



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:25 am BST

PDB ID : 1LCU  
Title : Polylysine Induces an Antiparallel Actin Dimer that Nucleates Filament Assembly: Crystal Structure at 3.5 Å Resolution  
Authors : Bubb, M.R.; Govindasamy, L.; Yarmola, E.G.; Vorobiev, S.M.; Almo, S.C.; Somasundaram, T.; Chapman, M.S.; Agbandje-Mckenna, M.; McKenna, R.  
Deposited on : 2002-04-06  
Resolution : 3.50 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](mailto: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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

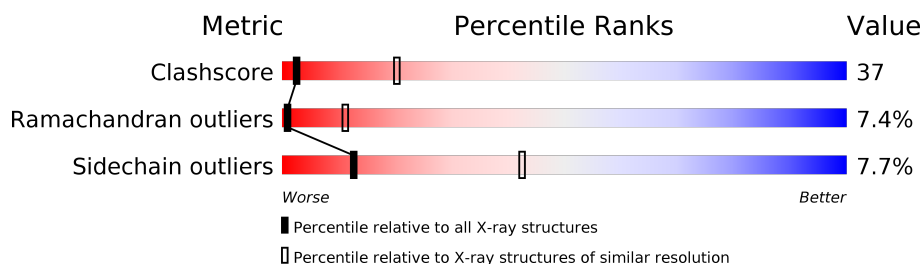
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	371	
1	B	371	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5936 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2829	1794	476	540	19			
1	B	371	Total	C	N	O	S	0	0	0
			2896	1835	488	552	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	VAL	GLY	CONFLICT	UNP P68135
A	60	GLY	LYS	CONFLICT	UNP P68135
B	1056	VAL	GLY	CONFLICT	UNP P68135
B	1060	GLY	LYS	CONFLICT	UNP P68135

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	3	Total	Ca	0	0
			3	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

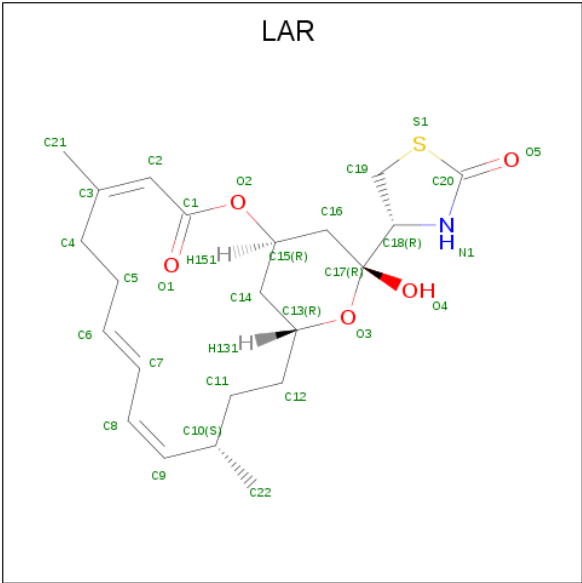
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is LATRUNCULIN A (three-letter code: LAR) (formula: C<sub>22</sub>H<sub>31</sub>NO<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			29	22	1	5	1		
5	B	1	Total	C	N	O	S	0	0
			29	22	1	5	1		

- Molecule 6 is water.

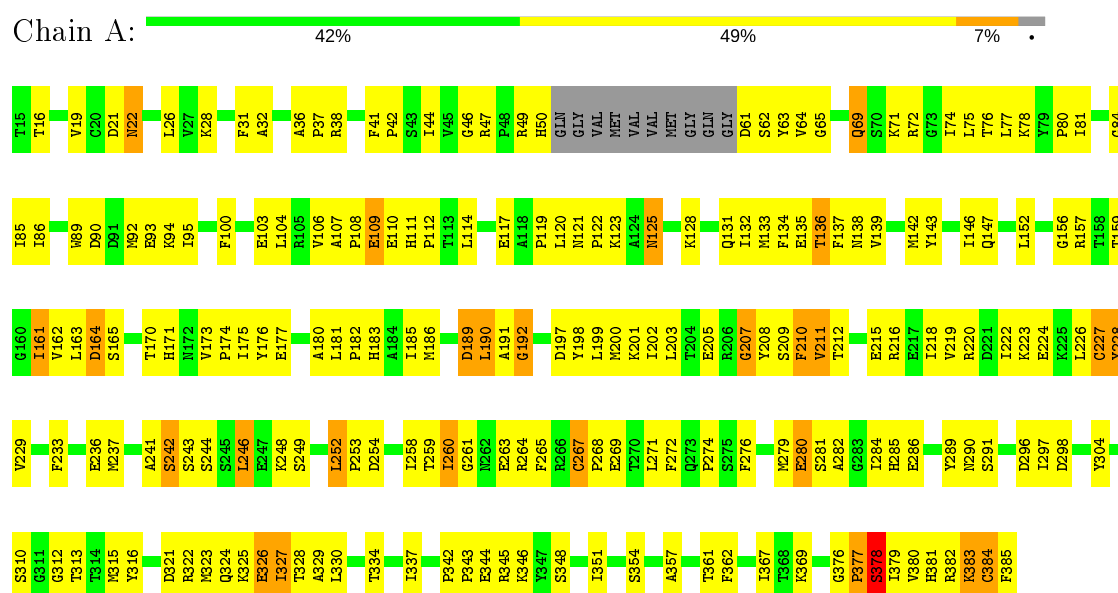
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	41	Total 41	O 41	0	0
6	B	43	Total 43	O 43	0	0

### 3 Residue-property plots

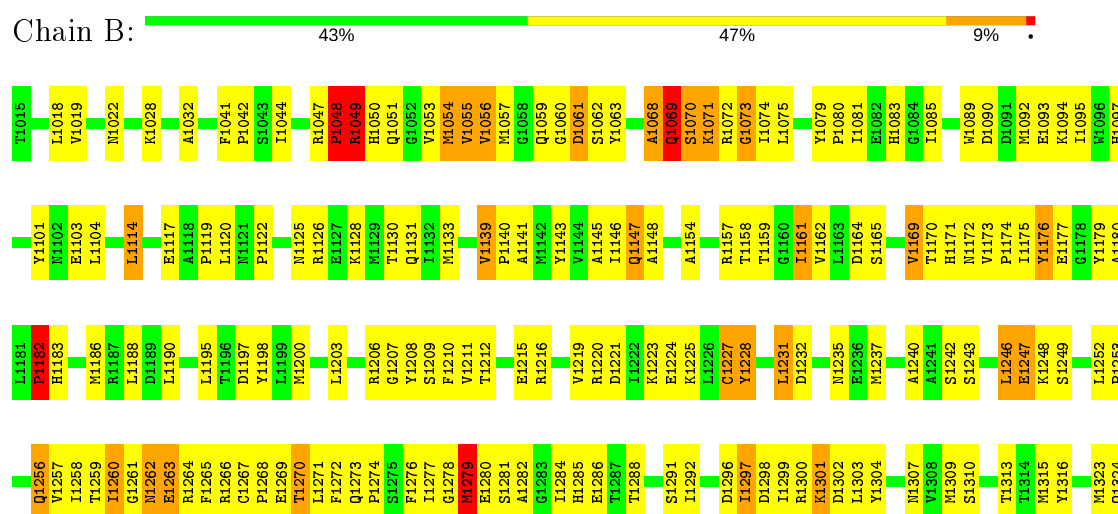
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle



K1325	E1326	I1327	T1328	A1329	L1330	A1331	F1332	I1337	I1340	A1341	P1342	P1343	E1344	R1345	K1346	V1347	S1348	V1349	M1350	I1351	G1352	G1353	S1354	I1355	L1356	A1357	S1358	T1361	F1362	Q1363	Q1364	M1365	T1368	K1369	Q1370	E1371	Y1372	G1376	P1377	S1378	I1379	V1380	H1381	R1382	K1383	C1384	F1385
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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.46Å 103.03Å 126.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50	Depositor
% Data completeness (in resolution range)	88.8 (30.00-3.50)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.196 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5936	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ATP, LAR, CL

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	0.43	0/2891	0.67	0/3919
1	B	0.42	0/2959	0.65	0/4011
All	All	0.42	0/5850	0.66	0/7930

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2829	0	2795	216	0
1	B	2896	0	2866	209	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	12	2	0
4	B	31	0	12	1	0
5	A	29	0	31	1	0
5	B	29	0	31	1	0
6	A	41	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	43	0	0	11	0
All	All	5936	0	5747	427	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 37.

All (427) 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:383:LYS:HD2	1:A:384:CYS:H	0.92	1.08
1:A:383:LYS:H	1:A:383:LYS:HE2	1.23	1.02
1:A:383:LYS:HD2	1:A:384:CYS:N	1.77	0.98
1:B:1351:ILE:HD12	1:B:1351:ILE:H	1.32	0.93
1:B:1376:GLY:O	1:B:1379:ILE:HG22	1.69	0.93
1:A:22:ASN:ND2	1:A:22:ASN:H	1.63	0.92
1:B:1200:MET:HE2	1:B:1216:ARG:HA	1.51	0.91
1:B:1055:VAL:HG12	1:B:1056:VAL:H	1.36	0.90
1:A:22:ASN:HD22	1:A:22:ASN:H	1.18	0.88
1:A:197:ASP:HA	1:A:200:MET:HE3	1.59	0.84
1:A:383:LYS:CD	1:A:384:CYS:H	1.86	0.82
1:B:1368:THR:HG23	1:B:1371:GLU:HG3	1.61	0.82
1:B:1247:GLU:HA	1:B:1264:ARG:HH11	1.47	0.78
1:B:1200:MET:CE	1:B:1216:ARG:HA	2.13	0.78
1:A:159:THR:HG23	1:A:176:TYR:HA	1.66	0.77
1:A:248:LYS:HG3	1:A:249:SER:H	1.50	0.77
1:A:86:ILE:HD13	1:A:92:MET:HG2	1.68	0.75
1:B:1051:GLN:HE22	1:B:1056:VAL:HB	1.52	0.74
1:B:1252:LEU:H	1:B:1252:LEU:HD23	1.52	0.74
1:A:180:ALA:O	1:A:182:PRO:HD3	1.86	0.74
1:B:1221:ASP:O	1:B:1225:LYS:HG2	1.86	0.74
1:B:1143:TYR:OH	1:B:1385:PHE:HA	1.86	0.74
1:B:1157:ARG:CZ	1:B:1340:ILE:HD13	2.17	0.74
1:A:190:LEU:C	1:A:190:LEU:HD12	2.09	0.73
1:A:80:PRO:HG2	1:A:95:ILE:HD11	1.70	0.73
1:B:1133:MET:O	1:B:1139:VAL:HG22	1.89	0.73
1:A:228:TYR:HE2	1:A:265:PHE:HD2	1.34	0.73
1:A:246:LEU:HD13	1:A:246:LEU:H	1.54	0.73
1:B:1053:VAL:HG12	1:B:1054:MET:H	1.54	0.72
1:B:1212:THR:HG23	1:B:1215:GLU:OE1	1.87	0.72
1:A:200:MET:HG2	1:A:219:VAL:HG21	1.72	0.72
1:A:279:MET:O	1:A:280:GLU:HB2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1117:GLU:OE1	1:B:1126:ARG:HD3	1.91	0.71
1:B:1271:LEU:HB3	1:B:1284:ILE:HD13	1.71	0.71
1:B:1228:TYR:CE2	1:B:1265:PHE:HB3	2.26	0.71
1:A:117:GLU:O	1:A:147:GLN:HG3	1.90	0.71
1:B:1164:ASP:HA	1:B:1310:SER:O	1.90	0.70
1:A:22:ASN:HB2	1:A:81:ILE:HD11	1.73	0.70
1:B:1069:GLN:HE21	1:B:1069:GLN:HA	1.55	0.70
1:B:1344:GLU:O	1:B:1346:LYS:N	2.25	0.69
1:A:321:ASP:O	1:A:324:GLN:HB3	1.93	0.69
1:A:114:LEU:HD12	1:A:357:ALA:HB2	1.75	0.69
1:A:274:PRO:O	1:A:279:MET:HB3	1.93	0.68
1:A:85:ILE:N	1:A:85:ILE:HD12	2.08	0.68
1:B:1203:LEU:O	1:B:1208:TYR:HB2	1.94	0.68
1:A:132:ILE:O	1:A:136:THR:HG23	1.93	0.68
1:A:203:LEU:O	1:A:208:TYR:HB2	1.92	0.67
1:B:1208:TYR:OH	1:B:1258:ILE:HG23	1.95	0.67
1:A:74:ILE:O	1:A:75:LEU:HD12	1.95	0.67
1:B:1175:ILE:N	1:B:1175:ILE:HD12	2.10	0.67
1:A:22:ASN:N	1:A:22:ASN:HD22	1.88	0.66
1:A:164:ASP:O	1:A:170:THR:HA	1.96	0.66
1:A:72:ARG:HD2	1:A:72:ARG:O	1.95	0.66
1:A:109:GLU:HA	1:A:138:ASN:O	1.96	0.66
1:A:26:LEU:HB2	1:A:28:LYS:HZ2	1.61	0.66
1:A:383:LYS:O	1:A:384:CYS:HB2	1.95	0.65
1:B:1248:LYS:HG3	1:B:1249:SER:H	1.62	0.65
1:B:1206:ARG:O	1:B:1206:ARG:HG2	1.97	0.65
1:A:69:GLN:HE21	1:A:69:GLN:HA	1.60	0.64
1:B:1288:THR:O	1:B:1292:ILE:HG13	1.97	0.64
1:B:1252:LEU:HB2	1:B:1253:PRO:CD	2.27	0.64
1:A:227:CYS:HA	1:A:264:ARG:O	1.98	0.63
1:A:252:LEU:HD12	1:A:253:PRO:N	2.13	0.63
1:B:1206:ARG:HH12	1:B:1261:GLY:H	1.45	0.63
1:A:47:ARG:HD3	1:A:62:SER:HB3	1.79	0.63
1:B:1246:LEU:HD21	1:B:1261:GLY:HA2	1.81	0.63
1:A:345:ARG:HA	1:A:348:SER:HB2	1.79	0.63
1:B:1261:GLY:O	1:B:1263:GLU:N	2.32	0.63
1:B:1377:PRO:O	1:B:1380:VAL:HG12	1.98	0.63
1:A:199:LEU:HD23	1:A:219:VAL:HG12	1.80	0.63
1:A:190:LEU:HD12	1:A:191:ALA:N	2.14	0.63
1:A:346:LYS:HE3	4:A:390:ATP:N7	2.14	0.63
1:A:36:ALA:HB1	1:A:37:PRO:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ILE:CD1	1:A:92:MET:HG2	2.28	0.62
1:B:1053:VAL:HG12	1:B:1054:MET:N	2.14	0.62
1:B:1380:VAL:HG22	1:B:1380:VAL:O	1.98	0.62
1:A:228:TYR:CE2	1:A:265:PHE:HD2	2.16	0.62
1:A:161:ILE:HD11	1:A:174:PRO:HG3	1.82	0.62
1:B:1277:ILE:HG13	1:B:1277:ILE:O	2.00	0.62
1:A:383:LYS:H	1:A:383:LYS:CE	2.06	0.62
1:A:261:GLY:N	1:A:263:GLU:OE2	2.33	0.61
1:A:377:PRO:O	1:A:379:ILE:HG22	2.01	0.61
1:A:197:ASP:HA	1:A:200:MET:CE	2.30	0.61
1:B:1158:THR:O	1:B:1177:GLU:N	2.33	0.61
1:B:1260:ILE:HD12	1:B:1260:ILE:H	1.65	0.61
1:B:1232:ASP:OD2	1:B:1235:ASN:HB2	2.01	0.60
1:B:1278:GLY:O	1:B:1280:GLU:N	2.34	0.60
1:A:41:PHE:CE2	1:A:103:GLU:HG3	2.37	0.60
1:B:1351:ILE:N	1:B:1351:ILE:HD12	2.12	0.59
1:A:164:ASP:HA	1:A:310:SER:O	2.03	0.59
1:A:377:PRO:HD2	6:A:533:HOH:O	2.02	0.59
1:A:208:TYR:OH	1:A:258:ILE:HG23	2.02	0.59
1:B:1228:TYR:HE2	1:B:1265:PHE:HB3	1.65	0.58
1:B:1351:ILE:H	1:B:1351:ILE:CD1	2.09	0.58
1:A:351:ILE:H	1:A:351:ILE:HD12	1.67	0.58
1:A:159:THR:HA	1:A:175:ILE:O	2.03	0.58
1:A:357:ALA:HA	1:A:362:PHE:CD2	2.39	0.58
1:A:134:PHE:CE1	1:A:369:LYS:HA	2.39	0.58
1:B:1055:VAL:O	1:B:1057:MET:N	2.37	0.58
1:A:367:ILE:CD1	1:A:380:VAL:HA	2.33	0.58
1:B:1069:GLN:HB3	6:B:49:HOH:O	2.04	0.57
1:A:383:LYS:O	1:A:384:CYS:CB	2.52	0.57
1:B:1368:THR:HG23	1:B:1371:GLU:CG	2.32	0.57
1:A:343:PRO:HG2	1:A:344:GLU:OE2	2.04	0.57
1:B:1072:ARG:O	1:B:1072:ARG:HD2	2.04	0.57
1:B:1186:MET:HG2	1:B:1291:SER:OG	2.05	0.57
1:B:1285:HIS:CE1	1:B:1286:GLU:HG3	2.39	0.57
1:B:1220:ARG:O	1:B:1224:GLU:HG3	2.04	0.57
1:A:377:PRO:O	1:A:379:ILE:N	2.38	0.57
1:A:260:ILE:HD12	1:A:260:ILE:H	1.70	0.56
1:A:376:GLY:O	1:A:379:ILE:HG22	2.05	0.56
1:B:1206:ARG:NH1	1:B:1261:GLY:H	2.02	0.56
1:B:1059:GLN:HB3	6:B:6:HOH:O	2.06	0.56
1:A:312:GLY:O	1:A:315:MET:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1063:TYR:HA	6:B:74:HOH:O	2.06	0.56
1:B:1117:GLU:OE2	1:B:1126:ARG:NH1	2.39	0.56
1:B:1262:ASN:HD21	1:B:1266:ARG:NE	2.03	0.56
1:B:1061:ASP:OD1	1:B:1062:SER:N	2.39	0.55
1:A:74:ILE:C	1:A:75:LEU:HD12	2.26	0.55
1:A:246:LEU:H	1:A:246:LEU:CD1	2.20	0.55
1:A:61:ASP:N	6:A:526:HOH:O	2.40	0.55
1:A:223:LYS:HD3	1:A:316:TYR:OH	2.07	0.55
1:B:1212:THR:OG1	1:B:1215:GLU:HG3	2.06	0.55
1:B:1228:TYR:CD2	1:B:1228:TYR:C	2.80	0.55
1:A:220:ARG:HD3	5:A:411:LAR:O4	2.07	0.55
1:A:252:LEU:HG	1:A:254:ASP:HB3	1.89	0.54
1:A:334:THR:HG23	1:A:334:THR:O	2.08	0.54
1:B:1081:ILE:HG13	1:B:1092:MET:HE3	1.89	0.54
1:B:1247:GLU:HA	1:B:1264:ARG:NH1	2.20	0.54
1:B:1055:VAL:O	1:B:1056:VAL:C	2.45	0.54
1:B:1081:ILE:CG1	1:B:1092:MET:HE3	2.37	0.54
1:B:1231:LEU:N	1:B:1231:LEU:HD12	2.21	0.54
1:A:289:TYR:O	1:A:291:SER:N	2.41	0.54
1:A:81:ILE:HG13	1:A:92:MET:CE	2.38	0.54
1:B:1097:HIS:CE1	1:B:1101:TYR:CD1	2.95	0.54
1:B:1176:TYR:HD2	1:B:1177:GLU:N	2.05	0.54
1:A:165:SER:O	1:A:313:THR:HB	2.08	0.54
1:B:1228:TYR:HD2	1:B:1228:TYR:C	2.11	0.54
1:B:1342:PRO:O	1:B:1345:ARG:HG2	2.07	0.54
1:A:63:TYR:HE1	1:A:71:LYS:HZ2	1.53	0.54
1:A:22:ASN:ND2	1:A:22:ASN:N	2.37	0.53
1:A:286:GLU:O	1:A:289:TYR:HB3	2.07	0.53
1:B:1272:PHE:C	1:B:1274:PRO:HD3	2.28	0.53
1:B:1055:VAL:HG12	1:B:1056:VAL:N	2.15	0.53
1:B:1070:SER:O	1:B:1071:LYS:HB2	2.08	0.53
1:B:1081:ILE:HG13	1:B:1092:MET:CE	2.38	0.53
1:B:1068:ALA:O	1:B:1069:GLN:C	2.46	0.53
1:A:208:TYR:CZ	1:A:258:ILE:HG23	2.43	0.53
1:A:208:TYR:CE1	1:A:258:ILE:HG12	2.44	0.53
1:A:380:VAL:O	1:A:380:VAL:HG22	2.09	0.53
1:B:1085:ILE:N	1:B:1085:ILE:HD12	2.24	0.53
1:B:1206:ARG:CG	1:B:1206:ARG:O	2.57	0.53
1:A:49:ARG:HG3	1:A:76:THR:HG23	1.91	0.52
1:A:44:ILE:O	1:A:44:ILE:HD12	2.09	0.52
1:B:1200:MET:HE1	1:B:1216:ARG:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1343:PRO:HG2	1:B:1344:GLU:OE2	2.09	0.52
1:A:276:PHE:N	1:A:276:PHE:CD2	2.75	0.52
1:B:1237:MET:O	1:B:1240:ALA:HB3	2.10	0.52
1:A:327:ILE:HD12	1:A:327:ILE:C	2.30	0.52
1:B:1180:ALA:O	1:B:1182:PRO:HD3	2.10	0.52
1:A:74:ILE:HG13	1:A:75:LEU:CD1	2.40	0.52
1:A:16:THR:O	1:A:111:HIS:ND1	2.43	0.52
1:A:200:MET:HE1	1:A:216:ARG:HG3	1.91	0.52
1:B:1267:CYS:HB3	1:B:1268:PRO:CD	2.40	0.52
1:B:1304:TYR:HB3	1:B:1337:ILE:CD1	2.40	0.52
1:A:252:LEU:HD12	1:A:253:PRO:CD	2.40	0.51
1:A:131:GLN:HG2	1:A:135:GLU:HG3	1.91	0.51
1:A:119:PRO:HD2	1:A:171:HIS:ND1	2.25	0.51
1:A:351:ILE:N	1:A:351:ILE:HD12	2.25	0.51
1:B:1119:PRO:HB2	1:B:1171:HIS:CD2	2.44	0.51
1:A:31:PHE:HE2	1:A:38:ARG:HE	1.59	0.51
1:A:246:LEU:HD22	1:A:246:LEU:C	2.30	0.51
1:A:289:TYR:C	1:A:291:SER:H	2.14	0.51
1:B:1072:ARG:O	1:B:1073:GLY:C	2.49	0.51
1:A:133:MET:HB3	1:A:139:VAL:HG21	1.91	0.51
1:A:108:PRO:C	1:A:110:GLU:H	2.13	0.51
1:A:226:LEU:N	1:A:226:LEU:HD22	2.25	0.51
1:A:267:CYS:HB3	1:A:268:PRO:CD	2.41	0.51
1:B:1054:MET:O	1:B:1055:VAL:O	2.28	0.51
1:B:1154:ALA:HB2	1:B:1352:GLY:CA	2.41	0.51
1:B:1252:LEU:HB2	1:B:1253:PRO:HD2	1.92	0.51
1:A:265:PHE:C	1:A:267:CYS:H	2.12	0.51
1:A:276:PHE:HD2	1:A:276:PHE:N	2.09	0.51
1:B:1032:ALA:HB1	1:B:1358:SER:OG	2.11	0.51
1:B:1018:LEU:HD22	1:B:1104:LEU:HD23	1.93	0.51
1:B:1074:ILE:O	1:B:1074:ILE:HG13	2.11	0.50
1:A:26:LEU:HB2	1:A:28:LYS:NZ	2.27	0.50
1:B:1061:ASP:HA	6:B:6:HOH:O	2.12	0.50
1:A:71:LYS:O	1:A:75:LEU:HD13	2.11	0.50
1:A:107:ALA:O	1:A:110:GLU:HB3	2.11	0.50
1:A:190:LEU:HD11	1:A:271:LEU:HD23	1.93	0.50
1:B:1260:ILE:HG22	1:B:1263:GLU:OE2	2.12	0.50
1:A:143:TYR:OH	1:A:383:LYS:HB2	2.11	0.50
1:A:86:ILE:HG12	1:A:92:MET:HE3	1.93	0.50
1:B:1141:ALA:HB2	1:B:1368:THR:HA	1.94	0.50
1:B:1327:ILE:O	1:B:1330:LEU:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:CD2	1:A:175:ILE:HD12	2.41	0.50
1:B:1176:TYR:HE1	1:B:1299:ILE:HG21	1.76	0.50
1:B:1246:LEU:O	1:B:1264:ARG:HD3	2.12	0.50
1:B:1164:ASP:O	1:B:1170:THR:HA	2.12	0.49
1:B:1198:TYR:HH	1:B:1276:PHE:HD1	1.56	0.49
1:A:198:TYR:CZ	1:A:276:PHE:HB3	2.48	0.49
1:B:1068:ALA:O	1:B:1070:SER:N	2.45	0.49
1:A:69:GLN:HE21	1:A:69:GLN:CA	2.22	0.49
1:B:1092:MET:O	1:B:1093:GLU:C	2.50	0.49
1:B:1055:VAL:HA	1:B:1057:MET:CE	2.42	0.49
1:B:1072:ARG:HA	1:B:1075:LEU:CD1	2.43	0.49
1:B:1114:LEU:HD23	1:B:1143:TYR:O	2.12	0.49
1:A:342:PRO:O	1:A:345:ARG:HG2	2.12	0.49
1:A:252:LEU:HD12	1:A:253:PRO:HD2	1.94	0.49
1:A:383:LYS:HD3	1:A:385:PHE:HE1	1.78	0.49
1:B:1042:PRO:HB3	5:B:1411:LAR:H141	1.94	0.49
1:B:1159:THR:HG23	1:B:1176:TYR:HA	1.95	0.49
1:B:1246:LEU:HD22	1:B:1246:LEU:C	2.33	0.49
1:B:1044:ILE:HG23	1:B:1079:TYR:CD2	2.48	0.49
1:B:1228:TYR:CD2	1:B:1265:PHE:HB3	2.47	0.49
1:A:248:LYS:H	1:A:260:ILE:HD11	1.77	0.48
1:B:1089:TRP:CD2	1:B:1128:LYS:HG2	2.47	0.48
1:B:1209:SER:O	1:B:1210:PHE:HB2	2.12	0.48
1:A:186:MET:HG2	1:A:291:SER:HB2	1.95	0.48
1:B:1208:TYR:CZ	1:B:1258:ILE:HG23	2.48	0.48
1:A:289:TYR:C	1:A:291:SER:N	2.64	0.48
1:A:298:ASP:HB2	6:A:543:HOH:O	2.13	0.48
1:A:85:ILE:CD1	1:A:85:ILE:N	2.76	0.48
1:A:89:TRP:O	1:A:93:GLU:HG3	2.13	0.48
1:B:1069:GLN:O	1:B:1071:LYS:N	2.37	0.48
1:A:233:PHE:O	1:A:237:MET:HB2	2.13	0.48
1:B:1157:ARG:NH1	1:B:1340:ILE:HD13	2.28	0.48
1:A:198:TYR:OH	1:A:276:PHE:HB3	2.14	0.48
4:A:390:ATP:H1'	6:A:517:HOH:O	2.14	0.48
1:B:1279:MET:O	1:B:1280:GLU:HB3	2.13	0.48
1:B:1195:LEU:HD23	1:B:1316:TYR:OH	2.13	0.48
1:A:41:PHE:HB2	1:A:42:PRO:HD2	1.95	0.48
1:B:1197:ASP:O	1:B:1200:MET:HB3	2.13	0.48
1:B:1344:GLU:C	1:B:1346:LYS:N	2.67	0.48
1:B:1348:SER:HA	1:B:1351:ILE:HD13	1.95	0.48
1:B:1165:SER:O	1:B:1313:THR:HB	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:HD13	1:A:174:PRO:HA	1.96	0.48
1:A:212:THR:OG1	1:A:215:GLU:HG3	2.14	0.48
1:B:1080:PRO:HB2	1:B:1092:MET:HE2	1.96	0.48
1:B:1125:ASN:O	1:B:1126:ARG:C	2.52	0.48
1:B:1344:GLU:C	1:B:1346:LYS:H	2.17	0.47
1:A:265:PHE:C	1:A:267:CYS:N	2.68	0.47
1:A:22:ASN:HB2	1:A:81:ILE:CD1	2.44	0.47
1:B:1313:THR:O	1:B:1313:THR:HG22	2.14	0.47
1:A:94:LYS:NZ	6:A:540:HOH:O	2.48	0.47
1:B:1247:GLU:HG2	1:B:1248:LYS:N	2.30	0.47
1:B:1053:VAL:CG1	1:B:1054:MET:H	2.27	0.46
1:A:248:LYS:HG3	1:A:249:SER:N	2.24	0.46
1:B:1055:VAL:C	1:B:1057:MET:N	2.68	0.46
1:B:1072:ARG:HA	1:B:1075:LEU:HD11	1.96	0.46
1:B:1315:MET:HE2	1:B:1346:LYS:HD2	1.97	0.46
1:A:248:LYS:H	1:A:260:ILE:CD1	2.29	0.46
1:B:1282:ALA:HB1	1:B:1286:GLU:CB	2.45	0.46
1:B:1198:TYR:OH	1:B:1276:PHE:HD1	1.97	0.46
1:B:1362:PHE:O	1:B:1365:MET:N	2.49	0.46
1:A:285:HIS:CG	1:A:286:GLU:N	2.83	0.46
1:A:63:TYR:N	1:A:63:TYR:CD2	2.84	0.46
1:B:1228:TYR:HD2	1:B:1228:TYR:O	1.97	0.46
1:B:1256:GLN:HG2	1:B:1257:VAL:H	1.81	0.46
1:B:1296:ASP:O	1:B:1298:ASP:N	2.48	0.46
1:B:1055:VAL:O	1:B:1057:MET:HG3	2.16	0.46
1:B:1080:PRO:HB2	1:B:1092:MET:CE	2.46	0.46
1:A:361:THR:O	1:A:361:THR:HG22	2.16	0.46
1:A:64:VAL:HG22	1:A:65:GLY:N	2.30	0.46
1:A:74:ILE:HG13	1:A:75:LEU:HD13	1.98	0.46
1:B:1146:ILE:HG13	1:B:1385:PHE:CZ	2.50	0.46
1:A:351:ILE:H	1:A:351:ILE:CD1	2.30	0.45
1:B:1231:LEU:HD12	1:B:1231:LEU:H	1.81	0.45
1:B:1247:GLU:OE1	1:B:1247:GLU:N	2.49	0.45
1:B:1270:THR:HG23	1:B:1276:PHE:HB2	1.97	0.45
1:A:152:LEU:HD11	1:A:157:ARG:HB2	1.97	0.45
1:A:181:LEU:HB3	1:A:183:HIS:CE1	2.51	0.45
1:A:384:CYS:O	1:A:385:PHE:HB2	2.16	0.45
1:B:1161:ILE:HD13	1:B:1162:VAL:N	2.31	0.45
1:B:1176:TYR:CE1	1:B:1299:ILE:HG21	2.51	0.45
1:B:1327:ILE:HD11	1:B:1337:ILE:HG13	1.99	0.45
1:A:85:ILE:HG23	1:A:125:ASN:ND2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1188:LEU:HG	1:B:1190:LEU:HB3	1.99	0.45
1:B:1262:ASN:N	6:B:56:HOH:O	2.48	0.45
1:B:1272:PHE:CD1	1:B:1272:PHE:N	2.85	0.45
1:B:1146:ILE:HG13	1:B:1385:PHE:HZ	1.81	0.45
1:A:207:GLY:O	1:A:208:TYR:CG	2.69	0.45
1:A:269:GLU:O	1:A:272:PHE:N	2.40	0.45
1:A:323:MET:O	1:A:324:GLN:C	2.54	0.45
1:B:1301:LYS:HD2	1:B:1302:ASP:OD2	2.15	0.45
1:A:146:ILE:O	1:A:147:GLN:C	2.54	0.45
1:A:19:VAL:HG21	1:A:354:SER:HA	1.97	0.45
1:B:1258:ILE:HG22	1:B:1259:THR:N	2.32	0.45
1:B:1228:TYR:HE2	1:B:1265:PHE:CD2	2.35	0.45
1:B:1173:VAL:HA	1:B:1174:PRO:HD3	1.60	0.45
1:B:1297:ILE:HD12	1:B:1300:ARG:HD2	1.99	0.45
1:B:1369:LYS:O	1:B:1370:GLN:C	2.55	0.45
1:A:133:MET:O	1:A:139:VAL:HG22	2.16	0.44
1:A:246:LEU:O	1:A:264:ARG:NH1	2.47	0.44
1:A:186:MET:CG	1:A:291:SER:HB2	2.47	0.44
1:A:85:ILE:HG22	1:A:86:ILE:N	2.32	0.44
1:B:1028:LYS:N	1:B:1028:LYS:HD3	2.31	0.44
1:B:1041:PHE:CE2	1:B:1103:GLU:HG3	2.52	0.44
1:B:1130:THR:OG1	1:B:1380:VAL:HG21	2.17	0.44
1:A:156:GLY:O	1:A:157:ARG:HG3	2.18	0.44
1:A:198:TYR:O	1:A:202:ILE:HG23	2.17	0.44
1:A:21:ASP:HB3	1:A:28:LYS:HB2	1.98	0.44
1:A:248:LYS:CG	1:A:249:SER:H	2.25	0.44
1:A:81:ILE:HG13	1:A:92:MET:HE3	1.98	0.44
1:B:1019:VAL:HG21	1:B:1354:SER:HA	1.99	0.44
1:B:1327:ILE:O	1:B:1328:THR:C	2.55	0.44
1:A:344:GLU:C	1:A:346:LYS:H	2.20	0.44
1:A:81:ILE:HG13	1:A:92:MET:HE1	1.98	0.44
1:B:1119:PRO:O	1:B:1120:LEU:HB2	2.17	0.44
1:B:1363:GLN:HB2	6:B:17:HOH:O	2.18	0.44
1:B:1175:ILE:N	1:B:1175:ILE:CD1	2.80	0.44
1:B:1131:GLN:HG3	1:B:1372:TYR:OH	2.17	0.44
1:B:1383:LYS:C	1:B:1385:PHE:H	2.21	0.44
1:A:161:ILE:HG22	1:A:161:ILE:O	2.16	0.44
1:B:1049:ARG:HH11	1:B:1049:ARG:CB	2.30	0.44
1:B:1265:PHE:C	1:B:1267:CYS:N	2.70	0.44
1:B:1059:GLN:C	1:B:1061:ASP:H	2.21	0.44
1:B:1157:ARG:HG3	1:B:1157:ARG:HH21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:PHE:HE1	1:A:137:PHE:CD2	2.36	0.44
1:A:122:PRO:O	1:A:125:ASN:HB2	2.17	0.44
1:A:44:ILE:HD12	1:A:44:ILE:C	2.38	0.44
1:A:161:ILE:HA	1:A:161:ILE:HD13	1.76	0.44
1:A:241:ALA:O	1:A:242:SER:O	2.36	0.44
1:A:326:GLU:O	1:A:330:LEU:HD23	2.18	0.44
1:B:1055:VAL:C	1:B:1057:MET:HG3	2.38	0.44
1:B:1080:PRO:HG2	1:B:1095:ILE:CD1	2.48	0.44
1:B:1292:ILE:H	1:B:1292:ILE:HG13	1.57	0.44
1:B:1309:MET:HG3	1:B:1341:ALA:HB2	1.99	0.44
1:A:176:TYR:O	1:A:177:GLU:C	2.56	0.43
1:B:1210:PHE:CD2	1:B:1210:PHE:N	2.85	0.43
1:B:1231:LEU:CD1	1:B:1231:LEU:H	2.31	0.43
1:B:1362:PHE:O	1:B:1363:GLN:C	2.56	0.43
1:A:324:GLN:O	1:A:328:THR:HG23	2.18	0.43
1:A:84:GLY:C	1:A:85:ILE:HD12	2.38	0.43
1:B:1022:ASN:HB3	1:B:1081:ILE:HD11	2.00	0.43
1:B:1297:ILE:HA	1:B:1300:ARG:HG3	1.99	0.43
1:B:1304:TYR:HB3	1:B:1337:ILE:HD13	2.01	0.43
1:B:1145:ALA:HA	1:B:1385:PHE:HE2	1.84	0.43
1:A:152:LEU:CD1	1:A:157:ARG:HB2	2.47	0.43
1:A:279:MET:O	1:A:280:GLU:CB	2.61	0.43
1:B:1362:PHE:CD1	1:B:1365:MET:HG3	2.54	0.43
1:A:121:ASN:HD22	1:A:125:ASN:HB3	1.83	0.43
1:B:1075:LEU:O	1:B:1075:LEU:HD12	2.18	0.43
1:B:1258:ILE:HB	6:B:62:HOH:O	2.17	0.43
1:B:1383:LYS:C	1:B:1384:CYS:SG	2.97	0.43
1:A:119:PRO:O	1:A:120:LEU:HB2	2.18	0.43
1:A:327:ILE:C	1:A:329:ALA:N	2.72	0.43
1:A:252:LEU:HD12	1:A:254:ASP:H	1.84	0.43
1:A:72:ARG:HD2	1:A:72:ARG:C	2.39	0.43
1:B:1228:TYR:CE2	1:B:1265:PHE:HD2	2.36	0.43
1:A:63:TYR:HE1	1:A:71:LYS:NZ	2.16	0.43
1:B:1047:ARG:CD	1:B:1062:SER:HB3	2.49	0.43
1:B:1383:LYS:N	6:B:23:HOH:O	2.48	0.43
1:A:258:ILE:CG2	1:A:259:THR:N	2.82	0.42
1:B:1246:LEU:HD21	1:B:1261:GLY:CA	2.48	0.42
1:A:122:PRO:O	1:A:123:LYS:C	2.58	0.42
1:A:252:LEU:CD1	1:A:254:ASP:H	2.31	0.42
1:A:104:LEU:O	1:A:106:VAL:HG13	2.19	0.42
1:A:77:LEU:O	1:A:78:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:PRO:HB2	1:A:92:MET:HE1	2.01	0.42
1:A:176:TYR:CE2	1:A:177:GLU:HG3	2.54	0.42
1:A:220:ARG:NH1	1:A:224:GLU:OE2	2.53	0.42
1:A:296:ASP:O	1:A:298:ASP:N	2.53	0.42
1:A:304:TYR:HB3	1:A:337:ILE:HD13	2.02	0.42
1:B:1069:GLN:CA	1:B:1069:GLN:HE21	2.22	0.42
1:B:1122:PRO:O	1:B:1125:ASN:HB2	2.19	0.42
1:B:1157:ARG:HG3	1:B:1157:ARG:NH2	2.35	0.42
1:A:200:MET:CE	1:A:216:ARG:HG3	2.49	0.42
1:A:271:LEU:O	1:A:284:ILE:HG23	2.19	0.42
1:B:1269:GLU:OE2	1:B:1273:GLN:HG3	2.20	0.42
1:B:1323:MET:O	1:B:1324:GLN:C	2.57	0.42
1:A:199:LEU:HD22	1:A:223:LYS:HB2	2.02	0.42
1:B:1223:LYS:HA	1:B:1227:CYS:SG	2.60	0.42
1:B:1265:PHE:C	1:B:1267:CYS:H	2.23	0.42
1:A:210:PHE:O	1:A:211:VAL:HB	2.19	0.41
1:A:248:LYS:HD2	1:A:248:LYS:HA	1.86	0.41
1:A:28:LYS:HD3	1:A:28:LYS:N	2.34	0.41
1:B:1083:HIS:O	1:B:1169:VAL:HG21	2.20	0.41
1:B:1179:TYR:HB3	6:B:501:HOH:O	2.19	0.41
1:B:1265:PHE:O	1:B:1267:CYS:N	2.53	0.41
1:A:134:PHE:CD1	1:A:369:LYS:HG3	2.55	0.41
1:A:199:LEU:CD2	1:A:223:LYS:HB2	2.50	0.41
1:A:327:ILE:C	1:A:329:ALA:H	2.24	0.41
1:A:379:ILE:HG23	1:A:380:VAL:N	2.35	0.41
1:A:49:ARG:HG3	1:A:76:THR:CG2	2.49	0.41
1:A:111:HIS:HA	1:A:112:PRO:HD3	1.93	0.41
1:A:152:LEU:HD23	1:A:175:ILE:HD12	2.02	0.41
1:B:1071:LYS:HA	6:B:25:HOH:O	2.20	0.41
1:A:173:VAL:HG22	1:A:185:ILE:HG23	2.03	0.41
1:A:229:VAL:CG1	1:A:322:ARG:HG2	2.50	0.41
1:A:46:GLY:O	1:A:47:ARG:HG2	2.20	0.41
1:B:1200:MET:HE3	1:B:1219:VAL:HG21	2.03	0.41
1:A:282:ALA:HB1	1:A:286:GLU:HB3	2.02	0.41
1:A:377:PRO:HB2	1:A:378:SER:H	1.70	0.41
1:A:47:ARG:HD3	1:A:62:SER:CB	2.47	0.41
1:B:1018:LEU:HD22	1:B:1104:LEU:CD2	2.50	0.41
1:A:152:LEU:HD22	1:A:175:ILE:HD12	2.02	0.41
1:A:236:GLU:HG3	1:A:265:PHE:CE2	2.56	0.41
1:A:378:SER:HA	1:A:381:HIS:CD2	2.56	0.41
1:B:1147:GLN:O	1:B:1148:ALA:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1265:PHE:CD1	1:B:1266:ARG:N	2.88	0.41
1:B:1362:PHE:CD1	1:B:1365:MET:HB2	2.56	0.41
1:A:100:PHE:CE1	1:A:137:PHE:CD2	3.08	0.41
1:A:191:ALA:O	1:A:192:GLY:C	2.59	0.41
1:A:377:PRO:O	1:A:378:SER:C	2.59	0.41
1:A:89:TRP:CE3	1:A:128:LYS:HG2	2.55	0.41
1:A:132:ILE:HA	1:A:136:THR:CG2	2.51	0.41
1:B:1053:VAL:CG1	1:B:1054:MET:N	2.83	0.41
1:B:1141:ALA:CB	1:B:1368:THR:HA	2.50	0.41
1:B:1303:LEU:HA	1:B:1303:LEU:HD12	1.91	0.41
4:B:1390:ATP:H1'	6:B:64:HOH:O	2.21	0.41
1:A:205:GLU:C	1:A:207:GLY:H	2.23	0.41
1:A:248:LYS:O	1:A:260:ILE:HD11	2.20	0.41
1:A:121:ASN:ND2	1:A:125:ASN:HB3	2.35	0.40
1:A:81:ILE:CG1	1:A:92:MET:HE3	2.51	0.40
1:B:1248:LYS:HG3	1:B:1249:SER:N	2.33	0.40
1:A:218:ILE:O	1:A:222:ILE:HG13	2.21	0.40
1:A:162:VAL:HG12	1:A:163:LEU:N	2.36	0.40
1:A:211:VAL:N	1:A:215:GLU:OE1	2.53	0.40
1:B:1092:MET:O	1:B:1095:ILE:N	2.55	0.40
1:B:1140:PRO:O	1:B:1141:ALA:HB2	2.21	0.40
1:B:1146:ILE:O	1:B:1147:GLN:C	2.59	0.40
1:B:1089:TRP:CE3	1:B:1128:LYS:HG2	2.57	0.40
1:A:26:LEU:C	1:A:28:LYS:HZ3	2.24	0.40
1:B:1047:ARG:O	1:B:1048:PRO:C	2.60	0.40
1:B:1274:PRO:HG2	1:B:1281:SER:O	2.21	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	357/371 (96%)	277 (78%)	58 (16%)	22 (6%)	1	15
1	B	369/371 (100%)	277 (75%)	60 (16%)	32 (9%)	1	9
All	All	726/742 (98%)	554 (76%)	118 (16%)	54 (7%)	1	11

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	PHE
1	A	211	VAL
1	A	242	SER
1	A	280	GLU
1	A	281	SER
1	A	326	GLU
1	A	377	PRO
1	A	378	SER
1	A	384	CYS
1	B	1049	ARG
1	B	1054	MET
1	B	1055	VAL
1	B	1068	ALA
1	B	1069	GLN
1	B	1070	SER
1	B	1071	LYS
1	B	1182	PRO
1	B	1227	CYS
1	B	1279	MET
1	B	1345	ARG
1	A	192	GLY
1	A	209	SER
1	A	227	CYS
1	A	243	SER
1	A	297	ILE
1	B	1183	HIS
1	B	1207	GLY
1	B	1211	VAL
1	B	1231	LEU
1	B	1242	SER
1	B	1263	GLU
1	B	1297	ILE
1	B	1326	GLU
1	B	1378	SER
1	B	1380	VAL

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Mol	Chain	Res	Type
1	A	32	ALA
1	A	201	LYS
1	A	207	GLY
1	A	244	SER
1	A	290	ASN
1	A	325	LYS
1	B	1050	HIS
1	B	1256	GLN
1	B	1348	SER
1	A	189	ASP
1	B	1048	PRO
1	B	1060	GLY
1	B	1243	SER
1	B	1262	ASN
1	B	1090	ASP
1	B	1147	GLN
1	B	1073	GLY
1	A	267	CYS
1	B	1056	VAL

### 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	307/314 (98%)	287 (94%)	20 (6%)	17	50
1	B	314/314 (100%)	286 (91%)	28 (9%)	9	37
All	All	621/628 (99%)	573 (92%)	48 (8%)	13	42

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	50	HIS
1	A	69	GLN
1	A	90	ASP

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Mol	Chain	Res	Type
1	A	109	GLU
1	A	125	ASN
1	A	136	THR
1	A	142	MET
1	A	161	ILE
1	A	164	ASP
1	A	189	ASP
1	A	190	LEU
1	A	228	TYR
1	A	246	LEU
1	A	252	LEU
1	A	260	ILE
1	A	327	ILE
1	A	378	SER
1	A	382	ARG
1	A	383	LYS
1	B	1048	PRO
1	B	1049	ARG
1	B	1061	ASP
1	B	1069	GLN
1	B	1094	LYS
1	B	1114	LEU
1	B	1139	VAL
1	B	1161	ILE
1	B	1169	VAL
1	B	1172	ASN
1	B	1176	TYR
1	B	1182	PRO
1	B	1228	TYR
1	B	1246	LEU
1	B	1247	GLU
1	B	1260	ILE
1	B	1270	THR
1	B	1279	MET
1	B	1301	LYS
1	B	1307	ASN
1	B	1332	PRO
1	B	1349	VAL
1	B	1356	LEU
1	B	1361	THR
1	B	1368	THR
1	B	1378	SER

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Mol	Chain	Res	Type
1	B	1382	ARG
1	B	1384	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	69	GLN
1	A	102	ASN
1	A	121	ASN
1	A	125	ASN
1	A	131	GLN
1	A	290	ASN
1	A	307	ASN
1	A	363	GLN
1	A	364	GLN
1	A	381	HIS
1	B	1051	GLN
1	B	1069	GLN
1	B	1097	HIS
1	B	1102	ASN
1	B	1131	GLN
1	B	1171	HIS
1	B	1172	ASN
1	B	1290	ASN
1	B	1307	ASN
1	B	1363	GLN
1	B	1364	GLN

### 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 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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
5	LAR	A	411	-	30,31,31	1.14	3 (10%)	32,43,43	1.72	5 (15%)
5	LAR	B	1411	-	30,31,31	1.20	4 (13%)	32,43,43	1.53	3 (9%)
4	ATP	B	1390	2	26,33,33	2.23	12 (46%)	31,52,52	3.05	10 (32%)
4	ATP	A	390	2	26,33,33	2.18	11 (42%)	31,52,52	3.14	9 (29%)

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
5	LAR	A	411	-	-	4/23/51/51	0/2/3/3
5	LAR	B	1411	-	-	4/23/51/51	0/2/3/3
4	ATP	B	1390	2	-	2/18/38/38	0/3/3/3
4	ATP	A	390	2	-	1/18/38/38	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	390	ATP	C4-N3	5.54	1.43	1.35
4	B	1390	ATP	C4-N3	4.77	1.42	1.35
4	B	1390	ATP	O4'-C1'	4.75	1.47	1.41
4	B	1390	ATP	O5'-C5'	-4.40	1.27	1.44
4	A	390	ATP	O5'-C5'	-4.34	1.28	1.44
4	A	390	ATP	PA-O5'	-3.27	1.46	1.59
4	A	390	ATP	O4'-C1'	3.21	1.45	1.41
5	A	411	LAR	C18-N1	3.18	1.51	1.46
4	B	1390	ATP	PA-O5'	-3.02	1.47	1.59
5	B	1411	LAR	C20-N1	-2.90	1.30	1.34
5	B	1411	LAR	C18-N1	2.74	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	390	ATP	PB-O1B	-2.71	1.41	1.50
4	B	1390	ATP	C8-N7	-2.67	1.29	1.34
4	B	1390	ATP	PB-O1B	-2.63	1.41	1.50
4	A	390	ATP	C6-C5	2.35	1.52	1.43
4	B	1390	ATP	C3'-C4'	-2.33	1.47	1.53
5	A	411	LAR	C21-C3	2.22	1.56	1.50
5	B	1411	LAR	C21-C3	2.19	1.56	1.50
4	A	390	ATP	C2-N3	2.18	1.35	1.32
4	A	390	ATP	PA-O1A	-2.17	1.43	1.50
5	A	411	LAR	C20-N1	-2.11	1.31	1.34
4	A	390	ATP	PA-O2A	-2.11	1.45	1.55
5	B	1411	LAR	O3-C13	2.10	1.49	1.44
4	B	1390	ATP	C6-C5	2.06	1.50	1.43
4	B	1390	ATP	C2-N3	2.06	1.35	1.32
4	B	1390	ATP	PA-O1A	-2.05	1.43	1.50
4	B	1390	ATP	PA-O2A	-2.04	1.45	1.55
4	A	390	ATP	C8-N7	-2.04	1.31	1.34
4	A	390	ATP	PG-O2G	-2.01	1.47	1.54
4	B	1390	ATP	PG-O2G	-2.01	1.47	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	390	ATP	O5'-C5'-C4'	11.66	149.12	108.99
4	B	1390	ATP	O5'-C5'-C4'	11.59	148.89	108.99
4	A	390	ATP	O5'-PA-O1A	-7.11	81.27	109.07
4	B	1390	ATP	O5'-PA-O1A	-7.10	81.31	109.07
4	A	390	ATP	PA-O5'-C5'	5.90	156.28	121.68
4	B	1390	ATP	PA-O5'-C5'	5.72	155.20	121.68
5	A	411	LAR	C19-S1-C20	5.16	94.77	92.00
5	B	1411	LAR	C19-S1-C20	4.88	94.62	92.00
4	B	1390	ATP	C5'-C4'-C3'	-4.11	99.79	115.18
4	A	390	ATP	C5'-C4'-C3'	-4.04	100.04	115.18
5	A	411	LAR	C3-C2-C1	3.91	137.14	127.46
4	A	390	ATP	O4'-C4'-C3'	3.85	112.72	105.11
5	B	1411	LAR	C3-C2-C1	3.42	135.91	127.46
4	A	390	ATP	C3'-C2'-C1'	3.30	105.94	100.98
5	A	411	LAR	O5-C20-N1	3.12	130.21	126.81
4	A	390	ATP	C1'-N9-C4	-2.96	121.44	126.64
4	B	1390	ATP	C4-C5-N7	2.88	112.40	109.40
5	B	1411	LAR	O5-C20-N1	2.75	129.81	126.81
4	A	390	ATP	C4-C5-N7	2.70	112.21	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1390	ATP	C3'-C2'-C1'	2.31	104.46	100.98
4	B	1390	ATP	C1'-N9-C4	-2.30	122.61	126.64
4	B	1390	ATP	O4'-C4'-C3'	2.27	109.61	105.11
5	A	411	LAR	C21-C3-C2	-2.18	116.21	122.77
5	A	411	LAR	O2-C15-C16	2.15	112.94	107.59
4	B	1390	ATP	O2B-PB-O1B	2.11	122.69	112.24
4	A	390	ATP	O2B-PB-O1B	2.04	122.31	112.24
4	B	1390	ATP	O2A-PA-O1A	2.03	122.28	112.24

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1411	LAR	O3-C17-C18-C19
5	A	411	LAR	O3-C17-C18-C19
5	A	411	LAR	C3-C4-C5-C6
4	B	1390	ATP	PG-O3B-PB-O2B
4	A	390	ATP	PG-O3B-PB-O2B
5	B	1411	LAR	O2-C1-C2-C3
5	A	411	LAR	O2-C1-C2-C3
4	B	1390	ATP	PA-O3A-PB-O2B
5	B	1411	LAR	O1-C1-C2-C3
5	B	1411	LAR	C4-C5-C6-C7
5	A	411	LAR	C4-C5-C6-C7

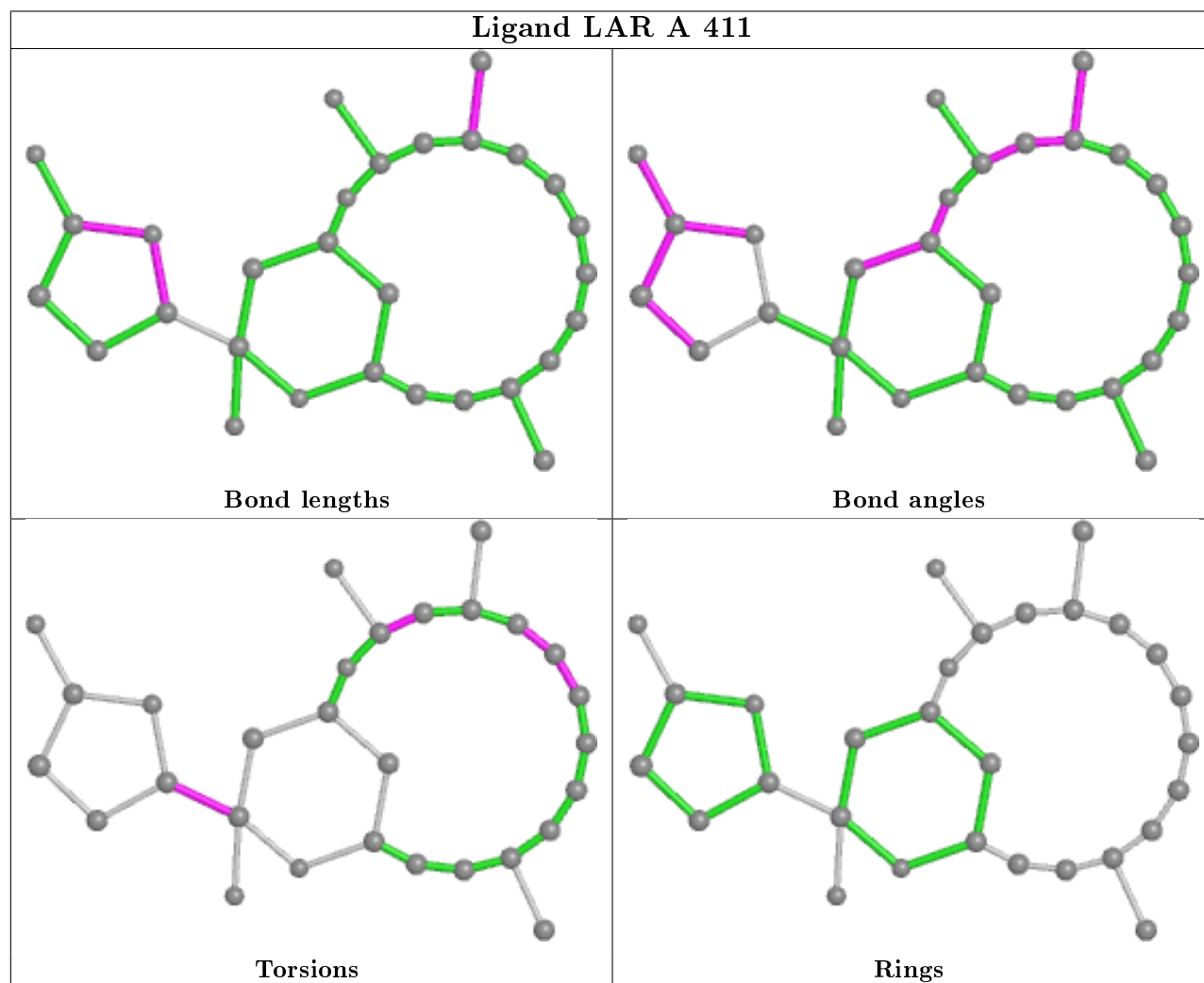
There are no ring outliers.

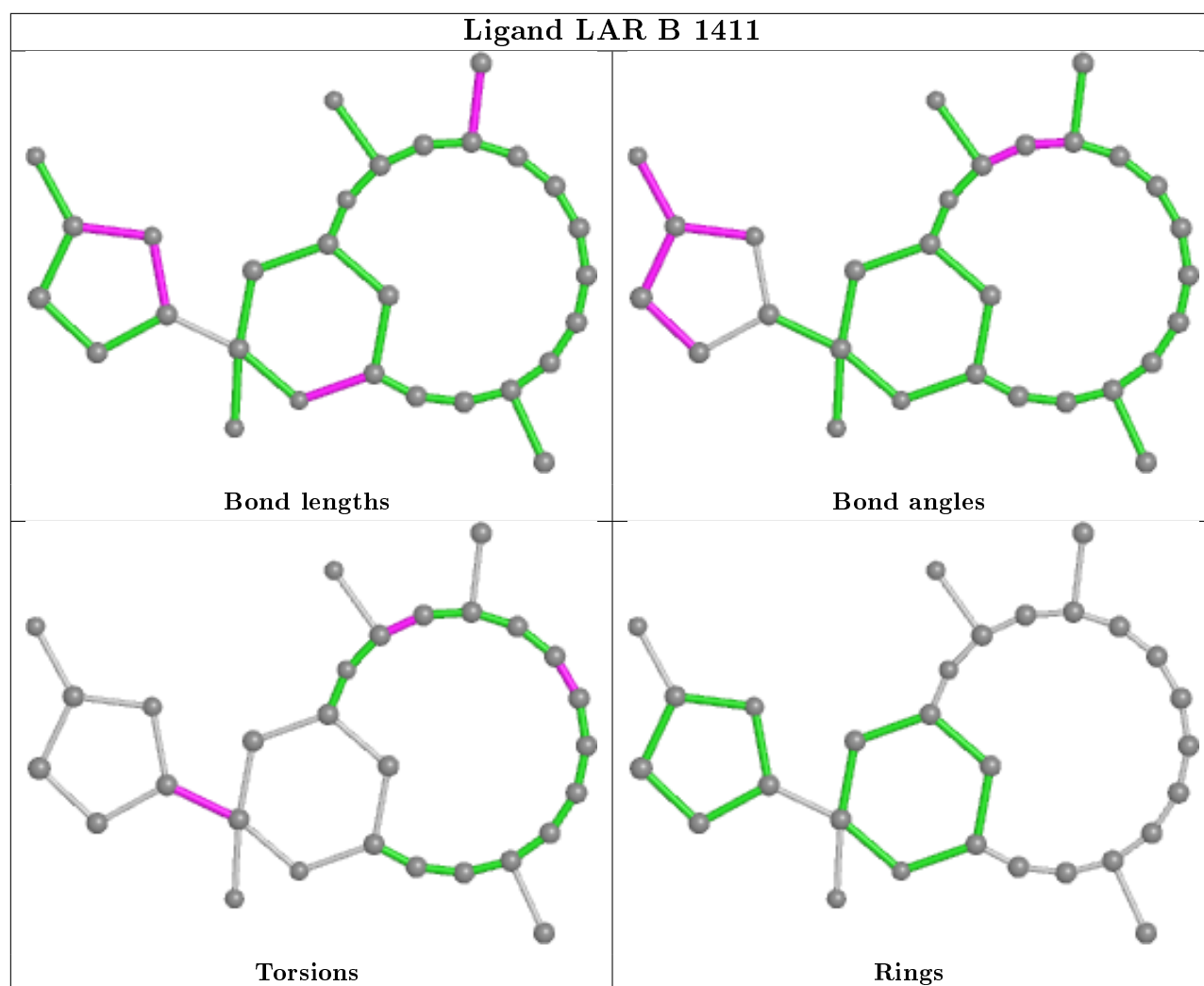
4 monomers are involved in 5 short contacts:

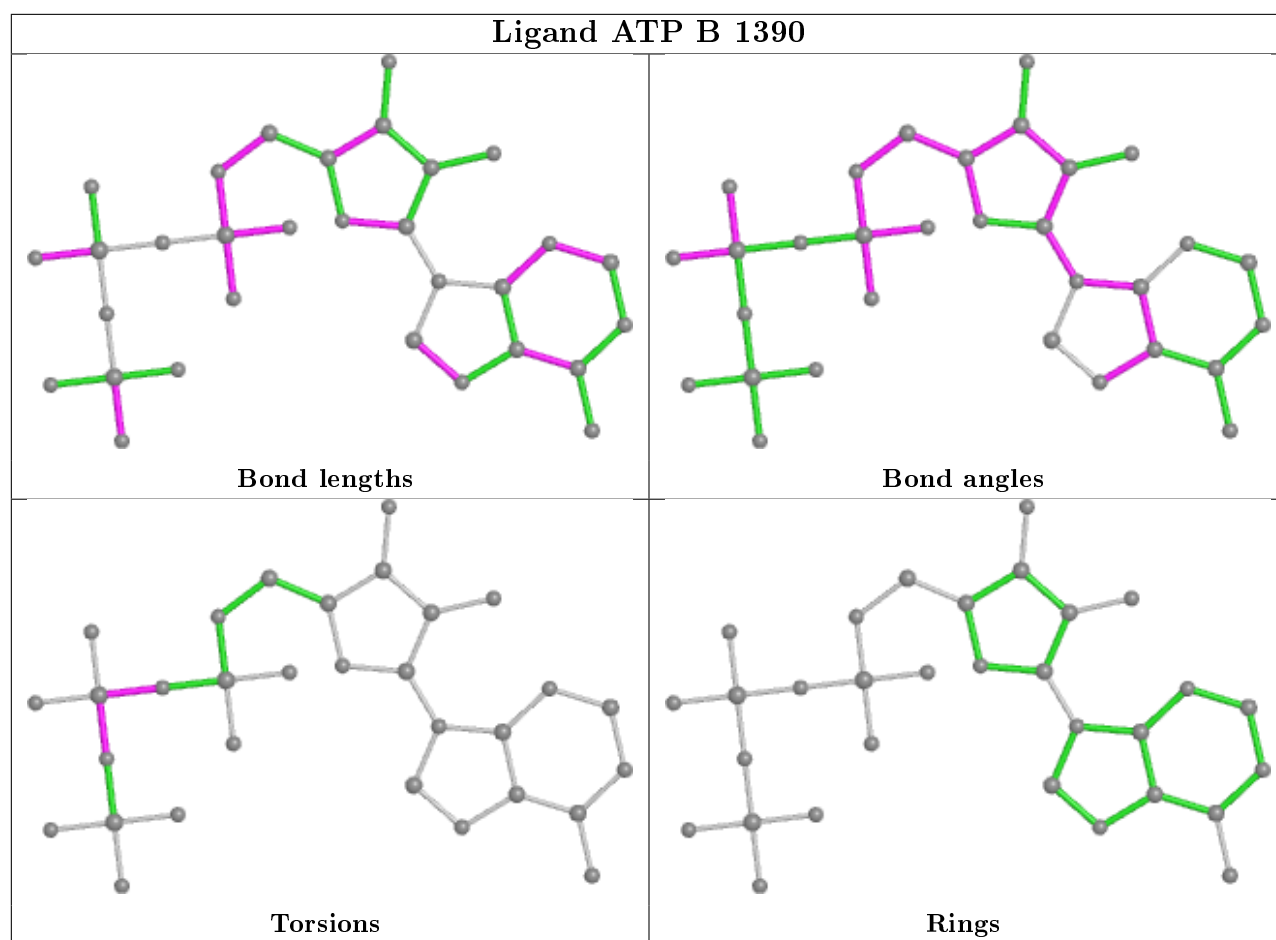
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	411	LAR	1	0
5	B	1411	LAR	1	0
4	B	1390	ATP	1	0
4	A	390	ATP	2	0

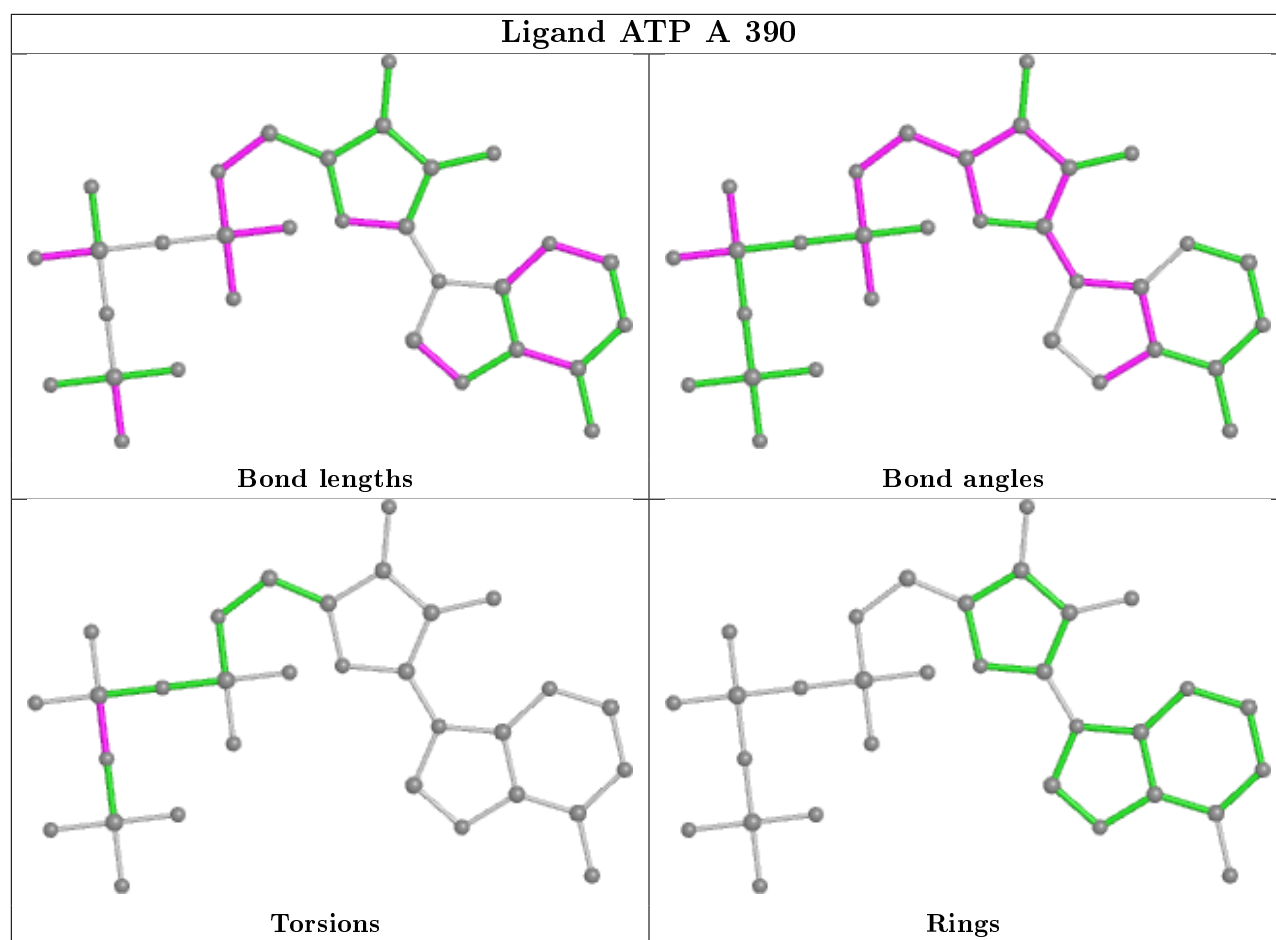
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.