



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:57 AM UTC

PDB ID : 1FP7 / pdb_00001fp7
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

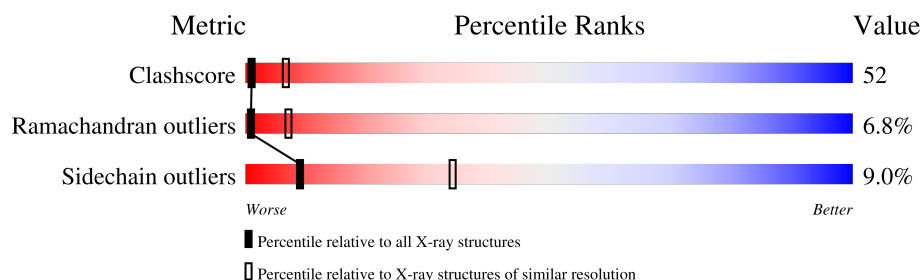
1 Overall quality at a glance

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	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	557	
1	B	557	

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	278	-	-	X	-
2	SO4	B	279	-	-	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.

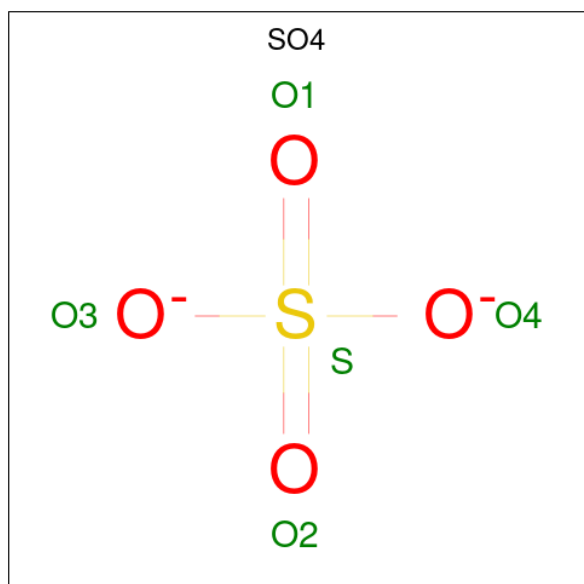
- Molecule 1 is a protein called FORMATE--TETRAHYDROFOLATE LIGASE.

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 (CCD ID: 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 (CCD ID: K) (formula: K).

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

- Molecule 4 is water.

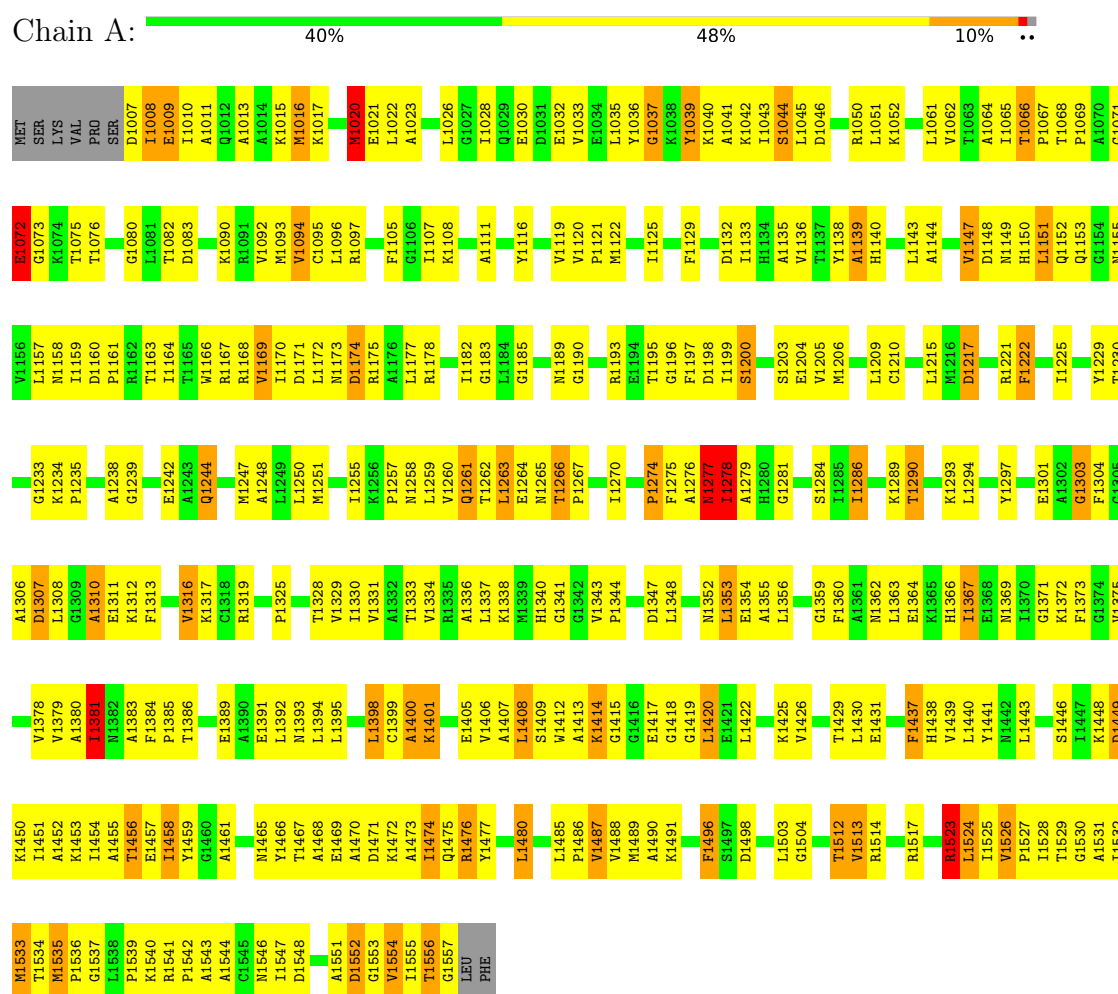
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	199	Total O 199 199	0	0
4	B	71	Total O 71 71	0	0

3 Residue-property plots

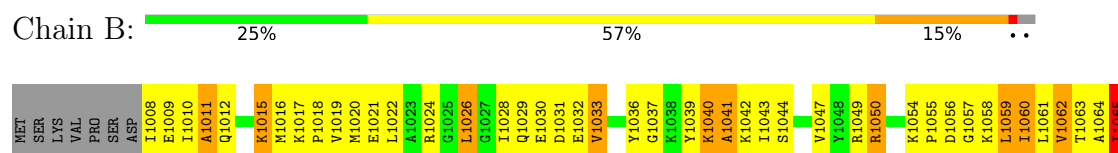
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: FORMATE--TETRAHYDROFOLATE LIGASE



• Molecule 1: FORMATE--TETRAHYDROFOLATE LIGASE



P1527	I1528	T1529	I1532	M1533	T1534	M1535	P1536	K1472	A1473	I1474	Q1475	R1476	Y1477	E1478	D1548	T1549	D1550	A1551	D1552	L1485	P1486	V1487	V1488	M1489	A1490	K1491	T1492	Q1493	Y1494	S1495	F1496	S1497	D1498	M1499	R1500	T1501	K1502	L1503	P1506	R1507	N1508	F1509	T1510	I1511	T1512	V1513	R1514	E1515	V1516	I1517	S1518	S1519	A1520	R1523	L1524	I1525	V1526	
I1391	L1392	N1393	L1394	L1395	Y1396	E1397	L1398	C1399	K1400	K1401	M1402	G1403	L1408	S1409	W1412	A1413	K1414	E1417	L1420	E1421	L1422	K1425	V1426	L1427	Q1428	T1429	L1430	E1431	S1432	R1433	P1434	S1435	R1436	F1437	H1438	V1439	L1440	Y1441	N1442	L1443	D1444	L1445	S1446	I1447	K1448	D1449	K1450	I1451	A1452	K1453	I1454	A1455	T1456	E1457	I1458			
V1329	T1330	V1331	A1332	T1333	V1334	R1335	A1336	L1337	M1338	M1339	H1340	G1341	G1342	V1343	P1344	D1347	L1348	E1351	M1352	L1353	E1354	A1355	L1356	R1357	E1358	G1359	F1360	A1361	M1362	L1363	E1364	H1366	I1367	E1368	N1369	I1370	G1371	K1372	F1373	G1374	V1375	P1376	A1377	V1378	V1379	A1380	I1381	M1382	A1383	F1384	P1385	K1386	D1387	T1388	E1389	A1390		
T1266	P1267	A1268	F1269	I1270	H1271	G1272	G1273	P1274	F1275	A1276	I1277	I1278	A1279	H1280	G1281	C1282	I1285	L1286	A1287	T1288	K1289	T1290	A1291	L1292	K1293	L1294	A1295	D1296	Y1297	V1298	V1299	T1300	G1303	F1304	G1305	A1306	D1307	L1308	G1309	A1310	E1311	K1312	F1313	Y1314	D1315	V1316	K1317	C1318	R1319	Y1320	F1323	K1324	P1325	D1326	E1327	T1328		
A1202	S1203	E1204	V1205	M1206	L1209	C1210	L1211	D1214	L1215	M1216	D1217	E1220	R1221	F1222	S1223	R1224	I1225	V1226	V1227	G1228	Y1229	T1230	Y1231	D1232	G1233	K1234	P1235	V1236	T1237	A1238	G1239	D1240	A1243	Q1244	G1245	S1246	M1247	A1248	L1249	L1250	M1251	K1252	D1253	I1254	I1255	K1256	P1257	N1258	L1259	V1260	Q1261	T1262	L1263	E1264	N1265			
T1066	P1067	T1068	P1069	A1070	G1071	E1072	G1073	L1074	T1075	T1076	T1077	S1078	V1079	G1080	L1081	T1082	D1083	A1084	L1085	A1086	R1087	L1088	G1089	K1090	R1091	V1092	M1093	V1094	C1095	R1096	L1097	E1098	P1103	S1104	F1105	G1106	I1107	K1108	G1109	G1110	A1111	A1112	G1113	G1114	G1115	Y1116	A1117	Q1118	V1119	V1120	P1121	M1122	E1123	G1124	I1125	F1129	S1200	V1201
G1131	D1132	I1133	H1134	A1135	V1136	H1140	L1143	A1144	V1147	D1148	M1149	H1150	Q1152	G1153	G1154	M1155	V1156	L1157	M1158	I1159	D1160	P1161	M1166	R1167	L1168	R1169	I1170	D1171	L1172	M1173	D1174	R1175	A1176	L1177	R1178	I1182	G1183	G1186	K1187	A1188	V1191	F1192	R1193	E1194	T1195	G1196	Q1197	D1198	I1199	S1200	V1201							

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: SO4, K

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	0/4201	1.11	31/5690 (0.5%)
1	B	0.52	0/4193	1.08	38/5679 (0.7%)
All	All	0.55	0/8394	1.10	69/11369 (0.6%)

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1476	ARG	N-CA-C	-10.22	99.95	111.71
1	A	1524	LEU	N-CA-C	10.08	125.44	108.20
1	B	1523	ARG	N-CA-C	8.61	118.39	108.49
1	B	1324	LYS	CA-C-N	8.04	129.88	119.84
1	B	1324	LYS	C-N-CA	8.04	129.88	119.84
1	B	1263	LEU	N-CA-C	-7.88	103.12	112.89
1	A	1553	GLY	N-CA-C	7.68	122.46	110.71
1	B	1204	GLU	N-CA-C	-7.40	102.91	112.23
1	A	1277	ASN	N-CA-C	-7.27	106.33	114.62
1	B	1169	VAL	N-CA-C	7.25	117.33	108.06
1	B	1217	ASP	N-CA-C	-7.19	102.85	111.69
1	A	1408	LEU	N-CA-C	-7.05	103.61	113.20
1	B	1011	ALA	N-CA-C	-6.76	105.15	113.19
1	A	1139	ALA	N-CA-C	-6.62	103.16	111.11
1	A	1169	VAL	N-CA-C	6.50	116.85	107.88
1	A	1009	GLU	N-CA-C	6.31	121.71	111.37
1	B	1384	PHE	CA-C-N	6.24	126.70	119.47
1	B	1384	PHE	C-N-CA	6.24	126.70	119.47
1	A	1217	ASP	N-CA-C	-6.15	104.49	112.23
1	B	1458	ILE	N-CA-C	6.14	116.26	110.30
1	A	1541	ARG	CA-C-N	6.11	127.47	119.84
1	A	1541	ARG	C-N-CA	6.11	127.47	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1451	ILE	N-CA-C	-6.09	104.57	110.72
1	A	1266	THR	N-CA-C	-5.90	101.62	110.24
1	B	1290	THR	N-CA-C	-5.82	104.31	111.40
1	A	1135	ALA	N-CA-C	-5.80	104.96	111.28
1	B	1174	ASP	N-CA-C	5.70	119.14	107.69
1	A	1458	ILE	N-CA-C	5.64	117.56	111.58
1	A	1026	LEU	N-CA-C	-5.63	107.06	114.04
1	B	1299	VAL	CB-CA-C	-5.60	106.29	112.68
1	B	1433	ARG	CA-C-N	5.58	126.05	120.14
1	B	1433	ARG	C-N-CA	5.58	126.05	120.14
1	A	1151	LEU	N-CA-C	-5.57	104.90	110.97
1	B	1554	VAL	N-CA-C	5.55	120.89	109.34
1	B	1037	GLY	N-CA-C	-5.51	103.45	112.83
1	B	1098	GLU	CA-C-N	5.51	125.27	119.76
1	B	1098	GLU	C-N-CA	5.51	125.27	119.76
1	A	1367	ILE	N-CA-C	-5.48	104.99	110.30
1	B	1340	HIS	N-CA-C	-5.46	106.46	113.01
1	A	1414	LYS	N-CA-C	5.45	118.75	112.97
1	B	1355	ALA	N-CA-C	-5.44	106.77	113.41
1	B	1553	GLY	N-CA-C	5.43	121.19	111.03
1	B	1136	VAL	N-CA-C	-5.43	105.21	110.42
1	B	1015	LYS	N-CA-C	5.42	122.35	110.80
1	B	1265	ASN	N-CA-C	5.40	118.88	111.54
1	B	1191	VAL	N-CA-C	5.35	114.37	108.05
1	B	1339	MET	N-CA-C	-5.35	105.55	111.71
1	B	1206	MET	N-CA-C	-5.34	105.82	112.93
1	A	1020	MET	N-CA-C	-5.34	105.36	111.07
1	A	1263	LEU	N-CA-C	-5.34	105.38	111.14
1	B	1129	PHE	CB-CA-C	-5.34	109.97	117.23
1	A	1535	MET	CA-C-N	5.33	126.51	119.84
1	A	1535	MET	C-N-CA	5.33	126.51	119.84
1	B	1437	PHE	N-CA-C	5.31	118.20	109.76
1	A	1147	VAL	N-CA-C	-5.26	105.19	110.30
1	B	1143	LEU	N-CA-C	-5.25	105.25	110.97
1	A	1496	PHE	N-CA-C	-5.25	106.72	113.02
1	A	1037	GLY	N-CA-C	-5.24	103.92	112.83
1	B	1381	ILE	N-CA-C	5.22	116.00	107.24
1	A	1406	VAL	N-CA-C	5.21	115.77	108.89
1	A	1413	ALA	N-CA-C	5.21	116.64	110.97
1	B	1226	VAL	N-CA-C	5.17	116.20	108.54
1	B	1041	ALA	N-CA-C	5.16	116.78	108.32
1	A	1039	TYR	N-CA-C	5.11	119.25	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1437	PHE	N-CA-C	5.09	117.86	109.76
1	B	1130	THR	N-CA-C	-5.05	105.59	112.26
1	A	1278	ILE	N-CA-C	-5.04	108.06	112.90
1	B	1427	LEU	N-CA-C	-5.04	105.87	111.36
1	A	1383	ALA	N-CA-C	5.01	117.00	110.43

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	372	1
1	B	4125	0	4211	492	0
2	A	35	0	0	15	1
2	B	20	0	0	4	0
3	A	2	0	0	1	0
4	A	199	0	0	29	0
4	B	71	0	0	17	0
All	All	8585	0	8430	865	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 52.

All (865) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1175:ARG:NH1	2:B:279:SO4:O3	1.58	1.33
1:A:1175:ARG:HD3	2:A:275:SO4:O3	1.40	1.22
1:B:1222:PHE:O	1:B:1225:ILE:HG22	1.40	1.19
1:A:1007:ASP:OD2	4:A:32:HOH:O	1.68	1.11
1:B:1079:VAL:HB	1:B:1117:ALA:HB1	1.34	1.08
1:B:1335:ARG:HD3	1:B:1348:LEU:HB3	1.33	1.07
1:A:1013:ALA:HB1	4:A:39:HOH:O	1.57	1.04
1:B:1557:GLY:CA	4:B:65:HOH:O	2.03	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1166:TRP:CH2	1:B:1225:ILE:HD11	1.95	1.02
1:A:1353:LEU:HD12	1:A:1353:LEU:H	1.25	1.02
1:A:1557:GLY:O	4:A:19:HOH:O	1.75	1.02
1:A:1405:GLU:CD	1:A:1422:LEU:HA	1.86	1.01
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:1469:GLU:HG3	4:A:175:HOH:O	1.64	0.95
1:A:1044:SER:OG	2:A:274:SO4:O4	1.84	0.94
1:A:1225:ILE:HG23	1:A:1238:ALA:HB2	1.48	0.94
1:A:1225:ILE:CG2	1:A:1238:ALA:CB	2.46	0.94
1:B:1417:GLU:HA	1:B:1420:LEU:HD23	1.52	0.91
1:A:1166:TRP:CZ3	1:A:1225:ILE:HD11	2.05	0.91
1:A:1277:ASN:HD22	1:A:1278:ILE:H	1.10	0.91
1:B:1455:ALA:HA	1:B:1459:TYR:HD2	1.34	0.91
1:B:1262:THR:HG22	1:B:1263:LEU:H	1.36	0.91
1:B:1329:VAL:HG12	1:B:1330:ILE:H	1.37	0.90
1:B:1451:ILE:HD11	1:B:1526:VAL:HG11	1.53	0.90
1:A:1375:VAL:O	4:A:103:HOH:O	1.87	0.90
1:B:1277:ASN:H	1:B:1277:ASN:HD22	1.15	0.90
1:B:1094:VAL:HG23	1:B:1268:ALA:HA	1.53	0.90
1:A:1125:ILE:HG12	1:A:1129:PHE:CE1	2.07	0.90
1:A:1210:CYS:O	4:A:62:HOH:O	1.89	0.89
1:B:1551:ALA:O	4:B:147:HOH:O	1.89	0.89
1:A:1277:ASN:HD22	1:A:1278:ILE:N	1.69	0.89
1:A:1476:ARG:O	1:A:1480:LEU:HB2	1.73	0.89
1:A:1301:GLU:OE1	4:A:197:HOH:O	1.91	0.89
1:B:1372:LYS:HZ3	1:B:1457:GLU:HG2	1.36	0.89
1:A:1185:GLY:HA3	1:A:1189:ASN:HD22	1.37	0.88
1:B:1169:VAL:CG2	1:B:1200:SER:HA	2.03	0.88
1:B:1086:ALA:HB2	1:B:1092:VAL:HG12	1.57	0.87
1:B:1543:ALA:O	1:B:1547:ILE:HG13	1.73	0.87
1:A:1082:THR:HG21	1:A:1094:VAL:HG22	1.56	0.86
1:A:1225:ILE:CG2	1:A:1238:ALA:HB3	2.05	0.86
1:B:1079:VAL:HG11	1:B:1117:ALA:O	1.76	0.85
1:B:1107:ILE:O	1:B:1108:LYS:HB2	1.73	0.85
1:A:1044:SER:OG	2:A:274:SO4:S	2.36	0.84
1:A:1020:MET:HE1	1:A:1030:GLU:HA	1.57	0.84
3:A:282[B]:K:K	4:A:186:HOH:O	0.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1069:PRO:HG2	1:B:1339:MET:HE1	1.65	0.78
1:B:1277:ASN:H	1:B:1277:ASN:ND2	1.81	0.78
1:B:1032:GLU:O	1:B:1033:VAL:HG23	1.84	0.77
1:B:1523:ARG:HD2	1:B:1523:ARG:H	1.50	0.77
1:A:1486:PRO:HD2	1:A:1523:ARG:HB3	1.65	0.77
1:A:1195:THR:HG21	4:A:35:HOH:O	1.83	0.77
1:A:1182:ILE:HG22	1:A:1183:GLY:N	1.99	0.77
1:B:1425:LYS:O	1:B:1429:THR:HG23	1.85	0.77
1:B:1065:ILE:HD13	1:B:1332:ALA:HA	1.67	0.76
1:A:1306:ALA:O	1:A:1310:ALA:HB3	1.86	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1075:THR:HG21	1:B:1113:GLY:HA2	1.69	0.74
1:B:1017:LYS:HB2	1:B:1261:GLN:HE22	1.51	0.74
1:B:1075:THR:CG2	1:B:1113:GLY:HA2	2.17	0.74
1:B:1323:PHE:O	1:B:1324:LYS:HG3	1.87	0.74
1:A:1068:THR:HB	1:A:1069:PRO:HD2	1.69	0.73
1:A:1175:ARG:HD3	2:A:275:SO4:S	2.28	0.73
1:A:1439:VAL:HG13	4:A:99:HOH:O	1.89	0.73
1:A:1136:VAL:HG13	1:A:1205:VAL:HG12	1.68	0.73
1:B:1262:THR:HG22	1:B:1263:LEU:N	2.03	0.72
1:A:1498:ASP:CB	1:A:1528:ILE:HG21	2.19	0.72
1:A:1532:ILE:O	1:A:1534:THR:N	2.22	0.72
1:A:1474:ILE:O	1:A:1474:ILE:HG22	1.91	0.71
1:A:1363:LEU:O	1:A:1367:ILE:HG12	1.91	0.71
1:A:1418:GLY:O	4:A:210:HOH:O	2.08	0.71
1:A:1526:VAL:HG22	1:A:1526:VAL:O	1.90	0.71
1:B:1278:ILE:O	1:B:1525:ILE:HD12	1.90	0.71
1:B:1515:GLU:HG2	1:B:1516:VAL:H	1.54	0.71
1:A:1303:GLY:O	4:A:86:HOH:O	2.08	0.71
1:B:1454:ILE:HG22	1:B:1459:TYR:CE2	2.25	0.70
1:B:1556:THR:HG22	1:B:1556:THR:O	1.89	0.70
1:A:1148:ASP:OD1	4:A:69:HOH:O	2.09	0.70
1:B:1058:LYS:HB3	1:B:1430:LEU:HD21	1.72	0.70
1:A:1175:ARG:HG2	1:A:1178:ARG:CZ	2.21	0.70
1:A:1556:THR:O	1:A:1556:THR:HG22	1.90	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:1473:ALA:C	1:A:1475:GLN:H	1.99	0.69
1:A:1042:LYS:HE2	1:A:1258:ASN:OD1	1.92	0.69
1:B:1557:GLY:HA2	4:B:65:HOH:O	1.81	0.69
1:A:1023:ALA:HB1	1:A:1028:ILE:HB	1.74	0.69
1:B:1324:LYS:HG2	1:B:1437:PHE:HB3	1.75	0.69
1:B:1042:LYS:NZ	1:B:1254:ALA:HA	2.08	0.69
1:A:1543:ALA:O	1:A:1547:ILE:HG12	1.91	0.69
1:B:1065:ILE:HG23	1:B:1332:ALA:HB2	1.75	0.69
1:B:1043:ILE:HD11	1:B:1259:LEU:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1308:LEU:O	1:A:1312:LYS:HG3	1.93	0.67
1:B:1083:ASP:HB3	1:B:1264:GLU:CD	2.20	0.67
1:A:1412:TRP:CD2	2:A:277:SO4:O4	2.46	0.67
1:A:1530:GLY:C	1:A:1532:ILE:H	2.02	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:1451:ILE:HG12	1:B:1489:MET:HE1	1.76	0.67
1:B:1043:ILE:HD11	1:B:1259:LEU:HD22	1.77	0.66
1:B:1149:ASN:O	1:B:1152:GLN:HB3	1.95	0.66
1:B:1360:PHE:CE2	1:B:1364:GLU:HB2	2.30	0.66
1:B:1417:GLU:O	1:B:1420:LEU:HB2	1.96	0.66
1:A:1116:TYR:CZ	2:A:278:SO4:O1	2.48	0.66
1:A:1092:VAL:HG23	1:A:1297:TYR:O	1.94	0.66
1:A:1150:HIS:CE1	1:A:1157:LEU:H	2.13	0.66
1:A:1171:ASP:HA	1:A:1199:ILE:HD12	1.77	0.66
1:A:1204:GLU:OE2	4:A:116:HOH:O	2.13	0.66
1:A:1262:THR:HG22	1:A:1263:LEU:N	2.05	0.66
1:A:1512:THR:O	1:A:1512:THR:HG22	1.94	0.66
1:A:1217:ASP:O	1:A:1221:ARG:HG3	1.95	0.66
1:B:1372:LYS:NZ	1:B:1457:GLU:HG2	2.10	0.66
1:B:1166:TRP:CH2	1:B:1225:ILE:CD1	2.76	0.66
1:A:1210:CYS:HA	1:A:1284:SER:HA	1.76	0.66
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:A:1158:ASN:O	1:A:1230:THR:HA	1.96	0.65
1:A:1389:GLU:C	1:A:1391:GLU:H	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1344:PRO:HD2	1:B:1347:ASP:HB2	1.79	0.65
1:B:1172:LEU:O	1:B:1535:MET:HE1	1.96	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:A:1407:ALA:C	1:A:1409:SER:H	2.05	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:1071:GLY:C	1:A:1072:GLU:HG3	2.22	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:1550:ASP:C	1:B:1552:ASP:H	2.06	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:A:1525:ILE:CG2	1:A:1526:VAL:N	2.62	0.62
1:B:1086:ALA:C	1:B:1088:LEU:H	2.08	0.62
1:B:1455:ALA:HA	1:B:1459:TYR:CD2	2.25	0.62
1:A:1229:TYR:HD2	1:A:1233:GLY:O	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:VAL:HG22	1:A:1093:MET:N	2.14	0.62
1:B:1072:GLU:CD	1:B:1073:GLY:H	2.07	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:1221:ARG:O	1:B:1222:PHE:C	2.44	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: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:B:1062:VAL:HG12	1:B:1300:THR:O	2.01	0.60
1:B:1499:ASP:C	1:B:1501:THR:H	2.09	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:1259:LEU:O	1:A:1260:VAL:HG13	2.01	0.60
1:A:1379:VAL:HG12	1:A:1381:ILE:HD13	1.84	0.60
1:A: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1306:ALA:HB3	1:A:1366:HIS:ND1	2.17	0.59
1:B:1092:VAL:HG23	1:B:1297:TYR:HB2	1.85	0.59
1:B:1155:ASN:HD21	1:B:1159:ILE:N	2.01	0.59
1:B:1451:ILE:HG12	1:B:1487:VAL:HG11	1.83	0.59
1:B:1133:ILE:HD13	1:B:1171:ASP:OD1	2.03	0.59
1:B:1408:LEU:HD13	1:B:1414:LYS:HE3	1.85	0.59
1:A:1008:ILE:HG12	1:A:1011:ALA:CB	2.33	0.59
1:A:1277:ASN:O	1:A:1490:ALA:HB2	2.03	0.59
1:A:1277:ASN:HD22	1:A:1277:ASN:H	1.50	0.59
1:A:1485:LEU:HD13	1:A:1523:ARG:HA	1.85	0.58
1:A:1325:PRO:HD2	1:A:1437:PHE:CD2	2.38	0.58
1:B:1204:GLU:C	1:B:1206:MET:H	2.11	0.58
1:B:1451:ILE:HG23	1:B:1489:MET:CE	2.33	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:B:1493:GLN:C	1:B:1495:SER:H	2.11	0.58
1:A:1182:ILE:HG22	1:A:1183:GLY:H	1.64	0.58
1:A:1173:ASN:HB3	1:A:1536:PRO:O	2.04	0.57
1:A:1334:VAL:HG12	1:A:1338:LYS:HE2	1.86	0.57
1:A:1408:LEU:HD13	1:A:1414:LYS:CE	2.34	0.57
1:A:1525:ILE:C	1:A:1526:VAL:HG12	2.27	0.57
1:B:1533:MET:HE1	2:B:279:SO4:O1	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:A:1367:ILE:HG22	1:A:1401:LYS:HE3	1.85	0.57
1:A:1391:GLU:O	1:A:1392:LEU:C	2.46	0.57
1:B:1199:ILE:HA	1:B:1535:MET:HE2	1.86	0.57
1:B:1515:GLU:HG2	1:B:1516:VAL:N	2.19	0.57
1:A:1170:ILE:HD12	1:A:1171:ASP:H	1.68	0.57
1:B:1079:VAL:CB	1:B:1117:ALA:HB1	2.22	0.57
1:A:1454:ILE:O	1:A:1458:ILE:HB	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1075:THR:O	1:B:1076:THR:C	2.48	0.57
1:B:1337:LEU:O	1:B:1359:GLY:HA3	2.04	0.57
1:B:1384:PHE:CD1	1:B:1385:PRO:HD2	2.40	0.57
1:A:1242:GLU:OE1	1:A:1242:GLU:HA	2.05	0.57
1:A:1408:LEU:HD13	1:A:1414:LYS:HE3	1.87	0.57
1:B:1276:ALA:HA	1:B:1279:ALA:O	2.05	0.57
1:B:1499:ASP:OD2	1:B:1502:LYS:HE3	2.05	0.57
1:B:1549:ILE:HG23	1:B:1549:ILE:O	2.03	0.57
1:B:1029:GLN:HB3	1:B:1031:ASP:OD2	2.05	0.56
1:B:1343:VAL:HG13	1:B:1347:ASP:O	2.05	0.56
1:B:1081:LEU:O	1:B:1085:LEU:HB2	2.04	0.56
1:B:1459:TYR:OH	1:B:1489:MET:HG3	2.05	0.56
1:A:1036:TYR:O	1:A:1040:LYS:NZ	2.38	0.56
1:A:1488:VAL:HG21	1:A:1523:ARG:CZ	2.35	0.56
1:B:1206:MET:O	1:B:1209:LEU:HB3	2.05	0.56
1:B:1276:ALA:HB3	1:B:1304:PHE:CD2	2.40	0.56
1:B:1445:LEU:O	1:B:1450:LYS:HE3	2.05	0.56
1:A:1384:PHE:CD2	1:A:1385:PRO:HD2	2.41	0.56
1:A:1523:ARG:HD2	1:A:1523:ARG:C	2.28	0.56
1:B:1044:SER:OG	2:B:280:SO4:O2	2.20	0.56
1:B:1054:LYS:HB3	1:B:1055:PRO:HD2	1.86	0.56
1:B:1066:THR:OG1	1:B:1366:HIS:NE2	2.32	0.56
1:B:1095:CYS:SG	1:B:1288:THR:HA	2.46	0.56
1:B:1277:ASN:ND2	1:B:1277:ASN:N	2.45	0.56
1:B:1178:ARG:HD3	1:B:1535:MET:HB3	1.86	0.56
1:A:1107:ILE:CG2	1:A:1539:PRO:HG2	2.35	0.56
1:A:1451:ILE:HG12	1:A:1489:MET:HE1	1.87	0.56
1:A:1473:ALA:O	1:A:1475:GLN:N	2.39	0.56
1:A:1555:ILE:HG23	1:A:1555:ILE:O	2.06	0.56
1:B:1017:LYS:N	1:B:1261:GLN:OE1	2.39	0.56
1:B:1042:LYS:HD3	1:B:1256:LYS:HB2	1.88	0.56
1:B:1058:LYS:CB	1:B:1430:LEU:HD21	2.36	0.56
1:B:1169:VAL:HG22	1:B:1200:SER:HA	1.84	0.56
1:A:1140:HIS:CD2	1:A:1203:SER:OG	2.54	0.56
1:B:1454:ILE:HG22	1:B:1459:TYR:HE2	1.70	0.56
1:A:1119:VAL:HG13	1:A:1261:GLN:O	2.06	0.56
1:A:1167:ARG:NH2	1:A:1178:ARG:O	2.39	0.56
1:B: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:1489:MET:HE1	1:B:1526:VAL:HG21	1.86	0.56
1:A:1525:ILE:HG22	1:A:1526:VAL:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1010:ILE:HA	1:B:1122:MET:HE1	1.86	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:B:1557:GLY:C	4:B:65:HOH:O	2.37	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:A:1473:ALA:C	1:A:1475:GLN:N	2.64	0.55
1:B:1093:MET:HE3	1:B:1267:PRO:HB3	1.89	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:1313:PHE:CD2	1:B:1313:PHE:C	2.84	0.55
1:B:1477:TYR:CE2	1:B:1516:VAL:HG12	2.33	0.55
1:B:1063:THR:HG22	1:B:1329:VAL:O	2.06	0.55
1:B:1211:LEU:HD21	1:B:1280:HIS:CD2	2.41	0.55
1:B:1398:LEU:C	1:B:1400:ALA:H	2.15	0.55
1:B:1487:VAL:HG12	1:B:1489:MET:HE2	1.89	0.55
1:B:1262:THR:CG2	1:B:1263:LEU:H	2.15	0.55
1:B:1338:LYS:C	1:B:1343:VAL:HB	2.32	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:A:1389:GLU:C	1:A:1391:GLU:N	2.61	0.54
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:A:1136:VAL:HG11	1:A:1206:MET:HE2	1.89	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:1293:LYS:C	1:B:1295:ALA:H	2.14	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:1542:PRO:C	1:A:1544:ALA:N	2.66	0.53
1:A:1042:LYS:NZ	1:A:1132:ASP:OD2	2.38	0.53
1:A:1155:ASN:OD1	1:A:1158:ASN:HA	2.09	0.53
1:A:1512:THR:HG22	1:A:1514:ARG:HE	1.74	0.53
1:B:1516:VAL:HG22	1:B:1526:VAL:HG12	1.91	0.53
1:B:1490:ALA:HB3	1:B:1527:PRO:HA	1.90	0.53
1:A:1488:VAL:CG2	1:A:1523:ARG:HD3	2.39	0.53
1:B:1133:ILE:HG22	1:B:1134:HIS:N	2.23	0.53
1:A:1175:ARG:HH11	1:A:1537:GLY:HA3	1.73	0.53
1:B:1225:ILE:HA	1:B:1520:ALA:HB3	1.89	0.53
1:B:1199:ILE:CA	1:B:1535:MET:HE2	2.40	0.52
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:1010:ILE:C	1:B:1012:GLN:H	2.17	0.52
1:B:1111:ALA:C	1:B:1113:GLY:H	2.17	0.52
1:B:1379:VAL:HG12	1:B:1380:ALA:N	2.24	0.52
1:B:1049:ARG:HD3	1:B:1049:ARG:C	2.33	0.52
1:B:1255:ILE:O	1:B:1255:ILE:HG13	2.10	0.52
1:A:1286:ILE:HD12	1:A:1286:ILE:C	2.34	0.52
1:A:1542:PRO:C	1:A:1544:ALA:H	2.16	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:B:1550:ASP:C	1:B:1552:ASP:N	2.66	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:1076:THR:O	1:B:1079:VAL:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1485:LEU:HD13	1:B:1523:ARG:HA	1.90	0.52
1:B:1517:ARG:HH12	1:B:1532:ILE:CD1	2.23	0.52
1:A:1533:MET:HB2	2:A:273:SO4:O2	2.09	0.52
1:B:1335:ARG:HD3	1:B:1348:LEU:CB	2.23	0.52
1:A:1136:VAL:HG21	1:A:1206:MET:HE2	1.92	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
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:B:1515:GLU:O	1:B:1527:PRO:HD2	2.10	0.51
1:B:1150:HIS:HE1	1:B:1156:VAL:N	2.08	0.51
1:B:1150:HIS:NE2	1:B:1157:LEU:HG	2.25	0.51
1:B:1448:LYS:HE2	1:B:1466:TYR:CD2	2.45	0.51
1:B:1043:ILE:O	1:B:1257:PRO:HD2	2.11	0.51
1:B:1154:GLY:O	1:B:1155:ASN:C	2.53	0.51
1:B:1178:ARG:O	1:B:1196:GLY:HA3	2.10	0.51
1:B:1247:MET:HA	1:B:1250:LEU:HD23	1.93	0.51
1:A:1044:SER:OG	2:A:274:SO4:O1	2.24	0.51
1:B:1077:THR:HG21	1:B:1331:VAL:HG22	1.91	0.51
1:B:1498:ASP:HB3	1:B:1528:ILE:HG21	1.92	0.51
1:B:1087:ARG:O	1:B:1088:LEU:HD23	2.10	0.51
1:A:1036:TYR:O	1:A:1040:LYS:HB2	2.11	0.51
1:A:1083:ASP:OD1	1:A:1262:THR:HG21	2.10	0.51
1:B:1318:CYS:HA	1:B:1323:PHE:HB2	1.92	0.51
1:A:1147:VAL:HG11	1:A:1164:ILE:HD13	1.91	0.51
1:B:1105:PHE:HB3	1:B:1544:ALA:HB2	1.93	0.51
1:A:1125:ILE:HG12	1:A:1129:PHE:CD1	2.43	0.51
1:A:1389:GLU:O	1:A:1393:ASN:HB2	2.11	0.51
1:B:1237:THR:O	1:B:1240:ASP:HB2	2.10	0.51
1:B:1279:ALA:HA	1:B:1523:ARG:NH2	2.26	0.51
1:B:1517:ARG:HH12	1:B:1532:ILE:HD12	1.75	0.51
1:A:1446:SER:HB3	1:A:1449:ASP:HB2	1.93	0.51
1:B:1360:PHE:O	1:B:1361:ALA:C	2.54	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:1016:MET:HE3	1:A:1039:TYR:CG	2.46	0.50
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:1138:TYR:O	1:A:1139:ALA:C	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1026:LEU:HD23	1:B:1028:ILE:HD11	1.94	0.50
1:B:1061:LEU:HD13	1:B:1313:PHE:CE1	2.46	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:1277:ASN:HD22	1:B:1278:ILE:N	2.09	0.50
1:B:1554:VAL:HG12	1:B:1555:ILE:N	2.27	0.50
1:A:1363:LEU:HD11	1:A:1367:ILE:HD11	1.93	0.50
1:B:1008:ILE:HG13	1:B:1011:ALA:CB	2.41	0.50
1:B:1124:ASP:O	1:B:1129:PHE:CA	2.59	0.50
1:B:1461:ALA:HB2	1:B:1509:PHE:HE1	1.77	0.50
1:B:1487:VAL:HG22	1:B:1524:LEU:HD12	1.94	0.50
1:B:1499:ASP:C	1:B:1501:THR:N	2.70	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:1351:GLU:OE1	1:B:1390:ALA:HB3	2.12	0.50
1:B:1491:LYS:C	1:B:1492:THR:O	2.52	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:1081:LEU:O	1:B:1081:LEU:HG	2.10	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:1198:ASP:C	1:A:1535:MET:HE2	2.37	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:1325:PRO:C	1:B:1327:ALA:H	2.20	0.49
1:B:1017:LYS:O	1:B:1018:PRO:C	2.55	0.49
1:B:1088:LEU:O	1:B:1090:LYS:HG2	2.12	0.49
1:A:1277:ASN:ND2	1:A:1277:ASN:N	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1453:LYS:HG2	4:A:111:HOH:O	2.13	0.48
1:B:1215:LEU:HD22	1:B:1215:LEU:O	2.13	0.48
1:B:1376:PRO:HG3	1:B:1433:ARG:HG2	1.95	0.48
1:B:1442:ASN:OD1	1:B:1443:LEU:N	2.46	0.48
1:B:1493:GLN:N	1:B:1493:GLN:OE1	2.46	0.48
1:A:1143:LEU:O	1:A:1144:ALA:C	2.56	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
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:1343:VAL:CG1	1:B:1348:LEU:HD23	2.44	0.48
1:A:1381:ILE:H	1:A:1381:ILE:CD1	2.19	0.48
1:A:1090:LYS:HB3	1:A:1297:TYR:CD2	2.48	0.48
1:A:1343:VAL:CG1	1:A:1348:LEU:HD23	2.43	0.48
1:A:1455:ALA:O	1:A:1461:ALA:HB3	2.13	0.48
1:A:1526:VAL:O	1:A:1526:VAL:CG2	2.61	0.48
1:B:1393:ASN:O	1:B:1396:TYR:HB2	2.13	0.48
1:A:1185:GLY:CA	1:A:1189:ASN:HD22	2.18	0.48
1:A:1290:THR:O	1:A:1294:LEU:HG	2.13	0.48
1:A:1369:ASN:C	1:A:1371:GLY:N	2.70	0.48
1:A:1178:ARG:NH2	2:A:275:SO4:O2	2.46	0.48
1:B:1086:ALA:C	1:B:1088:LEU:N	2.72	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:1019:VAL:HG23	1:B:1039:TYR:HA	1.95	0.48
1:B:1292:LEU:HD23	1:B:1298:VAL:CG2	2.43	0.48
1:B:1319:ARG:HG3	1:B:1439:VAL:HG11	1.96	0.48
1:A:1061:LEU:O	1:A:1328:THR:HA	2.14	0.47
1:A:1116:TYR:CE2	2:A:278:SO4:O1	2.67	0.47
1:A:1136:VAL:HG21	1:A:1206:MET:CE	2.44	0.47
1:A:1366:HIS:NE2	1:A:1496:PHE:CZ	2.82	0.47
1:A:1554:VAL:CG1	1:A:1555:ILE:N	2.77	0.47
1:B:1133:ILE:O	1:B:1136:VAL:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1216:MET:HE2	1:B:1216:MET:HA	1.95	0.47
1:B:1374:GLY:HA3	1:B:1438:HIS:HE1	1.78	0.47
1:B:1461:ALA:HA	1:B:1509:PHE:CE1	2.49	0.47
1:A:1360:PHE:CE2	1:A:1364:GLU:HB2	2.49	0.47
1:B:1313:PHE:CE2	1:B:1318:CYS:SG	3.07	0.47
1:A:1353:LEU:HD12	1:A:1353:LEU:N	2.09	0.47
1:A:1107:ILE:HG22	1:A:1539:PRO:HG2	1.94	0.47
1:A:1386:THR:HA	4:A:48:HOH:O	2.14	0.47
1:B:1143:LEU:O	1:B:1147:VAL:HG23	2.14	0.47
1:B:1220:GLU:O	1:B:1221:ARG:C	2.55	0.47
1:A:1555:ILE:O	1:A:1556:THR:CB	2.63	0.47
1:B:1155:ASN:OD1	1:B:1159:ILE:HB	2.14	0.47
1:B:1343:VAL:HG11	1:B:1348:LEU:HD23	1.96	0.47
1:A:1277:ASN:HD22	1:A:1277:ASN:N	2.08	0.47
1:A:1400:ALA:O	1:A:1401:LYS:HB2	2.15	0.47
1:A:1474:ILE:O	1:A:1474:ILE:CG2	2.61	0.47
1:B:1244:GLN:HG2	1:B:1245:GLY:H	1.79	0.47
1:A:1066:THR:H	1:A:1362:ASN:HD21	1.63	0.47
1:A:1259:LEU:O	1:A:1260:VAL:CG1	2.63	0.47
1:B:1009:GLU:HG2	1:B:1009:GLU:O	2.14	0.47
1:B:1257:PRO:HD3	1:B:1286:ILE:CD1	2.45	0.47
1:B:1507:ARG:O	1:B:1508:ASN:HB2	2.14	0.47
1:A:1457:GLU:OE2	4:A:218:HOH:O	2.20	0.47
1:B:1061:LEU:HD22	1:B:1313:PHE:CD1	2.50	0.47
1:B:1550:ASP:OD1	1:B:1551:ALA:N	2.47	0.47
1:A:1096:LEU:O	1:A:1270:ILE:HA	2.15	0.47
1:A:1366:HIS:CE1	1:A:1496:PHE:CZ	3.03	0.47
1:A:1533:MET:CB	2:A:273:SO4:O2	2.63	0.47
1: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:1245:GLY:O	1:B:1246:SER:C	2.57	0.46
1:B:1414:LYS:O	1:B:1417:GLU:HB3	2.15	0.46
1:A:1530:GLY:C	1:A:1532:ILE:N	2.70	0.46
1:B:1278:ILE:N	1:B:1278:ILE:HD12	2.31	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:B:1230:THR:C	1:B:1232:ASP:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1044:SER:C	1:A:1046:ASP:H	2.24	0.46
1:A:1247:MET:O	1:A:1248:ALA:C	2.58	0.46
1:B:1369:ASN:O	1:B:1370:ILE:C	2.56	0.46
1:B:1502:LYS:HB3	1:B:1506:PRO:HB3	1.98	0.46
1:B:1204:GLU:C	1:B:1206:MET:N	2.74	0.46
1:B:1492:THR:HG22	1:B:1498:ASP:HA	1.98	0.46
1:A:1140:HIS:C	1:A:1140:HIS:ND1	2.74	0.46
1:A:1448:LYS:HG2	1:A:1466:TYR:CZ	2.51	0.46
1:B:1136:VAL:HG13	1:B:1205:VAL:O	2.16	0.46
1:B:1150:HIS:O	1:B:1153:GLN:N	2.42	0.46
1:B:1451:ILE:CD1	1:B:1526:VAL:HG11	2.36	0.46
1:A:1023:ALA:HB1	1:A:1028:ILE:HD12	1.98	0.46
1:A:1151:LEU:O	1:A:1152:GLN:C	2.59	0.46
1:B:1120:VAL:HB	1:B:1121:PRO:HA	1.98	0.46
1:B:1369:ASN:CG	1:B:1458:ILE:HA	2.41	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:1175:ARG:C	1:A:1177:LEU:N	2.74	0.45
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: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:1412:TRP:CD1	4:B:139:HOH:O	2.70	0.45
1:B:1493:GLN:O	1:B:1495:SER:N	2.50	0.45
1:A:1105:PHE:HB3	1:A:1544:ALA:HB2	1.99	0.45
1:A:1107:ILE:O	1:A:1108:LYS:HB2	2.15	0.45
1:A:1381:ILE:CG2	1:A:1395:LEU:HD23	2.45	0.45
1:A:1498:ASP:HB2	1:A:1528:ILE:HG21	1.96	0.45
1:A:1523:ARG:HD2	1:A:1523:ARG:N	2.31	0.45
1:B:1293:LYS:C	1:B:1295:ALA:N	2.74	0.45
1:B:1323:PHE:C	1:B:1324:LYS:HG3	2.41	0.45
1:A:1071:GLY:O	1:A:1072:GLU:HG3	2.16	0.45
1:B:1205:VAL:O	1:B:1205:VAL:CG1	2.62	0.45
1:B:1488:VAL:HG23	1:B:1523:ARG:HG2	1.97	0.45
1:A:1408:LEU:HD13	1:A:1414:LYS:NZ	2.32	0.45
1:B:1026:LEU:HD21	1:B:1294:LEU:HB3	1.97	0.45
1:A:1199:ILE:O	1:A:1200:SER:C	2.60	0.45
1:B:1320:TYR:CZ	4:B:228:HOH:O	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1515:GLU:O	1:B:1516:VAL:HG23	2.16	0.45
1:B:1554:VAL:CG1	1:B:1555:ILE:N	2.80	0.45
1:A:1016:MET:HB3	1:A:1261:GLN:NE2	2.31	0.45
1:A:1052:LYS:HE3	4:A:227:HOH:O	2.15	0.45
1:A:1170:ILE:HG13	1:A:1171:ASP:N	2.32	0.45
1:A:1170:ILE:CD1	1:A:1171:ASP:H	2.29	0.45
1:B:1040:LYS:NZ	1:B:1040:LYS:HB2	2.31	0.45
1:B:1329:VAL:CG1	1:B:1330:ILE:H	2.18	0.45
1:B:1451:ILE:HG23	1:B:1489:MET:HE1	1.99	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:1032:GLU:CD	1:A:1050:ARG:NH1	2.75	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:1389:GLU:O	1:B:1390:ALA:C	2.60	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
1:A:1369:ASN:C	1:A:1371:GLY:H	2.25	0.44
1:A:1466:TYR:CE2	1:A:1513:VAL:HG11	2.52	0.44
1:B:1047:VAL:O	1:B:1050:ARG:HG3	2.17	0.44
1:B:1450:LYS:NZ	1:B:1485:LEU:O	2.50	0.44
1:B:1174:ASP:OD2	1:B:1176:ALA:HB3	2.17	0.44
1:B:1195:THR:HB	1:B:1196:GLY:H	1.29	0.44
1:B:1221:ARG:O	1:B:1223:SER:N	2.51	0.44
1:B:1382:ASN:HD22	1:B:1382:ASN:HA	1.60	0.44
1:B:1009:GLU:OE1	1:B:1115:GLY:N	2.33	0.44
1:B:1061:LEU:HD22	1:B:1313:PHE:CG	2.52	0.44
1:B:1257:PRO:HA	1:B:1271:HIS:CG	2.52	0.44
1:B:1311:GLU:C	1:B:1311:GLU:CD	2.85	0.44
1:B:1338:LYS:C	1:B:1341:GLY:H	2.24	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:B:1236:VAL:HG12	1:B:1237:THR:N	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1020:MET:HE3	1:A:1030:GLU:HG3	1.99	0.44
1:A:1340:HIS:HB3	1:A:1504:GLY:HA2	2.00	0.44
1:A:1489:MET:HE2	1:A:1526:VAL:HG11	1.99	0.44
1:B:1010:ILE:C	1:B:1012:GLN:N	2.72	0.44
1:B:1186:GLY:C	1:B:1188:ALA:H	2.25	0.44
1:B:1214:ASP:C	1:B:1216:MET:H	2.26	0.44
1:B:1221:ARG:O	1:B:1224:ARG:HG3	2.18	0.44
1:B:1312:LYS:O	1:B:1313:PHE:C	2.60	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: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:1473:ALA:O	1:B:1474:ILE:C	2.61	0.44
1:B:1523:ARG:N	1:B:1523:ARG:CD	2.63	0.44
1:A:1039:TYR:O	1:A:1260:VAL:HG12	2.17	0.44
1:A:1067:PRO:HB3	4:A:18:HOH:O	2.17	0.44
1:B:1043:ILE:CG2	1:B:1047:VAL:HG21	2.48	0.44
1:B:1065:ILE:HB	1:B:1066:THR:H	1.46	0.44
1:B: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:A:1407:ALA:C	1:A:1409:SER:N	2.70	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:1010:ILE:HB	1:A:1122:MET:HE1	2.00	0.43
1:A:1234:LYS:HA	1:A:1235:PRO:HD3	1.80	0.43
1:A:1556:THR:O	1:A:1556:THR:CG2	2.62	0.43
1:B:1086:ALA:O	1:B:1088:LEU:N	2.51	0.43
1:B:1166:TRP:HB2	1:B:1227:VAL:HA	1.99	0.43
1:B:1225:ILE:HG23	1:B:1225:ILE:O	2.18	0.43
1:B:1249:LEU:O	1:B:1249:LEU:HD12	2.17	0.43
1:B:1511:ILE:HG22	1:B:1528:ILE:HD12	1.99	0.43
1:A:1065:ILE:CD1	1:A:1337:LEU:HD13	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1075:THR:O	1:A:1076:THR:C	2.60	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:1243:ALA:O	1:B:1244:GLN:C	2.60	0.43
1:B:1395:LEU:O	1:B:1396:TYR:C	2.60	0.43
1:B:1493:GLN:C	1:B:1495:SER:N	2.76	0.43
1:B:1043:ILE:HG22	1:B:1047:VAL:HG21	2.00	0.43
1:B:1329:VAL:C	1:B:1330:ILE:HG22	2.43	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:A:1093:MET:HG2	1:A:1267:PRO:HB2	2.00	0.43
1:A:1160:ASP:HB3	1:A:1163:THR:HG23	2.00	0.43
1:A:1330:ILE:HG22	1:A:1379:VAL:HA	2.01	0.43
1:B:1016:MET:HB3	1:B:1261:GLN:OE1	2.17	0.43
1:B:1337:LEU:HA	1:B:1340:HIS:CD2	2.54	0.43
1:A:1551:ALA:C	4:A:259:HOH:O	2.61	0.43
1:B:1072:GLU:CD	1:B:1073:GLY:N	2.76	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:1149:ASN:O	1:B:1150:HIS:C	2.61	0.43
1:B:1206:MET:HE3	1:B:1273:GLY:N	2.34	0.43
1:B:1498:ASP:HB3	1:B:1528:ILE:CG2	2.49	0.43
1:A:1160:ASP:O	1:A:1161:PRO:C	2.61	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
1:B:1280:HIS:CD2	1:B:1282:CYS:HB2	2.54	0.43
1:B:1314:TYR:HD2	1:B:1437:PHE:HE2	1.67	0.43
1:B:1353:LEU:HB3	1:B:1394:LEU:HD22	2.01	0.43
1:B:1356:LEU:HD13	1:B:1356:LEU:O	2.18	0.43
1:B: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:B:1451:ILE:CG1	1:B:1489:MET:HE1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:ILE:O	1:A:1161:PRO:HD3	2.20	0.42
1:B:1047:VAL:HG11	1:B:1294:LEU:HD21	2.00	0.42
1:B:1286:ILE:C	1:B:1286:ILE:HD12	2.44	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:A:1414:LYS:O	1:A:1415:GLY:C	2.63	0.42
1:A:1471:ASP:O	1:A:1472:LYS:C	2.62	0.42
1:B:1076:THR:C	1:B:1078:SER:N	2.75	0.42
1:B:1159:ILE:O	1:B:1161:PRO:HD3	2.19	0.42
1:B:1250:LEU:H	1:B:1250:LEU:HD22	1.84	0.42
1:B:1453:LYS:NZ	1:B:1457:GLU:OE1	2.50	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:A:1475:GLN:O	1:A:1476:ARG:C	2.62	0.42
1:B:1030:GLU:C	1:B:1032:GLU:N	2.78	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:1229:TYR:CD2	1:B:1235:PRO:HG3	2.55	0.42
1:B:1360:PHE:C	1:B:1362:ASN:N	2.74	0.42
1:B:1390:ALA:HA	1:B:1393:ASN:HD22	1.84	0.42
1:B:1111:ALA:C	1:B:1113:GLY:N	2.78	0.42
1:B:1477:TYR:CZ	1:B:1518:LEU:HB3	2.54	0.42
1:A:1016:MET:HE3	1:A:1039:TYR:CD2	2.54	0.42
1:A:1108:LYS:HE2	1:A:1556:THR:HG23	2.01	0.42
1:A:1177:LEU:HB3	1:A:1197:PHE:HB2	2.01	0.42
1:A:1244:GLN:HE21	1:A:1244:GLN:N	2.13	0.42
1:B:1076:THR:O	1:B:1078:SER:N	2.52	0.42
1:B:1140:HIS:CE1	1:B:1167:ARG:O	2.73	0.42
1:B:1448:LYS:HE2	1:B:1466:TYR:CG	2.55	0.42
1:B:1465:ASN:C	1:B:1466:TYR:CD1	2.98	0.42
1:B:1148:ASP:OD2	1:B:1168:ARG:NH2	2.36	0.42
1:B:1486:PRO:C	1:B:1487:VAL:HG23	2.45	0.42
1:B:1009:GLU:HG2	1:B:1118:GLN:NE2	2.35	0.41
1:B:1012:GLN:HA	1:B:1012:GLN:OE1	2.19	0.41
1:B:1198:ASP:HA	1:B:1534:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1209:LEU:HD13	1:B:1251:MET:HE1	2.02	0.41
1:B:1308:LEU:O	1:B:1309:GLY:C	2.61	0.41
1:B:1336:ALA:O	1:B:1340:HIS:HD2	2.03	0.41
1:B:1518:LEU:HD12	1:B:1518:LEU:C	2.45	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:1259:LEU:C	1:A:1260:VAL:HG13	2.45	0.41
1:A:1490:ALA:HB3	1:A:1527:PRO:HA	2.02	0.41
1:B:1376:PRO:O	1:B:1377:ALA:HB2	2.21	0.41
1:A:1133:ILE:HG21	1:A:1171:ASP:OD1	2.20	0.41
1:A:1420:LEU:HA	1:A:1420:LEU:HD13	1.74	0.41
1:A:1555:ILE:O	1:A:1555:ILE:CG2	2.69	0.41
1:B:1085:LEU:C	1:B:1085:LEU:HD23	2.46	0.41
1:B:1154:GLY:C	1:B:1156:VAL:N	2.74	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:1307:ASP:OD1	1:A:1307:ASP:N	2.53	0.41
1:B:1017:LYS:H	1:B:1261:GLN:CD	2.26	0.41
1:B:1030:GLU:C	1:B:1032:GLU:H	2.28	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:A:1467:THR:O	1:A:1468:ALA:C	2.63	0.41
1:A:1475:GLN:C	1:A:1477:TYR:N	2.70	0.41
1:B:1047:VAL:CG1	1:B:1294:LEU:HD21	2.51	0.41
1:B:1249:LEU:C	1:B:1251:MET:N	2.78	0.41
1:B:1449:ASP:O	1:B:1452:ALA:HB3	2.20	0.41
1:A:1017:LYS:H	1:A:1261:GLN:NE2	2.18	0.41
1:A:1066:THR:HB	1:A:1362:ASN:ND2	2.34	0.41
1:A: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:A:1343:VAL:HG13	1:A:1344:PRO:HD2	2.02	0.41
1:A:1489:MET:HE1	1:A:1526:VAL:HG11	2.02	0.41
1:A:1491:LYS:HB3	1:A:1528:ILE:CG1	2.50	0.41
1:A:1552:ASP:OD1	1:A:1552:ASP:N	2.54	0.41
1:B:1061:LEU:HD22	1:B:1313:PHE:CE1	2.56	0.41
1:B:1420:LEU:O	1:B:1421:GLU:C	2.63	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:A:1330:ILE:CG2	1:A:1379:VAL:HG22	2.51	0.41
1:A:1452:ALA:O	1:A:1453:LYS:C	2.63	0.41
1:B:1029:GLN:H	1:B:1050:ARG:HH22	1.68	0.41
1:B:1193:ARG:HA	4:B:25:HOH:O	2.21	0.41
1:B:1412:TRP:CE3	1:B:1413:ALA:HB2	2.54	0.41
1:B:1417:GLU:HA	1:B:1420:LEU:CD2	2.38	0.41
1:B:1461:ALA:CA	1:B:1509:PHE:CE1	3.04	0.41
1:A:1209:LEU:HD13	1:A:1251:MET:HE3	2.03	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:1215:LEU:O	1:B:1216:MET:HE2	2.22	0.40
1:B:1398:LEU:C	1:B:1400:ALA:N	2.79	0.40
1:B:1402:ALA:O	1:B:1403:GLY:C	2.65	0.40
1:A:1333:THR:OG1	1:A:1336:ALA:HB3	2.21	0.40
1:B:1319:ARG:CZ	1:B:1443:LEU:HD13	2.51	0.40
1:B:1466:TYR:CD2	1:B:1513:VAL:HG11	2.56	0.40
1:A:1022:LEU:CD1	1:A:1261:GLN:HB3	2.51	0.40
1:A:1064:ALA:HB2	1:A:1331:VAL:HB	2.02	0.40
1:A:1221:ARG:HH11	1:A:1221:ARG:HD2	1.78	0.40
1:A:1354:GLU:OE2	1:A:1354:GLU:HA	2.21	0.40
1:A:1524:LEU:HA	1:A:1524:LEU:HD23	1.87	0.40
1:B:1116:TYR:HA	1:B:1263:LEU:HD12	2.03	0.40
1:B:1220:GLU:O	1:B:1223:SER:OG	2.35	0.40
1:A:1022:LEU:HD11	1:A:1261:GLN:OE1	2.21	0.40
1:A:1066:THR:N	1:A:1362:ASN:HD21	2.19	0.40
1:A:1097:ARG:HE	1:A:1097:ARG:HB2	1.61	0.40
1:A:1105:PHE:CD1	1:A:1105:PHE:N	2.89	0.40
1:A:1379:VAL:CG1	1:A:1380:ALA:N	2.84	0.40
1:A:1459:TYR:N	1:A:1459:TYR:CD1	2.87	0.40
1:B:1232:ASP:OD2	1:B:1232:ASP:N	2.55	0.40
1:B:1337:LEU:HD12	1:B:1337:LEU:N	2.36	0.40
1:A:1363:LEU:CD1	1:A:1367:ILE:HD11	2.51	0.40
1:A:1389:GLU:O	1:A:1391:GLU:N	2.54	0.40
1:B:1237:THR:H	1:B:1240:ASP:HB2	1.87	0.40
1:B:1389:GLU:C	1:B:1393:ASN:ND2	2.80	0.40

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

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

All (74) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	394 (91%)	38 (9%)	9	35
1	B	431/440 (98%)	391 (91%)	40 (9%)	8	33
All	All	863/880 (98%)	785 (91%)	78 (9%)	9	34

All (78) 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	1066	THR
1	A	1072	GLU
1	A	1094	VAL
1	A	1174	ASP
1	A	1215	LEU
1	A	1244	GLN

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Mol	Chain	Res	Type
1	A	1261	GLN
1	A	1274	PRO
1	A	1277	ASN
1	A	1278	ILE
1	A	1286	ILE
1	A	1290	THR
1	A	1307	ASP
1	A	1347	ASP
1	A	1353	LEU
1	A	1356	LEU
1	A	1381	ILE
1	A	1398	LEU
1	A	1420	LEU
1	A	1431	GLU
1	A	1438	HIS
1	A	1443	LEU
1	A	1449	ASP
1	A	1456	THR
1	A	1480	LEU
1	A	1487	VAL
1	A	1503	LEU
1	A	1512	THR
1	A	1513	VAL
1	A	1523	ARG
1	A	1526	VAL
1	A	1546	ASN
1	A	1552	ASP
1	B	1020	MET
1	B	1040	LYS
1	B	1050	ARG
1	B	1059	LEU
1	B	1060	ILE
1	B	1062	VAL
1	B	1065	ILE
1	B	1072	GLU
1	B	1094	VAL
1	B	1195	THR
1	B	1200	SER
1	B	1201	VAL
1	B	1215	LEU
1	B	1229	TYR
1	B	1232	ASP

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Mol	Chain	Res	Type
1	B	1244	GLN
1	B	1260	VAL
1	B	1266	THR
1	B	1269	PHE
1	B	1270	ILE
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	1443	LEU
1	B	1462	ASP
1	B	1480	LEU
1	B	1503	LEU
1	B	1518	LEU
1	B	1523	ARG
1	B	1529	THR
1	B	1535	MET
1	B	1546	ASN
1	B	1555	ILE

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

Mol	Chain	Res	Type
1	A	1140	HIS
1	A	1150	HIS
1	A	1153	GLN
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	A	1484	ASN
1	B	1029	GLN

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Mol	Chain	Res	Type
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	1277	ASN
1	B	1283	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	271	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	B	272	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	278	-	4,4,4	0.69	0	6,6,6	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	279	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	275	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	276	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	A	277	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	B	280	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	B	281	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	273	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	A	274	-	4,4,4	0.69	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 20 short contacts:

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