Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 07:22 AM EDT

PDB ID	:	1QR6
Title	:	HUMAN MITOCHONDRIAL NAD(P)-DEPENDENT MALIC ENZYME
Authors	:	Xu, Y.; Bhargava, G.; Wu, H.; Loeber, G.; Tong, L.
Deposited on	:	1999-06-18
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

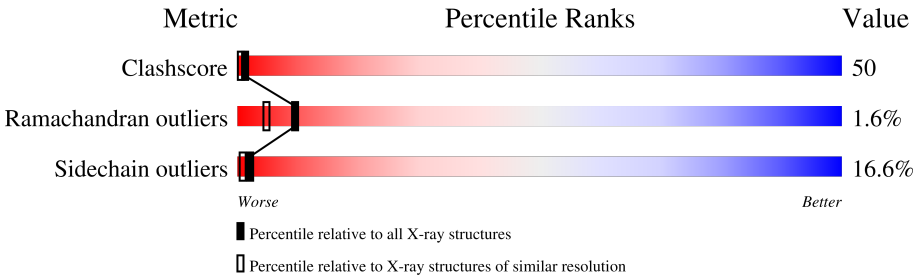
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	584	36% 49% 9% • 6%
1	B	584	37% 47% 11% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9620 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 MALIC ENZYME 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	Se	10	0	0
			4342	2779	739	801	9	14			
1	B	551	Total	C	N	O	S	Se	0	0	0
			4342	2779	739	801	9	14			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	38	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	47	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	75	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	86	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	108	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	177	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	219	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	239	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	325	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	327	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	343	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	407	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	539	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1029	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1038	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1047	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1075	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1086	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1108	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1177	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1219	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1239	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1325	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1327	MSE	MET	MODIFIED RESIDUE	UNP P23368

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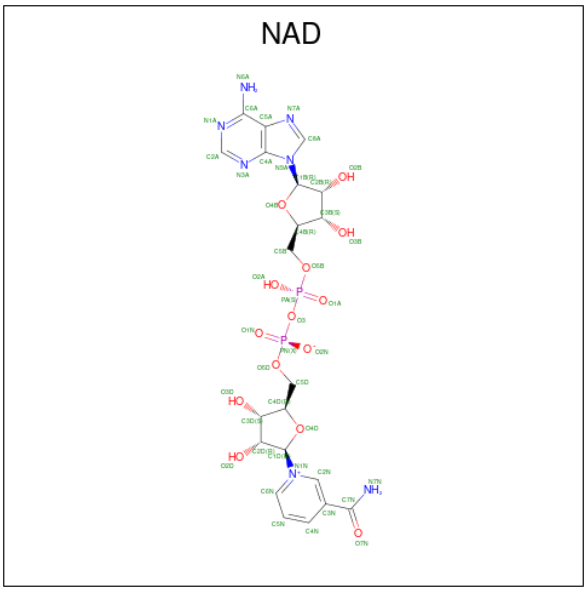
Chain	Residue	Modelled	Actual	Comment	Reference
B	1343	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1407	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1539	MSE	MET	MODIFIED RESIDUE	UNP P23368

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	374	Total	O	0	0
			374	374		
3	B	386	Total	O	0	0
			386	386		

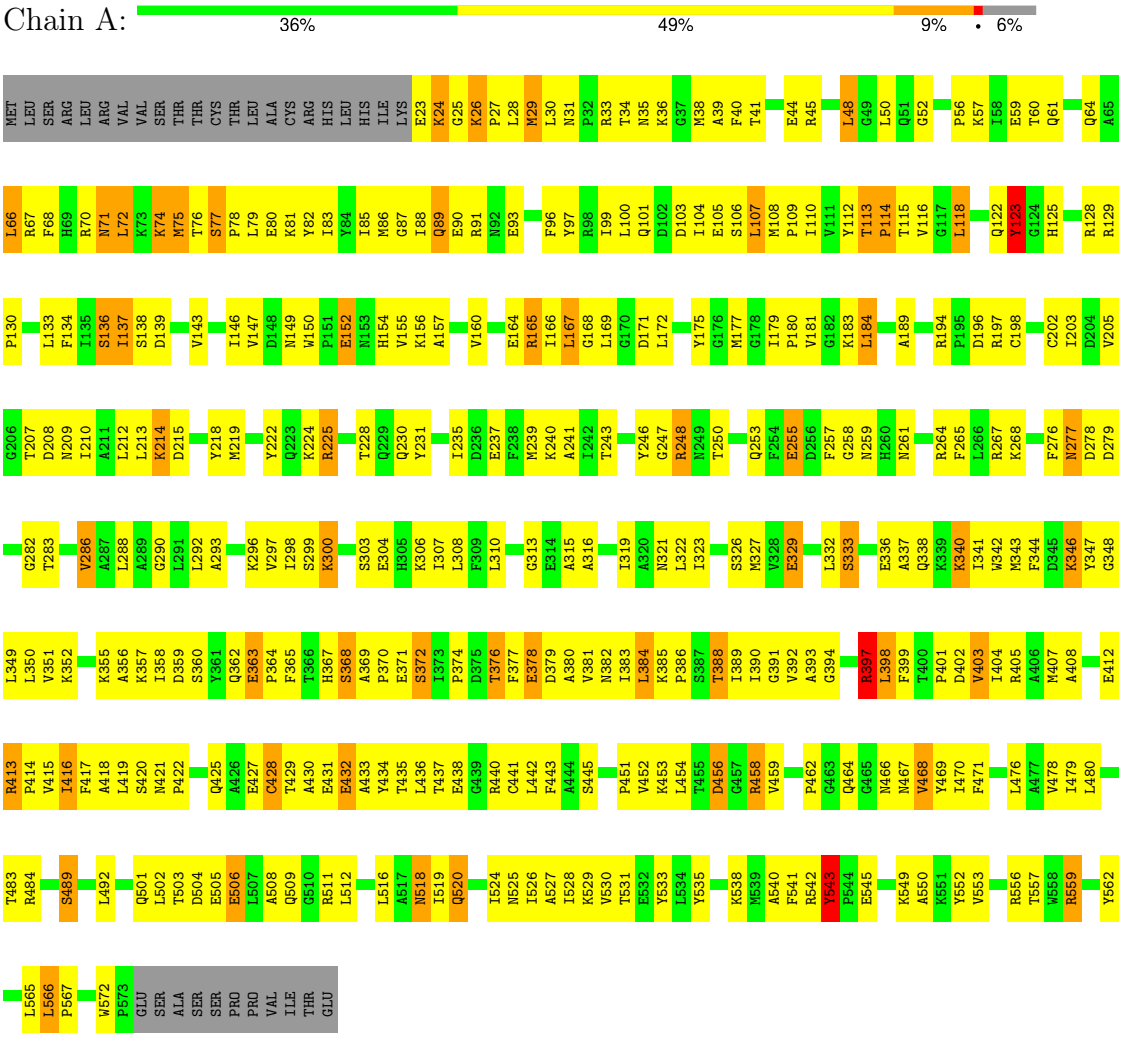
3 Residue-property plots (i)

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

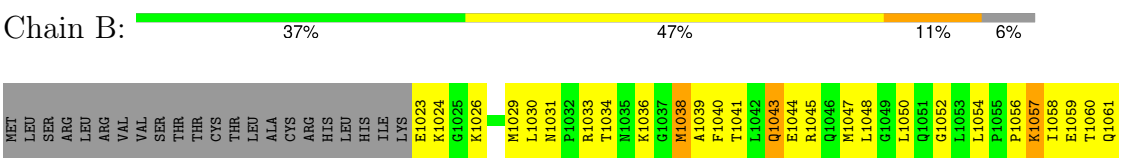
- Molecule 1: MALIC ENZYME 2

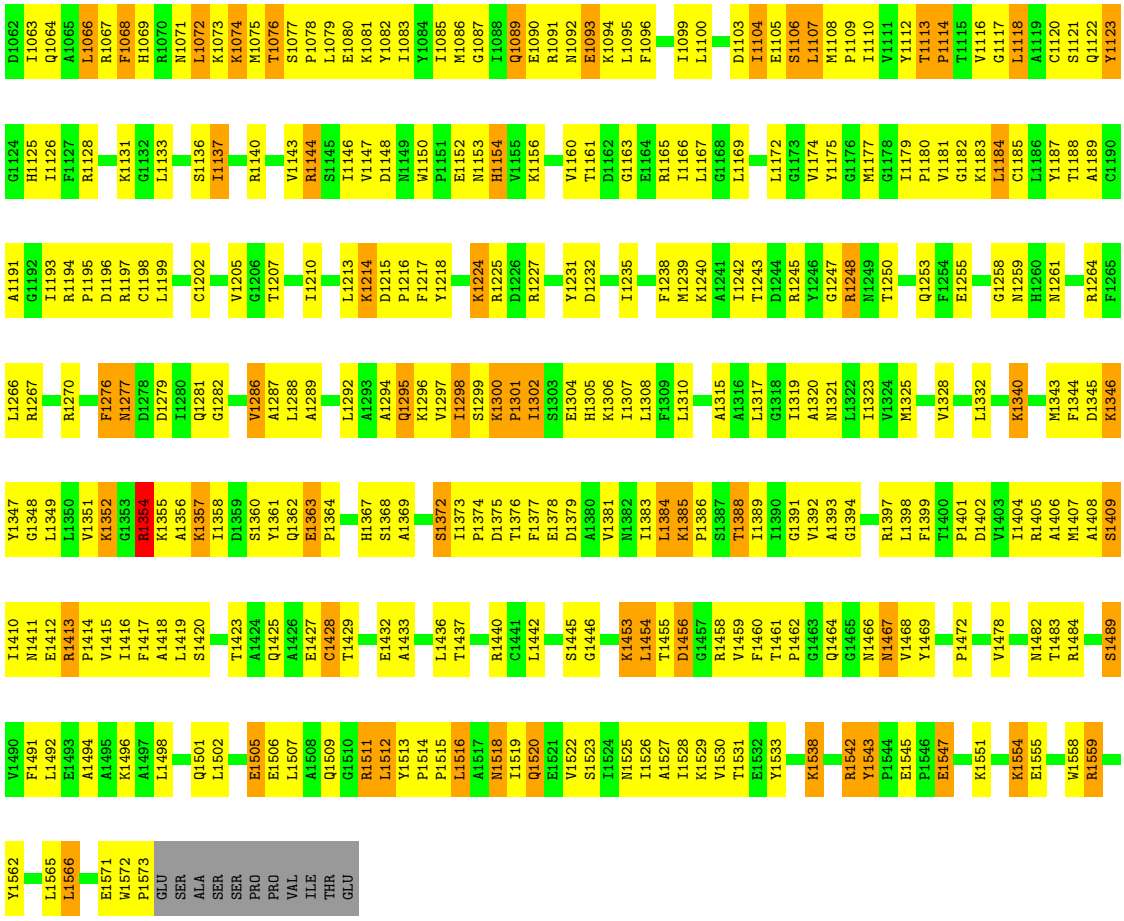
Chain A:



- Molecule 1: MALIC ENZYME 2

Chain B:




D1062 I1063 Q1064 A1065 L1066 R1067 F1068 H1069 R1070 N1071 L1072 K1073 K1074 M1075 T1076 S1077 P1078 L1079 E1080 K1081 Y1082 I1083 Y1084 I1085 M1086 G1087 I1088 Q1089 E1090 R1091 N1092 E1093 K1094 L1095 F1096 I1099 L1100 D1103 I1104 E1105 S1106 L1107 M1108 P1109 I1110 V1111 Y1112 T1113 P1114 T1115 V1116 G1117 L1118 A1119 C1120 S1121 Q1122 Y1123
G1124 H1125 I1126 F1127 R1128 K1131 G1132 L1133 S1136 I1137 R1140 V1143 R1144 S1145 I1146 V1147 D1148 N1149 W1150 P1151 E1152 N1153 H1154 V1155 K1156 V1160 T1161 D1162 G1163 E1164 R1165 I1166 L1167 G1168 L1169 L1172 G1173 V1174 Y1175 G1176 M1177 G1178 I1179 P1180 V1181 G1182 K1183 L1184 C1185 L1186 Y1187 T1188 A1189 C1190
A1191 G1192 I1193 R1194 P1195 D1196 R1197 C1198 L1199 C1202 V1205 G1206 T1207 I1210 L1213 K1214 D1215 P1216 F1217 Y1218 K1224 R1225 D1226 R1227 Y1231 D1232 I1235 F1238 M1239 K1240 A1241 I1242 T1243 D1244 R1245 Y1246 G1247 R1248 N1249 T1250 Q1253 F1254 E1255 G1258 N1259 H1260 N1261 R1264 F1265
L1266 R1267 R1270 F1276 N1277 D1278 D1279 I1280 Q1281 G1282 V1286 A1287 L1288 A1289 L1292 A1293 A1294 Q1295 K1296 V1297 I1298 S1299 K1300 P1301 I1302 S1303 E1304 H1305 K1306 I1307 L1308 F1309 L1310 A1315 A1316 L1317 G1318 I1319 A1320 N1321 L1322 I1323 V1324 M1325 V1328 L1332 K1340 M1343 F1344 D1345 K1346
Y1347 G1348 L1349 L1350 V1351 K1352 G1353 R1354 K1355 A1356 K1357 I1358 D1359 S1360 Y1361 Q1362 E1363 P1364 H1367 S1368 A1369 S1372 I1373 P1374 D1375 T1376 F1377 E1378 D1379 A1380 V1381 N1382 I1383 L1384 K1385 P1386 S1387 T1388 I1389 I1390 G1391 V1392 A1393 G1394 R1397 L1398 F1399 T1400 P1401 D1402 V1403 I1404 R1405 A1406 M1407 A1408 S1409
I1410 N1411 E1412 R1413 P1414 V1415 I1416 F1417 A1418 L1419 S1420 T1423 A1424 Q1425 A1426 E1427 C1428 T1429 E1432 A1433 L1436 T1437 R1440 C1441 L1442 S1445 G1446 K1453 L1454 T1455 D1456 G1457 R1458 V1459 F1460 T1461 P1462 G1463 Q1464 G1465 N1466 N1467 V1468 Y1469 P1472 V1478 N1482 T1483 R1484 S1489
V1490 F1491 L1492 E1493 A1494 A1495 K1496 A1497 L1498 Q1501 L1502 E1505 E1506 L1507 A1508 Q1509 G1510 R1511 L1512 Y1513 P1514 P1515 L1516 A1517 N1518 I1519 Q1520 E1521 V1522 S1523 I1524 N1525 I1526 A1527 I1528 K1529 V1530 T1531 E1532 Y1533 K1538 R1542 Y1543 P1544 E1545 P1546 E1547 K1551 K1554 E1555 W1558 R1559
Y1562 L1565 L1566 E1571 W1572 P1573 GLU SER ALA SER SER PRO PRO VAL ILE THR GLU

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α, β, γ	204.40Å 107.00Å 59.20Å 90.00° 90.00° 101.90°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	87.0 (20.00-2.10)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.228 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9620	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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: NAD

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	0.37	0/4422	0.64	2/5967 (0.0%)
1	B	0.37	0/4422	0.63	3/5967 (0.1%)
All	All	0.37	0/8844	0.63	5/11934 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1543	TYR	N-CA-C	7.24	130.53	111.00
1	A	543	TYR	N-CA-C	6.19	127.71	111.00
1	A	542	ARG	N-CA-C	-5.91	95.03	111.00
1	B	1542	ARG	N-CA-C	-5.62	95.81	111.00
1	B	1543	TYR	C-N-CD	5.00	138.90	128.40

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	4342	0	4366	455	0
1	B	4342	0	4366	441	0
2	A	88	0	52	2	0
2	B	88	0	52	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	374	0	0	145	0
3	B	386	0	0	155	0
All	All	9620	0	8836	884	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 50.

All (884) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1107:LEU:HD12	3:B:2496:HOH:O	1.42	1.19
1:A:218:TYR:HB2	3:A:2698:HOH:O	1.44	1.18
1:B:1472:PRO:HB2	3:B:2252:HOH:O	1.48	1.11
1:A:215:ASP:HB3	3:A:2698:HOH:O	1.51	1.10
1:B:1243:THR:HB	1:B:1248:ARG:HE	1.20	1.06
1:B:1513:TYR:HB3	3:B:2740:HOH:O	1.55	1.05
1:A:85:ILE:HG23	1:A:86:MSE:HE3	1.39	1.05
1:B:1113:THR:HB	1:B:1114:PRO:HD3	1.39	1.05
1:A:454:LEU:HD12	3:A:2700:HOH:O	1.58	1.03
1:B:1410:ILE:HG21	3:B:2585:HOH:O	1.60	1.01
1:B:1298:ILE:HG13	3:B:2614:HOH:O	1.61	1.00
1:B:1177:MSE:HG2	1:B:1202:CYS:HB2	1.46	0.97
1:B:1287:ALA:HA	3:B:2167:HOH:O	1.62	0.97
1:A:433:ALA:HB3	3:A:2670:HOH:O	1.62	0.97
1:B:1297:VAL:HG12	1:B:1298:ILE:HD13	1.48	0.96
1:B:1454:LEU:HD11	1:B:1460:PHE:HE2	1.31	0.95
1:B:1385:LYS:HB2	3:B:2680:HOH:O	1.65	0.94
1:A:72:LEU:HA	1:A:75:MSE:HE3	1.48	0.94
1:A:104:ILE:HG13	1:A:108:MSE:HE2	1.49	0.94
1:B:1310:LEU:HD12	3:B:2076:HOH:O	1.66	0.94
1:B:1492:LEU:HB2	3:B:2514:HOH:O	1.65	0.94
1:B:1543:TYR:O	1:B:1545:GLU:N	2.01	0.93
1:A:453:LYS:HE2	3:A:2688:HOH:O	1.67	0.93
1:A:86:MSE:HE2	1:A:86:MSE:HA	1.50	0.93
1:A:61:GLN:HA	1:A:64:GLN:HE21	1.31	0.92
1:B:1261:ASN:HD22	1:B:1264:ARG:HE	1.01	0.92
1:A:113:THR:HB	1:A:114:PRO:HD3	1.48	0.92
1:A:376:THR:HG22	1:A:379:ASP:H	1.36	0.91
1:A:543:TYR:O	1:A:545:GLU:N	2.05	0.90
1:A:393:ALA:HB3	3:A:2677:HOH:O	1.72	0.90
1:B:1526:ILE:HG23	3:B:2727:HOH:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ILE:HG23	1:A:388:THR:HG22	1.53	0.88
1:B:1177:MSE:HG2	1:B:1202:CYS:CB	2.02	0.88
1:A:349:LEU:HD23	3:A:2556:HOH:O	1.74	0.88
1:A:527:ALA:O	1:A:531:THR:HG23	1.74	0.87
1:B:1057:LYS:HB3	3:B:2238:HOH:O	1.75	0.86
1:B:1086:MSE:HE2	1:B:1086:MSE:HA	1.57	0.86
1:B:1527:ALA:O	1:B:1531:THR:HG23	1.76	0.86
1:A:44:GLU:O	1:A:48:LEU:HB2	1.75	0.85
1:A:277:ASN:HD21	1:A:279:ASP:HB2	1.39	0.85
1:A:431:GLU:HG2	1:A:452:VAL:HG22	1.58	0.85
1:B:1429:THR:HG23	1:B:1432:GLU:H	1.41	0.85
1:A:518:ASN:HB3	3:A:2661:HOH:O	1.75	0.85
1:A:91:ARG:HD2	3:B:2639:HOH:O	1.76	0.84
1:B:1308:LEU:HB3	1:B:1389:ILE:HD12	1.59	0.84
1:A:437:THR:HG23	3:A:2220:HOH:O	1.77	0.84
1:B:1547:GLU:HG2	3:B:2652:HOH:O	1.76	0.84
1:A:557:THR:HG22	3:A:2386:HOH:O	1.77	0.84
1:B:1515:PRO:HG2	1:B:1518:ASN:HD21	1.43	0.84
1:A:476:LEU:HD21	3:A:2386:HOH:O	1.77	0.84
1:B:1354:ARG:HD3	1:B:1358:ILE:HD11	1.58	0.84
1:A:167:LEU:HD11	3:A:2550:HOH:O	1.77	0.84
1:B:1058:ILE:HG13	3:B:2147:HOH:O	1.77	0.83
1:B:1194:ARG:HA	3:B:2518:HOH:O	1.79	0.83
1:A:374:PRO:HG3	1:A:380:ALA:HA	1.58	0.83
1:A:392:VAL:HG12	1:A:392:VAL:O	1.76	0.83
1:A:389:ILE:HG21	3:A:2333:HOH:O	1.77	0.83
1:B:1261:ASN:ND2	1:B:1264:ARG:HE	1.76	0.83
1:B:1319:ILE:HG23	3:B:2547:HOH:O	1.77	0.83
1:B:1558:TRP:HB3	3:B:2518:HOH:O	1.78	0.83
1:A:454:LEU:HA	3:A:2627:HOH:O	1.80	0.82
1:A:531:THR:HB	3:A:2234:HOH:O	1.78	0.82
1:B:1454:LEU:HD11	1:B:1460:PHE:CE2	2.13	0.82
1:A:429:THR:HG23	1:A:432:GLU:H	1.43	0.82
1:A:376:THR:HG23	1:A:378:GLU:H	1.44	0.82
1:B:1442:LEU:HD12	3:B:2614:HOH:O	1.79	0.82
1:A:109:PRO:O	1:A:114:PRO:HD2	1.79	0.82
1:A:24:LYS:HA	1:A:28:LEU:HD22	1.60	0.82
1:A:388:THR:HG23	3:A:2287:HOH:O	1.79	0.81
1:A:86:MSE:HE1	1:A:96:PHE:CE1	2.15	0.81
1:A:154:HIS:O	1:A:197:ARG:HG2	1.81	0.81
1:B:1405:ARG:HD2	3:B:2359:HOH:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ILE:HG21	3:A:2715:HOH:O	1.80	0.80
1:A:378:GLU:OE1	1:A:402:ASP:HB3	1.80	0.80
1:A:338:GLN:HB3	3:A:2569:HOH:O	1.80	0.80
1:B:1109:PRO:O	1:B:1114:PRO:HD2	1.82	0.80
1:B:1104:ILE:HG13	1:B:1108:MSE:HG3	1.63	0.80
1:B:1039:ALA:HA	1:B:1059:GLU:O	1.82	0.79
1:A:78:PRO:HG3	3:A:2628:HOH:O	1.81	0.79
1:A:327:MSE:HE3	1:A:337:ALA:HB1	1.65	0.79
1:A:372:SER:HB2	1:A:383:ILE:HG12	1.64	0.79
1:A:390:ILE:HG12	3:A:2571:HOH:O	1.83	0.79
1:B:1392:VAL:HG12	1:B:1392:VAL:O	1.82	0.79
1:A:128:ARG:HH22	1:B:1128:ARG:NH1	1.80	0.79
1:A:288:LEU:HG	3:A:2469:HOH:O	1.81	0.79
1:A:436:LEU:HB3	3:A:2512:HOH:O	1.83	0.79
1:B:1514:PRO:O	3:B:2740:HOH:O	2.01	0.78
1:A:471:PHE:CD1	3:A:2711:HOH:O	2.36	0.78
1:A:296:LYS:HE3	3:A:2737:HOH:O	1.83	0.78
1:B:1428:CYS:SG	3:B:2311:HOH:O	2.42	0.77
1:B:1351:VAL:HG11	1:B:1369:ALA:HB2	1.66	0.77
1:A:435:THR:HA	3:A:2229:HOH:O	1.83	0.77
1:B:1411:ASN:HB2	3:B:2146:HOH:O	1.84	0.77
1:A:437:THR:HG22	3:A:2063:HOH:O	1.83	0.77
1:A:310:LEU:HD23	1:A:427:GLU:HG2	1.68	0.76
1:B:1113:THR:CB	1:B:1114:PRO:HD3	2.15	0.76
1:A:386:PRO:HG2	3:A:2256:HOH:O	1.85	0.76
1:B:1085:ILE:HG23	1:B:1086:MSE:HE3	1.66	0.76
1:A:113:THR:CB	1:A:114:PRO:HD3	2.16	0.76
1:B:1406:ALA:C	3:B:2312:HOH:O	2.25	0.76
1:A:416:ILE:HD11	1:A:441:CYS:CB	2.16	0.75
1:A:437:THR:HG21	1:A:441:CYS:HB3	1.68	0.75
1:B:1240:LYS:HE2	3:B:2724:HOH:O	1.87	0.75
1:B:1294:ALA:HB1	1:B:1442:LEU:HD13	1.67	0.75
1:A:315:ALA:HA	3:A:2644:HOH:O	1.87	0.74
1:A:85:ILE:HG13	3:A:2715:HOH:O	1.87	0.74
1:B:1526:ILE:CG2	3:B:2727:HOH:O	2.32	0.74
1:B:1078:PRO:HB3	3:B:2741:HOH:O	1.87	0.74
1:A:212:LEU:O	3:A:2698:HOH:O	2.05	0.74
1:B:1207:THR:HG21	3:B:2716:HOH:O	1.85	0.74
1:A:308:LEU:HB3	1:A:389:ILE:HD12	1.67	0.74
1:A:250:THR:HB	3:A:2279:HOH:O	1.87	0.74
1:B:1399:PHE:HD1	3:B:2311:HOH:O	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1078:PRO:HD2	3:B:2507:HOH:O	1.87	0.73
1:B:1307:ILE:HG23	1:B:1388:THR:HG22	1.68	0.73
1:B:1411:ASN:ND2	3:B:2146:HOH:O	2.22	0.73
1:B:1320:ALA:HB2	3:B:2102:HOH:O	1.87	0.73
1:B:1340:LYS:HE3	3:B:2280:HOH:O	1.88	0.73
1:A:23:GLU:HG2	1:A:24:LYS:N	2.04	0.73
1:A:104:ILE:CG1	1:A:108:MSE:HE2	2.18	0.73
1:B:1513:TYR:OH	3:B:2167:HOH:O	2.05	0.73
1:A:440:ARG:HG2	3:A:2237:HOH:O	1.87	0.73
1:B:1308:LEU:HB2	1:B:1386:PRO:HG3	1.71	0.73
1:B:1414:PRO:HA	3:B:2146:HOH:O	1.89	0.73
1:B:1043:GLN:HB3	3:B:2742:HOH:O	1.87	0.73
1:B:1526:ILE:O	1:B:1530:VAL:HG23	1.87	0.73
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.71	0.72
1:A:376:THR:CG2	1:A:379:ASP:H	2.02	0.72
1:B:1308:LEU:HB3	1:B:1389:ILE:CD1	2.19	0.72
1:A:128:ARG:HH12	1:B:1128:ARG:HH12	1.34	0.72
1:B:1261:ASN:HD22	1:B:1264:ARG:NE	1.84	0.72
1:B:1386:PRO:HG2	3:B:2265:HOH:O	1.90	0.72
1:A:292:LEU:HD11	3:A:2469:HOH:O	1.89	0.72
1:B:1165:ARG:HD3	1:B:1258:GLY:HA2	1.71	0.72
1:B:1372:SER:O	1:B:1383:ILE:HD13	1.89	0.72
1:A:86:MSE:HE1	1:A:96:PHE:CZ	2.24	0.72
1:A:265:PHE:HD1	3:A:2457:HOH:O	1.72	0.72
1:A:416:ILE:HD11	1:A:441:CYS:HB2	1.70	0.72
1:A:433:ALA:O	1:A:437:THR:HG23	1.90	0.72
1:A:454:LEU:HD11	3:A:2178:HOH:O	1.89	0.72
1:B:1217:PHE:HB3	3:B:2107:HOH:O	1.90	0.71
1:B:1113:THR:HB	1:B:1114:PRO:CD	2.19	0.71
1:A:456:ASP:OD1	1:A:458:ARG:HB2	1.90	0.71
1:A:367:HIS:HE1	3:A:2569:HOH:O	1.71	0.71
1:B:1163:GLY:HA2	1:B:1166:ILE:HD11	1.72	0.71
1:A:82:TYR:HD2	1:A:83:ILE:HD13	1.54	0.71
1:A:454:LEU:HD22	3:A:2229:HOH:O	1.89	0.71
1:B:1183:LYS:HE2	1:B:1255:GLU:OE2	1.91	0.70
1:A:506:GLU:O	1:A:511:ARG:HB2	1.91	0.70
1:A:64:GLN:O	1:A:68:PHE:HD1	1.73	0.70
1:A:385:LYS:HG3	3:A:2226:HOH:O	1.91	0.70
1:A:553:VAL:HG13	3:A:2141:HOH:O	1.91	0.70
1:B:1302:ILE:HA	1:B:1305:HIS:CD2	2.27	0.70
1:A:466:ASN:CB	3:A:2681:HOH:O	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1378:GLU:OE1	1:B:1402:ASP:HB3	1.92	0.69
1:B:1523:SER:HB3	3:B:2252:HOH:O	1.91	0.69
1:A:26:LYS:HE3	3:B:2492:HOH:O	1.93	0.69
1:A:152:GLU:HG2	1:A:196:ASP:O	1.92	0.69
1:A:183:LYS:HG3	3:A:2534:HOH:O	1.92	0.69
1:A:243:THR:HG22	3:A:2279:HOH:O	1.92	0.69
1:B:1086:MSE:HE1	1:B:1096:PHE:CE1	2.27	0.69
1:A:374:PRO:HD3	1:A:383:ILE:HD13	1.73	0.69
1:A:471:PHE:CE2	3:A:2692:HOH:O	2.45	0.69
1:B:1152:GLU:HG2	1:B:1196:ASP:O	1.93	0.69
1:B:1090:GLU:HB3	3:B:2094:HOH:O	1.91	0.69
2:A:601:NAD:H4N	3:A:2275:HOH:O	1.93	0.69
1:B:1454:LEU:HD12	1:B:1458:ARG:HB2	1.75	0.69
1:A:79:LEU:O	1:A:83:ILE:HG12	1.93	0.68
1:A:404:ILE:CG2	3:A:2220:HOH:O	2.41	0.68
1:B:1060:THR:H	1:B:1063:ILE:HD12	1.58	0.68
1:B:1179:ILE:HB	1:B:1180:PRO:HD3	1.75	0.68
1:A:381:VAL:HG22	3:A:2256:HOH:O	1.91	0.68
1:B:1061:GLN:NE2	3:B:2583:HOH:O	2.25	0.68
1:A:307:ILE:HG23	1:A:388:THR:CG2	2.24	0.68
1:B:1558:TRP:CB	3:B:2518:HOH:O	2.40	0.68
1:A:464:GLN:HA	3:A:2143:HOH:O	1.91	0.68
1:B:1511:ARG:HG2	1:B:1511:ARG:HH11	1.58	0.68
1:A:303:SER:O	1:A:340:LYS:HE2	1.94	0.68
1:A:80:GLU:C	3:A:2308:HOH:O	2.32	0.68
1:B:1409:SER:N	3:B:2312:HOH:O	2.13	0.68
1:A:48:LEU:HD22	3:A:2081:HOH:O	1.94	0.68
1:B:1325:MSE:HE2	3:B:2514:HOH:O	1.94	0.68
1:B:1325:MSE:CE	3:B:2514:HOH:O	2.41	0.67
1:B:1381:VAL:HG22	3:B:2265:HOH:O	1.93	0.67
1:A:459:VAL:HA	3:A:2189:HOH:O	1.94	0.67
1:A:376:THR:HG23	1:A:378:GLU:N	2.09	0.67
1:A:401:PRO:HB3	1:A:436:LEU:HD21	1.76	0.67
1:B:1058:ILE:HG22	3:B:2329:HOH:O	1.95	0.67
1:B:1103:ASP:HB3	1:B:1107:LEU:HD22	1.77	0.67
1:B:1392:VAL:O	1:B:1392:VAL:CG1	2.42	0.67
1:B:1484:ARG:HB2	3:B:2087:HOH:O	1.95	0.66
1:A:85:ILE:HG23	1:A:86:MSE:CE	2.20	0.66
1:B:1110:ILE:HB	3:B:2496:HOH:O	1.95	0.66
1:B:1294:ALA:CB	1:B:1442:LEU:HD13	2.26	0.66
1:B:1519:ILE:HG23	3:B:2565:HOH:O	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ILE:O	1:A:239:MSE:HG2	1.95	0.66
1:A:327:MSE:HE1	1:A:337:ALA:O	1.94	0.66
1:A:183:LYS:NZ	3:A:2692:HOH:O	2.20	0.65
1:A:225:ARG:HB2	3:A:2531:HOH:O	1.95	0.65
1:B:1043:GLN:HE21	1:B:1566:LEU:HD11	1.61	0.65
1:A:415:VAL:N	3:A:2752:HOH:O	2.25	0.65
1:B:1153:ASN:HD22	1:B:1245:ARG:HH21	1.44	0.65
1:A:405:ARG:HA	3:A:2512:HOH:O	1.97	0.65
1:B:1086:MSE:HE1	1:B:1096:PHE:CZ	2.32	0.65
1:B:1277:ASN:C	1:B:1277:ASN:HD22	1.99	0.65
1:B:1551:LYS:O	1:B:1555:GLU:HG3	1.95	0.65
1:A:128:ARG:HH12	1:B:1128:ARG:NH1	1.94	0.65
1:B:1202:CYS:SG	3:B:2416:HOH:O	2.54	0.65
1:B:1104:ILE:HD13	3:B:2565:HOH:O	1.97	0.65
1:B:1207:THR:CB	3:B:2716:HOH:O	2.44	0.65
1:A:128:ARG:NH1	1:B:1128:ARG:HH12	1.95	0.65
1:B:1038:MSE:SE	3:B:2238:HOH:O	2.64	0.65
1:B:1294:ALA:HB1	1:B:1442:LEU:CD1	2.27	0.65
1:A:471:PHE:CG	3:A:2711:HOH:O	2.49	0.64
1:A:321:ASN:HB3	3:A:2678:HOH:O	1.96	0.64
1:A:467:ASN:OD1	3:A:2275:HOH:O	2.14	0.64
1:A:129:ARG:HG3	1:A:130:PRO:HD2	1.77	0.64
1:A:377:PHE:CZ	1:A:389:ILE:HD11	2.32	0.64
1:A:468:VAL:HA	1:A:471:PHE:CE2	2.32	0.64
1:B:1169:LEU:N	1:B:1169:LEU:HD12	2.13	0.64
1:A:347:TYR:CD1	1:A:356:ALA:HB1	2.32	0.64
1:B:1188:THR:CG2	3:B:2409:HOH:O	2.46	0.64
1:B:1137:ILE:O	1:B:1140:ARG:HG2	1.98	0.63
1:B:1250:THR:HB	3:B:2746:HOH:O	1.97	0.63
1:B:1308:LEU:HD23	1:B:1389:ILE:HD11	1.79	0.63
1:A:40:PHE:HE2	1:A:565:LEU:HD12	1.62	0.63
1:B:1538:LYS:HA	3:B:2213:HOH:O	1.97	0.63
1:B:1038:MSE:HG2	1:B:1057:LYS:O	1.99	0.63
1:A:413:ARG:HD2	3:A:2134:HOH:O	1.98	0.63
1:B:1376:THR:HG22	1:B:1379:ASP:H	1.63	0.63
1:B:1349:LEU:HD21	1:B:1384:LEU:HD21	1.79	0.63
1:B:1059:GLU:CD	1:B:1067:ARG:HH12	2.02	0.63
1:A:524:ILE:HD12	3:A:2386:HOH:O	1.97	0.63
1:B:1112:TYR:CG	1:B:1113:THR:N	2.66	0.63
1:A:184:LEU:HG	1:A:198:CYS:HB3	1.81	0.63
1:A:208:ASP:N	3:A:2531:HOH:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:MSE:CE	1:A:519:ILE:HG21	2.29	0.62
1:A:308:LEU:HB3	1:A:389:ILE:CD1	2.28	0.62
1:B:1103:ASP:O	1:B:1107:LEU:HB2	2.00	0.62
1:B:1243:THR:HB	1:B:1248:ARG:NE	2.04	0.62
1:B:1404:ILE:HD12	1:B:1436:LEU:HD12	1.80	0.62
1:B:1414:PRO:HB3	3:B:2146:HOH:O	1.99	0.62
1:B:1214:LYS:HD3	3:B:2156:HOH:O	2.00	0.62
1:A:136:SER:OG	1:A:138:SER:HB2	2.00	0.62
1:A:85:ILE:HA	1:A:88:ILE:HD12	1.81	0.62
1:A:434:TYR:HB3	3:A:2178:HOH:O	2.00	0.62
1:A:113:THR:HB	1:A:114:PRO:CD	2.27	0.62
1:B:1177:MSE:SE	3:B:2597:HOH:O	2.68	0.61
1:B:1024:LYS:HB2	3:B:2310:HOH:O	1.99	0.61
1:B:1188:THR:HG21	3:B:2409:HOH:O	1.99	0.61
1:A:277:ASN:ND2	1:A:279:ASP:HB2	2.14	0.61
1:B:1082:TYR:HD2	1:B:1083:ILE:HD13	1.65	0.61
1:B:1207:THR:CG2	3:B:2716:HOH:O	2.44	0.61
1:B:1357:LYS:NZ	1:B:1357:LYS:HB3	2.16	0.61
1:A:189:ALA:O	1:A:520:GLN:NE2	2.34	0.61
1:B:1024:LYS:HE3	3:B:2310:HOH:O	2.00	0.61
1:B:1075:MSE:HG2	1:B:1080:GLU:CD	2.21	0.61
1:A:228:THR:HG23	3:A:2560:HOH:O	2.00	0.61
1:A:86:MSE:HE2	1:A:86:MSE:CA	2.28	0.61
1:A:297:VAL:HG12	1:A:298:ILE:HD13	1.83	0.61
1:B:1494:ALA:HB1	3:B:2727:HOH:O	2.00	0.61
1:A:183:LYS:HE3	3:A:2711:HOH:O	2.00	0.61
1:A:374:PRO:CD	1:A:383:ILE:HD13	2.31	0.61
1:A:261:ASN:HD22	1:A:264:ARG:HE	1.47	0.60
1:B:1110:ILE:CB	3:B:2496:HOH:O	2.48	0.60
1:A:177:MSE:HE1	1:A:181:VAL:HG23	1.83	0.60
1:A:454:LEU:CD2	3:A:2229:HOH:O	2.47	0.60
1:B:1389:ILE:HG21	3:B:2538:HOH:O	1.99	0.60
1:B:1152:GLU:HG3	3:B:2660:HOH:O	2.02	0.60
1:B:1184:LEU:HG	1:B:1198:CYS:HB3	1.83	0.60
1:B:1392:VAL:HG12	3:B:2035:HOH:O	2.01	0.60
1:B:1394:GLY:HA2	1:B:1420:SER:HB3	1.84	0.60
1:A:218:TYR:O	1:B:1057:LYS:HE2	2.01	0.60
1:A:469:TYR:CE1	3:A:2681:HOH:O	2.52	0.60
1:A:505:GLU:H	1:A:505:GLU:CD	2.04	0.60
1:B:1089:GLN:HG3	1:B:1090:GLU:N	2.16	0.60
1:A:112:TYR:O	1:A:116:VAL:HG12	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:MSE:CE	1:A:181:VAL:HG23	2.31	0.60
1:B:1399:PHE:CD1	3:B:2311:HOH:O	2.51	0.60
1:A:489:SER:HB2	1:A:533:TYR:OH	2.02	0.59
1:A:518:ASN:HA	3:A:2214:HOH:O	2.03	0.59
1:B:1513:TYR:C	3:B:2740:HOH:O	2.40	0.59
1:B:1091:ARG:HD2	3:B:2640:HOH:O	2.02	0.59
1:B:1282:GLY:O	1:B:1286:VAL:HG22	2.03	0.59
1:A:177:MSE:HG2	1:A:202:CYS:CB	2.33	0.59
1:A:342:TRP:HA	3:A:2437:HOH:O	2.01	0.59
1:A:401:PRO:O	1:A:405:ARG:HG2	2.03	0.59
1:B:1150:TRP:CE2	1:B:1199:LEU:HD13	2.38	0.59
1:B:1288:LEU:N	3:B:2547:HOH:O	2.34	0.59
1:A:116:VAL:HG13	3:A:2550:HOH:O	2.03	0.59
1:B:1428:CYS:HB3	3:B:2311:HOH:O	2.02	0.59
1:B:1469:TYR:CZ	1:B:1516:LEU:HD13	2.37	0.59
1:A:407:MSE:HE1	3:A:2256:HOH:O	2.03	0.59
1:B:1079:LEU:HD21	1:B:1122:GLN:HG3	1.85	0.59
1:B:1433:ALA:O	1:B:1437:THR:HG23	2.03	0.59
1:B:1515:PRO:HG2	1:B:1518:ASN:ND2	2.15	0.59
1:A:112:TYR:CG	1:A:113:THR:N	2.71	0.59
1:B:1413:ARG:HA	1:B:1440:ARG:O	2.02	0.59
1:B:1086:MSE:CE	1:B:1096:PHE:CE1	2.86	0.58
1:B:1429:THR:HG22	1:B:1432:GLU:CG	2.33	0.58
1:B:1429:THR:HG22	1:B:1432:GLU:OE1	2.03	0.58
1:A:462:PRO:HG3	3:A:2582:HOH:O	2.02	0.58
1:A:108:MSE:N	1:A:109:PRO:HD2	2.18	0.58
1:A:505:GLU:HG2	3:A:2714:HOH:O	2.03	0.58
1:B:1277:ASN:ND2	1:B:1279:ASP:H	2.01	0.58
1:A:75:MSE:SE	3:A:2308:HOH:O	2.71	0.58
1:A:103:ASP:HB3	1:A:107:LEU:HD22	1.84	0.58
1:B:1286:VAL:HG11	1:B:1466:ASN:O	2.03	0.58
1:A:72:LEU:HA	1:A:75:MSE:CE	2.28	0.58
1:A:404:ILE:HG22	3:A:2220:HOH:O	2.02	0.58
1:B:1077:SER:O	1:B:1081:LYS:HG3	2.04	0.58
1:B:1207:THR:HB	3:B:2716:HOH:O	2.03	0.58
1:A:137:ILE:HG13	1:A:137:ILE:O	2.03	0.58
1:A:379:ASP:O	1:A:383:ILE:HD12	2.03	0.58
1:A:438:GLU:HA	3:A:2555:HOH:O	2.03	0.58
1:B:1153:ASN:ND2	1:B:1245:ARG:HH21	2.02	0.58
1:B:1298:ILE:HD11	1:B:1442:LEU:HD11	1.85	0.58
1:A:416:ILE:HD11	1:A:441:CYS:SG	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1298:ILE:O	1:B:1300:LYS:N	2.36	0.58
1:A:60:THR:O	1:A:64:GLN:HG3	2.03	0.58
1:B:1302:ILE:CD1	3:B:2722:HOH:O	2.52	0.58
1:B:1454:LEU:CD1	1:B:1458:ARG:HB2	2.34	0.58
1:B:1559:ARG:HG2	3:B:2338:HOH:O	2.04	0.58
1:A:286:VAL:HG13	1:A:470:ILE:HG12	1.84	0.58
1:A:458:ARG:NH2	3:A:2700:HOH:O	2.37	0.57
1:B:1525:ASN:O	1:B:1529:LYS:HG2	2.04	0.57
1:A:293:ALA:O	1:A:296:LYS:HB2	2.03	0.57
1:A:381:VAL:CG2	1:A:407:MSE:HE1	2.34	0.57
1:B:1573:PRO:HA	3:B:2734:HOH:O	2.03	0.57
1:A:86:MSE:CE	1:A:96:PHE:CE1	2.88	0.57
1:A:129:ARG:HB3	3:A:2434:HOH:O	2.03	0.57
1:B:1117:GLY:O	1:B:1169:LEU:HD21	2.04	0.57
1:B:1231:TYR:O	1:B:1235:ILE:HG12	2.04	0.57
1:A:405:ARG:CA	3:A:2512:HOH:O	2.52	0.57
1:B:1401:PRO:HA	1:B:1436:LEU:CD1	2.34	0.57
1:A:109:PRO:HA	1:A:113:THR:HB	1.86	0.57
1:A:505:GLU:O	1:A:509:GLN:HG3	2.04	0.57
1:B:1300:LYS:HD3	1:B:1304:GLU:HB3	1.86	0.57
1:B:1315:ALA:HB3	1:B:1392:VAL:CG1	2.34	0.57
1:A:36:LYS:O	1:A:39:ALA:HB3	2.05	0.57
1:A:166:ILE:N	1:A:166:ILE:HD12	2.20	0.57
1:A:277:ASN:ND2	1:A:279:ASP:H	2.03	0.57
1:B:1043:GLN:NE2	1:B:1566:LEU:HD11	2.20	0.57
1:B:1123:TYR:HB3	1:B:1175:TYR:CD2	2.39	0.57
1:B:1399:PHE:CG	1:B:1427:GLU:HB3	2.40	0.57
1:A:315:ALA:HB3	1:A:392:VAL:HG11	1.85	0.57
1:A:437:THR:CG2	3:A:2220:HOH:O	2.45	0.57
1:B:1073:LYS:HE2	1:B:1074:LYS:NZ	2.20	0.57
1:A:430:ALA:HB2	3:A:2582:HOH:O	2.05	0.56
1:B:1033:ARG:NH1	1:B:1093:GLU:OE1	2.38	0.56
1:A:41:THR:OG1	1:A:44:GLU:HG3	2.05	0.56
1:A:440:ARG:HB3	3:A:2134:HOH:O	2.05	0.56
1:B:1195:PRO:HG3	3:B:2409:HOH:O	2.06	0.56
1:A:248:ARG:HB3	1:A:484:ARG:NH2	2.21	0.56
1:A:397:ARG:NE	3:A:2162:HOH:O	2.37	0.56
1:A:52:GLY:HA3	1:B:1146:ILE:HG23	1.87	0.56
1:A:139:ASP:OD2	1:A:146:ILE:HD11	2.06	0.56
1:A:349:LEU:HD21	1:A:384:LEU:HD21	1.86	0.56
1:A:543:TYR:C	1:A:545:GLU:N	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1218:TYR:CZ	3:B:2716:HOH:O	2.53	0.56
1:B:1177:MSE:HG2	1:B:1202:CYS:HB3	1.88	0.56
1:A:526:ILE:O	1:A:530:VAL:HG23	2.05	0.55
1:B:1177:MSE:N	3:B:2416:HOH:O	2.39	0.55
1:B:1489:SER:HA	3:B:2514:HOH:O	2.06	0.55
1:A:431:GLU:HB3	3:A:2735:HOH:O	2.05	0.55
1:B:1319:ILE:HG22	1:B:1323:ILE:HD12	1.88	0.55
1:B:1194:ARG:HB2	1:B:1197:ARG:HG3	1.88	0.55
1:A:70:ARG:O	1:A:74:LYS:HG3	2.07	0.55
1:A:282:GLY:O	1:A:286:VAL:HG22	2.06	0.55
1:B:1385:LYS:HA	3:B:2585:HOH:O	2.06	0.55
1:A:381:VAL:HG13	3:A:2256:HOH:O	2.07	0.55
1:A:382:ASN:O	1:A:385:LYS:HG3	2.07	0.55
1:B:1057:LYS:CB	3:B:2238:HOH:O	2.44	0.55
1:A:381:VAL:HG22	1:A:407:MSE:HE1	1.87	0.55
1:A:394:GLY:HA2	1:A:420:SER:HB3	1.89	0.55
1:A:177:MSE:HG2	1:A:202:CYS:HB2	1.88	0.55
1:B:1023:GLU:HA	3:B:2347:HOH:O	2.07	0.55
1:A:139:ASP:CG	1:A:146:ILE:HD11	2.26	0.55
1:B:1294:ALA:O	1:B:1297:VAL:HB	2.07	0.55
1:A:342:TRP:CH2	1:A:367:HIS:HB2	2.42	0.55
1:A:57:LYS:HD2	1:B:1218:TYR:O	2.07	0.54
1:A:71:ASN:O	1:A:75:MSE:CE	2.55	0.54
1:B:1068:PHE:CZ	1:B:1072:LEU:HD13	2.42	0.54
1:B:1143:VAL:O	1:B:1147:VAL:HG23	2.07	0.54
1:A:219:MSE:HE3	3:A:2095:HOH:O	2.06	0.54
1:A:283:THR:HA	3:A:2275:HOH:O	2.07	0.54
1:A:315:ALA:O	1:A:319:ILE:HD12	2.06	0.54
1:A:346:LYS:HE3	1:A:347:TYR:CZ	2.41	0.54
1:A:370:PRO:HD2	3:A:2556:HOH:O	2.06	0.54
1:A:79:LEU:HD13	1:A:118:LEU:HD13	1.88	0.54
1:A:81:LYS:HE3	3:A:2451:HOH:O	2.07	0.54
1:B:1061:GLN:HA	1:B:1064:GLN:HE21	1.71	0.54
1:B:1064:GLN:OE1	3:B:2704:HOH:O	2.18	0.54
1:B:1131:LYS:HE3	3:B:2094:HOH:O	2.07	0.54
1:B:1243:THR:HG22	3:B:2746:HOH:O	2.06	0.54
1:B:1253:GLN:HG3	1:B:1276:PHE:CZ	2.43	0.54
1:B:1401:PRO:HA	1:B:1436:LEU:HD13	1.89	0.54
1:A:23:GLU:HG2	1:A:24:LYS:H	1.70	0.54
1:A:520:GLN:HG3	3:A:2214:HOH:O	2.06	0.54
1:A:412:GLU:HG3	1:A:413:ARG:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LEU:CD2	3:A:2386:HOH:O	2.45	0.54
1:A:484:ARG:HG3	1:A:541:PHE:CE1	2.42	0.54
1:B:1332:LEU:N	1:B:1332:LEU:HD12	2.22	0.54
1:A:283:THR:OG1	3:A:2275:HOH:O	2.19	0.54
1:B:1235:ILE:O	1:B:1239:MSE:HG2	2.07	0.54
1:B:1296:LYS:NZ	3:B:2480:HOH:O	2.39	0.54
1:A:416:ILE:HG22	3:A:2333:HOH:O	2.08	0.54
1:B:1344:PHE:CZ	1:B:1348:GLY:HA2	2.43	0.54
1:B:1104:ILE:HG12	1:B:1108:MSE:HE2	1.90	0.54
1:B:1047:MSE:HE3	3:B:2742:HOH:O	2.07	0.53
1:B:1144:ARG:NH1	1:B:1245:ARG:HB2	2.23	0.53
1:B:1248:ARG:HD2	1:B:1248:ARG:N	2.23	0.53
1:B:1414:PRO:CA	3:B:2146:HOH:O	2.49	0.53
1:A:225:ARG:CB	3:A:2531:HOH:O	2.54	0.53
1:A:261:ASN:ND2	1:A:264:ARG:HE	2.05	0.53
1:A:165:ARG:HD3	1:A:258:GLY:HA2	1.89	0.53
1:A:183:LYS:NZ	1:A:255:GLU:OE1	2.41	0.53
1:B:1036:LYS:NZ	3:B:2244:HOH:O	2.40	0.53
1:B:1346:LYS:HE2	1:B:1347:TYR:CZ	2.44	0.53
1:A:277:ASN:C	1:A:277:ASN:HD22	2.11	0.53
1:B:1043:GLN:CB	3:B:2742:HOH:O	2.53	0.53
1:B:1385:LYS:HD2	3:B:2680:HOH:O	2.07	0.53
1:B:1388:THR:OG1	1:B:1415:VAL:HB	2.08	0.53
1:A:372:SER:O	1:A:383:ILE:HG21	2.09	0.53
1:B:1261:ASN:ND2	1:B:1264:ARG:NE	2.52	0.53
1:B:1389:ILE:HG12	3:B:2538:HOH:O	2.09	0.53
1:A:343:MSE:HE2	1:A:365:PHE:HB2	1.91	0.53
1:A:344:PHE:CD1	1:A:349:LEU:N	2.76	0.53
1:B:1108:MSE:N	1:B:1109:PRO:HD2	2.23	0.53
1:B:1109:PRO:HA	1:B:1114:PRO:CD	2.39	0.53
1:B:1389:ILE:HG23	1:B:1399:PHE:CZ	2.44	0.53
1:A:213:LEU:HD11	1:A:224:LYS:HD3	1.89	0.53
1:A:374:PRO:HG3	1:A:380:ALA:CA	2.36	0.53
1:B:1177:MSE:CG	3:B:2597:HOH:O	2.57	0.53
1:B:1412:GLU:HG3	1:B:1413:ARG:HG2	1.90	0.53
1:A:177:MSE:HE1	1:A:181:VAL:CG2	2.38	0.52
1:A:452:VAL:HG12	1:A:452:VAL:O	2.09	0.52
3:A:2638:HOH:O	1:B:1125:HIS:HB3	2.09	0.52
1:A:129:ARG:HG3	1:A:130:PRO:CD	2.39	0.52
1:A:501:GLN:HE22	1:A:525:ASN:HD22	1.58	0.52
1:A:207:THR:C	3:A:2531:HOH:O	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:VAL:O	1:A:392:VAL:CG1	2.49	0.52
1:B:1205:VAL:HG22	3:B:2363:HOH:O	2.08	0.52
1:B:1310:LEU:HB3	1:B:1391:GLY:HA2	1.90	0.52
1:B:1407:MSE:HE3	3:B:2538:HOH:O	2.09	0.52
1:B:1514:PRO:N	3:B:2740:HOH:O	2.41	0.52
1:A:278:ASP:OD1	1:A:282:GLY:HA3	2.09	0.52
1:A:452:VAL:HG12	1:A:454:LEU:HD21	1.92	0.52
1:B:1289:ALA:HA	3:B:2674:HOH:O	2.09	0.52
1:A:143:VAL:O	1:A:147:VAL:HG23	2.09	0.52
1:B:1406:ALA:O	1:B:1410:ILE:HD12	2.09	0.52
1:B:1478:VAL:HG13	1:B:1483:THR:HB	1.92	0.52
1:A:552:TYR:O	1:A:556:ARG:HD2	2.10	0.52
1:B:1523:SER:CB	3:B:2252:HOH:O	2.52	0.52
1:A:437:THR:O	1:A:438:GLU:HB2	2.09	0.52
1:A:80:GLU:HG2	3:A:2308:HOH:O	2.09	0.52
1:B:1193:ILE:C	3:B:2518:HOH:O	2.46	0.52
1:B:1297:VAL:HG12	1:B:1298:ILE:CD1	2.32	0.52
1:A:128:ARG:NH2	1:B:1128:ARG:NH1	2.55	0.52
1:A:377:PHE:CE2	1:A:389:ILE:HD11	2.45	0.52
1:A:386:PRO:CG	3:A:2256:HOH:O	2.53	0.52
1:B:1086:MSE:HE2	1:B:1086:MSE:CA	2.34	0.52
1:B:1373:ILE:O	1:B:1373:ILE:HG22	2.08	0.52
1:A:103:ASP:HB3	1:A:107:LEU:CD2	2.39	0.51
1:A:347:TYR:HD1	1:A:356:ALA:HB1	1.76	0.51
1:A:435:THR:HG22	3:A:2229:HOH:O	2.10	0.51
1:B:1095:LEU:HG	1:B:1099:ILE:HD12	1.91	0.51
1:B:1099:ILE:HG22	1:B:1100:LEU:N	2.23	0.51
1:B:1286:VAL:HG12	3:B:2570:HOH:O	2.10	0.51
1:A:104:ILE:O	1:A:108:MSE:HG3	2.10	0.51
1:A:378:GLU:HG3	1:A:403:VAL:HG23	1.93	0.51
1:B:1110:ILE:HG13	3:B:2496:HOH:O	2.09	0.51
1:B:1165:ARG:CZ	3:B:2673:HOH:O	2.58	0.51
1:A:265:PHE:CD1	3:A:2457:HOH:O	2.53	0.51
1:B:1079:LEU:O	1:B:1083:ILE:HG12	2.10	0.51
1:B:1227:ARG:HG2	1:B:1227:ARG:HH11	1.75	0.51
1:B:1287:ALA:HB3	3:B:2547:HOH:O	2.10	0.51
1:B:1453:LYS:HB2	1:B:1459:VAL:HG13	1.92	0.51
1:B:1467:ASN:ND2	2:B:1601:NAD:H71N	2.09	0.51
1:B:1543:TYR:C	1:B:1545:GLU:N	2.63	0.51
1:A:277:ASN:HD22	1:A:279:ASP:N	2.09	0.51
1:A:310:LEU:CD2	1:A:427:GLU:HG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1086:MSE:CE	1:B:1096:PHE:HE1	2.23	0.51
1:B:1292:LEU:CD1	3:B:2674:HOH:O	2.59	0.51
1:B:1109:PRO:HA	1:B:1114:PRO:HD2	1.93	0.51
1:B:1292:LEU:HD12	3:B:2674:HOH:O	2.09	0.51
1:A:104:ILE:HG13	1:A:108:MSE:CE	2.33	0.51
1:A:346:LYS:HE3	1:A:347:TYR:CE2	2.46	0.51
1:B:1315:ALA:HB3	1:B:1392:VAL:HG11	1.91	0.51
1:A:329:GLU:O	1:A:329:GLU:HG3	2.11	0.51
1:A:333:SER:HB3	1:A:336:GLU:OE2	2.11	0.51
1:B:1047:MSE:HG3	3:B:2742:HOH:O	2.11	0.51
1:A:86:MSE:HA	1:A:86:MSE:CE	2.28	0.50
1:A:108:MSE:HE1	1:A:519:ILE:HG21	1.92	0.50
1:A:459:VAL:HG13	3:A:2189:HOH:O	2.11	0.50
1:B:1301:PRO:O	1:B:1304:GLU:HB2	2.11	0.50
1:A:24:LYS:HB2	1:A:48:LEU:O	2.12	0.50
1:A:404:ILE:HG22	3:A:2063:HOH:O	2.12	0.50
1:A:458:ARG:CZ	3:A:2700:HOH:O	2.58	0.50
1:B:1086:MSE:HA	1:B:1086:MSE:CE	2.38	0.50
1:A:39:ALA:HA	1:A:59:GLU:O	2.11	0.50
1:B:1378:GLU:CD	1:B:1402:ASP:HB3	2.31	0.50
1:B:1039:ALA:N	3:B:2704:HOH:O	2.44	0.50
1:B:1494:ALA:CB	3:B:2727:HOH:O	2.57	0.50
1:A:261:ASN:HD22	1:A:264:ARG:NE	2.09	0.50
1:A:352:LYS:HB2	1:A:368:SER:HA	1.93	0.50
1:B:1031:ASN:HB3	1:B:1034:THR:OG1	2.12	0.50
1:B:1068:PHE:HB2	3:B:2449:HOH:O	2.11	0.50
1:B:1354:ARG:HD3	1:B:1358:ILE:CD1	2.38	0.50
1:B:1428:CYS:CB	3:B:2311:HOH:O	2.58	0.50
1:A:175:TYR:HE2	1:A:219:MSE:HG3	1.77	0.50
1:A:408:ALA:HB2	3:A:2063:HOH:O	2.11	0.50
1:A:415:VAL:CG1	3:A:2287:HOH:O	2.59	0.50
1:B:1094:LYS:C	3:B:2583:HOH:O	2.50	0.50
1:A:78:PRO:HA	1:A:81:LYS:HG3	1.94	0.50
1:A:113:THR:CB	1:A:114:PRO:CD	2.88	0.50
1:B:1453:LYS:HA	1:B:1459:VAL:HA	1.93	0.50
1:A:45:ARG:HA	1:A:50:LEU:HD12	1.93	0.50
1:A:372:SER:O	1:A:383:ILE:HG12	2.12	0.50
1:B:1195:PRO:CG	3:B:2409:HOH:O	2.60	0.50
1:A:478:VAL:HG13	1:A:483:THR:HB	1.93	0.49
1:B:1154:HIS:O	1:B:1197:ARG:HD3	2.11	0.49
1:B:1469:TYR:HB3	1:B:1498:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1381:VAL:CG2	1:B:1407:MSE:HE1	2.43	0.49
1:A:183:LYS:NZ	1:A:255:GLU:OE2	2.44	0.49
1:A:418:ALA:O	1:A:445:SER:HA	2.12	0.49
1:A:462:PRO:CB	3:A:2582:HOH:O	2.59	0.49
1:B:1538:LYS:NZ	1:B:1543:TYR:OH	2.42	0.49
1:A:183:LYS:O	3:A:2534:HOH:O	2.20	0.49
1:B:1502:LEU:HD11	1:B:1512:LEU:C	2.32	0.49
1:B:1060:THR:O	1:B:1064:GLN:HG3	2.11	0.49
1:B:1277:ASN:HD21	1:B:1279:ASP:HB2	1.77	0.49
1:B:1310:LEU:HG	1:B:1393:ALA:HB2	1.95	0.49
1:A:23:GLU:CG	1:A:24:LYS:H	2.26	0.49
1:B:1489:SER:HB2	1:B:1533:TYR:OH	2.13	0.49
1:A:128:ARG:HG3	3:A:2271:HOH:O	2.12	0.49
1:A:467:ASN:ND2	3:A:2275:HOH:O	2.46	0.49
1:B:1140:ARG:HG2	1:B:1140:ARG:HH11	1.78	0.49
1:B:1357:LYS:NZ	1:B:1357:LYS:CB	2.75	0.49
1:B:1414:PRO:HD2	1:B:1440:ARG:O	2.13	0.49
1:B:1511:ARG:HH11	1:B:1511:ARG:CG	2.25	0.49
1:A:99:ILE:CG2	3:A:2715:HOH:O	2.50	0.49
1:A:323:ILE:HG22	1:A:327:MSE:HE2	1.94	0.49
1:B:1513:TYR:CB	3:B:2740:HOH:O	2.33	0.49
1:A:26:LYS:HA	1:A:29:MSE:HG3	1.95	0.48
1:A:327:MSE:HE3	1:A:337:ALA:CB	2.41	0.48
1:B:1061:GLN:NE2	3:B:2349:HOH:O	2.46	0.48
1:B:1294:ALA:CA	1:B:1442:LEU:HD13	2.43	0.48
1:A:35:ASN:ND2	1:A:91:ARG:O	2.44	0.48
1:A:399:PHE:HB2	1:A:428:CYS:HB3	1.94	0.48
1:A:408:ALA:HA	1:A:414:PRO:HG3	1.95	0.48
1:A:376:THR:HG22	1:A:379:ASP:N	2.18	0.48
1:A:100:LEU:HD12	1:A:100:LEU:O	2.13	0.48
1:A:443:PHE:CD2	3:A:2582:HOH:O	2.65	0.48
1:A:535:TYR:CD2	1:A:540:ALA:HB3	2.49	0.48
1:B:1169:LEU:N	1:B:1169:LEU:CD1	2.77	0.48
1:B:1069:HIS:O	1:B:1073:LYS:HB3	2.13	0.48
1:B:1144:ARG:NH1	1:B:1148:ASP:OD1	2.47	0.48
1:A:33:ARG:NH1	1:A:93:GLU:OE1	2.47	0.48
1:A:82:TYR:CD2	1:A:83:ILE:HD13	2.43	0.48
1:A:156:LYS:HD2	1:A:156:LYS:HA	1.70	0.48
1:A:157:ALA:HB2	1:A:479:ILE:HD11	1.95	0.48
1:A:415:VAL:HG12	3:A:2287:HOH:O	2.13	0.48
1:A:528:ILE:HD13	1:A:550:ALA:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1351:VAL:CG1	1:B:1369:ALA:HB2	2.40	0.48
1:B:1415:VAL:HG22	1:B:1442:LEU:HB2	1.96	0.48
1:B:1442:LEU:CD1	3:B:2614:HOH:O	2.48	0.48
1:A:377:PHE:O	1:A:381:VAL:HG23	2.13	0.48
1:A:31:ASN:HB3	1:A:34:THR:OG1	2.12	0.48
1:A:109:PRO:HA	1:A:114:PRO:CD	2.44	0.48
1:B:1277:ASN:C	1:B:1277:ASN:ND2	2.67	0.48
1:B:1363:GLU:N	1:B:1364:PRO:HD2	2.29	0.48
1:A:203:ILE:HG22	1:A:205:VAL:HG13	1.95	0.48
1:B:1213:LEU:HB2	3:B:2156:HOH:O	2.14	0.48
1:B:1345:ASP:HB2	2:B:1601:NAD:O2B	2.14	0.48
1:A:101:GLN:NE2	3:A:2709:HOH:O	2.28	0.47
1:B:1182:GLY:O	1:B:1185:CYS:HB2	2.14	0.47
1:A:118:LEU:O	1:A:122:GLN:HG2	2.13	0.47
1:B:1073:LYS:HE2	1:B:1074:LYS:CE	2.45	0.47
1:B:1202:CYS:HB2	3:B:2416:HOH:O	2.14	0.47
1:A:231:TYR:O	1:A:235:ILE:HG12	2.14	0.47
1:A:357:LYS:O	1:A:358:ILE:HD12	2.15	0.47
1:A:421:ASN:HB3	1:A:422:PRO:HA	1.97	0.47
1:B:1177:MSE:HA	3:B:2416:HOH:O	2.14	0.47
1:B:1372:SER:O	1:B:1374:PRO:HD3	2.15	0.47
1:A:401:PRO:HA	1:A:436:LEU:CD2	2.45	0.47
1:B:1131:LYS:NZ	3:B:2137:HOH:O	2.46	0.47
1:A:414:PRO:CA	3:A:2752:HOH:O	2.63	0.47
1:B:1105:GLU:HB3	3:B:2228:HOH:O	2.14	0.47
1:B:1165:ARG:NH2	3:B:2673:HOH:O	2.46	0.47
1:B:1301:PRO:HG3	3:B:2524:HOH:O	2.15	0.47
1:A:28:LEU:CD2	1:A:48:LEU:HG	2.45	0.47
1:A:177:MSE:CE	1:A:181:VAL:CG2	2.93	0.47
1:B:1109:PRO:CA	1:B:1114:PRO:HD2	2.44	0.47
1:B:1166:ILE:HG13	1:B:1172:LEU:HD12	1.95	0.47
1:B:1414:PRO:CB	3:B:2146:HOH:O	2.59	0.47
1:A:171:ASP:C	1:A:171:ASP:OD1	2.53	0.47
1:A:286:VAL:HG11	1:A:466:ASN:O	2.15	0.47
1:B:1558:TRP:CE3	3:B:2409:HOH:O	2.68	0.47
1:B:1137:ILE:O	1:B:1140:ARG:NH1	2.46	0.47
1:B:1179:ILE:HG21	3:B:2405:HOH:O	2.15	0.47
1:B:1267:ARG:CZ	1:B:1267:ARG:HB3	2.45	0.47
1:A:241:ALA:HA	3:A:2305:HOH:O	2.15	0.47
1:A:310:LEU:HD23	1:A:427:GLU:CG	2.42	0.47
1:A:435:THR:CA	3:A:2229:HOH:O	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1295:GLN:C	1:B:1297:VAL:H	2.18	0.47
1:A:194:ARG:NH2	1:A:196:ASP:OD2	2.48	0.46
1:B:1122:GLN:HB2	1:B:1126:ILE:HG12	1.97	0.46
1:A:133:LEU:HD13	1:A:150:TRP:HE3	1.81	0.46
1:B:1215:ASP:OD1	1:B:1216:PRO:HD2	2.15	0.46
1:B:1308:LEU:CB	1:B:1386:PRO:HG3	2.44	0.46
1:B:1328:VAL:HA	1:B:1332:LEU:O	2.16	0.46
1:A:110:ILE:O	1:A:115:THR:HB	2.15	0.46
1:A:553:VAL:HG22	3:A:2141:HOH:O	2.15	0.46
1:B:1321:ASN:HB3	3:B:2288:HOH:O	2.15	0.46
1:B:1429:THR:HG22	1:B:1432:GLU:CD	2.35	0.46
1:A:91:ARG:HH12	1:B:1090:GLU:CD	2.19	0.46
1:B:1156:LYS:HA	1:B:1156:LYS:HD2	1.74	0.46
1:A:57:LYS:NZ	1:A:59:GLU:OE2	2.44	0.46
1:A:225:ARG:HH11	1:A:225:ARG:HG2	1.80	0.46
1:A:344:PHE:CZ	1:A:348:GLY:HA2	2.50	0.46
1:A:417:PHE:HD2	3:A:2571:HOH:O	1.98	0.46
1:B:1068:PHE:CD2	1:B:1068:PHE:C	2.88	0.46
1:A:208:ASP:HA	1:A:224:LYS:HD2	1.97	0.46
1:A:323:ILE:O	1:A:327:MSE:HG3	2.15	0.46
1:A:524:ILE:O	1:A:527:ALA:HB3	2.16	0.46
2:A:602:NAD:H52N	3:A:2302:HOH:O	2.15	0.46
1:B:1277:ASN:HD22	1:B:1279:ASP:H	1.63	0.46
1:B:1288:LEU:HD21	1:B:1492:LEU:CD1	2.45	0.46
1:A:429:THR:HG22	1:A:432:GLU:OE1	2.15	0.46
1:B:1354:ARG:HG2	1:B:1356:ALA:O	2.16	0.46
1:A:483:THR:HG23	3:A:2032:HOH:O	2.15	0.46
1:B:1267:ARG:HG2	1:B:1267:ARG:HH11	1.81	0.46
1:B:1389:ILE:HG22	1:B:1416:ILE:HA	1.97	0.46
1:B:1393:ALA:HA	2:B:1601:NAD:O4B	2.16	0.46
1:A:129:ARG:HD3	3:B:2650:HOH:O	2.16	0.46
1:A:288:LEU:CG	3:A:2469:HOH:O	2.51	0.46
1:B:1325:MSE:HE1	3:B:2514:HOH:O	2.12	0.46
1:B:1502:LEU:HD23	1:B:1506:GLU:OE1	2.15	0.46
1:A:122:GLN:O	1:A:123:TYR:C	2.53	0.45
1:A:383:ILE:HG22	1:A:384:LEU:HD13	1.98	0.45
1:A:407:MSE:HE2	1:A:407:MSE:HB2	1.84	0.45
1:B:1315:ALA:HB3	1:B:1392:VAL:HG13	1.98	0.45
1:A:103:ASP:O	1:A:107:LEU:HB2	2.16	0.45
1:A:134:PHE:CE2	1:A:177:MSE:HG3	2.51	0.45
1:A:442:LEU:HA	3:A:2371:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1167:LEU:N	1:B:1167:LEU:HD23	2.30	0.45
1:B:1243:THR:HG22	1:B:1247:GLY:O	2.16	0.45
1:A:310:LEU:HD21	1:A:398:LEU:HB2	1.98	0.45
1:A:462:PRO:CG	3:A:2582:HOH:O	2.62	0.45
1:A:108:MSE:N	1:A:109:PRO:CD	2.79	0.45
1:A:172:LEU:O	1:A:175:TYR:HB2	2.16	0.45
1:A:288:LEU:HD22	1:A:322:LEU:HG	1.99	0.45
1:A:374:PRO:HB3	1:A:379:ASP:CB	2.47	0.45
1:A:407:MSE:SE	3:A:2256:HOH:O	2.85	0.45
1:B:1376:THR:HG22	1:B:1378:GLU:N	2.31	0.45
1:A:33:ARG:NH2	1:A:196:ASP:HA	2.32	0.45
1:B:1166:ILE:HG22	1:B:1167:LEU:HG	1.99	0.45
1:B:1250:THR:N	3:B:2746:HOH:O	2.49	0.45
1:A:71:ASN:O	1:A:75:MSE:HE3	2.16	0.45
1:A:212:LEU:HD22	1:A:218:TYR:CD2	2.50	0.45
1:A:466:ASN:HB3	3:A:2681:HOH:O	2.08	0.45
1:A:538:LYS:HA	3:A:2201:HOH:O	2.17	0.45
1:B:1076:THR:N	1:B:1080:GLU:OE2	2.49	0.45
1:B:1194:ARG:CA	3:B:2518:HOH:O	2.53	0.45
1:A:326:SER:HB2	1:A:492:LEU:HD11	1.99	0.45
1:A:97:TYR:O	1:A:101:GLN:HG3	2.17	0.45
1:A:208:ASP:OD1	1:A:224:LYS:HD2	2.17	0.45
1:A:253:GLN:HG3	1:A:276:PHE:CZ	2.52	0.45
1:B:1120:CYS:O	1:B:1175:TYR:HB3	2.16	0.45
1:B:1238:PHE:CE1	1:B:1242:ILE:HG13	2.52	0.45
1:A:300:LYS:HE3	1:A:304:GLU:HB3	1.99	0.45
3:A:2541:HOH:O	1:B:1026:LYS:HE3	2.17	0.45
1:B:1286:VAL:HG21	1:B:1467:ASN:ND2	2.32	0.45
1:B:1295:GLN:C	1:B:1297:VAL:N	2.71	0.45
1:B:1529:LYS:NZ	3:B:2699:HOH:O	2.49	0.45
1:A:164:GLU:O	1:A:164:GLU:HG3	2.16	0.45
1:A:315:ALA:HB3	1:A:392:VAL:CG1	2.45	0.45
1:A:467:ASN:C	1:A:469:TYR:H	2.18	0.45
1:B:1343:MSE:SE	3:B:2102:HOH:O	2.85	0.45
1:B:1466:ASN:OD1	1:B:1468:VAL:HG13	2.16	0.45
1:A:183:LYS:CE	3:A:2711:HOH:O	2.63	0.44
1:A:253:GLN:HG3	1:A:276:PHE:CE2	2.52	0.44
1:B:1041:THR:OG1	1:B:1044:GLU:HG3	2.18	0.44
1:B:1087:GLY:HA2	1:B:1090:GLU:HG2	1.99	0.44
1:B:1106:SER:C	1:B:1109:PRO:HD2	2.38	0.44
1:A:87:GLY:O	1:A:91:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1029:MSE:SE	1:B:1050:LEU:HD22	2.67	0.44
1:B:1407:MSE:N	3:B:2312:HOH:O	2.45	0.44
1:B:1043:GLN:CD	3:B:2742:HOH:O	2.56	0.44
1:B:1073:LYS:HG2	1:B:1074:LYS:N	2.33	0.44
1:B:1108:MSE:CE	1:B:1519:ILE:HG21	2.48	0.44
1:B:1118:LEU:HD22	1:B:1122:GLN:HE21	1.82	0.44
1:A:113:THR:CG2	1:A:114:PRO:HD3	2.47	0.44
1:A:183:LYS:NZ	1:A:255:GLU:CD	2.71	0.44
1:A:277:ASN:ND2	1:A:279:ASP:N	2.63	0.44
1:A:381:VAL:O	1:A:385:LYS:HA	2.16	0.44
1:A:557:THR:CG2	3:A:2386:HOH:O	2.47	0.44
1:B:1381:VAL:HG22	1:B:1407:MSE:HE1	1.99	0.44
1:A:66:LEU:O	1:A:70:ARG:HG3	2.17	0.44
1:A:214:LYS:NZ	3:A:2463:HOH:O	2.46	0.44
1:A:363:GLU:HG2	1:A:364:PRO:HD3	2.00	0.44
1:B:1376:THR:O	1:B:1379:ASP:HB2	2.17	0.44
1:A:112:TYR:O	1:A:113:THR:C	2.56	0.44
1:A:277:ASN:HD22	1:A:279:ASP:H	1.63	0.44
1:B:1109:PRO:C	1:B:1114:PRO:HD2	2.37	0.44
1:B:1383:ILE:HG22	1:B:1384:LEU:HD13	2.00	0.44
1:A:261:ASN:ND2	1:A:264:ARG:NE	2.65	0.44
1:B:1194:ARG:N	3:B:2518:HOH:O	2.50	0.44
1:A:225:ARG:HH11	1:A:225:ARG:CG	2.30	0.44
1:A:430:ALA:CB	3:A:2582:HOH:O	2.65	0.44
1:A:436:LEU:HB2	3:A:2220:HOH:O	2.16	0.44
1:A:452:VAL:C	3:A:2189:HOH:O	2.55	0.44
1:B:1153:ASN:HB2	3:B:2730:HOH:O	2.18	0.44
1:B:1187:TYR:O	1:B:1191:ALA:HB3	2.18	0.44
1:A:89:GLN:HG3	1:A:90:GLU:N	2.33	0.44
1:A:209:ASN:HB3	1:A:212:LEU:HD12	2.00	0.44
1:B:1294:ALA:HA	1:B:1442:LEU:HD13	2.00	0.44
1:A:67:ARG:CZ	3:A:2659:HOH:O	2.65	0.43
1:B:1038:MSE:HE3	1:B:1038:MSE:HB2	1.95	0.43
1:B:1089:GLN:OE1	1:B:1131:LYS:HE2	2.18	0.43
1:A:430:ALA:O	1:A:434:TYR:HD1	2.02	0.43
1:A:518:ASN:CB	3:A:2661:HOH:O	2.51	0.43
1:B:1385:LYS:CA	3:B:2585:HOH:O	2.64	0.43
1:A:167:LEU:HB2	1:A:168:GLY:H	1.58	0.43
1:A:397:ARG:HA	1:A:427:GLU:O	2.18	0.43
1:B:1177:MSE:CA	3:B:2416:HOH:O	2.66	0.43
1:B:1306:LYS:HB3	1:B:1386:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1408:ALA:HB2	1:B:1437:THR:HG22	2.01	0.43
1:A:64:GLN:HE22	1:A:562:TYR:HE1	1.65	0.43
1:A:109:PRO:CA	1:A:114:PRO:HD2	2.48	0.43
1:A:243:THR:HG22	1:A:247:GLY:O	2.19	0.43
1:A:327:MSE:HB3	1:A:332:LEU:HD22	2.00	0.43
1:B:1040:PHE:HE2	1:B:1565:LEU:HD11	1.84	0.43
1:A:467:ASN:C	1:A:469:TYR:N	2.71	0.43
1:B:1036:LYS:O	1:B:1039:ALA:HB3	2.19	0.43
1:B:1418:ALA:O	1:B:1445:SER:HA	2.19	0.43
1:A:128:ARG:HH22	1:B:1128:ARG:HH12	1.62	0.43
1:A:351:VAL:HG11	1:A:369:ALA:HB2	2.00	0.43
1:A:351:VAL:CG1	1:A:352:LYS:N	2.82	0.43
1:A:355:LYS:HA	1:A:355:LYS:HD3	1.87	0.43
1:A:383:ILE:C	3:A:2226:HOH:O	2.57	0.43
1:A:429:THR:HG22	1:A:432:GLU:HB2	1.99	0.43
1:A:344:PHE:CE1	1:A:348:GLY:HA2	2.54	0.43
1:A:298:ILE:HD11	1:A:413:ARG:HB2	2.01	0.43
1:B:1110:ILE:CG1	3:B:2496:HOH:O	2.67	0.43
1:B:1482:ASN:HD22	1:B:1542:ARG:HA	1.82	0.43
1:A:218:TYR:HB3	1:A:222:TYR:OH	2.19	0.43
1:B:1043:GLN:NE2	3:B:2742:HOH:O	2.52	0.43
1:B:1095:LEU:N	3:B:2583:HOH:O	2.51	0.43
1:B:1073:LYS:HG2	1:B:1074:LYS:HE2	2.01	0.42
1:B:1092:ASN:HD21	1:B:1562:TYR:HH	1.62	0.42
1:A:310:LEU:HB3	1:A:391:GLY:HA2	2.01	0.42
1:B:1108:MSE:N	1:B:1109:PRO:CD	2.82	0.42
1:B:1277:ASN:HD22	1:B:1279:ASP:N	2.18	0.42
1:A:136:SER:C	1:A:138:SER:N	2.72	0.42
1:A:405:ARG:N	3:A:2512:HOH:O	2.51	0.42
1:B:1113:THR:CB	1:B:1114:PRO:CD	2.84	0.42
1:B:1453:LYS:HG2	1:B:1459:VAL:HG22	2.00	0.42
1:B:1512:LEU:HD12	1:B:1512:LEU:HA	1.87	0.42
1:A:166:ILE:HD12	1:A:166:ILE:H	1.83	0.42
1:B:1091:ARG:NH2	3:B:2646:HOH:O	2.41	0.42
1:B:1467:ASN:HD21	2:B:1601:NAD:H71N	1.67	0.42
1:A:467:ASN:O	1:A:469:TYR:N	2.52	0.42
1:B:1031:ASN:HD21	1:B:1033:ARG:HB2	1.83	0.42
1:B:1177:MSE:O	1:B:1181:VAL:HG23	2.20	0.42
1:B:1538:LYS:HE3	1:B:1543:TYR:OH	2.18	0.42
1:A:404:ILE:HG22	3:A:2512:HOH:O	2.19	0.42
1:A:503:THR:O	1:A:506:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1133:LEU:HB2	1:B:1199:LEU:HD11	2.01	0.42
1:B:1161:THR:CG2	3:B:2416:HOH:O	2.67	0.42
1:A:104:ILE:HG23	1:A:105:GLU:N	2.35	0.42
1:A:146:ILE:HG23	1:B:1052:GLY:HA3	2.02	0.42
1:A:308:LEU:HB2	1:A:386:PRO:HG3	2.02	0.42
1:A:359:ASP:OD2	1:A:359:ASP:C	2.57	0.42
1:A:535:TYR:CD1	1:A:549:LYS:HE3	2.55	0.42
1:A:566:LEU:HD22	1:A:567:PRO:HD2	2.02	0.42
3:A:2408:HOH:O	1:B:1067:ARG:HD3	2.18	0.42
1:B:1038:MSE:HE3	3:B:2026:HOH:O	2.19	0.42
1:B:1118:LEU:O	1:B:1122:GLN:HG2	2.20	0.42
1:B:1401:PRO:O	1:B:1405:ARG:HG2	2.20	0.42
1:B:1446:GLY:O	1:B:1464:GLN:NE2	2.43	0.42
1:A:64:GLN:O	1:A:68:PHE:CD1	2.62	0.42
1:A:77:SER:HA	1:A:78:PRO:HD3	1.90	0.42
1:A:109:PRO:C	1:A:114:PRO:HD2	2.40	0.42
1:A:203:ILE:N	1:A:203:ILE:HD12	2.35	0.42
1:B:1167:LEU:HB2	1:B:1169:LEU:HD13	2.02	0.42
1:B:1407:MSE:SE	3:B:2265:HOH:O	2.87	0.42
1:B:1505:GLU:H	1:B:1505:GLU:HG2	1.45	0.42
1:A:86:MSE:HE1	1:A:96:PHE:HE1	1.79	0.42
1:A:466:ASN:OD1	1:A:468:VAL:HG13	2.19	0.42
1:B:1089:GLN:HE21	1:B:1089:GLN:HB2	1.57	0.42
1:B:1281:GLN:NE2	1:B:1491:PHE:CE1	2.88	0.42
1:B:1317:LEU:HD13	1:B:1361:TYR:HB3	2.02	0.42
1:B:1343:MSE:HE1	1:B:1362:GLN:HG2	2.02	0.42
1:B:1528:ILE:HD11	1:B:1554:LYS:CE	2.50	0.42
1:A:177:MSE:O	1:A:180:PRO:HD2	2.20	0.41
1:A:367:HIS:CE1	3:A:2569:HOH:O	2.58	0.41
1:B:1445:SER:O	1:B:1464:GLN:HA	2.19	0.41
1:B:1492:LEU:CB	3:B:2514:HOH:O	2.45	0.41
1:A:351:VAL:HG13	1:A:352:LYS:N	2.36	0.41
1:A:429:THR:HG22	1:A:432:GLU:CG	2.50	0.41
1:A:504:ASP:HB2	1:A:505:GLU:OE2	2.19	0.41
1:A:559:ARG:N	1:A:559:ARG:HD3	2.34	0.41
1:B:1352:LYS:HB2	1:B:1367:HIS:O	2.19	0.41
1:B:1460:PHE:O	1:B:1462:PRO:HD3	2.20	0.41
1:A:503:THR:OG1	1:A:506:GLU:HG2	2.19	0.41
1:B:1344:PHE:CD1	1:B:1349:LEU:N	2.88	0.41
1:B:1394:GLY:N	1:B:1420:SER:OG	2.47	0.41
1:B:1520:GLN:HB2	3:B:2219:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ILE:HD11	1:A:230:GLN:HB3	2.02	0.41
1:A:359:ASP:OD2	1:A:362:GLN:N	2.53	0.41
1:B:1310:LEU:CD2	1:B:1427:GLU:CG	2.98	0.41
1:B:1507:LEU:HD12	1:B:1507:LEU:HA	1.74	0.41
1:A:378:GLU:O	1:A:382:ASN:ND2	2.53	0.41
1:B:1112:TYR:HA	1:B:1116:VAL:HB	2.02	0.41
1:B:1227:ARG:HH11	1:B:1227:ARG:CG	2.33	0.41
1:B:1464:GLN:NE2	1:B:1466:ASN:HD22	2.19	0.41
1:A:30:LEU:HD12	3:B:2362:HOH:O	2.21	0.41
1:A:379:ASP:O	1:A:382:ASN:HB2	2.20	0.41
1:B:1066:LEU:HD12	1:B:1066:LEU:HA	1.85	0.41
1:B:1073:LYS:CG	1:B:1074:LYS:N	2.83	0.41
1:B:1317:LEU:HD13	1:B:1361:TYR:CB	2.50	0.41
1:B:1455:THR:HG23	1:B:1456:ASP:N	2.35	0.41
1:A:72:LEU:CA	1:A:75:MSE:HE3	2.35	0.41
1:B:1501:GLN:HE21	1:B:1522:VAL:HG22	1.86	0.41
1:B:1511:ARG:CG	1:B:1511:ARG:NH1	2.82	0.41
1:A:218:TYR:HB3	1:A:222:TYR:CZ	2.56	0.41
1:A:277:ASN:ND2	1:A:277:ASN:C	2.73	0.41
1:A:436:LEU:C	3:A:2220:HOH:O	2.58	0.41
1:A:505:GLU:O	1:A:508:ALA:HB3	2.20	0.41
1:B:1100:LEU:HD21	1:B:1189:ALA:HB2	2.02	0.41
1:B:1308:LEU:HG	1:B:1377:PHE:CE1	2.56	0.41
1:A:109:PRO:HA	1:A:114:PRO:HD2	2.02	0.41
1:A:130:PRO:HG2	1:B:1054:LEU:HD23	2.03	0.41
1:A:292:LEU:HD21	3:A:2469:HOH:O	2.21	0.41
1:A:313:GLY:O	1:A:316:ALA:N	2.54	0.41
1:A:363:GLU:N	1:A:364:PRO:HD2	2.35	0.41
1:A:374:PRO:HB3	1:A:379:ASP:HB3	2.03	0.41
1:A:402:ASP:HA	1:A:405:ARG:HD2	2.03	0.41
1:A:453:LYS:N	3:A:2189:HOH:O	2.53	0.41
1:A:476:LEU:O	1:A:480:LEU:HG	2.21	0.41
1:B:1071:ASN:O	1:B:1075:MSE:HE3	2.21	0.41
1:B:1202:CYS:CB	3:B:2416:HOH:O	2.69	0.41
1:B:1277:ASN:ND2	1:B:1279:ASP:N	2.69	0.41
1:B:1300:LYS:HD2	1:B:1305:HIS:CD2	2.56	0.41
1:B:1310:LEU:CD2	1:B:1427:GLU:HG2	2.51	0.41
1:B:1109:PRO:HA	1:B:1114:PRO:HD3	2.02	0.41
1:B:1456:ASP:OD1	1:B:1458:ARG:NH1	2.53	0.41
1:B:1501:GLN:NE2	1:B:1522:VAL:HA	2.36	0.41
1:A:128:ARG:NH2	1:B:1128:ARG:HH12	2.16	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:HB	1:A:246:TYR:CD2	2.56	0.40
1:A:290:GLY:O	1:A:293:ALA:HB3	2.21	0.40
1:B:1501:GLN:HE22	1:B:1525:ASN:HD22	1.69	0.40
1:A:76:THR:HG22	1:A:77:SER:N	2.36	0.40
1:A:146:ILE:O	1:A:149:ASN:HB2	2.22	0.40
1:A:230:GLN:HE21	1:A:230:GLN:HB2	1.63	0.40
1:A:384:LEU:C	3:A:2226:HOH:O	2.58	0.40
1:A:412:GLU:O	1:A:440:ARG:HB3	2.20	0.40
1:A:429:THR:CG2	1:A:432:GLU:H	2.24	0.40
1:B:1043:GLN:O	1:B:1047:MSE:HG3	2.21	0.40
1:B:1117:GLY:O	1:B:1169:LEU:CD2	2.70	0.40
1:B:1413:ARG:HE	1:B:1413:ARG:HB3	1.62	0.40
1:B:1416:ILE:C	1:B:1417:PHE:HD1	2.25	0.40
1:B:1565:LEU:HD21	3:B:2420:HOH:O	2.20	0.40
1:A:25:GLY:C	1:A:27:PRO:HD2	2.41	0.40
1:A:392:VAL:HG12	3:A:2008:HOH:O	2.22	0.40
1:A:432:GLU:O	1:A:436:LEU:HD13	2.21	0.40
1:A:438:GLU:O	1:A:458:ARG:NH2	2.53	0.40
1:B:1266:LEU:O	1:B:1270:ARG:HG2	2.20	0.40
1:A:341:ILE:O	1:A:367:HIS:NE2	2.42	0.40
1:A:480:LEU:HD12	3:A:2141:HOH:O	2.20	0.40
1:B:1196:ASP:O	3:B:2002:HOH:O	2.22	0.40
1:B:1224:LYS:NZ	3:B:2504:HOH:O	2.54	0.40
1:B:1281:GLN:NE2	1:B:1491:PHE:HE1	2.20	0.40
1:B:1300:LYS:CD	1:B:1304:GLU:HB3	2.52	0.40
1:B:1429:THR:CG2	1:B:1432:GLU:H	2.21	0.40
1:A:91:ARG:NH1	1:B:1090:GLU:OE1	2.53	0.40
1:A:109:PRO:HA	1:A:114:PRO:HD3	2.02	0.40
1:A:118:LEU:HD22	1:A:122:GLN:HE21	1.86	0.40
1:A:177:MSE:HE3	1:A:181:VAL:HG23	2.03	0.40
1:A:343:MSE:O	1:A:350:LEU:HD23	2.21	0.40
1:A:505:GLU:HB3	3:A:2714:HOH:O	2.21	0.40
1:B:1045:ARG:HA	1:B:1050:LEU:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	549/584 (94%)	505 (92%)	35 (6%)	9 (2%)	9 5
1	B	549/584 (94%)	502 (91%)	38 (7%)	9 (2%)	9 5
All	All	1098/1168 (94%)	1007 (92%)	73 (7%)	18 (2%)	9 5

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	THR
1	B	1113	THR
1	B	1299	SER
1	B	1571	GLU
1	A	259	ASN
1	A	432	GLU
1	B	1259	ASN
1	A	114	PRO
1	A	451	PRO
1	B	1114	PRO
1	A	56	PRO
1	A	123	TYR
1	A	397	ARG
1	B	1076	THR
1	B	1354	ARG
1	A	468	VAL
1	B	1301	PRO
1	B	1056	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	465/484 (96%)	390 (84%)	75 (16%)	2 1
1	B	465/484 (96%)	386 (83%)	79 (17%)	2 1
All	All	930/968 (96%)	776 (83%)	154 (17%)	2 1

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	26	LYS
1	A	29	MSE
1	A	38	MSE
1	A	48	LEU
1	A	66	LEU
1	A	71	ASN
1	A	72	LEU
1	A	74	LYS
1	A	75	MSE
1	A	77	SER
1	A	89	GLN
1	A	106	SER
1	A	107	LEU
1	A	118	LEU
1	A	123	TYR
1	A	125	HIS
1	A	136	SER
1	A	137	ILE
1	A	152	GLU
1	A	160	VAL
1	A	165	ARG
1	A	167	LEU
1	A	169	LEU
1	A	184	LEU
1	A	210	ILE
1	A	214	LYS
1	A	225	ARG
1	A	237	GLU
1	A	240	LYS
1	A	248	ARG
1	A	255	GLU
1	A	257	PHE

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Mol	Chain	Res	Type
1	A	267	ARG
1	A	268	LYS
1	A	277	ASN
1	A	286	VAL
1	A	299	SER
1	A	300	LYS
1	A	306	LYS
1	A	329	GLU
1	A	333	SER
1	A	340	LYS
1	A	346	LYS
1	A	360	SER
1	A	363	GLU
1	A	368	SER
1	A	371	GLU
1	A	372	SER
1	A	376	THR
1	A	378	GLU
1	A	384	LEU
1	A	388	THR
1	A	397	ARG
1	A	398	LEU
1	A	403	VAL
1	A	413	ARG
1	A	416	ILE
1	A	419	LEU
1	A	425	GLN
1	A	428	CYS
1	A	456	ASP
1	A	458	ARG
1	A	489	SER
1	A	502	LEU
1	A	506	GLU
1	A	512	LEU
1	A	516	LEU
1	A	518	ASN
1	A	520	GLN
1	A	529	LYS
1	A	543	TYR
1	A	559	ARG
1	A	566	LEU
1	A	572	TRP

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Mol	Chain	Res	Type
1	B	1030	LEU
1	B	1038	MSE
1	B	1043	GLN
1	B	1048	LEU
1	B	1057	LYS
1	B	1066	LEU
1	B	1068	PHE
1	B	1072	LEU
1	B	1074	LYS
1	B	1089	GLN
1	B	1093	GLU
1	B	1104	ILE
1	B	1106	SER
1	B	1107	LEU
1	B	1118	LEU
1	B	1121	SER
1	B	1123	TYR
1	B	1136	SER
1	B	1137	ILE
1	B	1144	ARG
1	B	1154	HIS
1	B	1160	VAL
1	B	1174	VAL
1	B	1184	LEU
1	B	1210	ILE
1	B	1214	LYS
1	B	1224	LYS
1	B	1225	ARG
1	B	1232	ASP
1	B	1248	ARG
1	B	1276	PHE
1	B	1277	ASN
1	B	1286	VAL
1	B	1295	GLN
1	B	1298	ILE
1	B	1300	LYS
1	B	1302	ILE
1	B	1340	LYS
1	B	1346	LYS
1	B	1352	LYS
1	B	1354	ARG
1	B	1355	LYS

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Mol	Chain	Res	Type
1	B	1357	LYS
1	B	1360	SER
1	B	1363	GLU
1	B	1368	SER
1	B	1372	SER
1	B	1375	ASP
1	B	1384	LEU
1	B	1385	LYS
1	B	1388	THR
1	B	1397	ARG
1	B	1398	LEU
1	B	1409	SER
1	B	1413	ARG
1	B	1419	LEU
1	B	1423	THR
1	B	1425	GLN
1	B	1428	CYS
1	B	1453	LYS
1	B	1454	LEU
1	B	1456	ASP
1	B	1461	THR
1	B	1467	ASN
1	B	1489	SER
1	B	1496	LYS
1	B	1505	GLU
1	B	1509	GLN
1	B	1511	ARG
1	B	1512	LEU
1	B	1516	LEU
1	B	1518	ASN
1	B	1520	GLN
1	B	1538	LYS
1	B	1547	GLU
1	B	1554	LYS
1	B	1559	ARG
1	B	1566	LEU
1	B	1572	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN

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Mol	Chain	Res	Type
1	A	46	GLN
1	A	64	GLN
1	A	71	ASN
1	A	122	GLN
1	A	230	GLN
1	A	261	ASN
1	A	277	ASN
1	A	295	GLN
1	A	330	ASN
1	A	382	ASN
1	A	425	GLN
1	A	482	ASN
1	A	485	HIS
1	A	501	GLN
1	A	509	GLN
1	A	520	GLN
1	B	1031	ASN
1	B	1043	GLN
1	B	1046	GLN
1	B	1064	GLN
1	B	1071	ASN
1	B	1122	GLN
1	B	1153	ASN
1	B	1261	ASN
1	B	1277	ASN
1	B	1330	ASN
1	B	1425	GLN
1	B	1464	GLN
1	B	1467	ASN
1	B	1482	ASN
1	B	1501	GLN
1	B	1509	GLN
1	B	1518	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	B	1601	-	42,48,48	1.85	10 (23%)	50,73,73	1.54	7 (14%)
2	NAD	B	1602	-	42,48,48	2.13	8 (19%)	50,73,73	1.51	5 (10%)
2	NAD	A	601	-	42,48,48	2.00	10 (23%)	50,73,73	1.50	7 (14%)
2	NAD	A	602	-	42,48,48	2.37	10 (23%)	50,73,73	1.56	5 (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
2	NAD	B	1601	-	-	0/26/62/62	0/5/5/5
2	NAD	B	1602	-	-	14/26/62/62	0/5/5/5
2	NAD	A	601	-	-	0/26/62/62	0/5/5/5
2	NAD	A	602	-	-	13/26/62/62	0/5/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	NAD	C2N-N1N	9.98	1.45	1.35
2	B	1602	NAD	C2N-N1N	7.77	1.43	1.35
2	A	601	NAD	C2N-N1N	7.55	1.43	1.35
2	B	1601	NAD	C2N-N1N	6.44	1.42	1.35
2	B	1602	NAD	O4D-C1D	5.19	1.47	1.40
2	A	602	NAD	O4B-C1B	4.95	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	NAD	O4D-C1D	4.91	1.47	1.40
2	A	601	NAD	O4D-C1D	4.66	1.47	1.40
2	B	1602	NAD	O4B-C1B	4.62	1.47	1.40
2	B	1602	NAD	C6N-N1N	4.27	1.45	1.35
2	A	602	NAD	C3N-C7N	4.05	1.56	1.50
2	B	1601	NAD	O4D-C1D	4.03	1.46	1.40
2	A	601	NAD	O4B-C1B	4.00	1.46	1.40
2	B	1601	NAD	O4B-C1B	3.72	1.45	1.40
2	B	1601	NAD	C2A-N3A	3.70	1.37	1.32
2	A	602	NAD	C2A-N3A	3.70	1.37	1.32
2	B	1601	NAD	C6N-N1N	3.69	1.43	1.35
2	B	1602	NAD	C2A-N3A	3.50	1.37	1.32
2	A	602	NAD	C6N-N1N	3.47	1.43	1.35
2	A	601	NAD	C2A-N3A	3.43	1.37	1.32
2	A	601	NAD	C6N-N1N	3.32	1.42	1.35
2	B	1602	NAD	C3N-C7N	3.28	1.55	1.50
2	A	602	NAD	C2N-C3N	2.61	1.43	1.39
2	A	601	NAD	PA-O3	-2.58	1.56	1.59
2	B	1601	NAD	C3N-C7N	2.56	1.54	1.50
2	A	602	NAD	C2A-N1A	2.44	1.38	1.33
2	A	601	NAD	C5A-N7A	-2.42	1.31	1.39
2	A	601	NAD	C2A-N1A	2.35	1.38	1.33
2	A	601	NAD	C3N-C7N	2.32	1.54	1.50
2	A	602	NAD	PN-O3	2.28	1.62	1.59
2	B	1601	NAD	C5A-N7A	-2.21	1.31	1.39
2	B	1601	NAD	C2A-N1A	2.20	1.37	1.33
2	B	1601	NAD	C4N-C3N	2.18	1.42	1.39
2	A	601	NAD	PN-O3	-2.16	1.57	1.59
2	B	1602	NAD	C5A-N7A	-2.16	1.32	1.39
2	B	1601	NAD	C5N-C4N	2.13	1.42	1.38
2	A	602	NAD	C4A-N3A	2.09	1.38	1.35
2	B	1602	NAD	C2A-N1A	2.07	1.37	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	602	NAD	N3A-C2A-N1A	-6.08	120.42	128.67
2	B	1602	NAD	N3A-C2A-N1A	-6.07	120.44	128.67
2	A	601	NAD	N3A-C2A-N1A	-5.76	120.85	128.67
2	B	1601	NAD	N3A-C2A-N1A	-5.74	120.88	128.67
2	A	601	NAD	C4A-C5A-N7A	4.25	113.83	109.34
2	B	1601	NAD	C4A-C5A-N7A	4.21	113.78	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1602	NAD	C4A-C5A-N7A	4.14	113.71	109.34
2	A	602	NAD	C6N-N1N-C2N	-3.96	118.51	121.88
2	A	602	NAD	C4A-C5A-N7A	3.85	113.41	109.34
2	B	1601	NAD	C4D-O4D-C1D	-3.25	106.95	109.92
2	B	1601	NAD	C6A-C5A-C4A	3.22	124.17	117.90
2	A	601	NAD	C6A-C5A-C4A	3.21	124.14	117.90
2	B	1602	NAD	C6A-C5A-C4A	3.07	123.87	117.90
2	A	602	NAD	C6A-C5A-C4A	3.04	123.82	117.90
2	B	1602	NAD	C6N-N1N-C2N	-3.03	119.30	121.88
2	B	1601	NAD	C4B-O4B-C1B	-2.98	107.19	109.92
2	A	601	NAD	C6N-N1N-C2N	-2.50	119.75	121.88
2	A	601	NAD	C4B-O4B-C1B	-2.50	107.64	109.92
2	A	602	NAD	C2D-C3D-C4D	2.28	107.01	102.61
2	A	601	NAD	C4D-O4D-C1D	-2.14	107.96	109.92
2	A	601	NAD	O4B-C1B-N9A	2.14	111.58	108.75
2	B	1601	NAD	C6N-N1N-C2N	-2.09	120.10	121.88
2	B	1601	NAD	O4B-C1B-N9A	2.08	111.50	108.75
2	B	1602	NAD	C2D-C3D-C4D	2.05	106.58	102.61

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	NAD	C5B-O5B-PA-O1A
2	A	602	NAD	C5B-O5B-PA-O2A
2	A	602	NAD	C5B-O5B-PA-O3
2	A	602	NAD	C5D-O5D-PN-O3
2	A	602	NAD	C5D-O5D-PN-O1N
2	A	602	NAD	C5D-O5D-PN-O2N
2	A	602	NAD	O4D-C4D-C5D-O5D
2	A	602	NAD	O4D-C1D-N1N-C2N
2	A	602	NAD	O4D-C1D-N1N-C6N
2	A	602	NAD	C2D-C1D-N1N-C2N
2	A	602	NAD	C2D-C1D-N1N-C6N
2	B	1602	NAD	C5B-O5B-PA-O1A
2	B	1602	NAD	C5B-O5B-PA-O3
2	B	1602	NAD	C5D-O5D-PN-O3
2	B	1602	NAD	C5D-O5D-PN-O1N
2	B	1602	NAD	C5D-O5D-PN-O2N
2	B	1602	NAD	O4D-C1D-N1N-C2N
2	B	1602	NAD	O4D-C1D-N1N-C6N
2	B	1602	NAD	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	B	1602	NAD	C2D-C1D-N1N-C6N
2	A	602	NAD	C3D-C4D-C5D-O5D
2	B	1602	NAD	O4D-C4D-C5D-O5D
2	B	1602	NAD	C3D-C4D-C5D-O5D
2	B	1602	NAD	C5B-O5B-PA-O2A
2	B	1602	NAD	C4D-C5D-O5D-PN
2	A	602	NAD	PA-O3-PN-O2N
2	B	1602	NAD	PN-O3-PA-O2A

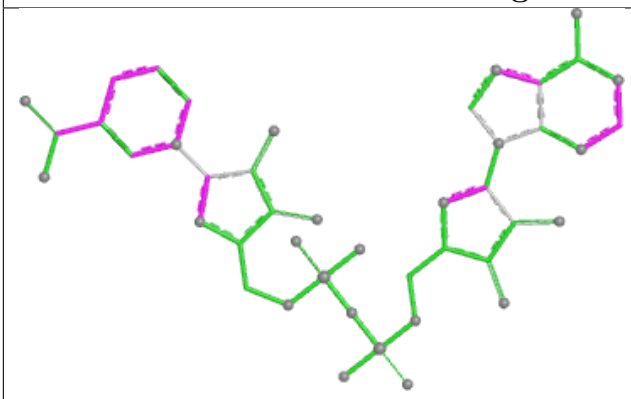
There are no ring outliers.

3 monomers are involved in 6 short contacts:

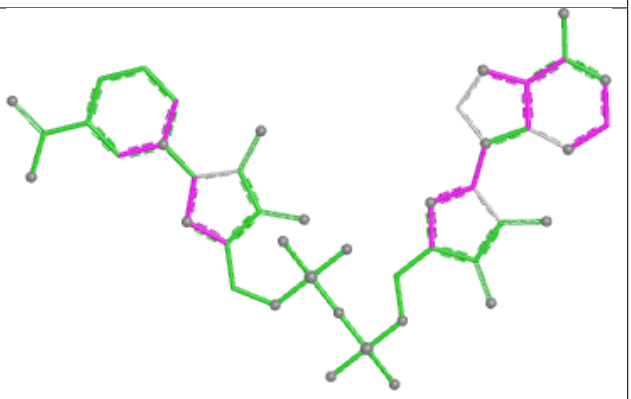
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1601	NAD	4	0
2	A	601	NAD	1	0
2	A	602	NAD	1	0

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 then 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.

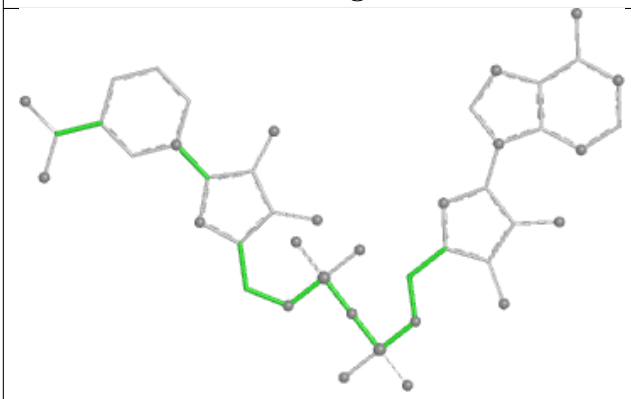
Ligand NAD B 1601



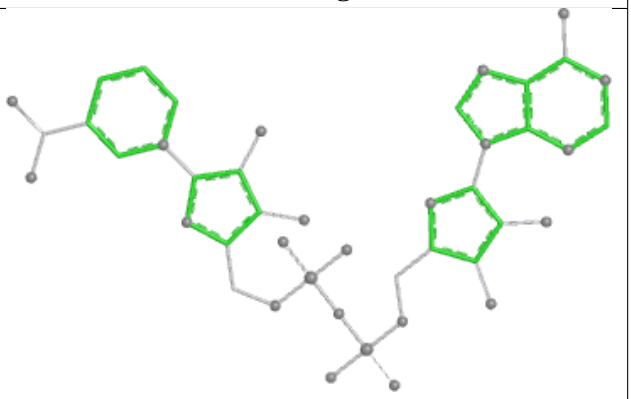
Bond lengths



Bond angles

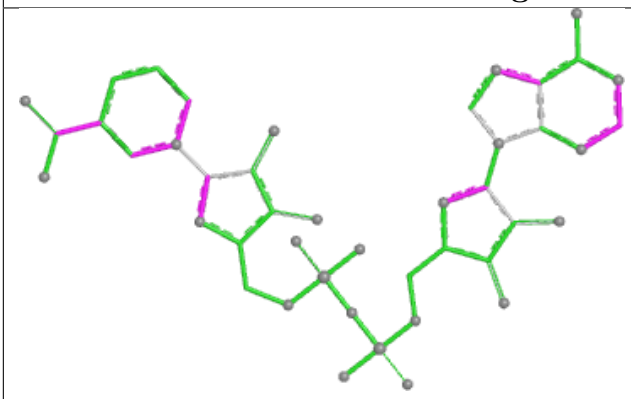


Torsions

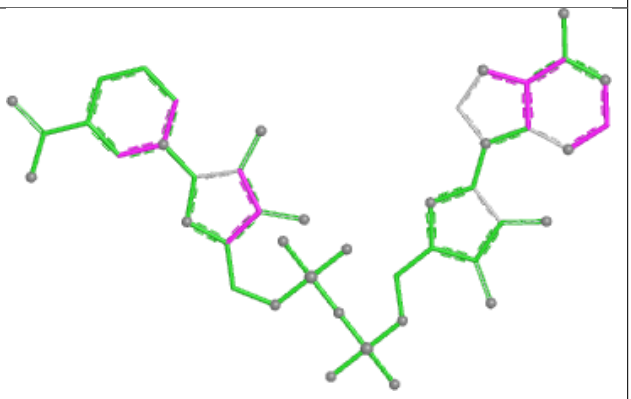


Rings

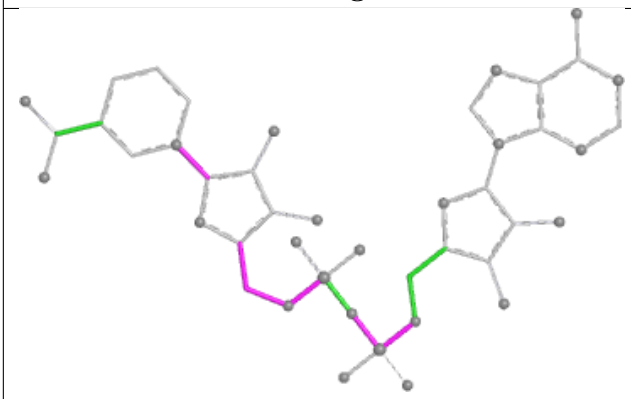
Ligand NAD B 1602



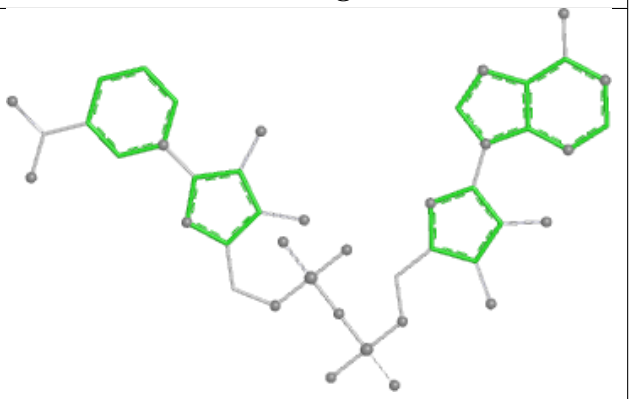
Bond lengths



Bond angles

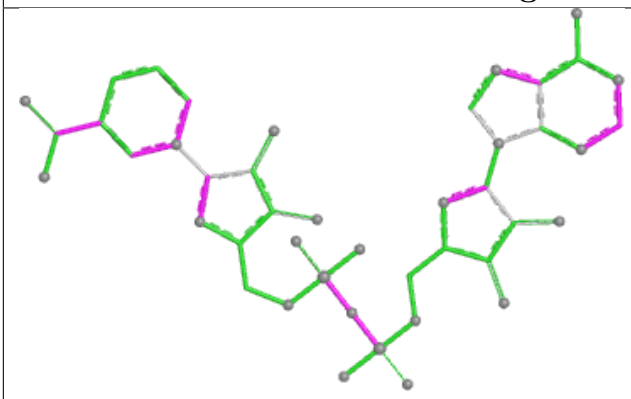


Torsions

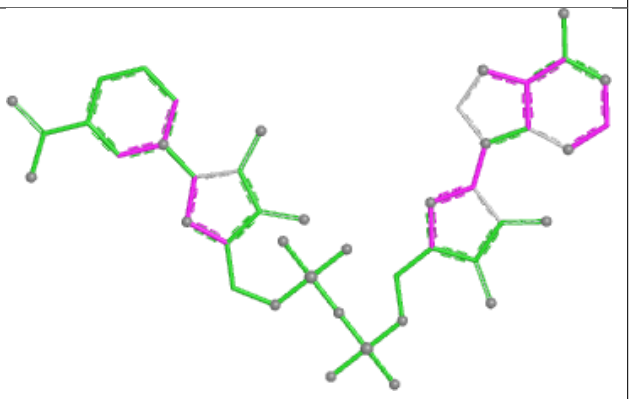


Rings

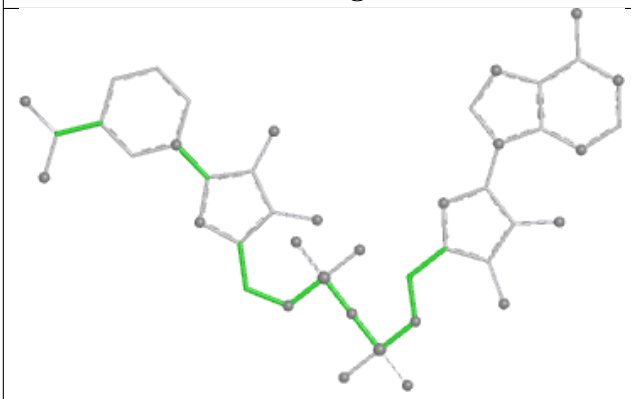
Ligand NAD A 601



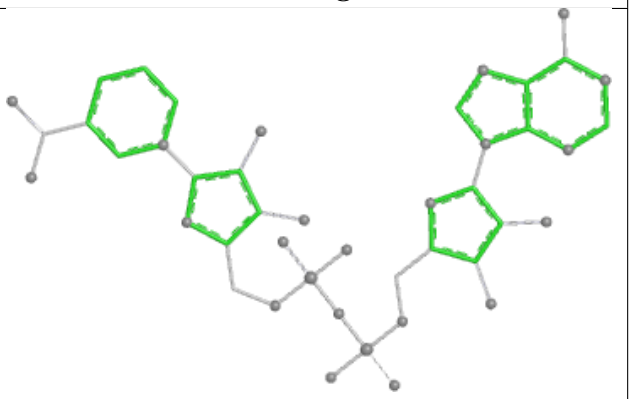
Bond lengths



Bond angles

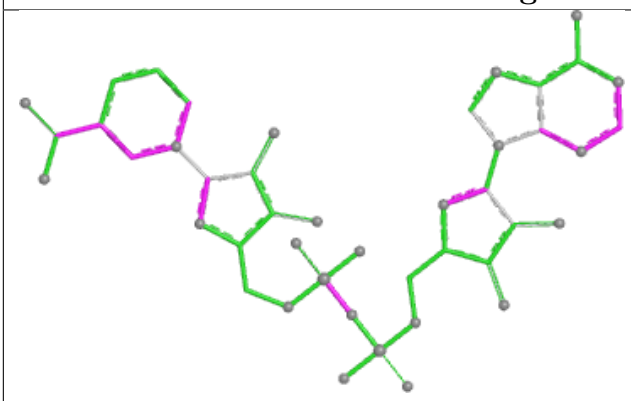


Torsions

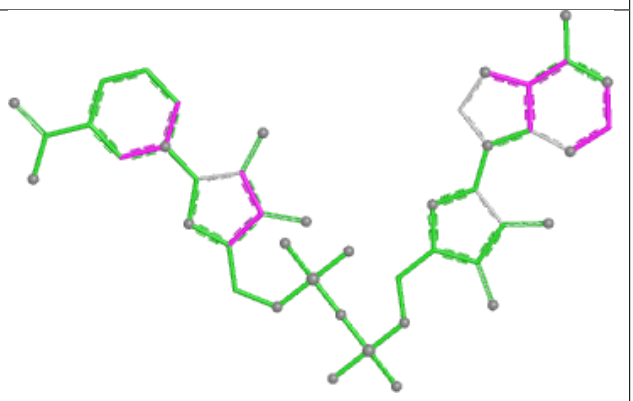


Rings

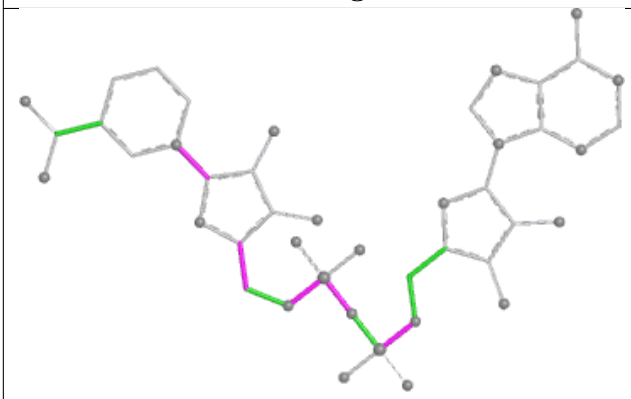
Ligand NAD A 602



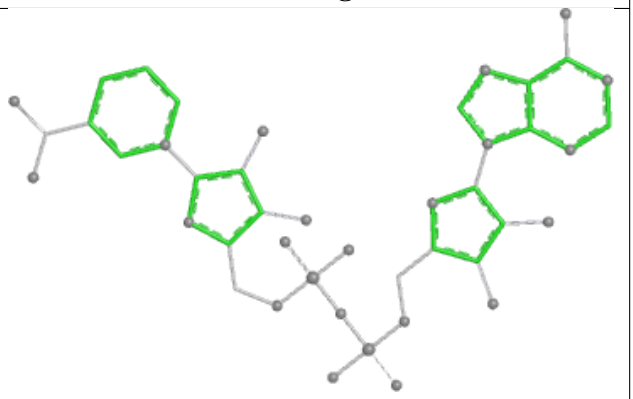
Bond lengths



Bond angles



Torsions



Rings

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.