



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:27 PM GMT

PDB ID : 1FP7  
Title : MONOVALENT CATION BINDING SITES IN N10-FORMYLTETRAHYDROFOLATE SYNTHETASE FROM MOORELLA THERMOACETICA  
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Deposited on : 2000-08-30  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

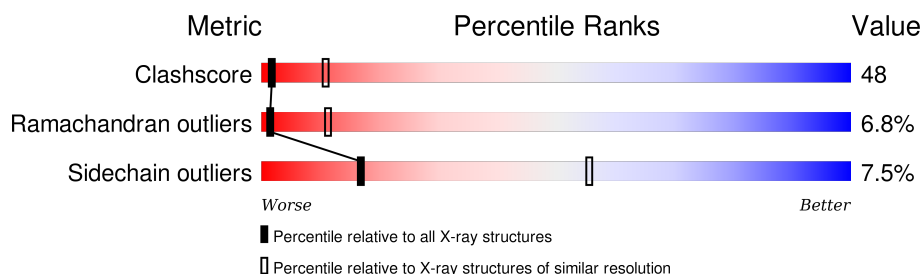
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.


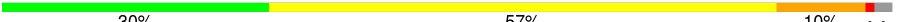
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	 43% 49% 6% ..
1	B	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	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: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

- 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.

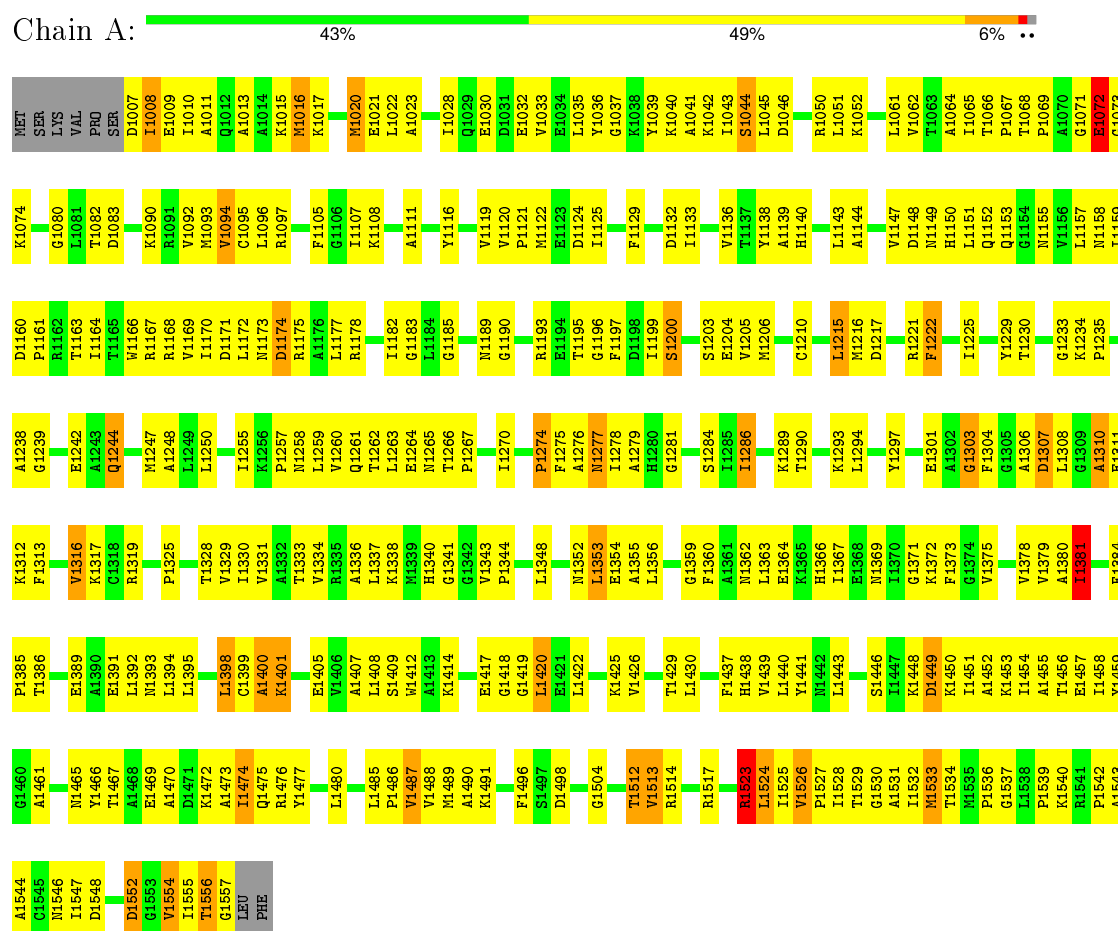
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	199	Total O 199 199	0	0
4	B	71	Total O 71 71	0	0

### 3 Residue-property plots

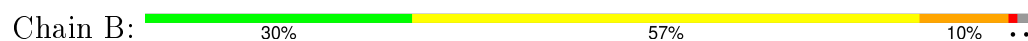
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



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A1551	G1483	L1408	H1340	M1277	C1210	A1135	P1067
D1552	M1484	L1409	G1341	I1278	L1211	V1136	T1068
G1553	L1485	M1412	G1342	A1279	L1215	H1140	P1069
V1554	L1486	A1413	V1343	H1280	G1281	L1143	A1070
T1555	P1486	A1413	P1344	G1282	E1220	A1144	G1071
T1556	V1487	K1414	D1347	L1285	R1221	L1152	E1072
G1557	V1488	E1417	L1346	I1286	F1222	A1154	G1073
LEU	M1489	L1420	E1351	A1287	S1223	V1147	R1074
PHE	A1490	E1421	L1352	T1288	R1224	D1148	T1075
	K1491	L1422	L1353	K1289	R1225	N1149	T1076
	Q1493	K1425	L1356	T1290	V1226	H1150	T1077
	Y1494	V1426	R1357	A1291	G1226	L1151	S1078
	S1495	L1427	E1358	L1292	O1229	Q1152	V1079
	F1496	L1428	G1359	K1293	T1230	G1153	G1080
	D1498	Q1428	F1360	L1294	Y1231	G1154	L1081
	D1499	T1429	F1361	A1295	D1232	N1155	T1082
	M1500	L1430	A1361	D1296	G1233	V1156	D1083
	T1501	E1431	M1362	Y1297	K1234	L1157	A1084
	K1502	S1432	L1363	V1298	P1235	N1158	L1085
		R1433	E1364	V1299	V1236	I1159	A1086
		P1434	K1365	T1300	T1237	D1160	R1087
		S1435	H1366		G1238	L1161	L1088
	P1506	H1367	L1367	G1303	A1239		K1090
	R1507	M1436	E1368	F1304	D1240		R1091
	M1508	F1437	M1369	G1305			V1092
	F1509	H1438	L1370	A1306	Q1244		M1093
	T1510	V1439	I1371	D1307	G1245		V1094
	I1511	L1440	K1372	L1308	S1246		C1095
	T1512	Y1441	K1373	G1309	M1247		L1096
	V1513	N1442	G1374	A1310	A1248		R1097
	V1514	L1443	V1375	E1311	L1249		
	E1515	D1444	P1376	K1312	L1250		P1103
	V1516	L1445	A1377	F1313	M1251		S1104
	V1517	S1446	V1378	Y1314	K1252		F1105
	R1518	I1447	V1379	D1315	D1263		G1106
	S1519	K1448	A1380	V1316	A1254		I1107
	A1520	D1449	L1381	K1317	I1255		K1108
		I1450	M1382	C1318	G1183		G1109
	R1523	A1452	A1383	R1319	P1257		G1110
	L1524	K1453	F1384	Y1320	G1186		A1111
	I1525	I1454	P1385		K1187		A1112
	V1526	A1455	T1386	F1323	A1188		G1113
	P1527	T1456	D1387	K1324	Q1261		G1114
	I1528	E1457		P1325	T1262		G1115
	T1529	I1458	A1390	D1326	L1263		Y1116
		Y1459	E1391	A1327	L1264		A1117
		G1460	L1392	T1328	N1265		Q1118
	T1534	A1461	N1393	V1329	T1266		V1119
	M1535	D1462	L1394	I1330	P1267		V1120
	P1536		L1395	V1331	A1268		P1121
			Y1396	A1332	F1269		
	A1543	M1465	E1397	T1333	I1270		D1124
	A1544	Y1466	L1398	V1334	H1271		I1125
	C1545	K1472	C1399	R1335	G1272		F1129
	N1546		A1400	A1336	G1273		
	I1547		K1401	L1337	P1274		D1132
	D1548		A1402	K1338	F1275		I1133
	I1549		G1403	M1339	L1276		H1134
	D1550						

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.88Å 160.88Å 256.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 3.20	Depositor
% Data completeness (in resolution range)	87.2 (19.99-3.20)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.285 , 0.355	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8585	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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 [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	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:1557:GLY:O	4:A:19:HOH:O	1.75	1.02
1:A:1353:LEU:H	1:A:1353:LEU:HD12	1.25	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:1405:GLU:CD	1:A:1422:LEU:HA	1.86	0.96
1:A:1262:THR:HG22	1:A:1263:LEU:H	1.31	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:B:1372:LYS:HZ3	1:B:1457:GLU:HG2	1.36	0.89
1:A:1301:GLU:OE1	4:A:197:HOH:O	1.91	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: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:1526:VAL:HG22	1:A:1526:VAL:O	1.90	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: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:1337:LEU:O	1:A:1359:GLY:HA3	1.92	0.70
1:A:1319:ARG:NH2	1:A:1441:TYR:O	2.24	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:B:1557:GLY:HA2	4:B:65:HOH:O	1.81	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:LYS:HE2	1:A:1258:ASN:OD1	1.92	0.69
1:B:1324:LYS:HG2	1:B:1437:PHE:HB3	1.75	0.69
1:A:1023:ALA:HB1	1:A:1028:ILE:HB	1.74	0.69
1:B:1042:LYS:NZ	1:B:1254:ALA:HA	2.08	0.69
1:B:1065:ILE:HG23	1:B:1332:ALA:HB2	1.75	0.69
1:A:1543:ALA:O	1:A:1547:ILE:HG12	1.91	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:1182:ILE:CG2	1:A:1183:GLY:N	2.56	0.68
1:A:1035:LEU:HD22	1:A:1037:GLY:O	1.92	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:HB3	1:B:1264:GLU:OE1	1.95	0.67
1:B:1083:ASP:O	1:B:1087:ARG:HB2	1.95	0.67
1:B:1489:MET:HE1	1:B:1526:VAL:HG21	1.76	0.67
1:B:1417:GLU:O	1:B:1420:LEU:HB2	1.96	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:1149:ASN:O	1:B:1152:GLN:HB3	1.95	0.66
1:A:1116:TYR:CZ	2:A:278:SO4:O1	2.48	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:1204:GLU:OE2	4:A:116:HOH:O	2.13	0.66
1:A:1512:THR:HG22	1:A:1512:THR: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: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:B:1383:ALA:HB3	1:B:1408:LEU:HG	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1210:CYS:HA	1:A:1284:SER:HA	1.76	0.66
1:B:1351:GLU:HG3	1:B:1391:GLU:HG3	1.78	0.66
1:B: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:1344:PRO:HD2	1:B:1347:ASP:HB2	1.79	0.65
1:B:1086:ALA:HB2	1:B:1092:VAL:CG1	2.26	0.65
1:B:1363:LEU:O	1:B:1367:ILE:HG12	1.96	0.65
1:A:1473:ALA:C	1:A:1475:GLN:H	1.99	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:B:1557:GLY:HA3	4:B:65:HOH:O	1.82	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:1319:ARG:NE	1:B:1443:LEU:HD13	2.12	0.64
1:A:1540:LYS:O	1:A:1542:PRO:HD3	1.98	0.64
1:B:1125:ILE:HA	1:B:1129:PHE:CD1	2.32	0.64
1:A:1257:PRO:HD3	1:A:1286:ILE:CD1	2.28	0.64
1:B:1526:VAL:HG23	1:B:1526:VAL:O	1.98	0.64
1:A:1090:LYS:HD2	1:A:1297:TYR:HE2	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:1066:THR:HB	1:A:1362:ASN:HD21	1.62	0.64
1:B:1442:ASN:O	1:B:1450:LYS:HE2	1.98	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: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:B:1143:LEU:HD23	1:B:1166:TRP:CE2	2.33	0.63
1:A:1111:ALA:HB2	1:A:1122:MET:SD	2.38	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

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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:B:1090:LYS:HB3	1:B:1297:TYR:HE2	1.64	0.62
1:A:1286:ILE:HG23	4:A:70:HOH:O	1.99	0.62
1:B:1339:MET:HA	1:B:1343:VAL:O	1.99	0.62
1:B:1059:LEU:HD12	1:B:1060:ILE:H	1.62	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:B:1070:ALA:HB2	1:B:1339:MET:SD	2.41	0.61
1:A:1389:GLU:C	1:A:1391:GLU:H	2.04	0.61
1:B:1017:LYS:HG3	1:B:1265:ASN:OD1	2.00	0.60
1:A:1470:ALA:O	1:A:1474:ILE:HG13	2.01	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:1275:PHE:HB3	1:B:1277:ASN:ND2	2.16	0.60
1:B:1043:ILE:HD12	1:B:1269:PHE:HE1	1.66	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:1379:VAL:HG12	1:A:1381:ILE:HD13	1.84	0.60
1:A:1259:LEU:O	1:A:1260:VAL:HG13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:1193:ARG:NH2	1:B:1195:THR:HG23	2.17	0.59
1:A:1090:LYS:HD2	1:A:1297:TYR:CE2	2.37	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:B:1550:ASP:C	1:B:1552:ASP:H	2.06	0.59
1:B:1124:ASP:O	1:B:1129:PHE:HA	2.02	0.59
1:A:1381:ILE:HD13	1:A:1381:ILE:N	2.17	0.59
1:A:1306:ALA:HB3	1:A:1366:HIS:ND1	2.17	0.59
1:B:1451:ILE:HG12	1:B:1487:VAL:HG11	1.83	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: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:1277:ASN:O	1:A:1490:ALA:HB2	2.03	0.59
1:A:1008:ILE:HG12	1:A:1011:ALA:CB	2.33	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:1488:VAL:HA	4:A:14:HOH:O	2.04	0.58
1:A:1230:THR:HG23	1:A:1234:LYS: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:1408:LEU:HD13	1:A:1414:LYS:CE	2.34	0.57
1:A:1334:VAL:HG12	1:A:1338:LYS:HE2	1.86	0.57
1:A:1173:ASN:HB3	1:A:1536:PRO:O	2.04	0.57
1:B:1063:THR:HG23	1:B:1064:ALA:N	2.19	0.57
1:A:1311:GLU:HG3	1:A:1312:LYS:N	2.17	0.57
1:B:1072:GLU:CD	1:B:1073:GLY:H	2.07	0.57
1:B:1515:GLU:HG2	1:B:1516:VAL:N	2.19	0.57
1:A:1367:ILE:HG22	1:A:1401:LYS:HE3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1079:VAL:CB	1:B:1117:ALA:HB1	2.22	0.57
1:A:1170:ILE:HD12	1:A:1171:ASP:H	1.68	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: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:A:1408:LEU:HD13	1:A:1414:LYS:HE3	1.87	0.57
1:A:1242:GLU:HA	1:A:1242:GLU:OE1	2.05	0.57
1:B:1549:ILE:O	1:B:1549:ILE:HG23	2.03	0.57
1:B:1343:VAL:HG13	1:B:1347:ASP:O	2.05	0.56
1:B:1029:GLN:HB3	1:B:1031:ASP:OD2	2.05	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:B:1081:LEU:O	1:B:1085:LEU:HB2	2.04	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:1445:LEU:O	1:B:1450:LYS:HE3	2.05	0.56
1:B:1276:ALA:HB3	1:B:1304:PHE:CD2	2.40	0.56
1:B:1206:MET:O	1:B:1209:LEU:HB3	2.05	0.56
1:A:1036:TYR:O	1:A:1040:LYS:NZ	2.38	0.56
1:B:1277:ASN:N	1:B:1277:ASN:ND2	2.45	0.56
1:B:1066:THR:OG1	1:B:1366:HIS:NE2	2.32	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:1095:CYS:SG	1:B:1288:THR:HA	2.46	0.56
1:B:1054:LYS:HB3	1:B:1055:PRO:HD2	1.86	0.56
1:B:1178:ARG:HD3	1:B:1535:MET:HB3	1.86	0.56
1:B:1169:VAL:HG22	1:B:1200:SER:HA	1.84	0.56
1:B:1017:LYS:N	1:B:1261:GLN:OE1	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:1058:LYS:CB	1:B:1430:LEU:HD21	2.36	0.56
1:B:1042:LYS:HD3	1:B:1256:LYS:HB2	1.88	0.56
1:A:1473:ALA:O	1:A:1475:GLN:N	2.39	0.56
1:B:1454:ILE:HG22	1:B:1459:TYR:HE2	1.70	0.56
1:A:1140:HIS:CD2	1:A:1203:SER:OG	2.54	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:1499:ASP:C	1:B:1501:THR:H	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1334:VAL:HB	1:B:1387:ASP:OD1	2.06	0.56
1:B:1009:GLU:HG2	1:B:1118:GLN:HE22	1.71	0.56
1:B:1075:THR:O	1:B:1078:SER:N	2.29	0.55
1:A:1525:ILE:HG22	1:A:1526:VAL:N	2.21	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: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:1150:HIS:HE1	1:A:1157:LEU:H	1.54	0.55
1:B:1331:VAL:HG12	1:B:1332:ALA:N	2.15	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:1477:TYR:CE2	1:B:1516:VAL:HG12	2.33	0.55
1:A:1381:ILE:HG21	1:A:1395:LEU:HD23	1.87	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:B:1076:THR:HG23	1:B:1114:GLY:O	2.07	0.54
1:A:1166:TRP:CZ3	1:A:1225:ILE:CD1	2.86	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:1376:PRO:CD	1:B:1435:SER:HB3	2.30	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:1090:LYS:HB3	1:B:1297:TYR:CE2	2.43	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:A:1286:ILE:HA	1:A:1289:LYS:HG2	1.90	0.54
1:A:1043:ILE:HD11	1:A:1259:LEU:HB2	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:B:1119:VAL:HG13	1:B:1261:GLN:O	2.07	0.53
1:A:1343:VAL:HG12	1:A:1344:PRO:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1489:MET:CE	1:A:1526:VAL:HG11	2.39	0.53
1:A:1453:LYS:O	1:A:1457:GLU:HB2	2.08	0.53
1:B:1182:ILE:HG13	1:B:1183:GLY:N	2.24	0.53
1:B:1193:ARG:NH2	1:B:1195:THR:CG2	2.71	0.53
1:A:1525:ILE:C	1:A:1526:VAL:HG12	2.27	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:B:1516:VAL:HG22	1:B:1526:VAL:HG12	1.91	0.53
1:A:1042:LYS:NZ	1:A:1132:ASP:OD2	2.38	0.53
1:A:1512:THR:HG22	1:A:1514:ARG:HE	1.74	0.53
1:A:1155:ASN:OD1	1:A:1158:ASN:HA	2.09	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:B:1225:ILE:HA	1:B:1520:ALA:HB3	1.89	0.53
1:A:1391:GLU:O	1:A:1392:LEU:C	2.46	0.53
1:B:1408:LEU:HD13	1:B:1414:LYS:CE	2.39	0.52
1:A:1175:ARG:HA	1:A:1178:ARG:HG3	1.91	0.52
1:A:1023:ALA:CB	1:A:1028:ILE:HD12	2.40	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:1384:PHE:CG	1:B:1385:PRO:HD2	2.44	0.52
1:B:1093:MET:HG2	1:B:1267:PRO:HB2	1.91	0.52
1:A:1065:ILE:HB	1:A:1362:ASN:HD22	1.75	0.52
1:B:1557:GLY:C	4:B:65:HOH:O	2.37	0.52
1:A:1488:VAL:HG23	1:A:1523:ARG:HD3	1.90	0.52
1:A:1009:GLU:HG3	4:A:151:HOH:O	2.09	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:B:1335:ARG:HD3	1:B:1348:LEU:CB	2.23	0.52
1:A:1523:ARG:C	1:A:1523:ARG:HD2	2.28	0.52
1:B:1204:GLU:C	1:B:1206:MET:H	2.11	0.52
1:A:1533:MET:HB2	2:A:273:SO4:O2	2.09	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: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:A:1379:VAL:HG12	1:A:1380:ALA:N	2.24	0.51
1:A:1373:PHE:CE2	1:A:1440:LEU:HB2	2.44	0.51
1:B:1448:LYS:HE2	1:B:1466:TYR:CD2	2.45	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:1178:ARG:O	1:B:1196:GLY:HA3	2.10	0.51
1:B:1081:LEU:O	1:B:1081:LEU:HG	2.10	0.51
1:B:1043:ILE:O	1:B:1257:PRO:HD2	2.11	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:1487:VAL:HG12	1:B:1489:MET:HE2	1.93	0.51
1:B:1087:ARG:O	1:B:1088:LEU:HD23	2.10	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:1036:TYR:O	1:A:1040:LYS:HB2	2.11	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:B:1279:ALA:HA	1:B:1523:ARG:NH2	2.26	0.51
1:A:1125:ILE:HG12	1:A:1129:PHE:CD1	2.43	0.51
1:B:1517:ARG:HH12	1:B:1532:ILE:HD12	1.75	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:A:1446:SER:HB3	1:A:1449:ASP:HB2	1.93	0.51
1:B:1489:MET:CE	1:B:1526:VAL:HG21	2.41	0.51
1:B:1331:VAL:O	1:B:1332:ALA:HB2	2.10	0.51
1:B:1042:LYS:NZ	1:B:1132:ASP:OD2	2.39	0.50
1:A:1329:VAL:HA	1:A:1378:VAL:O	2.10	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:A:1473:ALA:C	1:A:1475:GLN:N	2.64	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: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:1008:ILE:HG13	1:B:1011:ALA:CB	2.41	0.50
1:B:1487:VAL:HG22	1:B:1524:LEU:HD12	1.94	0.50
1:B:1338:LYS:C	1:B:1343:VAL:HB	2.32	0.50
1:A:1277:ASN:ND2	1:A:1277:ASN:H	2.10	0.50
1:A:1136:VAL:HG13	1:A:1205:VAL:CG1	2.41	0.50
1:B:1351:GLU:OE1	1:B:1390:ALA:HB3	2.12	0.50
1:B:1221:ARG:O	1:B:1224:ARG:N	2.37	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:1556:THR:O	1:B:1556:THR:CG2	2.58	0.49
1:A:1171:ASP:HA	1:A:1199:ILE:CD1	2.42	0.49
1:B:1229:TYR:N	1:B:1229:TYR:CD1	2.80	0.49
1:B:1261:GLN:HB2	1:B:1265:ASN:HA	1.94	0.49
1:A:1419:GLY:HA2	4:A:210:HOH:O	2.12	0.49
1:A:1472:LYS:O	1:A:1476:ARG:HG3	2.12	0.49
1:B:1447:ILE:HD12	1:B:1478:GLU:HG3	1.93	0.49
1:B:1446:SER:HB3	1:B:1449:ASP:OD2	2.12	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: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:B:1057:GLY:HA3	1:B:1296:ASP:O	2.12	0.49
1:A:1512:THR:O	1:A:1512:THR:CG2	2.59	0.49
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: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:1493:GLN:N	1:B:1493:GLN:OE1	2.46	0.48
1:B:1215:LEU:O	1:B:1215:LEU:HD22	2.13	0.48
1:B:1143:LEU:HD23	1:B:1166:TRP:NE1	2.28	0.48
1:B:1338:LYS:O	1:B:1341:GLY:N	2.45	0.48
1:B:1155:ASN:ND2	1:B:1159:ILE:N	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1550:ASP:C	1:B:1552:ASP:N	2.66	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:A:1344:PRO:O	1:A:1348:LEU:HG	2.13	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:1526:VAL:CG2	1:A:1526:VAL:O	2.61	0.48
1:A:1090:LYS:HB3	1:A:1297:TYR:CD2	2.48	0.48
1:B:1393:ASN:O	1:B:1396:TYR:HB2	2.13	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:1185:GLY:CA	1:A:1189:ASN:HD22	2.18	0.48
1:A:1542:PRO:C	1:A:1544:ALA:N	2.66	0.48
1:A:1290:THR:O	1:A:1294:LEU:HG	2.13	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:1443:LEU:HG	1:B:1484:ASN:O	2.14	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:1111:ALA:C	1:B:1113:GLY:H	2.17	0.48
1:B:1319:ARG:HG3	1:B:1439:VAL:HG11	1.96	0.48
1:A:1195:THR:HG22	1:A:1196:GLY:H	1.77	0.48
1:B:1292:LEU:HD23	1:B:1298:VAL:CG2	2.43	0.48
1:B:1019:VAL:HG23	1:B:1039:TYR:HA	1.95	0.48
1:B:1010:ILE:C	1:B:1012:GLN:H	2.17	0.48
1:B:1049:ARG:C	1:B:1049:ARG:HD3	2.33	0.47
1:A:1366:HIS:NE2	1:A:1496:PHE:CZ	2.82	0.47
1:A:1136:VAL:HG21	1:A:1206:MET:CE	2.44	0.47
1:A:1554:VAL:CG1	1:A:1555:ILE:N	2.77	0.47
1:B:1133:ILE:O	1:B:1136:VAL:N	2.46	0.47
1:A:1116:TYR:CE2	2:A:278:SO4:O1	2.67	0.47
1:A:1061:LEU:O	1:A:1328:THR:HA	2.14	0.47
1:A:1286:ILE:HD12	1:A:1286:ILE:C	2.34	0.47
1:B:1461:ALA:HA	1:B:1509:PHE:CE1	2.49	0.47
1:B:1374:GLY:HA3	1:B:1438:HIS:HE1	1.78	0.47
1:B:1313:PHE:CE2	1:B:1318:CYS:SG	3.07	0.47
1:A:1360:PHE:CE2	1:A:1364:GLU:HB2	2.49	0.47
1:A:1353:LEU:HD12	1:A:1353:LEU:N	2.09	0.47
1:B:1143:LEU:O	1:B:1147:VAL:HG23	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:A:1386:THR:HA	4:A:48:HOH:O	2.14	0.47
1:B:1343:VAL:HG11	1:B:1348:LEU:HD23	1.96	0.47
1:A:1555:ILE:O	1:A:1556:THR:CB	2.63	0.47
1:A:1542:PRO:C	1:A:1544:ALA:H	2.16	0.47
1:B:1155:ASN:OD1	1:B:1159:ILE:HB	2.14	0.47
1:B:1244:GLN:HG2	1:B:1245:GLY:H	1.79	0.47
1:A:1277:ASN:N	1:A:1277:ASN:HD22	2.08	0.47
1:A:1474:ILE:O	1:A:1474:ILE:CG2	2.61	0.47
1:A:1400:ALA:O	1:A:1401:LYS:HB2	2.15	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: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:O	1:B:1009:GLU:HG2	2.14	0.47
1:B:1507:ARG:O	1:B:1508:ASN:HB2	2.14	0.47
1:B:1550:ASP:OD1	1:B:1551:ALA:N	2.47	0.47
1:B:1061:LEU:HD22	1:B:1313:PHE:CD1	2.50	0.47
1:A:1457:GLU:OE2	4:A:218:HOH:O	2.20	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: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:A:1160:ASP:HB3	1:A:1163:THR:CG2	2.45	0.46
1:B:1278:ILE:HD12	1:B:1278:ILE:N	2.31	0.46
1:A:1532:ILE:O	1:A:1534:THR:HG23	2.15	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:B:1338:LYS:HB3	1:B:1343:VAL:HG21	1.97	0.46
1:B:1277:ASN:HD22	1:B:1277:ASN:N	1.85	0.46
1:A:1555:ILE:O	1:A:1556:THR:HB	2.16	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:B:1451:ILE:CD1	1:B:1526:VAL:HG11	2.36	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:A:1448:LYS:HG2	1:A:1466:TYR:CZ	2.51	0.46
1:A:1138:TYR:O	1:A:1139:ALA:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:1450:LYS:HB2	1:A:1487:VAL:HG21	1.97	0.45
1:A:1276:ALA:HB2	1:A:1281:GLY:HA3	1.98	0.45
1:B:1276:ALA:HB3	1:B:1304:PHE:CE2	2.51	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: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:1523:ARG:N	1:A:1523:ARG:HD2	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:1381:ILE:CG2	1:A:1395:LEU:HD23	2.45	0.45
1:B:1488:VAL:HG23	1:B:1523:ARG:HG2	1.97	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:1026:LEU:HD21	1:B:1294:LEU:HB3	1.97	0.45
1:A:1408:LEU:HD13	1:A:1414:LYS:NZ	2.32	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:B:1320:TYR:CZ	4:B:228:HOH:O	2.55	0.45
1:A:1016:MET:HB3	1:A:1261:GLN:NE2	2.31	0.45
1:B:1329:VAL:CG1	1:B:1330:ILE:H	2.18	0.45
1:B:1040:LYS:NZ	1:B:1040:LYS:HB2	2.31	0.45
1:A:1170:ILE:CD1	1:A:1171:ASP:H	2.29	0.45
1:A:1170:ILE:HG13	1:A:1171:ASP:N	2.32	0.45
1:A:1052:LYS:HE3	4:A:227:HOH:O	2.15	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:1488:VAL:HG21	1:A:1523:ARG:NH1	2.32	0.45
1:B:1488:VAL:CG2	1:B:1523:ARG:HG2	2.47	0.45
1:A:1152:GLN:OE1	1:A:1190:GLY:HA2	2.17	0.45
1:B:1432:SER:O	1:B:1434:PRO:HD3	2.16	0.45
1:A:1247:MET:O	1:A:1250:LEU:N	2.46	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: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:A:1466:TYR:CE2	1:A:1513:VAL:HG11	2.52	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:1174:ASP:OD2	1:B:1176:ALA:HB3	2.17	0.44
1:B:1382:ASN:HD22	1:B:1382:ASN:HA	1.60	0.44
1:B:1375:VAL:O	1:B:1376:PRO:O	2.35	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:1009:GLU:OE1	1:B:1115:GLY:N	2.33	0.44
1:A:1225:ILE:HG23	1:A:1225:ILE:O	2.17	0.44
1:B:1486:PRO:HD2	1:B:1523:ARG:HB3	1.99	0.44
1:A:1407:ALA:C	1:A:1409:SER:N	2.70	0.44
1:B:1325:PRO:C	1:B:1327:ALA:H	2.20	0.44
1:B:1236:VAL:HG12	1:B:1237:THR:N	2.32	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:1132:ASP:O	1:A:1136:VAL:HG23	2.18	0.44
1:A:1544:ALA:HA	1:A:1547:ILE:CG1	2.47	0.44
1:A:1465:ASN:HB2	1:A:1512:THR:OG1	2.17	0.44
1:A:1372:LYS:HE2	4:A:218:HOH:O	2.17	0.44
1:A:1341:GLY:HA3	1:A:1355:ALA:O	2.17	0.44
1:B:1221:ARG:O	1:B:1224:ARG:HG3	2.18	0.44
1:A:1017:LYS:H	1:A:1261:GLN:HE22	1.66	0.44
1:B:1447:ILE:CD1	1:B:1478:GLU:HG3	2.47	0.44
1:A:1530:GLY:C	1:A:1532:ILE:N	2.70	0.44
1:A:1340:HIS:HB3	1:A:1504:GLY:HA2	2.00	0.44
1:A:1264:GLU:O	1:A:1265:ASN:HB2	2.18	0.44
1:B:1439:VAL:HG23	1:B:1441:TYR:O	2.18	0.44
1:B:1523:ARG:N	1:B:1523:ARG:CD	2.63	0.44
1:B:1265:ASN:N	1:B:1265:ASN:ND2	2.65	0.44
1:A:1475:GLN:C	1:A:1477:TYR:N	2.70	0.44
1:B:1466:TYR:CD2	1:B:1513:VAL:CG1	3.00	0.44
1:A:1033:VAL:HG13	1:A:1041:ALA:HB1	2.00	0.44
1:B:1069:PRO:HG2	1:B:1339:MET:CE	2.48	0.44
1:B:1065:ILE:HB	1:B:1066:THR:H	1.46	0.44
1:B:1043:ILE:CG2	1:B:1047:VAL:HG21	2.48	0.44
1:B:1293:LYS:H	1:B:1293:LYS:HD2	1.82	0.44
1:B:1209:LEU:HD13	1:B:1251:MET:CE	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:TYR:O	1:A:1260:VAL:HG12	2.17	0.44
1:B:1155:ASN:ND2	1:B:1158:ASN:HA	2.33	0.44
1:B:1397:GLU:O	1:B:1399:CYS:N	2.50	0.44
1:A:1143:LEU:O	1:A:1144:ALA:C	2.56	0.44
1:A:1067:PRO:HB3	4:A:18:HOH:O	2.17	0.44
1:B:1532:ILE:O	1:B:1534:THR:N	2.48	0.44
1:B:1351:GLU:HA	1:B:1391:GLU:OE2	2.18	0.44
1:A:1343:VAL:HG12	1:A:1348:LEU:HD23	2.00	0.44
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:1086:ALA:O	1:B:1088:LEU:N	2.51	0.43
1:A:1556:THR:O	1:A:1556:THR:CG2	2.62	0.43
1:A:1234:LYS:HA	1:A:1235:PRO:HD3	1.80	0.43
1:B:1511:ILE:HG22	1:B:1528:ILE:HD12	1.99	0.43
1:B:1249:LEU:O	1:B:1249:LEU:HD12	2.17	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:1086:ALA:C	1:B:1088:LEU:N	2.72	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:1337:LEU:HA	1:B:1340:HIS:CD2	2.54	0.43
1:B:1016:MET:HB3	1:B:1261:GLN:OE1	2.17	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:A:1160:ASP:HB3	1:A:1163:THR:HG23	2.00	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:B:1498:ASP:HB3	1:B:1528:ILE:CG2	2.49	0.43
1:A:1369:ASN:C	1:A:1371:GLY:N	2.70	0.43
1:B:1526:VAL:O	1:B:1526:VAL:CG2	2.66	0.43
1:B:1314:TYR:HD2	1:B:1437:PHE:HE2	1.67	0.43
1:B:1042:LYS:HZ1	1:B:1254:ALA:HA	1.81	0.43
1:A:1544:ALA:HA	1:A:1547:ILE:HG12	2.01	0.43
1:B:1353:LEU:HB3	1:B:1394:LEU:HD22	2.01	0.43
1:A:1257:PRO:HD3	1:A:1286:ILE:HD13	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1010:ILE:HG13	1:A:1122:MET:HE2	1.99	0.43
1:A:1330:ILE:CG2	1:A:1379:VAL:HA	2.49	0.43
1:B:1021:GLU:O	1:B:1024:ARG:N	2.51	0.43
1:B:1369:ASN:O	1:B:1370:ILE:C	2.56	0.43
1:B:1280:HIS:CD2	1:B:1282:CYS:HB2	2.54	0.43
1:B:1356:LEU:O	1:B:1356:LEU:HD13	2.18	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:A:1399:CYS:O	1:A:1401:LYS:N	2.52	0.43
1:B:1305:GLY:O	1:B:1307:ASP:N	2.51	0.43
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:B:1047:VAL:HG11	1:B:1294:LEU:HD21	2.00	0.42
1:A:1159:ILE:O	1:A:1161:PRO:HD3	2.20	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:A:1149:ASN:ND2	1:A:1153:GLN:HE21	2.16	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:1517:ARG:HH22	1:B:1532:ILE:HG13	1.85	0.42
1:B:1029:GLN:HG3	1:B:1050:ARG:HH12	1.84	0.42
1:B:1555:ILE:O	1:B:1556:THR:HB	2.19	0.42
1:B:1193:ARG:HH21	1:B:1195:THR:HG23	1.83	0.42
1:A:1425:LYS:O	1:A:1429:THR:HG23	2.19	0.42
1:A:1175:ARG:HG2	1:A:1178:ARG:NH2	2.34	0.42
1:B:1390:ALA:HA	1:B:1393:ASN:HD22	1.84	0.42
1:A:1257:PRO:HD3	1:A:1286:ILE:HD11	1.99	0.42
1:B:1229:TYR:CD2	1:B:1235:PRO:HG3	2.55	0.42
1:B:1010:ILE:C	1:B:1012:GLN:N	2.72	0.42
1:B:1477:TYR:CZ	1:B:1518:LEU:HB3	2.54	0.42
1:B:1230:THR:C	1:B:1232:ASP:H	2.21	0.42
1:A:1177:LEU:HB3	1:A:1197:PHE:HB2	2.01	0.42
1:B:1076:THR:O	1:B:1078:SER:N	2.52	0.42
1:B:1245:GLY:O	1:B:1246:SER:C	2.57	0.42
1:A:1244:GLN:HE21	1:A:1244:GLN:N	2.13	0.42
1:A:1108:LYS:HE2	1:A:1556:THR:HG23	2.01	0.42
1:B:1140:HIS:CE1	1:B:1167:ARG:O	2.73	0.42
1:B:1448:LYS:HE2	1:B:1466:TYR:CG	2.55	0.42
1:B:1069:PRO:HG2	1:B:1339:MET:HE2	2.01	0.42
1:A:1044:SER:C	1:A:1046:ASP:H	2.24	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: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: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:1443:LEU:HD11	1:B:1486:PRO:HG3	2.02	0.41
1:A:1125:ILE:HD13	1:A:1270:ILE:CD1	2.50	0.41
1:B:1376:PRO:O	1:B:1377:ALA:HB2	2.21	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:A:1420:LEU:HD13	1:A:1420:LEU:HA	1.74	0.41
1:B:1450:LYS:O	1:B:1454:ILE:HG13	2.20	0.41
1:A:1555:ILE:CG2	1:A:1555:ILE:O	2.69	0.41
1:A:1133:ILE:HG21	1:A:1171:ASP:OD1	2.20	0.41
1:A:1239:GLY:HA2	1:A:1244:GLN:NE2	2.35	0.41
1:B:1313:PHE:HE2	1:B:1318:CYS:SG	2.44	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: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:1073:GLY:HA2	4:A:172:HOH:O	2.19	0.41
1:A:1422:LEU:O	1:A:1426:VAL:HG23	2.20	0.41
1:A:1017:LYS:H	1:A:1261:GLN:NE2	2.18	0.41
1:A:1140:HIS:C	1:A:1140:HIS:ND1	2.74	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:B:1265:ASN:N	1:B:1265:ASN:HD22	2.17	0.41
1:A:1066:THR:HB	1:A:1362:ASN:ND2	2.34	0.41
1:A:1313:PHE:CE1	1:A:1317:LYS:HD3	2.56	0.41
1:B:1061:LEU:HD22	1:B:1313:PHE:CE1	2.56	0.41
1:A:1491:LYS:HB3	1:A:1528:ILE:CG1	2.50	0.41
1:B:1369:ASN:CG	1:B:1458:ILE:HA	2.41	0.41
1:A:1343:VAL:HG13	1:A:1344:PRO:HD2	2.02	0.41
1:A:1151:LEU:O	1:A:1152:GLN:C	2.59	0.41
1:A:1552:ASP:N	1:A:1552:ASP:OD1	2.54	0.41
1:B:1193:ARG:HA	4:B:25:HOH:O	2.21	0.41
1:A:1175:ARG:C	1:A:1177:LEU:N	2.74	0.41
1:B:1417:GLU:HA	1:B:1420:LEU:CD2	2.38	0.41
1:B:1029:GLN:H	1:B:1050:ARG:HH22	1.68	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:1461:ALA:CA	1:B:1509:PHE:CE1	3.04	0.41
1:A:1330:ILE:CG2	1:A:1379:VAL:HG22	2.51	0.41
1:B:1412:TRP:CE3	1:B:1413:ALA:HB2	2.54	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:B:1323:PHE:C	1:B:1324:LYS:HG3	2.41	0.40
1:B:1293:LYS:C	1:B:1295:ALA:N	2.74	0.40
1:A:1316:VAL:HG12	1:A:1317:LYS:N	2.36	0.40
1:A:1172:LEU:O	1:A:1199:ILE:HD13	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:1333:THR:OG1	1:A:1336:ALA:HB3	2.21	0.40
1:A:1022:LEU:CD1	1:A:1261:GLN:HB3	2.51	0.40
1:B:1116:TYR:HA	1:B:1263:LEU:HD12	2.03	0.40
1:A:1221:ARG:HH11	1:A:1221:ARG:HD2	1.78	0.40
1:A:1524:LEU:HD23	1:A:1524:LEU:HA	1.87	0.40
1:A:1354:GLU:HA	1:A:1354:GLU:OE2	2.21	0.40
1:A:1064:ALA:HB2	1:A:1331:VAL:HB	2.02	0.40
1:A:1022:LEU:HD11	1:A:1261:GLN:OE1	2.21	0.40
1:B:1337:LEU:N	1:B:1337:LEU:HD12	2.36	0.40
1:A:1066:THR:N	1:A:1362:ASN:HD21	2.19	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:1379:VAL:CG1	1:A:1380:ALA:N	2.84	0.40
1:B:1232:ASP:N	1:B:1232:ASP:OD2	2.55	0.40
1:A:1459:TYR:CD1	1:A:1459:TYR:N	2.87	0.40
1:A:1097:ARG:HB2	1:A:1097:ARG:HE	1.61	0.40
1:A:1451:ILE:HG12	1:A:1489:MET:HE1	2.02	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: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	29
1	B	546/557 (98%)	385 (70%)	107 (20%)	54 (10%)	1	4
All	All	1093/1114 (98%)	822 (75%)	197 (18%)	74 (7%)	1	11

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%)	18	57
1	B	431/440 (98%)	397 (92%)	34 (8%)	15	53
All	All	863/880 (98%)	798 (92%)	65 (8%)	17	55

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	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	A	273	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	A	274	1	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	A	275	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	A	276	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	A	277	-	4,4,4	1.62	1 (25%)	6,6,6	0.49	0
2	SO4	A	278	1	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	B	272	1	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	B	279	1	4,4,4	1.62	1 (25%)	6,6,6	0.49	0
2	SO4	B	280	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	SO4	B	281	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	278	SO4	O1-S	-2.22	1.39	1.47
2	B	281	SO4	O1-S	-2.21	1.39	1.47
2	A	277	SO4	O1-S	-2.21	1.39	1.47
2	B	279	SO4	O1-S	-2.21	1.39	1.47
2	A	275	SO4	O1-S	-2.21	1.39	1.47
2	A	274	SO4	O1-S	-2.21	1.39	1.47
2	B	272	SO4	O1-S	-2.20	1.39	1.47
2	A	276	SO4	O1-S	-2.20	1.39	1.47
2	B	280	SO4	O1-S	-2.20	1.39	1.47
2	A	271	SO4	O1-S	-2.18	1.39	1.47
2	A	273	SO4	O1-S	-2.18	1.39	1.47

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.