



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 10:41 AM EST

PDB ID : 1FP7  
Title : MONOVALENT CATION BINDING SITES IN N10-FORMYLTETRAHYDROFOLATE SYNTHETASE FROM MOORELLA THERMOACETICA  
Authors : Radfar, R.; Leapheart, A.; Brewer, J.M.; Minor, W.; Odom, J.D.  
Deposited on : 2000-08-30  
Resolution : 3.20 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.

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
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

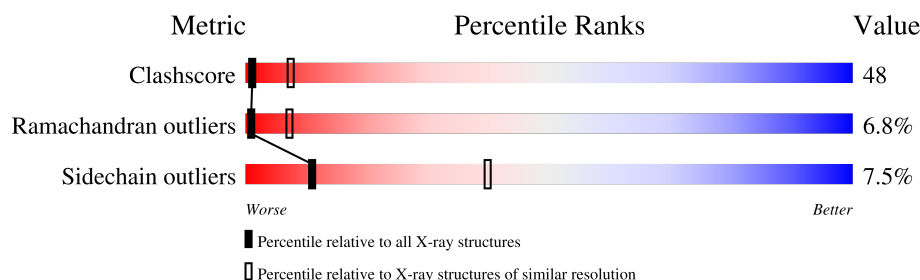
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)

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  $\geq 3$ , 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	557	
1	B	557	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	273	-	-	X	-
2	SO4	A	274	-	-	X	-
2	SO4	A	275	-	-	X	-
2	SO4	A	277	-	-	X	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	278	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8585 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.

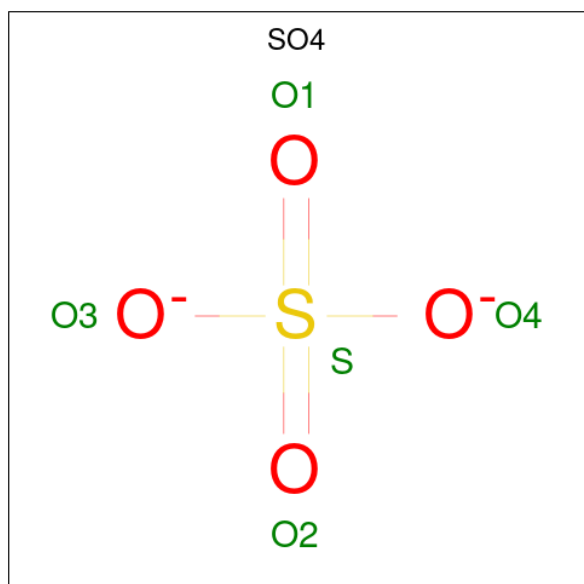
- Molecule 1 is a protein called FORMATE--TETRAHYDROFOLATE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4133	2617	715	780	21			
1	B	548	Total	C	N	O	S	0	0	0
			4125	2613	714	777	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P21164
A	?	-	VAL	deletion	UNP P21164
B	?	-	GLU	deletion	UNP P21164
B	?	-	VAL	deletion	UNP P21164

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	199	Total O 199 199	0	0
4	B	71	Total O 71 71	0	0



A1551	G1483	L1408	H1340	M1277	C1210	A1135	P1067
D1552	N1484	L1408	G1341	I1278	L1211	V1136	T1068
G1553	S1409	L1408	G1342	A1279	L1215	H1140	P1069
V1554	W1412	V1343	P1344	H1280	L1215	L1143	A1070
T1555	A1413	K1414	D1347	G1281	E1220	A1144	G1071
T1556	V1487	E1417	L1348	G1282	R1221	V1147	E1072
G1557	V1488	L1420	E1351	I1285	F1222	D1148	G1073
LEU	M1489	L1421	N1352	I1286	S1223	N1149	R1074
PHE	A1490	L1422	L1353	A1287	R1224	H1150	T1075
	Q1493	K1425	L1356	T1288	I1225	H1151	T1077
	Y1494	V1426	R1357	K1289	V1226	S1078	S1078
S1495	F1496	L1427	E1358	T1290	G1227	I1151	V1079
F1497	S1497	Q1428	G1359	A1291	G1228	Q1152	G1080
Q1498	D1498	T1429	F1360	K1292	Y1229	L1153	L1081
D1499	M1500	L1430	A1361	L1293	T1230	G1154	T1082
M1500	T1501	E1431	N1362	A1295	Y1231	N1155	D1083
K1502	S1432	S1432	L1363	A1296	D1232	V1156	A1084
P1506	P1434	P1434	K1365	D1296	G1233	L1157	L1085
R1507	S1435	S1435	H1366	Y1297	K1234	N1158	A1086
N1508	N1436	N1436	H1367	V1298	P1235	I1159	R1087
F1509	F1437	F1437	E1368	V1299	T1236	D1160	G1088
T1510	H1438	H1438	N1369	T1300	P1237	T1237	G1089
I1511	V1439	L1440	I1370	G1303	A1238	K1090	K1090
T1512	L1440	L1440	G1371	F1304	G1239	R1091	R1091
V1513	Y1441	Y1441	K1372	G1305	D1240	V1092	V1092
R1514	N1442	N1442	F1373	A1306	Q1244	R1166	R1092
E1515	L1443	L1443	G1374	D1307	S1246	R1167	V1092
V1516	D1444	D1444	V1375	L1308	M1247	R1168	M1093
R1517	S1445	S1445	P1376	G1309	A1248	V1169	V1094
L1518	S1446	S1446	A1377	A1310	L1249	I1170	C1095
S1519	I1447	I1447	V1378	E1311	L1250	D1174	L1096
A1520	K1448	K1448	V1379	F1312	M1251	R1175	G1106
	D1449	D1449	A1380	Y1314	K1252	A1176	L1107
R1523	K1450	K1450	I1381	G1315	D1253	R1178	I1107
L1524	I1451	I1451	N1382	V1316	A1254	K1108	K1108
V1525	A1452	A1452	A1383	K1317	I1255	G1109	G1109
V1526	K1453	K1453	F1384	C1318	K1256	G1110	G1110
P1527	I1454	I1454	P1385	R1319	P1257	A1111	A1111
I1528	A1455	A1455	T1386	Y1320	N1258	G1112	A1112
T1529	T1456	T1456	D1387	F1323	L1259	K1187	G1113
	E1457	E1457		K1324	V1260	A1183	G1114
M1533	I1458	I1458	A1390	P1325	Q1261	G1115	G1115
T1534	Y1459	Y1459	E1391	D1326	T1262	R1193	Y1116
M1535	G1460	G1460	L1392	L1263	L1263	E1194	A1117
P1536	A1461	A1461	N1393	A1327	E1264	T1195	Q1118
	D1462	D1462	L1394	T1328	N1265	G1196	V1119
	N1465	N1465	L1395	V1329	T1266	F1197	V1120
A1543	Y1466	Y1466	Y1396	I1330	P1267	D1198	P1121
A1544	K1472	K1472	E1397	V1331	A1268	I1199	
N1546			L1398	T1332	F1269	S1200	D1124
T1547			C1399	T1333	I1270	I1125	I1125
D1548	R1476	R1476	A1400	V1334	H1271	S1203	F1129
I1549	Y1477	Y1477	K1401	R1335	G1273	E1204	
D1550	E1478	E1478	G1403	A1336	P1274	V1205	D1132
				L1337	F1275	M1206	I1133
				M1339	A1276		H1134

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.88Å 160.88Å 256.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 3.20	Depositor
% Data completeness (in resolution range)	87.2 (19.99-3.20)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.285 , 0.355	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8585	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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: K, SO4

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	0.44	0/4201	0.72	1/5690 (0.0%)
1	B	0.40	0/4193	0.68	0/5679
All	All	0.42	0/8394	0.70	1/11369 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1524	LEU	N-CA-C	5.35	125.44	111.00

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	4133	0	4219	358	1
1	B	4125	0	4211	449	0
2	A	35	0	0	15	1
2	B	20	0	0	3	0
3	A	2	0	0	1	0
4	A	199	0	0	28	0
4	B	71	0	0	16	0
All	All	8585	0	8430	808	1

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 48.

All (808) 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:1175:ARG:NH1	2:B:279:SO4:O3	1.58	1.33
1:A:1175:ARG:HD3	2:A:275:SO4:O3	1.40	1.22
1:B:1222:PHE:O	1:B:1225:ILE:HG22	1.40	1.19
1:A:1007:ASP:OD2	4:A:32:HOH:O	1.68	1.11
1:B:1079:VAL:HB	1:B:1117:ALA:HB1	1.34	1.08
1:B:1335:ARG:HD3	1:B:1348:LEU:HB3	1.33	1.07
1:A:1013:ALA:HB1	4:A:39:HOH:O	1.57	1.04
1:B:1557:GLY:CA	4:B:65:HOH:O	2.03	1.04
1:B:1166:TRP:CH2	1:B:1225:ILE:HD11	1.95	1.02
1:A:1353:LEU:HD12	1:A:1353:LEU:H	1.25	1.02
1:A:1557:GLY:O	4:A:19:HOH:O	1.75	1.02
1:B:1239:GLY:HA2	1:B:1244:GLN:HE22	1.18	1.01
1:B:1376:PRO:HD3	1:B:1435:SER:HB3	1.45	0.97
1:B:1166:TRP:CZ3	1:B:1225:ILE:HD11	2.00	0.97
1:A:1417:GLU:HA	1:A:1420:LEU:HD23	1.45	0.97
1:A:1262:THR:HG22	1:A:1263:LEU:H	1.31	0.96
1:A:1405:GLU:CD	1:A:1422:LEU:HA	1.86	0.96
1:A:1469:GLU:HG3	4:A:175:HOH:O	1.64	0.95
1:A:1044:SER:OG	2:A:274:SO4:O4	1.84	0.94
1:A:1225:ILE:HG23	1:A:1238:ALA:HB2	1.48	0.94
1:A:1225:ILE:CG2	1:A:1238:ALA:CB	2.46	0.94
1:B:1417:GLU:HA	1:B:1420:LEU:HD23	1.52	0.91
1:A:1166:TRP:CZ3	1:A:1225:ILE:HD11	2.05	0.91
1:A:1277:ASN:HD22	1:A:1278:ILE:H	1.10	0.91
1:B:1455:ALA:HA	1:B:1459:TYR:HD2	1.34	0.91
1:B:1262:THR:HG22	1:B:1263:LEU:H	1.36	0.91
1:B:1329:VAL:HG12	1:B:1330:ILE:H	1.37	0.90
1:B:1451:ILE:HD11	1:B:1526:VAL:HG11	1.53	0.90
1:A:1375:VAL:O	4:A:103:HOH:O	1.87	0.90
1:B:1277:ASN:H	1:B:1277:ASN:HD22	1.15	0.90
1:B:1094:VAL:HG23	1:B:1268:ALA:HA	1.53	0.90
1:A:1125:ILE:HG12	1:A:1129:PHE:CE1	2.07	0.90
1:A:1210:CYS:O	4:A:62:HOH:O	1.89	0.89
1:B:1551:ALA:O	4:B:147:HOH:O	1.89	0.89
1:A:1277:ASN:HD22	1:A:1278:ILE:N	1.69	0.89
1:A:1476:ARG:O	1:A:1480:LEU:HB2	1.73	0.89
1:A:1301:GLU:OE1	4:A:197:HOH:O	1.91	0.89

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1372:LYS:HZ3	1:B:1457:GLU:HG2	1.36	0.89
1:A:1185:GLY:HA3	1:A:1189:ASN:HD22	1.37	0.88
1:B:1169:VAL:CG2	1:B:1200:SER:HA	2.03	0.88
1:B:1086:ALA:HB2	1:B:1092:VAL:HG12	1.57	0.87
1:B:1543:ALA:O	1:B:1547:ILE:HG13	1.73	0.87
1:A:1082:THR:HG21	1:A:1094:VAL:HG22	1.56	0.86
1:A:1225:ILE:CG2	1:A:1238:ALA:HB3	2.05	0.86
1:B:1079:VAL:HG11	1:B:1117:ALA:O	1.76	0.85
1:B:1107:ILE:O	1:B:1108:LYS:HB2	1.73	0.85
1:A:1044:SER:OG	2:A:274:SO4:S	2.36	0.84
3:A:282[B]:K:K	4:A:186:HOH:O	0.77	0.84
1:A:1225:ILE:HG23	1:A:1238:ALA:CB	2.05	0.83
1:B:1085:LEU:HD13	1:B:1092:VAL:HG21	1.60	0.83
1:B:1331:VAL:HG12	1:B:1332:ALA:H	1.42	0.83
1:B:1478:GLU:OE2	4:B:236:HOH:O	1.95	0.83
1:B:1523:ARG:NH1	1:B:1525:ILE:HD11	1.93	0.83
1:B:1447:ILE:HD11	1:B:1483:GLY:HA2	1.59	0.83
1:A:1072:GLU:OE1	4:A:191:HOH:O	1.98	0.82
1:A:1412:TRP:CG	2:A:277:SO4:O4	2.32	0.82
1:A:1244:GLN:H	1:A:1244:GLN:NE2	1.78	0.82
1:B:1239:GLY:HA2	1:B:1244:GLN:NE2	1.96	0.81
1:B:1523:ARG:N	1:B:1523:ARG:HD2	1.94	0.81
1:A:1225:ILE:HG22	1:A:1238:ALA:HB3	1.62	0.80
1:B:1477:TYR:HE2	1:B:1516:VAL:HG12	1.44	0.80
1:B:1049:ARG:O	1:B:1049:ARG:HD3	1.82	0.80
1:A:1008:ILE:HG12	1:A:1011:ALA:HB3	1.63	0.80
1:A:1166:TRP:CE3	1:A:1225:ILE:HD11	2.16	0.80
1:B:1169:VAL:HG21	1:B:1200:SER:HA	1.61	0.80
1:A:1140:HIS:HD2	1:A:1203:SER:OG	1.64	0.80
1:A:1175:ARG:CD	2:A:275:SO4:O3	2.27	0.79
1:A:1225:ILE:CG2	1:A:1238:ALA:HB2	2.07	0.79
1:B:1277:ASN:ND2	1:B:1278:ILE:H	1.81	0.79
1:A:1080:GLY:HA3	1:A:1409:SER:OG	1.82	0.79
1:B:1422:LEU:O	1:B:1426:VAL:HG23	1.82	0.79
1:B:1277:ASN:H	1:B:1277:ASN:ND2	1.81	0.78
1:B:1032:GLU:O	1:B:1033:VAL:HG23	1.84	0.77
1:B:1523:ARG:HD2	1:B:1523:ARG:H	1.50	0.77
1:A:1486:PRO:HD2	1:A:1523:ARG:HB3	1.65	0.77
1:A:1195:THR:HG21	4:A:35:HOH:O	1.83	0.77
1:A:1182:ILE:HG22	1:A:1183:GLY:N	1.99	0.77
1:B:1425:LYS:O	1:B:1429:THR:HG23	1.85	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1065:ILE:HD13	1:B:1332:ALA:HA	1.67	0.76
1:A:1306:ALA:O	1:A:1310:ALA:HB3	1.86	0.76
1:B:1110:GLY:HA2	4:B:92:HOH:O	1.84	0.76
1:B:1059:LEU:HD12	1:B:1060:ILE:N	2.01	0.75
1:A:1394:LEU:O	1:A:1398:LEU:HB2	1.86	0.75
1:A:1082:THR:HG21	1:A:1094:VAL:CG2	2.15	0.75
1:B:1325:PRO:HD2	1:B:1437:PHE:CD2	2.21	0.75
1:B:1103:PRO:CG	4:B:181:HOH:O	2.34	0.75
1:B:1337:LEU:HD23	1:B:1360:PHE:HA	1.69	0.75
1:A:1164:ILE:HG21	1:A:1193:ARG:NH2	2.02	0.74
1:B:1075:THR:HG21	1:B:1113:GLY:HA2	1.69	0.74
1:B:1017:LYS:HB2	1:B:1261:GLN:HE22	1.51	0.74
1:B:1075:THR:CG2	1:B:1113:GLY:HA2	2.17	0.74
1:B:1323:PHE:O	1:B:1324:LYS:HG3	1.87	0.74
1:A:1068:THR:HB	1:A:1069:PRO:HD2	1.69	0.73
1:A:1175:ARG:HD3	2:A:275:SO4:S	2.28	0.73
1:A:1439:VAL:HG13	4:A:99:HOH:O	1.89	0.73
1:A:1136:VAL:HG13	1:A:1205:VAL:HG12	1.68	0.73
1:B:1262:THR:HG22	1:B:1263:LEU:N	2.03	0.72
1:A:1498:ASP:CB	1:A:1528:ILE:HG21	2.19	0.72
1:A:1532:ILE:O	1:A:1534:THR:N	2.22	0.72
1:A:1556:THR:O	1:A:1556:THR:HG22	1.90	0.71
1:A:1474:ILE:O	1:A:1474:ILE:HG22	1.91	0.71
1:A:1363:LEU:O	1:A:1367:ILE:HG12	1.91	0.71
1:A:1418:GLY:O	4:A:210:HOH:O	2.08	0.71
1:A:1526:VAL:HG22	1:A:1526:VAL:O	1.90	0.71
1:B:1278:ILE:O	1:B:1525:ILE:HD12	1.90	0.71
1:B:1515:GLU:HG2	1:B:1516:VAL:H	1.54	0.71
1:A:1303:GLY:O	4:A:86:HOH:O	2.08	0.71
1:B:1454:ILE:HG22	1:B:1459:TYR:CE2	2.25	0.70
1:B:1556:THR:HG22	1:B:1556:THR:O	1.89	0.70
1:A:1148:ASP:OD1	4:A:69:HOH:O	2.09	0.70
1:B:1058:LYS:HB3	1:B:1430:LEU:HD21	1.72	0.70
1:A:1175:ARG:HG2	1:A:1178:ARG:CZ	2.21	0.70
1:B:1042:LYS:HE2	1:B:1258:ASN:OD1	1.92	0.70
1:A:1051:LEU:O	1:A:1293:LYS:HG2	1.92	0.70
1:B:1103:PRO:HG3	4:B:181:HOH:O	1.91	0.70
1:A:1319:ARG:NH2	1:A:1441:TYR:O	2.24	0.70
1:A:1337:LEU:O	1:A:1359:GLY:HA3	1.92	0.70
1:B:1306:ALA:O	1:B:1310:ALA:HB3	1.91	0.70
1:B:1417:GLU:CA	1:B:1420:LEU:HD23	2.22	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1182:ILE:CG2	1:A:1183:GLY:H	2.05	0.69
1:A:1042:LYS:HE2	1:A:1258:ASN:OD1	1.92	0.69
1:B:1557:GLY:HA2	4:B:65:HOH:O	1.81	0.69
1:A:1023:ALA:HB1	1:A:1028:ILE:HB	1.74	0.69
1:B:1324:LYS:HG2	1:B:1437:PHE:HB3	1.75	0.69
1:B:1042:LYS:NZ	1:B:1254:ALA:HA	2.08	0.69
1:A:1543:ALA:O	1:A:1547:ILE:HG12	1.91	0.69
1:B:1065:ILE:HG23	1:B:1332:ALA:HB2	1.75	0.69
1:B:1043:ILE:HD11	1:B:1259:LEU:HB2	1.74	0.68
1:A:1244:GLN:H	1:A:1244:GLN:HE21	1.42	0.68
1:B:1109:GLY:O	4:B:92:HOH:O	2.10	0.68
1:A:1035:LEU:HD22	1:A:1037:GLY:O	1.92	0.68
1:A:1182:ILE:CG2	1:A:1183:GLY:N	2.56	0.68
1:A:1082:THR:CG2	1:A:1094:VAL:HG22	2.24	0.68
1:A:1517:ARG:HH22	1:A:1532:ILE:HG13	1.59	0.68
1:B:1394:LEU:O	1:B:1398:LEU:HD23	1.92	0.68
1:B:1293:LYS:N	1:B:1293:LYS:HD2	2.09	0.68
1:A:1020:MET:HE3	1:A:1030:GLU:HG3	1.76	0.67
1:A:1308:LEU:O	1:A:1312:LYS:HG3	1.93	0.67
1:A:1412:TRP:CD2	2:A:277:SO4:O4	2.46	0.67
1:B:1125:ILE:HG12	1:B:1129:PHE:CE1	2.30	0.67
1:B:1205:VAL:HG12	1:B:1205:VAL:O	1.93	0.67
1:B:1065:ILE:CD1	1:B:1332:ALA:HA	2.25	0.67
1:B:1091:ARG:HB3	1:B:1296:ASP:H	1.60	0.67
1:A:1275:PHE:HB3	1:A:1277:ASN:ND2	2.10	0.67
1:B:1083:ASP:O	1:B:1087:ARG:HB2	1.95	0.67
1:B:1083:ASP:HB3	1:B:1264:GLU:OE1	1.95	0.67
1:B:1489:MET:HE1	1:B:1526:VAL:HG21	1.76	0.67
1:B:1043:ILE:HD11	1:B:1259:LEU:HD22	1.77	0.66
1:B:1149:ASN:O	1:B:1152:GLN:HB3	1.95	0.66
1:B:1360:PHE:CE2	1:B:1364:GLU:HB2	2.30	0.66
1:B:1417:GLU:O	1:B:1420:LEU:HB2	1.96	0.66
1:A:1116:TYR:CZ	2:A:278:SO4:O1	2.48	0.66
1:A:1092:VAL:HG23	1:A:1297:TYR:O	1.94	0.66
1:A:1150:HIS:CE1	1:A:1157:LEU:H	2.13	0.66
1:A:1171:ASP:HA	1:A:1199:ILE:HD12	1.77	0.66
1:A:1204:GLU:OE2	4:A:116:HOH:O	2.13	0.66
1:A:1262:THR:HG22	1:A:1263:LEU:N	2.05	0.66
1:A:1512:THR:O	1:A:1512:THR:HG22	1.94	0.66
1:A:1217:ASP:O	1:A:1221:ARG:HG3	1.95	0.66
1:B:1372:LYS:NZ	1:B:1457:GLU:HG2	2.10	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1166:TRP:CH2	1:B:1225:ILE:CD1	2.76	0.66
1:A:1210:CYS:HA	1:A:1284:SER:HA	1.76	0.66
1:B:1351:GLU:HG3	1:B:1391:GLU:HG3	1.78	0.66
1:B:1383:ALA:HB3	1:B:1408:LEU:HG	1.78	0.66
1:B:1206:MET:HE2	1:B:1273:GLY:O	1.96	0.65
1:A:1158:ASN:O	1:A:1230:THR:HA	1.96	0.65
1:B:1144:ALA:HB1	1:B:1168:ARG:HH21	1.60	0.65
1:B:1086:ALA:HB2	1:B:1092:VAL:CG1	2.26	0.65
1:B:1344:PRO:HD2	1:B:1347:ASP:HB2	1.79	0.65
1:A:1473:ALA:C	1:A:1475:GLN:H	1.99	0.65
1:B:1363:LEU:O	1:B:1367:ILE:HG12	1.96	0.65
1:A:1426:VAL:O	1:A:1430:LEU:HB2	1.97	0.65
1:B:1329:VAL:HG12	1:B:1330:ILE:N	2.11	0.65
1:A:1175:ARG:NH1	1:A:1537:GLY:HA3	2.11	0.64
1:A:1277:ASN:ND2	1:A:1278:ILE:N	2.45	0.64
1:B:1173:ASN:OD1	1:B:1536:PRO:HB2	1.97	0.64
1:B:1557:GLY:HA3	4:B:65:HOH:O	1.82	0.64
1:A:1540:LYS:O	1:A:1542:PRO:HD3	1.98	0.64
1:B:1319:ARG:NE	1:B:1443:LEU:HD13	2.12	0.64
1:A:1257:PRO:HD3	1:A:1286:ILE:CD1	2.28	0.64
1:B:1125:ILE:HA	1:B:1129:PHE:CD1	2.32	0.64
1:A:1090:LYS:HD2	1:A:1297:TYR:HE2	1.62	0.64
1:B:1526:VAL:HG23	1:B:1526:VAL:O	1.98	0.64
1:A:1066:THR:HB	1:A:1362:ASN:HD21	1.62	0.64
1:B:1175:ARG:O	1:B:1178:ARG:HG3	1.98	0.64
1:B:1222:PHE:O	1:B:1225:ILE:CG2	2.34	0.64
1:A:1121:PRO:O	1:A:1125:ILE:HG13	1.98	0.64
1:A:1491:LYS:HB3	1:A:1528:ILE:HG13	1.79	0.64
1:B:1442:ASN:O	1:B:1450:LYS:HE2	1.98	0.64
1:A:1082:THR:HG22	1:A:1266:THR:HG21	1.80	0.64
1:B:1337:LEU:O	1:B:1340:HIS:HB2	1.98	0.64
1:A:1111:ALA:HB2	1:A:1122:MET:SD	2.38	0.63
1:B:1143:LEU:HD23	1:B:1166:TRP:CE2	2.33	0.63
1:B:1472:LYS:O	1:B:1476:ARG:HG3	1.98	0.63
1:B:1496:PHE:HD2	1:B:1506:PRO:HD2	1.63	0.63
1:B:1292:LEU:HD23	1:B:1298:VAL:HG21	1.79	0.63
1:B:1186:GLY:O	1:B:1188:ALA:N	2.31	0.63
1:B:1275:PHE:O	1:B:1279:ALA:HB3	1.98	0.63
1:A:1452:ALA:O	1:A:1456:THR:N	2.30	0.63
1:B:1082:THR:HG22	1:B:1266:THR:HG21	1.80	0.63
1:B:1097:ARG:NH2	2:B:272:SO4:O1	2.24	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1083:ASP:HB3	1:B:1264:GLU:CD	2.20	0.63
1:B:1136:VAL:HG13	1:B:1205:VAL:HG12	1.81	0.63
1:A:1525:ILE:CG2	1:A:1526:VAL:N	2.62	0.62
1:B:1455:ALA:HA	1:B:1459:TYR:CD2	2.25	0.62
1:A:1530:GLY:C	1:A:1532:ILE:H	2.02	0.62
1:A:1092:VAL:HG22	1:A:1093:MET:N	2.14	0.62
1:A:1229:TYR:HD2	1:A:1233:GLY:O	1.82	0.62
1:B:1335:ARG:HH21	1:B:1386:THR:HG21	1.65	0.62
1:B:1488:VAL:HG21	1:B:1523:ARG:NE	2.15	0.62
1:A:1275:PHE:HB3	1:A:1277:ASN:HD21	1.65	0.62
1:A:1548:ASP:O	1:A:1555:ILE:HG22	2.00	0.62
1:A:1286:ILE:HG23	4:A:70:HOH:O	1.99	0.62
1:B:1090:LYS:HB3	1:B:1297:TYR:HE2	1.64	0.62
1:B:1059:LEU:HD12	1:B:1060:ILE:H	1.62	0.62
1:B:1339:MET:HA	1:B:1343:VAL:O	1.99	0.62
1:A:1095:CYS:O	1:A:1096:LEU:HD23	1.99	0.61
1:A:1119:VAL:HA	1:A:1262:THR:HA	1.82	0.61
1:A:1381:ILE:HD13	1:A:1381:ILE:H	1.65	0.61
1:A:1405:GLU:OE2	1:A:1422:LEU:HA	2.00	0.61
1:B:1021:GLU:O	1:B:1024:ARG:HB2	2.01	0.61
1:B:1451:ILE:HG12	1:B:1489:MET:HE1	1.82	0.61
1:B:1319:ARG:HE	1:B:1443:LEU:HD13	1.65	0.61
1:A:1120:VAL:HB	1:A:1121:PRO:HA	1.82	0.61
1:A:1405:GLU:OE2	1:A:1425:LYS:HB2	2.01	0.61
1:B:1059:LEU:HB3	1:B:1325:PRO:HA	1.83	0.61
1:A:1389:GLU:C	1:A:1391:GLU:H	2.04	0.61
1:B:1070:ALA:HB2	1:B:1339:MET:SD	2.41	0.61
1:A:1470:ALA:O	1:A:1474:ILE:HG13	2.01	0.60
1:B:1017:LYS:HG3	1:B:1265:ASN:OD1	2.00	0.60
1:B:1365:LYS:HE3	1:B:1369:ASN:HD21	1.64	0.60
1:A:1498:ASP:HB3	1:A:1528:ILE:HG21	1.80	0.60
1:B:1351:GLU:HG3	1:B:1391:GLU:CG	2.31	0.60
1:B:1303:GLY:O	1:B:1309:GLY:HA3	2.00	0.60
1:B:1293:LYS:O	1:B:1295:ALA:N	2.34	0.60
1:B:1043:ILE:HD12	1:B:1269:PHE:HE1	1.66	0.60
1:B:1275:PHE:HB3	1:B:1277:ASN:ND2	2.16	0.60
1:A:1071:GLY:C	1:A:1072:GLU:HG3	2.22	0.60
1:B:1062:VAL:HG12	1:B:1300:THR:O	2.01	0.60
1:A:1533:MET:HA	2:A:273:SO4:O2	2.00	0.60
1:A:1017:LYS:N	1:A:1261:GLN:HE22	2.00	0.60
1:A:1136:VAL:HG21	1:A:1206:MET:HE2	1.84	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1259:LEU:O	1:A:1260:VAL:HG13	2.01	0.60
1:A:1379:VAL:HG12	1:A:1381:ILE:HD13	1.84	0.60
1:A:1407:ALA:C	1:A:1409:SER:H	2.05	0.59
1:A:1446:SER:N	4:A:23:HOH:O	2.28	0.59
1:A:1488:VAL:HB	1:A:1525:ILE:HD13	1.84	0.59
1:B:1066:THR:HG23	4:B:179:HOH:O	2.01	0.59
1:A:1090:LYS:HD2	1:A:1297:TYR:CE2	2.37	0.59
1:B:1193:ARG:NH2	1:B:1195:THR:HG23	2.17	0.59
1:B:1312:LYS:O	1:B:1316:VAL:HG23	2.02	0.59
1:A:1554:VAL:HG12	1:A:1555:ILE:N	2.16	0.59
1:B:1159:ILE:HA	1:B:1230:THR:HA	1.84	0.59
1:A:1381:ILE:HD13	1:A:1381:ILE:N	2.17	0.59
1:B:1124:ASP:O	1:B:1129:PHE:HA	2.02	0.59
1:B:1550:ASP:C	1:B:1552:ASP:H	2.06	0.59
1:A:1306:ALA:HB3	1:A:1366:HIS:ND1	2.17	0.59
1:B:1092:VAL:HG23	1:B:1297:TYR:HB2	1.85	0.59
1:B:1155:ASN:HD21	1:B:1159:ILE:N	2.01	0.59
1:B:1451:ILE:HG12	1:B:1487:VAL:HG11	1.83	0.59
1:B:1133:ILE:HD13	1:B:1171:ASP:OD1	2.03	0.59
1:B:1408:LEU:HD13	1:B:1414:LYS:HE3	1.85	0.59
1:A:1008:ILE:HG12	1:A:1011:ALA:CB	2.33	0.59
1:A:1277:ASN:O	1:A:1490:ALA:HB2	2.03	0.59
1:A:1277:ASN:HD22	1:A:1277:ASN:H	1.50	0.59
1:A:1485:LEU:HD13	1:A:1523:ARG:HA	1.85	0.58
1:A:1325:PRO:HD2	1:A:1437:PHE:CD2	2.38	0.58
1:B:1451:ILE:HG23	1:B:1489:MET:CE	2.33	0.58
1:A:1020:MET:HE1	1:A:1030:GLU:HA	1.85	0.58
1:A:1045:LEU:HD11	1:A:1255:ILE:O	2.03	0.58
1:B:1275:PHE:HB3	1:B:1277:ASN:HD21	1.67	0.58
1:A:1230:THR:HG23	1:A:1234:LYS:O	2.04	0.58
1:A:1488:VAL:HA	4:A:14:HOH:O	2.04	0.58
1:B:1140:HIS:HD2	1:B:1203:SER:OG	1.85	0.58
1:A:1275:PHE:O	1:A:1279:ALA:HB3	2.04	0.58
1:B:1091:ARG:NH1	4:B:118:HOH:O	2.32	0.58
1:A:1182:ILE:HG22	1:A:1183:GLY:H	1.64	0.58
1:A:1173:ASN:HB3	1:A:1536:PRO:O	2.04	0.57
1:A:1334:VAL:HG12	1:A:1338:LYS:HE2	1.86	0.57
1:A:1408:LEU:HD13	1:A:1414:LYS:CE	2.34	0.57
1:A:1311:GLU:HG3	1:A:1312:LYS:N	2.17	0.57
1:B:1063:THR:HG23	1:B:1064:ALA:N	2.19	0.57
1:B:1072:GLU:CD	1:B:1073:GLY:H	2.07	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1367:ILE:HG22	1:A:1401:LYS:HE3	1.85	0.57
1:B:1515:GLU:HG2	1:B:1516:VAL:N	2.19	0.57
1:A:1170:ILE:HD12	1:A:1171:ASP:H	1.68	0.57
1:B:1079:VAL:CB	1:B:1117:ALA:HB1	2.22	0.57
1:A:1454:ILE:O	1:A:1458:ILE:HB	2.04	0.57
1:B:1337:LEU:O	1:B:1359:GLY:HA3	2.04	0.57
1:B:1384:PHE:CD1	1:B:1385:PRO:HD2	2.40	0.57
1:A:1242:GLU:OE1	1:A:1242:GLU:HA	2.05	0.57
1:A:1408:LEU:HD13	1:A:1414:LYS:HE3	1.87	0.57
1:B:1276:ALA:HA	1:B:1279:ALA:O	2.05	0.57
1:B:1499:ASP:OD2	1:B:1502:LYS:HE3	2.05	0.57
1:B:1549:ILE:HG23	1:B:1549:ILE:O	2.03	0.57
1:B:1029:GLN:HB3	1:B:1031:ASP:OD2	2.05	0.56
1:B:1343:VAL:HG13	1:B:1347:ASP:O	2.05	0.56
1:B:1081:LEU:O	1:B:1085:LEU:HB2	2.04	0.56
1:B:1221:ARG:O	1:B:1222:PHE:C	2.44	0.56
1:B:1459:TYR:OH	1:B:1489:MET:HG3	2.05	0.56
1:A:1036:TYR:O	1:A:1040:LYS:NZ	2.38	0.56
1:A:1488:VAL:HG21	1:A:1523:ARG:CZ	2.35	0.56
1:A:1489:MET:HE1	1:A:1526:VAL:HG11	1.86	0.56
1:B:1206:MET:O	1:B:1209:LEU:HB3	2.05	0.56
1:B:1276:ALA:HB3	1:B:1304:PHE:CD2	2.40	0.56
1:B:1445:LEU:O	1:B:1450:LYS:HE3	2.05	0.56
1:A:1384:PHE:CD2	1:A:1385:PRO:HD2	2.41	0.56
1:B:1044:SER:OG	2:B:280:SO4:O2	2.20	0.56
1:B:1054:LYS:HB3	1:B:1055:PRO:HD2	1.86	0.56
1:B:1066:THR:OG1	1:B:1366:HIS:NE2	2.32	0.56
1:B:1095:CYS:SG	1:B:1288:THR:HA	2.46	0.56
1:B:1277:ASN:ND2	1:B:1277:ASN:N	2.45	0.56
1:B:1178:ARG:HD3	1:B:1535:MET:HB3	1.86	0.56
1:A:1107:ILE:CG2	1:A:1539:PRO:HG2	2.35	0.56
1:A:1473:ALA:O	1:A:1475:GLN:N	2.39	0.56
1:A:1555:ILE:HG23	1:A:1555:ILE:O	2.06	0.56
1:B:1017:LYS:N	1:B:1261:GLN:OE1	2.39	0.56
1:B:1042:LYS:HD3	1:B:1256:LYS:HB2	1.88	0.56
1:B:1058:LYS:CB	1:B:1430:LEU:HD21	2.36	0.56
1:B:1169:VAL:HG22	1:B:1200:SER:HA	1.84	0.56
1:A:1140:HIS:CD2	1:A:1203:SER:OG	2.54	0.56
1:B:1454:ILE:HG22	1:B:1459:TYR:HE2	1.70	0.56
1:A:1119:VAL:HG13	1:A:1261:GLN:O	2.06	0.56
1:A:1167:ARG:NH2	1:A:1178:ARG:O	2.39	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1086:ALA:C	1:B:1088:LEU:H	2.08	0.56
1:B:1334:VAL:HB	1:B:1387:ASP:OD1	2.06	0.56
1:B:1499:ASP:C	1:B:1501:THR:H	2.09	0.56
1:B:1009:GLU:HG2	1:B:1118:GLN:HE22	1.71	0.56
1:A:1525:ILE:HG22	1:A:1526:VAL:N	2.21	0.55
1:B:1075:THR:O	1:B:1078:SER:N	2.29	0.55
1:B:1285:ILE:N	4:B:184:HOH:O	2.34	0.55
1:A:1451:ILE:HG12	1:A:1489:MET:CE	2.37	0.55
1:B:1277:ASN:HD22	1:B:1278:ILE:H	1.53	0.55
1:A:1150:HIS:HE1	1:A:1157:LEU:H	1.54	0.55
1:A:1222:PHE:O	1:A:1225:ILE:HG22	2.05	0.55
1:B:1518:LEU:HD12	1:B:1519:SER:N	2.21	0.55
1:A:1032:GLU:OE2	1:A:1050:ARG:NH1	2.39	0.55
1:B:1233:GLY:O	1:B:1235:PRO:HD3	2.07	0.55
1:B:1331:VAL:HG12	1:B:1332:ALA:N	2.15	0.55
1:A:1381:ILE:HG21	1:A:1395:LEU:HD23	1.87	0.55
1:B:1477:TYR:CE2	1:B:1516:VAL:HG12	2.33	0.55
1:B:1063:THR:HG22	1:B:1329:VAL:O	2.06	0.55
1:B:1211:LEU:HD21	1:B:1280:HIS:CD2	2.41	0.55
1:B:1262:THR:CG2	1:B:1263:LEU:H	2.15	0.55
1:B:1115:GLY:O	1:B:1118:GLN:HG2	2.07	0.55
1:A:1277:ASN:ND2	1:A:1278:ILE:H	1.92	0.55
1:B:1466:TYR:CE2	1:B:1513:VAL:HG11	2.42	0.55
1:B:1132:ASP:OD2	1:B:1254:ALA:HA	2.07	0.54
1:A:1166:TRP:CZ3	1:A:1225:ILE:CD1	2.86	0.54
1:B:1076:THR:HG23	1:B:1114:GLY:O	2.07	0.54
1:B:1043:ILE:HD12	1:B:1269:PHE:CE1	2.42	0.54
1:B:1380:ALA:O	1:B:1381:ILE:HD13	2.07	0.54
1:B:1357:ARG:O	1:B:1360:PHE:HB3	2.08	0.54
1:B:1374:GLY:HA3	1:B:1438:HIS:CE1	2.42	0.54
1:B:1376:PRO:CD	1:B:1435:SER:HB3	2.30	0.54
1:A:1389:GLU:C	1:A:1391:GLU:N	2.61	0.54
1:A:1533:MET:CA	2:A:273:SO4:O2	2.56	0.54
1:B:1090:LYS:HB3	1:B:1297:TYR:CE2	2.43	0.54
1:A:1043:ILE:HD11	1:A:1259:LEU:HB2	1.90	0.54
1:A:1286:ILE:HA	1:A:1289:LYS:HG2	1.90	0.54
1:A:1013:ALA:CB	4:A:39:HOH:O	2.32	0.54
1:B:1210:CYS:SG	1:B:1274:PRO:HD3	2.48	0.54
1:A:1278:ILE:CG2	1:A:1278:ILE:O	2.55	0.54
1:B:1085:LEU:HD21	1:B:1297:TYR:CD2	2.43	0.54
1:B:1155:ASN:O	1:B:1158:ASN:N	2.36	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1343:VAL:HG12	1:A:1344:PRO:O	2.09	0.53
1:B:1119:VAL:HG13	1:B:1261:GLN:O	2.07	0.53
1:A:1453:LYS:O	1:A:1457:GLU:HB2	2.08	0.53
1:A:1489:MET:CE	1:A:1526:VAL:HG11	2.39	0.53
1:B:1182:ILE:HG13	1:B:1183:GLY:N	2.24	0.53
1:A:1525:ILE:C	1:A:1526:VAL:HG12	2.27	0.53
1:B:1193:ARG:NH2	1:B:1195:THR:CG2	2.71	0.53
1:A:1169:VAL:HG21	1:A:1200:SER:HA	1.91	0.53
1:B:1493:GLN:C	1:B:1495:SER:H	2.11	0.53
1:A:1042:LYS:NZ	1:A:1132:ASP:OD2	2.38	0.53
1:A:1155:ASN:OD1	1:A:1158:ASN:HA	2.09	0.53
1:A:1512:THR:HG22	1:A:1514:ARG:HE	1.74	0.53
1:B:1516:VAL:HG22	1:B:1526:VAL:HG12	1.91	0.53
1:B:1490:ALA:HB3	1:B:1527:PRO:HA	1.90	0.53
1:A:1488:VAL:CG2	1:A:1523:ARG:HD3	2.39	0.53
1:B:1133:ILE:HG22	1:B:1134:HIS:N	2.23	0.53
1:A:1175:ARG:HH11	1:A:1537:GLY:HA3	1.73	0.53
1:A:1391:GLU:O	1:A:1392:LEU:C	2.46	0.53
1:B:1225:ILE:HA	1:B:1520:ALA:HB3	1.89	0.53
1:B:1408:LEU:HD13	1:B:1414:LYS:CE	2.39	0.52
1:A:1023:ALA:CB	1:A:1028:ILE:HD12	2.40	0.52
1:A:1175:ARG:HA	1:A:1178:ARG:HG3	1.91	0.52
1:B:1379:VAL:HG12	1:B:1380:ALA:N	2.24	0.52
1:B:1075:THR:O	1:B:1076:THR:C	2.48	0.52
1:B:1255:ILE:O	1:B:1255:ILE:HG13	2.10	0.52
1:B:1076:THR:OG1	1:B:1114:GLY:HA3	2.09	0.52
1:B:1093:MET:HG2	1:B:1267:PRO:HB2	1.91	0.52
1:B:1384:PHE:CG	1:B:1385:PRO:HD2	2.44	0.52
1:A:1065:ILE:HB	1:A:1362:ASN:HD22	1.75	0.52
1:A:1009:GLU:HG3	4:A:151:HOH:O	2.09	0.52
1:A:1488:VAL:HG23	1:A:1523:ARG:HD3	1.90	0.52
1:B:1557:GLY:C	4:B:65:HOH:O	2.37	0.52
1:B:1076:THR:O	1:B:1079:VAL:N	2.42	0.52
1:B:1485:LEU:HD13	1:B:1523:ARG:HA	1.90	0.52
1:B:1517:ARG:HH12	1:B:1532:ILE:CD1	2.23	0.52
1:A:1523:ARG:HD2	1:A:1523:ARG:C	2.28	0.52
1:A:1533:MET:HB2	2:A:273:SO4:O2	2.09	0.52
1:B:1204:GLU:C	1:B:1206:MET:H	2.11	0.52
1:B:1335:ARG:HD3	1:B:1348:LEU:CB	2.23	0.52
1:A:1169:VAL:CG2	1:A:1200:SER:HA	2.40	0.52
1:A:1092:VAL:CG2	1:A:1093:MET:N	2.73	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1008:ILE:HG13	1:B:1011:ALA:HB2	1.91	0.52
1:A:1174:ASP:HB3	1:A:1177:LEU:HG	1.91	0.51
1:A:1277:ASN:ND2	1:A:1277:ASN:N	2.58	0.51
1:A:1373:PHE:CE2	1:A:1440:LEU:HB2	2.44	0.51
1:A:1379:VAL:HG12	1:A:1380:ALA:N	2.24	0.51
1:A:1451:ILE:HG12	1:A:1489:MET:HE3	1.92	0.51
1:B:1515:GLU:O	1:B:1527:PRO:HD2	2.10	0.51
1:B:1150:HIS:HE1	1:B:1156:VAL:N	2.08	0.51
1:B:1150:HIS:NE2	1:B:1157:LEU:HG	2.25	0.51
1:B:1448:LYS:HE2	1:B:1466:TYR:CD2	2.45	0.51
1:B:1043:ILE:O	1:B:1257:PRO:HD2	2.11	0.51
1:B:1081:LEU:O	1:B:1081:LEU:HG	2.10	0.51
1:B:1178:ARG:O	1:B:1196:GLY:HA3	2.10	0.51
1:B:1247:MET:HA	1:B:1250:LEU:HD23	1.93	0.51
1:A:1044:SER:OG	2:A:274:SO4:O1	2.24	0.51
1:B:1077:THR:HG21	1:B:1331:VAL:HG22	1.91	0.51
1:B:1498:ASP:HB3	1:B:1528:ILE:HG21	1.92	0.51
1:B:1087:ARG:O	1:B:1088:LEU:HD23	2.10	0.51
1:B:1487:VAL:HG12	1:B:1489:MET:HE2	1.93	0.51
1:A:1036:TYR:O	1:A:1040:LYS:HB2	2.11	0.51
1:A:1083:ASP:OD1	1:A:1262:THR:HG21	2.10	0.51
1:B:1318:CYS:HA	1:B:1323:PHE:HB2	1.92	0.51
1:A:1147:VAL:HG11	1:A:1164:ILE:HD13	1.91	0.51
1:B:1105:PHE:HB3	1:B:1544:ALA:HB2	1.93	0.51
1:A:1125:ILE:HG12	1:A:1129:PHE:CD1	2.43	0.51
1:A:1389:GLU:O	1:A:1393:ASN:HB2	2.11	0.51
1:B:1237:THR:O	1:B:1240:ASP:HB2	2.10	0.51
1:B:1279:ALA:HA	1:B:1523:ARG:NH2	2.26	0.51
1:B:1517:ARG:HH12	1:B:1532:ILE:HD12	1.75	0.51
1:A:1446:SER:HB3	1:A:1449:ASP:HB2	1.93	0.51
1:B:1331:VAL:O	1:B:1332:ALA:HB2	2.10	0.51
1:B:1489:MET:CE	1:B:1526:VAL:HG21	2.41	0.51
1:A:1329:VAL:HA	1:A:1378:VAL:O	2.10	0.50
1:B:1042:LYS:NZ	1:B:1132:ASP:OD2	2.39	0.50
1:A:1473:ALA:C	1:A:1475:GLN:N	2.64	0.50
1:B:1026:LEU:HD23	1:B:1028:ILE:HD11	1.94	0.50
1:B:1293:LYS:C	1:B:1295:ALA:H	2.14	0.50
1:B:1061:LEU:HD13	1:B:1313:PHE:CE1	2.46	0.50
1:B:1313:PHE:CD2	1:B:1313:PHE:C	2.84	0.50
1:B:1337:LEU:HA	1:B:1340:HIS:HD2	1.77	0.50
1:B:1353:LEU:N	1:B:1353:LEU:HD12	2.26	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1398:LEU:C	1:B:1400:ALA:H	2.15	0.50
1:B:1277:ASN:HD22	1:B:1278:ILE:N	2.09	0.50
1:B:1554:VAL:HG12	1:B:1555:ILE:N	2.27	0.50
1:A:1363:LEU:HD11	1:A:1367:ILE:HD11	1.93	0.50
1:B:1008:ILE:HG13	1:B:1011:ALA:CB	2.41	0.50
1:B:1124:ASP:O	1:B:1129:PHE:CA	2.59	0.50
1:B:1461:ALA:HB2	1:B:1509:PHE:HE1	1.77	0.50
1:B:1487:VAL:HG22	1:B:1524:LEU:HD12	1.94	0.50
1:A:1136:VAL:HG13	1:A:1205:VAL:CG1	2.41	0.50
1:A:1277:ASN:ND2	1:A:1277:ASN:H	2.10	0.50
1:B:1338:LYS:C	1:B:1343:VAL:HB	2.32	0.50
1:B:1351:GLU:OE1	1:B:1390:ALA:HB3	2.12	0.50
1:A:1171:ASP:HA	1:A:1199:ILE:CD1	2.42	0.49
1:A:1486:PRO:HD2	1:A:1523:ARG:CB	2.40	0.49
1:B:1083:ASP:HA	4:B:190:HOH:O	2.11	0.49
1:B:1221:ARG:O	1:B:1224:ARG:N	2.37	0.49
1:B:1229:TYR:CD1	1:B:1229:TYR:N	2.80	0.49
1:B:1556:THR:O	1:B:1556:THR:CG2	2.58	0.49
1:A:1419:GLY:HA2	4:A:210:HOH:O	2.12	0.49
1:B:1261:GLN:HB2	1:B:1265:ASN:HA	1.94	0.49
1:A:1472:LYS:O	1:A:1476:ARG:HG3	2.12	0.49
1:B:1446:SER:HB3	1:B:1449:ASP:OD2	2.12	0.49
1:B:1447:ILE:HD12	1:B:1478:GLU:HG3	1.93	0.49
1:A:1467:THR:O	1:A:1470:ALA:HB3	2.13	0.49
1:B:1019:VAL:HG11	1:B:1041:ALA:HB3	1.94	0.49
1:B:1491:LYS:HG3	1:B:1492:THR:O	2.13	0.49
1:B:1277:ASN:ND2	1:B:1278:ILE:N	2.55	0.49
1:B:1440:LEU:HD22	1:B:1458:ILE:HD11	1.95	0.49
1:B:1082:THR:OG1	1:B:1094:VAL:HG13	2.13	0.49
1:B:1088:LEU:O	1:B:1090:LYS:HG2	2.12	0.49
1:A:1512:THR:O	1:A:1512:THR:CG2	2.59	0.49
1:B:1057:GLY:HA3	1:B:1296:ASP:O	2.12	0.49
1:B:1244:GLN:HG2	1:B:1245:GLY:N	2.28	0.49
1:B:1486:PRO:O	1:B:1524:LEU:HD12	2.12	0.49
1:A:1136:VAL:HG11	1:A:1206:MET:HE2	1.94	0.48
1:A:1453:LYS:HG2	4:A:111:HOH:O	2.13	0.48
1:B:1215:LEU:HD22	1:B:1215:LEU:O	2.13	0.48
1:B:1376:PRO:HG3	1:B:1433:ARG:HG2	1.95	0.48
1:B:1442:ASN:OD1	1:B:1443:LEU:N	2.46	0.48
1:B:1493:GLN:N	1:B:1493:GLN:OE1	2.46	0.48
1:B:1143:LEU:HD23	1:B:1166:TRP:NE1	2.28	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1155:ASN:ND2	1:B:1159:ILE:N	2.61	0.48
1:B:1338:LYS:O	1:B:1341:GLY:N	2.45	0.48
1:A:1344:PRO:O	1:A:1348:LEU:HG	2.13	0.48
1:B:1036:TYR:CE1	1:B:1042:LYS:HG3	2.49	0.48
1:B:1133:ILE:O	1:B:1135:ALA:N	2.46	0.48
1:B:1465:ASN:O	1:B:1513:VAL:HG12	2.14	0.48
1:B:1550:ASP:C	1:B:1552:ASP:N	2.66	0.48
1:B:1343:VAL:CG1	1:B:1348:LEU:HD23	2.44	0.48
1:A:1381:ILE:H	1:A:1381:ILE:CD1	2.19	0.48
1:A:1090:LYS:HB3	1:A:1297:TYR:CD2	2.48	0.48
1:A:1343:VAL:CG1	1:A:1348:LEU:HD23	2.43	0.48
1:A:1455:ALA:O	1:A:1461:ALA:HB3	2.13	0.48
1:A:1526:VAL:O	1:A:1526:VAL:CG2	2.61	0.48
1:B:1393:ASN:O	1:B:1396:TYR:HB2	2.13	0.48
1:A:1185:GLY:CA	1:A:1189:ASN:HD22	2.18	0.48
1:A:1290:THR:O	1:A:1294:LEU:HG	2.13	0.48
1:A:1542:PRO:C	1:A:1544:ALA:N	2.66	0.48
1:A:1178:ARG:NH2	2:A:275:SO4:O2	2.46	0.48
1:B:1125:ILE:HG12	1:B:1129:PHE:HE1	1.79	0.48
1:B:1169:VAL:HG23	1:B:1198:ASP:O	2.13	0.48
1:B:1440:LEU:CD2	1:B:1458:ILE:HD11	2.44	0.48
1:B:1443:LEU:HG	1:B:1484:ASN:O	2.14	0.48
1:A:1195:THR:HG22	1:A:1196:GLY:H	1.77	0.48
1:B:1010:ILE:C	1:B:1012:GLN:H	2.17	0.48
1:B:1019:VAL:HG23	1:B:1039:TYR:HA	1.95	0.48
1:B:1111:ALA:C	1:B:1113:GLY:H	2.17	0.48
1:B:1292:LEU:HD23	1:B:1298:VAL:CG2	2.43	0.48
1:B:1319:ARG:HG3	1:B:1439:VAL:HG11	1.96	0.48
1:A:1061:LEU:O	1:A:1328:THR:HA	2.14	0.47
1:A:1116:TYR:CE2	2:A:278:SO4:O1	2.67	0.47
1:A:1136:VAL:HG21	1:A:1206:MET:CE	2.44	0.47
1:A:1366:HIS:NE2	1:A:1496:PHE:CZ	2.82	0.47
1:A:1554:VAL:CG1	1:A:1555:ILE:N	2.77	0.47
1:B:1049:ARG:HD3	1:B:1049:ARG:C	2.33	0.47
1:B:1133:ILE:O	1:B:1136:VAL:N	2.46	0.47
1:A:1286:ILE:HD12	1:A:1286:ILE:C	2.34	0.47
1:B:1374:GLY:HA3	1:B:1438:HIS:HE1	1.78	0.47
1:B:1461:ALA:HA	1:B:1509:PHE:CE1	2.49	0.47
1:A:1360:PHE:CE2	1:A:1364:GLU:HB2	2.49	0.47
1:B:1313:PHE:CE2	1:B:1318:CYS:SG	3.07	0.47
1:A:1353:LEU:HD12	1:A:1353:LEU:N	2.09	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1107:ILE:HG22	1:A:1539:PRO:HG2	1.94	0.47
1:A:1386:THR:HA	4:A:48:HOH:O	2.14	0.47
1:B:1143:LEU:O	1:B:1147:VAL:HG23	2.14	0.47
1:A:1542:PRO:C	1:A:1544:ALA:H	2.16	0.47
1:A:1555:ILE:O	1:A:1556:THR:CB	2.63	0.47
1:B:1155:ASN:OD1	1:B:1159:ILE:HB	2.14	0.47
1:B:1343:VAL:HG11	1:B:1348:LEU:HD23	1.96	0.47
1:A:1277:ASN:HD22	1:A:1277:ASN:N	2.08	0.47
1:A:1400:ALA:O	1:A:1401:LYS:HB2	2.15	0.47
1:A:1474:ILE:O	1:A:1474:ILE:CG2	2.61	0.47
1:B:1244:GLN:HG2	1:B:1245:GLY:H	1.79	0.47
1:A:1066:THR:H	1:A:1362:ASN:HD21	1.63	0.47
1:A:1259:LEU:O	1:A:1260:VAL:CG1	2.63	0.47
1:B:1009:GLU:HG2	1:B:1009:GLU:O	2.14	0.47
1:B:1199:ILE:HA	1:B:1535:MET:HE2	1.97	0.47
1:B:1257:PRO:HD3	1:B:1286:ILE:CD1	2.45	0.47
1:B:1507:ARG:O	1:B:1508:ASN:HB2	2.14	0.47
1:A:1457:GLU:OE2	4:A:218:HOH:O	2.20	0.47
1:B:1061:LEU:HD22	1:B:1313:PHE:CD1	2.50	0.47
1:B:1550:ASP:OD1	1:B:1551:ALA:N	2.47	0.47
1:A:1096:LEU:O	1:A:1270:ILE:HA	2.15	0.47
1:A:1366:HIS:CE1	1:A:1496:PHE:CZ	3.03	0.47
1:A:1533:MET:CB	2:A:273:SO4:O2	2.63	0.47
1:B:1154:GLY:O	1:B:1155:ASN:C	2.53	0.47
1:A:1160:ASP:HB3	1:A:1163:THR:CG2	2.45	0.46
1:A:1353:LEU:H	1:A:1353:LEU:CD1	2.04	0.46
1:B:1414:LYS:O	1:B:1417:GLU:HB3	2.15	0.46
1:B:1278:ILE:N	1:B:1278:ILE:HD12	2.31	0.46
1:A:1107:ILE:O	1:A:1108:LYS:HB2	2.15	0.46
1:A:1149:ASN:O	1:A:1152:GLN:HB3	2.16	0.46
1:A:1532:ILE:O	1:A:1534:THR:HG23	2.15	0.46
1:A:1555:ILE:O	1:A:1556:THR:HB	2.16	0.46
1:B:1277:ASN:HD22	1:B:1277:ASN:N	1.85	0.46
1:B:1338:LYS:HB3	1:B:1343:VAL:HG21	1.97	0.46
1:B:1492:THR:HG23	1:B:1493:GLN:N	2.31	0.46
1:B:1360:PHE:O	1:B:1361:ALA:C	2.54	0.46
1:B:1502:LYS:HB3	1:B:1506:PRO:HB3	1.98	0.46
1:B:1492:THR:HG22	1:B:1498:ASP:HA	1.98	0.46
1:A:1138:TYR:O	1:A:1139:ALA:C	2.53	0.46
1:A:1448:LYS:HG2	1:A:1466:TYR:CZ	2.51	0.46
1:B:1136:VAL:HG13	1:B:1205:VAL:O	2.16	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1150:HIS:O	1:B:1153:GLN:N	2.42	0.46
1:B:1451:ILE:CD1	1:B:1526:VAL:HG11	2.36	0.46
1:A:1023:ALA:HB1	1:A:1028:ILE:HD12	1.98	0.46
1:B:1120:VAL:HB	1:B:1121:PRO:HA	1.98	0.46
1:B:1378:VAL:HG11	1:B:1422:LEU:CD1	2.46	0.46
1:B:1425:LYS:HA	1:B:1428:GLN:HB3	1.97	0.46
1:A:1276:ALA:HB2	1:A:1281:GLY:HA3	1.98	0.45
1:A:1450:LYS:HB2	1:A:1487:VAL:HG21	1.97	0.45
1:B:1331:VAL:CG1	1:B:1332:ALA:H	2.23	0.45
1:B:1499:ASP:C	1:B:1501:THR:N	2.70	0.45
1:B:1036:TYR:HB3	1:B:1040:LYS:NZ	2.30	0.45
1:B:1121:PRO:HG2	1:B:1124:ASP:HB2	1.98	0.45
1:B:1276:ALA:HB3	1:B:1304:PHE:CE2	2.51	0.45
1:B:1373:PHE:CE2	1:B:1440:LEU:HB2	2.51	0.45
1:B:1491:LYS:C	1:B:1492:THR:O	2.52	0.45
1:B:1493:GLN:O	1:B:1495:SER:N	2.50	0.45
1:A:1105:PHE:HB3	1:A:1544:ALA:HB2	1.99	0.45
1:A:1381:ILE:CG2	1:A:1395:LEU:HD23	2.45	0.45
1:A:1498:ASP:HB2	1:A:1528:ILE:HG21	1.96	0.45
1:A:1523:ARG:HD2	1:A:1523:ARG:N	2.31	0.45
1:A:1071:GLY:O	1:A:1072:GLU:HG3	2.16	0.45
1:B:1205:VAL:O	1:B:1205:VAL:CG1	2.62	0.45
1:B:1488:VAL:HG23	1:B:1523:ARG:HG2	1.97	0.45
1:A:1408:LEU:HD13	1:A:1414:LYS:NZ	2.32	0.45
1:B:1026:LEU:HD21	1:B:1294:LEU:HB3	1.97	0.45
1:B:1320:TYR:CZ	4:B:228:HOH:O	2.55	0.45
1:B:1515:GLU:O	1:B:1516:VAL:HG23	2.16	0.45
1:B:1554:VAL:CG1	1:B:1555:ILE:N	2.80	0.45
1:A:1016:MET:HB3	1:A:1261:GLN:NE2	2.31	0.45
1:A:1052:LYS:HE3	4:A:227:HOH:O	2.15	0.45
1:A:1170:ILE:HG13	1:A:1171:ASP:N	2.32	0.45
1:A:1170:ILE:CD1	1:A:1171:ASP:H	2.29	0.45
1:B:1040:LYS:NZ	1:B:1040:LYS:HB2	2.31	0.45
1:B:1329:VAL:CG1	1:B:1330:ILE:H	2.18	0.45
1:A:1125:ILE:HA	1:A:1129:PHE:CD1	2.51	0.45
1:B:1060:ILE:HD12	1:B:1299:VAL:HG22	1.98	0.45
1:B:1140:HIS:HE1	1:B:1167:ARG:O	1.99	0.45
1:A:1152:GLN:OE1	1:A:1190:GLY:HA2	2.17	0.45
1:A:1247:MET:O	1:A:1250:LEU:N	2.46	0.45
1:A:1488:VAL:HG21	1:A:1523:ARG:NH1	2.32	0.45
1:B:1432:SER:O	1:B:1434:PRO:HD3	2.16	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1488:VAL:CG2	1:B:1523:ARG:HG2	2.47	0.45
1:A:1083:ASP:HB3	1:A:1264:GLU:OE1	2.17	0.44
1:A:1466:TYR:CE2	1:A:1513:VAL:HG11	2.52	0.44
1:B:1020:MET:HE2	1:B:1033:VAL:HG11	1.99	0.44
1:B:1047:VAL:O	1:B:1050:ARG:HG3	2.17	0.44
1:B:1174:ASP:OD2	1:B:1176:ALA:HB3	2.17	0.44
1:B:1195:THR:HB	1:B:1196:GLY:H	1.29	0.44
1:B:1221:ARG:O	1:B:1223:SER:N	2.51	0.44
1:B:1382:ASN:HD22	1:B:1382:ASN:HA	1.60	0.44
1:B:1009:GLU:OE1	1:B:1115:GLY:N	2.33	0.44
1:B:1061:LEU:HD22	1:B:1313:PHE:CG	2.52	0.44
1:B:1257:PRO:HA	1:B:1271:HIS:CG	2.52	0.44
1:B:1369:ASN:OD1	1:B:1458:ILE:HA	2.18	0.44
1:B:1375:VAL:O	1:B:1376:PRO:O	2.35	0.44
1:A:1225:ILE:HG23	1:A:1225:ILE:O	2.17	0.44
1:A:1407:ALA:C	1:A:1409:SER:N	2.70	0.44
1:B:1236:VAL:HG12	1:B:1237:THR:N	2.32	0.44
1:B:1325:PRO:C	1:B:1327:ALA:H	2.20	0.44
1:B:1486:PRO:HD2	1:B:1523:ARG:HB3	1.99	0.44
1:A:1132:ASP:O	1:A:1136:VAL:HG23	2.18	0.44
1:A:1341:GLY:HA3	1:A:1355:ALA:O	2.17	0.44
1:A:1372:LYS:HE2	4:A:218:HOH:O	2.17	0.44
1:A:1465:ASN:HB2	1:A:1512:THR:OG1	2.17	0.44
1:A:1544:ALA:HA	1:A:1547:ILE:CG1	2.47	0.44
1:B:1017:LYS:O	1:B:1018:PRO:C	2.55	0.44
1:B:1022:LEU:HD11	1:B:1261:GLN:NE2	2.33	0.44
1:A:1017:LYS:H	1:A:1261:GLN:HE22	1.66	0.44
1:A:1340:HIS:HB3	1:A:1504:GLY:HA2	2.00	0.44
1:A:1530:GLY:C	1:A:1532:ILE:N	2.70	0.44
1:B:1221:ARG:O	1:B:1224:ARG:HG3	2.18	0.44
1:B:1447:ILE:CD1	1:B:1478:GLU:HG3	2.47	0.44
1:A:1033:VAL:HG13	1:A:1041:ALA:HB1	2.00	0.44
1:A:1264:GLU:O	1:A:1265:ASN:HB2	2.18	0.44
1:A:1475:GLN:C	1:A:1477:TYR:N	2.70	0.44
1:B:1265:ASN:N	1:B:1265:ASN:ND2	2.65	0.44
1:B:1439:VAL:HG23	1:B:1441:TYR:O	2.18	0.44
1:B:1466:TYR:CD2	1:B:1513:VAL:CG1	3.00	0.44
1:B:1523:ARG:N	1:B:1523:ARG:CD	2.63	0.44
1:A:1039:TYR:O	1:A:1260:VAL:HG12	2.17	0.44
1:A:1067:PRO:HB3	4:A:18:HOH:O	2.17	0.44
1:A:1143:LEU:O	1:A:1144:ALA:C	2.56	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1043:ILE:CG2	1:B:1047:VAL:HG21	2.48	0.44
1:B:1065:ILE:HB	1:B:1066:THR:H	1.46	0.44
1:B:1069:PRO:HG2	1:B:1339:MET:CE	2.48	0.44
1:B:1155:ASN:ND2	1:B:1158:ASN:HA	2.33	0.44
1:B:1209:LEU:HD13	1:B:1251:MET:CE	2.48	0.44
1:B:1293:LYS:HD2	1:B:1293:LYS:H	1.82	0.44
1:B:1397:GLU:O	1:B:1399:CYS:N	2.50	0.44
1:A:1343:VAL:HG12	1:A:1348:LEU:HD23	2.00	0.44
1:B:1351:GLU:HA	1:B:1391:GLU:OE2	2.18	0.44
1:B:1532:ILE:O	1:B:1534:THR:N	2.48	0.44
1:A:1234:LYS:HA	1:A:1235:PRO:HD3	1.80	0.43
1:A:1556:THR:O	1:A:1556:THR:CG2	2.62	0.43
1:B:1086:ALA:O	1:B:1088:LEU:N	2.51	0.43
1:B:1166:TRP:HB2	1:B:1227:VAL:HA	1.99	0.43
1:B:1225:ILE:HG23	1:B:1225:ILE:O	2.18	0.43
1:B:1249:LEU:O	1:B:1249:LEU:HD12	2.17	0.43
1:B:1511:ILE:HG22	1:B:1528:ILE:HD12	1.99	0.43
1:A:1065:ILE:CD1	1:A:1337:LEU:HD13	2.47	0.43
1:A:1312:LYS:O	1:A:1316:VAL:HB	2.18	0.43
1:B:1168:ARG:HB3	1:B:1197:PHE:CE1	2.53	0.43
1:B:1043:ILE:HG22	1:B:1047:VAL:HG21	2.00	0.43
1:A:1239:GLY:HA2	1:A:1244:GLN:HE22	1.82	0.43
1:B:1326:ASP:O	1:B:1430:LEU:HD13	2.18	0.43
1:B:1465:ASN:HB2	1:B:1512:THR:HG23	2.01	0.43
1:B:1029:GLN:HG3	1:B:1050:ARG:NH1	2.32	0.43
1:B:1032:GLU:OE1	1:B:1050:ARG:NH1	2.52	0.43
1:B:1086:ALA:C	1:B:1088:LEU:N	2.72	0.43
1:A:1093:MET:HG2	1:A:1267:PRO:HB2	2.00	0.43
1:A:1160:ASP:HB3	1:A:1163:THR:HG23	2.00	0.43
1:A:1330:ILE:HG22	1:A:1379:VAL:HA	2.01	0.43
1:B:1016:MET:HB3	1:B:1261:GLN:OE1	2.17	0.43
1:B:1337:LEU:HA	1:B:1340:HIS:CD2	2.54	0.43
1:A:1215:LEU:HB3	1:A:1216:MET:HE3	2.00	0.43
1:A:1168:ARG:HG2	1:A:1197:PHE:CE2	2.54	0.43
1:A:1262:THR:CG2	1:A:1263:LEU:H	2.14	0.43
1:A:1369:ASN:C	1:A:1371:GLY:N	2.70	0.43
1:B:1498:ASP:HB3	1:B:1528:ILE:CG2	2.49	0.43
1:A:1010:ILE:HG13	1:A:1122:MET:HE2	1.99	0.43
1:A:1257:PRO:HD3	1:A:1286:ILE:HD13	1.98	0.43
1:A:1330:ILE:CG2	1:A:1379:VAL:HA	2.49	0.43
1:A:1544:ALA:HA	1:A:1547:ILE:HG12	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1021:GLU:O	1:B:1024:ARG:N	2.51	0.43
1:B:1042:LYS:HZ1	1:B:1254:ALA:HA	1.81	0.43
1:B:1280:HIS:CD2	1:B:1282:CYS:HB2	2.54	0.43
1:B:1314:TYR:HD2	1:B:1437:PHE:HE2	1.67	0.43
1:B:1353:LEU:HB3	1:B:1394:LEU:HD22	2.01	0.43
1:B:1356:LEU:HD13	1:B:1356:LEU:O	2.18	0.43
1:B:1369:ASN:O	1:B:1370:ILE:C	2.56	0.43
1:B:1526:VAL:O	1:B:1526:VAL:CG2	2.66	0.43
1:A:1399:CYS:O	1:A:1401:LYS:N	2.52	0.43
1:A:1525:ILE:HG22	1:A:1527:PRO:HD3	2.01	0.43
1:A:1532:ILE:O	1:A:1532:ILE:HG12	2.17	0.43
1:B:1305:GLY:O	1:B:1307:ASP:N	2.51	0.43
1:A:1159:ILE:O	1:A:1161:PRO:HD3	2.20	0.42
1:B:1047:VAL:HG11	1:B:1294:LEU:HD21	2.00	0.42
1:B:1220:GLU:O	1:B:1221:ARG:C	2.55	0.42
1:B:1408:LEU:O	1:B:1414:LYS:HB2	2.20	0.42
1:A:1149:ASN:ND2	1:A:1153:GLN:HE21	2.16	0.42
1:B:1159:ILE:O	1:B:1161:PRO:HD3	2.19	0.42
1:B:1250:LEU:H	1:B:1250:LEU:HD22	1.84	0.42
1:B:1143:LEU:HD11	1:B:1238:ALA:CB	2.49	0.42
1:B:1499:ASP:O	1:B:1501:THR:N	2.52	0.42
1:B:1506:PRO:HB2	1:B:1509:PHE:CD2	2.55	0.42
1:B:1029:GLN:HG3	1:B:1050:ARG:HH12	1.84	0.42
1:B:1517:ARG:HH22	1:B:1532:ILE:HG13	1.85	0.42
1:B:1555:ILE:O	1:B:1556:THR:HB	2.19	0.42
1:A:1425:LYS:O	1:A:1429:THR:HG23	2.19	0.42
1:B:1193:ARG:HH21	1:B:1195:THR:HG23	1.83	0.42
1:A:1175:ARG:HG2	1:A:1178:ARG:NH2	2.34	0.42
1:A:1257:PRO:HD3	1:A:1286:ILE:HD11	1.99	0.42
1:B:1010:ILE:C	1:B:1012:GLN:N	2.72	0.42
1:B:1229:TYR:CD2	1:B:1235:PRO:HG3	2.55	0.42
1:B:1390:ALA:HA	1:B:1393:ASN:HD22	1.84	0.42
1:B:1230:THR:C	1:B:1232:ASP:H	2.21	0.42
1:B:1477:TYR:CZ	1:B:1518:LEU:HB3	2.54	0.42
1:A:1108:LYS:HE2	1:A:1556:THR:HG23	2.01	0.42
1:A:1177:LEU:HB3	1:A:1197:PHE:HB2	2.01	0.42
1:A:1244:GLN:HE21	1:A:1244:GLN:N	2.13	0.42
1:B:1076:THR:O	1:B:1078:SER:N	2.52	0.42
1:B:1140:HIS:CE1	1:B:1167:ARG:O	2.73	0.42
1:B:1245:GLY:O	1:B:1246:SER:C	2.57	0.42
1:B:1448:LYS:HE2	1:B:1466:TYR:CG	2.55	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1044:SER:C	1:A:1046:ASP:H	2.24	0.42
1:B:1069:PRO:HG2	1:B:1339:MET:HE2	2.01	0.42
1:B:1148:ASP:OD2	1:B:1168:ARG:NH2	2.36	0.42
1:B:1009:GLU:HG2	1:B:1118:GLN:NE2	2.35	0.41
1:B:1012:GLN:HA	1:B:1012:GLN:OE1	2.19	0.41
1:B:1198:ASP:HA	1:B:1534:THR:O	2.20	0.41
1:B:1336:ALA:O	1:B:1340:HIS:HD2	2.03	0.41
1:A:1125:ILE:HD13	1:A:1270:ILE:CD1	2.50	0.41
1:B:1443:LEU:HD11	1:B:1486:PRO:HG3	2.02	0.41
1:A:1022:LEU:HD11	1:A:1261:GLN:HB3	2.01	0.41
1:A:1490:ALA:HB3	1:A:1527:PRO:HA	2.02	0.41
1:B:1376:PRO:O	1:B:1377:ALA:HB2	2.21	0.41
1:A:1133:ILE:HG21	1:A:1171:ASP:OD1	2.20	0.41
1:A:1420:LEU:HA	1:A:1420:LEU:HD13	1.74	0.41
1:A:1555:ILE:O	1:A:1555:ILE:CG2	2.69	0.41
1:B:1450:LYS:O	1:B:1454:ILE:HG13	2.20	0.41
1:A:1239:GLY:HA2	1:A:1244:GLN:NE2	2.35	0.41
1:A:1247:MET:O	1:A:1248:ALA:C	2.58	0.41
1:A:1307:ASP:OD1	1:A:1307:ASP:N	2.53	0.41
1:B:1313:PHE:HE2	1:B:1318:CYS:SG	2.44	0.41
1:A:1073:GLY:HA2	4:A:172:HOH:O	2.19	0.41
1:B:1047:VAL:CG1	1:B:1294:LEU:HD21	2.51	0.41
1:B:1449:ASP:O	1:B:1452:ALA:HB3	2.20	0.41
1:A:1017:LYS:H	1:A:1261:GLN:NE2	2.18	0.41
1:A:1066:THR:HB	1:A:1362:ASN:ND2	2.34	0.41
1:A:1140:HIS:C	1:A:1140:HIS:ND1	2.74	0.41
1:A:1313:PHE:CE1	1:A:1317:LYS:HD3	2.56	0.41
1:A:1422:LEU:O	1:A:1426:VAL:HG23	2.20	0.41
1:B:1265:ASN:N	1:B:1265:ASN:HD22	2.17	0.41
1:B:1269:PHE:HD1	1:B:1269:PHE:HA	1.71	0.41
1:B:1336:ALA:O	1:B:1340:HIS:CD2	2.74	0.41
1:B:1360:PHE:C	1:B:1362:ASN:N	2.74	0.41
1:A:1151:LEU:O	1:A:1152:GLN:C	2.59	0.41
1:A:1343:VAL:HG13	1:A:1344:PRO:HD2	2.02	0.41
1:A:1491:LYS:HB3	1:A:1528:ILE:CG1	2.50	0.41
1:A:1552:ASP:OD1	1:A:1552:ASP:N	2.54	0.41
1:B:1061:LEU:HD22	1:B:1313:PHE:CE1	2.56	0.41
1:B:1369:ASN:CG	1:B:1458:ILE:HA	2.41	0.41
1:A:1170:ILE:CG1	1:A:1171:ASP:N	2.84	0.41
1:A:1175:ARG:C	1:A:1177:LEU:N	2.74	0.41
1:A:1330:ILE:CG2	1:A:1379:VAL:HG22	2.51	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1029:GLN:H	1:B:1050:ARG:HH22	1.68	0.41
1:B:1193:ARG:HA	4:B:25:HOH:O	2.21	0.41
1:B:1412:TRP:CE3	1:B:1413:ALA:HB2	2.54	0.41
1:B:1417:GLU:HA	1:B:1420:LEU:CD2	2.38	0.41
1:B:1461:ALA:CA	1:B:1509:PHE:CE1	3.04	0.41
1:B:1456:THR:HB	1:B:1457:GLU:H	1.64	0.41
1:A:1017:LYS:HD3	1:A:1021:GLU:OE2	2.20	0.40
1:A:1172:LEU:O	1:A:1199:ILE:HD13	2.21	0.40
1:A:1316:VAL:HG12	1:A:1317:LYS:N	2.36	0.40
1:B:1293:LYS:C	1:B:1295:ALA:N	2.74	0.40
1:B:1323:PHE:C	1:B:1324:LYS:HG3	2.41	0.40
1:A:1333:THR:OG1	1:A:1336:ALA:HB3	2.21	0.40
1:B:1319:ARG:CZ	1:B:1443:LEU:HD13	2.51	0.40
1:B:1466:TYR:CD2	1:B:1513:VAL:HG11	2.56	0.40
1:A:1022:LEU:CD1	1:A:1261:GLN:HB3	2.51	0.40
1:A:1064:ALA:HB2	1:A:1331:VAL:HB	2.02	0.40
1:A:1221:ARG:HH11	1:A:1221:ARG:HD2	1.78	0.40
1:A:1354:GLU:OE2	1:A:1354:GLU:HA	2.21	0.40
1:A:1524:LEU:HA	1:A:1524:LEU:HD23	1.87	0.40
1:B:1116:TYR:HA	1:B:1263:LEU:HD12	2.03	0.40
1:A:1022:LEU:HD11	1:A:1261:GLN:OE1	2.21	0.40
1:A:1066:THR:N	1:A:1362:ASN:HD21	2.19	0.40
1:A:1097:ARG:HE	1:A:1097:ARG:HB2	1.61	0.40
1:A:1105:PHE:CD1	1:A:1105:PHE:N	2.89	0.40
1:A:1199:ILE:O	1:A:1200:SER:C	2.60	0.40
1:A:1379:VAL:CG1	1:A:1380:ALA:N	2.84	0.40
1:A:1459:TYR:N	1:A:1459:TYR:CD1	2.87	0.40
1:B:1232:ASP:N	1:B:1232:ASP:OD2	2.55	0.40
1:B:1337:LEU:HD12	1:B:1337:LEU:N	2.36	0.40
1:A:1363:LEU:CD1	1:A:1367:ILE:HD11	2.51	0.40
1:A:1389:GLU:O	1:A:1391:GLU:N	2.54	0.40
1:A:1451:ILE:HG12	1:A:1489:MET:HE1	2.02	0.40
1:B:1237:THR:H	1:B:1240:ASP:HB2	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:ASP:OD1	2:A:278:SO4:O3[3_665]	1.60	0.60

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	547/557 (98%)	437 (80%)	90 (16%)	20 (4%)	2	19
1	B	546/557 (98%)	385 (70%)	107 (20%)	54 (10%)	0	2
All	All	1093/1114 (98%)	822 (75%)	197 (18%)	74 (7%)	1	7

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1015	LYS
1	A	1304	PHE
1	A	1533	MET
1	A	1556	THR
1	B	1056	ASP
1	B	1065	ILE
1	B	1187	LYS
1	B	1294	LEU
1	B	1304	PHE
1	B	1325	PRO
1	B	1330	ILE
1	B	1332	ALA
1	B	1376	PRO
1	B	1456	THR
1	B	1509	PHE
1	A	1200	SER
1	A	1303	GLY
1	A	1401	LYS
1	A	1474	ILE
1	B	1077	THR
1	B	1087	ARG
1	B	1108	LYS
1	B	1134	HIS
1	B	1222	PHE
1	B	1252	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1267	PRO
1	B	1306	ALA
1	B	1317	LYS
1	B	1398	LEU
1	B	1401	LYS
1	B	1403	GLY
1	B	1494	TYR
1	B	1554	VAL
1	A	1072	GLU
1	A	1352	ASN
1	A	1400	ALA
1	B	1067	PRO
1	B	1076	THR
1	B	1156	VAL
1	B	1326	ASP
1	B	1362	ASN
1	B	1399	CYS
1	B	1452	ALA
1	B	1500	MET
1	A	1274	PRO
1	B	1015	LYS
1	B	1026	LEU
1	B	1244	GLN
1	B	1440	LEU
1	B	1492	THR
1	A	1531	ALA
1	B	1112	ALA
1	B	1195	THR
1	B	1221	ARG
1	B	1274	PRO
1	B	1550	ASP
1	B	1551	ALA
1	A	1222	PHE
1	A	1310	ALA
1	A	1381	ILE
1	A	1523	ARG
1	A	1529	THR
1	B	1072	GLU
1	B	1113	GLY
1	B	1215	LEU
1	B	1260	VAL
1	B	1453	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1486	PRO
1	B	1033	VAL
1	A	1554	VAL
1	A	1316	VAL
1	B	1154	GLY
1	B	1161	PRO
1	B	1331	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	432/440 (98%)	401 (93%)	31 (7%)	12	41
1	B	431/440 (98%)	397 (92%)	34 (8%)	10	38
All	All	863/880 (98%)	798 (92%)	65 (8%)	11	40

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1008	ILE
1	A	1016	MET
1	A	1020	MET
1	A	1044	SER
1	A	1062	VAL
1	A	1072	GLU
1	A	1074	LYS
1	A	1094	VAL
1	A	1124	ASP
1	A	1174	ASP
1	A	1215	LEU
1	A	1244	GLN
1	A	1274	PRO
1	A	1277	ASN
1	A	1286	ILE
1	A	1307	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1353	LEU
1	A	1356	LEU
1	A	1381	ILE
1	A	1398	LEU
1	A	1420	LEU
1	A	1438	HIS
1	A	1443	LEU
1	A	1449	ASP
1	A	1487	VAL
1	A	1512	THR
1	A	1513	VAL
1	A	1523	ARG
1	A	1526	VAL
1	A	1546	ASN
1	A	1552	ASP
1	B	1020	MET
1	B	1050	ARG
1	B	1059	LEU
1	B	1065	ILE
1	B	1072	GLU
1	B	1094	VAL
1	B	1124	ASP
1	B	1193	ARG
1	B	1195	THR
1	B	1200	SER
1	B	1215	LEU
1	B	1229	TYR
1	B	1232	ASP
1	B	1244	GLN
1	B	1260	VAL
1	B	1266	THR
1	B	1269	PHE
1	B	1277	ASN
1	B	1280	HIS
1	B	1285	ILE
1	B	1290	THR
1	B	1311	GLU
1	B	1313	PHE
1	B	1330	ILE
1	B	1353	LEU
1	B	1356	LEU
1	B	1382	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1462	ASP
1	B	1499	ASP
1	B	1518	LEU
1	B	1523	ARG
1	B	1529	THR
1	B	1535	MET
1	B	1546	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1029	GLN
1	A	1140	HIS
1	A	1149	ASN
1	A	1150	HIS
1	A	1189	ASN
1	A	1244	GLN
1	A	1261	GLN
1	A	1265	ASN
1	A	1277	ASN
1	A	1283	ASN
1	A	1362	ASN
1	A	1465	ASN
1	B	1029	GLN
1	B	1118	GLN
1	B	1140	HIS
1	B	1150	HIS
1	B	1153	GLN
1	B	1189	ASN
1	B	1244	GLN
1	B	1265	ASN
1	B	1277	ASN
1	B	1369	ASN
1	B	1382	ASN
1	B	1393	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\# Z  > 2$
2	SO4	B	281	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	278	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	274	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	B	279	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	275	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	277	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	276	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	B	272	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	271	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	B	280	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	A	273	-	4,4,4	0.68	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	278	SO4	2	1
2	A	274	SO4	3	0
2	B	279	SO4	1	0
2	A	275	SO4	4	0
2	A	277	SO4	2	0
2	B	272	SO4	1	0
2	B	280	SO4	1	0
2	A	273	SO4	4	0

## 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.