



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:49 PM GMT

PDB ID : 1QR6
Title : HUMAN MITOCHONDRIAL NAD(P)-DEPENDENT MALIC ENZYME
Authors : Xu, Y.; Bhargava, G.; Wu, H.; Loeber, G.; Tong, L.
Deposited on : 1999-06-18
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

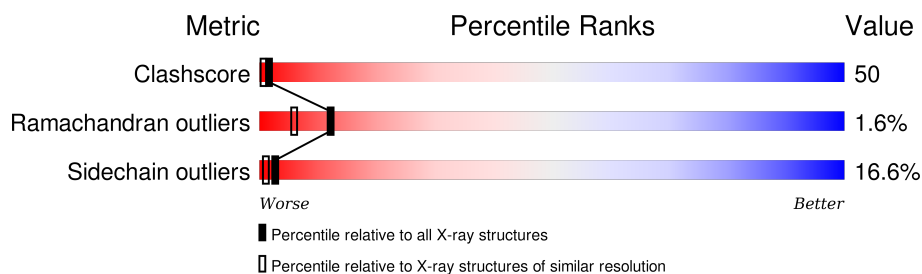
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	584	
1	B	584	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9620 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 MALIC ENZYME 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	Se	10	0	0
			4342	2779	739	801	9	14			
1	B	551	Total	C	N	O	S	Se	0	0	0
			4342	2779	739	801	9	14			

There are 28 discrepancies between the modelled and reference sequences:

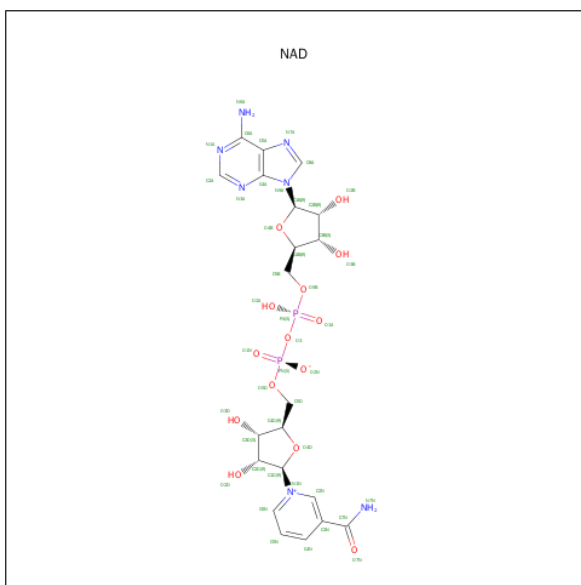
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	38	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	47	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	75	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	86	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	108	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	177	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	219	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	239	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	325	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	327	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	343	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	407	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	539	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1029	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1038	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1047	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1075	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1086	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1108	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1177	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1219	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1239	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1325	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1327	MSE	MET	MODIFIED RESIDUE	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1343	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1407	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1539	MSE	MET	MODIFIED RESIDUE	UNP P23368

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

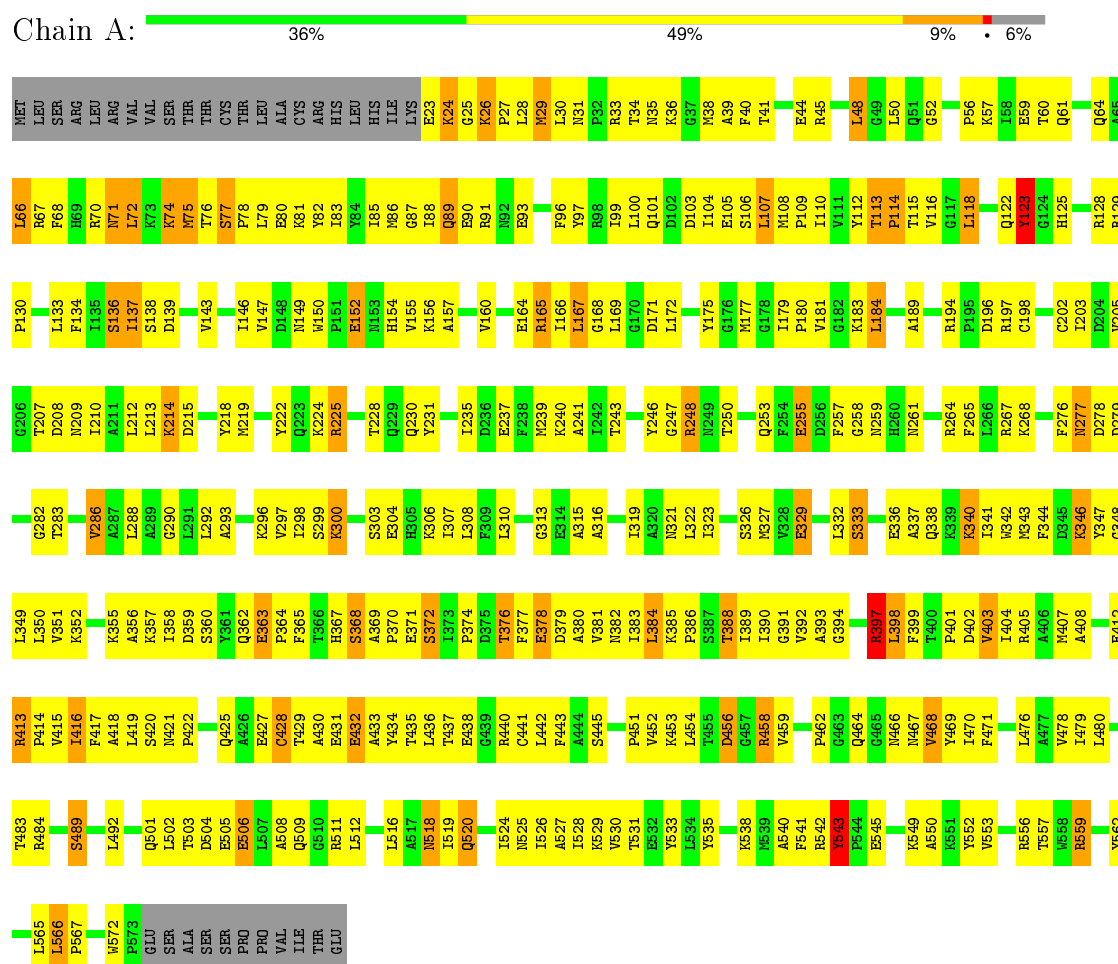
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	374	Total	O	0	0
			374	374		
3	B	386	Total	O	0	0
			386	386		

3 Residue-property plots

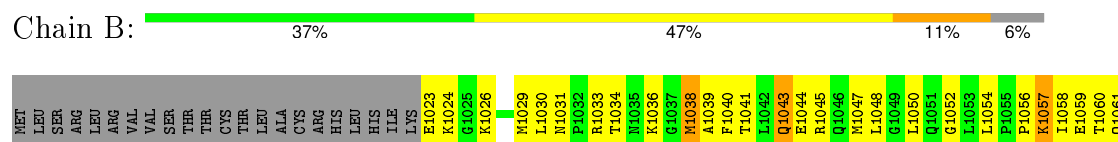
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: MALIC ENZYME 2



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Y1562	W490	I1410	Y1347	L1266	A1191	G1124	D1062
L1565	F1491	M4411	G1348	R1267	G1192	H1125	I1063
L1566	E1492	E1413	L1349	R1270	R1193	I1126	Q1064
E1571	E1493	R1413	L1350	F1276	R1194	F1127	A1065
H1572	A1494	P1414	V1351	M1277	P1195	R1128	L1066
P1573	A1495	V1415	K1352	D1278	R1196	K1131	R1067
GLU	K1496	I1416	G1353	D1276	R1197	G1132	F1068
SER	A1497	F1417	R1354	D1279	C1198	L1133	H1069
SER	L1498	A1418	K1355	I1280	C1202	S1136	R1070
SER	Q1501	L1419	A1356	I1281	S1137	M1071	N1071
SER	L1502	S1420	K1357	G1282	V1205	S1136	L1072
PRO	E1505	T1423	I1358	V1286	G1206	I1140	K1073
PRO	E1506	A1424	D1359	L1287	T1207	R1143	K1074
VAL	L1507	Q1425	S1360	L1288	V1143	S1145	M1075
ILE	A1508	E1427	Y1361	A1289	R1144	P1078	S1077
THR	Q1509	C1428	A1369	L1292	I1210	L1079	P1078
GLU	G1510	T1429	H1367	L1293	L1213	I1146	E1080
R1511	R1511	E1432	S1368	A1293	K1214	V1147	K1081
L1512	L1512	A1433	A1361	A1294	D1215	I1148	I1082
Y1513	Y1513	A1433	Q1295	K1296	P1216	M1149	I1083
P1514	P1514	E1427	K1296	K1296	F1217	W1150	Y1084
P1515	P1515	L1436	V1297	V1297	Y1218	P1151	I1085
L1516	L1516	T1437	I1298	I1298	E1152	M1086	M1086
A1517	A1517	R1440	S1299	S1299	N1153	G1087	G1087
M1518	M1518	C1441	K1300	K1300	H1154	I1088	I1088
I1519	I1519	L1442	P1301	P1301	V1155	Q1089	Q1089
Q1520	Q1520	L1442	F1377	F1377	K1156	E1090	E1090
E1521	E1521	S1445	E1378	E1378	V1160	R1091	R1091
V1522	V1522	G1446	D1379	D1379	T1161	N1092	N1092
S1523	S1523	K1453	A1380	A1380	I1162	E1093	E1093
I1524	I1524	L1454	V1381	V1381	G1163	K1094	K1094
M1525	M1525	T1455	N1382	N1382	L1164	L1095	L1095
I1526	I1526	T1455	L1383	L1383	R1165	I1099	I1099
A1527	A1527	D1456	L1384	L1384	L1166	L1100	L1100
I1528	I1528	G1457	K1385	K1385	G1168	D1103	D1103
K1529	K1529	R1458	P1386	P1386	L1169	I1104	I1104
V1530	V1530	V1459	S1397	S1397	L1172	E1105	E1105
T1531	T1531	F1460	T1388	T1388	G1173	S1106	S1106
E1532	E1532	T1461	I1390	I1390	V1174	L1107	L1107
Y1533	Y1533	P1462	G1391	G1391	Y1175	M1108	M1108
K1538	K1538	Q1463	V1392	V1392	G1176	P1109	P1109
R1542	R1542	G1465	A1393	A1393	M1177	I1110	I1110
Y1543	Y1543	N1466	L1322	L1322	G1178	V1111	V1111
P1544	P1544	M1467	V1324	V1324	I1179	Y1112	Y1112
E1545	E1545	V1468	M1325	M1325	P1180	T1113	T1113
P1546	P1546	Y1469	V1328	V1328	V1181	P1114	P1114
E1547	E1547	P1472	L1332	L1332	G1182	T1115	T1115
K1551	K1551	V1478	V1403	V1403	K1183	G1117	G1117
E1554	E1554	N1482	I1404	I1404	L1184	V1116	V1116
E1555	E1555	R1405	V1403	V1403	C1185	G1117	G1117
W1558	W1558	T1483	M1343	M1343	L1185	L1118	L1118
R1559	R1559	R1484	F1344	F1344	Y1187	C1120	C1120
		S1489	D1345	D1345	T1188	S1121	S1121
			A1408	A1408	R1264	Q1122	Q1122
			S1409	S1409	F1265	Y1123	Y1123

4 Data and refinement statistics

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

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α , β , γ	204.40 Å 107.00 Å 59.20 Å 90.00° 90.00° 101.90°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	87.0 (20.00-2.10)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.228 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9620	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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:
NAD

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	0.37	0/4422	0.64	2/5967 (0.0%)
1	B	0.37	0/4422	0.63	3/5967 (0.1%)
All	All	0.37	0/8844	0.63	5/11934 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1543	TYR	N-CA-C	7.24	130.53	111.00
1	A	543	TYR	N-CA-C	6.19	127.71	111.00
1	A	542	ARG	N-CA-C	-5.91	95.03	111.00
1	B	1542	ARG	N-CA-C	-5.62	95.81	111.00
1	B	1543	TYR	C-N-CD	5.00	138.90	128.40

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	4342	0	4366	455	0
1	B	4342	0	4366	441	0
2	A	88	0	52	2	0
2	B	88	0	52	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	374	0	0	145	0
3	B	386	0	0	155	0
All	All	9620	0	8836	884	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 50.

All (884) 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:1107:LEU:HD12	3:B:2496:HOH:O	1.42	1.19
1:A:218:TYR:HB2	3:A:2698:HOH:O	1.44	1.18
1:B:1472:PRO:HB2	3:B:2252:HOH:O	1.48	1.11
1:A:215:ASP:HB3	3:A:2698:HOH:O	1.51	1.10
1:B:1243:THR:HB	1:B:1248:ARG:HE	1.20	1.06
1:B:1513:TYR:HB3	3:B:2740:HOH:O	1.55	1.05
1:B:1113:THR:HB	1:B:1114:PRO:HD3	1.39	1.05
1:A:85:ILE:HG23	1:A:86:MSE:HE3	1.39	1.05
1:A:454:LEU:HD12	3:A:2700:HOH:O	1.58	1.03
1:B:1410:ILE:HG21	3:B:2585:HOH:O	1.60	1.01
1:B:1298:ILE:HG13	3:B:2614:HOH:O	1.61	1.00
1:B:1177:MSE:HG2	1:B:1202:CYS:HB2	1.46	0.97
1:B:1287:ALA:HA	3:B:2167:HOH:O	1.62	0.97
1:A:433:ALA:HB3	3:A:2670:HOH:O	1.62	0.97
1:B:1297:VAL:HG12	1:B:1298:ILE:HD13	1.48	0.96
1:B:1454:LEU:HD11	1:B:1460:PHE:HE2	1.31	0.95
1:B:1385:LYS:HB2	3:B:2680:HOH:O	1.65	0.94
1:A:104:ILE:HG13	1:A:108:MSE:HE2	1.49	0.94
1:A:72:LEU:HA	1:A:75:MSE:HE3	1.48	0.94
1:B:1310:LEU:HD12	3:B:2076:HOH:O	1.66	0.94
1:B:1492:LEU:HB2	3:B:2514:HOH:O	1.65	0.94
1:B:1543:TYR:O	1:B:1545:GLU:N	2.01	0.93
1:A:453:LYS:HE2	3:A:2688:HOH:O	1.67	0.93
1:A:86:MSE:HA	1:A:86:MSE:HE2	1.50	0.93
1:B:1261:ASN:HD22	1:B:1264:ARG:HE	1.01	0.92
1:A:61:GLN:HA	1:A:64:GLN:HE21	1.31	0.92
1:A:113:THR:HB	1:A:114:PRO:HD3	1.48	0.92
1:A:376:THR:HG22	1:A:379:ASP:H	1.36	0.91
1:A:543:TYR:O	1:A:545:GLU:N	2.05	0.90
1:A:393:ALA:HB3	3:A:2677:HOH:O	1.72	0.90
1:B:1526:ILE:HG23	3:B:2727:HOH:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ILE:HG23	1:A:388:THR:HG22	1.53	0.88
1:B:1177:MSE:HG2	1:B:1202:CYS:CB	2.02	0.88
1:A:349:LEU:HD23	3:A:2556:HOH:O	1.74	0.88
1:A:527:ALA:O	1:A:531:THR:HG23	1.74	0.87
1:B:1057:LYS:HB3	3:B:2238:HOH:O	1.75	0.86
1:B:1086:MSE:HA	1:B:1086:MSE:HE2	1.57	0.86
1:B:1527:ALA:O	1:B:1531:THR:HG23	1.76	0.86
1:A:277:ASN:HD21	1:A:279:ASP:HB2	1.39	0.85
1:A:44:GLU:O	1:A:48:LEU:HB2	1.75	0.85
1:A:431:GLU:HG2	1:A:452:VAL:HG22	1.58	0.85
1:B:1429:THR:HG23	1:B:1432:GLU:H	1.41	0.85
1:A:518:ASN:HB3	3:A:2661:HOH:O	1.75	0.85
1:B:1308:LEU:HB3	1:B:1389:ILE:HD12	1.59	0.84
1:A:91:ARG:HD2	3:B:2639:HOH:O	1.76	0.84
1:A:437:THR:HG23	3:A:2220:HOH:O	1.77	0.84
1:B:1547:GLU:HG2	3:B:2652:HOH:O	1.76	0.84
1:A:557:THR:HG22	3:A:2386:HOH:O	1.77	0.84
1:B:1515:PRO:HG2	1:B:1518:ASN:HD21	1.43	0.84
1:A:476:LEU:HD21	3:A:2386:HOH:O	1.77	0.84
1:B:1354:ARG:HD3	1:B:1358:ILE:HD11	1.58	0.84
1:A:167:LEU:HD11	3:A:2550:HOH:O	1.77	0.84
1:B:1058:ILE:HG13	3:B:2147:HOH:O	1.77	0.83
1:B:1194:ARG:HA	3:B:2518:HOH:O	1.79	0.83
1:A:374:PRO:HG3	1:A:380:ALA:HA	1.58	0.83
1:A:392:VAL:O	1:A:392:VAL:HG12	1.76	0.83
1:B:1319:ILE:HG23	3:B:2547:HOH:O	1.77	0.83
1:A:389:ILE:HG21	3:A:2333:HOH:O	1.77	0.83
1:B:1261:ASN:ND2	1:B:1264:ARG:HE	1.76	0.83
1:B:1558:TRP:HB3	3:B:2518:HOH:O	1.78	0.83
1:A:454:LEU:HA	3:A:2627:HOH:O	1.80	0.82
1:B:1454:LEU:HD11	1:B:1460:PHE:CE2	2.13	0.82
1:A:531:THR:HB	3:A:2234:HOH:O	1.78	0.82
1:A:429:THR:HG23	1:A:432:GLU:H	1.43	0.82
1:A:376:THR:HG23	1:A:378:GLU:H	1.44	0.82
1:B:1442:LEU:HD12	3:B:2614:HOH:O	1.79	0.82
1:A:109:PRO:O	1:A:114:PRO:HD2	1.79	0.82
1:A:24:LYS:HA	1:A:28:LEU:HD22	1.60	0.82
1:A:388:THR:HG23	3:A:2287:HOH:O	1.79	0.81
1:A:86:MSE:HE1	1:A:96:PHE:CE1	2.15	0.81
1:A:154:HIS:O	1:A:197:ARG:HG2	1.81	0.81
1:B:1405:ARG:HD2	3:B:2359:HOH:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ILE:HG21	3:A:2715:HOH:O	1.80	0.80
1:A:378:GLU:OE1	1:A:402:ASP:HB3	1.80	0.80
1:A:338:GLN:HB3	3:A:2569:HOH:O	1.80	0.80
1:B:1109:PRO:O	1:B:1114:PRO:HD2	1.82	0.80
1:B:1104:ILE:HG13	1:B:1108:MSE:HG3	1.63	0.80
1:B:1039:ALA:HA	1:B:1059:GLU:O	1.82	0.79
1:A:78:PRO:HG3	3:A:2628:HOH:O	1.81	0.79
1:A:372:SER:HB2	1:A:383:ILE:HG12	1.64	0.79
1:A:327:MSE:HE3	1:A:337:ALA:HB1	1.65	0.79
1:B:1392:VAL:O	1:B:1392:VAL:HG12	1.82	0.79
1:A:390:ILE:HG12	3:A:2571:HOH:O	1.83	0.79
1:A:128:ARG:HH22	1:B:1128:ARG:NH1	1.80	0.79
1:A:288:LEU:HG	3:A:2469:HOH:O	1.81	0.79
1:A:436:LEU:HB3	3:A:2512:HOH:O	1.83	0.79
1:B:1514:PRO:O	3:B:2740:HOH:O	2.01	0.78
1:A:471:PHE:CD1	3:A:2711:HOH:O	2.36	0.78
1:A:296:LYS:HE3	3:A:2737:HOH:O	1.83	0.78
1:B:1428:CYS:SG	3:B:2311:HOH:O	2.42	0.77
1:B:1351:VAL:HG11	1:B:1369:ALA:HB2	1.66	0.77
1:A:435:THR:HA	3:A:2229:HOH:O	1.83	0.77
1:B:1411:ASN:HB2	3:B:2146:HOH:O	1.84	0.77
1:A:437:THR:HG22	3:A:2063:HOH:O	1.83	0.77
1:A:310:LEU:HD23	1:A:427:GLU:HG2	1.68	0.76
1:B:1113:THR:CB	1:B:1114:PRO:HD3	2.15	0.76
1:A:386:PRO:HG2	3:A:2256:HOH:O	1.85	0.76
1:B:1085:ILE:HG23	1:B:1086:MSE:HE3	1.66	0.76
1:A:113:THR:CB	1:A:114:PRO:HD3	2.16	0.76
1:B:1406:ALA:C	3:B:2312:HOH:O	2.25	0.76
1:A:437:THR:HG21	1:A:441:CYS:HB3	1.68	0.75
1:A:416:ILE:HD11	1:A:441:CYS:CB	2.16	0.75
1:B:1240:LYS:HE2	3:B:2724:HOH:O	1.87	0.75
1:B:1294:ALA:HB1	1:B:1442:LEU:HD13	1.67	0.75
1:A:315:ALA:HA	3:A:2644:HOH:O	1.87	0.74
1:A:85:ILE:HG13	3:A:2715:HOH:O	1.87	0.74
1:B:1526:ILE:CG2	3:B:2727:HOH:O	2.32	0.74
1:B:1078:PRO:HB3	3:B:2741:HOH:O	1.87	0.74
1:A:212:LEU:O	3:A:2698:HOH:O	2.05	0.74
1:B:1207:THR:HG21	3:B:2716:HOH:O	1.85	0.74
1:A:308:LEU:HB3	1:A:389:ILE:HD12	1.67	0.74
1:A:250:THR:HB	3:A:2279:HOH:O	1.87	0.74
1:B:1399:PHE:HD1	3:B:2311:HOH:O	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1307:ILE:HG23	1:B:1388:THR:HG22	1.68	0.73
1:B:1078:PRO:HD2	3:B:2507:HOH:O	1.87	0.73
1:B:1411:ASN:ND2	3:B:2146:HOH:O	2.22	0.73
1:B:1340:LYS:HE3	3:B:2280:HOH:O	1.88	0.73
1:B:1320:ALA:HB2	3:B:2102:HOH:O	1.87	0.73
1:A:104:ILE:CG1	1:A:108:MSE:HE2	2.18	0.73
1:A:23:GLU:HG2	1:A:24:LYS:N	2.04	0.73
1:B:1513:TYR:OH	3:B:2167:HOH:O	2.05	0.73
1:B:1308:LEU:HB2	1:B:1386:PRO:HG3	1.71	0.73
1:A:440:ARG:HG2	3:A:2237:HOH:O	1.87	0.73
1:B:1414:PRO:HA	3:B:2146:HOH:O	1.89	0.73
1:B:1043:GLN:HB3	3:B:2742:HOH:O	1.87	0.73
1:B:1526:ILE:O	1:B:1530:VAL:HG23	1.87	0.73
1:A:376:THR:CG2	1:A:379:ASP:H	2.02	0.72
1:B:1308:LEU:HB3	1:B:1389:ILE:CD1	2.19	0.72
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.71	0.72
1:A:128:ARG:HH12	1:B:1128:ARG:HH12	1.34	0.72
1:B:1386:PRO:HG2	3:B:2265:HOH:O	1.90	0.72
1:B:1261:ASN:HD22	1:B:1264:ARG:NE	1.84	0.72
1:A:292:LEU:HD11	3:A:2469:HOH:O	1.89	0.72
1:B:1372:SER:O	1:B:1383:ILE:HD13	1.89	0.72
1:B:1165:ARG:HD3	1:B:1258:GLY:HA2	1.71	0.72
1:A:86:MSE:HE1	1:A:96:PHE:CZ	2.24	0.72
1:A:416:ILE:HD11	1:A:441:CYS:HB2	1.70	0.72
1:A:433:ALA:O	1:A:437:THR:HG23	1.90	0.72
1:A:454:LEU:HD11	3:A:2178:HOH:O	1.89	0.72
1:A:265:PHE:HD1	3:A:2457:HOH:O	1.72	0.72
1:B:1217:PHE:HB3	3:B:2107:HOH:O	1.90	0.71
1:B:1113:THR:HB	1:B:1114:PRO:CD	2.19	0.71
1:A:456:ASP:OD1	1:A:458:ARG:HB2	1.90	0.71
1:A:367:HIS:HE1	3:A:2569:HOH:O	1.71	0.71
1:B:1163:GLY:HA2	1:B:1166:ILE:HD11	1.72	0.71
1:A:82:TYR:HD2	1:A:83:ILE:HD13	1.54	0.71
1:A:454:LEU:HD22	3:A:2229:HOH:O	1.89	0.71
1:B:1183:LYS:HE2	1:B:1255:GLU:OE2	1.91	0.70
1:A:506:GLU:O	1:A:511:ARG:HB2	1.91	0.70
1:A:64:GLN:O	1:A:68:PHE:HD1	1.73	0.70
1:A:385:LYS:HG3	3:A:2226:HOH:O	1.91	0.70
1:A:553:VAL:HG13	3:A:2141:HOH:O	1.91	0.70
1:B:1302:ILE:HA	1:B:1305:HIS:CD2	2.27	0.70
1:B:1523:SER:HB3	3:B:2252:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ASN:CB	3:A:2681:HOH:O	2.40	0.69
1:B:1378:GLU:OE1	1:B:1402:ASP:HB3	1.92	0.69
1:A:26:LYS:HE3	3:B:2492:HOH:O	1.93	0.69
1:A:183:LYS:HG3	3:A:2534:HOH:O	1.92	0.69
1:A:243:THR:HG22	3:A:2279:HOH:O	1.92	0.69
1:A:152:GLU:HG2	1:A:196:ASP:O	1.92	0.69
1:B:1086:MSE:HE1	1:B:1096:PHE:CE1	2.27	0.69
1:A:374:PRO:HD3	1:A:383:ILE:HD13	1.73	0.69
1:A:471:PHE:CE2	3:A:2692:HOH:O	2.45	0.69
1:B:1152:GLU:HG2	1:B:1196:ASP:O	1.93	0.69
1:B:1090:GLU:HB3	3:B:2094:HOH:O	1.91	0.69
2:A:601:NAD:H4N	3:A:2275:HOH:O	1.93	0.69
1:B:1454:LEU:HD12	1:B:1458:ARG:HB2	1.75	0.69
1:A:404:ILE:CG2	3:A:2220:HOH:O	2.41	0.68
1:B:1060:THR:H	1:B:1063:ILE:HD12	1.58	0.68
1:A:79:LEU:O	1:A:83:ILE:HG12	1.93	0.68
1:B:1179:ILE:HB	1:B:1180:PRO:HD3	1.75	0.68
1:A:381:VAL:HG22	3:A:2256:HOH:O	1.91	0.68
1:B:1061:GLN:NE2	3:B:2583:HOH:O	2.25	0.68
1:A:307:ILE:HG23	1:A:388:THR:CG2	2.24	0.68
1:B:1558:TRP:CB	3:B:2518:HOH:O	2.40	0.68
1:A:464:GLN:HA	3:A:2143:HOH:O	1.91	0.68
1:B:1511:ARG:HH11	1:B:1511:ARG:HG2	1.58	0.68
1:A:303:SER:O	1:A:340:LYS:HE2	1.94	0.68
1:B:1409:SER:N	3:B:2312:HOH:O	2.13	0.68
1:A:80:GLU:C	3:A:2308:HOH:O	2.32	0.68
1:B:1325:MSE:HE2	3:B:2514:HOH:O	1.94	0.68
1:A:48:LEU:HD22	3:A:2081:HOH:O	1.94	0.68
1:B:1325:MSE:CE	3:B:2514:HOH:O	2.41	0.67
1:B:1381:VAL:HG22	3:B:2265:HOH:O	1.93	0.67
1:A:459:VAL:HA	3:A:2189:HOH:O	1.94	0.67
1:B:1103:ASP:HB3	1:B:1107:LEU:HD22	1.77	0.67
1:A:376:THR:HG23	1:A:378:GLU:N	2.09	0.67
1:A:401:PRO:HB3	1:A:436:LEU:HD21	1.76	0.67
1:B:1058:ILE:HG22	3:B:2329:HOH:O	1.95	0.67
1:B:1392:VAL:O	1:B:1392:VAL:CG1	2.42	0.67
1:B:1484:ARG:HB2	3:B:2087:HOH:O	1.95	0.66
1:B:1110:ILE:HB	3:B:2496:HOH:O	1.95	0.66
1:B:1519:ILE:HG23	3:B:2565:HOH:O	1.93	0.66
1:A:85:ILE:HG23	1:A:86:MSE:CE	2.20	0.66
1:B:1294:ALA:CB	1:B:1442:LEU:HD13	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ILE:O	1:A:239:MSE:HG2	1.95	0.66
1:A:327:MSE:HE1	1:A:337:ALA:O	1.94	0.66
1:A:183:LYS:NZ	3:A:2692:HOH:O	2.20	0.65
1:B:1043:GLN:HE21	1:B:1566:LEU:HD11	1.61	0.65
1:A:225:ARG:HB2	3:A:2531:HOH:O	1.95	0.65
1:A:415:VAL:N	3:A:2752:HOH:O	2.25	0.65
1:B:1153:ASN:HD22	1:B:1245:ARG:HH21	1.44	0.65
1:A:405:ARG:HA	3:A:2512:HOH:O	1.97	0.65
1:B:1086:MSE:HE1	1:B:1096:PHE:CZ	2.32	0.65
1:B:1277:ASN:HD22	1:B:1277:ASN:C	1.99	0.65
1:B:1551:LYS:O	1:B:1555:GLU:HG3	1.95	0.65
1:B:1202:CYS:SG	3:B:2416:HOH:O	2.54	0.65
1:A:128:ARG:HH12	1:B:1128:ARG:NH1	1.94	0.65
1:B:1104:ILE:HD13	3:B:2565:HOH:O	1.97	0.65
1:B:1207:THR:CB	3:B:2716:HOH:O	2.44	0.65
1:B:1038:MSE:SE	3:B:2238:HOH:O	2.64	0.65
1:B:1294:ALA:HB1	1:B:1442:LEU:CD1	2.27	0.65
1:A:128:ARG:NH1	1:B:1128:ARG:HH12	1.95	0.65
1:A:471:PHE:CG	3:A:2711:HOH:O	2.49	0.64
1:A:467:ASN:OD1	3:A:2275:HOH:O	2.14	0.64
1:A:321:ASN:HB3	3:A:2678:HOH:O	1.96	0.64
1:A:129:ARG:HG3	1:A:130:PRO:HD2	1.77	0.64
1:A:377:PHE:CZ	1:A:389:ILE:HD11	2.32	0.64
1:A:468:VAL:HA	1:A:471:PHE:CE2	2.32	0.64
1:B:1169:LEU:N	1:B:1169:LEU:HD12	2.13	0.64
1:A:347:TYR:CD1	1:A:356:ALA:HB1	2.32	0.64
1:B:1188:THR:CG2	3:B:2409:HOH:O	2.46	0.64
1:B:1250:THR:HB	3:B:2746:HOH:O	1.97	0.63
1:B:1308:LEU:HD23	1:B:1389:ILE:HD11	1.79	0.63
1:B:1137:ILE:O	1:B:1140:ARG:HG2	1.98	0.63
1:B:1538:LYS:HA	3:B:2213:HOH:O	1.97	0.63
1:A:40:PHE:HE2	1:A:565:LEU:HD12	1.62	0.63
1:B:1038:MSE:HG2	1:B:1057:LYS:O	1.99	0.63
1:A:413:ARG:HD2	3:A:2134:HOH:O	1.98	0.63
1:B:1376:THR:HG22	1:B:1379:ASP:H	1.63	0.63
1:B:1349:LEU:HD21	1:B:1384:LEU:HD21	1.79	0.63
1:B:1059:GLU:CD	1:B:1067:ARG:HH12	2.02	0.63
1:B:1112:TYR:CG	1:B:1113:THR:N	2.66	0.63
1:A:524:ILE:HD12	3:A:2386:HOH:O	1.97	0.63
1:A:208:ASP:N	3:A:2531:HOH:O	2.31	0.63
1:A:184:LEU:HG	1:A:198:CYS:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:MSE:CE	1:A:519:ILE:HG21	2.29	0.62
1:B:1103:ASP:O	1:B:1107:LEU:HB2	2.00	0.62
1:B:1243:THR:HB	1:B:1248:ARG:NE	2.04	0.62
1:A:308:LEU:HB3	1:A:389:ILE:CD1	2.28	0.62
1:B:1404:ILE:HD12	1:B:1436:LEU:HD12	1.80	0.62
1:B:1414:PRO:HB3	3:B:2146:HOH:O	1.99	0.62
1:B:1214:LYS:HD3	3:B:2156:HOH:O	2.00	0.62
1:A:136:SER:OG	1:A:138:SER:HB2	2.00	0.62
1:A:85:ILE:HA	1:A:88:ILE:HD12	1.81	0.62
1:A:434:TYR:HB3	3:A:2178:HOH:O	2.00	0.62
1:A:113:THR:HB	1:A:114:PRO:CD	2.27	0.62
1:B:1177:MSE:SE	3:B:2597:HOH:O	2.68	0.61
1:B:1188:THR:HG21	3:B:2409:HOH:O	1.99	0.61
1:B:1024:LYS:HB2	3:B:2310:HOH:O	1.99	0.61
1:A:277:ASN:ND2	1:A:279:ASP:HB2	2.14	0.61
1:B:1207:THR:CG2	3:B:2716:HOH:O	2.44	0.61
1:B:1082:TYR:HD2	1:B:1083:ILE:HD13	1.65	0.61
1:B:1357:LYS:HB3	1:B:1357:LYS:NZ	2.16	0.61
1:A:189:ALA:O	1:A:520:GLN:NE2	2.34	0.61
1:B:1024:LYS:HE3	3:B:2310:HOH:O	2.00	0.61
1:B:1075:MSE:HG2	1:B:1080:GLU:CD	2.21	0.61
1:A:228:THR:HG23	3:A:2560:HOH:O	2.00	0.61
1:A:86:MSE:HE2	1:A:86:MSE:CA	2.28	0.61
1:B:1494:ALA:HB1	3:B:2727:HOH:O	2.00	0.61
1:A:297:VAL:HG12	1:A:298:ILE:HD13	1.83	0.61
1:A:374:PRO:CD	1:A:383:ILE:HD13	2.31	0.61
1:A:183:LYS:HE3	3:A:2711:HOH:O	2.00	0.61
1:B:1110:ILE:CB	3:B:2496:HOH:O	2.48	0.60
1:A:261:ASN:HD22	1:A:264:ARG:HE	1.47	0.60
1:A:177:MSE:HE1	1:A:181:VAL:HG23	1.83	0.60
1:A:454:LEU:CD2	3:A:2229:HOH:O	2.47	0.60
1:B:1389:ILE:HG21	3:B:2538:HOH:O	1.99	0.60
1:B:1152:GLU:HG3	3:B:2660:HOH:O	2.02	0.60
1:B:1392:VAL:HG12	3:B:2035:HOH:O	2.01	0.60
1:B:1184:LEU:HG	1:B:1198:CYS:HB3	1.83	0.60
1:B:1394:GLY:HA2	1:B:1420:SER:HB3	1.84	0.60
1:A:218:TYR:O	1:B:1057:LYS:HE2	2.01	0.60
1:B:1089:GLN:HG3	1:B:1090:GLU:N	2.16	0.60
1:A:469:TYR:CE1	3:A:2681:HOH:O	2.52	0.60
1:A:505:GLU:H	1:A:505:GLU:CD	2.04	0.60
1:B:1399:PHE:CD1	3:B:2311:HOH:O	2.51	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:TYR:O	1:A:116:VAL:HG12	2.01	0.60
1:A:177:MSE:CE	1:A:181:VAL:HG23	2.31	0.60
1:A:518:ASN:HA	3:A:2214:HOH:O	2.03	0.59
1:A:489:SER:HB2	1:A:533:TYR:OH	2.02	0.59
1:B:1513:TYR:C	3:B:2740:HOH:O	2.40	0.59
1:B:1282:GLY:O	1:B:1286:VAL:HG22	2.03	0.59
1:B:1091:ARG:HD2	3:B:2640:HOH:O	2.02	0.59
1:A:177:MSE:HG2	1:A:202:CYS:CB	2.33	0.59
1:B:1288:LEU:N	3:B:2547:HOH:O	2.34	0.59
1:A:401:PRO:O	1:A:405:ARG:HG2	2.03	0.59
1:A:342:TRP:HA	3:A:2437:HOH:O	2.01	0.59
1:B:1150:TRP:CE2	1:B:1199:LEU:HD13	2.38	0.59
1:B:1428:CYS:HB3	3:B:2311:HOH:O	2.02	0.59
1:A:116:VAL:HG13	3:A:2550:HOH:O	2.03	0.59
1:B:1469:TYR:CZ	1:B:1516:LEU:HD13	2.37	0.59
1:A:407:MSE:HE1	3:A:2256:HOH:O	2.03	0.59
1:B:1515:PRO:HG2	1:B:1518:ASN:ND2	2.15	0.59
1:B:1079:LEU:HD21	1:B:1122:GLN:HG3	1.85	0.59
1:B:1433:ALA:O	1:B:1437:THR:HG23	2.03	0.59
1:A:112:TYR:CG	1:A:113:THR:N	2.71	0.59
1:B:1413:ARG:HA	1:B:1440:ARG:O	2.02	0.59
1:B:1086:MSE:CE	1:B:1096:PHE:CE1	2.86	0.58
1:B:1429:THR:HG22	1:B:1432:GLU:CG	2.33	0.58
1:B:1429:THR:HG22	1:B:1432:GLU:OE1	2.03	0.58
1:A:462:PRO:HG3	3:A:2582:HOH:O	2.02	0.58
1:A:108:MSE:N	1:A:109:PRO:HD2	2.18	0.58
1:B:1277:ASN:ND2	1:B:1279:ASP:H	2.01	0.58
1:A:505:GLU:HG2	3:A:2714:HOH:O	2.03	0.58
1:B:1286:VAL:HG11	1:B:1466:ASN:O	2.03	0.58
1:A:75:MSE:SE	3:A:2308:HOH:O	2.71	0.58
1:A:103:ASP:HB3	1:A:107:LEU:HD22	1.84	0.58
1:A:404:ILE:HG22	3:A:2220:HOH:O	2.02	0.58
1:A:72:LEU:HA	1:A:75:MSE:CE	2.28	0.58
1:B:1207:THR:HB	3:B:2716:HOH:O	2.03	0.58
1:B:1077:SER:O	1:B:1081:LYS:HG3	2.04	0.58
1:A:379:ASP:O	1:A:383:ILE:HD12	2.03	0.58
1:A:438:GLU:HA	3:A:2555:HOH:O	2.03	0.58
1:B:1298:ILE:HD11	1:B:1442:LEU:HD11	1.85	0.58
1:B:1153:ASN:ND2	1:B:1245:ARG:HH21	2.02	0.58
1:A:137:ILE:HG13	1:A:137:ILE:O	2.03	0.58
1:A:416:ILE:HD11	1:A:441:CYS:SG	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1298:ILE:O	1:B:1300:LYS:N	2.36	0.58
1:B:1302:ILE:CD1	3:B:2722:HOH:O	2.52	0.58
1:B:1454:LEU:CD1	1:B:1458:ARG:HB2	2.34	0.58
1:A:60:THR:O	1:A:64:GLN:HG3	2.03	0.58
1:B:1559:ARG:HG2	3:B:2338:HOH:O	2.04	0.58
1:A:286:VAL:HG13	1:A:470:ILE:HG12	1.84	0.58
1:A:458:ARG:NH2	3:A:2700:HOH:O	2.37	0.57
1:B:1525:ASN:O	1:B:1529:LYS:HG2	2.04	0.57
1:A:381:VAL:CG2	1:A:407:MSE:HE1	2.34	0.57
1:A:293:ALA:O	1:A:296:LYS:HB2	2.03	0.57
1:B:1573:PRO:HA	3:B:2734:HOH:O	2.03	0.57
1:A:86:MSE:CE	1:A:96:PHE:CE1	2.88	0.57
1:B:1117:GLY:O	1:B:1169:LEU:HD21	2.04	0.57
1:A:129:ARG:HB3	3:A:2434:HOH:O	2.03	0.57
1:B:1231:TYR:O	1:B:1235:ILE:HG12	2.04	0.57
1:A:405:ARG:CA	3:A:2512:HOH:O	2.52	0.57
1:B:1401:PRO:HA	1:B:1436:LEU:CD1	2.34	0.57
1:B:1300:LYS:HD3	1:B:1304:GLU:HB3	1.86	0.57
1:A:109:PRO:HA	1:A:113:THR:HB	1.86	0.57
1:B:1315:ALA:HB3	1:B:1392:VAL:CG1	2.34	0.57
1:A:505:GLU:O	1:A:509:GLN:HG3	2.04	0.57
1:B:1399:PHE:CG	1:B:1427:GLU:HB3	2.40	0.57
1:A:277:ASN:ND2	1:A:279:ASP:H	2.03	0.57
1:A:36:LYS:O	1:A:39:ALA:HB3	2.05	0.57
1:B:1043:GLN:NE2	1:B:1566:LEU:HD11	2.20	0.57
1:B:1123:TYR:HB3	1:B:1175:TYR:CD2	2.39	0.57
1:A:166:ILE:N	1:A:166:ILE:HD12	2.20	0.57
1:A:437:THR:CG2	3:A:2220:HOH:O	2.45	0.57
1:A:315:ALA:HB3	1:A:392:VAL:HG11	1.85	0.57
1:B:1073:LYS:HE2	1:B:1074:LYS:NZ	2.20	0.57
1:A:430:ALA:HB2	3:A:2582:HOH:O	2.05	0.56
1:B:1033:ARG:NH1	1:B:1093:GLU:OE1	2.38	0.56
1:A:41:THR:OG1	1:A:44:GLU:HG3	2.05	0.56
1:B:1195:PRO:HG3	3:B:2409:HOH:O	2.06	0.56
1:A:440:ARG:HB3	3:A:2134:HOH:O	2.05	0.56
1:A:397:ARG:NE	3:A:2162:HOH:O	2.37	0.56
1:A:248:ARG:HB3	1:A:484:ARG:NH2	2.21	0.56
1:A:349:LEU:HD21	1:A:384:LEU:HD21	1.86	0.56
1:A:139:ASP:OD2	1:A:146:ILE:HD11	2.06	0.56
1:A:52:GLY:HA3	1:B:1146:ILE:HG23	1.87	0.56
1:A:543:TYR:C	1:A:545:GLU:N	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1218:TYR:CZ	3:B:2716:HOH:O	2.53	0.56
1:B:1177:MSE:HG2	1:B:1202:CYS:HB3	1.88	0.56
1:B:1489:SER:HA	3:B:2514:HOH:O	2.06	0.55
1:B:1177:MSE:N	3:B:2416:HOH:O	2.39	0.55
1:A:526:ILE:O	1:A:530:VAL:HG23	2.05	0.55
1:B:1319:ILE:HG22	1:B:1323:ILE:HD12	1.88	0.55
1:A:431:GLU:HB3	3:A:2735:HOH:O	2.05	0.55
1:B:1194:ARG:HB2	1:B:1197:ARG:HG3	1.88	0.55
1:B:1385:LYS:HA	3:B:2585:HOH:O	2.06	0.55
1:A:282:GLY:O	1:A:286:VAL:HG22	2.06	0.55
1:A:70:ARG:O	1:A:74:LYS:HG3	2.07	0.55
1:B:1057:LYS:CB	3:B:2238:HOH:O	2.44	0.55
1:A:381:VAL:HG13	3:A:2256:HOH:O	2.07	0.55
1:A:382:ASN:O	1:A:385:LYS:HG3	2.07	0.55
1:A:381:VAL:HG22	1:A:407:MSE:HE1	1.87	0.55
1:A:394:GLY:HA2	1:A:420:SER:HB3	1.89	0.55
1:A:177:MSE:HG2	1:A:202:CYS:HB2	1.88	0.55
1:B:1023:GLU:HA	3:B:2347:HOH:O	2.07	0.55
1:B:1294:ALA:O	1:B:1297:VAL:HB	2.07	0.55
1:A:139:ASP:CG	1:A:146:ILE:HD11	2.26	0.55
1:A:342:TRP:CH2	1:A:367:HIS:HB2	2.42	0.55
1:A:71:ASN:O	1:A:75:MSE:CE	2.55	0.54
1:A:57:LYS:HD2	1:B:1218:TYR:O	2.07	0.54
1:B:1143:VAL:O	1:B:1147:VAL:HG23	2.07	0.54
1:B:1068:PHE:CZ	1:B:1072:LEU:HD13	2.42	0.54
1:A:370:PRO:HD2	3:A:2556:HOH:O	2.06	0.54
1:A:315:ALA:O	1:A:319:ILE:HD12	2.06	0.54
1:A:283:THR:HA	3:A:2275:HOH:O	2.07	0.54
1:A:346:LYS:HE3	1:A:347:TYR:CZ	2.41	0.54
1:A:219:MSE:HE3	3:A:2095:HOH:O	2.06	0.54
1:B:1243:THR:HG22	3:B:2746:HOH:O	2.06	0.54
1:B:1131:LYS:HE3	3:B:2094:HOH:O	2.07	0.54
1:B:1401:PRO:HA	1:B:1436:LEU:HD13	1.89	0.54
1:B:1061:GLN:HA	1:B:1064:GLN:HE21	1.71	0.54
1:B:1064:GLN:OE1	3:B:2704:HOH:O	2.18	0.54
1:A:81:LYS:HE3	3:A:2451:HOH:O	2.07	0.54
1:A:79:LEU:HD13	1:A:118:LEU:HD13	1.88	0.54
1:B:1253:GLN:HG3	1:B:1276:PHE:CZ	2.43	0.54
1:A:23:GLU:HG2	1:A:24:LYS:H	1.70	0.54
1:A:520:GLN:HG3	3:A:2214:HOH:O	2.06	0.54
1:A:476:LEU:CD2	3:A:2386:HOH:O	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:GLU:HG3	1:A:413:ARG:HG2	1.88	0.54
1:A:484:ARG:HG3	1:A:541:PHE:CE1	2.42	0.54
1:B:1332:LEU:HD12	1:B:1332:LEU:N	2.22	0.54
1:A:283:THR:OG1	3:A:2275:HOH:O	2.19	0.54
1:B:1235:ILE:O	1:B:1239:MSE:HG2	2.07	0.54
1:B:1296:LYS:NZ	3:B:2480:HOH:O	2.39	0.54
1:A:416:ILE:HG22	3:A:2333:HOH:O	2.08	0.54
1:B:1344:PHE:CZ	1:B:1348:GLY:HA2	2.43	0.54
1:B:1104:ILE:HG12	1:B:1108:MSE:HE2	1.90	0.54
1:B:1248:ARG:HD2	1:B:1248:ARG:N	2.23	0.53
1:B:1414:PRO:CA	3:B:2146:HOH:O	2.49	0.53
1:B:1047:MSE:HE3	3:B:2742:HOH:O	2.07	0.53
1:B:1144:ARG:NH1	1:B:1245:ARG:HB2	2.23	0.53
1:A:225:ARG:CB	3:A:2531:HOH:O	2.54	0.53
1:A:261:ASN:ND2	1:A:264:ARG:HE	2.05	0.53
1:B:1036:LYS:NZ	3:B:2244:HOH:O	2.40	0.53
1:A:183:LYS:NZ	1:A:255:GLU:OE1	2.41	0.53
1:B:1346:LYS:HE2	1:B:1347:TYR:CZ	2.44	0.53
1:A:165:ARG:HD3	1:A:258:GLY:HA2	1.89	0.53
1:A:277:ASN:HD22	1:A:277:ASN:C	2.11	0.53
1:B:1385:LYS:HD2	3:B:2680:HOH:O	2.07	0.53
1:B:1388:THR:OG1	1:B:1415:VAL:HB	2.08	0.53
1:B:1043:GLN:CB	3:B:2742:HOH:O	2.53	0.53
1:A:372:SER:O	1:A:383:ILE:HG21	2.09	0.53
1:B:1389:ILE:HG12	3:B:2538:HOH:O	2.09	0.53
1:B:1261:ASN:ND2	1:B:1264:ARG:NE	2.52	0.53
1:B:1108:MSE:N	1:B:1109:PRO:HD2	2.23	0.53
1:B:1109:PRO:HA	1:B:1114:PRO:CD	2.39	0.53
1:A:344:PHE:CD1	1:A:349:LEU:N	2.76	0.53
1:B:1389:ILE:HG23	1:B:1399:PHE:CZ	2.44	0.53
1:A:343:MSE:HE2	1:A:365:PHE:HB2	1.91	0.53
1:A:213:LEU:HD11	1:A:224:LYS:HD3	1.89	0.53
1:A:374:PRO:HG3	1:A:380:ALA:CA	2.36	0.53
1:B:1177:MSE:CG	3:B:2597:HOH:O	2.57	0.53
1:B:1412:GLU:HG3	1:B:1413:ARG:HG2	1.90	0.53
1:A:452:VAL:O	1:A:452:VAL:HG12	2.09	0.52
1:A:177:MSE:HE1	1:A:181:VAL:CG2	2.38	0.52
3:A:2638:HOH:O	1:B:1125:HIS:HB3	2.09	0.52
1:A:129:ARG:HG3	1:A:130:PRO:CD	2.39	0.52
1:A:501:GLN:HE22	1:A:525:ASN:HD22	1.58	0.52
1:B:1514:PRO:N	3:B:2740:HOH:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1310:LEU:HB3	1:B:1391:GLY:HA2	1.90	0.52
1:B:1407:MSE:HE3	3:B:2538:HOH:O	2.09	0.52
1:A:392:VAL:CG1	1:A:392:VAL:O	2.49	0.52
1:A:207:THR:C	3:A:2531:HOH:O	2.47	0.52
1:B:1205:VAL:HG22	3:B:2363:HOH:O	2.08	0.52
1:A:452:VAL:HG12	1:A:454:LEU:HD21	1.92	0.52
1:A:278:ASP:OD1	1:A:282:GLY:HA3	2.09	0.52
1:B:1289:ALA:HA	3:B:2674:HOH:O	2.09	0.52
1:B:1406:ALA:O	1:B:1410:ILE:HD12	2.09	0.52
1:A:143:VAL:O	1:A:147:VAL:HG23	2.09	0.52
1:B:1478:VAL:HG13	1:B:1483:THR:HB	1.92	0.52
1:B:1523:SER:CB	3:B:2252:HOH:O	2.52	0.52
1:A:552:TYR:O	1:A:556:ARG:HD2	2.10	0.52
1:A:437:THR:O	1:A:438:GLU:HB2	2.09	0.52
1:B:1297:VAL:HG12	1:B:1298:ILE:CD1	2.32	0.52
1:A:80:GLU:HG2	3:A:2308:HOH:O	2.09	0.52
1:B:1193:ILE:C	3:B:2518:HOH:O	2.46	0.52
1:A:377:PHE:CE2	1:A:389:ILE:HD11	2.45	0.52
1:A:386:PRO:CG	3:A:2256:HOH:O	2.53	0.52
1:B:1086:MSE:CA	1:B:1086:MSE:HE2	2.34	0.52
1:A:128:ARG:NH2	1:B:1128:ARG:NH1	2.55	0.52
1:B:1373:ILE:HG22	1:B:1373:ILE:O	2.08	0.52
1:A:103:ASP:HB3	1:A:107:LEU:CD2	2.39	0.51
1:A:435:THR:HG22	3:A:2229:HOH:O	2.10	0.51
1:B:1286:VAL:HG12	3:B:2570:HOH:O	2.10	0.51
1:B:1095:LEU:HG	1:B:1099:ILE:HD12	1.91	0.51
1:B:1099:ILE:HG22	1:B:1100:LEU:N	2.23	0.51
1:A:347:TYR:HD1	1:A:356:ALA:HB1	1.76	0.51
1:B:1110:ILE:HG13	3:B:2496:HOH:O	2.09	0.51
1:A:378:GLU:HG3	1:A:403:VAL:HG23	1.93	0.51
1:A:104:ILE:O	1:A:108:MSE:HG3	2.10	0.51
1:B:1165:ARG:CZ	3:B:2673:HOH:O	2.58	0.51
1:B:1287:ALA:HB3	3:B:2547:HOH:O	2.10	0.51
1:B:1467:ASN:ND2	2:B:1601:NAD:H71N	2.09	0.51
1:B:1543:TYR:C	1:B:1545:GLU:N	2.63	0.51
1:A:265:PHE:CD1	3:A:2457:HOH:O	2.53	0.51
1:B:1079:LEU:O	1:B:1083:ILE:HG12	2.10	0.51
1:B:1453:LYS:HB2	1:B:1459:VAL:HG13	1.92	0.51
1:B:1227:ARG:HG2	1:B:1227:ARG:HH11	1.75	0.51
1:A:277:ASN:HD22	1:A:279:ASP:N	2.09	0.51
1:A:310:LEU:CD2	1:A:427:GLU:HG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1086:MSE:CE	1:B:1096:PHE:HE1	2.23	0.51
1:B:1292:LEU:CD1	3:B:2674:HOH:O	2.59	0.51
1:B:1109:PRO:HA	1:B:1114:PRO:HD2	1.93	0.51
1:B:1292:LEU:HD12	3:B:2674:HOH:O	2.09	0.51
1:A:104:ILE:HG13	1:A:108:MSE:CE	2.33	0.51
1:B:1315:ALA:HB3	1:B:1392:VAL:HG11	1.91	0.51
1:A:346:LYS:HE3	1:A:347:TYR:CE2	2.46	0.51
1:A:329:GLU:HG3	1:A:329:GLU:O	2.11	0.51
1:B:1047:MSE:HG3	3:B:2742:HOH:O	2.11	0.51
1:A:333:SER:HB3	1:A:336:GLU:OE2	2.11	0.51
1:A:86:MSE:CE	1:A:86:MSE:HA	2.28	0.50
1:A:459:VAL:HG13	3:A:2189:HOH:O	2.11	0.50
1:B:1301:PRO:O	1:B:1304:GLU:HB2	2.11	0.50
1:A:108:MSE:HE1	1:A:519:ILE:HG21	1.92	0.50
1:A:404:ILE:HG22	3:A:2063:HOH:O	2.12	0.50
1:A:458:ARG:CZ	3:A:2700:HOH:O	2.58	0.50
1:B:1086:MSE:HA	1:B:1086:MSE:CE	2.38	0.50
1:A:24:LYS:HB2	1:A:48:LEU:O	2.12	0.50
1:A:39:ALA:HA	1:A:59:GLU:O	2.11	0.50
1:B:1378:GLU:CD	1:B:1402:ASP:HB3	2.31	0.50
1:B:1494:ALA:CB	3:B:2727:HOH:O	2.57	0.50
1:B:1039:ALA:N	3:B:2704:HOH:O	2.44	0.50
1:B:1354:ARG:HD3	1:B:1358:ILE:CD1	2.38	0.50
1:A:261:ASN:HD22	1:A:264:ARG:NE	2.09	0.50
1:B:1031:ASN:HB3	1:B:1034:THR:OG1	2.12	0.50
1:B:1068:PHE:HB2	3:B:2449:HOH:O	2.11	0.50
1:A:352:LYS:HB2	1:A:368:SER:HA	1.93	0.50
1:B:1428:CYS:CB	3:B:2311:HOH:O	2.58	0.50
1:A:408:ALA:HB2	3:A:2063:HOH:O	2.11	0.50
1:A:415:VAL:CG1	3:A:2287:HOH:O	2.59	0.50
1:B:1094:LYS:C	3:B:2583:HOH:O	2.50	0.50
1:A:175:TYR:HE2	1:A:219:MSE:HG3	1.77	0.50
1:A:113:THR:CB	1:A:114:PRO:CD	2.88	0.50
1:A:78:PRO:HA	1:A:81:LYS:HG3	1.94	0.50
1:B:1453:LYS:HA	1:B:1459:VAL:HA	1.93	0.50
1:A:372:SER:O	1:A:383:ILE:HG12	2.12	0.50
1:B:1195:PRO:CG	3:B:2409:HOH:O	2.60	0.50
1:A:45:ARG:HA	1:A:50:LEU:HD12	1.93	0.50
1:B:1154:HIS:O	1:B:1197:ARG:HD3	2.11	0.49
1:B:1469:TYR:HB3	1:B:1498:LEU:HD22	1.94	0.49
1:A:478:VAL:HG13	1:A:483:THR:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1381:VAL:CG2	1:B:1407:MSE:HE1	2.43	0.49
1:A:462:PRO:CB	3:A:2582:HOH:O	2.59	0.49
1:B:1538:LYS:NZ	1:B:1543:TYR:OH	2.42	0.49
1:A:183:LYS:NZ	1:A:255:GLU:OE2	2.44	0.49
1:A:418:ALA:O	1:A:445:SER:HA	2.12	0.49
1:A:183:LYS:O	3:A:2534:HOH:O	2.20	0.49
1:B:1502:LEU:HD11	1:B:1512:LEU:C	2.32	0.49
1:B:1310:LEU:HG	1:B:1393:ALA:HB2	1.95	0.49
1:B:1060:THR:O	1:B:1064:GLN:HG3	2.11	0.49
1:B:1277:ASN:HD21	1:B:1279:ASP:HB2	1.77	0.49
1:A:23:GLU:CG	1:A:24:LYS:H	2.26	0.49
1:B:1489:SER:HB2	1:B:1533:TYR:OH	2.13	0.49
1:A:128:ARG:HG3	3:A:2271:HOH:O	2.12	0.49
1:A:467:ASN:ND2	3:A:2275:HOH:O	2.46	0.49
1:B:1140:ARG:HH11	1:B:1140:ARG:HG2	1.78	0.49
1:B:1357:LYS:CB	1:B:1357:LYS:NZ	2.75	0.49
1:B:1414:PRO:HD2	1:B:1440:ARG:O	2.13	0.49
1:B:1511:ARG:CG	1:B:1511:ARG:HH11	2.25	0.49
1:B:1513:TYR:CB	3:B:2740:HOH:O	2.33	0.49
1:A:99:ILE:CG2	3:A:2715:HOH:O	2.50	0.49
1:A:323:ILE:HG22	1:A:327:MSE:HE2	1.94	0.49
1:B:1294:ALA:CA	1:B:1442:LEU:HD13	2.43	0.48
1:B:1061:GLN:NE2	3:B:2349:HOH:O	2.46	0.48
1:A:327:MSE:HE3	1:A:337:ALA:CB	2.41	0.48
1:A:26:LYS:HA	1:A:29:MSE:HG3	1.95	0.48
1:A:408:ALA:HA	1:A:414:PRO:HG3	1.95	0.48
1:A:35:ASN:ND2	1:A:91:ARG:O	2.44	0.48
1:A:399:PHE:HB2	1:A:428:CYS:HB3	1.94	0.48
1:A:376:THR:HG22	1:A:379:ASP:N	2.18	0.48
1:A:443:PHE:CD2	3:A:2582:HOH:O	2.65	0.48
1:B:1169:LEU:N	1:B:1169:LEU:CD1	2.77	0.48
1:A:535:TYR:CD2	1:A:540:ALA:HB3	2.49	0.48
1:A:100:LEU:HD12	1:A:100:LEU:O	2.13	0.48
1:B:1144:ARG:NH1	1:B:1148:ASP:OD1	2.47	0.48
1:B:1069:HIS:O	1:B:1073:LYS:HB3	2.13	0.48
1:A:415:VAL:HG12	3:A:2287:HOH:O	2.13	0.48
1:B:1442:LEU:CD1	3:B:2614:HOH:O	2.48	0.48
1:B:1415:VAL:HG22	1:B:1442:LEU:HB2	1.96	0.48
1:B:1351:VAL:CG1	1:B:1369:ALA:HB2	2.40	0.48
1:A:82:TYR:CD2	1:A:83:ILE:HD13	2.43	0.48
1:A:33:ARG:NH1	1:A:93:GLU:OE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LYS:HD2	1:A:156:LYS:HA	1.70	0.48
1:A:157:ALA:HB2	1:A:479:ILE:HD11	1.95	0.48
1:A:528:ILE:HD13	1:A:550:ALA:HA	1.95	0.48
1:A:377:PHE:O	1:A:381:VAL:HG23	2.13	0.48
1:A:109:PRO:HA	1:A:114:PRO:CD	2.44	0.48
1:A:31:ASN:HB3	1:A:34:THR:OG1	2.12	0.48
1:B:1277:ASN:C	1:B:1277:ASN:ND2	2.67	0.48
1:B:1363:GLU:N	1:B:1364:PRO:HD2	2.29	0.48
1:B:1345:ASP:HB2	2:B:1601:NAD:O2B	2.14	0.48
1:B:1213:LEU:HB2	3:B:2156:HOH:O	2.14	0.48
1:A:203:ILE:HG22	1:A:205:VAL:HG13	1.95	0.48
1:B:1182:GLY:O	1:B:1185:CYS:HB2	2.14	0.47
1:A:101:GLN:NE2	3:A:2709:HOH:O	2.28	0.47
1:B:1202:CYS:HB2	3:B:2416:HOH:O	2.14	0.47
1:A:118:LEU:O	1:A:122:GLN:HG2	2.13	0.47
1:B:1073:LYS:HE2	1:B:1074:LYS:CE	2.45	0.47
1:B:1177:MSE:HA	3:B:2416:HOH:O	2.14	0.47
1:B:1372:SER:O	1:B:1374:PRO:HD3	2.15	0.47
1:A:231:TYR:O	1:A:235:ILE:HG12	2.14	0.47
1:A:357:LYS:O	1:A:358:ILE:HD12	2.15	0.47
1:A:421:ASN:HB3	1:A:422:PRO:HA	1.97	0.47
1:A:401:PRO:HA	1:A:436:LEU:CD2	2.45	0.47
1:B:1131:LYS:NZ	3:B:2137:HOH:O	2.46	0.47
1:A:414:PRO:CA	3:A:2752:HOH:O	2.63	0.47
1:B:1301:PRO:HG3	3:B:2524:HOH:O	2.15	0.47
1:B:1165:ARG:NH2	3:B:2673:HOH:O	2.46	0.47
1:B:1105:GLU:HB3	3:B:2228:HOH:O	2.14	0.47
1:B:1109:PRO:CA	1:B:1114:PRO:HD2	2.44	0.47
1:A:28:LEU:CD2	1:A:48:LEU:HG	2.45	0.47
1:B:1414:PRO:CB	3:B:2146:HOH:O	2.59	0.47
1:A:177:MSE:CE	1:A:181:VAL:CG2	2.93	0.47
1:B:1166:ILE:HG13	1:B:1172:LEU:HD12	1.95	0.47
1:B:1558:TRP:CE3	3:B:2409:HOH:O	2.68	0.47
1:A:286:VAL:HG11	1:A:466:ASN:O	2.15	0.47
1:A:171:ASP:OD1	1:A:171:ASP:C	2.53	0.47
1:B:1179:ILE:HG21	3:B:2405:HOH:O	2.15	0.47
1:B:1137:ILE:O	1:B:1140:ARG:NH1	2.46	0.47
1:B:1267:ARG:CZ	1:B:1267:ARG:HB3	2.45	0.47
1:A:435:THR:CA	3:A:2229:HOH:O	2.55	0.47
1:B:1295:GLN:C	1:B:1297:VAL:H	2.18	0.47
1:A:310:LEU:HD23	1:A:427:GLU:CG	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ALA:HA	3:A:2305:HOH:O	2.15	0.47
1:A:194:ARG:NH2	1:A:196:ASP:OD2	2.48	0.46
1:B:1122:GLN:HB2	1:B:1126:ILE:HG12	1.97	0.46
1:B:1308:LEU:CB	1:B:1386:PRO:HG3	2.44	0.46
1:B:1328:VAL:HA	1:B:1332:LEU:O	2.16	0.46
1:B:1215:ASP:OD1	1:B:1216:PRO:HD2	2.15	0.46
1:A:133:LEU:HD13	1:A:150:TRP:HE3	1.81	0.46
1:A:553:VAL:HG22	3:A:2141:HOH:O	2.15	0.46
1:B:1429:THR:HG22	1:B:1432:GLU:CD	2.35	0.46
1:A:110:ILE:O	1:A:115:THR:HB	2.15	0.46
1:B:1321:ASN:HB3	3:B:2288:HOH:O	2.15	0.46
1:A:91:ARG:HH12	1:B:1090:GLU:CD	2.19	0.46
1:B:1156:LYS:HA	1:B:1156:LYS:HD2	1.74	0.46
1:A:344:PHE:CZ	1:A:348:GLY:HA2	2.50	0.46
1:A:417:PHE:HD2	3:A:2571:HOH:O	1.98	0.46
1:A:57:LYS:NZ	1:A:59:GLU:OE2	2.44	0.46
1:A:225:ARG:HG2	1:A:225:ARG:HH11	1.80	0.46
1:B:1068:PHE:CD2	1:B:1068:PHE:C	2.88	0.46
1:B:1288:LEU:HD21	1:B:1492:LEU:CD1	2.45	0.46
1:A:524:ILE:O	1:A:527:ALA:HB3	2.16	0.46
1:A:323:ILE:O	1:A:327:MSE:HG3	2.15	0.46
1:A:208:ASP:HA	1:A:224:LYS:HD2	1.97	0.46
1:B:1277:ASN:HD22	1:B:1279:ASP:H	1.63	0.46
2:A:602:NAD:H52N	3:A:2302:HOH:O	2.15	0.46
1:A:429:THR:HG22	1:A:432:GLU:OE1	2.15	0.46
1:B:1354:ARG:HG2	1:B:1356:ALA:O	2.16	0.46
1:B:1389:ILE:HG22	1:B:1416:ILE:HA	1.97	0.46
1:B:1393:ALA:HA	2:B:1601:NAD:O4B	2.16	0.46
1:A:483:THR:HG23	3:A:2032:HOH:O	2.15	0.46
1:B:1267:ARG:HH11	1:B:1267:ARG:HG2	1.81	0.46
1:B:1325:MSE:HE1	3:B:2514:HOH:O	2.12	0.46
1:A:288:LEU:CG	3:A:2469:HOH:O	2.51	0.46
1:A:129:ARG:HD3	3:B:2650:HOH:O	2.16	0.46
1:B:1502:LEU:HD23	1:B:1506:GLU:OE1	2.15	0.46
1:A:383:ILE:HG22	1:A:384:LEU:HD13	1.98	0.45
1:A:407:MSE:HB2	1:A:407:MSE:HE2	1.84	0.45
1:B:1315:ALA:HB3	1:B:1392:VAL:HG13	1.98	0.45
1:A:122:GLN:O	1:A:123:TYR:C	2.53	0.45
1:B:1243:THR:HG22	1:B:1247:GLY:O	2.16	0.45
1:A:134:PHE:CE2	1:A:177:MSE:HG3	2.51	0.45
1:B:1167:LEU:N	1:B:1167:LEU:HD23	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASP:O	1:A:107:LEU:HB2	2.16	0.45
1:A:442:LEU:HA	3:A:2371:HOH:O	2.16	0.45
1:A:462:PRO:CG	3:A:2582:HOH:O	2.62	0.45
1:A:310:LEU:HD21	1:A:398:LEU:HB2	1.98	0.45
1:A:374:PRO:HB3	1:A:379:ASP:CB	2.47	0.45
1:A:407:MSE:SE	3:A:2256:HOH:O	2.85	0.45
1:A:108:MSE:N	1:A:109:PRO:CD	2.79	0.45
1:A:288:LEU:HD22	1:A:322:LEU:HG	1.99	0.45
1:B:1376:THR:HG22	1:B:1378:GLU:N	2.31	0.45
1:A:172:LEU:O	1:A:175:TYR:HB2	2.16	0.45
1:B:1250:THR:N	3:B:2746:HOH:O	2.49	0.45
1:B:1166:ILE:HG22	1:B:1167:LEU:HG	1.99	0.45
1:A:33:ARG:NH2	1:A:196:ASP:HA	2.32	0.45
1:A:212:LEU:HD22	1:A:218:TYR:CD2	2.50	0.45
1:A:71:ASN:O	1:A:75:MSE:HE3	2.16	0.45
1:B:1194:ARG:CA	3:B:2518:HOH:O	2.53	0.45
1:A:466:ASN:HB3	3:A:2681:HOH:O	2.08	0.45
1:B:1076:THR:N	1:B:1080:GLU:OE2	2.49	0.45
1:A:538:LYS:HA	3:A:2201:HOH:O	2.17	0.45
1:A:326:SER:HB2	1:A:492:LEU:HD11	1.99	0.45
1:A:208:ASP:OD1	1:A:224:LYS:HD2	2.17	0.45
1:B:1120:CYS:O	1:B:1175:TYR:HB3	2.16	0.45
1:A:97:TYR:O	1:A:101:GLN:HG3	2.17	0.45
1:A:253:GLN:HG3	1:A:276:PHE:CZ	2.52	0.45
1:B:1238:PHE:CE1	1:B:1242:ILE:HG13	2.52	0.45
1:B:1286:VAL:HG21	1:B:1467:ASN:ND2	2.32	0.45
1:B:1295:GLN:C	1:B:1297:VAL:N	2.71	0.45
1:B:1529:LYS:NZ	3:B:2699:HOH:O	2.49	0.45
3:A:2541:HOH:O	1:B:1026:LYS:HE3	2.17	0.45
1:A:300:LYS:HE3	1:A:304:GLU:HB3	1.99	0.45
1:B:1466:ASN:OD1	1:B:1468:VAL:HG13	2.16	0.45
1:A:315:ALA:HB3	1:A:392:VAL:CG1	2.45	0.45
1:A:467:ASN:C	1:A:469:TYR:H	2.18	0.45
1:B:1343:MSE:SE	3:B:2102:HOH:O	2.85	0.45
1:A:164:GLU:O	1:A:164:GLU:HG3	2.16	0.45
1:B:1106:SER:C	1:B:1109:PRO:HD2	2.38	0.44
1:B:1087:GLY:HA2	1:B:1090:GLU:HG2	1.99	0.44
1:A:183:LYS:CE	3:A:2711:HOH:O	2.63	0.44
1:A:253:GLN:HG3	1:A:276:PHE:CE2	2.52	0.44
1:B:1041:THR:OG1	1:B:1044:GLU:HG3	2.18	0.44
1:B:1407:MSE:N	3:B:2312:HOH:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLY:O	1:A:91:ARG:HG3	2.17	0.44
1:B:1029:MSE:SE	1:B:1050:LEU:HD22	2.67	0.44
1:B:1108:MSE:CE	1:B:1519:ILE:HG21	2.48	0.44
1:B:1043:GLN:CD	3:B:2742:HOH:O	2.56	0.44
1:B:1118:LEU:HD22	1:B:1122:GLN:HE21	1.82	0.44
1:B:1073:LYS:HG2	1:B:1074:LYS:N	2.33	0.44
1:A:381:VAL:O	1:A:385:LYS:HA	2.16	0.44
1:B:1381:VAL:HG22	1:B:1407:MSE:HE1	1.99	0.44
1:A:113:THR:CG2	1:A:114:PRO:HD3	2.47	0.44
1:A:557:THR:CG2	3:A:2386:HOH:O	2.47	0.44
1:A:277:ASN:ND2	1:A:279:ASP:N	2.63	0.44
1:A:183:LYS:NZ	1:A:255:GLU:CD	2.71	0.44
1:B:1376:THR:O	1:B:1379:ASP:HB2	2.17	0.44
1:A:66:LEU:O	1:A:70:ARG:HG3	2.17	0.44
1:A:363:GLU:HG2	1:A:364:PRO:HD3	2.00	0.44
1:A:214:LYS:NZ	3:A:2463:HOH:O	2.46	0.44
1:B:1109:PRO:C	1:B:1114:PRO:HD2	2.37	0.44
1:A:112:TYR:O	1:A:113:THR:C	2.56	0.44
1:A:277:ASN:HD22	1:A:279:ASP:H	1.63	0.44
1:B:1383:ILE:HG22	1:B:1384:LEU:HD13	2.00	0.44
1:B:1194:ARG:N	3:B:2518:HOH:O	2.50	0.44
1:A:261:ASN:ND2	1:A:264:ARG:NE	2.65	0.44
1:A:430:ALA:CB	3:A:2582:HOH:O	2.65	0.44
1:A:436:LEU:HB2	3:A:2220:HOH:O	2.16	0.44
1:A:452:VAL:C	3:A:2189:HOH:O	2.55	0.44
1:A:225:ARG:CG	1:A:225:ARG:HH11	2.30	0.44
1:B:1153:ASN:HB2	3:B:2730:HOH:O	2.18	0.44
1:B:1187:TYR:O	1:B:1191:ALA:HB3	2.18	0.44
1:A:209:ASN:HB3	1:A:212:LEU:HD12	2.00	0.44
1:B:1294:ALA:HA	1:B:1442:LEU:HD13	2.00	0.44
1:A:89:GLN:HG3	1:A:90:GLU:N	2.33	0.44
1:B:1038:MSE:HB2	1:B:1038:MSE:HE3	1.95	0.43
1:B:1089:GLN:OE1	1:B:1131:LYS:HE2	2.18	0.43
1:A:67:ARG:CZ	3:A:2659:HOH:O	2.65	0.43
1:A:430:ALA:O	1:A:434:TYR:HD1	2.02	0.43
1:B:1385:LYS:CA	3:B:2585:HOH:O	2.64	0.43
1:A:518:ASN:CB	3:A:2661:HOH:O	2.51	0.43
1:B:1306:LYS:HB3	1:B:1386:PRO:HA	2.00	0.43
1:B:1177:MSE:CA	3:B:2416:HOH:O	2.66	0.43
1:A:167:LEU:HB2	1:A:168:GLY:H	1.58	0.43
1:A:397:ARG:HA	1:A:427:GLU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1408:ALA:HB2	1:B:1437:THR:HG22	2.01	0.43
1:A:109:PRO:CA	1:A:114:PRO:HD2	2.48	0.43
1:A:64:GLN:HE22	1:A:562:TYR:HE1	1.65	0.43
1:A:327:MSE:HB3	1:A:332:LEU:HD22	2.00	0.43
1:A:243:THR:HG22	1:A:247:GLY:O	2.19	0.43
1:B:1040:PHE:HE2	1:B:1565:LEU:HD11	1.84	0.43
1:B:1418:ALA:O	1:B:1445:SER:HA	2.19	0.43
1:B:1036:LYS:O	1:B:1039:ALA:HB3	2.19	0.43
1:A:467:ASN:C	1:A:469:TYR:N	2.71	0.43
1:A:383:ILE:C	3:A:2226:HOH:O	2.57	0.43
1:A:429:THR:HG22	1:A:432:GLU:HB2	1.99	0.43
1:A:128:ARG:HH22	1:B:1128:ARG:HH12	1.62	0.43
1:A:351:VAL:HG11	1:A:369:ALA:HB2	2.00	0.43
1:A:351:VAL:CG1	1:A:352:LYS:N	2.82	0.43
1:A:355:LYS:HD3	1:A:355:LYS:HA	1.87	0.43
1:A:344:PHE:CE1	1:A:348:GLY:HA2	2.54	0.43
1:B:1110:ILE:CG1	3:B:2496:HOH:O	2.67	0.43
1:A:298:ILE:HD11	1:A:413:ARG:HB2	2.01	0.43
1:B:1482:ASN:HD22	1:B:1542:ARG:HA	1.82	0.43
1:A:218:TYR:HB3	1:A:222:TYR:OH	2.19	0.43
1:B:1095:LEU:N	3:B:2583:HOH:O	2.51	0.43
1:B:1043:GLN:NE2	3:B:2742:HOH:O	2.52	0.43
1:B:1073:LYS:HG2	1:B:1074:LYS:HE2	2.01	0.42
1:B:1092:ASN:HD21	1:B:1562:TYR:HH	1.62	0.42
1:B:1108:MSE:N	1:B:1109:PRO:CD	2.82	0.42
1:A:310:LEU:HB3	1:A:391:GLY:HA2	2.01	0.42
1:B:1277:ASN:HD22	1:B:1279:ASP:N	2.18	0.42
1:B:1113:THR:CB	1:B:1114:PRO:CD	2.84	0.42
1:A:405:ARG:N	3:A:2512:HOH:O	2.51	0.42
1:A:136:SER:C	1:A:138:SER:N	2.72	0.42
1:B:1453:LYS:HG2	1:B:1459:VAL:HG22	2.00	0.42
1:B:1512:LEU:HA	1:B:1512:LEU:HD12	1.87	0.42
1:B:1467:ASN:HD21	2:B:1601:NAD:H71N	1.67	0.42
1:B:1091:ARG:NH2	3:B:2646:HOH:O	2.41	0.42
1:A:166:ILE:H	1:A:166:ILE:HD12	1.83	0.42
1:B:1177:MSE:O	1:B:1181:VAL:HG23	2.20	0.42
1:B:1538:LYS:HE3	1:B:1543:TYR:OH	2.18	0.42
1:A:467:ASN:O	1:A:469:TYR:N	2.52	0.42
1:B:1031:ASN:HD21	1:B:1033:ARG:HB2	1.83	0.42
1:A:404:ILE:HG22	3:A:2512:HOH:O	2.19	0.42
1:B:1161:THR:CG2	3:B:2416:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:THR:O	1:A:506:GLU:HG3	2.20	0.42
1:B:1133:LEU:HB2	1:B:1199:LEU:HD11	2.01	0.42
1:B:1038:MSE:HE3	3:B:2026:HOH:O	2.19	0.42
1:A:308:LEU:HB2	1:A:386:PRO:HG3	2.02	0.42
1:B:1446:GLY:O	1:B:1464:GLN:NE2	2.43	0.42
1:A:104:ILE:HG23	1:A:105:GLU:N	2.35	0.42
1:B:1401:PRO:O	1:B:1405:ARG:HG2	2.20	0.42
3:A:2408:HOH:O	1:B:1067:ARG:HD3	2.18	0.42
1:B:1118:LEU:O	1:B:1122:GLN:HG2	2.20	0.42
1:A:146:ILE:HG23	1:B:1052:GLY:HA3	2.02	0.42
1:A:535:TYR:CD1	1:A:549:LYS:HE3	2.55	0.42
1:A:359:ASP:OD2	1:A:359:ASP:C	2.57	0.42
1:A:566:LEU:HD22	1:A:567:PRO:HD2	2.02	0.42
1:B:1407:MSE:SE	3:B:2265:HOH:O	2.87	0.42
1:A:109:PRO:C	1:A:114:PRO:HD2	2.40	0.42
1:A:64:GLN:O	1:A:68:PHE:CD1	2.62	0.42
1:A:77:SER:HA	1:A:78:PRO:HD3	1.90	0.42
1:B:1167:LEU:HB2	1:B:1169:LEU:HD13	2.02	0.42
1:A:203:ILE:HD12	1:A:203:ILE:N	2.35	0.42
1:B:1505:GLU:H	1:B:1505:GLU:HG2	1.45	0.42
1:A:86:MSE:HE1	1:A:96:PHE:HE1	1.79	0.42
1:B:1089:GLN:HE21	1:B:1089:GLN:HB2	1.57	0.42
1:A:466:ASN:OD1	1:A:468:VAL:HG13	2.19	0.42
1:B:1343:MSE:HE1	1:B:1362:GLN:HG2	2.02	0.42
1:B:1528:ILE:HD11	1:B:1554:LYS:CE	2.50	0.42
1:B:1281:GLN:NE2	1:B:1491:PHE:CE1	2.88	0.42
1:B:1317:LEU:HD13	1:B:1361:TYR:HB3	2.02	0.42
1:B:1492:LEU:CB	3:B:2514:HOH:O	2.45	0.41
1:B:1445:SER:O	1:B:1464:GLN:HA	2.19	0.41
1:A:367:HIS:CE1	3:A:2569:HOH:O	2.58	0.41
1:A:177:MSE:O	1:A:180:PRO:HD2	2.20	0.41
1:A:429:THR:HG22	1:A:432:GLU:CG	2.50	0.41
1:B:1460:PHE:O	1:B:1462:PRO:HD3	2.20	0.41
1:A:504:ASP:HB2	1:A:505:GLU:OE2	2.19	0.41
1:A:351:VAL:HG13	1:A:352:LYS:N	2.36	0.41
1:B:1352:LYS:HB2	1:B:1367:HIS:O	2.19	0.41
1:A:559:ARG:N	1:A:559:ARG:HD3	2.34	0.41
1:B:1344:PHE:CD1	1:B:1349:LEU:N	2.88	0.41
1:A:503:THR:OG1	1:A:506:GLU:HG2	2.19	0.41
1:B:1394:GLY:N	1:B:1420:SER:OG	2.47	0.41
1:B:1520:GLN:HB2	3:B:2219:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1310:LEU:CD2	1:B:1427:GLU:CG	2.98	0.41
1:A:137:ILE:HD11	1:A:230:GLN:HB3	2.02	0.41
1:A:359:ASP:OD2	1:A:362:GLN:N	2.53	0.41
1:B:1507:LEU:HD12	1:B:1507:LEU:HA	1.74	0.41
1:B:1112:TYR:HA	1:B:1116:VAL:HB	2.02	0.41
1:A:378:GLU:O	1:A:382:ASN:ND2	2.53	0.41
1:B:1464:GLN:NE2	1:B:1466:ASN:HD22	2.19	0.41
1:B:1227:ARG:CG	1:B:1227:ARG:HH11	2.33	0.41
1:A:379:ASP:O	1:A:382:ASN:HB2	2.20	0.41
1:B:1455:THR:HG23	1:B:1456:ASP:N	2.35	0.41
1:B:1073:LYS:CG	1:B:1074:LYS:N	2.83	0.41
1:B:1317:LEU:HD13	1:B:1361:TYR:CB	2.50	0.41
1:A:30:LEU:HD12	3:B:2362:HOH:O	2.21	0.41
1:B:1066:LEU:HD12	1:B:1066:LEU:HA	1.85	0.41
1:A:72:LEU:CA	1:A:75:MSE:HE3	2.35	0.41
1:B:1511:ARG:CG	1:B:1511:ARG:NH1	2.82	0.41
1:B:1501:GLN:HE21	1:B:1522:VAL:HG22	1.86	0.41
1:A:218:TYR:HB3	1:A:222:TYR:CZ	2.56	0.41
1:A:436:LEU:C	3:A:2220:HOH:O	2.58	0.41
1:B:1308:LEU:HG	1:B:1377:PHE:CE1	2.56	0.41
1:A:277:ASN:ND2	1:A:277:ASN:C	2.73	0.41
1:B:1100:LEU:HD21	1:B:1189:ALA:HB2	2.02	0.41
1:A:505:GLU:O	1:A:508:ALA:HB3	2.20	0.41
1:A:374:PRO:HB3	1:A:379:ASP:HB3	2.03	0.41
1:A:402:ASP:HA	1:A:405:ARG:HD2	2.03	0.41
1:A:453:LYS:N	3:A:2189:HOH:O	2.53	0.41
1:B:1310:LEU:CD2	1:B:1427:GLU:HG2	2.51	0.41
1:B:1300:LYS:HD2	1:B:1305:HIS:CD2	2.56	0.41
1:B:1202:CYS:CB	3:B:2416:HOH:O	2.69	0.41
1:A:109:PRO:HA	1:A:114:PRO:HD2	2.02	0.41
1:A:476:LEU:O	1:A:480:LEU:HG	2.21	0.41
1:A:292:LEU:HD21	3:A:2469:HOH:O	2.21	0.41
1:B:1277:ASN:ND2	1:B:1279:ASP:N	2.69	0.41
1:A:130:PRO:HG2	1:B:1054:LEU:HD23	2.03	0.41
1:B:1071:ASN:O	1:B:1075:MSE:HE3	2.21	0.41
1:A:363:GLU:N	1:A:364:PRO:HD2	2.35	0.41
1:A:313:GLY:O	1:A:316:ALA:N	2.54	0.41
1:B:1109:PRO:HA	1:B:1114:PRO:HD3	2.02	0.41
1:B:1456:ASP:OD1	1:B:1458:ARG:NH1	2.53	0.41
1:B:1501:GLN:NE2	1:B:1522:VAL:HA	2.36	0.41
1:A:128:ARG:NH2	1:B:1128:ARG:HH12	2.16	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLY:O	1:A:293:ALA:HB3	2.21	0.40
1:B:1501:GLN:HE22	1:B:1525:ASN:HD22	1.69	0.40
1:A:155:VAL:HB	1:A:246:TYR:CD2	2.56	0.40
1:A:384:LEU:C	3:A:2226:HOH:O	2.58	0.40
1:A:429:THR:CG2	1:A:432:GLU:H	2.24	0.40
1:B:1416:ILE:C	1:B:1417:PHE:HD1	2.25	0.40
1:A:76:THR:HG22	1:A:77:SER:N	2.36	0.40
1:B:1413:ARG:HB3	1:B:1413:ARG:HE	1.62	0.40
1:A:412:GLU:O	1:A:440:ARG:HB3	2.20	0.40
1:B:1043:GLN:O	1:B:1047:MSE:HG3	2.21	0.40
1:B:1117:GLY:O	1:B:1169:LEU:CD2	2.70	0.40
1:A:230:GLN:HE21	1:A:230:GLN:HB2	1.63	0.40
1:A:146:ILE:O	1:A:149:ASN:HB2	2.22	0.40
1:B:1565:LEU:HD21	3:B:2420:HOH:O	2.20	0.40
1:A:432:GLU:O	1:A:436:LEU:HD13	2.21	0.40
1:A:438:GLU:O	1:A:458:ARG:NH2	2.53	0.40
1:A:392:VAL:HG12	3:A:2008:HOH:O	2.22	0.40
1:A:25:GLY:C	1:A:27:PRO:HD2	2.41	0.40
1:B:1266:LEU:O	1:B:1270:ARG:HG2	2.20	0.40
1:B:1300:LYS:CD	1:B:1304:GLU:HB3	2.52	0.40
1:A:480:LEU:HD12	3:A:2141:HOH:O	2.20	0.40
1:B:1429:THR:CG2	1:B:1432:GLU:H	2.21	0.40
1:A:341:ILE:O	1:A:367:HIS:NE2	2.42	0.40
1:B:1196:ASP:O	3:B:2002:HOH:O	2.22	0.40
1:B:1281:GLN:NE2	1:B:1491:PHE:HE1	2.20	0.40
1:B:1224:LYS:NZ	3:B:2504:HOH:O	2.54	0.40
1:A:109:PRO:HA	1:A:114:PRO:HD3	2.02	0.40
1:A:91:ARG:NH1	1:B:1090:GLU:OE1	2.53	0.40
1:A:177:MSE:HE3	1:A:181:VAL:HG23	2.03	0.40
1:A:118:LEU:HD22	1:A:122:GLN:HE21	1.86	0.40
1:A:505:GLU:HB3	3:A:2714:HOH:O	2.21	0.40
1:A:343:MSE:O	1:A:350:LEU:HD23	2.21	0.40
1:B:1045:ARG:HA	1:B:1050:LEU:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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	549/584 (94%)	505 (92%)	35 (6%)	9 (2%)	12	6
1	B	549/584 (94%)	502 (91%)	38 (7%)	9 (2%)	12	6
All	All	1098/1168 (94%)	1007 (92%)	73 (7%)	18 (2%)	12	6

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	THR
1	B	1113	THR
1	B	1299	SER
1	B	1571	GLU
1	A	259	ASN
1	A	432	GLU
1	B	1259	ASN
1	A	114	PRO
1	A	451	PRO
1	B	1114	PRO
1	A	56	PRO
1	A	123	TYR
1	A	397	ARG
1	B	1076	THR
1	B	1354	ARG
1	A	468	VAL
1	B	1301	PRO
1	B	1056	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	465/484 (96%)	390 (84%)	75 (16%)	3	1
1	B	465/484 (96%)	386 (83%)	79 (17%)	2	1
All	All	930/968 (96%)	776 (83%)	154 (17%)	3	1

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	26	LYS
1	A	29	MSE
1	A	38	MSE
1	A	48	LEU
1	A	66	LEU
1	A	71	ASN
1	A	72	LEU
1	A	74	LYS
1	A	75	MSE
1	A	77	SER
1	A	89	GLN
1	A	106	SER
1	A	107	LEU
1	A	118	LEU
1	A	123	TYR
1	A	125	HIS
1	A	136	SER
1	A	137	ILE
1	A	152	GLU
1	A	160	VAL
1	A	165	ARG
1	A	167	LEU
1	A	169	LEU
1	A	184	LEU
1	A	210	ILE
1	A	214	LYS
1	A	225	ARG
1	A	237	GLU
1	A	240	LYS
1	A	248	ARG
1	A	255	GLU
1	A	257	PHE

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Mol	Chain	Res	Type
1	A	267	ARG
1	A	268	LYS
1	A	277	ASN
1	A	286	VAL
1	A	299	SER
1	A	300	LYS
1	A	306	LYS
1	A	329	GLU
1	A	333	SER
1	A	340	LYS
1	A	346	LYS
1	A	360	SER
1	A	363	GLU
1	A	368	SER
1	A	371	GLU
1	A	372	SER
1	A	376	THR
1	A	378	GLU
1	A	384	LEU
1	A	388	THR
1	A	397	ARG
1	A	398	LEU
1	A	403	VAL
1	A	413	ARG
1	A	416	ILE
1	A	419	LEU
1	A	425	GLN
1	A	428	CYS
1	A	456	ASP
1	A	458	ARG
1	A	489	SER
1	A	502	LEU
1	A	506	GLU
1	A	512	LEU
1	A	516	LEU
1	A	518	ASN
1	A	520	GLN
1	A	529	LYS
1	A	543	TYR
1	A	559	ARG
1	A	566	LEU
1	A	572	TRP

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Mol	Chain	Res	Type
1	B	1030	LEU
1	B	1038	MSE
1	B	1043	GLN
1	B	1048	LEU
1	B	1057	LYS
1	B	1066	LEU
1	B	1068	PHE
1	B	1072	LEU
1	B	1074	LYS
1	B	1089	GLN
1	B	1093	GLU
1	B	1104	ILE
1	B	1106	SER
1	B	1107	LEU
1	B	1118	LEU
1	B	1121	SER
1	B	1123	TYR
1	B	1136	SER
1	B	1137	ILE
1	B	1144	ARG
1	B	1154	HIS
1	B	1160	VAL
1	B	1174	VAL
1	B	1184	LEU
1	B	1210	ILE
1	B	1214	LYS
1	B	1224	LYS
1	B	1225	ARG
1	B	1232	ASP
1	B	1248	ARG
1	B	1276	PHE
1	B	1277	ASN
1	B	1286	VAL
1	B	1295	GLN
1	B	1298	ILE
1	B	1300	LYS
1	B	1302	ILE
1	B	1340	LYS
1	B	1346	LYS
1	B	1352	LYS
1	B	1354	ARG
1	B	1355	LYS

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Mol	Chain	Res	Type
1	B	1357	LYS
1	B	1360	SER
1	B	1363	GLU
1	B	1368	SER
1	B	1372	SER
1	B	1375	ASP
1	B	1384	LEU
1	B	1385	LYS
1	B	1388	THR
1	B	1397	ARG
1	B	1398	LEU
1	B	1409	SER
1	B	1413	ARG
1	B	1419	LEU
1	B	1423	THR
1	B	1425	GLN
1	B	1428	CYS
1	B	1453	LYS
1	B	1454	LEU
1	B	1456	ASP
1	B	1461	THR
1	B	1467	ASN
1	B	1489	SER
1	B	1496	LYS
1	B	1505	GLU
1	B	1509	GLN
1	B	1511	ARG
1	B	1512	LEU
1	B	1516	LEU
1	B	1518	ASN
1	B	1520	GLN
1	B	1538	LYS
1	B	1547	GLU
1	B	1554	LYS
1	B	1559	ARG
1	B	1566	LEU
1	B	1572	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN

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Mol	Chain	Res	Type
1	A	46	GLN
1	A	64	GLN
1	A	71	ASN
1	A	122	GLN
1	A	230	GLN
1	A	261	ASN
1	A	277	ASN
1	A	295	GLN
1	A	330	ASN
1	A	382	ASN
1	A	425	GLN
1	A	482	ASN
1	A	485	HIS
1	A	501	GLN
1	A	509	GLN
1	A	520	GLN
1	B	1031	ASN
1	B	1043	GLN
1	B	1046	GLN
1	B	1064	GLN
1	B	1071	ASN
1	B	1122	GLN
1	B	1153	ASN
1	B	1261	ASN
1	B	1277	ASN
1	B	1330	ASN
1	B	1425	GLN
1	B	1464	GLN
1	B	1467	ASN
1	B	1482	ASN
1	B	1501	GLN
1	B	1509	GLN
1	B	1518	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

4 ligands are modelled in this entry.

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	NAD	A	601	-	38,48,48	1.59	8 (21%)	47,73,73	1.97	4 (8%)
2	NAD	A	602	-	38,48,48	1.83	8 (21%)	47,73,73	1.97	4 (8%)
2	NAD	B	1601	-	38,48,48	1.59	9 (23%)	47,73,73	1.99	6 (12%)
2	NAD	B	1602	-	38,48,48	1.80	7 (18%)	47,73,73	1.97	4 (8%)

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	NAD	A	601	-	-	0/22/62/62	0/5/5/5
2	NAD	A	602	-	-	0/22/62/62	0/5/5/5
2	NAD	B	1601	-	-	0/22/62/62	0/5/5/5
2	NAD	B	1602	-	-	0/22/62/62	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1602	NAD	C5A-C4A	-3.15	1.33	1.40
2	A	602	NAD	C5A-C4A	-3.05	1.33	1.40
2	A	601	NAD	C5A-C4A	-2.82	1.34	1.40
2	B	1601	NAD	C5A-C4A	-2.79	1.34	1.40
2	A	601	NAD	C5A-N7A	-2.43	1.31	1.39
2	B	1601	NAD	C5A-N7A	-2.21	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1602	NAD	C5A-N7A	-2.16	1.32	1.39
2	B	1601	NAD	C4N-C3N	2.01	1.42	1.39
2	B	1601	NAD	C2A-N1A	2.07	1.37	1.33
2	A	601	NAD	C2A-N1A	2.21	1.38	1.33
2	A	601	NAD	C3N-C7N	2.23	1.54	1.50
2	A	602	NAD	C2A-N1A	2.30	1.38	1.33
2	B	1601	NAD	C3N-C7N	2.46	1.54	1.50
2	A	602	NAD	C2N-C3N	2.73	1.43	1.39
2	A	601	NAD	C6N-N1N	2.77	1.42	1.35
2	A	602	NAD	C6N-N1N	2.90	1.43	1.35
2	A	601	NAD	C2A-N3A	2.95	1.37	1.32
2	B	1602	NAD	C2A-N3A	3.01	1.37	1.32
2	B	1601	NAD	C6N-N1N	3.09	1.43	1.35
2	B	1602	NAD	C3N-C7N	3.14	1.55	1.50
2	A	602	NAD	C2A-N3A	3.18	1.37	1.32
2	B	1601	NAD	C2A-N3A	3.19	1.37	1.32
2	B	1602	NAD	C6N-N1N	3.58	1.45	1.35
2	B	1601	NAD	O4B-C1B	3.62	1.45	1.41
2	A	602	NAD	C3N-C7N	3.87	1.56	1.50
2	A	601	NAD	O4B-C1B	3.90	1.46	1.41
2	B	1601	NAD	O4D-C1D	3.94	1.46	1.41
2	B	1602	NAD	O4B-C1B	4.55	1.47	1.41
2	A	601	NAD	O4D-C1D	4.59	1.47	1.41
2	A	602	NAD	O4D-C1D	4.85	1.47	1.41
2	A	602	NAD	O4B-C1B	4.90	1.47	1.41
2	B	1602	NAD	O4D-C1D	5.14	1.47	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	NAD	N3A-C2A-N1A	-11.06	120.42	128.89
2	B	1602	NAD	N3A-C2A-N1A	-11.05	120.44	128.89
2	A	601	NAD	N3A-C2A-N1A	-10.50	120.85	128.89
2	B	1601	NAD	N3A-C2A-N1A	-10.47	120.88	128.89
2	B	1601	NAD	C4D-O4D-C1D	-2.52	106.95	109.72
2	B	1601	NAD	C4B-O4B-C1B	-2.30	107.19	109.72
2	B	1601	NAD	C3N-C7N-N7N	-2.16	115.46	117.82
2	A	602	NAD	C3N-C7N-N7N	-2.08	115.54	117.82
2	B	1602	NAD	C3N-C7N-N7N	-2.08	115.54	117.82
2	A	601	NAD	C3N-C7N-N7N	-2.02	115.61	117.82
2	B	1602	NAD	O4D-C1D-N1N	2.08	110.41	108.13
2	A	602	NAD	C2D-C3D-C4D	2.14	107.01	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1601	NAD	O4D-C1D-N1N	3.54	112.02	108.13
2	A	601	NAD	O4D-C1D-N1N	3.92	112.43	108.13
2	A	602	NAD	C4A-C5A-N7A	4.27	113.41	109.48
2	B	1602	NAD	C4A-C5A-N7A	4.60	113.71	109.48
2	B	1601	NAD	C4A-C5A-N7A	4.68	113.78	109.48
2	A	601	NAD	C4A-C5A-N7A	4.73	113.83	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAD	1	0
2	A	602	NAD	1	0
2	B	1601	NAD	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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