



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:08 AM UTC

PDB ID : 1FC0 / pdb_00001fc0
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

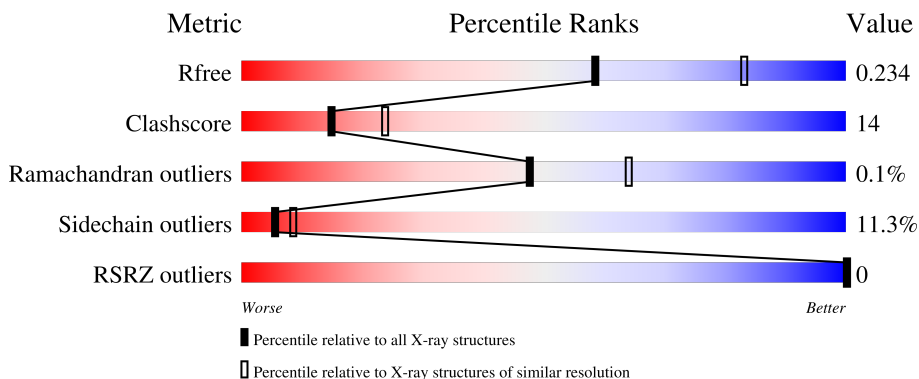
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	
1	B	846	

2 Entry composition [i](#)

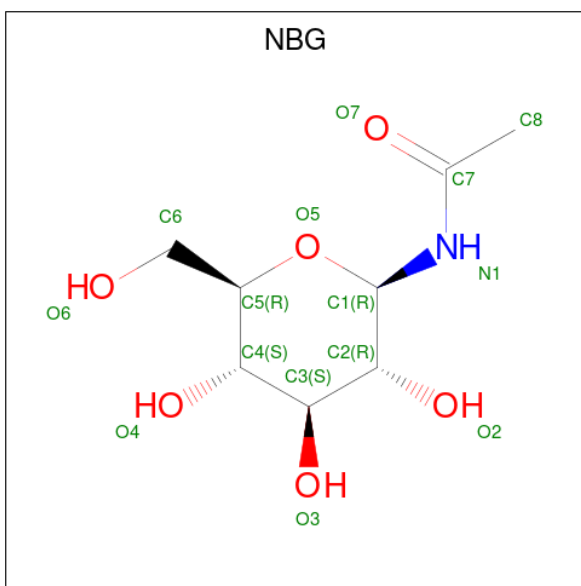
There are 4 unique types of molecules in this entry. The entry contains 13169 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

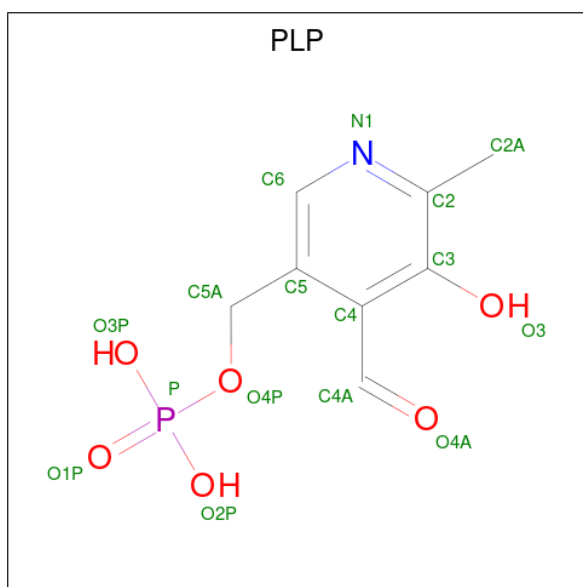
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	792	Total 6425	C 4129	N 1090	O 1177	S 29	0	0	0
1	B	793	Total 6429	C 4131	N 1091	O 1178	S 29	0	0	0

- Molecule 2 is N-acetyl-beta-D-glucopyranosylamine (CCD ID: NBG) (formula: C₈H₁₅NO₆).



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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

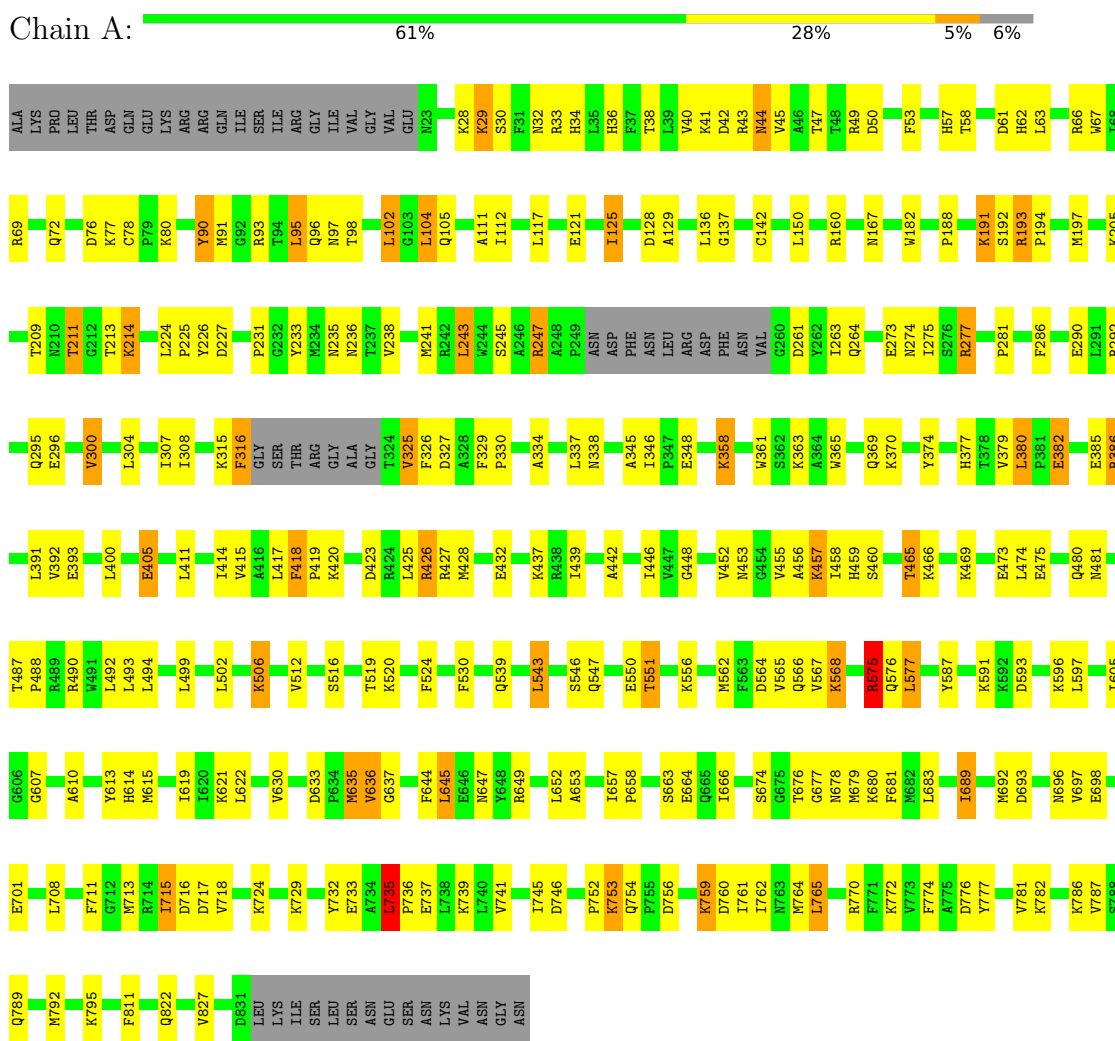
- Molecule 4 is water.

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

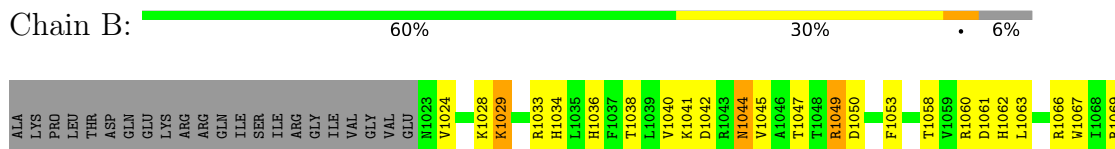
3 Residue-property plots i

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



• Molecule 1: GLYCOGEN PHOSPHORYLASE, LIVER FORM



Q1072	M1197	E1290	R1386	Q1480	P1594	L1683	F1774
D1076	K1205	L1291	L1391	M1481	K1596	I1689	A1775
C1078	V1206	R1292	V1392	E1393	L1597	M1692	D1776
P1079	E1207	Q1295	E1393	T1487	I1605	D1693	Y1777
K1080	H1208	E1296	P1397	P1488	G1606	M1696	V1781
R1093	T1203	V1300	L1400	E1489	G1607	V1697	K1782
T1094	M1210	L1304	E1405	V1491	A1610	E1698	K1786
L1095	K1214	I1308	L4411	L1492	Y1613	Q1788	V1787
T1098	W1215	F1316	I4414	L1494	H1614	Q1789	S1788
L1102	D1217	GLY	I4415	L1499	M1615	M1792	Q1789
G1103	L1224	SER	V414	L1502	I1619	K1795	V1827
L1104	P1225	THR	V415	L1502	I1620	F1711	E1828
E1110	Y1226	ARG	L1417	K1506	K1621	G1712	P1829
A1111	D1227	GLY	F1418	S1516	L1622	M1713	S1830
Y1112	P1231	ALA	P1419	T1519	V1630	I1715	D1831
Y1113	M1235	T1324	K1420	K1520	M1635	D1716	V1827
Q1114	M1236	V1325	D1423	F1524	V1636	V1717	E1828
I1119	T1237	F1329	L1425	D1527	L1640	V1718	P1829
L1122	V1238	P1330	R1426	F1527	F1644	K1724	S1830
I1125	M1241	A1334	M1427	F1530	F1644	K1729	D1831
E1126	R1242	L1337	M1428	Q1539	L1645	E1730	LEU
E1127	W1244	N1338	E1432	K1542	E1646	Y1731	LYS
D1128	S1245	D1339	K1437	L1543	N1647	Y1732	ILE
G1135	A1246	P1342	R1438	L1543	Y1648	E1733	SER
L1136	R1247	A1345	I1439	S1546	R1649	A1734	LEU
C1142	A1248	I1346	A1442	Q1547	V1650	L1738	SER
L1150	ASN	E1348	I1446	E1550	P1658	P1736	SER
R1160	ASP	K1358	V1448	T1551	D1661	E1737	ASN
N1167	ASP	W1361	V1452	K1556	L1662	K1739	LYS
I1170	PHE	W1365	V1455	M1562	S1663	L1740	VAL
W1174	ASN	Q1369	A1456	F1563	E1664	V1741	ASN
D1261	VAL	K1370	K1457	D1564	Q1665	I1745	ASN
W1182	G1260	Y1374	H1459	V1565	I1666	P1752	LYS
Y1185	Y1262	H1377	S1460	V1567	T1668	K1753	ASN
P1188	I1263	T1378	I1462	K1568	A1673	Q1754	GLY
S1275	Q1264	V1379	T1465	R1575	S1674	D1756	ASN
R1192	E1273	L1380	K1466	Q1576	G1675	K1759	ASN
P1194	I1275	P1381	K1469	L1577	T1676	I1761	GLY
S1276	S1276	E1382	E1473	Y1587	G1677	I1762	ASN
R1277	R1277	A1383	E1474	K1587	M1678	M1763	ASN
F1286	F1286	L1384	L474	K1591	M1679	M1764	ASN
		E1385	E1475	K1592	K1680	L1765	ASN
				K1593	F1681	L1770	ASN
				D1593	K1592	F1771	ASN
					L1474	K1772	ASN
					E1475	V1773	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 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.1 (30.00-2.40) 95.1 (30.00-2.40)	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 0.195 , 0.234	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)	0.33 , 25.4	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	0.96	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, 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	0.41	0/6569	0.88	15/8884 (0.2%)
1	B	0.40	0/6573	0.88	13/8889 (0.1%)
All	All	0.41	0/13142	0.88	28/17773 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ALA	N-CA-C	-7.45	99.21	109.71
1	B	1576	GLN	N-CA-C	-6.91	104.12	112.54
1	B	1575	ARG	N-CA-C	6.86	121.12	111.52
1	A	576	GLN	N-CA-C	-6.67	104.41	112.54
1	A	575	ARG	N-CA-C	6.58	120.74	111.52
1	A	565	VAL	N-CA-C	6.13	116.69	108.11
1	B	1565	VAL	N-CA-C	5.99	116.49	108.11
1	B	1418	PHE	CA-C-N	5.90	125.38	119.24
1	B	1418	PHE	C-N-CA	5.90	125.38	119.24
1	A	91	MET	N-CA-C	5.83	120.12	112.89
1	B	1455	VAL	N-CA-C	5.74	117.68	112.29
1	B	1277	ARG	N-CA-C	5.71	117.31	111.14
1	A	418	PHE	CA-C-N	5.71	125.18	119.24
1	A	418	PHE	C-N-CA	5.71	125.18	119.24
1	A	677	GLY	N-CA-C	-5.59	105.91	113.24
1	A	465	THR	N-CA-C	5.38	117.23	111.36
1	B	1650	VAL	N-CA-C	5.38	116.01	110.36
1	B	1465	THR	N-CA-C	5.37	117.22	111.36
1	A	182	TRP	N-CA-C	5.20	119.25	113.01
1	A	746	ASP	N-CA-C	5.15	117.63	111.71
1	B	1677	GLY	N-CA-C	-5.11	106.54	113.24
1	A	214	LYS	N-CA-C	5.11	116.72	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1182	TRP	N-CA-C	5.11	119.14	113.01
1	B	1735	LEU	CA-C-N	5.10	124.54	119.24
1	B	1735	LEU	C-N-CA	5.10	124.54	119.24
1	A	735	LEU	CA-C-N	5.04	124.48	119.24
1	A	735	LEU	C-N-CA	5.04	124.48	119.24
1	A	453	ASN	N-CA-C	5.00	117.41	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	167	0
1	B	6429	0	6422	189	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	355	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 14.

All (355) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1547:GLN:O	1:B:1551:THR:HG23	1.69	0.93
1:B:1615:MET:HE1	1:B:1761:ILE:HA	1.48	0.93
1:A:615:MET:HE1	1:A:761:ILE:HA	1.48	0.92
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: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:1615:MET:HE2	1:B:1764:MET:HE2	1.74	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:A:615:MET:HE2	1:A:764:MET:HE2	1.75	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:1615:MET:HE2	1:B:1764:MET:CE	2.26	0.66
1:B:1292:ARG:O	1:B:1296:GLU:HG3	1.96	0.66
1:A:591:LYS:HD2	1:A:635:MET:HG2	1.77	0.65
1:A:615:MET:HE2	1:A:764:MET:CE	2.26	0.65
1:B:1206:VAL:HG23	1:B:1397:PRO:HB2	1.79	0.65
1:A:292:ARG:O	1:A:296:GLU:HG3	1.96	0.65
1:B:1170:ILE:HG13	1:B:1646:GLU:HG3	1.79	0.65
1:B:1197:MET:HE3	1:B:1224:LEU:HB2	1.78	0.64
1:B:1777:TYR:O	1:B:1781:VAL:HG23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:197:MET:HE3	1:A:224:LEU:HB2	1.81	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:80:LYS:HB3	1:A:827:VAL:HG12	1.85	0.58
1:A:539:GLN:HE21	1:A:543:LEU:HD12	1.68	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:1615:MET:HE1	1:B:1761:ILE:HG12	1.85	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:615:MET:HE1	1:A:761:ILE:HG12	1.85	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:B:1593:ASP:CG	1:B:1596:LYS:HB2	2.30	0.57
1:A:593:ASP:CG	1:A:596:LYS:HB2	2.31	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: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
1:A:442:ALA:O	1:A:446:ILE:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1575:ARG:NH2	1:B:1776:ASP:HB2	2.22	0.55
1:B:1697:VAL:O	1:B:1701:GLU:HG3	2.06	0.55
1:B:1080:LYS:HE2	1:B:1334:ALA:HB2	1.88	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:1338:ASN:OD1	1:B:1377:HIS:NE2	2.40	0.55
1:B:1428:MET:HE1	1:B:1474:LEU:HD22	1.89	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:1216:ILE:HD12	1:B:1217:ASP:CG	2.31	0.55
1:B:1261:ASP:OD1	1:B:1264:GLN:HB2	2.07	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:1615:MET:HE1	1:B:1761:ILE:CA	2.31	0.54
1:B:1029:LYS:HB3	1:B:1033:ARG:HH21	1.72	0.54
1:A:575:ARG:HH22	1:A:776:ASP:CG	2.16	0.54
1:B:1575:ARG:HH22	1:B:1776:ASP:CG	2.14	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:1382:GLU:CD	1:B:1770:ARG:HH22	2.15	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:A:615:MET:HE1	1:A:761:ILE:CA	2.30	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1732:TYR:CE1	1:B:1739:LYS:HG3	2.44	0.52
1:A:649:ARG:HG2	1:A:649:ARG:HH11	1.75	0.52
1:B:1274:ASN:ND2	1:B:1277:ARG:HD2	2.24	0.52
1:A:98:THR:HG22	1:A:102:LEU:HD22	1.91	0.52
1:B:1649:ARG:HH11	1:B:1649:ARG:HG2	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:A:428:MET:HE1	1:A:474:LEU:HD22	1.92	0.51
1:B:1415:VAL:HG23	1:B:1425:LEU:HD21	1.93	0.51
1:B:1457:LYS:HG3	1:B:1698:GLU:CD	2.36	0.51
1:A:415:VAL:HG23	1:A:425:LEU:HD21	1.92	0.51
1:B:1789:GLN:HA	1:B:1792:MET:HE2	1.93	0.51
1:B:1679:MET:HE2	1:B:1811:PHE:CD1	2.46	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:A:789:GLN:HA	1:A:792:MET:HE2	1.93	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: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: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: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:286:PHE:CD1	1:A:385:GLU:HG2	2.46	0.49
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.95	0.49
1:A:330:PRO:HB3	1:A:370:LYS:HB3	1.93	0.49
1:B:1047:THR:O	1:B:1050:ASP:HB2	2.11	0.49
1:A:689:ILE:HG23	1:A:689:ILE:O	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HG23	1:B:1689:ILE:O	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:A:679:MET:HE2	1:A:811:PHE:CD1	2.47	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:A:759:LYS:HA	1:A:759:LYS:HD3	1.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:A:72:GLN:HE21	1:A:76:ASP:CG	2.23	0.46
1:B:1224:LEU:HD12	1:B:1225:PRO:CD	2.45	0.46
1:A:386:ARG:HH11	1:A:386:ARG:HB2	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: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: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:HH11	1:B:1386:ARG:HB2	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:B:1562:MET:HE1	1:B:1787:VAL:HG12	1.99	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:A:417:LEU:C	1:A:419:PRO:HD3	2.43	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: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:A:562:MET:HE1	1:A:787:VAL:HG12	1.99	0.44
1:B:1063:LEU:HG	1:B:1102:LEU:HD21	1.99	0.44
1:A:386:ARG:HH11	1:A:386:ARG:CB	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:HG22	1:A:711:PHE:CE2	2.53	0.44
1:A:575:ARG:HH22	1:A:776:ASP:CB	2.31	0.44
1:A:645:LEU:HD23	1:A:645:LEU:HA	1.86	0.44
1:A:663:SER:HB2	1:A:681:PHE:CG	2.52	0.44
1:B:1072:GLN:HE21	1:B:1076:ASP:CG	2.25	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
1:A:43:ARG:HD2	1:A:43:ARG:HA	1.85	0.44
1:B:1024:VAL:HG13	1:B:1111:ALA:HA	1.99	0.44
1:B:1241:MET:HE3	1:B:1243:LEU:HD22	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:90:TYR:HB2	1:A:137:GLY:C	2.44	0.43
1:A:315:LYS:O	1:A:316:PHE:C	2.61	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:1494:LEU:C	1:B:1494:LEU:HD23	2.44	0.43
1:A:494:LEU:HD23	1:A:494:LEU:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:615:MET:CE	1:A:761:ILE:HG12	2.48	0.42
1:B:1053:PHE:CE1	1:B:1188:PRO:HD3	2.52	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: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:B:1417:LEU:C	1:B:1419:PRO:HD3	2.44	0.42
1:A:457:LYS:HG3	1:A:698:GLU:CD	2.45	0.41
1:A:735:LEU:HA	1:A:736:PRO:HD2	1.78	0.41
1:B:1300:VAL:CG1	1:B:1345:ALA:HA	2.50	0.41
1:B:1542:LYS:NZ	1:B:1661:ASP:OD2	2.47	0.41
1:A:66:ARG:HD3	1:A:236:ASN:HA	2.02	0.41
1:A:241:MET:HE3	1:A:243:LEU:HD22	2.02	0.41
1:A:636:VAL:CG2	1:A:637:GLY:N	2.83	0.41
1:B:1041:LYS:NZ	1:B:1050:ASP:OD2	2.49	0.41
1:B:1564:ASP:OD1	1:B:1664:GLU:OE2	2.38	0.41
1:B:1594:PRO:HG3	1:B:1635:MET:SD	2.60	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:1615:MET:CE	1:B:1761:ILE:HG12	2.49	0.41
1:A:192:SER:C	1:A:194:PRO:HD3	2.45	0.41
1:B:1610:ALA:HB3	1:B:1613:TYR:HB2	2.02	0.41
1:B:1192:SER:C	1:B:1194:PRO:HD3	2.45	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:1125:ILE:HD13	1:B:1125:ILE:HA	1.90	0.41
1:B:1191:LYS:HD2	1:B:1191:LYS:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1060:ARG:O	1:B:1063:LEU:HB2	2.21	0.41
1:B:1615:MET:HE2	1:B:1764:MET:HE3	2.03	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:1382:GLU:OE2	1:B:1770:ARG:NH2	2.54	0.40
1:B:1546:SER:O	1:B:1550:GLU:HG3	2.20	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:HD22	1:A:32:ASN:HA	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

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%)	48 64
1	B	787/846 (93%)	738 (94%)	48 (6%)	1 (0%)	48 64
All	All	1573/1692 (93%)	1477 (94%)	94 (6%)	2 (0%)	48 64

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%)	613 (88%)	80 (12%)	5 8
1	B	693/739 (94%)	617 (89%)	76 (11%)	6 9
All	All	1386/1478 (94%)	1230 (89%)	156 (11%)	5 8

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	30	SER
1	A	44	ASN
1	A	69	ARG
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	121	GLU
1	A	125	ILE
1	A	128	ASP
1	A	150	LEU
1	A	191	LYS
1	A	193	ARG
1	A	205	LYS
1	A	209	THR
1	A	211	THR
1	A	213	THR
1	A	214	LYS

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Mol	Chain	Res	Type
1	A	243	LEU
1	A	245	SER
1	A	247	ARG
1	A	277	ARG
1	A	300	VAL
1	A	308	ILE
1	A	316	PHE
1	A	325	VAL
1	A	337	LEU
1	A	358	LYS
1	A	377	HIS
1	A	379	VAL
1	A	380	LEU
1	A	382	GLU
1	A	386	ARG
1	A	405	GLU
1	A	420	LYS
1	A	426	ARG
1	A	457	LYS
1	A	466	LYS
1	A	473	GLU
1	A	475	GLU
1	A	480	GLN
1	A	493	LEU
1	A	499	LEU
1	A	502	LEU
1	A	506	LYS
1	A	520	LYS
1	A	543	LEU
1	A	551	THR
1	A	556	LYS
1	A	567	VAL
1	A	568	LYS
1	A	575	ARG
1	A	577	LEU
1	A	597	LEU
1	A	621	LYS
1	A	622	LEU
1	A	635	MET
1	A	636	VAL
1	A	645	LEU
1	A	652	LEU

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Mol	Chain	Res	Type
1	A	683	LEU
1	A	689	ILE
1	A	708	LEU
1	A	715	ILE
1	A	724	LYS
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	A	822	GLN
1	B	1029	LYS
1	B	1044	ASN
1	B	1049	ARG
1	B	1069	ARG
1	B	1077	LYS
1	B	1078	CYS
1	B	1095	LEU
1	B	1102	LEU
1	B	1104	LEU
1	B	1110	GLU
1	B	1125	ILE
1	B	1128	ASP
1	B	1150	LEU
1	B	1191	LYS
1	B	1205	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	1300	VAL
1	B	1308	ILE
1	B	1316	PHE

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Mol	Chain	Res	Type
1	B	1337	LEU
1	B	1358	LYS
1	B	1379	VAL
1	B	1386	ARG
1	B	1405	GLU
1	B	1420	LYS
1	B	1426	ARG
1	B	1457	LYS
1	B	1466	LYS
1	B	1473	GLU
1	B	1475	GLU
1	B	1480	GLN
1	B	1493	LEU
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	1597	LEU
1	B	1621	LYS
1	B	1622	LEU
1	B	1635	MET
1	B	1636	VAL
1	B	1640	LEU
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	1724	LYS
1	B	1729	LYS
1	B	1733	GLU
1	B	1735	LEU
1	B	1753	LYS
1	B	1756	ASP

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Mol	Chain	Res	Type
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	1822	GLN
1	B	1830	SER
1	B	1831	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) 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	71	GLN
1	A	72	GLN
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	408	GLN
1	A	450	HIS
1	A	459	HIS
1	A	484	ASN
1	A	522	HIS
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	A	763	ASN
1	B	1034	HIS

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Mol	Chain	Res	Type
1	B	1044	ASN
1	B	1062	HIS
1	B	1071	GLN
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	1408	GLN
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
1	B	1763	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 oligosaccharides 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	B	1860	1	15,15,16	1.99	4 (26%)	21,22,23	0.99	2 (9%)
3	PLP	A	860	1	15,15,16	1.90	3 (20%)	21,22,23	1.27	3 (14%)
2	NBG	A	861	-	15,15,15	1.19	1 (6%)	21,21,21	1.54	4 (19%)
2	NBG	B	1861	-	15,15,15	1.41	2 (13%)	21,21,21	1.28	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	B	1860	1	-	0/6/6/8	0/1/1/1
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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1860	PLP	C4A-C4	-5.69	1.40	1.51
3	A	860	PLP	C4A-C4	-4.53	1.42	1.51
3	A	860	PLP	C3-C2	-3.83	1.37	1.41
2	B	1861	NBG	C2-C1	3.63	1.56	1.53
2	A	861	NBG	C2-C1	3.45	1.56	1.53
2	B	1861	NBG	C1-N1	2.45	1.46	1.43
3	B	1860	PLP	C5A-C5	2.33	1.57	1.50
3	A	860	PLP	P-O3P	-2.20	1.46	1.54
3	B	1860	PLP	P-O2P	-2.14	1.46	1.54
3	B	1860	PLP	C3-C2	-2.02	1.38	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	861	NBG	C5-O5-C1	4.65	118.93	112.47
2	B	1861	NBG	C5-O5-C1	3.91	117.90	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	861	NBG	C3-C2-C1	2.82	114.00	109.86
2	B	1861	NBG	C3-C2-C1	2.47	113.49	109.86
2	A	861	NBG	C2-C1-N1	-2.38	108.19	111.25
3	B	1860	PLP	O2P-P-O4P	-2.33	100.60	106.67
2	A	861	NBG	O5-C1-C2	2.19	112.19	109.72
3	A	860	PLP	O3P-P-O2P	2.13	115.79	107.80
2	B	1861	NBG	C2-C1-N1	-2.07	108.58	111.25
3	A	860	PLP	C5A-C5-C6	-2.07	115.99	119.36
3	B	1860	PLP	O3P-P-O2P	2.07	115.55	107.80
3	A	860	PLP	C5-C6-N1	-2.00	120.57	123.83

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%)	-1.74	0 100 100	15, 31, 57, 101	0
1	B	793/846 (93%)	-1.71	0 100 100	16, 32, 60, 101	0
All	All	1585/1692 (93%)	-1.73	0 100 100	15, 32, 59, 101	0

There are no RSRZ outliers to report.

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 oligosaccharides 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(Å ²)	Q<0.9
2	NBG	A	861	15/15	1.00	0.02	14,23,31,32	0
2	NBG	B	1861	15/15	1.00	0.02	17,31,35,38	0
3	PLP	A	860	15/16	1.00	0.02	3,13,26,31	0
3	PLP	B	1860	15/16	1.00	0.02	14,19,31,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.