



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:59 AM GMT

PDB ID : 1JM6
Title : Pyruvate dehydrogenase kinase, isozyme 2, containing ADP
Authors : Steussy, C.N.; Popov, K.M.; Bowker-Kinley, M.M.; Sloan, R.B.; Harris, R.A.;
Hamilton, J.A.
Deposited on : 2001-07-17
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

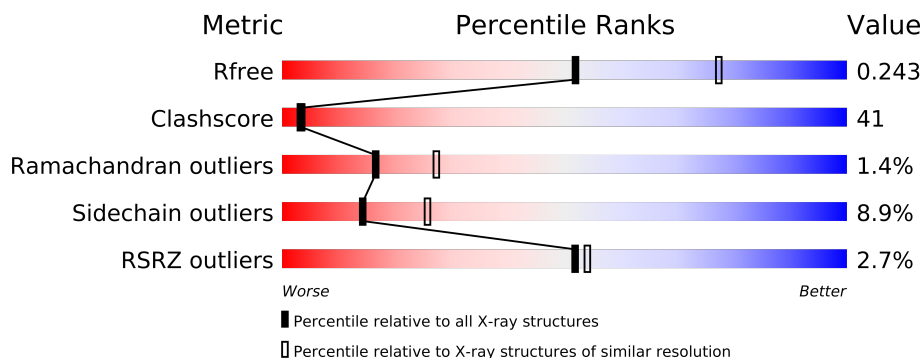
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	407	
1	B	407	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5677 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

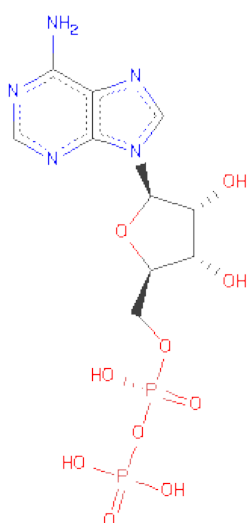
- Molecule 1 is a protein called Pyruvate dehydrogenase kinase, isozyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2709	1743	444	505	17			
1	B	336	Total	C	N	O	S	0	0	0
			2684	1728	441	498	17			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

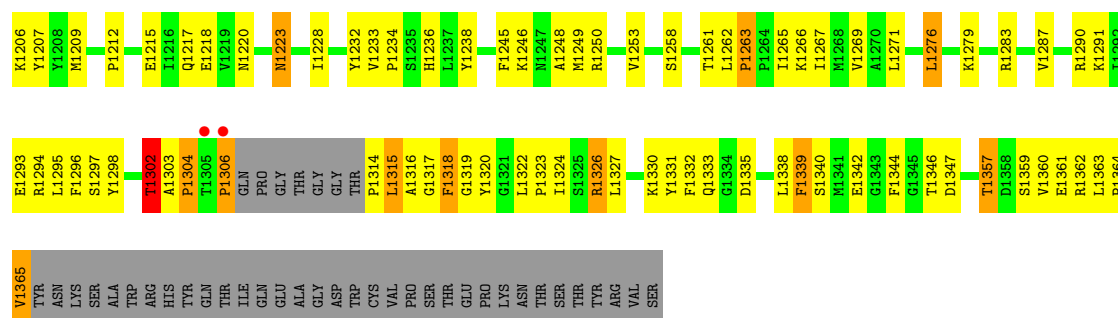
- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		
4	B	109	Total	O	0	0
			109	109		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.42Å 109.87Å 71.41Å 90.00° 104.52° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50 29.26 – 2.40	Depositor EDS
% Data completeness (in resolution range)	84.2 (6.00-2.50) 85.4 (29.26-2.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.39Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.202 , 0.262 0.191 , 0.243	Depositor DCC
R_{free} test set	1626 reflections (4.78%)	DCC
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.5	EDS
Estimated twinning fraction	0.478 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 35644 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5677	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: MG, ADP

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	0.78	6/2771 (0.2%)	1.14	16/3752 (0.4%)
1	B	0.65	5/2745 (0.2%)	0.94	6/3715 (0.2%)
All	All	0.72	11/5516 (0.2%)	1.05	22/7467 (0.3%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1090	PHE	C-N	-8.56	1.14	1.34
1	A	1178	LYS	C-N	-7.66	1.16	1.34
1	B	1306	PRO	CA-C	7.37	1.67	1.52
1	A	1215	GLU	CB-CG	7.13	1.65	1.52
1	B	1215	GLU	CD-OE2	6.47	1.32	1.25
1	B	1306	PRO	C-O	6.01	1.35	1.23
1	A	1215	GLU	CG-CD	5.98	1.60	1.51
1	A	1096	GLU	C-O	5.94	1.34	1.23
1	B	1302	THR	CB-OG1	5.71	1.54	1.43
1	B	1039	LYS	CD-CE	5.42	1.64	1.51
1	A	1366	TYR	C-O	5.22	1.33	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1090	PHE	O-C-N	-12.48	102.73	122.70
1	A	1137	PRO	C-N-CA	10.68	148.39	121.70
1	A	1138	VAL	N-CA-C	10.08	138.22	111.00
1	A	1006	ALA	C-N-CA	-9.54	102.27	122.30
1	A	1090	PHE	CA-C-N	9.25	137.55	117.20
1	B	1059	GLU	OE1-CD-OE2	-7.68	114.09	123.30
1	B	1326	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	A	1090	PHE	C-N-CA	7.45	140.33	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1223	ASN	N-CA-CB	7.43	123.97	110.60
1	A	1137	PRO	CA-C-N	-7.00	101.79	117.20
1	A	1137	PRO	N-CA-C	6.88	129.98	112.10
1	B	1223	ASN	N-CA-C	-6.30	93.99	111.00
1	A	1096	GLU	CA-C-N	6.13	130.68	117.20
1	A	1096	GLU	O-C-N	-5.99	113.12	122.70
1	A	1127	LEU	CA-C-N	-5.80	104.45	117.20
1	A	1026	LYS	C-N-CA	-5.79	107.22	121.70
1	B	1326	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	1099	ARG	CA-C-N	5.42	129.12	117.20
1	B	1263	PRO	CA-N-CD	-5.22	104.20	111.50
1	A	1128	GLU	N-CA-C	-5.16	97.07	111.00
1	A	1195	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	1305	THR	C-N-CD	-5.05	109.48	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2709	0	2692	254	0
1	B	2684	0	2679	192	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	1	0
3	B	27	0	12	9	0
4	A	119	0	0	17	0
4	B	109	0	0	16	0
All	All	5677	0	5395	442	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 41.

All (442) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1042:PHE:CE2	1:A:1095:PRO:HG3	1.64	1.33
1:A:1138:VAL:CG1	1:A:1138:VAL:O	1.75	1.29
1:A:1223:ASN:HD22	1:A:1226:GLN:CB	1.58	1.16
1:A:1031:PHE:HA	1:A:1036:ALA:N	1.60	1.15
1:A:1177:PRO:HD2	1:A:1179:HIS:NE2	1.62	1.14
1:A:1070:THR:HG21	1:A:1125:GLY:HA2	1.30	1.13
1:A:1005:LEU:O	1:A:1005:LEU:HG	1.36	1.12
1:B:1306:PRO:O	1:B:1317:GLY:HA3	1.49	1.11
1:A:1225:THR:O	1:A:1225:THR:HG22	1.44	1.10
1:A:1138:VAL:HG12	1:A:1138:VAL:O	1.30	1.10
1:A:1112:ARG:HH12	1:A:1165:THR:HG21	0.95	1.08
1:A:1038:GLU:HG2	1:A:1168:PHE:CD2	1.89	1.07
1:A:1223:ASN:HD22	1:A:1226:GLN:HB3	0.96	1.06
1:B:1218:GLU:HG2	1:B:1269:VAL:HB	1.39	1.05
1:A:1177:PRO:CD	1:A:1179:HIS:NE2	2.23	1.01
1:A:1112:ARG:NH1	1:A:1165:THR:HG21	1.74	0.99
1:A:1223:ASN:ND2	1:A:1226:GLN:HB3	1.76	0.99
1:A:1042:PHE:HE2	1:A:1095:PRO:CG	1.73	0.99
1:A:1066:ARG:HG2	1:A:1136:ASP:OD2	1.64	0.96
1:A:1042:PHE:HE2	1:A:1095:PRO:HG3	0.81	0.96
1:B:1144:GLN:HE22	1:B:1297:SER:HA	1.31	0.95
1:A:1085:LEU:HA	1:A:1088:MET:HE3	1.48	0.95
1:A:1005:LEU:O	1:A:1005:LEU:CG	2.15	0.94
1:A:1225:THR:CG2	1:A:1225:THR:O	2.16	0.94
1:A:1177:PRO:HD2	1:A:1179:HIS:CE1	2.02	0.94
1:A:1271:LEU:HD13	1:A:1276:LEU:HD22	1.47	0.94
1:A:1178:LYS:O	1:A:1178:LYS:HG3	1.65	0.93
1:A:1138:VAL:HG13	1:A:1138:VAL:O	1.69	0.92
1:B:1144:GLN:NE2	1:B:1297:SER:HA	1.85	0.91
1:B:1152:LEU:HD13	1:B:1364:PRO:CD	2.02	0.90
1:A:1031:PHE:CA	1:A:1036:ALA:N	2.35	0.89
1:B:1346:THR:HG21	3:B:3510:ADP:N6	1.86	0.89
1:B:1258:SER:O	1:B:1262:LEU:CD1	2.21	0.88
1:A:1093:LYS:O	1:A:1095:PRO:HD3	1.73	0.88
1:A:1041:SER:O	1:A:1045:LEU:HB2	1.74	0.88
1:B:1061:ASN:HA	1:B:1068:LEU:HD11	1.54	0.87
1:A:1084:LEU:HG	1:A:1088:MET:CE	2.06	0.86
1:B:1095:PRO:HD3	4:B:6192:HOH:O	1.75	0.84
1:A:1084:LEU:HG	1:A:1088:MET:HE2	1.58	0.84
1:B:1113:ASN:HA	1:B:1116:ASN:HD22	1.41	0.84
1:A:1306:PRO:HG2	4:A:6188:HOH:O	1.77	0.84
1:A:1038:GLU:HG2	1:A:1168:PHE:CE2	2.13	0.83
1:A:1084:LEU:O	1:A:1088:MET:HE2	1.77	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1013:GLU:HG3	4:B:6051:HOH:O	1.78	0.83
1:B:1152:LEU:CD1	1:B:1364:PRO:HD3	2.09	0.82
1:A:1223:ASN:ND2	1:A:1226:GLN:CB	2.38	0.82
1:A:1086:ASP:O	1:A:1089:GLU:HG2	1.79	0.81
1:B:1025:MET:O	1:B:1029:LEU:HD13	1.81	0.80
1:B:1024:SER:H	1:B:1027:GLN:HE21	1.30	0.80
1:B:1002:ASN:HB3	1:B:1082:GLN:HE22	1.48	0.79
1:A:1148:ASP:HA	1:A:1327:LEU:HD11	1.64	0.79
1:B:1152:LEU:HD13	1:B:1364:PRO:HD3	1.64	0.78
1:A:1302:THR:HG22	1:A:1302:THR:O	1.83	0.78
1:A:1067:VAL:O	1:A:1073:VAL:HG21	1.85	0.77
1:B:1022:PRO:HB3	1:B:1361:GLU:O	1.84	0.77
1:A:1084:LEU:C	1:A:1088:MET:HE2	2.05	0.77
1:A:1085:LEU:HD23	1:A:1088:MET:HE3	1.67	0.77
1:B:1097:ASP:O	1:B:1100:THR:HG22	1.85	0.76
1:A:1074:GLN:O	1:A:1075:LEU:C	2.20	0.76
1:A:1177:PRO:CG	1:A:1179:HIS:NE2	2.48	0.76
1:A:1178:LYS:O	1:A:1178:LYS:CG	2.33	0.76
1:A:1012:ILE:HG23	1:A:1054:ALA:HB1	1.67	0.76
1:A:1042:PHE:CE2	1:A:1095:PRO:CG	2.58	0.75
1:A:1163:GLN:NE2	1:A:1182:SER:H	1.85	0.75
1:A:1093:LYS:O	1:A:1095:PRO:CD	2.35	0.74
1:B:1306:PRO:O	1:B:1317:GLY:CA	2.32	0.74
1:B:1258:SER:O	1:B:1262:LEU:HD13	1.86	0.74
1:A:1228:ILE:HD13	1:A:1269:VAL:HG12	1.69	0.74
1:A:1012:ILE:O	1:A:1016:SER:HB3	1.88	0.74
1:A:1037:CYS:HB3	1:A:1040:THR:HG23	1.68	0.74
1:A:1085:LEU:HD23	1:A:1088:MET:CE	2.18	0.74
1:A:1119:VAL:HG12	1:A:1120:PRO:HD3	1.69	0.74
1:B:1250:ARG:NH2	1:B:1303:ALA:HB2	2.03	0.73
1:B:1012:ILE:O	1:B:1016:SER:HB3	1.87	0.73
1:A:1138:VAL:HG22	1:A:1141:GLN:NE2	2.03	0.73
1:B:1152:LEU:HD13	1:B:1364:PRO:HD2	1.69	0.73
1:B:1029:LEU:HD11	1:B:1183:ILE:HG21	1.69	0.73
1:A:1105:THR:O	1:A:1109:VAL:HG23	1.89	0.73
1:A:1041:SER:OG	1:A:1164:HIS:HD2	1.72	0.73
1:A:1089:GLU:OE2	1:A:1090:PHE:CE1	2.42	0.72
1:B:1182:SER:O	1:B:1234:PRO:HD2	1.89	0.72
1:A:1089:GLU:OE2	1:A:1090:PHE:HE1	1.71	0.72
1:B:1271:LEU:HD13	1:B:1276:LEU:HD22	1.70	0.72
1:A:1177:PRO:HB2	1:A:1179:HIS:CD2	2.24	0.72
1:A:1163:GLN:HE22	1:A:1182:SER:H	1.35	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1257:GLU:HG3	4:A:6020:HOH:O	1.90	0.71
1:B:1038:GLU:OE1	1:B:1101:LEU:HD12	1.90	0.71
1:A:1158:ARG:HD2	4:A:6149:HOH:O	1.91	0.71
1:A:1212:PRO:HG3	1:A:1252:THR:HG21	1.71	0.71
1:A:1088:MET:HA	1:A:1091:LEU:HD12	1.72	0.71
1:B:1142:ASN:O	1:B:1143:ILE:C	2.28	0.71
1:A:1070:THR:HG23	1:A:1071:PRO:HD2	1.73	0.71
1:B:1319:GLY:N	3:B:3510:ADP:O1B	2.20	0.70
1:A:1299:MET:HG2	4:A:6187:HOH:O	1.91	0.70
1:B:1152:LEU:CD1	1:B:1364:PRO:CD	2.69	0.70
1:A:1063:LEU:CD2	1:A:1067:VAL:HG21	2.22	0.69
1:B:1346:THR:HG21	3:B:3510:ADP:HN62	1.56	0.69
1:B:1249:MET:O	1:B:1253:VAL:HG23	1.93	0.69
1:B:1094:ASP:O	1:B:1100:THR:HG21	1.92	0.69
1:A:1138:VAL:HG22	1:A:1141:GLN:HE22	1.57	0.69
1:A:1020:PRO:HD2	1:A:1366:TYR:HB2	1.74	0.69
1:A:1112:ARG:HH12	1:A:1165:THR:CG2	1.90	0.68
1:A:1199:MET:HG3	1:A:1238:TYR:OH	1.93	0.68
1:A:1063:LEU:CD2	1:A:1067:VAL:CG2	2.72	0.68
1:A:1020:PRO:HD2	1:A:1366:TYR:CB	2.25	0.67
1:A:1066:ARG:NE	1:A:1136:ASP:OD1	2.28	0.67
1:A:1083:SER:OG	1:A:1111:ILE:HG23	1.94	0.67
1:A:1037:CYS:HB3	1:A:1040:THR:CG2	2.23	0.67
1:B:1346:THR:CG2	3:B:3510:ADP:HN62	2.08	0.66
1:B:1142:ASN:OD1	1:B:1145:TYR:HB3	1.95	0.66
1:B:1106:ASP:HA	4:B:6193:HOH:O	1.93	0.66
1:A:1113:ASN:HA	1:A:1116:ASN:ND2	2.11	0.66
1:B:1022:PRO:HG3	1:B:1363:LEU:HD12	1.78	0.65
1:B:1295:LEU:HD22	3:B:3510:ADP:O4'	1.97	0.65
1:A:1220:ASN:OD1	1:A:1223:ASN:N	2.25	0.65
1:A:1112:ARG:HD2	1:A:1162:ASN:HD21	1.61	0.65
1:A:1088:MET:HG2	1:A:1091:LEU:CD1	2.27	0.65
1:B:1068:LEU:O	1:B:1074:GLN:HG3	1.97	0.65
1:B:1291:LYS:HG2	1:B:1294:ARG:NH1	2.12	0.65
1:B:1163:GLN:OE1	1:B:1181:GLY:HA3	1.97	0.65
1:A:1118:VAL:HG21	4:A:6148:HOH:O	1.95	0.64
1:B:1123:ALA:O	1:B:1126:VAL:HG22	1.96	0.64
1:A:1165:THR:HG22	4:A:6183:HOH:O	1.97	0.64
1:B:1116:ASN:ND2	4:B:6234:HOH:O	2.30	0.64
1:A:1089:GLU:HG3	1:A:1090:PHE:CD1	2.33	0.64
1:A:1279:LYS:NZ	4:A:6186:HOH:O	2.31	0.64
1:B:1220:ASN:CG	1:B:1223:ASN:O	2.35	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1088:MET:HA	1:A:1091:LEU:CD1	2.28	0.63
1:A:1053:LEU:HD22	1:A:1080:TYR:CD2	2.33	0.63
1:B:1119:VAL:HG22	1:B:1151:TYR:CE2	2.34	0.63
1:A:1237:LEU:HA	1:A:1240:MET:HE2	1.81	0.63
1:B:1093:LYS:NZ	1:B:1103:GLN:OE1	2.31	0.62
1:B:1331:TYR:CE1	1:B:1361:GLU:HB2	2.34	0.62
1:B:1038:GLU:CD	1:B:1101:LEU:HD12	2.18	0.62
1:B:1346:THR:HG21	3:B:3510:ADP:C6	2.34	0.62
1:A:1112:ARG:O	1:A:1116:ASN:ND2	2.32	0.62
1:A:1272:GLY:HA3	1:B:1342:GLU:HG2	1.82	0.62
1:B:1113:ASN:HA	1:B:1116:ASN:ND2	2.13	0.62
1:B:1197:TYR:CE2	1:B:1201:LYS:HD3	2.34	0.62
1:A:1296:PHE:O	1:A:1323:PRO:HG3	1.99	0.62
1:A:1153:SER:O	1:A:1157:ILE:HD12	2.01	0.61
1:A:1084:LEU:O	1:A:1088:MET:CE	2.49	0.61
1:B:1261:THR:O	1:B:1263:PRO:HD3	2.00	0.61
1:A:1156:SER:O	1:A:1160:LEU:HG	2.01	0.60
1:B:1290:ARG:HH11	1:B:1294:ARG:HH22	1.47	0.60
1:B:1326:ARG:HD2	4:B:6042:HOH:O	2.01	0.60
1:A:1152:LEU:CD1	1:A:1364:PRO:HD3	2.31	0.60
1:B:1038:GLU:CG	1:B:1101:LEU:HD12	2.31	0.60
1:A:1316:ALA:HB3	4:A:4603:HOH:O	2.02	0.60
1:A:1320:TYR:O	1:A:1323:PRO:HD2	2.02	0.60
1:A:1063:LEU:HD11	1:A:1146:PHE:CD2	2.37	0.60
1:A:1228:ILE:CD1	1:A:1269:VAL:HG12	2.32	0.59
1:B:1023:LEU:HD11	1:B:1044:PHE:HZ	1.67	0.59
1:B:1266:LYS:HD2	4:B:6090:HOH:O	2.01	0.59
1:A:1089:GLU:CG	1:A:1090:PHE:CD1	2.86	0.59
1:B:1207:TYR:CD1	1:B:1314:PRO:HB3	2.37	0.59
1:B:1057:MET:SD	1:B:1080:TYR:HB3	2.43	0.59
1:A:1063:LEU:HD22	1:A:1067:VAL:HG22	1.83	0.59
1:A:1067:VAL:HG12	1:A:1129:TYR:CE1	2.38	0.59
1:B:1144:GLN:HE22	1:B:1297:SER:CA	2.12	0.59
1:A:1302:THR:CG2	1:A:1302:THR:O	2.51	0.58
1:A:1163:GLN:O	1:A:1167:ILE:HG13	2.01	0.58
1:B:1258:SER:HB3	4:B:6012:HOH:O	2.02	0.58
1:B:1063:LEU:HG	1:B:1064:PRO:HD2	1.86	0.58
1:A:1331:TYR:CE1	1:A:1361:GLU:HG2	2.39	0.58
1:A:1250:ARG:HD3	4:A:6072:HOH:O	2.03	0.58
1:A:1116:ASN:ND2	4:A:6081:HOH:O	2.29	0.58
1:A:1112:ARG:HD2	1:A:1162:ASN:ND2	2.19	0.57
1:A:1020:PRO:CD	1:A:1366:TYR:HB2	2.34	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1159:MET:HG3	1:B:1331:TYR:OH	2.04	0.57
1:A:1088:MET:HG2	1:A:1091:LEU:HD11	1.86	0.57
1:B:1038:GLU:HG2	1:B:1101:LEU:CD1	2.34	0.57
1:A:1025:MET:HG3	1:A:1029:LEU:HD12	1.86	0.57
1:A:1152:LEU:HD12	1:A:1364:PRO:HD3	1.87	0.57
1:A:1084:LEU:CG	1:A:1088:MET:HE2	2.33	0.57
1:A:1249:MET:O	1:A:1253:VAL:HG23	2.05	0.57
1:A:1294:ARG:O	1:A:1296:PHE:N	2.37	0.57
1:A:1215:GLU:OE1	1:A:1266:LYS:HD2	2.05	0.57
1:A:1097:ASP:O	1:A:1098:HIS:C	2.41	0.57
1:A:1039:LYS:O	1:A:1043:THR:HB	2.05	0.56
1:B:1250:ARG:HH12	1:B:1302:THR:HG22	1.69	0.56
1:A:1072:SER:HB3	1:A:1121:THR:O	2.05	0.56
1:A:1063:LEU:HD22	1:A:1067:VAL:CG2	2.36	0.56
1:B:1250:ARG:NH1	1:B:1302:THR:HG22	2.21	0.56
1:A:1293:GLU:HG3	4:A:6221:HOH:O	2.04	0.56
1:A:1046:ARG:O	1:A:1091:LEU:HD21	2.06	0.56
1:B:1084:LEU:O	1:B:1088:MET:HG3	2.04	0.56
1:B:1144:GLN:HE22	1:B:1298:TYR:H	1.54	0.56
1:B:1063:LEU:HD23	1:B:1067:VAL:HG13	1.87	0.56
1:A:1042:PHE:CD2	1:A:1095:PRO:HG3	2.34	0.56
1:A:1031:PHE:C	1:A:1036:ALA:N	2.59	0.56
1:A:1045:LEU:HB3	1:A:1104:PHE:HZ	1.70	0.55
1:A:1143:ILE:HG22	1:A:1147:LEU:HD22	1.88	0.55
1:B:1002:ASN:CB	1:B:1082:GLN:HE22	2.18	0.55
1:A:1099:ARG:HA	1:A:1102:SER:OG	2.07	0.55
1:A:1177:PRO:HB2	1:A:1179:HIS:HD2	1.70	0.55
1:A:1063:LEU:HD23	1:A:1067:VAL:CG2	2.35	0.55
1:B:1207:TYR:CE1	1:B:1314:PRO:HB3	2.41	0.55
1:B:1228:ILE:CD1	1:B:1269:VAL:HG12	2.36	0.55
1:A:1146:PHE:HD2	1:A:1147:LEU:HD12	1.70	0.55
1:A:1146:PHE:CD2	1:A:1147:LEU:HD12	2.41	0.55
1:A:1113:ASN:HA	1:A:1116:ASN:HD22	1.70	0.55
1:B:1117:ASP:O	1:B:1120:PRO:HD2	2.07	0.55
1:B:1039:LYS:NZ	1:B:1096:GLU:OE1	2.30	0.55
1:A:1168:PHE:O	1:A:1169:ASP:C	2.46	0.55
1:A:1167:ILE:O	1:A:1167:ILE:HG22	2.05	0.55
1:B:1059:GLU:CD	1:B:1149:ARG:HH21	2.10	0.55
1:A:1186:ASN:O	1:A:1186:ASN:ND2	2.40	0.55
1:B:1228:ILE:HD13	1:B:1269:VAL:HG12	1.88	0.54
1:B:1029:LEU:HA	1:B:1180:ILE:HG21	1.88	0.54
1:A:1353:LYS:HG2	1:A:1358:ASP:HB2	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1064:PRO:HD2	1:B:1067:VAL:CG1	2.38	0.54
1:A:1023:LEU:HD11	1:A:1044:PHE:HZ	1.72	0.54
1:A:1038:GLU:CG	1:A:1168:PHE:CD2	2.77	0.54
1:B:1346:THR:CG2	3:B:3510:ADP:N6	2.62	0.54
1:B:1022:PRO:HG3	1:B:1363:LEU:CD1	2.36	0.54
1:A:1023:LEU:HD11	1:A:1044:PHE:CZ	2.42	0.54
1:B:1081:VAL:O	1:B:1085:LEU:HG	2.08	0.54
1:A:1063:LEU:HD23	1:A:1067:VAL:HG21	1.89	0.54
1:B:1061:ASN:CB	4:B:6231:HOH:O	2.56	0.54
1:A:1294:ARG:C	1:A:1296:PHE:H	2.11	0.54
1:B:1320:TYR:HB2	1:B:1324:ILE:CD1	2.37	0.54
1:B:1100:THR:CG2	1:B:1101:LEU:HD23	2.38	0.54
1:A:1279:LYS:HG3	1:A:1349:VAL:HG22	1.89	0.53
1:B:1304:PRO:CB	1:B:1306:PRO:HD2	2.39	0.53
1:A:1063:LEU:CD2	1:A:1067:VAL:HG22	2.38	0.53
1:B:1100:THR:HG23	1:B:1101:LEU:HD23	1.91	0.53
1:A:1152:LEU:HD13	1:A:1363:LEU:HA	1.91	0.53
1:A:1297:SER:HB3	1:A:1300:TYR:CB	2.38	0.53
1:B:1304:PRO:O	1:B:1317:GLY:CA	2.56	0.53
1:B:1246:LYS:HD2	1:B:1315:LEU:HD22	1.91	0.53
1:A:1212:PRO:HG3	1:A:1252:THR:CG2	2.37	0.53
1:B:1119:VAL:HG22	1:B:1151:TYR:HE2	1.73	0.53
1:A:1099:ARG:O	1:A:1100:THR:C	2.46	0.53
1:B:1041:SER:HB3	1:B:1164:HIS:CE1	2.44	0.53
1:A:1364:PRO:O	1:A:1366:TYR:HD2	1.92	0.53
1:B:1302:THR:HB	3:B:3510:ADP:O2'	2.10	0.52
1:A:1177:PRO:HG2	1:A:1179:HIS:NE2	2.22	0.52
1:B:1070:THR:HG23	1:B:1128:GLU:HG3	1.90	0.52
1:A:1063:LEU:HD11	1:A:1146:PHE:CE2	2.43	0.52
1:A:1019:SER:OG	1:A:1366:TYR:C	2.48	0.52
1:B:1058:LYS:NZ	4:B:6230:HOH:O	2.42	0.52
1:A:1025:MET:HG3	1:A:1029:LEU:CD1	2.39	0.52
1:A:1355:LEU:HB2	1:A:1358:ASP:OD2	2.09	0.52
1:A:1084:LEU:HG	1:A:1088:MET:HE1	1.87	0.52
1:B:1152:LEU:HD12	1:B:1364:PRO:HD3	1.89	0.52
1:A:1223:ASN:ND2	1:A:1226:GLN:HB2	2.24	0.51
1:A:1038:GLU:HB3	1:A:1101:LEU:HD13	1.91	0.51
1:A:1163:GLN:NE2	1:A:1182:SER:OG	2.42	0.51
1:B:1159:MET:HG3	1:B:1331:TYR:CE2	2.45	0.51
1:A:1038:GLU:O	1:A:1041:SER:N	2.43	0.51
1:A:1020:PRO:HG2	1:A:1366:TYR:HB3	1.93	0.51
1:B:1024:SER:HB3	1:B:1027:GLN:HG3	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1070:THR:CG2	1:B:1128:GLU:HG3	2.40	0.51
1:B:1051:VAL:O	1:B:1055:ASN:OD1	2.29	0.51
1:B:1220:ASN:OD1	1:B:1223:ASN:O	2.28	0.51
1:B:1165:THR:O	1:B:1169:ASP:OD2	2.28	0.51
1:B:1119:VAL:HB	1:B:1120:PRO:HD3	1.93	0.50
1:B:1163:GLN:O	1:B:1167:ILE:HG13	2.11	0.50
1:A:1193:VAL:HA	1:A:1241:LEU:HD13	1.92	0.50
1:A:1061:ASN:HD22	1:A:1061:ASN:H	1.57	0.50
1:A:1112:ARG:HB2	1:A:1161:ILE:HG21	1.93	0.50
1:B:1038:GLU:CG	1:B:1101:LEU:CD1	2.89	0.50
1:A:1146:PHE:CZ	1:A:1150:PHE:HB2	2.47	0.50
1:B:1189:VAL:O	1:B:1193:VAL:HG23	2.12	0.49
1:B:1316:ALA:HB2	4:B:6087:HOH:O	2.11	0.49
1:A:1061:ASN:HD22	1:A:1061:ASN:N	2.10	0.49
1:A:1247:ASN:ND2	3:A:3500:ADP:O2A	2.45	0.49
1:B:1031:PHE:O	1:B:1032:GLY:O	2.30	0.49
1:A:1167:ILE:CG2	1:A:1167:ILE:O	2.60	0.49
1:A:1020:PRO:HB3	1:A:1363:LEU:HD13	1.95	0.49
1:A:1318:PHE:HE1	4:A:6218:HOH:O	1.94	0.49
1:A:1190:SER:OG	1:A:1218:GLU:OE2	2.29	0.49
1:B:1008:ALA:HB3	1:B:1009:PRO:HD3	1.94	0.49
1:A:1180:ILE:HD12	1:A:1185:PRO:HG3	1.95	0.49
1:B:1144:GLN:HE22	1:B:1298:TYR:N	2.10	0.49
1:A:1212:PRO:HB3	1:A:1263:PRO:O	2.12	0.49
1:B:1111:ILE:O	1:B:1115:HIS:HD2	1.96	0.49
1:A:1053:LEU:CD1	1:A:1083:SER:O	2.61	0.49
1:A:1019:SER:OG	1:A:1366:TYR:HB2	2.13	0.49
1:B:1197:TYR:O	1:B:1201:LYS:HB2	2.13	0.48
1:A:1066:ARG:CG	1:A:1136:ASP:OD2	2.50	0.48
1:A:1038:GLU:CB	1:A:1101:LEU:HD13	2.43	0.48
1:A:1067:VAL:HG12	1:A:1129:TYR:HE1	1.77	0.48
1:A:1042:PHE:CE2	1:A:1046:ARG:NH1	2.81	0.48
1:A:1119:VAL:HG22	1:A:1151:TYR:CE2	2.49	0.48
1:B:1250:ARG:CZ	1:B:1303:ALA:HB2	2.44	0.48
1:A:1148:ASP:OD1	1:A:1327:LEU:HD21	2.14	0.48
1:A:1294:ARG:C	1:A:1296:PHE:N	2.66	0.47
1:B:1003:ALA:H	1:B:1085:LEU:HB3	1.79	0.47
1:A:1084:LEU:C	1:A:1088:MET:CE	2.81	0.47
1:A:1363:LEU:HB2	1:A:1366:TYR:CE2	2.49	0.47
1:A:1341:MET:CE	1:B:1279:LYS:HE2	2.43	0.47
1:A:1136:ASP:N	1:A:1137:PRO:CD	2.76	0.47
1:B:1012:ILE:HG23	1:B:1054:ALA:HB1	1.95	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1046:ARG:NH1	1:B:1090:PHE:O	2.45	0.47
1:A:1085:LEU:HD23	1:A:1088:MET:HE1	1.95	0.47
1:B:1061:ASN:HB2	4:B:6231:HOH:O	2.12	0.47
1:B:1159:MET:HE3	1:B:1233:VAL:HG21	1.95	0.47
1:B:1149:ARG:HH22	1:B:1365:VAL:HB	1.78	0.47
1:A:1081:VAL:O	1:A:1085:LEU:HG	2.13	0.47
1:A:1129:TYR:C	1:A:1136:ASP:HB3	2.35	0.47
1:B:1346:THR:HG22	4:B:6060:HOH:O	2.14	0.47
1:B:1258:SER:HB3	1:B:1261:THR:OG1	2.15	0.47
1:A:1075:LEU:HD23	1:A:1121:THR:HG21	1.96	0.47
1:A:1200:ALA:C	1:A:1249:MET:HE1	2.35	0.47
1:A:1163:GLN:HE22	1:A:1182:SER:N	2.08	0.47
1:A:1058:LYS:O	1:A:1062:LEU:HD13	2.14	0.47
1:A:1092:ASP:OD1	1:A:1093:LYS:N	2.48	0.47
1:A:1042:PHE:CZ	1:A:1046:ARG:NH1	2.82	0.47
1:B:1038:GLU:O	1:B:1041:SER:N	2.48	0.47
1:B:1199:MET:HG3	1:B:1238:TYR:OH	2.15	0.46
1:B:1304:PRO:O	1:B:1317:GLY:HA3	2.16	0.46
1:A:1305:THR:HG23	1:A:1306:PRO:HD2	1.96	0.46
1:A:1042:PHE:CZ	1:A:1046:ARG:HD3	2.51	0.46
1:B:1060:ILE:O	1:B:1063:LEU:HB2	2.15	0.46
1:B:1002:ASN:HB3	1:B:1082:GLN:NE2	2.25	0.46
1:B:1044:PHE:CD2	1:B:1045:LEU:HD13	2.51	0.46
1:A:1070:THR:HG23	1:A:1071:PRO:CD	2.45	0.46
1:A:1339:PHE:CE1	1:B:1339:PHE:HB3	2.51	0.46
1:B:1052:ARG:CZ	1:B:1160:LEU:HD11	2.46	0.46
1:B:1267:ILE:HA	1:B:1279:LYS:O	2.16	0.46
1:A:1143:ILE:O	1:A:1147:LEU:HB2	2.16	0.46
1:A:1353:LYS:HG2	1:A:1358:ASP:CB	2.46	0.46
1:B:1061:ASN:HA	1:B:1068:LEU:CD1	2.38	0.45
1:B:1198:ASP:O	1:B:1199:MET:O	2.33	0.45
1:B:1332:PHE:O	1:B:1333:GLN:HB2	2.16	0.45
1:A:1053:LEU:CD2	1:A:1080:TYR:CD2	2.99	0.45
1:A:1042:PHE:O	1:A:1043:THR:C	2.54	0.45
1:B:1263:PRO:HB3	1:B:1283:ARG:NE	2.32	0.45
1:A:1320:TYR:C	1:A:1323:PRO:HD2	2.36	0.45
1:B:1094:ASP:OD2	1:B:1097:ASP:HB2	2.16	0.45
1:B:1098:HIS:HB2	4:B:6117:HOH:O	2.16	0.45
1:B:1245:PHE:O	1:B:1249:MET:HG3	2.17	0.45
1:A:1196:ALA:HA	1:A:1238:TYR:CE1	2.51	0.45
1:A:1012:ILE:HG23	1:A:1054:ALA:CB	2.41	0.45
1:A:1089:GLU:CG	1:A:1090:PHE:CE1	3.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1020:PRO:CD	1:A:1366:TYR:CB	2.92	0.44
1:B:1333:GLN:HG2	1:B:1360:VAL:O	2.18	0.44
1:A:1045:LEU:HD12	1:A:1045:LEU:HA	1.78	0.44
1:B:1212:PRO:HD2	1:B:1249:MET:HB3	2.00	0.44
1:B:1233:VAL:HG11	1:B:1236:HIS:CD2	2.53	0.44
1:A:1158:ARG:NH1	4:A:6082:HOH:O	2.51	0.44
1:A:1318:PHE:HB2	1:A:1320:TYR:CE2	2.53	0.44
1:A:1152:LEU:HD13	1:A:1364:PRO:HD3	2.00	0.44
1:B:1106:ASP:CA	4:B:6193:HOH:O	2.59	0.44
1:A:1200:ALA:HB1	1:A:1249:MET:CE	2.47	0.44
1:A:1297:SER:HB3	1:A:1300:TYR:HB3	1.98	0.44
1:A:1330:LYS:HA	1:A:1334:GLY:O	2.17	0.44
1:A:1223:ASN:ND2	1:A:1226:GLN:OE1	2.50	0.44
1:A:1053:LEU:O	1:A:1057:MET:HG3	2.18	0.44
1:B:1023:LEU:HD11	1:B:1044:PHE:CZ	2.49	0.44
1:B:1324:ILE:O	1:B:1327:LEU:HB2	2.18	0.43
1:A:1143:ILE:O	1:A:1147:LEU:HD13	2.18	0.43
1:B:1203:LEU:HB3	1:B:1315:LEU:HD23	1.99	0.43
1:B:1322:LEU:N	3:B:3510:ADP:O1A	2.43	0.43
1:B:1068:LEU:HA	1:B:1073:VAL:HG11	2.00	0.43
1:B:1331:TYR:O	1:B:1361:GLU:HA	2.18	0.43
1:A:1166:LEU:HA	1:A:1166:LEU:HD23	1.87	0.43
1:A:1177:PRO:CB	1:A:1179:HIS:CD2	3.00	0.43
4:A:6186:HOH:O	1:B:1344:PHE:HE2	2.01	0.43
1:B:1015:PHE:HB3	1:B:1051:VAL:HA	2.00	0.43
1:B:1038:GLU:HG2	1:B:1101:LEU:HD13	1.99	0.43
1:A:1072:SER:OG	1:A:1124:GLN:HB3	2.18	0.43
1:A:1158:ARG:NH2	4:A:6153:HOH:O	2.45	0.43
1:A:1199:MET:CG	1:A:1238:TYR:OH	2.64	0.43
1:A:1070:THR:HG21	1:A:1125:GLY:CA	2.22	0.43
1:B:1043:THR:O	4:B:6190:HOH:O	2.21	0.43
1:B:1012:ILE:O	1:B:1016:SER:N	2.50	0.43
1:B:1059:GLU:OE1	1:B:1149:ARG:NH2	2.50	0.43
1:A:1188:SER:O	1:A:1189:VAL:C	2.55	0.43
1:B:1082:GLN:HB3	1:B:1114:ARG:NH1	2.33	0.42
1:A:1074:GLN:O	1:A:1077:GLN:N	2.52	0.42
1:A:1250:ARG:HH22	1:A:1302:THR:C	2.22	0.42
1:B:1318:PHE:HB3	1:B:1320:TYR:CE2	2.54	0.42
1:B:1041:SER:HB3	1:B:1164:HIS:ND1	2.34	0.42
1:B:1057:MET:HA	1:B:1060:ILE:HD12	2.01	0.42
1:B:1330:LYS:HE2	1:B:1335:ASP:OD2	2.19	0.42
1:A:1291:LYS:O	1:A:1294:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1297:SER:HB3	1:A:1300:TYR:HB2	2.01	0.42
1:B:1124:GLN:HE22	1:B:1127:LEU:HD23	1.85	0.42
1:B:1164:HIS:NE2	4:B:6027:HOH:O	2.25	0.42
1:B:1049:LEU:HB3	1:B:1087:ILE:HD13	2.01	0.42
1:B:1246:LYS:HA	1:B:1249:MET:HE2	2.01	0.42
1:B:1287:VAL:HG12	1:B:1291:LYS:HB2	2.02	0.42
1:A:1341:MET:HE1	1:B:1279:LYS:HE2	2.01	0.42
1:A:1067:VAL:N	1:A:1129:TYR:HE1	2.18	0.42
1:B:1023:LEU:N	1:B:1023:LEU:HD12	2.35	0.42
1:B:1202:LEU:O	1:B:1206:LYS:HG3	2.20	0.42
1:A:1159:MET:O	1:A:1163:GLN:HG2	2.19	0.42
1:B:1128:GLU:HA	1:B:1128:GLU:OE1	2.20	0.42
1:B:1250:ARG:HB2	1:B:1315:LEU:HD12	2.02	0.42
1:A:1060:ILE:O	1:A:1060:ILE:CG2	2.68	0.42
1:A:1070:THR:HG23	1:A:1128:GLU:OE1	2.20	0.41
1:A:1068:LEU:HA	1:A:1073:VAL:HG11	2.02	0.41
1:A:1020:PRO:HD2	1:A:1366:TYR:HB3	2.00	0.41
1:B:1044:PHE:HD2	1:B:1045:LEU:HD13	1.85	0.41
1:A:1029:LEU:HD23	1:A:1180:ILE:HD13	2.02	0.41
1:A:1193:VAL:HG22	1:A:1241:LEU:HD13	2.01	0.41
1:B:1202:LEU:HA	1:B:1202:LEU:HD12	1.87	0.41
1:A:1129:TYR:O	1:A:1136:ASP:HB3	2.20	0.41
1:A:1262:LEU:HA	1:A:1263:PRO:HD3	1.90	0.41
1:B:1290:ARG:NH1	1:B:1294:ARG:HH22	2.16	0.41
1:B:1159:MET:HE2	1:B:1182:SER:OG	2.20	0.41
1:B:1339:PHE:CD1	1:B:1347:ASP:HB2	2.55	0.41
1:A:1265:ILE:HG21	1:A:1265:ILE:HD13	1.90	0.41
1:B:1218:GLU:HA	1:B:1269:VAL:O	2.20	0.41
1:B:1190:SER:OG	1:B:1218:GLU:OE1	2.31	0.41
1:B:1096:GLU:OE1	1:B:1096:GLU:HA	2.20	0.41
1:B:1049:LEU:HB2	1:B:1050:PRO:HD3	2.03	0.41
1:B:1357:THR:HG23	1:B:1357:THR:O	2.21	0.41
1:B:1159:MET:HG3	1:B:1331:TYR:CZ	2.56	0.41
1:A:1187:CYS:O	1:A:1229:HIS:HA	2.20	0.41
1:A:1144:GLN:OE1	1:A:1298:TYR:CD1	2.74	0.41
1:A:1332:PHE:O	1:A:1333:GLN:HB2	2.21	0.41
1:A:1039:LYS:O	1:A:1043:THR:CB	2.68	0.41
1:B:1030:ASP:O	1:B:1036:ALA:N	2.54	0.41
1:A:1324:ILE:CG2	4:A:6096:HOH:O	2.68	0.41
1:A:1220:ASN:HB3	1:A:1223:ASN:O	2.21	0.41
1:A:1086:ASP:O	1:A:1089:GLU:CG	2.59	0.41
1:A:1154:ARG:HD2	4:A:6148:HOH:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1197:TYR:CZ	1:B:1201:LYS:HD3	2.56	0.41
1:A:1331:TYR:OH	1:A:1361:GLU:OE2	2.39	0.41
1:B:1296:PHE:O	1:B:1323:PRO:HG3	2.21	0.41
1:A:1008:ALA:HB3	1:A:1009:PRO:HD3	2.02	0.41
1:B:1042:PHE:HE1	1:B:1090:PHE:HB3	1.86	0.41
1:B:1304:PRO:O	1:B:1317:GLY:HA2	2.20	0.40
1:B:1111:ILE:O	1:B:1115:HIS:CD2	2.74	0.40
1:B:1205:ASP:O	1:B:1209:MET:HA	2.21	0.40
1:A:1140:ASN:HB3	1:A:1142:ASN:ND2	2.36	0.40
1:B:1203:LEU:HD23	1:B:1203:LEU:HA	1.78	0.40
1:A:1047:GLN:O	1:A:1051:VAL:HG23	2.21	0.40
1:A:1085:LEU:HA	1:A:1088:MET:CE	2.32	0.40
1:B:1002:ASN:OD1	1:B:1082:GLN:NE2	2.54	0.40
1:A:1012:ILE:HD11	1:A:1057:MET:SD	2.61	0.40
1:B:1248:ALA:CB	1:B:1265:ILE:HD12	2.51	0.40
1:A:1250:ARG:NH2	1:A:1302:THR:O	2.54	0.40
1:B:1232:TYR:O	1:B:1234:PRO:HD3	2.21	0.40
1:B:1053:LEU:HD23	1:B:1080:TYR:CD2	2.56	0.40
1:B:1063:LEU:HG	1:B:1064:PRO:CD	2.52	0.40
1:A:1203:LEU:N	1:A:1203:LEU:HD23	2.36	0.40
1:A:1182:SER:O	1:A:1233:VAL:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	329/407 (81%)	290 (88%)	32 (10%)	7 (2%)	11	16
1	B	326/407 (80%)	306 (94%)	18 (6%)	2 (1%)	33	55
All	All	655/814 (80%)	596 (91%)	50 (8%)	9 (1%)	16	27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1138	VAL
1	A	1224	ALA
1	A	1295	LEU
1	A	1039	LYS
1	B	1199	MET
1	A	1137	PRO
1	A	1304	PRO
1	B	1304	PRO
1	A	1095	PRO

5.3.2 Protein sidechains ⓘ

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	305/363 (84%)	277 (91%)	28 (9%)	13	24
1	B	302/363 (83%)	276 (91%)	26 (9%)	15	27
All	All	607/726 (84%)	553 (91%)	54 (9%)	14	26

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1004	SER
1	A	1005	LEU
1	A	1013	GLU
1	A	1016	SER
1	A	1024	SER
1	A	1026	LYS
1	A	1045	LEU
1	A	1047	GLN
1	A	1061	ASN
1	A	1063	LEU
1	A	1067	VAL
1	A	1068	LEU
1	A	1078	SER
1	A	1128	GLU
1	A	1152	LEU
1	A	1153	SER
1	A	1217	GLN

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Mol	Chain	Res	Type
1	A	1257	GLU
1	A	1262	LEU
1	A	1266	LYS
1	A	1268	MET
1	A	1273	GLU
1	A	1276	LEU
1	A	1318	PHE
1	A	1353	LYS
1	A	1357	THR
1	A	1358	ASP
1	A	1362	ARG
1	B	1002	ASN
1	B	1013	GLU
1	B	1016	SER
1	B	1019	SER
1	B	1030	ASP
1	B	1041	SER
1	B	1045	LEU
1	B	1101	LEU
1	B	1152	LEU
1	B	1158	ARG
1	B	1159	MET
1	B	1169	ASP
1	B	1188	SER
1	B	1217	GLN
1	B	1276	LEU
1	B	1293	GLU
1	B	1302	THR
1	B	1315	LEU
1	B	1318	PHE
1	B	1338	LEU
1	B	1339	PHE
1	B	1340	SER
1	B	1357	THR
1	B	1359	SER
1	B	1362	ARG
1	B	1365	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1047	GLN

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Mol	Chain	Res	Type
1	A	1061	ASN
1	A	1116	ASN
1	A	1142	ASN
1	A	1162	ASN
1	A	1163	GLN
1	A	1164	HIS
1	A	1217	GLN
1	A	1223	ASN
1	A	1236	HIS
1	A	1239	HIS
1	B	1002	ASN
1	B	1027	GLN
1	B	1055	ASN
1	B	1061	ASN
1	B	1077	GLN
1	B	1082	GLN
1	B	1116	ASN
1	B	1144	GLN
1	B	1256	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	ADP	A	3500	2	29,29,29	1.50	5 (17%)	45,45,45	2.46	7 (15%)
3	ADP	B	3510	2	29,29,29	1.49	5 (17%)	45,45,45	2.46	7 (15%)

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	ADP	A	3500	2	-	0/16/32/32	0/1/3/3
3	ADP	B	3510	2	-	0/16/32/32	0/1/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3500	ADP	C4-N9	-3.98	1.31	1.37
3	B	3510	ADP	C4-N9	-3.96	1.32	1.37
3	A	3500	ADP	PB-O3A	-2.85	1.55	1.60
3	B	3510	ADP	PB-O2B	2.84	1.65	1.54
3	A	3500	ADP	PB-O2B	2.84	1.65	1.54
3	B	3510	ADP	PB-O3A	-2.81	1.55	1.60
3	B	3510	ADP	O4'-C1'	2.77	1.45	1.41
3	A	3500	ADP	O4'-C1'	2.75	1.45	1.41
3	A	3500	ADP	PA-O3A	-2.52	1.55	1.59
3	B	3510	ADP	PA-O3A	-2.50	1.55	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3500	ADP	N3-C2-N1	-11.30	119.27	128.71
3	B	3510	ADP	N3-C2-N1	-11.29	119.27	128.71
3	B	3510	ADP	O4'-C1'-N9	6.12	114.14	108.44
3	A	3500	ADP	O4'-C1'-N9	6.11	114.12	108.44
3	A	3500	ADP	C4-C5-N7	-5.59	104.73	109.52
3	B	3510	ADP	C4-C5-N7	-5.58	104.74	109.52
3	B	3510	ADP	N3-C4-N9	4.65	133.83	125.43
3	A	3500	ADP	N3-C4-N9	4.65	133.82	125.43
3	B	3510	ADP	C5-C4-N3	-3.59	117.87	125.70
3	A	3500	ADP	C5-C4-N3	-3.59	117.89	125.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3510	ADP	C2-N3-C4	3.54	124.10	114.01
3	A	3500	ADP	C2-N3-C4	3.54	124.09	114.01
3	B	3510	ADP	N7-C8-N9	-2.25	108.00	114.36
3	A	3500	ADP	N7-C8-N9	-2.25	108.01	114.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	339/407 (83%)	0.21	10 (2%) 49 51	19, 41, 80, 117	0
1	B	336/407 (82%)	0.19	8 (2%) 56 58	20, 40, 70, 107	0
All	All	675/814 (82%)	0.20	18 (2%) 52 54	19, 41, 74, 117	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1366	TYR	7.1
1	A	1177	PRO	6.1
1	A	1036	ALA	5.6
1	B	1002	ASN	5.5
1	A	1003	ALA	4.5
1	B	1003	ALA	3.7
1	B	1306	PRO	3.4
1	B	1305	THR	3.3
1	B	1141	GLN	2.8
1	A	1037	CYS	2.7
1	B	1129	TYR	2.7
1	A	1304	PRO	2.7
1	A	1129	TYR	2.6
1	B	1142	ASN	2.3
1	A	1099	ARG	2.2
1	A	1224	ALA	2.2
1	A	1032	GLY	2.1
1	B	1180	ILE	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

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ADP	A	3500	27/27	0.15	-0.31	16,26,35,38	0
3	ADP	B	3510	27/27	0.15	-0.44	16,26,35,38	0
2	MG	B	4611	1/1	0.12	-1.60	47,47,47,47	0
2	MG	A	4601	1/1	0.09	-8.24	44,44,44,44	0

6.5 Other polymers

There are no such residues in this entry.