



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 01:24 am BST

PDB ID : 1JM6
Title : Pyruvate dehydrogenase kinase, isozyme 2, containing ADP
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Hamilton, J.A.
Deposited on : 2001-07-17
Resolution : 2.50 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 : 2.11
buster-report : 1.1.7 (2018)
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) : 2.11

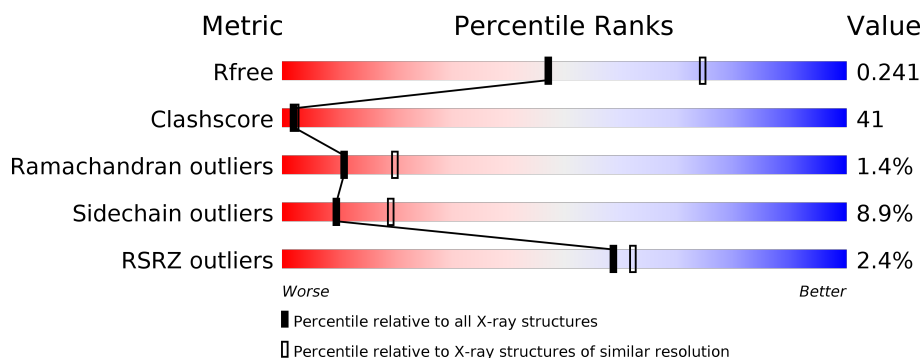
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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	407	<div> <div>2%</div> <div> <div></div> <div>34%</div> <div>42%</div> <div>6%</div> <div>17%</div> </div> </div>
1	B	407	<div> <div>2%</div> <div> <div></div> <div>37%</div> <div>39%</div> <div>6%</div> <div>17%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	B	3510	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5677 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.

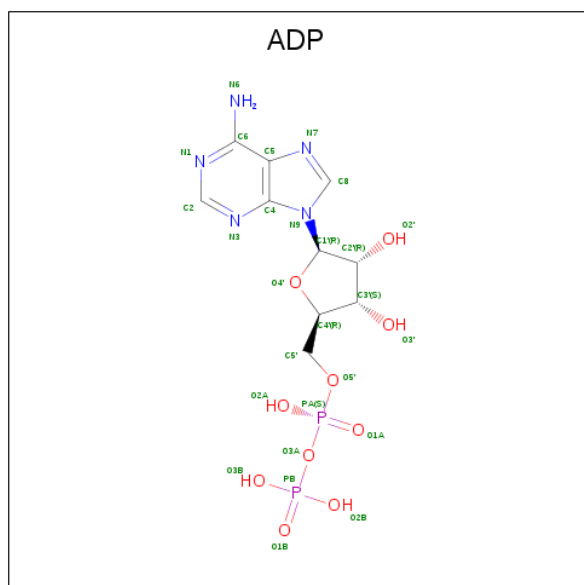
- Molecule 1 is a protein called Pyruvate dehydrogenase kinase, isozyme 2.

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: $C_{10}H_{15}N_5O_{10}P_2$).



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		

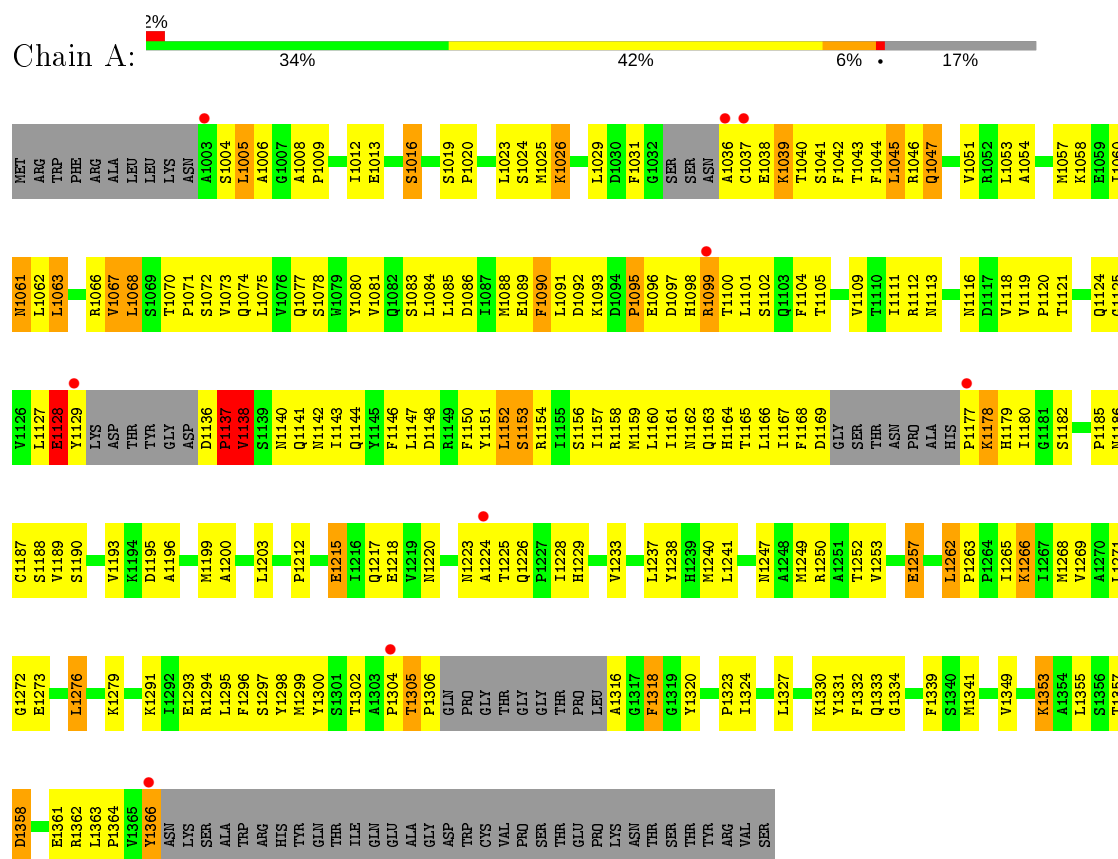
- Molecule 4 is water.

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

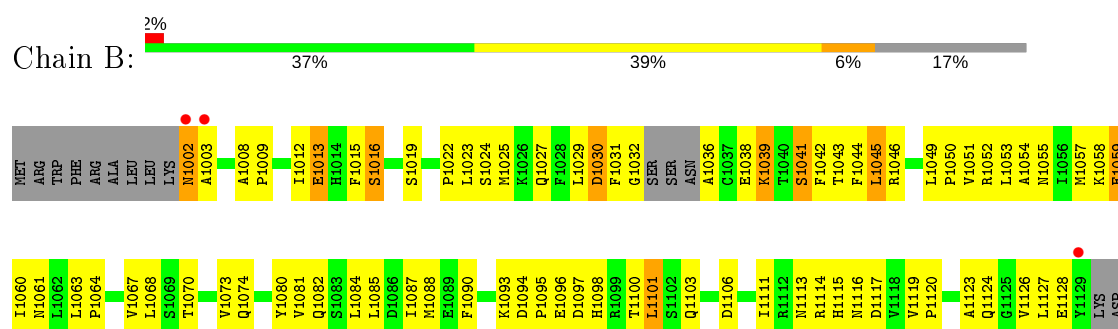
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Pyruvate dehydrogenase kinase, isozyme 2



• Molecule 1: Pyruvate dehydrogenase kinase, isozyme 2



THR	K1206	E1293	V1365
TYR	Y1207	R1294	TYR
GLY	Y1208	L1295	ASN
ASP	M1209	F1296	LYS
ASP	S1297	SER	LYS
PRO	P1212	ALA	ALA
VAL		TRP	TRP
SER		ANG	ANG
ASN	E1215	T1302	HIS
Q1141	I1216	A1303	TYR
N1142	Q1217	P1304	TYR
I1143	E1218	T1305	GLN
Q1144	V1219	P1306	THR
Y1145	M1220	GLN	ILE
		PRO	GLN
R1149	N1223	GLY	GLU
F1150	I1228	THR	ALA
Y1151		GLY	ALA
L1152		GLY	ASP
		THR	ASP
R1188	Y1232	THR	TRP
M1159	V1233	P1314	CYS
L1160	P1234	L1315	VAL
	S1235	A1316	PRO
Q1163	H1236	G1317	SER
H1164	L1237	F1318	THR
T1165	Y1238	G1319	GLU
L1166		Y1320	PRO
I1167	F1245	G1321	LYS
F1168	K1246	L1322	ASN
D1169	M1247	P1323	THR
GLY	A1248	I1324	SER
SER	M1249	S1325	SER
THR	R1250	R1326	THR
ASN		L1327	TYR
PRO	V1253	K1330	ARG
ALA	S1258	Y1331	VAL
HIS	T1261	F1332	SER
P1177	L1262	Q1333	
	P1263	G1334	
I1180	P1264	D1335	
G1181	I1265	L1338	
S1182	K1266	F1339	
I1183	I1267	S1340	
	M1268	R1341	
S1188	V1269	E1342	
V1189	A1270	G1343	
S1190	L1271	F1344	
		G1345	
V1193	L1276	T1346	
		D1347	
Y1197	K1279	T1357	
D1198		D1358	
M1199	R1283	S1359	
A1200		V1360	
K1201	V1287	E1361	
L1202		R1362	
L1203	R1290	L1363	
G1204	K1291	P1364	
D1205	I1292		

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 0.188 , 0.241	Depositor DCC
R_{free} test set	1626 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.478 for l,-k,h	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.

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: 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 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	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

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 41.

All (442) 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: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:1271:LEU:HD13	1:A:1276:LEU:HD22	1.47	0.94
1:A:1177:PRO:HD2	1:A:1179:HIS:CE1	2.02	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:1041:SER:O	1:A:1045:LEU:HB2	1.74	0.88
1:A:1093:LYS:O	1:A:1095:PRO:HD3	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:LEU:O	1:A:1088:MET:HE2	1.77	0.83
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:A:1074:GLN:O	1:A:1075:LEU:C	2.20	0.76
1:B:1097:ASP:O	1:B:1100:THR:HG22	1.85	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:1258:SER:O	1:B:1262:LEU:HD13	1.86	0.74
1:B:1306:PRO:O	1:B:1317:GLY:CA	2.32	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:1012:ILE:O	1:B:1016:SER:HB3	1.87	0.73
1:B:1250:ARG:NH2	1:B:1303:ALA:HB2	2.03	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:A:1105:THR:O	1:A:1109:VAL:HG23	1.89	0.73
1:B:1029:LEU:HD11	1:B:1183:ILE:HG21	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1257:GLU:HG3	4:A:6020:HOH:O	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:B:1038:GLU:OE1	1:B:1101:LEU:HD12	1.90	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:1094:ASP:O	1:B:1100:THR:HG21	1.92	0.69
1:B:1249:MET:O	1:B:1253:VAL:HG23	1.93	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:1037:CYS:HB3	1:A:1040:THR:CG2	2.23	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:B:1346:THR:CG2	3:B:3510:ADP:HN62	2.08	0.66
1:B:1106:ASP:HA	4:B:6193:HOH:O	1.93	0.66
1:B:1142:ASN:OD1	1:B:1145:TYR:HB3	1.95	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:1163:GLN:OE1	1:B:1181:GLY:HA3	1.97	0.65
1:B:1291:LYS:HG2	1:B:1294:ARG:NH1	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1038:GLU:CD	1:B:1101:LEU:HD12	2.18	0.62
1:B:1331:TYR:CE1	1:B:1361:GLU:HB2	2.34	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:A:1296:PHE:O	1:A:1323:PRO:HG3	1.99	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: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:A:1316:ALA:HB3	4:A:4603:HOH:O	2.02	0.60
1:B:1038:GLU:CG	1:B:1101:LEU:HD12	2.31	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:1163:GLN:O	1:A:1167:ILE:HG13	2.01	0.58
1:A:1302:THR:CG2	1:A:1302:THR:O	2.51	0.58
1:B:1063:LEU:HG	1:B:1064:PRO:HD2	1.86	0.58
1:B:1258:SER:HB3	4:B:6012:HOH:O	2.02	0.58
1:A:1331:TYR:CE1	1:A:1361:GLU:HG2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1020:PRO:CD	1:A:1366:TYR:HB2	2.34	0.57
1:A:1112:ARG:HD2	1:A:1162:ASN:ND2	2.19	0.57
1:B:1159:MET:HG3	1:B:1331:TYR:OH	2.04	0.57
1:A:1025:MET:HG3	1:A:1029:LEU:HD12	1.86	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: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:1097:ASP:O	1:A:1098:HIS:C	2.41	0.57
1:A:1215:GLU:OE1	1:A:1266:LYS:HD2	2.05	0.57
1:A:1294:ARG:O	1:A:1296:PHE:N	2.37	0.57
1:A:1039:LYS:O	1:A:1043:THR:HB	2.05	0.56
1:A:1072:SER:HB3	1:A:1121:THR:O	2.05	0.56
1:B:1250:ARG:HH12	1:B:1302:THR:HG22	1.69	0.56
1:A:1063:LEU:HD22	1:A:1067:VAL:CG2	2.36	0.56
1:A:1293:GLU:HG3	4:A:6221:HOH:O	2.04	0.56
1:B:1250:ARG:NH1	1:B:1302:THR:HG22	2.21	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:1063:LEU:HD23	1:B:1067:VAL:HG13	1.87	0.56
1:B:1144:GLN:HE22	1:B:1298:TYR:H	1.54	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:1099:ARG:HA	1:A:1102:SER:OG	2.07	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:1063:LEU:HD23	1:A:1067:VAL:CG2	2.35	0.55
1:A:1177:PRO:HB2	1:A:1179:HIS:HD2	1.70	0.55
1:B:1207:TYR:CE1	1:B:1314:PRO:HB3	2.41	0.55
1:A:1146:PHE:CD2	1:A:1147:LEU:HD12	2.41	0.55
1:A:1146:PHE:HD2	1:A:1147:LEU:HD12	1.70	0.55
1:B:1228:ILE:CD1	1:B:1269:VAL:HG12	2.36	0.55
1:A:1113:ASN:HA	1:A:1116:ASN:HD22	1.70	0.55
1:B:1039:LYS:NZ	1:B:1096:GLU:OE1	2.30	0.55
1:B:1117:ASP:O	1:B:1120:PRO:HD2	2.07	0.55
1:A:1167:ILE:O	1:A:1167:ILE:HG22	2.05	0.55
1:A:1168:PHE:O	1:A:1169:ASP:C	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1353:LYS:HG2	1:A:1358:ASP:HB2	1.89	0.54
1:B:1029:LEU:HA	1:B:1180:ILE:HG21	1.88	0.54
1:B:1228:ILE:HD13	1:B:1269:VAL:HG12	1.88	0.54
1:A:1023:LEU:HD11	1:A:1044:PHE:HZ	1.72	0.54
1:B:1064:PRO:HD2	1:B:1067:VAL:CG1	2.38	0.54
1:A:1023:LEU:HD11	1:A:1044:PHE:CZ	2.42	0.54
1:A:1038:GLU:CG	1:A:1168:PHE:CD2	2.77	0.54
1:B:1022:PRO:HG3	1:B:1363:LEU:CD1	2.36	0.54
1:B:1081:VAL:O	1:B:1085:LEU:HG	2.08	0.54
1:B:1346:THR:CG2	3:B:3510:ADP:N6	2.62	0.54
1:A:1063:LEU:HD23	1:A:1067:VAL:HG21	1.89	0.54
1:A:1294:ARG:C	1:A:1296:PHE:H	2.11	0.54
1:B:1061:ASN:CB	4:B:6231:HOH:O	2.56	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:A:1063:LEU:CD2	1:A:1067:VAL:HG22	2.38	0.53
1:A:1152:LEU:HD13	1:A:1363:LEU:HA	1.91	0.53
1:B:1100:THR:HG23	1:B:1101:LEU:HD23	1.91	0.53
1:B:1304:PRO:CB	1:B:1306:PRO:HD2	2.39	0.53
1:A:1297:SER:HB3	1:A:1300:TYR:CB	2.38	0.53
1:B:1246:LYS:HD2	1:B:1315:LEU:HD22	1.91	0.53
1:B:1304:PRO:O	1:B:1317:GLY:CA	2.56	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:A:1364:PRO:O	1:A:1366:TYR:HD2	1.92	0.53
1:B:1041:SER:HB3	1:B:1164:HIS:CE1	2.44	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:1019:SER:OG	1:A:1366:TYR:C	2.48	0.52
1:A:1063:LEU:HD11	1:A:1146:PHE:CE2	2.43	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:1038:GLU:HB3	1:A:1101:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1163:GLN:NE2	1:A:1182:SER:OG	2.42	0.51
1:A:1223:ASN:ND2	1:A:1226:GLN:HB2	2.24	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
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:1165:THR:O	1:B:1169:ASP:OD2	2.28	0.51
1:B:1220:ASN:OD1	1:B:1223:ASN:O	2.28	0.51
1:B:1119:VAL:HB	1:B:1120:PRO:HD3	1.93	0.50
1:A:1193:VAL:HA	1:A:1241:LEU:HD13	1.92	0.50
1:B:1163:GLN:O	1:B:1167:ILE:HG13	2.11	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:1190:SER:OG	1:A:1218:GLU:OE2	2.29	0.49
1:A:1318:PHE:HE1	4:A:6218:HOH:O	1.94	0.49
1:A:1020:PRO:HB3	1:A:1363:LEU:HD13	1.95	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: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:B:1144:GLN:HE22	1:B:1298:TYR:N	2.10	0.49
1:A:1019:SER:OG	1:A:1366:TYR:HB2	2.13	0.49
1:A:1053:LEU:CD1	1:A:1083:SER:O	2.61	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:A:1148:ASP:OD1	1:A:1327:LEU:HD21	2.14	0.48
1:B:1250:ARG:CZ	1:B:1303:ALA:HB2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:1258:SER:HB3	1:B:1261:THR:OG1	2.15	0.47
1:A:1058:LYS:O	1:A:1062:LEU:HD13	2.14	0.47
1:A:1163:GLN:HE22	1:A:1182:SER:N	2.08	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:A:1305:THR:HG23	1:A:1306:PRO:HD2	1.96	0.46
1:B:1304:PRO:O	1:B:1317:GLY:HA3	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1320:TYR:C	1:A:1323:PRO:HD2	2.36	0.45
1:B:1263:PRO:HB3	1:B:1283:ARG:NE	2.32	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:A:1196:ALA:HA	1:A:1238:TYR:CE1	2.51	0.45
1:B:1245:PHE:O	1:B:1249:MET:HG3	2.17	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
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: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:B:1233:VAL:HG11	1:B:1236:HIS:CD2	2.53	0.44
1:B:1212:PRO:HD2	1:B:1249:MET:HB3	2.00	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: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:1053:LEU:O	1:A:1057:MET:HG3	2.18	0.44
1:A:1223:ASN:ND2	1:A:1226:GLN:OE1	2.50	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:A:1166:LEU:HA	1:A:1166:LEU:HD23	1.87	0.43
1:B:1068:LEU:HA	1:B:1073:VAL:HG11	2.00	0.43
1:B:1203:LEU:HB3	1:B:1315:LEU:HD23	1.99	0.43
1:B:1331:TYR:O	1:B:1361:GLU:HA	2.18	0.43
1:B:1322:LEU:N	3:B:3510:ADP:O1A	2.43	0.43
1:A:1177:PRO:CB	1:A:1179:HIS:CD2	3.00	0.43
1:B:1015:PHE:HB3	1:B:1051:VAL:HA	2.00	0.43
4:A:6186:HOH:O	1:B:1344:PHE:HE2	2.01	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:B:1038:GLU:HG2	1:B:1101:LEU:HD13	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1188:SER:O	1:A:1189:VAL:C	2.55	0.43
1:A:1074:GLN:O	1:A:1077:GLN:N	2.52	0.42
1:B:1082:GLN:HB3	1:B:1114:ARG:NH1	2.33	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
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:1049:LEU:HB3	1:B:1087:ILE:HD13	2.01	0.42
1:B:1164:HIS:NE2	4:B:6027:HOH:O	2.25	0.42
1:B:1246:LYS:HA	1:B:1249:MET:HE2	2.01	0.42
1:A:1341:MET:HE1	1:B:1279:LYS:HE2	2.01	0.42
1:B:1287:VAL:HG12	1:B:1291:LYS:HB2	2.02	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:A:1060:ILE:O	1:A:1060:ILE:CG2	2.68	0.42
1:B:1250:ARG:HB2	1:B:1315:LEU:HD12	2.02	0.42
1:A:1070:THR:HG23	1:A:1128:GLU:OE1	2.20	0.41
1:A:1020:PRO:HD2	1:A:1366:TYR:HB3	2.00	0.41
1:A:1029:LEU:HD23	1:A:1180:ILE:HD13	2.02	0.41
1:A:1068:LEU:HA	1:A:1073:VAL:HG11	2.02	0.41
1:A:1193:VAL:HG22	1:A:1241:LEU:HD13	2.01	0.41
1:B:1044:PHE:HD2	1:B:1045:LEU:HD13	1.85	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:A:1265:ILE:HG21	1:A:1265:ILE:HD13	1.90	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:B:1049:LEU:HB2	1:B:1050:PRO:HD3	2.03	0.41
1:B:1096:GLU:OE1	1:B:1096:GLU:HA	2.20	0.41
1:B:1190:SER:OG	1:B:1218:GLU:OE1	2.31	0.41
1:B:1218:GLU:HA	1:B:1269:VAL:O	2.20	0.41
1:B:1357:THR:HG23	1:B:1357:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1159:MET:HG3	1:B:1331:TYR:CZ	2.56	0.41
1:A:1039:LYS:O	1:A:1043:THR:CB	2.68	0.41
1:A:1324:ILE:CG2	4:A:6096:HOH:O	2.68	0.41
1:B:1030:ASP:O	1:B:1036:ALA:N	2.54	0.41
1:A:1220:ASN:HB3	1:A:1223:ASN:O	2.21	0.41
1:A:1331:TYR:OH	1:A:1361:GLU:OE2	2.39	0.41
1:B:1197:TYR:CZ	1:B:1201:LYS:HD3	2.56	0.41
1:A:1008:ALA:HB3	1:A:1009:PRO:HD3	2.02	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
1:B:1296:PHE:O	1:B:1323:PRO:HG3	2.21	0.41
1:B:1042:PHE:HE1	1:B:1090:PHE:HB3	1.86	0.41
1:A:1140:ASN:HB3	1:A:1142:ASN:ND2	2.36	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:B:1304:PRO:O	1:B:1317:GLY:HA2	2.20	0.40
1:A:1047:GLN:O	1:A:1051:VAL:HG23	2.21	0.40
1:B:1203:LEU:HA	1:B:1203:LEU:HD23	1.78	0.40
1:A:1012:ILE:HD11	1:A:1057:MET:SD	2.61	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:B:1248:ALA:CB	1:B:1265:ILE:HD12	2.51	0.40
1:A:1203:LEU:N	1:A:1203:LEU:HD23	2.36	0.40
1:A:1250:ARG:NH2	1:A:1302:THR:O	2.54	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:B:1232:TYR:O	1:B:1234:PRO:HD3	2.21	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%)	7	11
1	B	326/407 (80%)	306 (94%)	18 (6%)	2 (1%)	25	43
All	All	655/814 (80%)	596 (91%)	50 (8%)	9 (1%)	11	20

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%)	9	18
1	B	302/363 (83%)	276 (91%)	26 (9%)	10	20
All	All	607/726 (84%)	553 (91%)	54 (9%)	9	19

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 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 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	24,29,29	1.24	2 (8%)	29,45,45	1.59	3 (10%)
3	ADP	B	3510	2	24,29,29	1.24	2 (8%)	29,45,45	1.59	3 (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	ADP	A	3500	2	-	7/12/32/32	0/3/3/3
3	ADP	B	3510	2	-	7/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3510	ADP	O4'-C1'	3.24	1.45	1.41
3	A	3500	ADP	O4'-C1'	3.22	1.45	1.41
3	B	3510	ADP	PB-O2B	2.66	1.65	1.54
3	A	3500	ADP	PB-O2B	2.66	1.65	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3500	ADP	N3-C2-N1	-6.02	119.27	128.68
3	B	3510	ADP	N3-C2-N1	-6.02	119.27	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3500	ADP	C4-C5-N7	-4.48	104.73	109.40
3	B	3510	ADP	C4-C5-N7	-4.47	104.74	109.40
3	B	3510	ADP	C3'-C2'-C1'	2.03	104.03	100.98
3	A	3500	ADP	C3'-C2'-C1'	2.01	104.00	100.98

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3500	ADP	PA-O3A-PB-O3B
3	A	3500	ADP	C5'-O5'-PA-O1A
3	A	3500	ADP	C5'-O5'-PA-O3A
3	B	3510	ADP	PA-O3A-PB-O3B
3	B	3510	ADP	C5'-O5'-PA-O1A
3	B	3510	ADP	C5'-O5'-PA-O3A
3	A	3500	ADP	PB-O3A-PA-O1A
3	B	3510	ADP	PB-O3A-PA-O1A
3	A	3500	ADP	C5'-O5'-PA-O2A
3	B	3510	ADP	C5'-O5'-PA-O2A
3	A	3500	ADP	PB-O3A-PA-O2A
3	B	3510	ADP	PB-O3A-PA-O2A
3	A	3500	ADP	PA-O3A-PB-O1B
3	B	3510	ADP	PA-O3A-PB-O1B

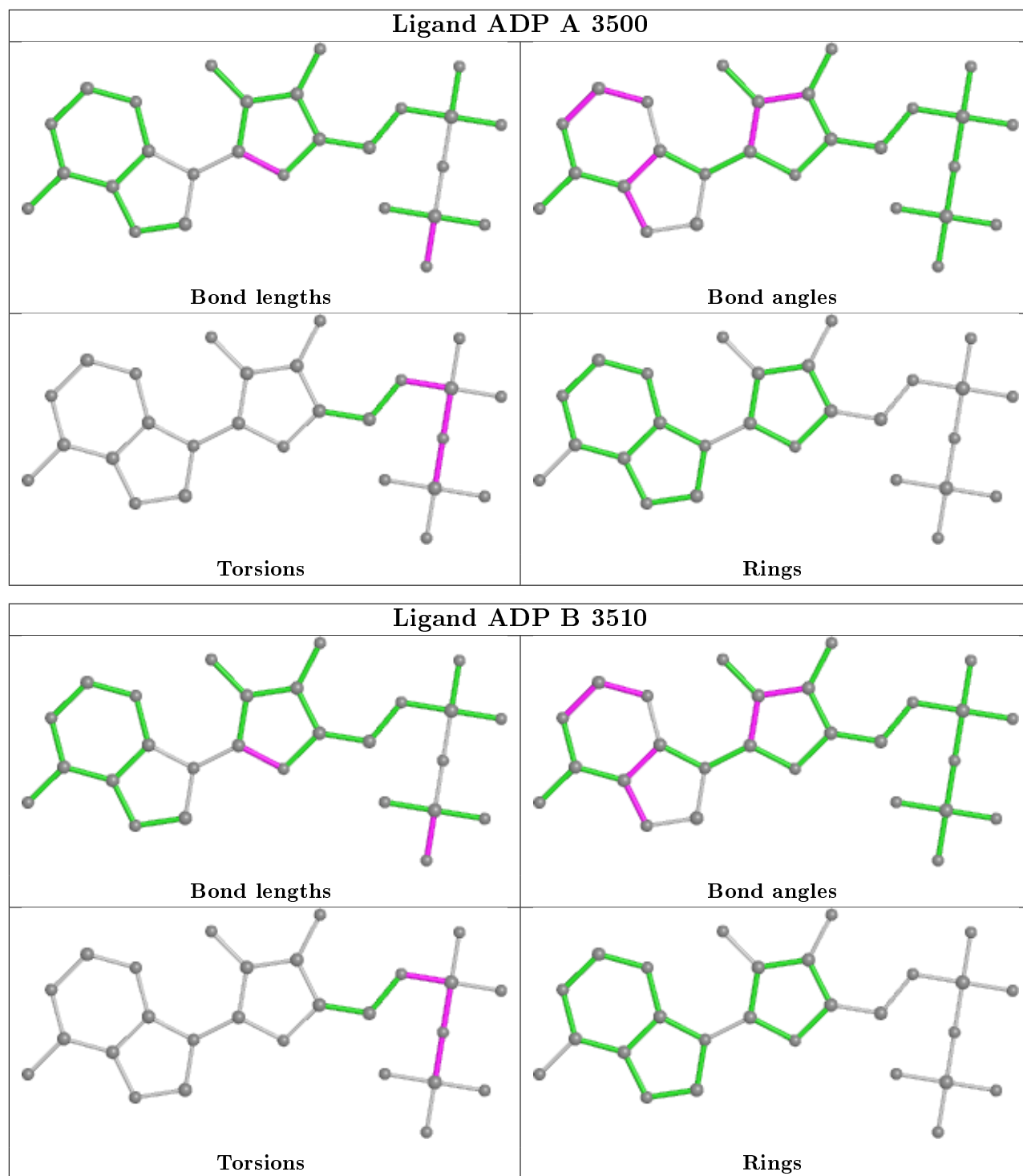
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3500	ADP	1	0
3	B	3510	ADP	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1178:LYS	C	1179:HIS	N	1.16
1	A	1090:PHE	C	1091:LEU	N	1.14

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	339/407 (83%)	-0.05	9 (2%) 54 58	19, 41, 80, 117	0
1	B	336/407 (82%)	-0.07	7 (2%) 63 66	20, 40, 70, 107	0
All	All	675/814 (82%)	-0.06	16 (2%) 59 62	19, 41, 74, 117	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1366	TYR	6.8
1	A	1177	PRO	6.0
1	A	1036	ALA	5.4
1	B	1002	ASN	5.2
1	A	1003	ALA	4.4
1	B	1003	ALA	3.7
1	B	1305	THR	3.0
1	B	1306	PRO	2.9
1	B	1141	GLN	2.8
1	A	1304	PRO	2.6
1	B	1129	TYR	2.5
1	A	1099	ARG	2.4
1	A	1037	CYS	2.3
1	A	1224	ALA	2.2
1	A	1129	TYR	2.2
1	B	1142	ASN	2.1

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](#)

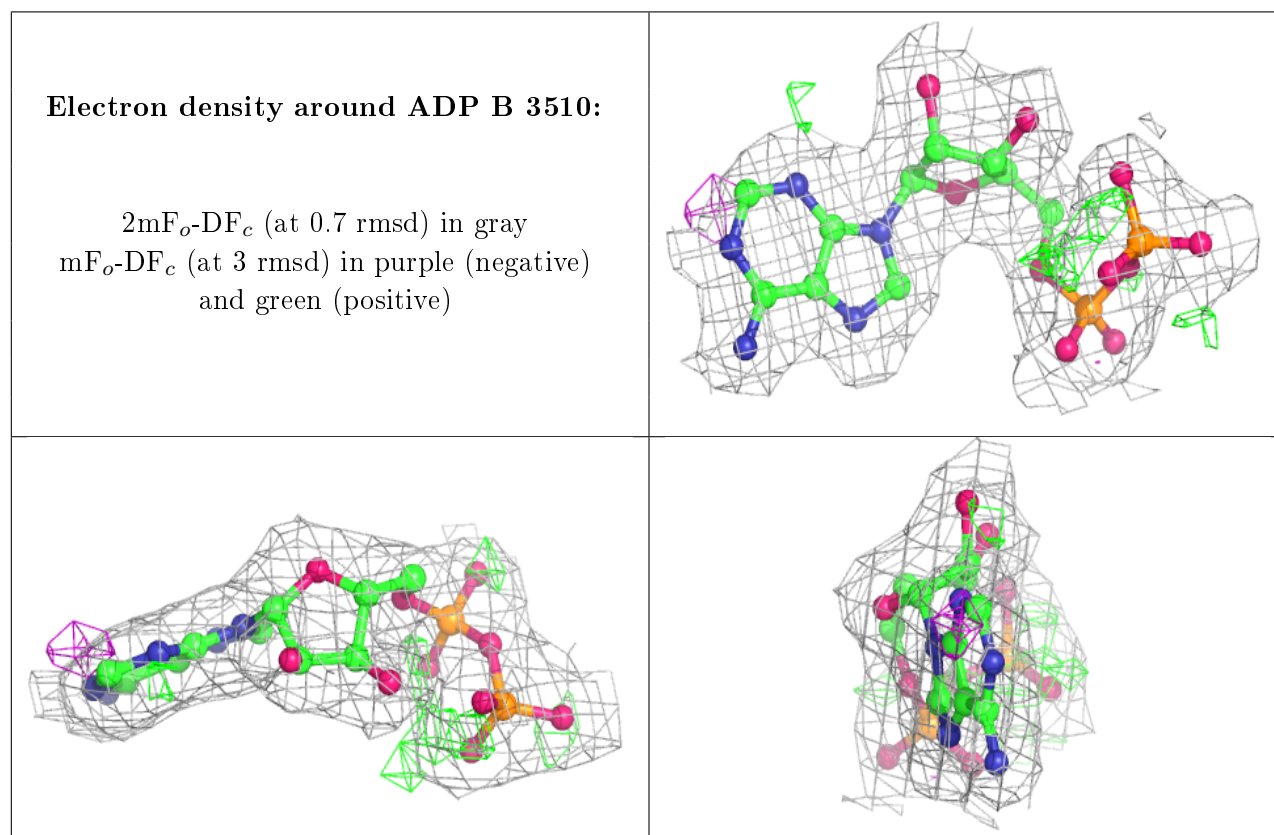
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

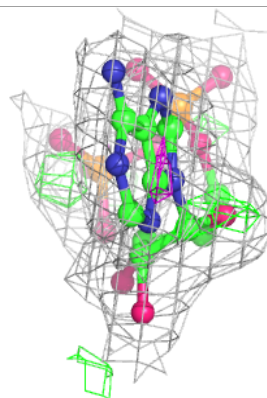
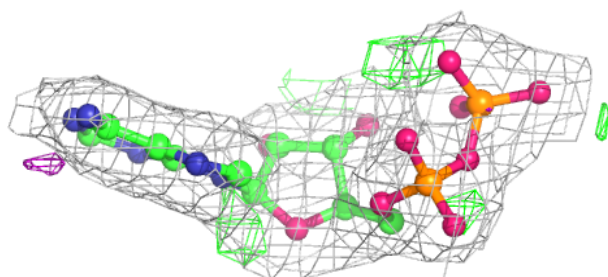
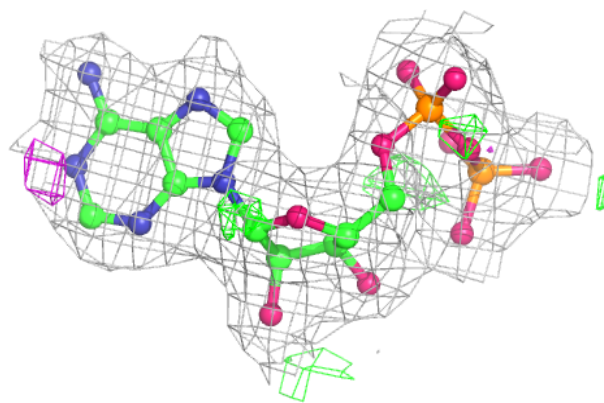
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	B	4611	1/1	0.96	0.10	47,47,47,47	0
3	ADP	B	3510	27/27	0.97	0.14	16,26,35,38	0
2	MG	A	4601	1/1	0.97	0.09	44,44,44,44	0
3	ADP	A	3500	27/27	0.98	0.13	16,26,35,38	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around ADP A 3500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.