



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2018 – 10:29 pm GMT

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

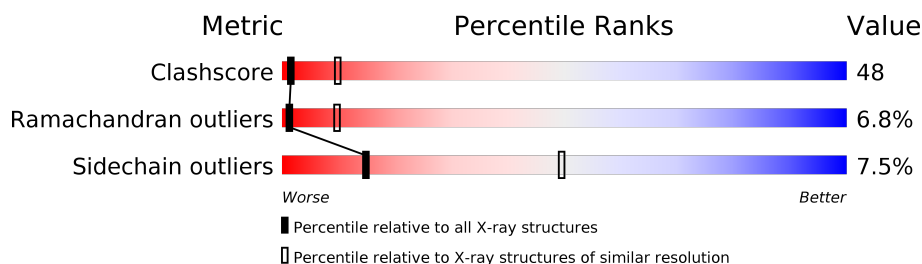
1 Overall quality at a glance

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	122078	1092 (3.20-3.20)
Ramachandran outliers	120005	1075 (3.20-3.20)
Sidechain outliers	119972	1074 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	277	-	-	X	-
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: SO₄) (formula: O₄S).



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.

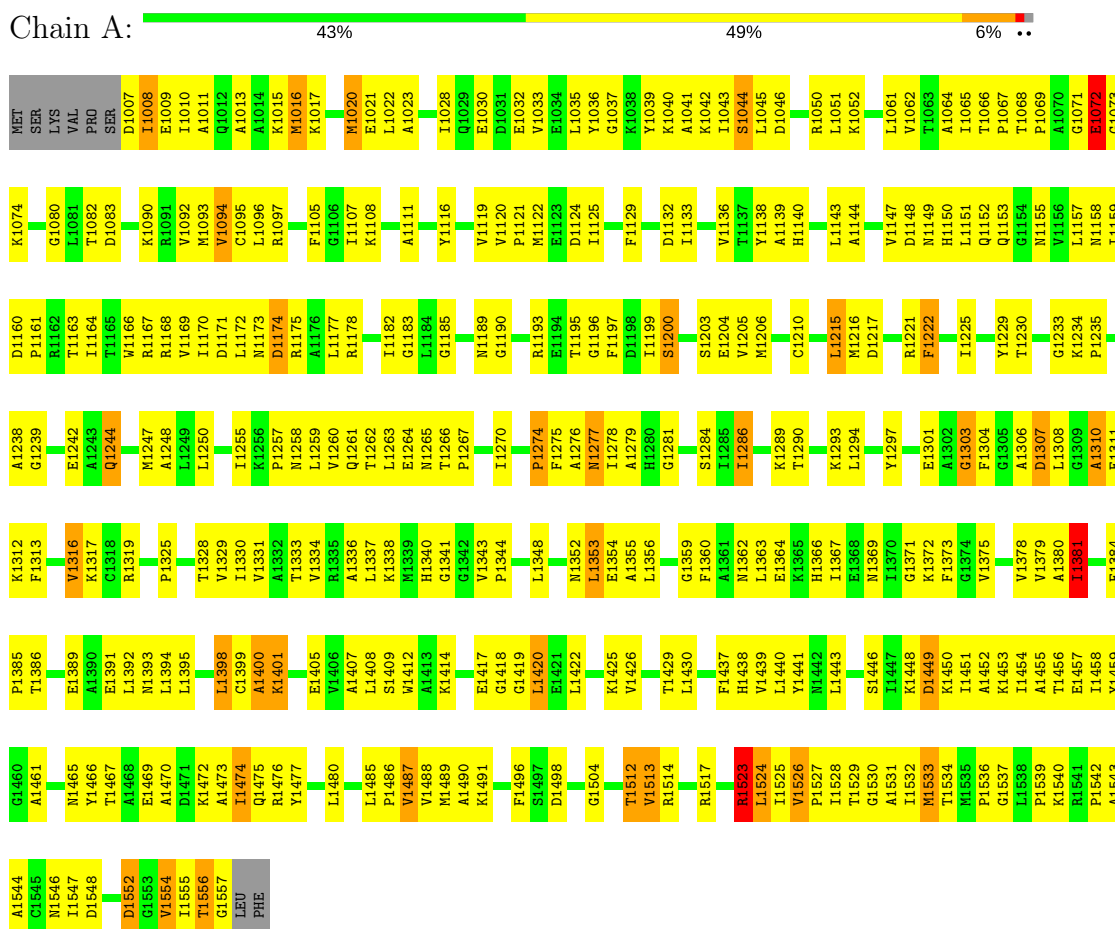
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	199	Total O 199 199	0	0
4	B	71	Total O 71 71	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: FORMATE--TETRAHYDROFOLATE LIGASE



• Molecule 1: FORMATE--TETRAHYDROFOLATE LIGASE



A1551	G1483	L1408	H1340	M1277	G1210	A1135	P1067
D1552	M1484	L1409	G1341	I1278	L1211	V1136	T1068
G1553	L1485	S1409	G1342	A1279	L1215	H1140	P1069
V1554	P1486	W1412	V1343	H1280	G1281	L1143	A1070
T1555	A1487	A1413	P1344	G1282	L1215	A1144	G1071
T1556	V1488	K1414	D1347	L1285	E1220	L1143	S1072
G1557	V1489	E1417	L1346	I1286	R1221	A1144	G1073
LEU	A1490	L1420	E1351	I1287	F1222	V1147	K1074
PHE	K1491	E1421	N1352	A1287	S1223	D1148	T1075
	T1492	L1422	L1353	T1288	I1225	N1149	T1076
	Q1493			K1289	V1226	H1150	T1077
	Y1494			T1290	L1151	V1078	S1078
	S1495			A1291	Q1152	V1079	V1079
	S1496	K1425	L1356	L1292	G1228	Q1152	G1080
	S1497	V1426	R1357	L1293	Y1229	L1160	L1081
	S1498	L1427	E1358	K1293	T1230	G1154	T1082
	D1498	Q1428	G1359	L1294	Y1231	N1155	D1083
	D1499	T1429	F1360	A1295	D1232	V1156	A1084
	M1500	L1430	A1361	D1296	G1233	L1157	L1085
	T1501	E1431	N1362	Y1297	K1234	N1158	A1086
	K1502	S1432	L1363	V1298	P1235	I1159	R1087
		P1433	E1364	V1299	V1236	D1160	L1088
		P1434	K1365	T1300	T1237	P1161	G1089
		S1435	H1366		A1238		K1090
P1506		N1436	I1367	G1303	G1239	W1166	R1091
R1507		F1437	E1368	F1304	D1240	R1167	V1092
M1508		H1438	N1369	G1305		R1168	M1093
F1509		V1439	I1370	A1306	G1244	V1169	V1094
T1510		L1440	G1371	D1307	G1245	I1170	C1095
T1511		Y1441	K1372	L1308	S1246	D1171	L1096
V1512		L1442	F1373	G1309	M1247	L1172	T1097
V1513		L1443	G1374	A1310	A1248	N1173	
R1514		D1444	V1375	E1311	L1249	D1174	P1103
E1515		L1445	A1376	K1312	L1250	R1175	S1104
V1516		S1446	A1377	F1313	M1251	A1176	F1105
R1517		T1447	V1378	Y1314	K1252	L1177	G1106
S1518		K1448	V1379	D1315	D1253	R1178	I1107
S1519		D1449	A1380	V1316	A1254	I1182	K1108
A1520		K1450	I1381	K1317	I1255	G1183	G1109
		T1451	N1382	C1318	K1256	G1110	G1110
R1523		A1452	A1383	R1319	P1257	A1111	A1111
L1524		K1453	F1384	Y1320	N1258	G1186	A1112
I1525		T1454	P1385		L1259	K1187	G1113
V1526		A1455	T1386	F1323	V1260	A1188	G1114
P1527		T1456	D1387	K1324	Q1261		G1115
I1528		E1457		P1325	T1262	R1193	G1116
T1529		I1458	A1390	D1326	L1263	E1194	A1117
		Y1459	E1391	A1327	E1264	T1195	Q1118
		G1460	L1392	T1328	N1265	G1196	V1119
		A1461	N1393	V1329	T1266	F1197	V1120
		D1462	L1394	I1330	P1267	D1198	P1121
			L1395	V1331	A1269	I1199	
			Y1396	A1332	F1269	S1200	D1124
			E1397	T1333	I1270	I1125	I1125
			L1398	V1334	H1271	S1203	F1129
			O1399	R1335	G1272	E1204	
			A1400	A1336	G1273	V1205	
			K1401	L1337	P1274	M1206	D1132
			A1402	K1338	F1275	I1133	I1133
			G1403	M1339	A1276	L1209	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, α , β , γ	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 ²)	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	357	0
1	B	4125	0	4211	448	0
2	A	35	0	0	14	0
2	B	20	0	0	2	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	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 distance (Å)	Clash 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:H	1:A:1353:LEU:HD12	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:HD22	1:B:1277:ASN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:H	1:B:1523:ARG:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:1075:THR:CG2	1:B:1113:GLY:HA2	2.17	0.74
1:B:1017:LYS:HB2	1:B:1261:GLN:HE22	1.51	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:HG22	1:A:1556:THR:O	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:1515:GLU:HG2	1:B:1516:VAL:H	1.54	0.71
1:B:1278:ILE:O	1:B:1525:ILE:HD12	1.90	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:O	1:B:1556:THR:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:1091:ARG:HB3	1:B:1296:ASP:H	1.60	0.67
1:B:1065:ILE:CD1	1:B:1332:ALA:HA	2.25	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:1149:ASN:O	1:B:1152:GLN:HB3	1.95	0.66
1:B:1043:ILE:HD11	1:B:1259:LEU:HD22	1.77	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: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:1092:VAL:HG23	1:A:1297:TYR:O	1.94	0.66
1:A:1512:THR:HG22	1:A:1512:THR:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:1136:VAL:HG13	1:B:1205:VAL:HG12	1.81	0.63
1:B:1083:ASP:HB3	1:B:1264:GLU:CD	2.20	0.63

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:1155:ASN:HD21	1:B:1159:ILE:N	2.01	0.59
1:B:1092:VAL:HG23	1:B:1297:TYR:HB2	1.85	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:H	1:A:1277:ASN:HD22	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: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:1173:ASN:HB3	1:A:1536:PRO:O	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:HA	1:A:1242:GLU:OE1	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: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:1445:LEU:O	1:B:1450:LYS:HE3	2.05	0.56
1:A:1036:TYR:O	1:A:1040:LYS:NZ	2.38	0.56
1:B:1276:ALA:HB3	1:B:1304:PHE:CD2	2.40	0.56
1:A:1384:PHE:CD2	1:A:1385:PRO:HD2	2.41	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:N	1:B:1277:ASN:ND2	2.45	0.56
1:B:1044:SER:OG	2:B:280:SO4:O2	2.20	0.56
1:B:1178:ARG:HD3	1:B:1535:MET:HB3	1.86	0.56
1:A:1473:ALA:O	1:A:1475:GLN:N	2.39	0.56
1:A:1107:ILE:CG2	1:A:1539:PRO:HG2	2.35	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:1169:VAL:HG22	1:B:1200:SER:HA	1.84	0.56
1:B:1058:LYS:CB	1:B:1430:LEU:HD21	2.36	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:1167:ARG:NH2	1:A:1178:ARG:O	2.39	0.56
1:A:1119:VAL:HG13	1:A:1261:GLN:O	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:1211:LEU:HD21	1:B:1280:HIS:CD2	2.41	0.55
1:B:1063:THR:HG22	1:B:1329:VAL:O	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:1391:GLU:O	1:A:1392:LEU:C	2.46	0.53
1:A:1175:ARG:HH11	1:A:1537:GLY:HA3	1.73	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:1517:ARG:HH12	1:B:1532:ILE:CD1	2.23	0.52
1:B:1485:LEU:HD13	1:B:1523:ARG:HA	1.90	0.52
1:A:1523:ARG:C	1:A:1523:ARG:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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: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:B:1043:ILE:O	1:B:1257:PRO:HD2	2.11	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:1517:ARG:HH12	1:B:1532:ILE:HD12	1.75	0.51
1:B:1279:ALA:HA	1:B:1523:ARG:NH2	2.26	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:C	1:B:1313:PHE:CD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:O	1:B:1215:LEU:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:CD1	1:A:1381:ILE:H	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:CG2	1:A:1526:VAL:O	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: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:1061:LEU:O	1:A:1328:THR:HA	2.14	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:C	1:B:1049:ARG:HD3	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:1386:THR:HA	4:A:48:HOH:O	2.14	0.47
1:A:1107:ILE:HG22	1:A:1539:PRO:HG2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:N	1:A:1277:ASN:HD22	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: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:B:1199:ILE:HA	1:B:1535:MET:HE2	1.97	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:HD12	1:B:1278:ILE:N	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:1150:HIS:O	1:B:1153:GLN:N	2.42	0.46
1:B:1136:VAL:HG13	1:B:1205:VAL:O	2.16	0.46
1:B:1451:ILE:CD1	1:B:1526:VAL:HG11	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:1381:ILE:CG2	1:A:1395:LEU:HD23	2.45	0.45
1:A:1523:ARG:HD2	1:A:1523:ARG:N	2.31	0.45
1:A:1498:ASP:HB2	1:A:1528:ILE:HG21	1.96	0.45
1:A:1105:PHE:HB3	1:A:1544:ALA:HB2	1.99	0.45
1:A:1071:GLY:O	1:A:1072:GLU:HG3	2.16	0.45
1:B:1205:VAL:CG1	1:B:1205:VAL:O	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:HB2	1:B:1040:LYS:NZ	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:1257:PRO:HA	1:B:1271:HIS:CG	2.52	0.44
1:B:1061:LEU:HD22	1:B:1313:PHE: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: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:A:1039:TYR:O	1:A:1260:VAL:HG12	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:HD12	1:B:1249:LEU:O	2.17	0.43
1:B:1511:ILE:HG22	1:B:1528:ILE:HD12	1.99	0.43
1:A:1312:LYS:O	1:A:1316:VAL:HB	2.18	0.43
1:A:1065:ILE:CD1	1:A:1337:LEU:HD13	2.47	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:1160:ASP:HB3	1:A:1163:THR:HG23	2.00	0.43
1:A:1093:MET:HG2	1:A:1267:PRO:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1280:HIS:CD2	1:B:1282:CYS:HB2	2.54	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:1353:LEU:HB3	1:B:1394:LEU:HD22	2.01	0.43
1:B:1314:TYR:HD2	1:B:1437:PHE:HE2	1.67	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:1220:GLU:O	1:B:1221:ARG:C	2.55	0.42
1:B:1047:VAL:HG11	1:B:1294:LEU:HD21	2.00	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:HD22	1:B:1250:LEU:H	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:N	1:A:1244:GLN:HE21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:OE1	1:B:1012:GLN:HA	2.19	0.41
1:B:1336:ALA:O	1:B:1340:HIS:HD2	2.03	0.41
1:B:1198:ASP:HA	1:B:1534:THR:O	2.20	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:HD13	1:A:1420:LEU:HA	1.74	0.41
1:A:1555:ILE:CG2	1:A:1555:ILE:O	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:N	1:A:1307:ASP:OD1	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:1066:THR:HB	1:A:1362:ASN:ND2	2.34	0.41
1:A:1140:HIS:ND1	1:A:1140:HIS:C	2.74	0.41
1:A:1017:LYS:H	1:A:1261:GLN:NE2	2.18	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:N	1:A:1552:ASP:OD1	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: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: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:A:1170:ILE:CG1	1:A:1171:ASP:N	2.84	0.41

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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: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:1221:ARG:HD2	1:A:1221:ARG:HH11	1.78	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:1354:GLU:HA	1:A:1354:GLU:OE2	2.21	0.40
1:A:1524:LEU:HD23	1:A:1524:LEU:HA	1.87	0.40
1:B:1116:TYR:HA	1:B:1263:LEU:HD12	2.03	0.40
1:A:1097:ARG:HB2	1:A:1097:ARG:HE	1.61	0.40
1:A:1105:PHE:N	1:A:1105:PHE:CD1	2.89	0.40
1:A:1199:ILE:O	1:A:1200:SER:C	2.60	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:1379:VAL:CG1	1:A:1380:ALA:N	2.84	0.40
1:A:1459:TYR:CD1	1:A:1459:TYR:N	2.87	0.40
1:B:1232:ASP:N	1:B:1232:ASP:OD2	2.55	0.40
1:B:1337:LEU:N	1:B:1337:LEU:HD12	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

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%)	4	25
1	B	546/557 (98%)	385 (70%)	107 (20%)	54 (10%)	0	3
All	All	1093/1114 (98%)	822 (75%)	197 (18%)	74 (7%)	1	10

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
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

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Mol	Chain	Res	Type
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
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%)	16	51
1	B	431/440 (98%)	397 (92%)	34 (8%)	13	46
All	All	863/880 (98%)	798 (92%)	65 (8%)	15	49

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
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

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Mol	Chain	Res	Type
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
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

Some 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 [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 carbohydrates 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	A	271	-	4,4,4	0.73	0	6,6,6	0.50	0
2	SO4	A	273	-	4,4,4	0.74	0	6,6,6	0.51	0
2	SO4	A	274	1	4,4,4	0.74	0	6,6,6	0.51	0
2	SO4	A	275	-	4,4,4	0.74	0	6,6,6	0.50	0
2	SO4	A	276	-	4,4,4	0.73	0	6,6,6	0.50	0
2	SO4	A	277	-	4,4,4	0.74	0	6,6,6	0.50	0
2	SO4	A	278	1	4,4,4	0.74	0	6,6,6	0.50	0
2	SO4	B	272	1	4,4,4	0.74	0	6,6,6	0.51	0
2	SO4	B	279	1	4,4,4	0.74	0	6,6,6	0.50	0
2	SO4	B	280	-	4,4,4	0.74	0	6,6,6	0.51	0
2	SO4	B	281	-	4,4,4	0.74	0	6,6,6	0.50	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	271	-	-	0/0/0/0	0/0/0/0
2	SO4	A	273	-	-	0/0/0/0	0/0/0/0
2	SO4	A	274	1	-	0/0/0/0	0/0/0/0
2	SO4	A	275	-	-	0/0/0/0	0/0/0/0
2	SO4	A	276	-	-	0/0/0/0	0/0/0/0
2	SO4	A	277	-	-	0/0/0/0	0/0/0/0
2	SO4	A	278	1	-	0/0/0/0	0/0/0/0
2	SO4	B	272	1	-	0/0/0/0	0/0/0/0
2	SO4	B	279	1	-	0/0/0/0	0/0/0/0
2	SO4	B	280	-	-	0/0/0/0	0/0/0/0
2	SO4	B	281	-	-	0/0/0/0	0/0/0/0

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	A	273	SO4	4	0
2	A	274	SO4	2	0
2	A	275	SO4	4	0
2	A	277	SO4	2	0
2	A	278	SO4	2	0
2	B	272	SO4	1	0
2	B	280	SO4	1	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.