593:ASP:CG	1:B:1596:LYS:HB2	2.30	0.52
1:A:98:THR:HG22	1:A:102:LEU:HD22	1.91	0.52
1:A:593:ASP:CG	1:A:596:LYS:HB2	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1649:ARG:HG2	1:B:1649:ARG:HH11	1.75	0.52
1:A:316:PHE:CE1	1:A:325:VAL:HB	2.45	0.51
1:A:737:GLU:O	1:A:741:VAL:HG23	2.11	0.51
1:B:1411:LEU:HD23	1:B:1414:ILE:HD13	1.91	0.51
1:B:1415:VAL:HG23	1:B:1425:LEU:HD21	1.93	0.51
1:A:47:THR:H	1:A:50:ASP:HB2	1.76	0.51
1:A:415:VAL:HG23	1:A:425:LEU:HD21	1.92	0.51
1:B:1442:ALA:O	1:B:1446:ILE:HG13	2.10	0.51
1:B:1737:GLU:O	1:B:1741:VAL:HG23	2.11	0.51
1:A:274:ASN:ND2	1:A:277:ARG:HD2	2.25	0.51
1:A:167:ASN:ND2	1:A:647:ASN:HD21	2.09	0.51
1:B:1036:HIS:O	1:B:1040:VAL:HA	2.11	0.51
1:A:261:ASP:OD1	1:A:264:GLN:HB2	2.11	0.51
1:B:1028:LYS:HE2	1:B:1114:GLN:NE2	2.26	0.51
1:B:1300:VAL:HG13	1:B:1345:ALA:HA	1.92	0.51
1:A:80:LYS:HE2	1:A:334:ALA:HB2	1.92	0.50
1:A:307:ILE:HG23	4:A:2226:HOH:O	2.10	0.50
1:B:1382:GLU:CD	1:B:1770:ARG:HH22	2.15	0.50
1:A:325:VAL:CG2	1:A:326:PHE:N	2.74	0.50
1:B:1361:TRP:CH2	1:B:1405:GLU:HB3	2.46	0.50
1:B:1216:ILE:HD12	1:B:1217:ASP:CG	2.31	0.50
1:A:47:THR:O	1:A:50:ASP:HB2	2.12	0.50
1:A:97:ASN:HA	1:A:494:LEU:HD12	1.94	0.50
1:A:281:PRO:HG3	1:B:1262:TYR:CE2	2.46	0.50
1:A:192:SER:HB3	1:A:226:TYR:CE1	2.47	0.50
1:A:286:PHE:CD1	1:A:385:GLU:HG2	2.46	0.49
1:A:330:PRO:HB3	1:A:370:LYS:HB3	1.93	0.49
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.95	0.49
1:B:1047:THR:O	1:B:1050:ASP:HB2	2.11	0.49
1:A:689:ILE:O	1:A:689:ILE:HG23	2.13	0.49
1:B:1575:ARG:HH22	1:B:1776:ASP:CG	2.14	0.49
1:A:136:LEU:HD11	1:A:338:ASN:OD1	2.13	0.49
1:A:36:HIS:O	1:A:40:VAL:HA	2.12	0.49
1:B:1568:LYS:O	1:B:1607:GLY:HA3	2.12	0.49
1:A:193:ARG:HD2	1:A:227:ASP:OD1	2.13	0.49
1:A:263:ILE:HG12	4:A:2177:HOH:O	2.12	0.49
1:A:29:LYS:HB3	1:A:33:ARG:HH21	1.77	0.49
1:A:789:GLN:O	1:A:792:MET:HB2	2.13	0.49
1:B:1047:THR:H	1:B:1050:ASP:HB2	1.78	0.49
1:A:58:THR:O	1:A:62:HIS:HD2	1.96	0.49
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:LYS:O	1:A:607:GLY:HA3	2.13	0.49
1:B:1330:PRO:HB3	1:B:1370:LYS:HB3	1.94	0.48
1:A:142:CYS:SG	1:A:487:THR:HG22	2.53	0.48
1:A:28:LYS:HG2	1:A:111:ALA:HB1	1.94	0.48
1:B:1058:THR:O	1:B:1062:HIS:HD2	1.97	0.48
1:A:411:LEU:HD23	1:A:414:ILE:HD13	1.95	0.48
1:B:1174:TRP:CH2	1:B:1621:LYS:HG3	2.48	0.48
1:B:1455:VAL:H	1:B:1459:HIS:CD2	2.29	0.48
1:B:1689:ILE:O	1:B:1689:ILE:HG23	2.13	0.48
1:B:1300:VAL:HG22	1:B:1345:ALA:HB2	1.95	0.48
1:B:1274:ASN:HD22	1:B:1277:ARG:NH1	1.99	0.48
1:A:193:ARG:HH11	1:A:193:ARG:HA	1.78	0.48
1:B:1718:VAL:HG13	1:B:1772:LYS:HE2	1.96	0.48
1:A:605:ILE:O	1:A:644:PHE:HA	2.14	0.48
1:A:753:LYS:O	1:A:754:GLN:HG3	2.14	0.48
1:A:455:VAL:H	1:A:459:HIS:CD2	2.29	0.48
1:A:300:VAL:HG13	1:A:345:ALA:HA	1.95	0.48
1:B:1324:THR:CG2	1:B:1325:VAL:N	2.76	0.48
1:B:1605:ILE:O	1:B:1644:PHE:HA	2.14	0.48
1:A:167:ASN:ND2	4:A:2154:HOH:O	2.46	0.47
1:B:1049:ARG:NH2	1:B:1053:PHE:HE2	2.12	0.47
1:A:300:VAL:HG22	1:A:345:ALA:HB2	1.96	0.47
1:B:1142:CYS:SG	1:B:1487:THR:HG22	2.54	0.47
1:B:1034:HIS:HE1	1:B:1061:ASP:OD2	1.97	0.47
1:A:423:ASP:OD1	1:A:427:ARG:HD3	2.14	0.47
1:A:423:ASP:O	1:A:426:ARG:HG3	2.15	0.47
1:B:1167:ASN:ND2	1:B:1647:ASN:HD21	2.13	0.47
1:B:1247:ARG:HA	1:B:1273:GLU:HG2	1.97	0.47
1:A:380:LEU:HD13	1:A:382:GLU:OE2	2.14	0.47
1:B:1381:PRO:HA	1:B:1384:LEU:CD1	2.45	0.47
1:B:1676:THR:O	1:B:1680:LYS:HG3	2.15	0.47
1:A:759:LYS:HA	1:A:759:LYS:HD3	1.40	0.47
1:B:1459:HIS:HB2	1:B:1673:ALA:O	2.14	0.47
1:A:49:ARG:HG2	4:A:2211:HOH:O	2.14	0.47
1:A:304:LEU:HD12	1:A:348:GLU:CG	2.45	0.47
1:B:1423:ASP:OD1	1:B:1427:ARG:HD3	2.15	0.47
1:B:1066:ARG:CD	1:B:1236:ASN:HA	2.44	0.46
1:B:1692:MET:HG3	1:B:1697:VAL:HG22	1.97	0.46
1:B:1457:LYS:HG3	1:B:1698:GLU:CD	2.36	0.46
1:B:1789:GLN:O	1:B:1792:MET:HB2	2.15	0.46
1:A:456:ALA:HB2	1:A:674:SER:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1577:LEU:HG	1:B:1619:ILE:HG12	1.98	0.46
1:B:1304:LEU:HD12	1:B:1348:GLU:CG	2.46	0.46
1:A:577:LEU:HG	1:A:619:ILE:HG12	1.96	0.46
1:A:41:LYS:HD2	1:A:45:VAL:HG23	1.98	0.46
1:B:1423:ASP:O	1:B:1426:ARG:HG3	2.15	0.46
1:B:1224:LEU:HD12	1:B:1225:PRO:CD	2.45	0.46
1:A:614:HIS:HE1	1:A:760:ASP:OD1	1.99	0.46
1:A:386:ARG:HB2	1:A:386:ARG:HH11	1.81	0.46
1:A:112:ILE:HG23	1:A:117:LEU:HB2	1.97	0.45
1:A:66:ARG:CD	1:A:236:ASN:HA	2.46	0.45
1:A:575:ARG:HH22	1:A:776:ASP:CG	2.16	0.45
1:B:1080:LYS:HB3	1:B:1827:VAL:HG12	1.99	0.45
1:B:1456:ALA:HB2	1:B:1674:SER:HB2	1.99	0.45
1:B:1614:HIS:HE1	1:B:1760:ASP:OD1	1.99	0.45
1:B:1102:LEU:HB3	1:B:1104:LEU:HD23	1.98	0.45
1:B:1828:GLU:HA	1:B:1829:PRO:HD3	1.85	0.45
1:A:587:TYR:CD1	1:A:630:VAL:HG22	2.51	0.45
1:A:63:LEU:HD21	1:A:231:PRO:HB3	1.97	0.45
1:B:1374:TYR:CD2	1:B:1452:VAL:HG13	2.51	0.45
1:A:361:TRP:CH2	1:A:405:GLU:HB3	2.52	0.45
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.99	0.45
1:B:1587:TYR:CD1	1:B:1630:VAL:HG22	2.52	0.45
1:B:1386:ARG:HB2	1:B:1386:ARG:HH11	1.81	0.45
1:B:1049:ARG:HH22	1:B:1185:TYR:HB3	1.80	0.45
1:A:374:TYR:CD2	1:A:452:VAL:HG13	2.52	0.45
1:A:191:LYS:HA	1:A:191:LYS:HD2	1.78	0.45
1:B:1663:SER:HB2	1:B:1681:PHE:CG	2.52	0.45
1:A:789:GLN:HA	1:A:792:MET:HE2	2.00	0.44
1:A:247:ARG:HA	1:A:273:GLU:HG2	1.99	0.44
1:B:1135:GLY:HA3	4:B:2153:HOH:O	2.17	0.44
1:A:745:ILE:HG22	1:A:762:ILE:HD11	1.99	0.44
1:B:1063:LEU:HG	1:B:1102:LEU:HD21	1.99	0.44
1:A:666:ILE:HG22	1:A:711:PHE:CE2	2.53	0.44
1:A:386:ARG:CB	1:A:386:ARG:HH11	2.31	0.44
1:A:575:ARG:HH22	1:A:776:ASP:CB	2.31	0.44
1:A:663:SER:HB2	1:A:681:PHE:CG	2.52	0.44
1:B:1745:ILE:CG2	1:B:1762:ILE:HD11	2.48	0.44
1:A:645:LEU:HA	1:A:645:LEU:HD23	1.86	0.44
1:B:1753:LYS:O	1:B:1754:GLN:HG3	2.18	0.44
1:B:1028:LYS:HG2	1:B:1111:ALA:HB1	2.00	0.44
1:A:102:LEU:HB3	1:A:104:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1024:VAL:HG13	1:B:1111:ALA:HA	1.99	0.44
1:A:43:ARG:HA	1:A:43:ARG:HD2	1.85	0.44
1:B:1136:LEU:HD11	1:B:1338:ASN:OD1	2.18	0.43
1:A:745:ILE:CG2	1:A:762:ILE:HD11	2.47	0.43
1:B:1067:TRP:HA	1:B:1238:VAL:HB	2.00	0.43
1:A:67:TRP:HA	1:A:238:VAL:HB	2.00	0.43
1:B:1657:ILE:HB	1:B:1658:PRO:HD3	1.99	0.43
1:B:1041:LYS:HD2	1:B:1045:VAL:HG23	2.00	0.43
1:A:460:SER:CB	1:A:481:ASN:HB2	2.49	0.43
1:B:1765:LEU:HG	1:B:1774:PHE:CZ	2.53	0.43
1:A:233:TYR:CE2	1:A:512:VAL:HG11	2.53	0.43
1:A:543:LEU:O	1:A:547:GLN:HG3	2.19	0.43
1:A:458:ILE:HG23	1:A:459:HIS:N	2.34	0.43
1:B:1365:TRP:CD1	1:B:1369:GLN:NE2	2.87	0.43
1:A:524:PHE:N	1:A:524:PHE:CD1	2.87	0.43
1:A:718:VAL:HG13	1:A:772:LYS:HE2	2.01	0.43
1:A:676:THR:O	1:A:680:LYS:HG3	2.19	0.43
1:B:1575:ARG:HH22	1:B:1776:ASP:CB	2.31	0.42
1:B:1392:VAL:HG21	1:B:1439:ILE:HD12	2.01	0.42
1:A:516:SER:O	1:A:519:THR:HG23	2.19	0.42
1:A:224:LEU:HD12	1:A:225:PRO:CD	2.46	0.42
1:B:1460:SER:CB	1:B:1481:ASN:HB2	2.49	0.42
1:B:1524:PHE:CD1	1:B:1524:PHE:N	2.86	0.42
1:B:1077:LYS:HD3	1:B:1077:LYS:HA	1.57	0.42
1:B:1458:ILE:HG23	1:B:1459:HIS:N	2.34	0.42
1:B:1731:TYR:O	1:B:1735:LEU:HD12	2.20	0.42
1:A:392:VAL:HG21	1:A:439:ILE:HD12	2.00	0.42
1:A:211:THR:O	1:A:358:LYS:NZ	2.52	0.42
1:A:365:TRP:CD1	1:A:369:GLN:NE2	2.88	0.42
1:A:678:ASN:OD1	1:A:679:MET:N	2.53	0.42
1:B:1066:ARG:HG2	1:B:1236:ASN:O	2.19	0.42
1:B:1053:PHE:CE1	1:B:1188:PRO:HD3	2.52	0.42
1:B:1102:LEU:HB3	1:B:1104:LEU:CD2	2.49	0.42
1:A:41:LYS:NZ	1:A:50:ASP:OD2	2.51	0.42
1:B:1543:LEU:O	1:B:1547:GLN:HG3	2.19	0.42
1:B:1386:ARG:HH11	1:B:1386:ARG:CB	2.32	0.42
1:B:1745:ILE:HG22	1:B:1762:ILE:HD11	2.00	0.42
1:A:546:SER:O	1:A:550:GLU:HG3	2.20	0.42
1:B:1049:ARG:NH1	1:B:1053:PHE:HE2	2.18	0.42
1:B:1063:LEU:HD21	1:B:1231:PRO:HB3	2.01	0.42
1:B:1300:VAL:CG1	1:B:1345:ALA:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:LEU:HA	1:A:736:PRO:HD2	1.78	0.41
1:B:1594:PRO:HG3	1:B:1635:MET:SD	2.60	0.41
1:A:66:ARG:HD3	1:A:236:ASN:HA	2.02	0.41
1:B:1564:ASP:OD1	1:B:1664:GLU:OE2	2.38	0.41
1:B:1041:LYS:NZ	1:B:1050:ASP:OD2	2.49	0.41
1:A:636:VAL:CG2	1:A:637:GLY:N	2.83	0.41
1:B:1207:GLU:O	1:B:1213:THR:HA	2.21	0.41
1:B:1170:ILE:HG12	1:B:1646:GLU:CG	2.49	0.41
1:A:53:PHE:CE1	1:A:188:PRO:HD3	2.54	0.41
1:B:1112:ILE:HG13	1:B:1119:ILE:HD13	2.02	0.41
1:A:610:ALA:HB3	1:A:613:TYR:HB2	2.01	0.41
1:B:1610:ALA:HB3	1:B:1613:TYR:HB2	2.02	0.41
1:B:1462:ILE:HD11	1:B:1715:ILE:CD1	2.51	0.41
1:A:72:GLN:HE21	1:A:76:ASP:CG	2.23	0.41
1:B:1516:SER:O	1:B:1519:THR:HG23	2.19	0.41
1:B:1666:ILE:HG22	1:B:1711:PHE:CE2	2.55	0.41
1:A:564:ASP:OD1	1:A:664:GLU:OE2	2.39	0.41
1:A:66:ARG:HG2	1:A:236:ASN:O	2.21	0.41
1:B:1049:ARG:CZ	1:B:1053:PHE:HE2	2.34	0.41
1:B:1125:ILE:HA	1:B:1125:ILE:HD13	1.90	0.41
1:B:1191:LYS:HA	1:B:1191:LYS:HD2	1.80	0.41
1:B:1060:ARG:O	1:B:1063:LEU:HB2	2.21	0.41
1:B:1527:ASP:HB3	1:B:1530:PHE:HB3	2.03	0.40
1:A:49:ARG:HA	1:A:125:ILE:HG21	2.03	0.40
1:A:96:GLN:HE21	1:A:105:GLN:HE22	1.69	0.40
1:B:1382:GLU:OE2	1:B:1770:ARG:NH2	2.54	0.40
1:B:1167:ASN:HD22	1:B:1647:ASN:HD21	1.69	0.40
1:A:327:ASP:OD1	1:A:363:LYS:HE2	2.21	0.40
1:A:418:PHE:CE1	1:A:474:LEU:HD11	2.57	0.40
1:B:1546:SER:O	1:B:1550:GLU:HG3	2.20	0.40
1:A:765:LEU:HG	1:A:774:PHE:CZ	2.56	0.40
1:B:1066:ARG:HD3	1:B:1236:ASN:HA	2.02	0.40
1:B:1458:ILE:HG22	4:B:2076:HOH:O	2.21	0.40
1:B:1668:THR:OG1	1:B:1771:PHE:HB3	2.22	0.40
1:B:1418:PHE:CE1	1:B:1474:LEU:HD11	2.56	0.40
1:A:715:ILE:HG23	1:A:716:ASP:N	2.36	0.40
1:A:633:ASP:OD2	1:A:635:MET:HB3	2.22	0.40
1:B:1789:GLN:HA	1:B:1792:MET:HE2	2.04	0.40
1:B:1095:LEU:HB2	1:B:1126:GLU:OE1	2.22	0.40
1:A:57:HIS:HD2	4:A:2064:HOH:O	2.04	0.40
1:A:32:ASN:HA	1:A:32:ASN:HD22	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1339:ASP:O	1:B:1342:PRO:HD2	2.22	0.40

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%)	56 74
1	B	787/846 (93%)	738 (94%)	48 (6%)	1 (0%)	56 74
All	All	1573/1692 (93%)	1477 (94%)	94 (6%)	2 (0%)	56 74

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%)	8 11
1	B	693/739 (94%)	622 (90%)	71 (10%)	9 13
All	All	1386/1478 (94%)	1240 (90%)	146 (10%)	8 12

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	30	SER
1	A	42	ASP
1	A	44	ASN
1	A	77	LYS
1	A	78	CYS
1	A	90	TYR
1	A	95	LEU
1	A	102	LEU
1	A	104	LEU
1	A	128	ASP
1	A	138	ARG
1	A	150	LEU
1	A	191	LYS
1	A	193	ARG
1	A	205	LYS
1	A	211	THR
1	A	213	THR
1	A	214	LYS
1	A	243	LEU
1	A	245	SER
1	A	247	ARG
1	A	277	ARG
1	A	308	ILE
1	A	316	PHE
1	A	325	VAL
1	A	337	LEU
1	A	377	HIS
1	A	379	VAL
1	A	380	LEU
1	A	382	GLU
1	A	386	ARG
1	A	394	LYS
1	A	420	LYS
1	A	426	ARG
1	A	436	SER
1	A	453	ASN
1	A	466	LYS
1	A	475	GLU
1	A	480	GLN
1	A	499	LEU
1	A	502	LEU

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Mol	Chain	Res	Type
1	A	506	LYS
1	A	520	LYS
1	A	543	LEU
1	A	556	LYS
1	A	567	VAL
1	A	568	LYS
1	A	573	TYR
1	A	575	ARG
1	A	577	LEU
1	A	579	ASN
1	A	597	LEU
1	A	598	PHE
1	A	613	TYR
1	A	621	LYS
1	A	622	LEU
1	A	635	MET
1	A	645	LEU
1	A	652	LEU
1	A	683	LEU
1	A	689	ILE
1	A	708	LEU
1	A	715	ILE
1	A	729	LYS
1	A	733	GLU
1	A	735	LEU
1	A	753	LYS
1	A	756	ASP
1	A	759	LYS
1	A	765	LEU
1	A	770	ARG
1	A	782	LYS
1	A	786	LYS
1	A	795	LYS
1	B	1042	ASP
1	B	1044	ASN
1	B	1077	LYS
1	B	1078	CYS
1	B	1090	TYR
1	B	1095	LEU
1	B	1102	LEU
1	B	1104	LEU
1	B	1110	GLU

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Mol	Chain	Res	Type
1	B	1128	ASP
1	B	1138	ARG
1	B	1150	LEU
1	B	1191	LYS
1	B	1210	ASN
1	B	1214	LYS
1	B	1216	ILE
1	B	1243	LEU
1	B	1245	SER
1	B	1247	ARG
1	B	1277	ARG
1	B	1308	ILE
1	B	1316	PHE
1	B	1327	ASP
1	B	1337	LEU
1	B	1379	VAL
1	B	1386	ARG
1	B	1394	LYS
1	B	1420	LYS
1	B	1426	ARG
1	B	1436	SER
1	B	1453	ASN
1	B	1466	LYS
1	B	1475	GLU
1	B	1480	GLN
1	B	1499	LEU
1	B	1502	LEU
1	B	1506	LYS
1	B	1520	LYS
1	B	1543	LEU
1	B	1556	LYS
1	B	1567	VAL
1	B	1568	LYS
1	B	1575	ARG
1	B	1577	LEU
1	B	1579	ASN
1	B	1597	LEU
1	B	1598	PHE
1	B	1613	TYR
1	B	1621	LYS
1	B	1622	LEU
1	B	1635	MET

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Mol	Chain	Res	Type
1	B	1645	LEU
1	B	1652	LEU
1	B	1683	LEU
1	B	1689	ILE
1	B	1692	MET
1	B	1708	LEU
1	B	1715	ILE
1	B	1729	LYS
1	B	1733	GLU
1	B	1735	LEU
1	B	1753	LYS
1	B	1756	ASP
1	B	1759	LYS
1	B	1765	LEU
1	B	1770	ARG
1	B	1782	LYS
1	B	1786	LYS
1	B	1795	LYS
1	B	1830	SER
1	B	1831	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	34	HIS
1	A	44	ASN
1	A	62	HIS
1	A	72	GLN
1	A	97	ASN
1	A	105	GLN
1	A	106	ASN
1	A	114	GLN
1	A	167	ASN
1	A	239	ASN
1	A	270	ASN
1	A	274	ASN
1	A	284	ASN
1	A	305	GLN
1	A	369	GLN
1	A	410	HIS
1	A	450	HIS

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Mol	Chain	Res	Type
1	A	459	HIS
1	A	481	ASN
1	A	539	GLN
1	A	541	ASN
1	A	566	GLN
1	A	571	HIS
1	A	579	ASN
1	A	614	HIS
1	B	1032	ASN
1	B	1034	HIS
1	B	1044	ASN
1	B	1062	HIS
1	B	1072	GLN
1	B	1114	GLN
1	B	1167	ASN
1	B	1239	ASN
1	B	1270	ASN
1	B	1274	ASN
1	B	1284	ASN
1	B	1305	GLN
1	B	1369	GLN
1	B	1410	HIS
1	B	1459	HIS
1	B	1481	ASN
1	B	1539	GLN
1	B	1541	ASN
1	B	1566	GLN
1	B	1571	HIS
1	B	1579	ASN
1	B	1614	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates 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	$\#\|Z\| > 2$
3	PLP	A	860	1	15,15,16	2.11	3 (20%)	21,22,23	1.29	2 (9%)
2	NBG	A	861	-	15,15,15	1.22	1 (6%)	21,21,21	1.50	3 (14%)
3	PLP	B	1860	1	15,15,16	1.98	4 (26%)	21,22,23	1.00	3 (14%)
2	NBG	B	1861	-	15,15,15	1.48	2 (13%)	21,21,21	1.26	3 (14%)

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	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/5/26/26	0/1/1/1
3	PLP	B	1860	1	-	0/6/6/8	0/1/1/1
2	NBG	B	1861	-	-	0/5/26/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1860	PLP	C4A-C4	-5.59	1.40	1.51
3	A	860	PLP	C3-C2	-5.47	1.37	1.40
3	A	860	PLP	C4A-C4	-4.46	1.42	1.51
3	B	1860	PLP	C3-C2	-2.75	1.38	1.40
3	A	860	PLP	P-O3P	-2.25	1.46	1.54
3	B	1860	PLP	P-O2P	-2.19	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1860	PLP	C5A-C5	2.11	1.57	1.50
2	B	1861	NBG	C1-N1	2.95	1.46	1.43
2	A	861	NBG	C2-C1	3.58	1.56	1.53
2	B	1861	NBG	C2-C1	3.76	1.56	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	861	NBG	C2-C1-N1	-2.91	108.19	111.44
2	B	1861	NBG	C2-C1-N1	-2.56	108.58	111.44
3	B	1860	PLP	O2P-P-O4P	-2.07	100.60	106.56
3	A	860	PLP	C5A-C5-C4	2.03	124.34	121.65
3	B	1860	PLP	O3P-P-O1P	2.12	117.39	110.58
2	B	1861	NBG	C3-C2-C1	2.12	113.49	110.09
3	B	1860	PLP	O3P-P-O2P	2.15	115.55	107.38
3	A	860	PLP	O3P-P-O2P	2.21	115.79	107.38
2	A	861	NBG	C3-C2-C1	2.44	114.00	110.09
2	B	1861	NBG	C5-O5-C1	3.72	117.90	112.49
2	A	861	NBG	C5-O5-C1	4.43	118.93	112.49

There are no chirality outliers.

There are no torsion outliers.

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%)	-0.53	8 (1%) 84 83	15, 31, 57, 101	0
1	B	793/846 (93%)	-0.48	8 (1%) 84 83	16, 32, 60, 101	0
All	All	1585/1692 (93%)	-0.51	16 (1%) 84 83	15, 32, 59, 101	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1831	ASP	5.1
1	A	831	ASP	4.9
1	B	1316	PHE	4.8
1	B	1420	LYS	4.1
1	A	598	PHE	3.8
1	A	434	GLU	3.4
1	B	1554	LYS	3.2
1	B	1598	PHE	3.2
1	A	597	LEU	2.9
1	A	828	GLU	2.8
1	B	1830	SER	2.8
1	B	1597	LEU	2.5
1	A	316	PHE	2.4
1	B	1324	THR	2.2
1	A	420	LYS	2.1
1	A	830	SER	2.0

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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	NBG	B	1861	15/15	0.96	0.12	0.77	17,31,35,38	0
2	NBG	A	861	15/15	0.98	0.11	-0.23	14,23,31,32	0
3	PLP	B	1860	15/16	0.98	0.09	-0.79	14,19,31,34	0
3	PLP	A	860	15/16	0.99	0.09	-1.23	3,13,26,31	0

6.5 Other polymers (i)

There are no such residues in this entry.