

# Full wwPDB X-ray Structure Validation Report (i)

#### Apr 7, 2022 – 05:00 PM EDT

PDB ID	:	1FP7
Title	:	MONOVALENT CATION BINDING SITES IN N10-FORMYLTETRAHYD
		ROFOLATE SYNTHETASE FROM MOORELLA THERMOACETICA
Authors	:	Radfar, R.; Leaphart, 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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)	:	2.27

## 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 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.



Matria	Whole archive	Similar resolution		
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
Clashscore	141614	1253 (3.20-3.20)		
Ramachandran outliers	138981	1234 (3.20-3.20)		
Sidechain outliers	138945	1233 (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 >=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	А	557	43%	49%	6% ••		
1	В	557	30%	57%	10% ••		

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	А	273	-	-	Х	-
2	SO4	А	274	-	-	Х	-
2	SO4	А	275	-	-	Х	-
2	SO4	А	277	-	-	Х	-



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	А	278	-	-	Х	-



## 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	А	549	Total 4133	C 2617	N 715	O 780	S 21	0	0	0
1	В	548	Total 4125	C 2613	N 714	O 777	S 21	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	?	-	GLU	deletion	UNP P21164
А	?	-	VAL	deletion	UNP P21164
В	?	-	GLU	deletion	UNP P21164
В	?	-	VAL	deletion	UNP P21164

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

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

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

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	199	Total O 199 199	0	0
4	В	71	Total         O           71         71	0	0





## 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.

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Note EDS was not executed.

• Molecule 1: FORMATE--TETRAHYDROFOLATE LIGASE

• Molecule 1: FORMATE--TETRAHYDROFOLATE LIGASE





P1067	T1068	P1069	G1071	E1072	K1074	T1075	1 1070 T1077	<mark>S1078</mark>	V1079	L1081	T1082	D1083	A1084 L1085	A1086	R1087	L1088	K1090	R1091	V1092	M1093 V1094	C1095	L1096	R1097	P1103	S1104	F1105	G1106 11107	K1108	G1109	G1110 A1111	A1112	G1113	G1114 G1115	Y1116	A1117	Q1118 V1110	V1120	P1121		D1124	02111	F1129	D1132	I1133	H1134
A1135	V1136		0±111	L1143		V1147	N1149	H1150	L1151	q1153 Q1153	G1154	N1155	V1156 L1157	N1158	I1159	D1160 P1161		W1166	R1167	R1168 V1169	11170	D1171	L1172	D1173	R1175	A1176	L11// P1178	0/TTV	11182	G1183	G1186	K1187	A1188	R1193	E1194	T1195	F1197	D1198	11199 21222	S1200	81203	E1204	M1206		F1708
C1210	L1211	1 10 1		E1220 B1221	F1222	S1223	11225 III	V1226	V1227	Y1229	T1230	Y1231	01232 G1233	K1234	P1235	V1236 T1237	A1238	G1239	D1240	01244	G1245	<mark>S1246</mark>	M1247	A1248 11249	L1250	M1251	K1252	A1254	11255	K1256 D1257	N1258	L1259	V1260 01261	T1262	L1263	E1264 N1766	T1266	P1267	A1268	F1269	H1271	G1272	61273 P1274	F1275	A1276
N1277	11278	A1279 U1280	G1281	C1282	11285	I1286	A126/ T1288	K1289	T1290	A1291 L1292	K1293	L1294	A1295 D1296	Y1297	V1298	V1299 T1300		G1303	F1304	61305 41306	D1307	L1308	G1309	A1310 E1311	K1312	F1313	Y1314 D1215	V1316	K1317	C1318 R1319	Y1320		F1323 K1324	P1325	D1326	A1327	V1329	I1330	V1331	A1332 T1333	V1334	R1335	A1330 L1337	K1338	622TW
H1340	G1341	G1342	P1344	D1 247	L1348		E1351	L1353	T 1 DE C	L1330 R1357	E1358	G1359	F1360 A1361	N1362	L1363	E1364 K1365	H1366	11367	E1368	N1369 T1370	G1371	K1372	F1373	G1374 V1375	P1376	A1377	V13/8 V1370	413/9 A1380	11381	N1382 A1383	F1384	P1385	T1386 D1387		A1390	E1391	N1393	L1394	L1395	Y1396 F1397	L1398	C1399	A1400 K1401	A1402	G1403
	L1408	S1409	A1413	K1414	E1417		E1421	L1422	V110E	V1426	L1427	Q1428	11429 L1430	E1431	S1432	R1433 P1434	S1435	N1436	F1437	H1438 V1439	L1440	Y1441	N1442	L1443 D1444	L1445	S1446	1144/ V1008	D1449	K1450	11451 A1457	K1453	I1454	A1455 T1456	E1457	I1458	Y1459	A1461	D1462		N1465 V1466		K1472	R1476	Y1477	E1478
	G1483	N1484	P1486	V1487 V1488	M1489	A1490	T1492	Q1493	Y1494	51435 F1496	S1497	D1498	D1499 M1500	T1501	K1502	P1506	R1507	N1508	F1509	T1510 11511	T1512	V1513	R1514	E1515 V1516	R1517	L1518	81519 A1620	AL020	R1523	L1524 T1525	V1526	P1527	I1528 T1529		11532	M1533 T1624	M1535	P1536	1	A1543 A1544	C1545	N1546	1104/ D1548	11549	D1990
A1551	D1552	G1553 V1 66 A	11555	T1556 C1557	TEU	PHE																																							



## 4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants	160.88Å 160.88Å 256.12Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	19.99 - 3.20	Depositor
% Data completeness	87 2 (19 99-3 20)	Depositor
(in resolution range)	01.2 (15.55 5.20)	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 $(Å^2)$	40.0	wwPDB-VP



## 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, K

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).

Mal	Chain	Bond	lengths	Bond angles				
1VIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5			
1	А	0.44	0/4201	0.72	1/5690~(0.0%)			
1	В	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	$Observed(^{o})$	$Ideal(^{o})$
1	А	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 (i)

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	А	4133	0	4219	357	0
1	В	4125	0	4211	448	0
2	А	35	0	0	14	0
2	В	20	0	0	2	0
3	А	2	0	0	1	0
4	А	199	0	0	28	0
4	В	71	0	0	16	0
All	All	8585	0	8430	806	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 48.

All (806) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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: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
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



	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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
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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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
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



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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
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



A + 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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
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



	AL O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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
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



	<b>A t</b> area <b>D</b>	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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
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



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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
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



A + a 1	1 J	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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
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



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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
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



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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
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



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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
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



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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
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



A + a 1	1 J	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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
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



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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
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



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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
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



	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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
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



A + 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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
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



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
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
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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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

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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	547/557~(98%)	437 (80%)	90 (16%)	20~(4%)	3 22
1	В	546/557~(98%)	385 (70%)	107 (20%)	54 (10%)	0 3
All	All	1093/1114 (98%)	822 (75%)	197 (18%)	74 (7%)	1 9

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

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	1015	LYS
1	А	1304	PHE
1	А	1533	MET
1	А	1556	THR
1	В	1056	ASP
1	В	1065	ILE
1	В	1187	LYS
1	В	1294	LEU
1	В	1304	PHE
1	В	1325	PRO
1	В	1330	ILE
1	В	1332	ALA
1	В	1376	PRO
1	В	1456	THR
1	В	1509	PHE
1	А	1200	SER
1	А	1303	GLY
1	А	1401	LYS
1	А	1474	ILE
1	В	1077	THR
1	В	1087	ARG
1	В	1108	LYS
1	В	1134	HIS
1	В	1222	PHE
1	В	1252	LYS
1	В	1267	PRO
1	В	1306	ALA
1	В	1317	LYS
1	В	1398	LEU
1	В	1401	LYS
1	В	1403	GLY
1	В	1494	TYR
1	В	1554	VAL



Mol	Chain	Res	Type
1	А	1072	GLU
1	А	1352	ASN
1	А	1400	ALA
1	В	1067	PRO
1	В	1076	THR
1	В	1156	VAL
1	В	1326	ASP
1	В	1362	ASN
1	В	1399	CYS
1	В	1452	ALA
1	В	1500	MET
1	А	1274	PRO
1	В	1015	LYS
1	В	1026	LEU
1	В	1244	GLN
1	В	1440	LEU
1	В	1492	THR
1	А	1531	ALA
1	В	1112	ALA
1	В	1195	THR
1	В	1221	ARG
1	В	1274	PRO
1	В	1550	ASP
1	В	1551	ALA
1	А	1222	PHE
1	А	1310	ALA
1	А	1381	ILE
1	А	1523	ARG
1	A	1529	THR
1	В	1072	GLU
1	В	1113	GLY
1	В	1215	LEU
1	В	1260	VAL
1	В	1453	LYS
1	В	1486	PRO
1	В	1033	VAL
1	А	1554	VAL
1	А	1316	VAL
1	В	1154	GLY
1	В	1161	PRO
1	В	1331	VAL

Continued from previous page..



#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	432/440~(98%)	401 (93%)	31~(7%)	-	14	47
1	В	431/440 (98%)	397~(92%)	34 (8%)	-	12	43
All	All	863/880~(98%)	798~(92%)	65~(8%)	-	13	45

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

Mol	Chain	Res	Type
1	А	1008	ILE
1	А	1016	MET
1	А	1020	MET
1	А	1044	SER
1	А	1062	VAL
1	А	1072	GLU
1	А	1074	LYS
1	А	1094	VAL
1	А	1124	ASP
1	А	1174	ASP
1	А	1215	LEU
1	А	1244	GLN
1	А	1274	PRO
1	А	1277	ASN
1	А	1286	ILE
1	А	1307	ASP
1	А	1353	LEU
1	А	1356	LEU
1	А	1381	ILE
1	А	1398	LEU
1	А	1420	LEU
1	А	1438	HIS
1	А	1443	LEU
1	А	1449	ASP
1	А	1487	VAL
1	А	1512	THR
1	А	1513	VAL



Mol	Chain	Res	Type
1	А	1523	ARG
1	А	1526	VAL
1	А	1546	ASN
1	А	1552	ASP
1	В	1020	MET
1	В	1050	ARG
1	В	1059	LEU
1	В	1065	ILE
1	В	1072	GLU
1	В	1094	VAL
1	В	1124	ASP
1	В	1193	ARG
1	В	1195	THR
1	В	1200	SER
1	В	1215	LEU
1	В	1229	TYR
1	В	1232	ASP
1	В	1244	GLN
1	В	1260	VAL
1	В	1266	THR
1	В	1269	PHE
1	В	1277	ASN
1	В	1280	HIS
1	В	1285	ILE
1	В	1290	THR
1	В	1311	GLU
1	В	1313	PHE
1	В	1330	ILE
1	В	1353	LEU
1	В	1356	LEU
1	В	1382	ASN
1	В	1462	ASP
1	В	1499	ASP
1	В	1518	LEU
1	В	1523	ARG
1	В	1529	THR
1	В	1535	MET
1	В	1546	ASN

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



$\operatorname{Mol}$	Chain	Res	Type
1	А	1029	GLN
1	А	1140	HIS
1	А	1149	ASN
1	А	1150	HIS
1	А	1189	ASN
1	А	1244	GLN
1	А	1261	GLN
1	А	1265	ASN
1	А	1277	ASN
1	А	1283	ASN
1	А	1362	ASN
1	А	1465	ASN
1	В	1029	GLN
1	В	1118	GLN
1	В	1140	HIS
1	В	1150	HIS
1	В	1153	GLN
1	В	1189	ASN
1	В	1244	GLN
1	В	1265	ASN
1	В	1277	ASN
1	В	1369	ASN
1	В	1382	ASN
1	В	1393	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)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.



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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).

Mal	Turne	Chain	Dec	Tink	Bond lengths			E	Bond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	SO4	А	273	-	4,4,4	0.82	0	6,6,6	0.50	0
2	SO4	В	272	1	4,4,4	0.82	0	$6,\!6,\!6$	0.50	0
2	SO4	В	280	-	4,4,4	0.82	0	6,6,6	0.50	0
2	SO4	А	271	-	4,4,4	0.82	0	6,6,6	0.50	0
2	SO4	А	275	-	4,4,4	0.82	0	$6,\!6,\!6$	0.50	0
2	SO4	В	281	-	4,4,4	0.82	0	6,6,6	0.50	0
2	SO4	А	274	1	4,4,4	0.82	0	$6,\!6,\!6$	0.50	0
2	SO4	А	276	-	4,4,4	0.82	0	6,6,6	0.50	0
2	SO4	А	278	1	4,4,4	0.82	0	6,6,6	0.50	0
2	SO4	А	277	-	4,4,4	0.82	0	6,6,6	0.50	0
2	SO4	В	279	1	4,4,4	0.82	0	6,6,6	0.50	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.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	273	SO4	4	0
2	В	272	SO4	1	0
2	В	280	SO4	1	0
2	А	275	SO4	4	0
2	А	274	SO4	2	0
2	А	278	SO4	2	0
2	А	277	SO4	2	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 (i)

### 6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

#### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

#### 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

#### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

