



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:16 PM BST

PDB ID : 1FC0
Title : HUMAN LIVER GLYCOGEN PHOSPHORYLASE COMPLEXED WITH N-ACETYL-BETA-D-GLUCOPYRANOSYLAMINE
Authors : Rath, V.L.; Ammirati, M.; LeMotte, P.K.; Fennell, K.F.; Mansour, M.M.; Danley, D.E.; Hynes, T.R.; Schulte, G.K.; Wasilko, D.J.; Pandit, J.
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

<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)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

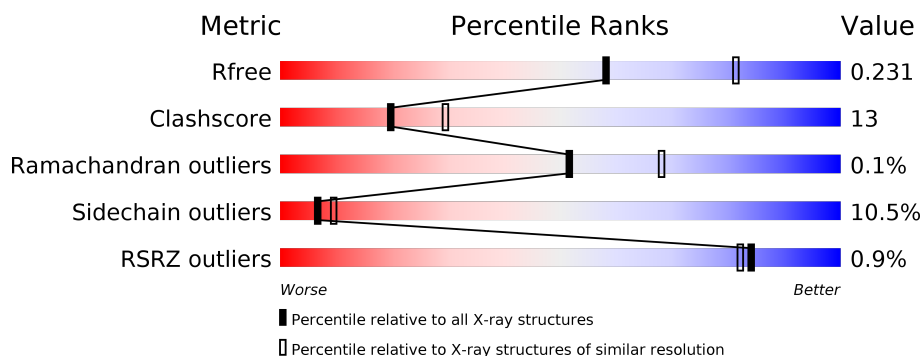
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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 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 $\leq 5\%$. 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	<div> <div></div> <div>63% 27% 6%</div> </div>
1	B	846	<div> <div></div> <div>62% 28% 6%</div> </div>

2 Entry composition [i](#)

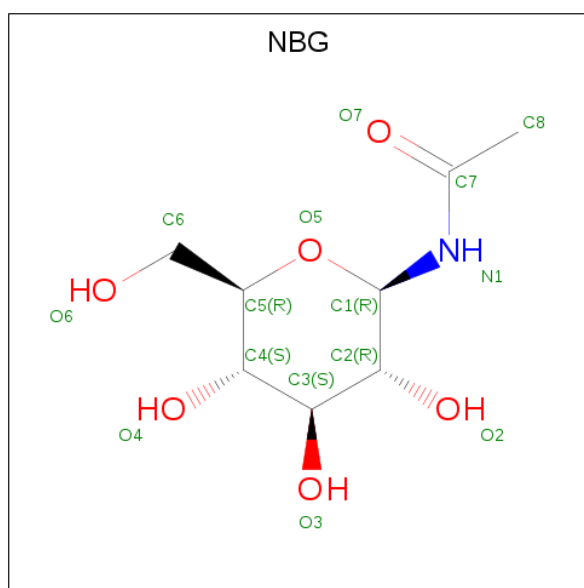
There are 4 unique types of molecules in this entry. The entry contains 13169 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

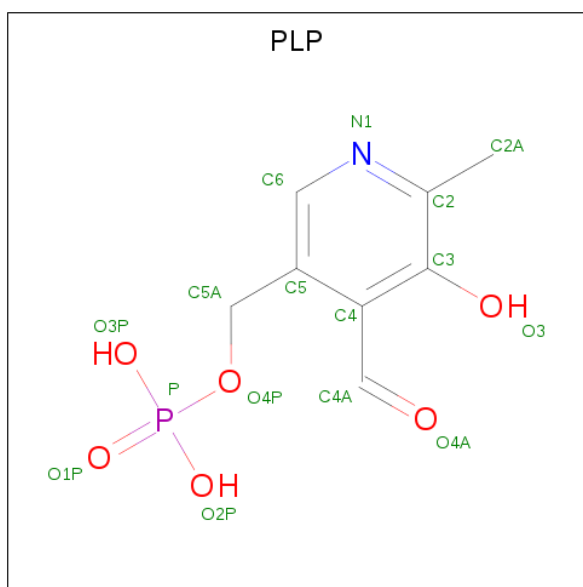
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	792	Total	C	N	O	S	0	0	0
			6425	4129	1090	1177	29			
1	B	793	Total	C	N	O	S	0	0	0
			6429	4131	1091	1178	29			

- 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	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		

- Molecule 1: GLYCOGEN PHOSPHORYLASE, LIVER FORM



S1830	G1712	A1610	L1492	L1400	L1304	N1210	G1078	ALA
D1831	M1713	Y1613	L1499	E1405	I1308	T1213	P1079	LYS
LEU	I1714	H1614	L1502	L1411	F1316	K1214	K1080	PRO
LYS	D1716	M1615	K1506	I1414	GLY	I1216	Y1090	LEU
ILE	D1717	I1619	S1516	V1415	THR	D1217	R1093	THR
SER	V1718	I1620	T1519	F1418	ARG	L1224	T1094	GLN
LEU	K1729	L1622	K1520	P1419	GLY	P1225	L1095	GLY
SER	E1730	V1630	F1524	K1420	ALA	Y1226	T1098	ARG
ASN	Y1731	M1635	D1527	D1423	T1324	D1227	GLN	ARG
ASN	Y1732	F1644	F1530	R1424	G1323	P1231	ILE	GLN
LYS	E1733	L1645	F1539	R1426	V1325	Y1237	SER	ILE
VAL	A1734	E1646	Q1547	R1427	F1326	N1235	ILE	ARG
ASN	L1735	E1647	Q1546	E1432	A1334	N1236	GLY	ARG
ASN	L1736	M1648	L1543	S1436	L1337	T1237	ILE	GLY
GLY	P1737	R1649	S1546	K1437	N1338	V1238	ILE	VAL
ASN	E1738	L1650	Q1547	I1439	D1339	L1243	GLY	GLY
ASN	L1739	S1651	Q1547	I1439	P1342	W1244	VAL	VAL
ASN	K1739	L1652	Q1547	I1439	N1338	A1246	GLU	GLU
ASN	L1740	L1653	Q1547	I1439	D1339	R1247	N1023	N1023
ASN	V1741	A1653	Q1547	I1439	P1330	A1248	Y1024	Y1024
ASN	I1745	I1657	E1550	A1442	A1334	P1249	K1028	K1028
ASN	P1752	P1658	T1551	I1446	L1337	ASN	K1029	K1029
ASN	K1753	S1663	K1554	I1446	A1345	ASP	H1033	H1033
ASN	Q1754	E1664	V1555	V1447	I1346	PHE	R1034	R1034
ASN	D1756	Q1665	K1556	G1448	P1347	ASN	H1035	H1035
ASN	K1759	L1666	D1564	V1452	E1348	LEU	H1036	H1036
ASN	D1760	I1666	V1565	N1453	W1361	ASP	F1037	F1037
ASN	I1761	S1667	Q1566	G1454	W1365	ASN	T1038	T1038
ASN	I1762	T1668	V1566	V1455	W1365	VAL	L1040	L1040
ASN	L1765	A1673	V1567	V1456	Q1369	G1260	K1041	K1041
ASN	R1770	S1674	K1568	K1457	K1370	D1261	D1042	D1042
ASN	F1771	G1675	R1575	I1458	A1370	Y1262	R1043	R1043
ASN	K1772	T1676	L1576	H1459	Y1374	I1263	N1044	N1044
ASN	F1773	K1680	L1577	S1460	I1377	Q1264	V1045	V1045
ASN	D1774	F1681	L1578	I1461	H1377	E1273	A1046	A1046
ASN	A1775	M1682	N1579	I1462	T1378	N1274	T1047	T1047
ASN	D1776	L1683	Y1587	T1465	V1379	I1275	T1048	T1048
ASN	Y1777	L1683	K1589	K1466	L1380	S1276	A1049	A1049
ASN	V1781	I1689	K1591	K1469	P1381	R1277	D1050	D1050
ASN	K1782	M1692	D1592	L1474	E1382	Y1185	F1053	F1053
ASN	K1786	D1693	P1594	E1475	E1385	F1286	T1058	T1058
ASN	Q1789	M1696	K1595	E1475	R1386	E1290	Y1059	Y1059
ASN	V1792	V1697	K1596	Q1480	L1291	L1291	R1060	R1060
ASN	M1795	E1698	L1597	N1481	R1292	R1292	D1061	D1061
ASN	K1795	E1701	F1598	T1487	L1391	Q1295	H1062	H1062
ASN	V1827	L1708	I1605	P1488	V1392	E1296	L1063	L1063
ASN	E1828	F1711	G1606	R1489	E1393	E1296	R1066	R1066
ASN	P1829	F1711	G1607	R1490	K1394	W1207	W1067	W1067
ASN					P1397	V1300	K1077	K1077

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ 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.

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:1591:LYS:HD2	1:B:1635:MET:HG2	1.77	0.67
1:B:1653:ALA:O	1:B:1657:ILE:HG13	1.95	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

Continued on next page...

Continued from previous page...

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:A:575:ARG:HD3	1:A:666:ILE:O	2.03	0.58
1:B:1346:ILE:HD13	1:B:1448:GLY:HA3	1.85	0.58
1:A:693:ASP:O	1:A:696:ASN:HB2	2.04	0.57
1:A:697:VAL:O	1:A:701:GLU:HG3	2.05	0.57
1:B:1411:LEU:HD23	1:B:1414:ILE:CD1	2.35	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:A:393:GLU:HB2	1:A:400:LEU:CD2	2.35	0.56
1:B:1432:GLU:O	1:B:1437:LYS:HA	2.06	0.56
1:B:1615:MET:CE	1:B:1761:ILE:HA	2.36	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

Continued on next page...

Continued from previous page...

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:A:346:ILE:HD13	1:A:448:GLY:HA3	1.89	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:B:1575:ARG:NH2	1:B:1776:ASP:HB2	2.22	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: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: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:1261:ASP:OD1	1:B:1264:GLN:HB2	2.07	0.55
1:B:1174:TRP:CZ2	1:B:1621:LYS:HG3	2.42	0.55
1:A:316:PHE:CZ	1:A:325:VAL:HB	2.41	0.54
1:A:732:TYR:CE1	1:A:739:LYS:HG3	2.43	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:432:GLU:O	1:A:437:LYS:HA	2.06	0.54
1:A:53:PHE:HE1	1:A:188:PRO:HD3	1.72	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:1286:PHE:CD1	1:B:1385:GLU:HG2	2.44	0.53
1:B:1393:GLU:HB2	1:B:1400:LEU:CD2	2.39	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:1465:THR:O	1:B:1469:LYS:HB2	2.10	0.52
1:B:1732:TYR:CE1	1:B:1739:LYS:HG3	2.44	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

Continued on next page...

Continued from previous page...

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:A:47:THR:H	1:A:50:ASP:HB2	1.76	0.51
1:B:1415:VAL:HG23	1:B:1425:LEU:HD21	1.93	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:167:ASN:ND2	1:A:647:ASN:HD21	2.09	0.51
1:A:261:ASP:OD1	1:A:264:GLN:HB2	2.11	0.51
1:A:274:ASN:ND2	1:A:277:ARG:HD2	2.25	0.51
1:B:1036:HIS:O	1:B:1040:VAL:HA	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:307:ILE:HG23	4:A:2226:HOH:O	2.10	0.50
1:A:80:LYS:HE2	1:A:334:ALA:HB2	1.92	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:192:SER:HB3	1:A:226:TYR:CE1	2.47	0.50
1:A:281:PRO:HG3	1:B:1262:TYR:CE2	2.46	0.50
1:A:97:ASN:HA	1:A:494:LEU:HD12	1.94	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:A:136:LEU:HD11	1:A:338:ASN:OD1	2.13	0.49
1:B:1575:ARG:HH22	1:B:1776:ASP:CG	2.14	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:A:58:THR:O	1:A:62:HIS:HD2	1.96	0.49
1:B:1047:THR:H	1:B:1050:ASP:HB2	1.78	0.49
1:A:568:LYS:O	1:A:607:GLY:HA3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.94	0.49
1:A:142:CYS:SG	1:A:487:THR:HG22	2.53	0.48
1:B:1330:PRO:HB3	1:B:1370:LYS:HB3	1.94	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:A:193:ARG:HH11	1:A:193:ARG:HA	1.78	0.48
1:A:605:ILE:O	1:A:644:PHE:HA	2.14	0.48
1:B:1274:ASN:HD22	1:B:1277:ARG:NH1	1.99	0.48
1:B:1718:VAL:HG13	1:B:1772:LYS:HE2	1.96	0.48
1:A:300:VAL:HG13	1:A:345:ALA:HA	1.95	0.48
1:A:455:VAL:H	1:A:459:HIS:CD2	2.29	0.48
1:A:753:LYS:O	1:A:754:GLN:HG3	2.14	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:A:300:VAL:HG22	1:A:345:ALA:HB2	1.96	0.47
1:B:1049:ARG:NH2	1:B:1053:PHE:HE2	2.12	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:A:380:LEU:HD13	1:A:382:GLU:OE2	2.14	0.47
1:B:1247:ARG:HA	1:B:1273:GLU:HG2	1.97	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:A:304:LEU:HD12	1:A:348:GLU:CG	2.45	0.47
1:A:49:ARG:HG2	4:A:2211:HOH:O	2.14	0.47
1:B:1459:HIS:HB2	1:B:1673:ALA:O	2.14	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

Continued on next page...

Continued from previous page...

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:386:ARG:HB2	1:A:386:ARG:HH11	1.81	0.46
1:A:614:HIS:HE1	1:A:760:ASP:OD1	1.99	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:1614:HIS:HE1	1:B:1760:ASP:OD1	1.99	0.45
1:B:1456:ALA:HB2	1:B:1674:SER:HB2	1.99	0.45
1:A:63:LEU:HD21	1:A:231:PRO:HB3	1.97	0.45
1:A:587:TYR:CD1	1:A:630:VAL:HG22	2.51	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:361:TRP:CH2	1:A:405:GLU:HB3	2.52	0.45
1:B:1374:TYR:CD2	1:B:1452:VAL:HG13	2.51	0.45
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.99	0.45
1:B:1386:ARG:HB2	1:B:1386:ARG:HH11	1.81	0.45
1:B:1587:TYR:CD1	1:B:1630:VAL:HG22	2.52	0.45
1:B:1049:ARG:HH22	1:B:1185:TYR:HB3	1.80	0.45
1:A:191:LYS:HA	1:A:191:LYS:HD2	1.78	0.45
1:A:374:TYR:CD2	1:A:452:VAL:HG13	2.52	0.45
1:B:1663:SER:HB2	1:B:1681:PHE:CG	2.52	0.45
1:A:247:ARG:HA	1:A:273:GLU:HG2	1.99	0.44
1:A:789:GLN:HA	1:A:792:MET:HE2	2.00	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:386:ARG:CB	1:A:386:ARG:HH11	2.31	0.44
1:A:666:ILE:HG22	1:A:711:PHE:CE2	2.53	0.44
1:A:645:LEU:HA	1:A:645:LEU:HD23	1.86	0.44
1:A:663:SER:HB2	1:A:681:PHE:CG	2.52	0.44
1:A:575:ARG:HH22	1:A:776:ASP:CB	2.31	0.44
1:B:1745:ILE:CG2	1:B:1762:ILE:HD11	2.48	0.44
1:A:102:LEU:HB3	1:A:104:LEU:HD22	1.99	0.44
1:B:1028:LYS:HG2	1:B:1111:ALA:HB1	2.00	0.44
1:B:1753:LYS:O	1:B:1754:GLN:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:HA	1:A:43:ARG:HD2	1.85	0.44
1:B:1024:VAL:HG13	1:B:1111:ALA:HA	1.99	0.44
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:B:1136:LEU:HD11	1:B:1338:ASN:OD1	2.18	0.43
1:A:67:TRP:HA	1:A:238:VAL:HB	2.00	0.43
1:A:460:SER:CB	1:A:481:ASN:HB2	2.49	0.43
1:B:1041:LYS:HD2	1:B:1045:VAL:HG23	2.00	0.43
1:B:1657:ILE:HB	1:B:1658:PRO:HD3	1.99	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:676:THR:O	1:A:680:LYS:HG3	2.19	0.43
1:A:718:VAL:HG13	1:A:772:LYS:HE2	2.01	0.43
1:A:516:SER:O	1:A:519:THR:HG23	2.19	0.42
1:B:1392:VAL:HG21	1:B:1439:ILE:HD12	2.01	0.42
1:B:1575:ARG:HH22	1:B:1776:ASP:CB	2.31	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:1077:LYS:HD3	1:B:1077:LYS:HA	1.57	0.42
1:B:1524:PHE:CD1	1:B:1524:PHE:N	2.86	0.42
1:A:211:THR:O	1:A:358:LYS:NZ	2.52	0.42
1:A:392:VAL:HG21	1:A:439:ILE:HD12	2.00	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: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:A:41:LYS:NZ	1:A:50:ASP:OD2	2.51	0.42
1:B:1066:ARG:HG2	1:B:1236:ASN:O	2.19	0.42
1:B:1102:LEU:HB3	1:B:1104:LEU:CD2	2.49	0.42
1:B:1053:PHE:CE1	1:B:1188:PRO:HD3	2.52	0.42
1:A:546:SER:O	1:A:550:GLU:HG3	2.20	0.42
1:B:1386:ARG:HH11	1:B:1386:ARG:CB	2.32	0.42
1:B:1543:LEU:O	1:B:1547:GLN:HG3	2.19	0.42
1:B:1745:ILE:HG22	1:B:1762:ILE:HD11	2.00	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:A:735:LEU:HA	1:A:736:PRO:HD2	1.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1300:VAL:CG1	1:B:1345:ALA:HA	2.50	0.41
1:A:636:VAL:CG2	1:A:637:GLY:N	2.83	0.41
1:A:66:ARG:HD3	1:A:236:ASN:HA	2.02	0.41
1:B:1041:LYS:NZ	1:B:1050:ASP:OD2	2.49	0.41
1:B:1594:PRO:HG3	1:B:1635:MET:SD	2.60	0.41
1:B:1564:ASP:OD1	1:B:1664:GLU:OE2	2.38	0.41
1:A:53:PHE:CE1	1:A:188:PRO:HD3	2.54	0.41
1:A:610:ALA:HB3	1:A:613:TYR:HB2	2.01	0.41
1:B:1112:ILE:HG13	1:B:1119:ILE:HD13	2.02	0.41
1:B:1170:ILE:HG12	1:B:1646:GLU:CG	2.49	0.41
1:B:1207:GLU:O	1:B:1213:THR:HA	2.21	0.41
1:B:1610:ALA:HB3	1:B:1613:TYR:HB2	2.02	0.41
1:A:72:GLN:HE21	1:A:76:ASP:CG	2.23	0.41
1:B:1462:ILE:HD11	1:B:1715:ILE:CD1	2.51	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:1191:LYS:HA	1:B:1191:LYS:HD2	1.80	0.41
1:B:1125:ILE:HA	1:B:1125:ILE:HD13	1.90	0.41
1:B:1060:ARG:O	1:B:1063:LEU:HB2	2.21	0.41
1:A:49:ARG:HA	1:A:125:ILE:HG21	2.03	0.40
1:B:1527:ASP:HB3	1:B:1530:PHE:HB3	2.03	0.40
1:A:96:GLN:HE21	1:A:105:GLN:HE22	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:A:765:LEU:HG	1:A:774:PHE:CZ	2.56	0.40
1:B:1167:ASN:HD22	1:B:1647:ASN:HD21	1.69	0.40
1:B:1546:SER:O	1:B:1550:GLU:HG3	2.20	0.40
1:B:1382:GLU:OE2	1:B:1770:ARG:NH2	2.54	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:A:715:ILE:HG23	1:A:716:ASP:N	2.36	0.40
1:B:1418:PHE:CE1	1:B:1474:LEU:HD11	2.56	0.40
1:A:32:ASN:HA	1:A:32:ASN:HD22	1.71	0.40
1:A:57:HIS:HD2	4:A:2064:HOH:O	2.04	0.40
1:A:633:ASP:OD2	1:A:635:MET:HB3	2.22	0.40
1:B:1095:LEU:HB2	1:B:1126:GLU:OE1	2.22	0.40
1:B:1339:ASP:O	1:B:1342:PRO:HD2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1789:GLN:HA	1:B:1792:MET:HE2	2.04	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%)	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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	1.86	3 (20%)	20,22,23	1.28	2 (10%)
2	NBG	A	861	-	15,15,15	1.22	1 (6%)	21,21,21	1.58	4 (19%)
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%)

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	-	2/6/6/8	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
3	PLP	B	1860	1	-	0/6/6/8	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	-5.47	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
2	B	1861	NBG	C1-N1	2.71	1.46	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1860	PLP	C5A-C5	2.24	1.57	1.50
3	A	860	PLP	P-O3P	-2.14	1.46	1.54
3	B	1860	PLP	P-O2P	-2.08	1.46	1.54
3	B	1860	PLP	C3-C2	-2.03	1.38	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
2	A	861	NBG	O5-C1-C2	2.35	112.19	109.83
2	B	1861	NBG	C2-C1-N1	-2.32	108.58	111.30
3	B	1860	PLP	O2P-P-O4P	-2.30	100.60	106.73
3	A	860	PLP	O3P-P-O2P	2.13	115.79	107.64
3	B	1860	PLP	O3P-P-O2P	2.07	115.55	107.64
3	A	860	PLP	C5A-C5-C6	-2.06	115.99	119.37

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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

All (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
1	A	434	GLU	3.3
1	B	1554	LYS	3.1
1	B	1598	PHE	3.1
1	A	597	LEU	2.8
1	A	828	GLU	2.7
1	B	1830	SER	2.7
1	B	1597	LEU	2.4
1	A	316	PHE	2.3
1	B	1324	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95th 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(\AA^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.