



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:07 AM GMT

PDB ID : 2VZ9
Title : CRYSTAL STRUCTURE OF MAMMALIAN FATTY ACID SYNTHASE IN
COMPLEX WITH NADP
Authors : Maier, T.; Leibundgut, M.; Ban, N.
Deposited on : 2008-07-31
Resolution : 3.30 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

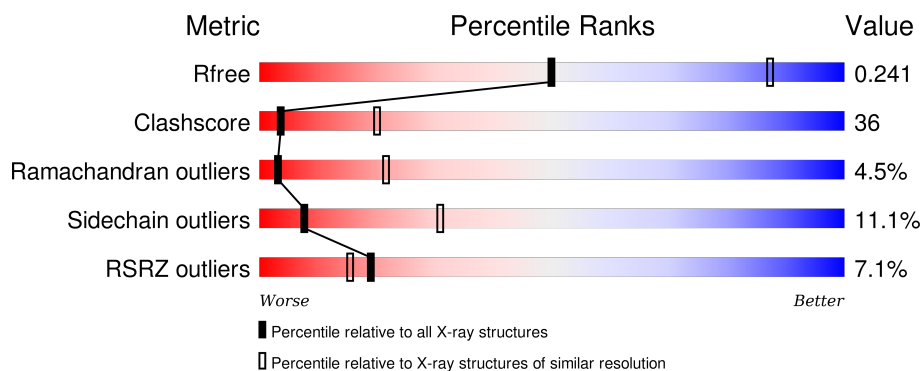
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	2512	<div> <div>5%</div> <div>38%</div> <div>38%</div> <div>7%</div> <div>17%</div> </div>
1	B	2512	<div> <div>7%</div> <div>36%</div> <div>40%</div> <div>7%</div> <div>17%</div> </div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 31949 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.

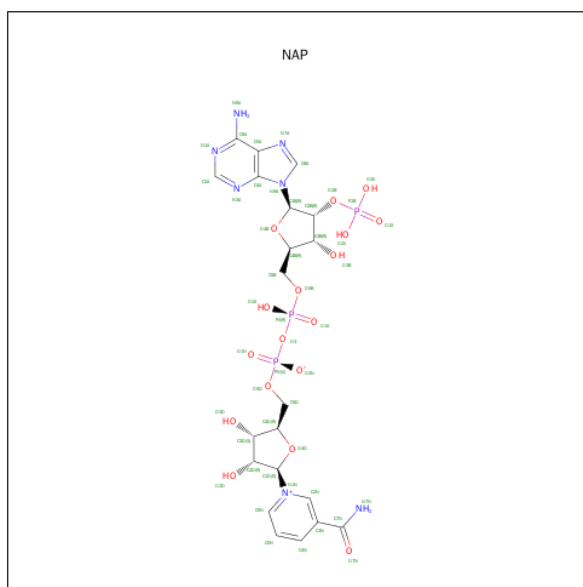
- Molecule 1 is a protein called FATTY ACID SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2081	Total	C	N	O	S	0	0	0
			15858	10015	2786	2973	84			
1	B	2086	Total	C	N	O	S	0	0	0
			15899	10041	2793	2981	84			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	834	ILE	UNK	CONFLICT SEE REMARK 9	UNP A5YV76
B	834	ILE	UNK	CONFLICT SEE REMARK 9	UNP A5YV76

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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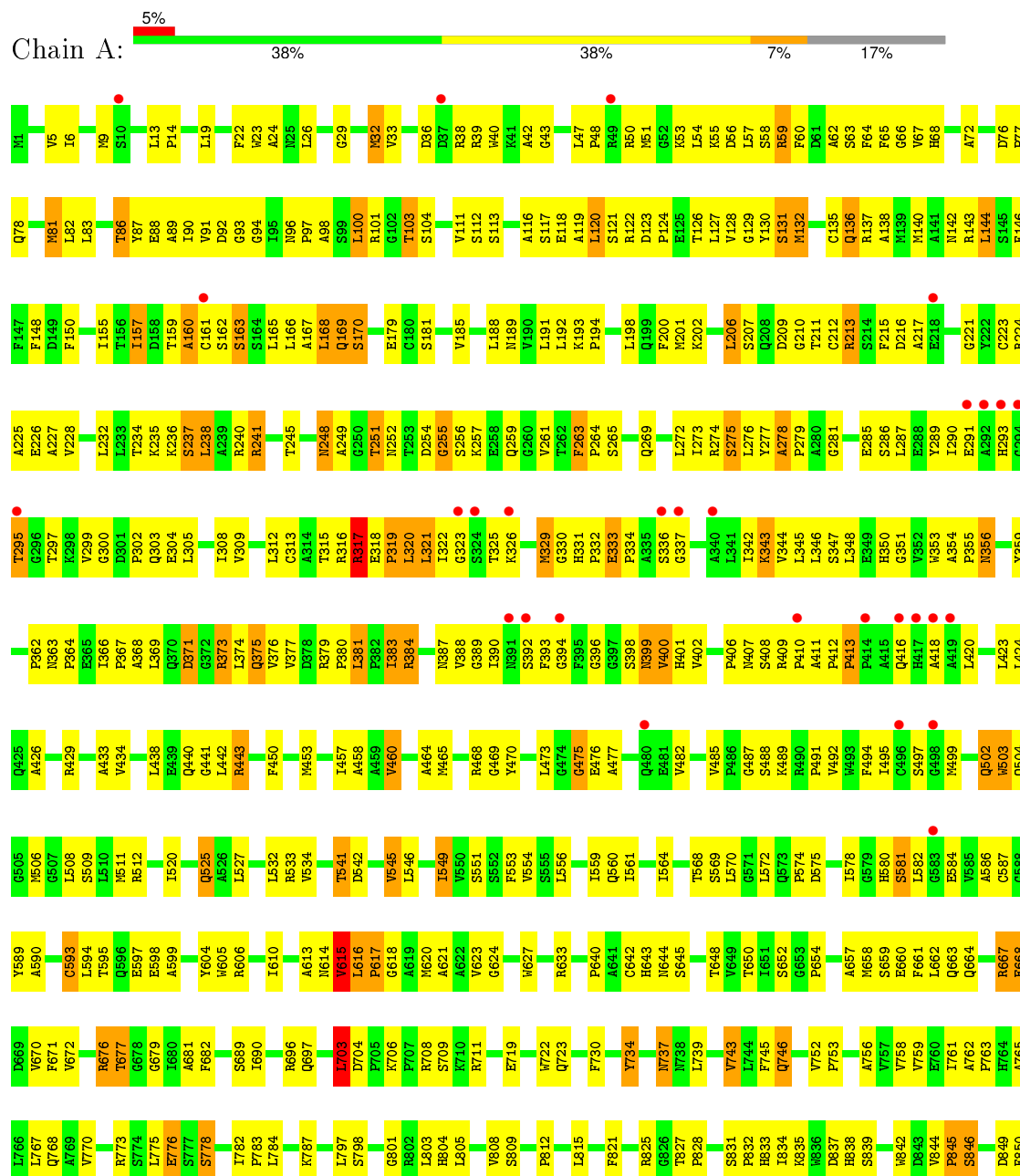
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

3 Residue-property plots

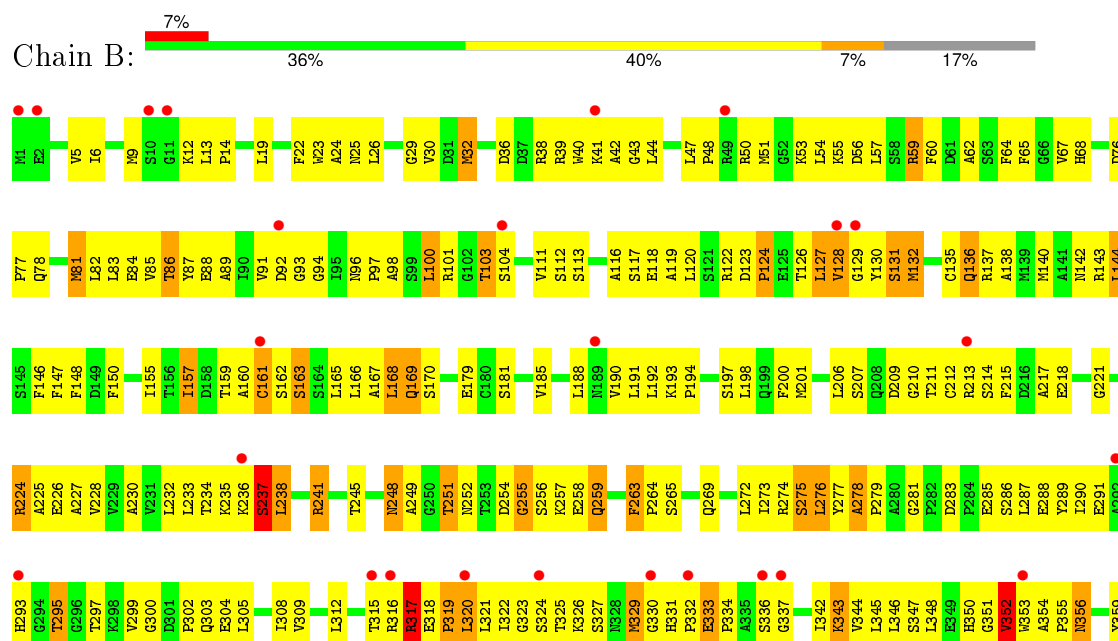
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: FATTY ACID SYNTHASE



G1781	M1782	A1783	V1784	F1785	L1786	K1787	H1788	V1789	F1790	F1791	A1792	H1793	L1794	L1795	S1796	D1797	S1798	L1799	F1800	E1801	E1802	G1803	H1807	V1810	S1811	E1812	L1813	L1814	K1815	I1818	V1823	Q1824	P1825	V1836	E1837	A1838	A1839	F1840	A1841	V1842	V1843	A1844	Q1845	H1848	K1851	V1852	V1853	L1854	Q1855	V1856	R1857	E1858												
E1703	K1704	R1705	A1706	R1711	F1712	C1719	F1720	F1721	A1721	R1724	D1725	T1726	S1727	F1728	E1729	V1732	L1733	H1734	R1735	T1736	K1739	G1740	V1741	L1742	L1743	H1746	E1750	L1753	S1756	V1757	R1758	C1759	L1760	A1761	Q1762	H1763	R1765	F1766	L1767	E1768	I1769	K1771	V1772	L1773	S1774	L1775	H1776	N1777	L1778															
S1625	V1626	L1627	L1628	L1629	T1633	V1636	T1639	E1644	V1648	P1649	S1650	V1651	V1652	T1653	T1654	A1655	S1656	V1657	T1658	L1659	V1661	R1662	G1663	L1664	V1665	Q1666	E1669	V1670	L1671	L1672	L1673	S1675	G1678	G1679	V1680	G1681	Q1682	A1683	A1684	I1687	G1692	C1693	R1694	V1695	F1696	E1697	G1698	L1699																
V1553	A1554	L1555	F1556	A1557	S1558	C1559	Q1560	D1561	R1562	L1563	C1564	S1565	V1566	V1567	V1568	L1569	S1570	F1573	R1574	L1578	A1579	G1580	G1581	L1582	F1583	S1584	P1585	D1586	S1587	L1588	T1594	R1595	D1596	G1597	M1598	M1601	E1602	F1603	S1604	G1605	R1606	R1611	M1614	G1615	M1616	V1617	P1618	A1619	E1620	G1621	L1622	A1623	T1624											
P1482	A1483	P1484	E1485	H1486	M1487	P1488	S1489	S1490	L1493	V1496	L1501	V1502	M1503	M1504	V1505	R1507	A1508	G1509	W1510	W1511	G1512	A1513	F1514	R1515	H1516	F1517	P1518	L1519	Q1520	D1522	R1523	P1524	E1525	K1526	Q1527	T1528	E1529	H1530	V1533	M1534	V1535	L1536	S1537	A1538	G1539	D1540	R1545	S1549	P1550	L1551	H1552													
T1421	S1422	F1423	V1424	W1425	L1426	D1427	L1428	L1429	L1432	L1433	A1434	D1435	A1436	S1437	S1438	R1439	P1440	V1441	W1442	L1443	M1444	A1445	A1446	G1447	C1448	A1449	L1450	T1451	H1452	V1453	V1454	G1455	V1456	V1457	N1458	C1459	L1460	R1461	K1462	E1463	P1464	G1465	G1466	H1467	R1468	T1469	R1470	C1471	V1472	V1473	V1474	S1475	A1476	L1477	S1478	S1479	L1480	L1481						
G1356	E1357	M1358	V1359	G1360	F1361	L1362	T1363	S1364	P1365	E1366	Q1367	G1368	G1369	H1370	H1371	L1372	L1373	A1374	Q1375	L1376	Q1377	W1378	E1379	S1380	L1381	F1382	G1383	S1384	L1385	L1386	L1387	L1388	L1389	V1390	S1395	L1396	Y1397	G1398	S1399	M1333	M1334	A1335	F1400	L1401	F1402	L1403	T1404	L1405	Q1406	T1407	P1408	P1409	L1410	L1411	L1412	L1413	P1414	P1415	L1416	S1417	V1418	E1419	P1420	D1421
L1289	E1290	Q1291	P1292	H1293	L1294	K1295	Q1296	G1297	P1298	W1299	D1300	P1301	A1302	M1303	P1304	L1305	P1306	G1307	S1308	L1309	G1310	K1311	A1312	L1315	L1316	C1317	M1318	C1319	A1320	L1321	L1324	P1327	P1329	A1330	M1333	M1334	A1335	F1400	L1401	F1402	L1403	T1404	L1405	Q1406	T1407	P1408	P1409	L1410	L1411	L1412	L1413	P1414	P1415	L1416	S1417	V1418	E1419	P1420	D1421					
L1221	D1222	A1223	P1224	L1225	L1226	K1227	A1228	L1229	G1230	T1231	T1232	A1233	L1234	E1235	M1236	M1237	P1240	K1241	M1242	K1243	V1244	V1245	E1246	V1247	L1248	D1251	P1252	G1253	L1254	Y1255	S1256	R1257	L1258	P1259	A1260	L1261	L1262	Q1265	P1266	V1267	M1268	D1271	Y1272	T1273	A1274	T1275	D1276	L1282	E1283	A1284	L1285	Q1286	G1287	K1288										
MET	VAL	VAL	PRO	GLY	LEU	ASP	GLY	ALA	GLN	ALA	PRO	ARG	GLU	ALA	PRO	GLN	SER	L1180	P1181	R1182	L1183	A1184	A1185	A1186	A1187	C1188	Q1189	L1190	V1191	L1192	M1193	G1194	M1195	LEU	GLN	LEU	L1200	G1201	Q1202	V1203	E1138	E1139	L1140	G1145	L1146	A1147	L1150	THR	LYS	VAL	ALA	GLN	GLY	LEU	LYS									
N1085	L1086	N1087	T1088	V1089	G1092	F1096	L1097	S1101	A1107	P1108	Q1109	E1110	H1111	L1112	I1115	K1118	F1119	C1120	F1121	T1122	H1124	V1125	E1126	C1129	L1130	A1131	G1132	M1133	T1134	A1135	Q1137	E1138	E1139	L1140	G1145	L1146	A1147	L1150	THR	LYS	VAL	ALA	GLN	GLY	LEU	LYS																		
Q1008	L1009	L1010	L1011	D1014	L1015	E1016	R1019	L1022	Q1023	V1029	F1031	L1032	D1033	A1034	L1036	H1037	M1038	S1039	I1040	L1041	P1043	P1051	F1054	T1055	S1056	I1057	D1060	P1061	T1062	H1063	H1064	R1065	Q1066	K1067	L1068	Y1069	L1071	Q1072	D1073	T1074	T1075	Q1076	A1077	A1078	V1082	D1083	R1084																	
P851	S852	M853	S854	S855	S856	S857	S858	V859	V861	F866	S867	P868	H873	Y874	L875	V876	D877	H878	D881	S882	R883	F886	P887	G888	T889	G890	A891	V892	S893	P894	S895	D896	S897	T898	L899	W899	L894	T895	H896	R897	S898	Q899	L907	T910	P911	V912	V913	F914	G915	D916	V917	I924	L925											
T928	V931	E934	V935	N936	L937	S941	F944	E945	S947	W962	E963	S964	P965	P967	F970	A974	A975	V976	D977	P978	A979	D980	S981	A983	E984	F985	L986	Y993	K994	R997	Y1001	D1002	Y1003	G1004	P1005	F1007																												

- Molecule 1: FATTY ACID SYNTHASE







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.15Å 244.89Å 135.37Å 90.00° 101.84° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 29.97 – 3.34	Depositor EDS
% Data completeness (in resolution range)	84.1 (30.00-3.30) 90.2 (29.97-3.34)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.31Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.193 , 0.244 0.198 , 0.241	Depositor DCC
R_{free} test set	4016 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	117.6	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 87.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 80013 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31949	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/16199	0.64	3/22016 (0.0%)
1	B	0.41	0/16240	0.61	1/22070 (0.0%)
All	All	0.43	0/32439	0.62	4/44086 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1216	LEU	CA-CB-CG	5.89	128.85	115.30
1	B	1216	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	703	LEU	N-CA-C	-5.16	97.08	111.00
1	A	321	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15858	0	15834	1137	0
1	B	15899	0	15882	1193	0
2	A	96	0	50	12	0
2	B	96	0	50	3	0
All	All	31949	0	31816	2282	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 36.

All (2282) 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:333:GLU:HB2	1:B:334:PRO:HD3	1.26	1.17
1:A:333:GLU:HB2	1:A:334:PRO:HD3	1.28	1.13
1:A:616:LEU:HD23	1:A:617:PRO:HD2	1.32	1.10
1:A:123:ASP:HB3	1:A:126:THR:HB	1.18	1.10
1:A:1477:LEU:HD11	1:A:2043:ARG:HD2	1.36	1.06
1:B:1662:ARG:HG2	1:B:1662:ARG:HH11	0.90	1.03
1:B:1216:LEU:HD12	1:B:1218:SER:H	1.20	1.03
1:A:343:LYS:HE3	1:A:354:ALA:HB3	1.40	1.03
1:A:1190:LEU:HD13	1:A:1206:GLN:HE21	1.23	1.02
1:A:112:SER:HB2	1:A:334:PRO:HG3	1.39	1.02
1:B:112:SER:HB2	1:B:334:PRO:HG3	1.38	1.02
1:A:384:ARG:HH11	1:A:384:ARG:HG3	1.22	1.02
1:B:384:ARG:HH11	1:B:384:ARG:HG3	1.20	1.02
1:B:278:ALA:HB3	1:B:279:PRO:HD3	1.40	1.01
1:A:165:LEU:HD23	1:A:400:VAL:HG22	1.42	1.00
1:B:643:HIS:HA	1:B:649:VAL:HG22	1.41	1.00
1:B:1616:MET:HB3	1:B:1800:PHE:CZ	1.97	0.99
1:A:278:ALA:HB3	1:A:279:PRO:HD3	1.44	0.99
1:B:1662:ARG:NH1	1:B:1662:ARG:HG2	1.65	0.98
1:B:1003:TYR:CZ	1:B:1037:HIS:HE1	1.82	0.97
1:B:1220:LEU:HB3	1:B:1257:ARG:HH22	1.30	0.96
1:A:1216:LEU:HD12	1:A:1218:SER:H	1.31	0.95
1:B:1653:THR:HG22	1:B:1810:VAL:HG12	1.48	0.94
1:A:166:LEU:HD12	1:A:251:THR:HG21	1.50	0.94
1:B:165:LEU:HD23	1:B:400:VAL:HG22	1.51	0.93
1:B:1418:VAL:HG13	1:B:1425:TRP:CE2	2.03	0.93
1:B:1184:LEU:H	1:B:1216:LEU:HD21	1.32	0.93
1:B:333:GLU:HB2	1:B:334:PRO:CD	1.99	0.92
1:B:166:LEU:HD12	1:B:251:THR:HG21	1.51	0.92
1:A:1624:THR:HG22	1:A:1857:ARG:HH21	1.35	0.92
1:A:1790:THR:HG22	1:B:1662:ARG:HH22	1.33	0.92
1:A:1003:TYR:CE2	1:A:1037:HIS:HE1	1.87	0.92
1:A:1528:THR:HG22	1:A:1530:HIS:H	1.35	0.91
1:B:1616:MET:HE2	1:B:1650:ILE:HD13	1.53	0.91
1:A:1003:TYR:CZ	1:A:1037:HIS:HE1	1.89	0.90
1:B:1662:ARG:HH11	1:B:1662:ARG:CG	1.82	0.90
1:B:1003:TYR:CE2	1:B:1037:HIS:HE1	1.88	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:ASN:HD22	1:A:1136:LEU:HD12	1.36	0.90
1:A:1182:ARG:HB3	1:A:1216:LEU:HB2	1.52	0.90
1:B:1628:LEU:HD13	1:B:1633:THR:HG21	1.54	0.90
1:A:443:ARG:HG3	1:A:443:ARG:HH11	1.38	0.88
1:A:1349:LEU:HD13	1:A:1359:VAL:HG21	1.56	0.88
1:A:126:THR:HG22	1:A:127:LEU:HG	1.56	0.88
1:B:1475:SER:HB3	1:B:1505:VAL:HG13	1.53	0.87
1:A:1545:ARG:HH11	1:A:1545:ARG:HG3	1.38	0.87
1:A:1082:VAL:HG22	1:A:1089:VAL:HG22	1.56	0.87
1:B:1208:ARG:HH11	1:B:1211:LEU:HD22	1.39	0.87
1:B:1838:ALA:HA	1:B:1841:ARG:HG3	1.57	0.87
1:A:333:GLU:HB2	1:A:334:PRO:CD	2.04	0.86
1:B:443:ARG:HH11	1:B:443:ARG:HG3	1.40	0.86
1:A:319:PRO:HD2	1:A:373:ARG:O	1.74	0.86
1:B:1232:THR:HA	1:B:1515:ARG:HH21	1.40	0.86
1:A:1222:ASP:HB3	1:A:1257:ARG:CZ	2.07	0.85
1:A:1838:ALA:HA	1:A:1841:ARG:HG3	1.58	0.85
1:B:1315:LEU:O	1:B:1344:LEU:HD13	1.76	0.85
1:A:123:ASP:CB	1:A:126:THR:HB	2.06	0.85
1:B:1569:THR:HG21	1:B:1622:LEU:HA	1.59	0.85
1:A:502:GLN:HG2	1:A:556:LEU:HD11	1.59	0.84
1:A:1893:LEU:HB3	1:A:1925:GLN:NE2	1.92	0.84
1:A:527:LEU:HD12	1:A:534:VAL:HG22	1.59	0.84
1:B:319:PRO:HD2	1:B:373:ARG:O	1.76	0.84
1:B:782:ILE:HD12	1:B:803:LEU:HD23	1.60	0.84
1:A:82:LEU:O	1:A:86:THR:HG23	1.78	0.84
1:B:1326:ASP:OD1	1:B:1327:PRO:HD2	1.76	0.84
1:B:527:LEU:HD12	1:B:534:VAL:HG22	1.56	0.84
1:A:1009:LEU:HD11	1:A:1030:SER:HB2	1.58	0.83
1:A:1124:HIS:CD2	1:A:1512:GLY:HA2	2.13	0.83
1:B:1651:VAL:HG13	1:B:1680:VAL:HA	1.60	0.83
1:B:87:TYR:O	1:B:91:VAL:HG22	1.77	0.83
1:A:1771:LYS:HE2	1:A:1795:LEU:HD22	1.61	0.83
1:A:1034:ALA:HA	1:A:1037:HIS:CD2	2.12	0.83
1:A:782:ILE:HD12	1:A:803:LEU:HD23	1.61	0.83
1:A:1662:ARG:HH11	1:A:1662:ARG:CG	1.91	0.83
1:A:976:VAL:HG22	1:A:977:ASP:H	1.44	0.82
1:B:82:LEU:O	1:B:86:THR:HG23	1.78	0.82
1:B:1486:MET:O	1:B:1488:PRO:HD3	1.78	0.82
1:A:1505:VAL:HG23	1:A:1513:ALA:HA	1.61	0.82
1:B:680:ILE:HG12	1:B:681:ALA:N	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1533:VAL:HG12	1:B:1622:LEU:HB3	1.61	0.82
1:B:1248:LEU:HD11	1:B:1324:LEU:HG	1.61	0.82
1:B:1642:LEU:HD12	1:B:1859:GLU:HG3	1.59	0.82
1:A:627:TRP:HB2	1:A:643:HIS:CD2	2.15	0.82
1:A:610:ILE:HA	1:A:690:ILE:HD13	1.60	0.82
1:B:1082:VAL:HG22	1:B:1089:VAL:HG22	1.60	0.81
1:B:1009:LEU:HD11	1:B:1030:SER:HB2	1.62	0.81
1:A:1252:GLY:HA3	1:A:1318:ASN:HB3	1.63	0.81
1:B:1216:LEU:HD12	1:B:1218:SER:N	1.95	0.81
1:A:1220:LEU:HB3	1:A:1257:ARG:HH22	1.42	0.81
1:A:1357:GLU:O	1:A:1361:PHE:HD1	1.62	0.81
1:A:132:MET:HE1	1:B:200:PHE:CE2	2.16	0.81
1:A:1190:LEU:HD13	1:A:1206:GLN:NE2	1.96	0.81
1:A:623:VAL:HG22	1:A:672:VAL:HG22	1.63	0.81
1:A:1418:VAL:HG13	1:A:1425:TRP:CE2	2.14	0.81
1:A:984:GLU:O	1:A:985:PHE:HB2	1.79	0.81
1:A:883:ARG:HH11	1:A:924:ILE:HD11	1.45	0.80
1:A:1428:SER:O	1:A:1432:ILE:HG13	1.82	0.80
1:B:502:GLN:HG2	1:B:556:LEU:HD11	1.61	0.80
1:B:278:ALA:CB	1:B:279:PRO:HD3	2.10	0.80
1:A:468:ARG:HD3	1:A:485:VAL:HG21	1.62	0.80
1:A:217:ALA:HB2	1:A:364:PRO:HD3	1.63	0.80
1:B:1073:ASP:O	1:B:1074:THR:HG22	1.81	0.80
1:B:944:PHE:CD2	1:B:959:VAL:HG22	2.17	0.80
1:B:1282:LEU:HD21	1:B:1296:GLN:HB2	1.64	0.80
1:A:861:VAL:HG22	1:A:934:GLU:HB3	1.64	0.80
1:B:1003:TYR:CZ	1:B:1037:HIS:CE1	2.69	0.79
1:B:1771:LYS:HE2	1:B:1795:LEU:HD22	1.63	0.79
1:A:278:ALA:CB	1:A:279:PRO:HD3	2.12	0.79
1:A:1211:LEU:O	1:A:1214:ASP:HB2	1.80	0.79
1:A:1887:TYR:HD2	1:A:1967:GLY:HA3	1.48	0.79
1:A:200:PHE:CE2	1:B:132:MET:HE1	2.16	0.79
1:B:420:LEU:HD11	1:B:512:ARG:HB3	1.62	0.79
1:A:19:LEU:HD11	1:A:342:ILE:HD13	1.62	0.79
1:A:1473:LEU:HD11	1:A:1503:MET:SD	2.22	0.79
1:A:1265:GLN:HE21	1:A:2026:ARG:HH11	1.30	0.79
1:B:668:GLU:O	1:B:669:ASP:HB2	1.80	0.79
1:B:143:ARG:HG2	1:B:143:ARG:HH11	1.47	0.79
1:A:6:ILE:HG21	1:A:345:LEU:HD11	1.64	0.79
1:B:1616:MET:HB3	1:B:1800:PHE:HZ	1.45	0.78
1:B:23:TRP:CE2	1:B:350:HIS:HD2	2.00	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:PHE:CE2	1:A:773:ARG:NH2	2.51	0.78
1:B:1541:LEU:HD13	1:B:1840:PHE:HB3	1.65	0.78
1:A:155:ILE:HD11	1:B:166:LEU:HD11	1.66	0.78
1:B:1299:TRP:HZ3	1:B:1301:PRO:HA	1.46	0.78
1:B:1996:TYR:HD1	1:B:2040:ALA:HB1	1.48	0.78
1:B:1364:SER:N	1:B:1365:PRO:HD2	1.98	0.78
1:A:23:TRP:CE2	1:A:350:HIS:HD2	2.02	0.78
1:B:1428:SER:O	1:B:1432:ILE:HG13	1.83	0.78
1:B:1119:PHE:HB3	1:B:2105:VAL:HB	1.63	0.77
1:A:1725:ASP:OD2	1:A:1727:SER:HB3	1.84	0.77
1:B:1139:GLU:OE2	1:B:1216:LEU:HD11	1.84	0.77
1:B:620:MET:HG3	1:B:677:THR:HG21	1.64	0.77
1:B:23:TRP:CE2	1:B:350:HIS:CD2	2.73	0.77
1:B:1887:TYR:HD2	1:B:1967:GLY:HA3	1.49	0.77
1:A:1616:MET:HE3	1:A:1650:ILE:HA	1.64	0.77
1:A:1996:TYR:HD1	1:A:2040:ALA:HB1	1.48	0.77
1:A:627:TRP:HB2	1:A:643:HIS:HD2	1.50	0.77
1:A:1254:LEU:HD13	1:A:1316:VAL:HG12	1.67	0.77
1:A:944:PHE:CD2	1:A:959:VAL:HG22	2.19	0.77
1:B:1184:LEU:H	1:B:1216:LEU:CD2	1.96	0.77
1:A:984:GLU:HG2	1:A:986:ARG:HE	1.49	0.77
1:B:1893:LEU:HB3	1:B:1925:GLN:NE2	2.00	0.77
1:B:6:ILE:HG21	1:B:345:LEU:HD11	1.67	0.77
1:A:1656:TYR:CE2	1:A:1687:ILE:HD13	2.19	0.77
1:B:1150:LEU:HD13	1:B:1192:LEU:HD23	1.65	0.77
1:A:368:ALA:H	1:A:371:ASP:HB3	1.49	0.77
1:B:1183:LEU:HD13	1:B:1210:LEU:HB3	1.65	0.76
1:A:1457:VAL:HG21	1:A:1473:LEU:HD22	1.67	0.76
1:A:87:TYR:O	1:A:91:VAL:HG22	1.85	0.76
1:A:2075:THR:HB	1:A:2077:ASP:H	1.51	0.76
1:A:309:VAL:HG11	1:A:373:ARG:HD2	1.67	0.76
1:B:861:VAL:HG22	1:B:934:GLU:HB3	1.66	0.76
1:A:168:LEU:HB2	1:A:185:VAL:HG11	1.68	0.76
1:A:1207:GLU:O	1:A:1211:LEU:HB2	1.86	0.76
1:B:883:ARG:HH11	1:B:924:ILE:HD11	1.51	0.76
1:B:1133:ASN:HD22	1:B:1136:LEU:HD12	1.51	0.76
1:B:1034:ALA:HA	1:B:1037:HIS:CD2	2.20	0.76
1:A:1073:ASP:O	1:A:1074:THR:HG22	1.84	0.76
1:A:504:GLN:HA	1:A:541:THR:HG21	1.67	0.76
1:B:1533:VAL:CG1	1:B:1622:LEU:HB3	2.16	0.76
1:A:112:SER:CB	1:A:334:PRO:HG3	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:SER:CB	1:B:334:PRO:HG3	2.14	0.76
1:B:384:ARG:HH11	1:B:384:ARG:CG	1.98	0.76
1:B:1456:MET:HG3	1:B:2036:PHE:HB2	1.68	0.76
1:B:343:LYS:HE3	1:B:354:ALA:HB3	1.65	0.76
1:A:1119:PHE:HB3	1:A:2105:VAL:HB	1.67	0.75
1:B:416:GLN:O	1:B:420:LEU:HB2	1.86	0.75
1:B:1974:VAL:HG22	1:B:1994:PRO:HG2	1.66	0.75
1:A:111:VAL:HG22	1:A:188:LEU:HB2	1.67	0.75
1:A:1429:LEU:HD11	1:A:1443:LEU:HD11	1.69	0.75
1:A:1569:THR:HG21	1:A:1622:LEU:HA	1.68	0.75
1:A:944:PHE:HD2	1:A:959:VAL:HG22	1.51	0.75
1:B:368:ALA:H	1:B:371:ASP:HB3	1.52	0.75
1:A:23:TRP:CE2	1:A:350:HIS:CD2	2.74	0.75
1:A:1182:ARG:HE	1:A:1217:LEU:H	1.34	0.75
1:A:963:GLU:O	1:A:965:PRO:HD3	1.86	0.75
1:A:1974:VAL:HG22	1:A:1994:PRO:HG2	1.69	0.75
1:B:944:PHE:HD2	1:B:959:VAL:HG22	1.52	0.74
1:A:416:GLN:O	1:A:420:LEU:HB2	1.87	0.74
1:B:1926:ALA:O	1:B:1930:ARG:HB2	1.87	0.74
1:A:14:PRO:HG2	1:A:329:MET:HG3	1.69	0.74
1:B:1430:LYS:HE3	1:B:1981:GLU:O	1.87	0.74
1:A:384:ARG:HH11	1:A:384:ARG:CG	1.99	0.74
1:B:1222:ASP:HB3	1:B:1257:ARG:CZ	2.17	0.74
1:A:1003:TYR:CZ	1:A:1037:HIS:CE1	2.73	0.74
1:B:1007:PHE:HE2	1:B:1030:SER:HA	1.53	0.74
1:B:1234:LEU:HD22	1:B:1262:LEU:HD22	1.69	0.74
1:B:14:PRO:HG2	1:B:329:MET:HG3	1.67	0.74
1:A:326:LYS:HE3	1:A:336:SER:HB2	1.70	0.74
1:B:168:LEU:HB2	1:B:185:VAL:HG11	1.69	0.74
1:B:1407:GLN:HE21	1:B:1439:ARG:NH2	1.85	0.74
1:B:1418:VAL:HG21	1:B:1443:LEU:HD13	1.70	0.74
1:B:326:LYS:HE3	1:B:336:SER:HB2	1.69	0.74
1:B:1476:ASN:O	1:B:1477:LEU:HD23	1.88	0.74
1:B:1231:ASP:HB3	1:B:1515:ARG:HD2	1.70	0.73
1:A:1460:LEU:HD11	1:A:1980:LEU:HD13	1.68	0.73
1:A:295:THR:HG22	1:A:331:HIS:HD2	1.52	0.73
1:B:1616:MET:CE	1:B:1650:ILE:HD13	2.17	0.73
1:B:982:THR:C	1:B:984:GLU:H	1.90	0.73
1:A:856:CYS:CB	1:B:856:CYS:SG	2.77	0.73
1:B:19:LEU:HD11	1:B:342:ILE:HD13	1.69	0.73
1:A:47:LEU:HA	1:A:201:MET:HE1	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1223:ALA:HB1	1:A:1224:PRO:HD2	1.70	0.73
1:B:136:GLN:HE22	1:B:138:ALA:H	1.35	0.73
1:B:1223:ALA:HB1	1:B:1224:PRO:HD2	1.68	0.73
1:B:322:ILE:HD12	1:B:374:LEU:HD13	1.69	0.73
1:A:1725:ASP:OD1	1:A:1726:THR:N	2.22	0.73
1:B:1641:THR:HG23	1:B:1644:GLU:OE1	1.87	0.73
1:A:616:LEU:CD2	1:A:617:PRO:HD2	2.15	0.73
1:A:1007:PHE:HE2	1:A:1030:SER:HA	1.54	0.72
1:B:1616:MET:HB3	1:B:1800:PHE:CE1	2.23	0.72
1:A:1208:ARG:HH11	1:A:1211:LEU:HD22	1.54	0.72
1:A:143:ARG:HG2	1:A:143:ARG:HH11	1.54	0.72
1:B:1205:ALA:O	1:B:1209:PRO:HG2	1.90	0.72
1:B:111:VAL:HG22	1:B:188:LEU:HB2	1.70	0.72
1:B:1407:GLN:HG2	1:B:1409:PRO:HD2	1.72	0.72
1:B:1247:VAL:HG11	1:B:1301:PRO:HG3	1.71	0.72
1:B:1732:VAL:O	1:B:1736:THR:HB	1.88	0.72
1:A:1545:ARG:CG	1:A:1545:ARG:HH11	2.02	0.72
1:B:1299:TRP:CZ3	1:B:1301:PRO:HA	2.24	0.72
1:A:1857:ARG:HG2	1:A:1871:ILE:HD11	1.72	0.72
1:B:309:VAL:HG11	1:B:373:ARG:HD2	1.69	0.72
1:A:504:GLN:HG2	1:A:541:THR:HG22	1.71	0.72
1:B:1725:ASP:OD2	1:B:1727:SER:HB3	1.89	0.72
1:A:1439:ARG:HB3	1:A:1440:PRO:HD3	1.72	0.72
1:A:1570:SER:OG	1:A:1602:GLU:HB3	1.90	0.72
1:A:2006:THR:HG21	1:A:2048:ARG:HH22	1.55	0.72
1:B:1254:LEU:HD13	1:B:1316:VAL:HG12	1.71	0.72
1:B:1408:THR:N	1:B:1409:PRO:HD3	2.05	0.71
1:A:136:GLN:HE22	1:A:138:ALA:H	1.37	0.71
1:B:1353:HIS:HB2	1:B:1354:PRO:HD2	1.72	0.71
1:B:1299:TRP:NE1	1:B:1306:PRO:HD2	2.04	0.71
1:A:1649:PRO:O	1:A:1653:THR:OG1	2.08	0.71
1:A:1661:VAL:HG21	1:A:1810:VAL:HG22	1.71	0.71
1:B:963:GLU:O	1:B:965:PRO:HD3	1.91	0.71
1:A:1299:TRP:HE1	1:A:1306:PRO:HD2	1.54	0.71
1:A:1903:TRP:HB2	1:A:2092:LEU:HD13	1.72	0.71
1:A:504:GLN:HG2	1:A:541:THR:CG2	2.20	0.71
1:A:1302:ALA:O	1:A:1304:PRO:HD3	1.91	0.71
1:B:112:SER:HB2	1:B:334:PRO:CG	2.19	0.71
1:A:443:ARG:NH1	1:A:443:ARG:HG3	2.05	0.71
1:B:982:THR:HG23	1:B:983:ALA:H	1.55	0.71
1:B:1903:TRP:HB2	1:B:2092:LEU:HD13	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1439:ARG:HB3	1:B:1440:PRO:HD3	1.73	0.71
1:A:112:SER:HB2	1:A:334:PRO:CG	2.18	0.71
1:B:50:ARG:HD3	1:B:210:GLY:O	1.90	0.71
1:A:1489:SER:H	1:A:1493:LEU:HD22	1.55	0.70
1:B:295:THR:HG22	1:B:331:HIS:HD2	1.55	0.70
1:A:1836:VAL:HG13	1:A:1854:ILE:HD13	1.73	0.70
1:A:166:LEU:HD11	1:B:155:ILE:HD11	1.71	0.70
1:B:1567:TYR:HA	1:B:1857:ARG:HG3	1.73	0.70
1:A:917:VAL:CG1	1:A:1054:PHE:HB2	2.22	0.70
1:B:165:LEU:HB2	1:B:337:GLY:HA3	1.74	0.70
1:B:1528:THR:HG22	1:B:1530:HIS:H	1.57	0.70
1:B:1139:GLU:CD	1:B:1218:SER:HB2	2.12	0.70
1:A:51:MET:HE2	1:A:191:LEU:HD13	1.74	0.70
1:A:215:PHE:CD2	1:A:305:LEU:HD11	2.26	0.70
1:B:1836:VAL:HG13	1:B:1854:ILE:HD13	1.74	0.70
1:A:502:GLN:CG	1:A:556:LEU:HD11	2.22	0.70
1:A:1186:ALA:HB1	1:A:1210:LEU:HD13	1.73	0.70
1:B:782:ILE:HD12	1:B:803:LEU:CD2	2.22	0.70
1:B:504:GLN:N	1:B:546:LEU:HD11	2.07	0.70
1:A:1036:LEU:HD21	1:A:1096:PHE:HE1	1.57	0.70
1:B:1371:HIS:O	1:B:1372:LEU:HG	1.92	0.69
1:A:368:ALA:N	1:A:371:ASP:HB3	2.08	0.69
1:B:1302:ALA:HB3	1:B:1304:PRO:HD2	1.74	0.69
1:A:1216:LEU:HD12	1:A:1218:SER:N	2.06	0.69
1:A:39:ARG:NH1	1:A:57:LEU:HD22	2.07	0.69
1:A:54:LEU:HG	1:A:226:GLU:HG3	1.74	0.69
1:B:913:VAL:HG23	1:B:962:TRP:HB2	1.74	0.69
1:A:1694:ARG:HH11	1:A:1694:ARG:HG3	1.57	0.69
1:B:2053:LEU:HD22	1:B:2054:PRO:HD2	1.74	0.69
1:A:853:GLY:O	1:A:854:SER:HB3	1.92	0.69
1:A:782:ILE:HD12	1:A:803:LEU:CD2	2.22	0.69
1:A:2064:GLY:O	1:A:2066:VAL:N	2.22	0.69
1:B:1034:ALA:O	1:B:1037:HIS:HB2	1.93	0.69
1:B:78:GLN:HB3	1:B:188:LEU:HD13	1.74	0.69
1:A:1777:ASN:HD22	1:B:1783:ALA:H	1.39	0.69
1:A:1782:MET:HB2	1:B:1778:HIS:O	1.92	0.69
1:A:159:THR:CG2	1:A:398:SER:HB3	2.23	0.69
1:A:1003:TYR:CE2	1:A:1037:HIS:CE1	2.78	0.69
1:B:1299:TRP:HE1	1:B:1306:PRO:HD2	1.57	0.69
1:A:1345:LEU:HD13	1:A:1403:LEU:HD13	1.74	0.69
1:A:913:VAL:HG23	1:A:962:TRP:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1662:ARG:HH11	1:A:1662:ARG:HG2	1.57	0.68
1:B:1180:LEU:HD23	1:B:1189:GLN:HE22	1.58	0.68
1:B:333:GLU:CB	1:B:334:PRO:HD3	2.15	0.68
1:B:54:LEU:HG	1:B:226:GLU:HG3	1.76	0.68
1:B:1036:LEU:HD21	1:B:1096:PHE:HE1	1.58	0.68
1:A:1034:ALA:O	1:A:1037:HIS:HB2	1.93	0.68
1:A:502:GLN:HG2	1:A:556:LEU:CD1	2.22	0.68
1:B:1361:PHE:O	1:B:1362:LEU:HD12	1.94	0.68
1:B:615:VAL:HG22	1:B:686:PHE:HD2	1.57	0.68
1:B:1554:ALA:HB2	1:B:1882:PRO:HG3	1.76	0.68
1:B:1703:GLU:O	1:B:1706:ALA:HB3	1.94	0.68
1:A:941:SER:HB2	1:B:945:GLU:OE2	1.93	0.68
1:B:420:LEU:HD11	1:B:512:ARG:HD2	1.76	0.68
1:A:808:VAL:HG12	1:A:809:SER:N	2.08	0.68
1:A:1146:LEU:HD13	1:A:1189:GLN:HG2	1.75	0.68
1:B:502:GLN:CG	1:B:556:LEU:HD11	2.23	0.68
1:B:1060:ASP:OD1	1:B:1062:VAL:HG23	1.93	0.68
1:B:159:THR:CG2	1:B:398:SER:HB3	2.22	0.68
1:B:1214:ASP:HB3	1:B:1215:PRO:HD3	1.74	0.68
1:A:50:ARG:HD3	1:A:210:GLY:O	1.94	0.68
1:A:1705:ARG:HG2	1:A:1720:PHE:HD2	1.59	0.68
1:A:1252:GLY:HA2	1:A:1318:ASN:HD22	1.59	0.68
1:A:953:LEU:HD12	1:A:954:ILE:N	2.09	0.68
1:B:1363:THR:HG22	1:B:1363:THR:O	1.93	0.68
1:B:1472:VAL:HG13	1:B:1502:VAL:O	1.94	0.68
1:B:1477:LEU:HD11	1:B:2043:ARG:HD2	1.74	0.68
1:A:976:VAL:O	1:A:978:PRO:HD3	1.93	0.68
1:A:1778:HIS:O	1:B:1782:MET:HB2	1.94	0.67
1:A:1732:VAL:O	1:A:1736:THR:HB	1.93	0.67
1:B:1003:TYR:CE2	1:B:1037:HIS:CE1	2.78	0.67
1:A:1009:LEU:CD1	1:A:1030:SER:HB2	2.23	0.67
1:A:1302:ALA:O	1:A:1303:ASN:HB2	1.92	0.67
1:B:159:THR:HG22	1:B:159:THR:O	1.94	0.67
1:B:917:VAL:CG1	1:B:1054:PHE:HB2	2.24	0.67
1:B:550:VAL:HG23	1:B:611:LYS:HD3	1.75	0.67
1:A:1248:LEU:HB3	1:A:1321:LEU:HD23	1.76	0.67
1:B:752:VAL:HG11	1:B:775:LEU:HD21	1.76	0.67
1:B:1457:VAL:HG21	1:B:1473:LEU:HD22	1.77	0.67
1:B:1252:GLY:HA3	1:B:1318:ASN:HB3	1.76	0.67
1:A:1275:THR:CG2	1:A:1299:TRP:HB2	2.24	0.67
1:B:1554:ALA:O	1:B:1556:PRO:HD3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1268:MET:HA	1:A:1268:MET:HE2	1.76	0.67
1:B:1454:VAL:HG13	1:B:1503:MET:CE	2.25	0.67
1:B:953:LEU:HD12	1:B:954:ILE:N	2.09	0.67
1:B:47:LEU:HA	1:B:201:MET:HE1	1.76	0.67
1:B:502:GLN:HG2	1:B:556:LEU:CD1	2.24	0.67
1:A:1234:LEU:HD22	1:A:1262:LEU:HD22	1.76	0.67
1:B:98:ALA:HA	1:B:101:ARG:HG3	1.77	0.67
1:A:254:ASP:HB2	1:A:257:LYS:HE2	1.76	0.67
1:A:1457:VAL:HG11	1:A:1473:LEU:HD22	1.76	0.67
1:A:1247:VAL:HG23	1:A:1315:LEU:HD11	1.75	0.67
1:B:1585:PRO:HB3	1:B:1598:MET:CE	2.25	0.67
1:B:1387:LEU:HD23	1:B:1406:GLN:HB3	1.76	0.67
1:A:157:ILE:HD11	1:A:167:ALA:HA	1.77	0.67
1:B:570:LEU:HB3	1:B:810:VAL:HB	1.77	0.67
1:B:1705:ARG:HG2	1:B:1720:PHE:HD2	1.60	0.67
1:A:2075:THR:HG22	1:A:2076:ASN:H	1.60	0.66
1:B:1887:TYR:CD2	1:B:1967:GLY:HA3	2.30	0.66
1:A:1353:HIS:HB3	1:A:1354:PRO:HD2	1.77	0.66
1:B:420:LEU:CD1	1:B:512:ARG:HD2	2.26	0.66
1:B:288:GLU:HG3	1:B:385:GLY:O	1.95	0.66
1:B:1344:LEU:HD12	1:B:1346:LEU:HD21	1.77	0.66
1:B:1725:ASP:OD1	1:B:1726:THR:N	2.28	0.66
1:A:1703:GLU:O	1:A:1706:ALA:HB3	1.94	0.66
1:A:460:VAL:HG21	1:A:465:MET:HG3	1.78	0.66
1:B:359:TYR:OH	1:B:362:PRO:HG3	1.95	0.66
1:B:581:SER:HB2	1:B:683:HIS:NE2	2.10	0.66
1:A:1350:LEU:O	1:A:1356:GLY:HA3	1.95	0.66
1:B:217:ALA:HB2	1:B:364:PRO:HD3	1.78	0.66
1:A:1350:LEU:HD22	1:A:1373:LEU:O	1.96	0.66
1:A:289:TYR:HB3	1:A:388:VAL:HG22	1.76	0.66
1:B:2006:THR:HG21	1:B:2048:ARG:HH22	1.60	0.66
1:B:2075:THR:HG22	1:B:2076:ASN:H	1.59	0.66
1:A:2053:LEU:HD22	1:A:2054:PRO:HD2	1.76	0.66
1:B:1653:THR:HG22	1:B:1810:VAL:CG1	2.25	0.66
1:B:499:MET:SD	1:B:502:GLN:NE2	2.68	0.66
1:B:289:TYR:HB3	1:B:388:VAL:HG22	1.78	0.66
1:A:78:GLN:HB3	1:A:188:LEU:HD13	1.77	0.66
1:B:1409:PRO:HB2	1:B:1439:ARG:HH12	1.61	0.66
1:A:56:ASP:OD2	1:A:59:ARG:HD3	1.96	0.66
1:A:77:PRO:O	1:A:81:MET:HG2	1.95	0.66
1:B:1036:LEU:CD2	1:B:1096:PHE:HE1	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1890:THR:HA	1:A:1915:THR:HB	1.76	0.66
1:A:1486:MET:CE	1:A:1506:TYR:HB3	2.26	0.66
1:B:215:PHE:CD2	1:B:305:LEU:HD11	2.31	0.65
1:A:1533:VAL:CG1	1:A:1622:LEU:HB3	2.25	0.65
1:A:545:VAL:HG22	1:A:551:SER:CB	2.26	0.65
1:B:263:PHE:HE2	1:B:303:GLN:HE21	1.44	0.65
1:A:64:PHE:HB2	1:A:429:ARG:HH21	1.61	0.65
1:A:1183:LEU:HB3	1:A:1216:LEU:HD23	1.78	0.65
1:B:82:LEU:HG	1:B:144:LEU:HD13	1.78	0.65
1:A:1357:GLU:O	1:A:1361:PHE:CD1	2.48	0.65
1:A:1783:ALA:H	1:B:1777:ASN:HD22	1.44	0.65
1:A:165:LEU:HB2	1:A:337:GLY:HA3	1.78	0.65
1:A:1484:PRO:O	1:A:1485:GLU:HB2	1.97	0.65
1:B:1009:LEU:CD1	1:B:1030:SER:HB2	2.26	0.65
1:A:503:TRP:CD1	1:A:787:LYS:HB2	2.32	0.65
1:B:1674:HIS:CD2	1:B:1698:THR:OG1	2.50	0.65
1:A:1060:ASP:OD1	1:A:1062:VAL:HG23	1.95	0.65
1:B:2064:GLY:O	1:B:2066:VAL:N	2.24	0.65
1:A:98:ALA:HA	1:A:101:ARG:HG3	1.79	0.65
1:A:1483:ALA:N	1:A:1484:PRO:HD3	2.11	0.65
1:A:254:ASP:CB	1:A:257:LYS:HE2	2.27	0.65
1:A:1888:VAL:HG22	1:A:1913:VAL:HB	1.78	0.65
1:A:118:GLU:HG3	1:B:118:GLU:HG3	1.77	0.65
1:B:1207:GLU:O	1:B:1211:LEU:HB2	1.96	0.65
1:B:443:ARG:HG3	1:B:443:ARG:NH1	2.08	0.65
1:B:368:ALA:N	1:B:371:ASP:HB3	2.11	0.65
1:B:1566:VAL:HG12	1:B:1856:VAL:HG21	1.77	0.65
1:B:254:ASP:CB	1:B:257:LYS:HE2	2.27	0.65
1:B:1374:SER:HB2	1:B:1377:GLN:HG3	1.79	0.65
1:A:1140:LEU:HD21	1:A:1354:PRO:HG2	1.77	0.65
1:B:1975:LEU:HD22	1:B:1977:ASP:OD1	1.96	0.65
1:A:1208:ARG:HH11	1:A:1211:LEU:CD2	2.11	0.64
1:B:1603:PHE:HE2	1:B:1615:GLY:C	2.00	0.64
1:A:1926:ALA:O	1:A:1930:ARG:HB2	1.95	0.64
1:B:662:LEU:HD13	1:B:672:VAL:HG12	1.79	0.64
1:A:1476:ASN:HA	1:A:1486:MET:SD	2.37	0.64
1:A:1574:ARG:HD2	1:A:1588:ILE:HD11	1.79	0.64
1:A:366:ILE:HD11	1:A:369:LEU:HD11	1.78	0.64
1:B:1470:ARG:HG3	1:B:1470:ARG:O	1.97	0.64
1:B:1766:PHE:HD2	1:B:1791:PHE:CE1	2.16	0.64
1:A:1887:TYR:CD2	1:A:1967:GLY:HA3	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1407:GLN:CG	1:B:1409:PRO:HD2	2.27	0.64
1:B:1374:SER:O	1:B:1378:TRP:HD1	1.81	0.64
1:B:1658:SER:O	1:B:1767:LEU:HD13	1.97	0.64
1:A:333:GLU:CB	1:A:334:PRO:HD3	2.18	0.64
1:B:157:ILE:HD11	1:B:167:ALA:HA	1.80	0.64
1:B:765:ALA:HB1	1:B:768:GLN:CG	2.28	0.64
1:B:527:LEU:HD13	1:B:532:LEU:HD23	1.80	0.64
1:A:1653:THR:HG22	1:A:1810:VAL:CG1	2.28	0.64
1:A:856:CYS:HB3	1:B:856:CYS:SG	2.37	0.64
1:A:1915:THR:CG2	2:A:3002:NAP:H2A	2.28	0.64
1:B:925:LEU:HD22	1:B:931:VAL:HG21	1.80	0.64
1:B:1211:LEU:O	1:B:1211:LEU:HG	1.98	0.64
1:B:13:LEU:HB3	1:B:14:PRO:HD2	1.79	0.64
1:A:51:MET:CE	1:A:191:LEU:HD13	2.27	0.64
1:B:64:PHE:CE2	1:B:464:ALA:HB1	2.33	0.64
1:A:1818:ILE:HA	1:A:1823:VAL:HG13	1.79	0.64
1:B:980:ASP:OD1	1:B:980:ASP:N	2.27	0.64
1:A:47:LEU:HA	1:A:201:MET:CE	2.27	0.64
1:B:64:PHE:HE2	1:B:464:ALA:HB1	1.63	0.64
1:B:1463:GLU:OE1	1:B:1980:LEU:HB2	1.98	0.64
1:B:1614:MET:O	1:B:1614:MET:HG2	1.98	0.64
1:A:1475:SER:HB3	1:A:1505:VAL:HG13	1.79	0.63
1:B:1799:LEU:O	1:B:1802:GLU:N	2.31	0.63
1:B:157:ILE:HD12	1:B:166:LEU:HD23	1.80	0.63
1:A:321:LEU:HD23	1:A:381:LEU:CD1	2.28	0.63
1:B:1338:LEU:HD13	1:B:1406:GLN:CG	2.29	0.63
1:A:93:GLY:HA2	1:A:241:ARG:HD2	1.80	0.63
1:A:2101:GLN:HG3	1:A:2102:PRO:HD2	1.80	0.63
1:A:157:ILE:HD12	1:A:166:LEU:HD23	1.79	0.63
1:B:1736:THR:HG23	1:B:1739:LYS:H	1.63	0.63
1:A:1475:SER:O	1:A:1486:MET:HE1	1.99	0.63
1:B:2075:THR:HG22	1:B:2076:ASN:N	2.14	0.63
1:A:1182:ARG:HE	1:A:1217:LEU:N	1.96	0.63
1:B:1532:PHE:HE1	1:B:1534:ASN:HB2	1.64	0.63
1:B:1585:PRO:HB3	1:B:1598:MET:HE3	1.79	0.63
1:A:1766:PHE:HD2	1:A:1791:PHE:CE1	2.16	0.63
1:B:1265:GLN:HG2	1:B:2026:ARG:HD2	1.80	0.63
1:A:82:LEU:HG	1:A:144:LEU:HD13	1.78	0.63
1:A:64:PHE:HE2	1:A:464:ALA:HB1	1.64	0.63
1:A:1180:LEU:HB2	1:A:1181:PRO:HD3	1.78	0.63
1:B:56:ASP:OD2	1:B:59:ARG:HD3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:LEU:HD23	1:A:617:PRO:CD	2.18	0.63
1:A:1216:LEU:CD1	1:A:1218:SER:H	2.08	0.63
1:A:499:MET:SD	1:A:502:GLN:NE2	2.71	0.63
1:B:1408:THR:N	1:B:1409:PRO:CD	2.61	0.63
1:B:1520:GLU:O	1:B:1522:ASP:N	2.32	0.63
1:A:1658:SER:O	1:A:1767:LEU:HD13	1.98	0.63
1:A:1570:SER:HB3	1:A:1853:VAL:HG22	1.81	0.63
1:B:1303:ASN:N	1:B:1304:PRO:CD	2.61	0.63
1:A:1476:ASN:O	1:A:1477:LEU:HD23	1.98	0.63
1:A:1215:PRO:HA	1:A:1220:LEU:CD1	2.29	0.63
1:B:1299:TRP:HZ2	1:B:1305:ALA:HA	1.63	0.63
1:B:1338:LEU:HB2	1:B:1406:GLN:HE21	1.64	0.63
1:A:945:GLU:OE2	1:B:941:SER:HB2	1.99	0.63
1:A:1126:GLU:HB3	1:A:1129:CYS:SG	2.38	0.63
1:A:2070:LEU:HD11	1:A:2076:ASN:HD21	1.63	0.62
1:B:259:GLN:HB2	1:B:263:PHE:CD1	2.34	0.62
1:B:1433:LEU:HD21	1:B:1465:GLY:HA3	1.81	0.62
1:A:252:ASN:ND2	1:A:272:LEU:HB2	2.13	0.62
1:A:1538:ARG:NH2	1:A:1585:PRO:HD3	2.14	0.62
1:A:48:PRO:HD3	1:A:201:MET:CE	2.29	0.62
1:A:344:VAL:HG11	1:A:388:VAL:HG11	1.79	0.62
1:A:1422:SER:O	1:A:1423:PHE:HB2	1.98	0.62
1:B:1617:VAL:HG21	1:B:1626:VAL:HG11	1.81	0.62
1:B:1818:ILE:HA	1:B:1823:VAL:HG13	1.81	0.62
1:A:606:ARG:NH1	1:A:739:LEU:HG	2.14	0.62
1:A:13:LEU:HB3	1:A:14:PRO:HD2	1.79	0.62
1:B:39:ARG:NH1	1:B:57:LEU:HD22	2.14	0.62
1:B:1890:THR:HA	1:B:1915:THR:HB	1.81	0.62
1:A:1454:VAL:HG13	1:A:1503:MET:CE	2.30	0.62
1:A:423:LEU:HB2	1:A:797:LEU:HD22	1.82	0.62
1:B:1036:LEU:HD21	1:B:1096:PHE:CE1	2.33	0.62
1:B:304:GLU:HG3	1:B:393:PHE:HE2	1.63	0.62
1:B:1455:GLY:HA3	1:B:2039:SER:HB2	1.81	0.62
1:B:627:TRP:HB2	1:B:643:HIS:ND1	2.13	0.62
1:B:47:LEU:HA	1:B:201:MET:CE	2.29	0.62
1:A:1036:LEU:HD21	1:A:1096:PHE:CE1	2.35	0.62
1:B:621:ALA:CB	1:B:662:LEU:HD11	2.30	0.62
1:A:304:GLU:HG3	1:A:393:PHE:HE2	1.63	0.62
1:A:359:TYR:OH	1:A:362:PRO:HG3	2.00	0.62
1:B:859:VAL:HG13	1:B:936:ARG:HG2	1.81	0.62
1:A:1461:ARG:O	1:A:1461:ARG:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1409:PRO:CB	1:B:1439:ARG:HH12	2.12	0.62
1:B:1422:SER:O	1:B:1423:PHE:HB2	2.00	0.62
1:A:263:PHE:HE2	1:A:303:GLN:HE21	1.48	0.62
1:A:142:ASN:HD22	1:B:396:GLY:HA3	1.64	0.62
1:B:1616:MET:HE3	1:B:1650:ILE:HA	1.81	0.62
1:B:319:PRO:HB2	1:B:320:LEU:HD23	1.82	0.62
1:A:765:ALA:HB1	1:A:768:GLN:CG	2.29	0.62
1:B:1016:GLU:HA	1:B:1043:PRO:HG3	1.81	0.62
1:A:1285:ALA:HB1	1:A:1289:LEU:HG	1.82	0.62
1:A:1016:GLU:HA	1:A:1043:PRO:HG3	1.81	0.62
1:A:64:PHE:CE2	1:A:464:ALA:HB1	2.34	0.62
1:A:1245:VAL:HG11	1:A:1309:LEU:HD11	1.81	0.62
1:A:1564:CYS:SG	1:A:1628:LEU:HD21	2.39	0.62
1:A:295:THR:HG22	1:A:331:HIS:CD2	2.35	0.61
1:B:1007:PHE:CE2	1:B:1030:SER:HA	2.35	0.61
1:B:1554:ALA:CB	1:B:1882:PRO:HB3	2.30	0.61
1:B:2101:GLN:HG3	1:B:2102:PRO:HD2	1.81	0.61
1:A:319:PRO:HB2	1:A:320:LEU:HD23	1.82	0.61
1:A:745:PHE:CE2	1:A:767:LEU:HD13	2.35	0.61
1:A:1318:ASN:O	1:A:1321:LEU:HD22	2.00	0.61
1:B:1628:LEU:CD1	1:B:1633:THR:HG21	2.29	0.61
1:A:1229:CYS:HB3	1:A:1403:LEU:HD22	1.82	0.61
1:A:1460:LEU:CD1	1:A:1980:LEU:HD13	2.30	0.61
1:A:1350:LEU:HD11	1:A:1375:GLN:HG2	1.82	0.61
1:B:1603:PHE:HD2	1:B:1603:PHE:N	1.97	0.61
1:A:302:PRO:HA	1:A:366:ILE:HG21	1.82	0.61
1:A:2098:PHE:O	1:A:2101:GLN:HB2	2.00	0.61
1:A:1252:GLY:H	1:A:1321:LEU:HD21	1.66	0.61
1:B:1273:THR:HA	1:B:1295:THR:O	2.00	0.61
1:B:207:SER:OG	1:B:209:ASP:HB3	2.01	0.61
1:A:1130:LEU:O	1:A:1131:ALA:HB3	2.00	0.61
1:B:82:LEU:HG	1:B:144:LEU:CD1	2.31	0.61
1:A:111:VAL:CG2	1:A:188:LEU:HB2	2.30	0.61
1:B:1720:PHE:HD1	1:B:1720:PHE:N	1.99	0.61
1:B:344:VAL:HG11	1:B:388:VAL:HG11	1.83	0.61
1:A:1036:LEU:CD2	1:A:1096:PHE:HE1	2.12	0.61
1:B:1991:VAL:HG21	1:B:2033:ASN:ND2	2.16	0.61
1:A:878:HIS:HB2	1:A:1007:PHE:CE1	2.34	0.61
1:A:1422:SER:CB	1:A:1424:ARG:HG3	2.30	0.61
1:B:1570:SER:HB3	1:B:1853:VAL:HG22	1.83	0.61
1:A:1007:PHE:CE2	1:A:1030:SER:HA	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1422:SER:HB3	1:A:1424:ARG:HG3	1.82	0.61
1:A:1995:LYS:HB3	1:A:2041:MET:SD	2.41	0.61
1:B:1216:LEU:CD1	1:B:1218:SER:H	2.04	0.61
1:A:159:THR:O	1:A:159:THR:HG22	2.00	0.61
1:B:1888:VAL:HG22	1:B:1913:VAL:HB	1.82	0.61
1:A:1802:GLU:O	1:A:1802:GLU:HG2	2.01	0.61
1:A:1528:THR:CG2	1:A:1530:HIS:H	2.12	0.60
1:A:1585:PRO:HB3	1:A:1598:MET:CE	2.30	0.60
1:A:259:GLN:HB2	1:A:263:PHE:CD1	2.35	0.60
1:A:890:GLY:HA2	1:A:1029:VAL:HG13	1.83	0.60
1:B:252:ASN:ND2	1:B:272:LEU:HB2	2.15	0.60
1:B:1200:LEU:O	1:B:1203:VAL:HG23	2.00	0.60
1:B:295:THR:HG22	1:B:331:HIS:CD2	2.36	0.60
1:B:994:LYS:HA	1:B:997:ARG:NH1	2.16	0.60
1:A:1316:VAL:HG13	1:A:1345:LEU:HB3	1.82	0.60
1:B:662:LEU:HD22	1:B:672:VAL:CG1	2.32	0.60
1:B:236:LYS:HG3	1:B:237:SER:H	1.64	0.60
1:B:1694:ARG:HH11	1:B:1694:ARG:HG3	1.67	0.60
1:B:215:PHE:CE2	1:B:305:LEU:HD11	2.36	0.60
1:B:1011:LEU:HD21	1:B:1023:GLN:HB2	1.83	0.60
1:B:491:PRO:HD2	1:B:756:ALA:HA	1.83	0.60
1:B:117:SER:HB3	1:B:135:CYS:HB3	1.82	0.60
1:A:671:PHE:HE2	1:A:773:ARG:NH2	1.95	0.60
1:A:1476:ASN:ND2	1:A:1486:MET:HE2	2.17	0.60
1:B:1429:LEU:HD11	1:B:1443:LEU:HD11	1.84	0.60
1:B:861:VAL:CG2	1:B:934:GLU:HB3	2.31	0.60
1:B:1736:THR:CG2	1:B:1740:GLY:H	2.14	0.60
1:B:1955:LEU:O	1:B:1958:GLU:HB2	2.01	0.60
1:A:861:VAL:CG2	1:A:934:GLU:HB3	2.32	0.60
1:B:64:PHE:HB2	1:B:429:ARG:HH21	1.65	0.60
1:B:442:LEU:HD23	1:B:473:LEU:HD22	1.84	0.60
1:B:1569:THR:CG2	1:B:1622:LEU:HD23	2.31	0.60
1:B:353:TRP:HH2	1:B:388:VAL:HG21	1.67	0.60
1:B:1423:PHE:O	1:B:1985:PRO:HB3	2.02	0.60
1:A:1259:PRO:HB2	1:A:1292:LEU:HD22	1.83	0.60
1:A:1182:ARG:NH2	1:A:1217:LEU:HB3	2.17	0.60
1:B:1857:ARG:CZ	1:B:1871:ILE:HD11	2.31	0.60
1:A:118:GLU:HG3	1:B:118:GLU:CG	2.32	0.60
1:A:207:SER:OG	1:A:209:ASP:HB3	2.02	0.60
1:B:1320:ALA:O	1:B:1321:LEU:HG	2.01	0.60
1:B:123:ASP:O	1:B:127:LEU:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ALA:HB3	1:B:279:PRO:CD	2.24	0.60
1:A:1349:LEU:CD1	1:A:1359:VAL:HG11	2.32	0.60
1:B:290:ILE:CG2	1:B:322:ILE:HG12	2.32	0.60
1:A:856:CYS:SG	1:A:856:CYS:O	2.60	0.60
1:A:118:GLU:CG	1:B:118:GLU:HG3	2.32	0.60
1:B:1126:GLU:HB3	1:B:1129:CYS:SG	2.42	0.60
1:A:925:LEU:HD22	1:A:931:VAL:HG21	1.84	0.60
1:B:460:VAL:HG21	1:B:465:MET:HG3	1.82	0.60
1:B:384:ARG:NH1	1:B:384:ARG:HG3	2.02	0.59
1:A:81:MET:HG3	1:A:228:VAL:HG11	1.83	0.59
1:B:1554:ALA:C	1:B:1556:PRO:HD3	2.23	0.59
1:B:273:ILE:O	1:B:277:TYR:HD1	1.85	0.59
1:B:1694:ARG:NH1	1:B:1694:ARG:HG3	2.16	0.59
1:A:1790:THR:CG2	1:B:1662:ARG:HH22	2.11	0.59
1:A:1437:SER:O	1:A:1439:ARG:N	2.35	0.59
1:A:663:GLN:O	1:A:667:ARG:HD2	2.03	0.59
1:B:1234:LEU:HD11	1:B:1268:MET:HE3	1.85	0.59
1:A:1644:GLU:HB3	1:A:1825:PRO:CB	2.33	0.59
1:A:1133:ASN:HD22	1:A:1136:LEU:CD1	2.12	0.59
1:A:527:LEU:HD13	1:A:532:LEU:HD23	1.85	0.59
1:A:1662:ARG:NH1	1:A:1662:ARG:HG2	2.17	0.59
1:A:1302:ALA:C	1:A:1304:PRO:HD3	2.21	0.59
1:B:2098:PHE:O	1:B:2101:GLN:HB2	2.02	0.59
1:A:396:GLY:HA3	1:B:142:ASN:HD22	1.68	0.59
1:B:1231:ASP:CB	1:B:1515:ARG:HD2	2.32	0.59
1:B:305:LEU:HD23	1:B:308:ILE:HD12	1.84	0.59
1:A:1344:LEU:HD12	1:A:1346:LEU:HD21	1.83	0.59
1:B:1566:VAL:HG12	1:B:1856:VAL:CG2	2.33	0.59
1:A:1043:PRO:HA	1:A:1927:ARG:NH1	2.18	0.59
1:B:515:ARG:HG2	1:B:815:LEU:O	2.02	0.59
1:A:1363:THR:O	1:A:1365:PRO:HD3	2.03	0.59
1:B:765:ALA:HB1	1:B:768:GLN:HG3	1.84	0.59
1:A:200:PHE:CB	1:A:206:LEU:HD12	2.33	0.59
1:B:620:MET:SD	1:B:682:PHE:HB2	2.43	0.59
1:B:581:SER:HB2	1:B:683:HIS:CE1	2.37	0.59
1:B:236:LYS:HG3	1:B:237:SER:N	2.17	0.59
1:B:93:GLY:HA2	1:B:241:ARG:HD2	1.84	0.59
1:A:137:ARG:HD2	1:B:137:ARG:NH1	2.17	0.59
1:A:1991:VAL:HG21	1:A:2033:ASN:ND2	2.18	0.59
1:A:1736:THR:HG23	1:A:1739:LYS:H	1.68	0.59
1:A:644:ASN:HB3	1:A:770:VAL:HG11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1456:MET:CG	1:B:2036:PHE:HB2	2.32	0.59
1:B:1574:ARG:HD2	1:B:1588:ILE:HD11	1.85	0.59
1:A:1496:VAL:HG21	1:A:1511:TRP:CH2	2.38	0.58
1:A:672:VAL:HG12	1:A:672:VAL:O	2.01	0.58
1:A:200:PHE:HB3	1:A:206:LEU:HD12	1.83	0.58
1:B:1361:PHE:CE2	1:B:1370:ARG:HD3	2.37	0.58
1:B:1351:ALA:HB3	1:B:1372:LEU:O	2.03	0.58
1:A:117:SER:HB2	1:A:135:CYS:HB3	1.85	0.58
1:A:1514:PHE:O	1:A:1515:ARG:NH1	2.35	0.58
1:A:1955:LEU:O	1:A:1958:GLU:HB2	2.02	0.58
1:B:2070:LEU:HD11	1:B:2076:ASN:HD21	1.68	0.58
1:B:1442:TRP:HB3	1:B:1444:MET:HE1	1.85	0.58
1:A:82:LEU:HG	1:A:144:LEU:CD1	2.33	0.58
1:B:1603:PHE:CD2	1:B:1603:PHE:N	2.69	0.58
1:A:442:LEU:HD23	1:A:473:LEU:HD22	1.84	0.58
1:A:1711:ARG:HG2	1:A:1712:PHE:CE1	2.37	0.58
1:B:1711:ARG:HG2	1:B:1712:PHE:CE1	2.38	0.58
1:A:859:VAL:HG13	1:A:936:ARG:HG2	1.84	0.58
1:A:1533:VAL:HG12	1:A:1622:LEU:HB3	1.85	0.58
1:B:1303:ASN:H	1:B:1304:PRO:CD	2.16	0.58
1:B:1720:PHE:N	1:B:1720:PHE:CD1	2.70	0.58
1:A:1204:LEU:HD11	1:A:1365:PRO:HG2	1.85	0.58
1:B:251:THR:HB	1:B:399:ASN:O	2.03	0.58
1:A:1001:TYR:HB3	1:A:1003:TYR:CD1	2.37	0.58
1:B:290:ILE:HD13	1:B:308:ILE:HD13	1.85	0.58
1:A:1472:VAL:HG12	1:A:1473:LEU:N	2.17	0.58
1:B:423:LEU:HB2	1:B:797:LEU:HD22	1.84	0.58
1:A:1528:THR:HG22	1:A:1530:HIS:N	2.14	0.58
1:A:322:ILE:O	1:A:377:VAL:HG23	2.03	0.58
1:B:1338:LEU:HD13	1:B:1406:GLN:HG3	1.85	0.58
1:B:594:LEU:HD13	1:B:599:ALA:HA	1.84	0.58
1:B:1794:ILE:O	1:B:1795:LEU:HD23	2.03	0.58
1:B:1276:ASP:O	1:B:1299:TRP:N	2.36	0.58
1:B:1364:SER:N	1:B:1365:PRO:CD	2.67	0.58
1:B:254:ASP:HB2	1:B:257:LYS:HE2	1.84	0.58
1:B:426:ALA:HA	1:B:458:ALA:HB2	1.86	0.58
1:A:36:ASP:HB3	1:A:38:ARG:HG3	1.86	0.58
1:A:553:PHE:CD2	1:A:582:LEU:HD13	2.38	0.58
1:A:1457:VAL:HG21	1:A:1473:LEU:HB3	1.86	0.58
1:A:423:LEU:HD23	1:A:812:PRO:HG3	1.85	0.58
1:B:234:THR:HG22	1:B:235:LYS:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1995:LYS:HB3	1:B:2041:MET:SD	2.44	0.58
1:A:997:ARG:HA	1:A:1001:TYR:O	2.04	0.58
1:A:200:PHE:CD2	1:B:132:MET:HE1	2.38	0.58
1:A:1656:TYR:CD2	1:A:1687:ILE:HD13	2.39	0.58
1:A:188:LEU:HD22	1:A:228:VAL:HG12	1.85	0.58
1:B:1824:GLN:HG3	1:B:1825:PRO:HD2	1.86	0.58
1:A:1842:TYR:CE2	1:A:1848:HIS:HB3	2.39	0.58
1:B:655:GLN:HG2	1:B:655:GLN:O	2.03	0.58
1:B:1322:ALA:HB1	1:B:1371:HIS:CE1	2.39	0.58
1:A:1275:THR:HG22	1:A:1299:TRP:HB2	1.85	0.58
1:B:640:PRO:HA	1:B:651:ILE:HG22	1.85	0.58
1:A:586:ALA:O	1:A:589:TYR:HB3	2.03	0.58
1:B:1461:ARG:HG3	1:B:1461:ARG:O	2.04	0.58
1:B:982:THR:O	1:B:984:GLU:N	2.34	0.57
1:A:856:CYS:CB	1:B:856:CYS:HG	2.16	0.57
1:B:1214:ASP:OD2	1:B:1321:LEU:HD21	2.04	0.57
1:B:1802:GLU:O	1:B:1804:GLY:N	2.37	0.57
1:A:426:ALA:HA	1:A:458:ALA:HB2	1.85	0.57
1:B:997:ARG:HA	1:B:1001:TYR:O	2.04	0.57
1:B:1222:ASP:HA	1:B:1226:LEU:CD1	2.34	0.57
1:B:1836:VAL:HG13	1:B:1854:ILE:CD1	2.33	0.57
1:A:765:ALA:HB1	1:A:768:GLN:HG3	1.85	0.57
1:B:111:VAL:CG2	1:B:188:LEU:HB2	2.33	0.57
1:B:48:PRO:HD3	1:B:201:MET:CE	2.34	0.57
1:B:993:TYR:CZ	1:B:1008:GLN:HA	2.39	0.57
1:A:1735:HIS:H	1:A:1735:HIS:CD2	2.21	0.57
1:A:331:HIS:CE1	1:A:333:GLU:HA	2.39	0.57
1:B:1220:LEU:CB	1:B:1257:ARG:HH22	2.10	0.57
1:A:1208:ARG:HA	1:A:1211:LEU:HB2	1.86	0.57
1:A:953:LEU:HD12	1:A:954:ILE:H	1.69	0.57
1:B:662:LEU:HD22	1:B:672:VAL:HG11	1.86	0.57
1:A:1273:THR:HA	1:A:1295:THR:O	2.02	0.57
1:A:1182:ARG:NE	1:A:1217:LEU:H	2.01	0.57
1:B:1208:ARG:HH11	1:B:1211:LEU:CD2	2.14	0.57
1:A:215:PHE:O	1:A:363:ASN:HB2	2.04	0.57
1:B:1353:HIS:NE2	1:B:1398:GLY:HA2	2.19	0.57
1:A:1137:GLN:NE2	1:A:1396:PHE:CE1	2.72	0.57
1:A:273:ILE:O	1:A:277:TYR:HD1	1.87	0.57
1:A:1345:LEU:HD12	1:A:1402:PHE:O	2.04	0.57
1:A:1476:ASN:HA	1:A:1486:MET:HE1	1.85	0.57
1:A:1528:THR:HG21	1:A:1552:HIS:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:THR:O	1:A:160:ALA:HB3	2.05	0.57
1:A:1824:GLN:HG3	1:A:1825:PRO:HD2	1.85	0.57
1:A:91:VAL:HG21	1:A:834:ILE:HD13	1.86	0.57
1:B:38:ARG:HB2	1:B:53:LYS:HD2	1.87	0.57
1:B:1762:GLN:NE2	1:B:1787:LYS:HA	2.19	0.57
1:B:1209:PRO:O	1:B:1210:LEU:HG	2.05	0.57
1:A:1418:VAL:O	1:A:1418:VAL:HG12	2.04	0.57
1:A:1673:ILE:HD13	1:A:1684:ALA:CB	2.35	0.57
1:A:633:ARG:O	1:A:633:ARG:HG2	2.04	0.57
1:A:1001:TYR:HB3	1:A:1003:TYR:CE1	2.39	0.57
1:A:305:LEU:HD23	1:A:308:ILE:HD12	1.85	0.57
1:B:1299:TRP:CZ2	1:B:1305:ALA:HA	2.40	0.57
1:A:643:HIS:O	1:A:745:PHE:HB3	2.05	0.57
1:B:51:MET:CE	1:B:191:LEU:HD13	2.35	0.57
1:B:188:LEU:HD22	1:B:228:VAL:HG12	1.87	0.57
1:A:1836:VAL:HG13	1:A:1854:ILE:CD1	2.35	0.57
1:B:100:LEU:O	1:B:103:THR:OG1	2.23	0.57
1:B:2101:GLN:HG3	1:B:2102:PRO:CD	2.35	0.57
1:B:1954:SER:O	1:B:1958:GLU:HG3	2.05	0.57
1:A:1674:HIS:NE2	1:A:1756:SER:OG	2.37	0.57
1:A:290:ILE:HD13	1:A:308:ILE:HD13	1.87	0.56
1:B:1405:ARG:HH22	1:B:1470:ARG:NH2	2.03	0.56
1:B:77:PRO:O	1:B:81:MET:HG2	2.04	0.56
1:B:1409:PRO:HB2	1:B:1439:ARG:NH1	2.20	0.56
1:A:1489:SER:N	1:A:1493:LEU:HD22	2.19	0.56
1:A:1762:GLN:NE2	1:A:1787:LYS:HA	2.20	0.56
1:B:1647:SER:HA	1:B:1851:LYS:HG3	1.87	0.56
1:A:627:TRP:CH2	1:A:640:PRO:HB2	2.40	0.56
1:B:1567:TYR:CE1	1:B:1606:ARG:HG3	2.40	0.56
1:B:1565:SER:HB2	1:B:1857:ARG:NH2	2.20	0.56
1:B:1180:LEU:HD23	1:B:1189:GLN:NE2	2.19	0.56
1:A:248:ASN:ND2	1:A:249:ALA:H	2.03	0.56
1:B:455:ASN:HB2	1:B:813:ASN:HD21	1.69	0.56
1:A:1477:LEU:CD1	1:A:2043:ARG:HD2	2.23	0.56
1:A:343:LYS:CE	1:A:354:ALA:HB3	2.26	0.56
1:B:627:TRP:HB2	1:B:643:HIS:CE1	2.40	0.56
1:A:1528:THR:HG22	1:A:1529:GLU:N	2.19	0.56
1:A:321:LEU:HD23	1:A:381:LEU:HD12	1.86	0.56
1:B:1570:SER:OG	1:B:1602:GLU:HB3	2.05	0.56
1:B:1409:PRO:HG2	1:B:1439:ARG:HH12	1.70	0.56
1:A:1736:THR:CG2	1:A:1740:GLY:H	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2101:GLN:HG3	1:A:2102:PRO:CD	2.35	0.56
1:B:1265:GLN:HE21	1:B:2026:ARG:HH11	1.54	0.56
1:B:302:PRO:HA	1:B:366:ILE:HG21	1.85	0.56
1:A:1768:GLU:OE1	1:A:1768:GLU:HA	2.05	0.56
1:B:623:VAL:HG12	1:B:624:GLY:N	2.19	0.56
1:A:1672:LEU:N	1:A:1741:VAL:HG11	2.19	0.56
1:A:1204:LEU:HD21	1:A:1365:PRO:CG	2.34	0.56
1:A:1442:TRP:HB3	1:A:1444:MET:HE1	1.88	0.56
1:A:564:ILE:HD13	1:A:590:ALA:HB2	1.87	0.56
1:B:440:GLN:HG3	1:B:833:HIS:CG	2.39	0.56
1:B:1183:LEU:HD22	1:B:1213:ASP:O	2.05	0.56
1:A:1529:GLU:O	1:A:1529:GLU:HG3	2.05	0.56
1:B:81:MET:HG3	1:B:228:VAL:HG11	1.87	0.56
1:A:1252:GLY:N	1:A:1321:LEU:HD11	2.20	0.56
1:A:1265:GLN:HE21	1:A:2026:ARG:NH1	2.01	0.56
1:B:209:ASP:OD2	1:B:213:ARG:NE	2.38	0.56
1:A:1664:ARG:NH1	1:B:1664:ARG:HD3	2.20	0.56
1:A:251:THR:HB	1:A:399:ASN:O	2.06	0.56
1:A:1794:ILE:O	1:A:1795:LEU:HD23	2.06	0.56
1:A:1657:TYR:CZ	1:A:1662:ARG:HD2	2.40	0.56
1:B:1413:PRO:CB	1:B:1440:PRO:HB2	2.36	0.56
1:A:1350:LEU:CD1	1:A:1375:GLN:HG2	2.35	0.56
1:A:1289:LEU:HD22	1:A:1294:VAL:HB	1.86	0.56
1:B:890:GLY:HA2	1:B:1029:VAL:HG13	1.88	0.56
1:A:889:THR:HG21	1:A:1032:LEU:HB2	1.87	0.56
1:A:1397:TYR:CE1	1:A:1399:SER:HB2	2.41	0.56
1:B:1109:GLN:HB3	1:B:1111:HIS:CE1	2.40	0.56
1:A:278:ALA:CB	1:A:279:PRO:CD	2.84	0.56
1:B:1275:THR:CG2	1:B:1299:TRP:HB2	2.36	0.56
1:A:883:ARG:HH21	1:A:1107:ARG:HD3	1.71	0.56
1:B:572:LEU:HD12	1:B:810:VAL:CG1	2.35	0.56
1:A:118:GLU:CD	1:B:118:GLU:HG3	2.26	0.56
1:B:248:ASN:ND2	1:B:249:ALA:H	2.04	0.56
1:B:1539:GLY:HA2	1:B:1580:THR:O	2.06	0.56
1:A:1851:LYS:HG3	1:A:1852:VAL:N	2.21	0.56
1:B:1373:LEU:N	1:B:1373:LEU:HD23	2.21	0.56
1:A:1408:THR:HG23	1:A:1409:PRO:HD2	1.87	0.56
1:B:1180:LEU:HB2	1:B:1181:PRO:HD3	1.88	0.56
1:A:1720:PHE:N	1:A:1720:PHE:HD1	2.04	0.56
1:B:468:ARG:HD3	1:B:485:VAL:HG21	1.88	0.56
1:B:527:LEU:HD12	1:B:534:VAL:CG2	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:MET:CG	1:B:677:THR:HG21	2.35	0.56
1:B:207:SER:HB2	1:B:221:GLY:O	2.06	0.56
1:B:1237:MET:SD	1:B:1242:MET:HG3	2.46	0.56
1:A:594:LEU:HD13	1:A:599:ALA:HA	1.88	0.56
1:A:1653:THR:HG22	1:A:1810:VAL:HG11	1.86	0.56
1:B:665:LEU:HB2	1:B:672:VAL:HG21	1.87	0.56
1:A:1644:GLU:HB3	1:A:1825:PRO:HB3	1.87	0.56
1:A:1109:GLN:HB3	1:A:1111:HIS:CE1	2.41	0.56
1:B:1661:VAL:HG21	1:B:1810:VAL:HG22	1.87	0.55
1:B:1275:THR:HG22	1:B:1299:TRP:HB2	1.87	0.55
1:B:1133:ASN:ND2	1:B:1136:LEU:HD12	2.18	0.55
1:B:982:THR:C	1:B:984:GLU:N	2.58	0.55
1:A:379:ARG:O	1:A:381:LEU:HG	2.06	0.55
1:A:132:MET:HE1	1:B:200:PHE:CD2	2.42	0.55
1:A:1652:TYR:CD1	1:A:1823:VAL:HB	2.40	0.55
1:A:1628:LEU:HD13	1:A:1633:THR:HG21	1.88	0.55
1:A:581:SER:OG	1:A:582:LEU:N	2.37	0.55
1:A:633:ARG:NH2	1:A:668:GLU:OE1	2.39	0.55
1:B:1138:GLU:HG3	1:B:1142:LEU:HD12	1.88	0.55
1:B:1611:ARG:HG2	1:B:1612:ARG:H	1.71	0.55
1:B:353:TRP:CH2	1:B:388:VAL:HG21	2.41	0.55
1:A:1969:PHE:CD2	1:A:2017:VAL:HB	2.41	0.55
1:A:1724:ARG:NH1	2:A:3001:NAP:C8A	2.70	0.55
1:A:122:ARG:O	1:A:124:PRO:HD3	2.05	0.55
1:A:1456:MET:HG3	1:A:2036:PHE:HB2	1.88	0.55
1:A:776:GLU:HB3	1:A:778:SER:OG	2.06	0.55
1:A:287:LEU:HA	1:A:387:ASN:O	2.07	0.55
1:A:128:VAL:HG11	1:A:130:TYR:CZ	2.40	0.55
1:A:1390:VAL:HG22	1:A:1501:LEU:HD21	1.89	0.55
1:A:1662:ARG:HG3	1:A:1662:ARG:HH11	1.68	0.55
1:B:438:LEU:O	1:B:442:LEU:HG	2.06	0.55
1:A:38:ARG:HB2	1:A:53:LYS:HD2	1.87	0.55
1:A:1674:HIS:O	1:A:1675:SER:HB2	2.07	0.55
1:A:1606:ARG:HH21	1:A:1860:GLU:HG3	1.71	0.55
1:B:1124:HIS:CD2	1:B:1512:GLY:HA2	2.41	0.55
1:B:1671:VAL:CG2	1:B:1743:LEU:HB2	2.37	0.55
1:A:2075:THR:HG22	1:A:2076:ASN:N	2.22	0.55
1:A:1549:SER:O	1:A:1552:HIS:HB3	2.06	0.55
1:B:1523:ARG:NH1	1:B:1545:ARG:HE	2.03	0.55
1:B:1374:SER:O	1:B:1378:TRP:CD1	2.60	0.55
1:A:241:ARG:NH2	1:A:827:THR:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1231:ASP:HB3	1:A:1515:ARG:HD2	1.89	0.55
1:B:1671:VAL:HG23	1:B:1743:LEU:HB2	1.88	0.55
1:B:1115:ILE:HD11	1:B:2111:LEU:HD12	1.88	0.55
1:B:1514:PHE:O	1:B:1515:ARG:NH1	2.40	0.55
1:B:1652:TYR:CD1	1:B:1823:VAL:HB	2.41	0.55
1:B:1422:SER:HB3	1:B:1424:ARG:HG3	1.87	0.55
1:B:1311:LYS:O	1:B:1312:ALA:HB2	2.07	0.55
1:A:293:HIS:O	1:A:326:LYS:HD2	2.06	0.55
1:B:1662:ARG:HD3	1:B:1794:ILE:HG12	1.88	0.55
1:B:1183:LEU:HB3	1:B:1216:LEU:HD23	1.89	0.55
1:A:1720:PHE:N	1:A:1720:PHE:CD1	2.75	0.55
1:A:207:SER:HB2	1:A:221:GLY:O	2.06	0.55
1:A:1419:GLU:CD	1:A:1447:GLY:HA3	2.28	0.55
1:B:128:VAL:HG11	1:B:130:TYR:CZ	2.41	0.55
1:B:1001:TYR:HB3	1:B:1003:TYR:CD1	2.42	0.55
1:B:1222:ASP:HA	1:B:1226:LEU:HD11	1.89	0.55
1:B:1418:VAL:CG1	1:B:1425:TRP:CE2	2.86	0.55
1:A:887:PRO:HB2	1:A:890:GLY:H	1.72	0.55
1:A:1842:TYR:HE2	1:A:1848:HIS:HB3	1.71	0.55
1:A:1041:LEU:O	1:A:1041:LEU:HG	2.07	0.55
1:B:1672:LEU:N	1:B:1741:VAL:HG11	2.22	0.55
1:B:162:SER:OG	1:B:163:SER:N	2.39	0.54
1:B:635:PRO:O	1:B:637:GLY:N	2.40	0.54
1:B:1735:HIS:CD2	1:B:1735:HIS:H	2.25	0.54
1:B:501:ALA:O	1:B:763:PRO:HG2	2.07	0.54
1:B:331:HIS:CE1	1:B:333:GLU:HA	2.42	0.54
1:A:1486:MET:HE3	1:A:1506:TYR:HB3	1.90	0.54
1:A:1614:MET:HG3	1:A:1649:PRO:CG	2.38	0.54
1:B:610:ILE:HG21	1:B:680:ILE:HD12	1.90	0.54
1:A:100:LEU:O	1:A:103:THR:OG1	2.24	0.54
1:A:1769:ILE:HG23	2:A:3001:NAP:C2N	2.38	0.54
1:A:527:LEU:HD12	1:A:534:VAL:CG2	2.34	0.54
1:B:136:GLN:NE2	1:B:138:ALA:H	2.04	0.54
1:A:598:GLU:OE1	1:A:706:LYS:NZ	2.39	0.54
1:A:353:TRP:NE1	1:A:383:ILE:HB	2.22	0.54
1:B:1611:ARG:HG2	1:B:1612:ARG:N	2.22	0.54
1:A:1354:PRO:O	1:A:1358:MET:HG3	2.06	0.54
1:A:1301:PRO:HG2	1:A:1324:LEU:CD2	2.38	0.54
1:A:1801:GLU:C	1:A:1803:GLY:H	2.10	0.54
1:A:384:ARG:NH1	1:A:384:ARG:HG3	2.03	0.54
1:A:1530:HIS:HB3	1:A:1549:SER:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:TYR:CE2	1:A:97:PRO:HG2	2.43	0.54
1:B:1316:VAL:HG13	1:B:1345:LEU:HB3	1.90	0.54
1:A:1338:LEU:HB2	1:A:1406:GLN:HE21	1.72	0.54
1:B:379:ARG:O	1:B:381:LEU:HG	2.07	0.54
1:B:525:GLN:NE2	1:B:525:GLN:HA	2.23	0.54
1:B:745:PHE:CE2	1:B:767:LEU:HD13	2.43	0.54
1:A:333:GLU:CB	1:A:334:PRO:CD	2.84	0.54
1:A:1220:LEU:CB	1:A:1257:ARG:HH22	2.17	0.54
1:A:1771:LYS:O	1:A:1775:SER:HB2	2.08	0.54
1:A:580:HIS:O	1:A:581:SER:HB3	2.07	0.54
1:A:1200:LEU:HA	1:A:1203:VAL:HB	1.88	0.54
1:B:293:HIS:O	1:B:326:LYS:HD2	2.08	0.54
1:B:1533:VAL:HG21	1:B:1836:VAL:HG11	1.89	0.54
1:B:200:PHE:HB3	1:B:206:LEU:HG	1.90	0.54
1:B:883:ARG:HE	1:B:1107:ARG:HD3	1.72	0.54
1:B:615:VAL:HG22	1:B:686:PHE:CD2	2.40	0.54
1:A:1734:ARG:C	1:A:1736:THR:H	2.10	0.54
1:B:36:ASP:HB3	1:B:38:ARG:HG3	1.90	0.54
1:B:348:LEU:HD13	1:B:406:PRO:HB3	1.89	0.54
1:A:348:LEU:HD13	1:A:406:PRO:HB3	1.89	0.54
1:A:1455:GLY:HA3	1:A:2039:SER:HB2	1.90	0.54
1:B:543:GLU:HA	1:B:543:GLU:OE1	2.07	0.54
1:B:1429:LEU:HD11	1:B:1443:LEU:HD21	1.88	0.54
1:B:953:LEU:HD12	1:B:954:ILE:H	1.70	0.54
1:A:889:THR:CG2	1:A:1032:LEU:HB2	2.38	0.54
1:A:1338:LEU:HD13	1:A:1406:GLN:CG	2.37	0.54
1:B:1330:ALA:O	1:B:1334:MET:HG2	2.08	0.54
1:B:166:LEU:CD1	1:B:251:THR:HG21	2.31	0.54
1:A:287:LEU:HD23	1:A:387:ASN:O	2.08	0.54
1:B:606:ARG:NH1	1:B:739:LEU:HG	2.23	0.54
1:A:1315:LEU:O	1:A:1344:LEU:HD13	2.07	0.54
1:A:941:SER:N	1:B:945:GLU:OE2	2.41	0.54
1:B:127:LEU:HG	1:B:127:LEU:O	2.07	0.54
1:A:1648:VAL:HB	1:A:1649:PRO:HD3	1.89	0.54
1:A:1147:ALA:HB2	1:A:1188:CYS:SG	2.48	0.54
1:B:1243:LYS:HA	1:B:1271:ASP:HB2	1.90	0.54
1:A:1301:PRO:HG2	1:A:1324:LEU:HD23	1.89	0.54
1:A:491:PRO:HD2	1:A:756:ALA:HA	1.90	0.54
1:B:137:ARG:O	1:B:140:MET:HG2	2.08	0.53
1:A:1893:LEU:HB3	1:A:1925:GLN:HE21	1.72	0.53
1:A:1472:VAL:HG12	1:A:1473:LEU:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1569:THR:HG23	1:A:1602:GLU:O	2.07	0.53
1:B:2002:LEU:O	1:B:2006:THR:HB	2.08	0.53
1:A:118:GLU:HG3	1:B:118:GLU:CD	2.29	0.53
1:A:275:SER:HB2	1:A:276:LEU:HD23	1.88	0.53
1:A:1011:LEU:HD21	1:A:1023:GLN:HB2	1.91	0.53
1:A:1652:TYR:CE1	1:A:1823:VAL:HB	2.43	0.53
1:A:1476:ASN:HA	1:A:1486:MET:CE	2.38	0.53
1:A:1476:ASN:HB3	1:A:1486:MET:SD	2.49	0.53
1:B:642:CYS:HB2	1:B:650:THR:HB	1.89	0.53
1:B:1420:ASP:HB3	1:B:1425:TRP:HZ3	1.72	0.53
1:B:1454:VAL:HG13	1:B:1503:MET:HE1	1.90	0.53
1:A:1222:ASP:HB3	1:A:1257:ARG:NH1	2.22	0.53
1:B:371:ASP:O	1:B:371:ASP:CG	2.46	0.53
1:A:606:ARG:HH12	1:A:739:LEU:HG	1.72	0.53
1:A:993:TYR:CZ	1:A:1008:GLN:HA	2.43	0.53
1:B:1540:ASP:HB3	1:B:1542:SER:OG	2.09	0.53
1:A:1594:THR:OG1	1:A:1596:ASP:HB2	2.08	0.53
1:A:1139:GLU:OE1	1:A:1182:ARG:NH2	2.38	0.53
1:A:371:ASP:CG	1:A:371:ASP:O	2.46	0.53
1:A:1227:LYS:HB2	1:A:1261:LEU:HD22	1.91	0.53
1:B:278:ALA:CB	1:B:279:PRO:CD	2.81	0.53
1:B:1349:LEU:O	1:B:1372:LEU:HD22	2.09	0.53
1:A:1353:HIS:CD2	1:A:1398:GLY:HA2	2.44	0.53
1:B:122:ARG:NH1	1:B:849:ASP:O	2.42	0.53
1:A:1567:TYR:CE1	1:A:1606:ARG:HG3	2.43	0.53
1:B:889:THR:HG21	1:B:1032:LEU:HB2	1.91	0.53
1:A:1466:GLY:O	1:A:1469:ILE:HB	2.09	0.53
1:A:326:LYS:CE	1:A:336:SER:HB2	2.38	0.53
1:B:1532:PHE:CD1	1:B:1532:PHE:C	2.81	0.53
1:B:23:TRP:CZ2	1:B:350:HIS:HD2	2.26	0.53
1:A:1569:THR:HG21	1:A:1622:LEU:CA	2.36	0.53
1:B:2006:THR:O	1:B:2010:CYS:HB2	2.08	0.53
1:A:438:LEU:O	1:A:442:LEU:HG	2.09	0.53
1:A:1746:ASN:ND2	1:A:1753:LEU:HD12	2.24	0.53
1:A:1477:LEU:HB3	1:A:1507:ARG:HE	1.73	0.53
1:A:1585:PRO:HB3	1:A:1598:MET:HE3	1.91	0.53
1:B:586:ALA:O	1:B:589:TYR:HB3	2.08	0.53
1:A:234:THR:HG22	1:A:235:LYS:O	2.09	0.53
1:B:1418:VAL:HG13	1:B:1425:TRP:NE1	2.23	0.53
1:B:1420:ASP:HB3	1:B:1425:TRP:CZ3	2.44	0.53
1:A:984:GLU:O	1:A:985:PHE:CB	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:917:VAL:HG12	1:B:1054:PHE:HB2	1.90	0.53
1:B:1719:CYS:C	1:B:1720:PHE:HD1	2.12	0.53
1:A:1973:MET:SD	2:A:3002:NAP:H3D	2.49	0.53
1:A:2018:ILE:HG12	1:A:2041:MET:HE2	1.91	0.53
1:B:1995:LYS:HD3	1:B:2038:ASN:OD1	2.09	0.53
1:A:1986:GLU:HB3	1:A:1989:GLN:NE2	2.24	0.53
1:A:1477:LEU:CD1	1:A:1507:ARG:HH21	2.22	0.53
1:B:1456:MET:HG3	1:B:2036:PHE:HD1	1.74	0.53
1:B:1121:PHE:HB2	1:B:1514:PHE:CE2	2.44	0.53
1:B:680:ILE:CG1	1:B:681:ALA:N	2.70	0.53
1:A:23:TRP:CZ2	1:A:350:HIS:HD2	2.26	0.53
1:A:1254:LEU:HD13	1:A:1316:VAL:CG1	2.38	0.53
1:B:39:ARG:NH1	1:B:226:GLU:OE2	2.41	0.53
1:B:1251:ASP:HB3	1:B:1321:LEU:CD2	2.39	0.53
1:B:287:LEU:HA	1:B:387:ASN:O	2.08	0.53
1:B:1768:GLU:HA	1:B:1768:GLU:OE1	2.08	0.53
1:A:112:SER:O	1:A:137:ARG:NH2	2.42	0.53
1:B:997:ARG:HH21	1:B:2070:LEU:HD12	1.73	0.53
1:B:1371:HIS:O	1:B:1371:HIS:CG	2.62	0.53
1:B:972:THR:HG23	1:B:1081:VAL:HG21	1.90	0.53
1:A:570:LEU:HD21	1:A:815:LEU:HD21	1.91	0.53
1:B:1656:TYR:CE1	1:B:1687:ILE:HD11	2.44	0.53
1:B:1231:ASP:HB3	1:B:1515:ARG:CD	2.39	0.52
1:A:6:ILE:HG21	1:A:345:LEU:CD1	2.38	0.52
1:A:1147:ALA:HB1	1:A:1358:MET:CE	2.39	0.52
1:B:1863:PRO:O	1:B:1865:PRO:HD3	2.09	0.52
1:B:1677:SER:CB	1:B:1704:LYS:HD3	2.38	0.52
1:B:424:LEU:CD2	1:B:441:GLY:HA3	2.39	0.52
1:A:1183:LEU:HD13	1:A:1210:LEU:O	2.09	0.52
1:A:1443:LEU:O	1:A:1473:LEU:HA	2.08	0.52
1:A:945:GLU:OE2	1:B:941:SER:N	2.42	0.52
1:B:624:GLY:O	1:B:625:LEU:HD23	2.09	0.52
1:A:1395:SER:HB3	1:A:1399:SER:O	2.09	0.52
1:B:321:LEU:HD12	1:B:321:LEU:N	2.24	0.52
1:A:162:SER:OG	1:A:163:SER:N	2.40	0.52
1:B:1842:TYR:CE2	1:B:1848:HIS:HB3	2.45	0.52
1:B:1456:MET:HG3	1:B:2036:PHE:CD1	2.45	0.52
1:B:1343:PHE:O	1:B:1344:LEU:HD22	2.10	0.52
1:A:1454:VAL:HG13	1:A:1503:MET:HE1	1.91	0.52
1:B:808:VAL:HG12	1:B:809:SER:N	2.25	0.52
1:A:831:SER:N	1:A:832:PRO:CD	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1560:GLN:C	1:A:1562:ARG:H	2.13	0.52
1:A:161:CYS:HB2	1:A:394:GLY:HA2	1.91	0.52
1:B:1657:TYR:HA	1:B:1661:VAL:HG23	1.90	0.52
1:B:1766:PHE:CD2	1:B:1791:PHE:CE1	2.97	0.52
1:B:1451:SER:O	1:B:1453:VAL:N	2.43	0.52
1:B:637:GLY:O	1:B:685:TYR:HE2	1.92	0.52
1:B:287:LEU:HD23	1:B:387:ASN:O	2.09	0.52
1:A:1602:GLU:OE2	1:A:1650:ILE:N	2.42	0.52
1:A:91:VAL:HG21	1:A:834:ILE:CD1	2.40	0.52
1:A:1719:CYS:C	1:A:1720:PHE:HD1	2.12	0.52
1:B:1363:THR:CG2	1:B:1363:THR:O	2.58	0.52
1:A:275:SER:C	1:A:276:LEU:HD23	2.30	0.52
1:A:1424:ARG:O	1:A:1426:VAL:N	2.42	0.52
1:B:1234:LEU:HD11	1:B:1268:MET:CE	2.40	0.52
1:B:1499:GLY:O	1:B:1500:ASP:HB3	2.09	0.52
1:A:1489:SER:HA	1:A:1493:LEU:HD22	1.91	0.52
1:B:670:VAL:O	1:B:672:VAL:HG23	2.10	0.52
1:B:297:THR:HB	1:B:300:GLY:H	1.74	0.52
1:B:1580:THR:HG22	1:B:1581:GLY:N	2.25	0.52
1:B:1656:TYR:CE2	1:B:1687:ILE:HD13	2.45	0.52
1:B:351:GLY:C	1:B:383:ILE:HG22	2.29	0.52
1:B:506:MET:HB3	1:B:559:ILE:HD11	1.90	0.52
1:A:734:TYR:CD2	1:A:734:TYR:C	2.83	0.52
1:A:137:ARG:NH1	1:B:137:ARG:HD2	2.24	0.52
1:B:2065:ASP:C	1:B:2070:LEU:HD12	2.30	0.52
1:A:1470:ARG:O	1:A:1470:ARG:HG3	2.10	0.52
1:A:1502:VAL:HG12	1:A:1503:MET:HG2	1.91	0.52
1:A:228:VAL:HG23	1:A:228:VAL:O	2.08	0.52
1:A:297:THR:HG22	1:A:299:VAL:H	1.75	0.52
1:A:1456:MET:HG3	1:A:2036:PHE:HD1	1.75	0.52
1:B:1670:SER:O	1:B:1742:ASP:HB2	2.10	0.52
1:B:1555:LEU:CD2	1:B:1560:GLN:HE21	2.22	0.52
1:B:1771:LYS:O	1:B:1775:SER:HB2	2.09	0.52
1:B:1011:LEU:CD2	1:B:1023:GLN:HB2	2.40	0.52
1:A:504:GLN:HG3	1:A:546:LEU:HD11	1.92	0.52
1:B:1734:ARG:C	1:B:1736:THR:H	2.12	0.52
1:A:98:ALA:O	1:A:101:ARG:HG3	2.10	0.52
1:A:2102:PRO:HD2	1:A:2103:HIS:CD2	2.45	0.52
1:B:275:SER:C	1:B:276:LEU:HD23	2.29	0.52
1:A:1986:GLU:HG2	1:A:1989:GLN:OE1	2.09	0.52
1:A:1300:ASP:O	1:A:1302:ALA:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:VAL:HG12	1:A:809:SER:H	1.74	0.52
1:A:1574:ARG:HD2	1:A:1588:ILE:CD1	2.39	0.52
1:A:1456:MET:CG	1:A:2036:PHE:HB2	2.39	0.52
1:B:776:GLU:HB3	1:B:778:SER:OG	2.10	0.52
1:B:1409:PRO:CG	1:B:1439:ARG:HH12	2.23	0.52
1:B:979:ALA:HB1	1:B:983:ALA:HB3	1.92	0.52
1:B:965:PRO:O	1:B:967:PRO:HD3	2.10	0.52
1:B:276:LEU:HD23	1:B:276:LEU:N	2.25	0.52
1:B:506:MET:HE1	1:B:555:SER:HB3	1.91	0.52
1:B:481:GLU:HB3	1:B:805:LEU:HD11	1.92	0.52
1:B:1055:THR:HB	1:B:1097:LEU:O	2.10	0.52
1:A:1528:THR:CG2	1:A:1552:HIS:HB2	2.40	0.51
1:B:1470:ARG:O	1:B:1470:ARG:CG	2.57	0.51
1:B:606:ARG:HH12	1:B:739:LEU:HG	1.75	0.51
1:B:504:GLN:H	1:B:546:LEU:HD11	1.75	0.51
1:B:655:GLN:O	1:B:659:SER:HB3	2.10	0.51
1:B:225:ALA:O	1:B:332:PRO:HA	2.10	0.51
1:A:525:GLN:HA	1:A:525:GLN:NE2	2.24	0.51
1:A:123:ASP:H	1:A:127:LEU:HD12	1.75	0.51
1:B:1451:SER:O	1:B:1452:GLY:C	2.49	0.51
1:A:309:VAL:HG22	1:A:374:LEU:HD21	1.93	0.51
1:B:254:ASP:HB3	1:B:257:LYS:HE2	1.92	0.51
1:A:1123:PRO:HB3	1:A:1510:ALA:HB1	1.92	0.51
1:A:399:ASN:N	1:A:399:ASN:ND2	2.57	0.51
1:A:994:LYS:HA	1:A:997:ARG:NH1	2.25	0.51
1:B:878:HIS:HB2	1:B:1007:PHE:CE1	2.45	0.51
1:B:1130:LEU:O	1:B:1131:ALA:HB3	2.09	0.51
1:B:325:THR:OG1	1:B:343:LYS:HG2	2.09	0.51
1:B:324:SER:O	1:B:356:ASN:ND2	2.43	0.51
1:A:866:VAL:HG13	1:A:866:VAL:O	2.10	0.51
1:B:217:ALA:CB	1:B:364:PRO:HD3	2.40	0.51
1:A:1539:GLY:HA2	1:A:1580:THR:O	2.10	0.51
1:A:1781:GLY:O	1:A:1784:VAL:HG23	2.09	0.51
1:A:506:MET:HE2	1:A:559:ILE:CD1	2.40	0.51
1:B:408:SER:O	1:B:409:ARG:HB2	2.11	0.51
1:A:709:SER:OG	1:A:711:ARG:HB2	2.10	0.51
1:A:1480:THR:HG22	1:A:1481:SER:H	1.74	0.51
1:B:326:LYS:CE	1:B:336:SER:HB2	2.39	0.51
1:B:1477:LEU:CD1	1:B:2043:ARG:HD2	2.40	0.51
1:B:420:LEU:HD11	1:B:512:ARG:CB	2.35	0.51
1:B:889:THR:CG2	1:B:1032:LEU:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:895:THR:HA	1:B:935:VAL:HG11	1.91	0.51
1:B:2102:PRO:HD2	1:B:2103:HIS:CD2	2.46	0.51
1:A:1673:ILE:HD13	1:A:1684:ALA:HB1	1.92	0.51
1:A:322:ILE:HG22	1:A:376:VAL:HA	1.92	0.51
1:B:1353:HIS:HB2	1:B:1354:PRO:CD	2.39	0.51
1:A:1766:PHE:CD2	1:A:1791:PHE:CE1	2.98	0.51
1:A:1420:ASP:HB3	1:A:1425:TRP:CZ3	2.46	0.51
1:A:143:ARG:NH1	1:A:143:ARG:HG2	2.25	0.51
1:A:1954:SER:O	1:A:1958:GLU:HG3	2.09	0.51
1:A:1122:THR:HG21	1:A:1517:PHE:HZ	1.76	0.51
1:B:876:VAL:HG12	1:B:876:VAL:O	2.11	0.51
1:B:433:ALA:HB2	1:B:835:LYS:O	2.10	0.51
1:A:1556:PRO:O	1:A:1557:ALA:C	2.49	0.51
1:A:469:GLY:HA2	1:A:805:LEU:HD21	1.93	0.51
1:A:1866:ARG:O	1:A:1867:GLY:O	2.29	0.51
1:B:1303:ASN:H	1:B:1304:PRO:HD3	1.74	0.51
1:B:515:ARG:HH22	1:B:817:PRO:HA	1.76	0.51
1:A:1390:VAL:HG22	1:A:1501:LEU:CD2	2.41	0.51
1:B:973:ARG:O	1:B:974:ALA:HB3	2.10	0.51
1:A:64:PHE:HB2	1:A:429:ARG:NH2	2.25	0.51
1:A:965:PRO:O	1:A:967:PRO:HD3	2.11	0.50
1:B:1430:LYS:CE	1:B:1981:GLU:O	2.56	0.50
1:B:1408:THR:H	1:B:1409:PRO:HD3	1.76	0.50
1:B:983:ALA:O	1:B:985:PHE:N	2.41	0.50
1:A:2002:LEU:O	1:A:2006:THR:HB	2.11	0.50
1:B:1624:THR:HG22	1:B:1857:ARG:HH21	1.74	0.50
1:B:1382:PHE:HA	1:B:1387:LEU:HD12	1.93	0.50
1:B:1889:ILE:HG23	1:B:1969:PHE:HB2	1.93	0.50
1:B:612:GLU:HG2	1:B:612:GLU:O	2.11	0.50
1:B:734:TYR:C	1:B:734:TYR:CD2	2.82	0.50
1:A:2065:ASP:C	1:A:2070:LEU:HD12	2.32	0.50
1:B:168:LEU:HA	1:B:185:VAL:HG21	1.93	0.50
1:B:1674:HIS:HE1	1:B:1756:SER:OG	1.94	0.50
1:A:1338:LEU:HD22	1:A:1406:GLN:HE21	1.76	0.50
1:B:265:SER:O	1:B:269:GLN:HG3	2.11	0.50
1:A:1487:HIS:NE2	1:A:1490:SER:HB2	2.26	0.50
1:A:325:THR:OG1	1:A:343:LYS:HG2	2.11	0.50
1:A:1454:VAL:HG13	1:A:1503:MET:HE3	1.94	0.50
1:B:6:ILE:HG21	1:B:345:LEU:CD1	2.39	0.50
1:A:1886:SER:HA	1:A:1911:LYS:HB2	1.92	0.50
1:B:1085:ASN:C	1:B:1086:LEU:HD23	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1279:PRO:HG3	1:B:1298:GLN:HE22	1.75	0.50
1:B:1001:TYR:HB3	1:B:1003:TYR:CE1	2.45	0.50
1:B:1363:THR:HG22	1:B:1367:GLN:HE21	1.76	0.50
1:A:297:THR:HB	1:A:300:GLY:H	1.76	0.50
1:B:248:ASN:HD22	1:B:249:ALA:H	1.59	0.50
1:B:564:ILE:HD13	1:B:590:ALA:HB2	1.91	0.50
1:A:1841:ARG:O	1:A:1844:ALA:HB3	2.12	0.50
1:A:1411:ASP:OD2	1:A:1439:ARG:HB2	2.12	0.50
1:B:143:ARG:CG	1:B:143:ARG:HH11	2.19	0.50
1:B:159:THR:O	1:B:160:ALA:HB3	2.12	0.50
1:B:1431:ASP:C	1:B:1433:LEU:H	2.14	0.50
1:B:1833:ARG:NH2	1:B:1872:ALA:O	2.45	0.50
1:A:289:TYR:HE2	1:A:291:GLU:CA	2.25	0.50
1:B:1894:GLY:O	1:B:1896:PHE:N	2.45	0.50
1:B:275:SER:HB2	1:B:276:LEU:HD23	1.93	0.50
1:A:1651:VAL:HG12	1:A:1683:ALA:HB2	1.94	0.50
1:B:866:VAL:HG13	1:B:866:VAL:O	2.12	0.50
1:A:878:HIS:HB2	1:A:1007:PHE:HE1	1.75	0.50
1:A:1896:PHE:HB2	2:A:3002:NAP:O2N	2.12	0.50
1:B:1422:SER:CB	1:B:1424:ARG:HG3	2.42	0.50
1:A:128:VAL:HG11	1:A:130:TYR:CE2	2.46	0.50
1:B:903:LEU:O	1:B:905:GLN:HG3	2.12	0.50
1:A:112:SER:CB	1:A:334:PRO:CG	2.85	0.50
1:B:1657:TYR:CZ	1:B:1662:ARG:HD2	2.47	0.50
1:B:1001:TYR:CD2	1:B:1003:TYR:HE1	2.30	0.50
1:A:1857:ARG:CG	1:A:1871:ILE:HD11	2.40	0.50
1:B:276:LEU:O	1:B:281:GLY:HA3	2.12	0.50
1:A:662:LEU:C	1:A:664:GLN:N	2.63	0.50
1:B:440:GLN:HG3	1:B:833:HIS:CD2	2.47	0.50
1:A:1556:PRO:O	1:A:1558:SER:N	2.45	0.50
1:B:1886:SER:HA	1:B:1911:LYS:HB2	1.93	0.50
1:A:286:SER:HB2	1:A:387:ASN:HD22	1.77	0.50
1:A:23:TRP:CZ2	1:A:350:HIS:CD2	3.00	0.50
1:A:1734:ARG:O	1:A:1736:THR:N	2.42	0.50
1:A:1735:HIS:N	1:A:1735:HIS:CD2	2.79	0.50
1:B:51:MET:HE2	1:B:191:LEU:HD13	1.93	0.50
1:A:72:ALA:HB3	1:A:842:TRP:CZ3	2.47	0.50
1:B:1041:LEU:HG	1:B:1041:LEU:O	2.12	0.50
1:A:1568:TYR:CE2	1:A:1855:GLN:HB2	2.47	0.50
1:B:1416:LEU:HD21	1:B:1425:TRP:HB2	1.93	0.49
1:A:1420:ASP:HB3	1:A:1425:TRP:HZ3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1343:PHE:O	1:A:1344:LEU:HD22	2.11	0.49
1:B:9:MET:HE3	1:B:345:LEU:HD12	1.94	0.49
1:B:1734:ARG:O	1:B:1736:THR:N	2.43	0.49
1:B:100:LEU:O	1:B:101:ARG:C	2.50	0.49
1:A:1894:GLY:O	1:A:1896:PHE:N	2.45	0.49
1:B:1652:TYR:CE1	1:B:1823:VAL:HB	2.47	0.49
1:A:1086:LEU:HB2	1:A:1088:THR:HG23	1.94	0.49
1:A:5:VAL:HG12	1:A:245:THR:HA	1.94	0.49
1:A:895:THR:HA	1:A:935:VAL:HG11	1.92	0.49
1:A:1504:ASN:HB3	1:A:1511:TRP:HZ3	1.77	0.49
1:A:1528:THR:HG23	1:A:1552:HIS:ND1	2.28	0.49
1:A:1470:ARG:O	1:A:1472:VAL:HG23	2.12	0.49
1:A:1303:ASN:HA	1:A:1333:ASN:HB2	1.94	0.49
1:A:59:ARG:HD2	1:A:59:ARG:N	2.26	0.49
1:A:1746:ASN:HD21	1:A:1753:LEU:HD12	1.77	0.49
1:A:1785:PHE:HB2	1:B:1774:LEU:CD2	2.43	0.49
1:B:495:ILE:CD1	1:B:578:ILE:HB	2.41	0.49
1:A:475:GLY:C	1:A:477:ALA:H	2.15	0.49
1:B:1458:ASN:O	1:B:2027:GLY:HA3	2.13	0.49
1:B:1285:ALA:HB1	1:B:1289:LEU:HG	1.94	0.49
1:B:112:SER:CB	1:B:334:PRO:CG	2.85	0.49
1:A:278:ALA:HB3	1:A:279:PRO:CD	2.29	0.49
1:A:309:VAL:CG2	1:A:374:LEU:HD11	2.42	0.49
1:A:983:ALA:O	1:A:984:GLU:HB3	2.11	0.49
1:A:276:LEU:N	1:A:276:LEU:HD23	2.27	0.49
1:B:272:LEU:O	1:B:276:LEU:HG	2.12	0.49
1:A:1672:LEU:HD12	1:A:1696:PHE:O	2.11	0.49
1:B:1568:TYR:CE2	1:B:1855:GLN:HB2	2.47	0.49
1:A:166:LEU:CD1	1:A:251:THR:HG21	2.32	0.49
1:B:1232:THR:HA	1:B:1515:ARG:NH2	2.20	0.49
1:B:309:VAL:HG22	1:B:374:LEU:HD21	1.94	0.49
1:B:228:VAL:O	1:B:228:VAL:HG23	2.11	0.49
1:B:967:PRO:HB3	1:B:1063:THR:OG1	2.13	0.49
1:A:2103:HIS:H	1:A:2103:HIS:CD2	2.30	0.49
1:B:59:ARG:N	1:B:59:ARG:HD2	2.28	0.49
1:B:2103:HIS:CD2	1:B:2103:HIS:H	2.29	0.49
1:A:1889:ILE:HG23	1:A:1969:PHE:HB2	1.93	0.49
1:A:1055:THR:HB	1:A:1097:LEU:O	2.13	0.49
1:B:1885:LYS:HE2	1:B:2012:GLU:HB3	1.95	0.49
1:B:2086:GLN:HG2	1:B:2110:VAL:HG23	1.93	0.49
1:A:1476:ASN:HD22	1:A:1486:MET:CE	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2076:ASN:HA	1:B:2085:PRO:HG2	1.94	0.49
1:B:1418:VAL:HG13	1:B:1425:TRP:CD2	2.46	0.49
1:B:1476:ASN:N	1:B:1476:ASN:OD1	2.44	0.49
1:B:143:ARG:HG2	1:B:143:ARG:NH1	2.21	0.49
1:B:1364:SER:OG	1:B:1370:ARG:HG2	2.12	0.49
1:A:1234:LEU:HD21	1:A:1268:MET:HE3	1.95	0.49
1:B:1123:PRO:HB3	1:B:1510:ALA:HB1	1.94	0.49
1:B:972:THR:HG23	1:B:1081:VAL:CG2	2.42	0.49
1:B:1863:PRO:O	1:B:1865:PRO:CD	2.61	0.49
1:B:1555:LEU:HD11	1:B:1563:LEU:HD22	1.92	0.49
1:A:1885:LYS:HE2	1:A:2012:GLU:HB3	1.94	0.49
1:A:1520:GLU:O	1:A:1522:ASP:N	2.44	0.49
1:A:1626:VAL:HG13	1:A:1627:LEU:N	2.27	0.49
1:A:1451:SER:O	1:A:1453:VAL:N	2.45	0.49
1:B:389:GLY:O	1:B:390:ILE:HG13	2.12	0.49
1:A:384:ARG:NH1	1:A:384:ARG:CG	2.66	0.49
1:A:1001:TYR:CD2	1:A:1003:TYR:HE1	2.29	0.49
1:B:305:LEU:O	1:B:309:VAL:HG23	2.13	0.49
1:A:497:SER:OG	1:A:767:LEU:HG	2.13	0.49
1:B:1150:LEU:HB2	1:B:1192:LEU:HD21	1.94	0.49
1:B:1603:PHE:H	1:B:1603:PHE:HD2	1.59	0.49
1:A:734:TYR:HD2	1:A:734:TYR:C	2.15	0.49
1:B:1569:THR:HG21	1:B:1622:LEU:CA	2.38	0.49
1:A:1454:VAL:HA	1:A:1473:LEU:HD13	1.95	0.49
1:B:1395:SER:HB3	1:B:1399:SER:O	2.13	0.49
1:A:1528:THR:HG22	1:A:1529:GLU:H	1.78	0.49
1:B:765:ALA:HB1	1:B:768:GLN:HG2	1.95	0.49
1:B:581:SER:OG	1:B:582:LEU:N	2.45	0.49
1:B:1694:ARG:HH11	1:B:1694:ARG:CG	2.26	0.49
1:A:1338:LEU:CB	1:A:1406:GLN:HE21	2.26	0.49
1:A:1339:LYS:O	1:A:1340:GLU:HB2	2.12	0.49
1:A:1378:TRP:O	1:A:1382:PHE:CD1	2.65	0.49
1:A:1476:ASN:N	1:A:1476:ASN:ND2	2.60	0.49
1:B:1453:VAL:HG12	1:B:1457:VAL:HG23	1.95	0.49
1:B:1236:ASN:ND2	1:B:1502:VAL:H	2.11	0.49
1:A:1545:ARG:CG	1:A:1545:ARG:NH1	2.69	0.49
1:A:975:ALA:O	1:A:976:VAL:HB	2.12	0.49
1:A:495:ILE:CD1	1:A:578:ILE:HB	2.42	0.49
1:B:491:PRO:HA	1:B:575:ASP:OD2	2.13	0.49
1:B:1842:TYR:HE2	1:B:1848:HIS:HB3	1.78	0.49
1:B:506:MET:HE2	1:B:559:ILE:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1969:PHE:CD2	1:B:2017:VAL:HB	2.48	0.49
1:B:734:TYR:HD2	1:B:734:TYR:C	2.16	0.49
1:A:1451:SER:O	1:A:1452:GLY:C	2.51	0.49
1:A:1433:LEU:HD21	1:A:1465:GLY:HA3	1.95	0.49
1:B:1117:GLU:HB2	1:B:2107:SER:HB2	1.94	0.49
1:A:1140:LEU:HD22	1:A:1140:LEU:O	2.12	0.49
1:B:1647:SER:HB2	1:B:1851:LYS:HG3	1.95	0.49
1:B:1086:LEU:N	1:B:1086:LEU:HD23	2.28	0.49
1:A:2086:GLN:HG2	1:A:2110:VAL:HG23	1.94	0.49
1:A:408:SER:O	1:A:409:ARG:HB2	2.12	0.49
1:A:997:ARG:HH21	1:A:2070:LEU:HD12	1.78	0.48
1:B:1247:VAL:HG23	1:B:1315:LEU:HD11	1.95	0.48
1:B:91:VAL:HG21	1:B:834:ILE:HD13	1.93	0.48
1:B:1642:LEU:HG	1:B:1859:GLU:OE2	2.12	0.48
1:B:1736:THR:HG23	1:B:1740:GLY:H	1.78	0.48
1:A:1989:GLN:HG2	1:A:1990:ASP:N	2.28	0.48
1:A:988:SER:O	1:A:989:GLN:C	2.51	0.48
1:B:896:TRP:CD2	1:B:907:LEU:HD11	2.48	0.48
1:A:137:ARG:O	1:A:140:MET:HG2	2.13	0.48
1:B:1252:GLY:HA2	1:B:1318:ASN:HD22	1.78	0.48
1:A:1214:ASP:O	1:A:1216:LEU:N	2.41	0.48
1:B:610:ILE:CG2	1:B:680:ILE:HD12	2.43	0.48
1:B:1413:PRO:HB3	1:B:1440:PRO:HB2	1.94	0.48
1:A:856:CYS:HB2	1:B:856:CYS:HG	1.77	0.48
1:A:2006:THR:O	1:A:2010:CYS:HB2	2.13	0.48
1:B:896:TRP:CG	1:B:907:LEU:HD11	2.49	0.48
1:B:970:PHE:O	1:B:1067:LYS:NZ	2.45	0.48
1:A:846:SER:O	1:A:849:ASP:HB2	2.13	0.48
1:B:475:GLY:C	1:B:477:ALA:H	2.17	0.48
1:B:112:SER:O	1:B:137:ARG:NH2	2.46	0.48
1:A:1429:LEU:HD21	1:A:1443:LEU:HD21	1.95	0.48
1:B:143:ARG:NH1	1:B:143:ARG:CG	2.76	0.48
1:A:2068:VAL:N	2:A:3002:NAP:O1N	2.46	0.48
1:A:276:LEU:O	1:A:281:GLY:HA3	2.12	0.48
1:A:506:MET:HB3	1:A:559:ILE:HD11	1.93	0.48
1:B:1504:ASN:HB3	1:B:1511:TRP:HZ3	1.77	0.48
1:B:1841:ARG:O	1:B:1844:ALA:HB3	2.14	0.48
1:B:1476:ASN:C	1:B:1477:LEU:HD23	2.33	0.48
1:A:1489:SER:CA	1:A:1493:LEU:HD22	2.43	0.48
1:B:98:ALA:O	1:B:101:ARG:HG3	2.13	0.48
1:B:662:LEU:HD13	1:B:672:VAL:CG1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1666:GLN:O	1:A:1669:GLU:HG3	2.13	0.48
1:B:988:SER:O	1:B:989:GLN:C	2.47	0.48
1:A:903:LEU:O	1:A:904:SER:HB3	2.13	0.48
1:B:87:TYR:CE2	1:B:97:PRO:HG2	2.48	0.48
1:A:1416:LEU:HD21	1:A:1425:TRP:HB2	1.94	0.48
1:B:342:ILE:O	1:B:346:LEU:HG	2.13	0.48
1:B:1246:GLU:CD	1:B:1254:LEU:HB2	2.34	0.48
1:B:191:LEU:O	1:B:192:LEU:HD23	2.13	0.48
1:B:1123:PRO:HA	1:B:1512:GLY:HA3	1.96	0.48
1:B:497:SER:HB2	1:B:762:ALA:HB2	1.94	0.48
1:A:353:TRP:CE2	1:A:383:ILE:HB	2.49	0.48
1:A:148:PHE:HB3	1:A:150:PHE:CE1	2.49	0.48
1:B:1729:GLU:OE1	1:B:1758:ARG:HD2	2.13	0.48
1:A:290:ILE:HG23	1:A:322:ILE:HG13	1.95	0.48
1:B:2046:GLU:HG2	1:B:2104:PRO:HG2	1.95	0.48
1:B:12:LYS:HD2	1:B:81:MET:CE	2.44	0.48
1:A:136:GLN:NE2	1:A:138:ALA:H	2.06	0.48
1:A:1694:ARG:HH11	1:A:1694:ARG:CG	2.26	0.48
1:B:1697:THR:CG2	1:B:1698:THR:N	2.76	0.48
1:B:1672:LEU:HD12	1:B:1696:PHE:O	2.14	0.48
1:A:1240:PRO:HD2	1:A:1462:LYS:HE3	1.95	0.48
1:B:1240:PRO:HD2	1:B:1462:LYS:HE3	1.96	0.48
1:A:642:CYS:HA	1:A:743:VAL:HG23	1.95	0.48
1:A:1483:ALA:N	1:A:1484:PRO:CD	2.76	0.48
1:B:1220:LEU:HB3	1:B:1257:ARG:NH2	2.14	0.48
1:A:1624:THR:HG22	1:A:1857:ARG:NH2	2.16	0.48
1:A:917:VAL:HG12	1:A:1054:PHE:HB2	1.93	0.48
1:A:39:ARG:NH1	1:A:226:GLU:OE2	2.47	0.48
1:A:1147:ALA:O	1:A:1358:MET:HE1	2.14	0.48
1:A:1671:VAL:HG13	1:A:1673:ILE:HG13	1.94	0.48
1:A:506:MET:HE2	1:A:559:ILE:HD12	1.96	0.48
1:A:450:PHE:CE2	1:A:828:PRO:HB2	2.49	0.48
1:A:645:SER:OG	1:A:648:THR:N	2.47	0.48
1:A:342:ILE:O	1:A:346:LEU:HG	2.13	0.48
1:B:289:TYR:HE2	1:B:291:GLU:CA	2.26	0.48
1:B:1567:TYR:C	1:B:1856:VAL:HG23	2.34	0.48
1:B:572:LEU:C	1:B:572:LEU:HD23	2.34	0.48
1:B:434:VAL:O	1:B:438:LEU:HG	2.14	0.48
1:A:662:LEU:O	1:A:663:GLN:C	2.52	0.48
1:A:438:LEU:N	1:A:438:LEU:HD23	2.28	0.48
1:B:128:VAL:HG11	1:B:130:TYR:OH	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LYS:C	1:A:238:LEU:H	2.17	0.48
1:A:236:LYS:O	1:A:238:LEU:N	2.42	0.48
1:B:1390:VAL:HG13	1:B:1501:LEU:HD22	1.95	0.48
1:B:1904:LEU:HA	1:B:1904:LEU:HD23	1.56	0.48
1:A:1252:GLY:CA	1:A:1318:ASN:HD22	2.25	0.48
1:B:23:TRP:CZ2	1:B:350:HIS:CD2	3.00	0.48
1:B:981:SER:HA	1:B:986:ARG:NH2	2.29	0.48
1:A:226:GLU:O	1:A:227:ALA:HB2	2.14	0.48
1:B:64:PHE:HB2	1:B:429:ARG:NH2	2.29	0.48
1:A:1299:TRP:NE1	1:A:1306:PRO:HD2	2.25	0.48
1:A:100:LEU:O	1:A:101:ARG:C	2.52	0.48
1:A:103:THR:HG22	1:A:104:SER:H	1.77	0.48
1:A:1580:THR:HG22	1:A:1581:GLY:N	2.29	0.48
1:A:1235:GLU:OE2	1:A:1515:ARG:NH1	2.47	0.48
1:B:2023:SER:O	1:B:2027:GLY:HA2	2.14	0.48
1:A:225:ALA:O	1:A:332:PRO:HA	2.14	0.48
1:A:937:LEU:HA	1:A:937:LEU:HD12	1.69	0.48
1:B:1069:TYR:CD1	1:B:1077:ALA:O	2.67	0.48
1:B:1636:VAL:HG22	1:B:1636:VAL:O	2.13	0.48
1:A:1121:PHE:CE2	1:A:1507:ARG:HB2	2.49	0.47
1:A:1265:GLN:HG2	1:A:1266:PRO:HD2	1.94	0.47
1:B:883:ARG:HH21	1:B:1107:ARG:HD3	1.79	0.47
1:A:1995:LYS:HD3	1:A:2038:ASN:OD1	2.13	0.47
1:A:886:PHE:HA	1:A:887:PRO:HD3	1.63	0.47
1:B:993:TYR:OH	1:B:1010:VAL:HG23	2.14	0.47
1:A:1762:GLN:O	1:A:1763:HIS:HB2	2.12	0.47
1:B:297:THR:HG22	1:B:299:VAL:H	1.79	0.47
1:B:887:PRO:HB2	1:B:890:GLY:H	1.79	0.47
1:B:1578:LEU:C	1:B:1580:THR:H	2.16	0.47
1:A:1085:ASN:C	1:A:1086:LEU:HD23	2.34	0.47
1:A:642:CYS:SG	1:A:743:VAL:CG2	3.02	0.47
1:A:146:PHE:O	1:B:256:SER:HB3	2.13	0.47
1:B:2003:ASP:O	1:B:2007:ARG:HG3	2.14	0.47
1:A:661:PHE:O	1:A:661:PHE:CG	2.67	0.47
1:A:1446:VAL:HA	1:A:1476:ASN:OD1	2.14	0.47
1:A:1476:ASN:HD22	1:A:1486:MET:HE2	1.79	0.47
1:B:1442:TRP:CB	1:B:1444:MET:HE1	2.43	0.47
1:A:2076:ASN:HA	1:A:2085:PRO:HG2	1.96	0.47
1:B:606:ARG:O	1:B:610:ILE:HG13	2.13	0.47
1:B:1363:THR:HG22	1:B:1367:GLN:NE2	2.29	0.47
1:B:1915:THR:CG2	2:B:3002:NAP:H2A	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:993:TYR:OH	1:A:1010:VAL:HG23	2.14	0.47
1:B:506:MET:CE	1:B:559:ILE:HD12	2.44	0.47
1:A:645:SER:C	1:A:746:GLN:HG3	2.35	0.47
1:A:1786:LEU:C	1:A:1788:ASN:H	2.17	0.47
1:B:1071:LEU:HD12	1:B:1075:THR:OG1	2.14	0.47
1:B:1183:LEU:HB3	1:B:1216:LEU:CD2	2.44	0.47
1:B:1327:PRO:O	1:B:1331:VAL:HG23	2.14	0.47
1:A:605:TRP:O	1:A:606:ARG:C	2.53	0.47
1:A:856:CYS:HB2	1:B:856:CYS:SG	2.53	0.47
1:A:330:GLY:O	1:A:332:PRO:HD3	2.13	0.47
1:B:211:THR:HG22	1:B:212:CYS:N	2.28	0.47
1:B:1228:ALA:HB2	1:B:1517:PHE:CZ	2.49	0.47
1:A:2046:GLU:HG2	1:A:2104:PRO:HG2	1.95	0.47
1:A:1616:MET:HB3	1:A:1800:PHE:CE2	2.49	0.47
1:A:1289:LEU:HD22	1:A:1294:VAL:CB	2.44	0.47
1:A:896:TRP:CG	1:A:907:LEU:HD11	2.49	0.47
1:A:620:MET:SD	1:A:677:THR:HG21	2.54	0.47
1:A:533:ARG:HB2	1:A:533:ARG:HH11	1.79	0.47
1:B:1221:LEU:O	1:B:1226:LEU:HD21	2.14	0.47
1:B:1477:LEU:HB3	1:B:1507:ARG:HE	1.79	0.47
1:A:1299:TRP:CH2	1:A:1333:ASN:CG	2.88	0.47
1:B:1338:LEU:HD22	1:B:1406:GLN:HG3	1.96	0.47
1:B:1814:LEU:O	1:B:1818:ILE:HG13	2.15	0.47
1:B:299:VAL:O	1:B:302:PRO:HD2	2.13	0.47
1:B:1735:HIS:N	1:B:1735:HIS:CD2	2.83	0.47
1:A:1067:LYS:HB3	1:A:1092:GLY:HA2	1.95	0.47
1:B:1153:LYS:HD3	1:B:1195:ASN:HD22	1.79	0.47
1:B:1769:ILE:HG23	2:B:3001:NAP:C2N	2.45	0.47
1:B:333:GLU:O	1:B:336:SER:HB3	2.14	0.47
1:A:277:TYR:CZ	1:A:287:LEU:HD11	2.49	0.47
1:B:1022:LEU:HD13	1:B:1034:ALA:HB3	1.97	0.47
1:B:1574:ARG:HD2	1:B:1588:ILE:CD1	2.45	0.47
1:B:873:HIS:O	1:B:876:VAL:HG23	2.14	0.47
1:A:1619:ALA:O	1:A:1620:GLU:HB2	2.15	0.47
1:A:433:ALA:HB2	1:A:835:LYS:O	2.15	0.47
1:B:331:HIS:C	1:B:333:GLU:H	2.18	0.47
1:A:1182:ARG:CB	1:A:1216:LEU:HB2	2.33	0.47
1:B:1276:ASP:OD2	1:B:1281:ALA:HB3	2.14	0.47
1:A:782:ILE:HG22	1:A:783:PRO:O	2.14	0.47
1:A:1473:LEU:HD23	1:A:1502:VAL:O	2.15	0.47
1:A:504:GLN:HG3	1:A:546:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1223:ALA:O	1:A:1225:ALA:N	2.48	0.47
1:A:941:SER:CB	1:B:945:GLU:OE2	2.63	0.47
1:B:1585:PRO:HB3	1:B:1598:MET:HE1	1.96	0.47
1:A:1578:LEU:C	1:A:1580:THR:H	2.17	0.47
1:B:274:ARG:O	1:B:276:LEU:N	2.47	0.47
1:B:330:GLY:O	1:B:332:PRO:HD3	2.14	0.47
1:A:970:PHE:O	1:A:1067:LYS:HE2	2.15	0.47
1:B:709:SER:OG	1:B:711:ARG:HB2	2.14	0.47
1:A:1774:LEU:CD2	1:B:1785:PHE:HB2	2.45	0.47
1:B:1469:ILE:O	1:B:1469:ILE:CG2	2.61	0.47
1:B:1781:GLY:O	1:B:1784:VAL:HG23	2.15	0.47
1:B:633:ARG:HG2	1:B:633:ARG:O	2.14	0.47
1:A:420:LEU:HD11	1:A:512:ARG:HB3	1.96	0.47
1:A:64:PHE:HB2	1:A:429:ARG:HE	1.80	0.47
1:A:1670:SER:OG	1:A:1741:VAL:HA	2.15	0.47
1:A:491:PRO:HA	1:A:575:ASP:OD2	2.15	0.47
1:B:285:GLU:HG3	1:B:315:THR:OG1	2.15	0.47
1:B:1766:PHE:O	1:B:1792:HIS:HB2	2.14	0.47
1:B:289:TYR:OH	1:B:323:GLY:HA3	2.13	0.47
1:A:912:VAL:HG22	1:A:913:VAL:N	2.29	0.47
1:B:1338:LEU:HD13	1:B:1406:GLN:HG2	1.95	0.47
1:A:36:ASP:CB	1:A:38:ARG:HG3	2.45	0.47
1:B:1762:GLN:O	1:B:1763:HIS:HB2	2.14	0.47
1:A:1680:VAL:N	2:A:3001:NAP:O1N	2.32	0.47
1:A:424:LEU:CD2	1:A:441:GLY:HA3	2.45	0.47
1:B:1277:ARG:NH2	1:B:1323:THR:O	2.47	0.47
1:A:1071:LEU:HD12	1:A:1075:THR:OG1	2.15	0.47
1:B:644:ASN:HB2	1:B:648:THR:O	2.14	0.47
1:A:1476:ASN:CB	1:A:1486:MET:SD	3.03	0.47
1:B:1257:ARG:O	1:B:1260:ALA:HB3	2.15	0.47
1:A:1653:THR:HG22	1:A:1810:VAL:HG12	1.96	0.47
1:A:561:ILE:HG23	1:A:589:TYR:CE2	2.50	0.47
1:A:88:GLU:HB3	1:A:831:SER:HB2	1.97	0.47
1:A:1433:LEU:HD11	1:A:1465:GLY:O	2.15	0.47
1:B:1504:ASN:HB3	1:B:1511:TRP:CZ3	2.50	0.47
1:B:831:SER:N	1:B:832:PRO:CD	2.77	0.47
1:A:1485:GLU:HG2	1:A:1506:TYR:OH	2.15	0.46
1:B:1515:ARG:HD3	1:B:1515:ARG:HA	1.56	0.46
1:A:765:ALA:HB1	1:A:768:GLN:HG2	1.96	0.46
1:A:1473:LEU:HD21	1:A:1503:MET:SD	2.55	0.46
1:B:556:LEU:O	1:B:560:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:VAL:CG2	1:A:834:ILE:CD1	2.94	0.46
1:B:980:ASP:CG	1:B:982:THR:HG22	2.35	0.46
1:B:226:GLU:O	1:B:227:ALA:HB2	2.14	0.46
1:A:289:TYR:HE2	1:A:291:GLU:HA	1.80	0.46
1:A:2017:VAL:HG21	1:A:2099:LEU:HD21	1.96	0.46
1:A:2099:LEU:HD23	1:A:2099:LEU:HA	1.70	0.46
1:A:1387:LEU:HD22	1:A:1404:CYS:HB3	1.96	0.46
1:B:286:SER:HB2	1:B:387:ASN:HD22	1.79	0.46
1:A:1348:THR:HG23	1:A:1372:LEU:HD22	1.97	0.46
1:A:331:HIS:C	1:A:333:GLU:H	2.18	0.46
1:B:1662:ARG:NH1	1:B:1662:ARG:CG	2.50	0.46
1:A:1133:ASN:ND2	1:A:1136:LEU:HD12	2.17	0.46
1:A:1183:LEU:N	1:A:1216:LEU:HD22	2.29	0.46
1:A:1420:ASP:CB	1:A:1425:TRP:HZ3	2.28	0.46
1:A:168:LEU:O	1:A:168:LEU:HG	2.14	0.46
1:A:509:SER:O	1:A:512:ARG:HG3	2.14	0.46
1:B:168:LEU:HG	1:B:168:LEU:O	2.14	0.46
1:A:1299:TRP:HE1	1:A:1306:PRO:CD	2.25	0.46
1:B:1857:ARG:CZ	1:B:1871:ILE:CD1	2.93	0.46
1:A:59:ARG:HG3	1:A:838:HIS:HB3	1.96	0.46
1:B:297:THR:HB	1:B:300:GLY:N	2.31	0.46
1:B:1014:ASP:OD1	1:B:1015:LEU:N	2.49	0.46
1:A:837:ASP:OD1	1:A:839:SER:HB3	2.16	0.46
1:B:1216:LEU:CD1	1:B:1217:LEU:N	2.78	0.46
1:B:2069:VAL:HG12	1:B:2070:LEU:HD23	1.97	0.46
1:A:1136:LEU:HD21	1:A:1217:LEU:HG	1.97	0.46
1:B:1444:MET:HE2	1:B:1444:MET:HB3	1.81	0.46
1:B:305:LEU:HD22	1:B:322:ILE:HD13	1.96	0.46
1:B:509:SER:O	1:B:512:ARG:HG3	2.15	0.46
1:A:188:LEU:CD2	1:A:228:VAL:HG12	2.44	0.46
1:A:48:PRO:HD3	1:A:201:MET:HE3	1.97	0.46
1:B:1762:GLN:HB3	1:B:1763:HIS:CD2	2.50	0.46
1:B:1568:TYR:HE2	1:B:1855:GLN:HB2	1.79	0.46
1:B:1239:SER:C	1:B:1241:LYS:H	2.19	0.46
1:A:1486:MET:HE1	1:A:1506:TYR:HB3	1.98	0.46
1:B:1420:ASP:CB	1:B:1425:TRP:HZ3	2.28	0.46
1:B:309:VAL:CG2	1:B:374:LEU:HD11	2.45	0.46
1:B:1603:PHE:CE2	1:B:1615:GLY:C	2.85	0.46
1:B:209:ASP:CG	1:B:213:ARG:HH21	2.18	0.46
1:A:1798:SER:O	1:A:1802:GLU:OE1	2.33	0.46
1:B:117:SER:CB	1:B:135:CYS:HB3	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:LEU:CD2	1:A:931:VAL:HG21	2.46	0.46
1:A:248:ASN:HD22	1:A:249:ALA:H	1.61	0.46
1:A:1573:PHE:HD2	2:A:3001:NAP:HO3N	1.61	0.46
1:B:1669:GLU:HG2	1:B:1742:ASP:OD2	2.15	0.46
1:A:1568:TYR:HE2	1:A:1855:GLN:HB2	1.80	0.46
1:A:1086:LEU:N	1:A:1086:LEU:HD23	2.31	0.46
1:A:1439:ARG:O	1:A:1470:ARG:HB3	2.15	0.46
1:B:934:GLU:CG	1:B:947:SER:HB2	2.46	0.46
1:B:506:MET:HB3	1:B:559:ILE:CD1	2.46	0.46
1:B:1460:LEU:O	1:B:1462:LYS:N	2.49	0.46
1:A:1347:HIS:HD1	1:A:1401:LEU:HD13	1.81	0.46
1:B:161:CYS:HB2	1:B:394:GLY:HA2	1.97	0.46
1:B:643:HIS:CD2	1:B:746:GLN:HB3	2.50	0.46
1:B:1452:GLY:O	1:B:2036:PHE:CD1	2.68	0.46
1:B:532:LEU:HD22	1:B:604:TYR:CE1	2.51	0.46
1:A:1657:TYR:HA	1:A:1661:VAL:HG23	1.98	0.46
1:A:976:VAL:HG13	1:A:977:ASP:N	2.30	0.46
1:A:934:GLU:CG	1:A:947:SER:HB2	2.46	0.46
1:A:1246:GLU:CD	1:A:1254:LEU:HB2	2.36	0.46
1:B:912:VAL:HG22	1:B:913:VAL:N	2.31	0.46
1:B:1697:THR:HG23	1:B:1698:THR:N	2.30	0.46
1:A:1671:VAL:HG23	1:A:1743:LEU:HD13	1.98	0.46
1:B:887:PRO:O	1:B:888:GLY:C	2.54	0.46
1:A:1466:GLY:HA2	1:A:1469:ILE:CG1	2.46	0.46
1:A:1122:THR:HG1	1:A:1517:PHE:HE1	1.60	0.46
1:A:900:ALA:HB1	1:A:905:GLN:O	2.16	0.46
1:A:494:PHE:CD1	1:A:574:PRO:HB3	2.50	0.46
1:B:533:ARG:HB2	1:B:533:ARG:HH11	1.81	0.46
1:B:2075:THR:CG2	1:B:2076:ASN:H	2.28	0.46
1:B:1245:VAL:HB	1:B:1315:LEU:HD13	1.97	0.46
1:B:1036:LEU:CD2	1:B:1096:PHE:CE1	2.94	0.46
1:B:1556:PRO:O	1:B:1558:SER:N	2.49	0.46
1:A:1894:GLY:O	1:A:1895:GLY:C	2.53	0.46
1:A:142:ASN:ND2	1:B:396:GLY:HA3	2.30	0.46
1:B:438:LEU:N	1:B:438:LEU:HD23	2.30	0.46
1:B:1647:SER:CB	1:B:1851:LYS:HG3	2.46	0.46
1:B:1311:LYS:O	1:B:1312:ALA:CB	2.63	0.46
1:A:1064:HIS:O	1:A:1065:ARG:C	2.54	0.46
1:A:440:GLN:HG3	1:A:833:HIS:CG	2.50	0.46
1:B:1531:ALA:HA	1:B:1549:SER:H	1.81	0.46
1:A:62:ALA:O	1:A:67:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ALA:HB2	1:B:850:PHE:CE2	2.51	0.46
1:B:384:ARG:NH1	1:B:384:ARG:CG	2.65	0.46
1:A:1416:LEU:HD23	1:A:1429:LEU:CD2	2.45	0.46
1:B:1567:TYR:O	1:B:1856:VAL:HG23	2.16	0.46
1:A:2058:VAL:HG11	1:A:2060:TRP:CE2	2.51	0.46
1:B:886:PHE:HA	1:B:887:PRO:HD3	1.64	0.46
1:A:1724:ARG:HH12	2:A:3001:NAP:C8A	2.27	0.46
1:B:1289:LEU:HD22	1:B:1294:VAL:HB	1.96	0.46
1:A:1554:ALA:CB	1:A:1882:PRO:HB3	2.46	0.46
1:A:556:LEU:O	1:A:560:GLN:HG3	2.15	0.46
1:B:1361:PHE:CZ	1:B:1370:ARG:HD3	2.51	0.46
1:A:1975:LEU:HD22	1:A:1977:ASP:OD1	2.16	0.46
1:B:1577:MET:CE	1:B:1582:LYS:HD3	2.46	0.46
1:A:2043:ARG:HD3	1:A:2043:ARG:HA	1.61	0.46
1:A:1208:ARG:H	1:A:1209:PRO:CD	2.29	0.46
1:A:578:ILE:CG2	1:A:745:PHE:HE1	2.29	0.46
1:A:9:MET:HE3	1:A:345:LEU:HD12	1.98	0.46
1:B:209:ASP:CG	1:B:213:ARG:NH2	2.70	0.46
1:B:127:LEU:HD12	1:B:127:LEU:C	2.36	0.46
1:A:506:MET:HB3	1:A:506:MET:HE2	1.85	0.46
1:B:2017:VAL:HG21	1:B:2099:LEU:HD21	1.97	0.46
1:B:2099:LEU:HA	1:B:2099:LEU:HD23	1.71	0.46
1:A:1669:GLU:O	1:A:1693:CYS:HB3	2.16	0.46
1:A:533:ARG:HB2	1:A:533:ARG:NH1	2.31	0.46
1:A:1904:LEU:HD23	1:A:1904:LEU:HA	1.58	0.46
1:B:737:ASN:C	1:B:737:ASN:ND2	2.70	0.46
1:B:530:LEU:HD13	1:B:604:TYR:CE2	2.51	0.45
1:B:201:MET:HA	1:B:206:LEU:HB2	1.97	0.45
1:B:23:TRP:O	1:B:24:ALA:C	2.54	0.45
1:B:1360:GLY:O	1:B:1364:SER:OG	2.25	0.45
1:B:103:THR:HG22	1:B:104:SER:H	1.81	0.45
1:A:1818:ILE:HG12	1:A:1823:VAL:CG1	2.47	0.45
1:A:426:ALA:HA	1:A:458:ALA:CB	2.46	0.45
1:B:468:ARG:HG2	1:B:804:HIS:NE2	2.31	0.45
1:A:1338:LEU:HG	1:A:1339:LYS:N	2.31	0.45
1:A:1360:GLY:CA	1:A:1369:GLY:O	2.64	0.45
1:A:240:ARG:HG2	1:A:821:PHE:CD2	2.51	0.45
1:B:1690:SER:HB3	1:B:1822:VAL:HG13	1.98	0.45
1:A:356:ASN:HA	1:A:356:ASN:HD22	1.50	0.45
1:B:1405:ARG:NH1	1:B:1500:ASP:OD1	2.49	0.45
1:A:984:GLU:HG2	1:A:986:ARG:NE	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1370:ARG:O	1:B:1371:HIS:HB3	2.16	0.45
1:B:1351:ALA:HB2	1:B:1372:LEU:HB3	1.96	0.45
1:B:1130:LEU:HD22	1:B:1133:ASN:HD21	1.80	0.45
1:B:1674:HIS:CE1	1:B:1756:SER:OG	2.68	0.45
1:A:1424:ARG:C	1:A:1426:VAL:N	2.70	0.45
1:B:1647:SER:CA	1:B:1851:LYS:HG3	2.46	0.45
1:B:1086:LEU:HB2	1:B:1088:THR:HG23	1.99	0.45
1:A:1785:PHE:HB2	1:B:1774:LEU:HD22	1.98	0.45
1:A:1371:HIS:O	1:A:1371:HIS:CD2	2.69	0.45
1:A:1330:ALA:O	1:A:1334:MET:HG2	2.16	0.45
1:B:1261:LEU:O	1:B:1264:THR:HB	2.16	0.45
1:A:1115:ILE:HD11	1:A:2111:LEU:HG	1.99	0.45
1:A:737:ASN:HD22	1:A:737:ASN:C	2.17	0.45
1:A:336:SER:OG	1:A:337:GLY:N	2.49	0.45
1:A:277:TYR:O	1:A:278:ALA:C	2.54	0.45
1:B:1418:VAL:HG12	1:B:1418:VAL:O	2.15	0.45
1:B:1442:TRP:CD2	1:B:1472:VAL:HB	2.51	0.45
1:B:1473:LEU:HD23	1:B:1473:LEU:N	2.32	0.45
1:B:1837:GLU:O	1:B:1840:PHE:HB2	2.16	0.45
1:B:1413:PRO:CA	1:B:1440:PRO:HB2	2.47	0.45
1:B:367:PRO:C	1:B:369:LEU:H	2.20	0.45
1:A:1130:LEU:O	1:A:1131:ALA:CB	2.65	0.45
1:B:122:ARG:HG3	1:B:123:ASP:H	1.80	0.45
1:A:1606:ARG:HH21	1:A:1860:GLU:CG	2.29	0.45
1:A:1338:LEU:HD13	1:A:1406:GLN:HG3	1.97	0.45
1:A:1618:PRO:O	1:A:1619:ALA:HB2	2.17	0.45
1:A:593:CYS:SG	1:A:708:ARG:HA	2.57	0.45
1:B:1746:ASN:ND2	1:B:1753:LEU:HD12	2.32	0.45
1:A:470:TYR:C	1:A:470:TYR:CD1	2.90	0.45
1:B:399:ASN:ND2	1:B:399:ASN:N	2.63	0.45
1:B:1216:LEU:HD12	1:B:1217:LEU:N	2.31	0.45
1:B:1616:MET:C	1:B:1800:PHE:HZ	2.20	0.45
1:A:1470:ARG:O	1:A:1470:ARG:CG	2.65	0.45
1:B:1282:LEU:HD21	1:B:1296:GLN:CB	2.41	0.45
1:A:1345:LEU:O	1:A:1346:LEU:HD23	2.17	0.45
1:B:581:SER:CB	1:B:683:HIS:NE2	2.78	0.45
1:B:925:LEU:CD2	1:B:931:VAL:HG21	2.45	0.45
1:A:1585:PRO:O	1:A:1595:ARG:NH1	2.49	0.45
1:A:621:ALA:O	1:A:650:THR:HA	2.15	0.45
1:A:892:LEU:HD22	1:A:1057:ILE:HD12	1.98	0.45
1:A:169:GLN:HE21	1:A:169:GLN:C	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:TRP:O	1:B:606:ARG:C	2.55	0.45
1:B:136:GLN:NE2	1:B:138:ALA:N	2.64	0.45
1:B:289:TYR:HH	1:B:323:GLY:HA3	1.82	0.45
1:B:19:LEU:HA	1:B:19:LEU:HD23	1.76	0.45
1:A:1237:MET:SD	1:A:1242:MET:HG3	2.56	0.45
1:B:1894:GLY:O	1:B:1895:GLY:C	2.54	0.45
1:B:51:MET:HE1	1:B:191:LEU:HD13	1.98	0.45
1:B:40:TRP:CZ3	1:B:194:PRO:HA	2.51	0.45
1:B:1572:ASN:OD1	1:B:1851:LYS:NZ	2.49	0.45
1:A:762:ALA:HB1	1:A:763:PRO:HD2	1.99	0.45
1:B:62:ALA:O	1:B:67:VAL:HG22	2.17	0.45
1:B:1454:VAL:HA	1:B:1473:LEU:HD13	1.98	0.45
1:B:782:ILE:CD1	1:B:803:LEU:HD23	2.40	0.45
1:A:1662:ARG:HH12	1:B:1790:THR:CG2	2.29	0.45
1:A:1251:ASP:HB2	1:A:1321:LEU:HG	1.97	0.45
1:B:1351:ALA:HB2	1:B:1372:LEU:CB	2.47	0.45
1:B:1538:ARG:NH2	1:B:1585:PRO:HG2	2.32	0.45
1:B:1631:HIS:CD2	1:B:1803:GLY:HA3	2.51	0.45
1:A:1766:PHE:O	1:A:1792:HIS:HB2	2.17	0.45
1:A:549:ILE:HG13	1:A:553:PHE:CE1	2.52	0.45
1:B:234:THR:HG22	1:B:235:LYS:N	2.31	0.45
1:A:1408:THR:CG2	1:A:1409:PRO:HD2	2.46	0.45
1:A:475:GLY:O	1:A:477:ALA:N	2.48	0.45
1:A:1369:GLY:C	1:A:1371:HIS:H	2.20	0.45
1:A:1236:ASN:HA	1:A:1502:VAL:HG21	1.98	0.45
1:A:23:TRP:O	1:A:24:ALA:C	2.54	0.45
1:B:1338:LEU:CB	1:B:1406:GLN:HE21	2.29	0.45
1:B:258:GLU:H	1:B:259:GLN:NE2	2.15	0.45
1:A:297:THR:HB	1:A:300:GLY:N	2.32	0.45
1:B:1801:GLU:C	1:B:1803:GLY:H	2.20	0.45
1:B:1339:LYS:O	1:B:1340:GLU:HB2	2.17	0.45
1:B:561:ILE:HG23	1:B:589:TYR:CE2	2.51	0.45
1:B:403:ILE:C	1:B:404:LEU:HD23	2.37	0.45
1:A:1118:LYS:HB3	1:A:1519:LEU:HD13	1.99	0.45
1:B:1627:LEU:HD22	1:B:1627:LEU:HA	1.67	0.45
1:B:1800:PHE:CD2	1:B:1800:PHE:C	2.90	0.45
1:A:157:ILE:HD11	1:A:167:ALA:CA	2.44	0.45
1:A:305:LEU:O	1:A:309:VAL:HG23	2.16	0.45
1:B:2104:PRO:HD2	1:B:2105:VAL:H	1.82	0.45
1:B:1326:ASP:HA	1:B:1327:PRO:HD2	1.70	0.45
1:A:1350:LEU:HD13	1:A:1374:SER:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1674:HIS:HD2	1:B:1698:THR:OG1	1.97	0.45
1:B:1067:LYS:HB3	1:B:1092:GLY:HA2	1.98	0.45
1:A:642:CYS:HB2	1:A:650:THR:HB	1.99	0.45
1:B:1786:LEU:C	1:B:1788:ASN:H	2.20	0.45
1:B:1419:GLU:CD	1:B:1447:GLY:HA3	2.37	0.45
1:A:759:VAL:HG23	1:A:759:VAL:O	2.17	0.45
1:A:572:LEU:C	1:A:572:LEU:HD23	2.37	0.45
1:A:984:GLU:HG2	1:A:986:ARG:HG3	1.99	0.45
1:A:168:LEU:HA	1:A:185:VAL:HG21	1.98	0.45
1:A:136:GLN:NE2	1:A:138:ALA:N	2.65	0.45
1:B:1387:LEU:HD22	1:B:1404:CYS:HB3	1.98	0.45
1:B:1424:ARG:O	1:B:1426:VAL:N	2.49	0.45
1:A:1272:TYR:HB3	1:A:1294:VAL:HG22	1.99	0.45
1:B:426:ALA:HA	1:B:458:ALA:CB	2.46	0.45
1:A:1387:LEU:HD23	1:A:1406:GLN:HB3	1.98	0.45
1:B:1560:GLN:HA	1:B:1563:LEU:HB2	1.98	0.45
1:A:737:ASN:ND2	1:A:737:ASN:C	2.69	0.45
1:A:873:HIS:O	1:A:876:VAL:HG23	2.16	0.45
1:B:1812:GLU:HA	1:B:1815:LYS:HB2	1.97	0.45
1:A:363:ASN:HA	1:A:364:PRO:HD3	1.81	0.45
1:A:768:GLN:CD	1:A:783:PRO:HG3	2.36	0.45
1:B:1412:SER:HA	1:B:1413:PRO:HD3	1.61	0.45
1:B:903:LEU:O	1:B:904:SER:HB3	2.17	0.45
1:A:1385:ALA:O	1:A:1386:SER:HB2	2.16	0.45
1:A:58:SER:HB3	1:A:844:VAL:CG2	2.47	0.45
1:B:1221:LEU:HG	1:B:1221:LEU:O	2.17	0.44
1:A:606:ARG:O	1:A:610:ILE:HG13	2.18	0.44
1:A:1147:ALA:HB1	1:A:1358:MET:HE2	2.00	0.44
1:A:1515:ARG:HD3	1:A:1515:ARG:HA	1.62	0.44
1:B:2018:ILE:HG12	1:B:2041:MET:HE2	1.99	0.44
1:A:1111:HIS:O	1:A:1112:LEU:HD23	2.17	0.44
1:B:1028:TRP:O	1:B:1032:LEU:HB2	2.17	0.44
1:B:506:MET:HE2	1:B:559:ILE:HD12	1.99	0.44
1:A:970:PHE:O	1:A:1067:LYS:NZ	2.48	0.44
1:A:94:GLY:HA3	1:A:453:MET:HG2	1.97	0.44
1:A:2003:ASP:O	1:A:2007:ARG:HG3	2.17	0.44
1:A:1535:VAL:HG12	1:A:1537:SER:H	1.82	0.44
1:B:542:ASP:O	1:B:545:VAL:HG12	2.17	0.44
1:B:1000:GLY:HA2	1:B:1106:ARG:NH2	2.32	0.44
1:B:1472:VAL:HG12	1:B:1473:LEU:N	2.32	0.44
1:A:1857:ARG:HH11	1:A:1869:PRO:HG2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:VAL:HG13	1:B:554:VAL:HG12	1.99	0.44
1:B:206:LEU:HA	1:B:206:LEU:HD23	1.70	0.44
1:A:1411:ASP:HB2	1:A:1440:PRO:HD3	2.00	0.44
1:A:1473:LEU:HD23	1:A:1473:LEU:N	2.32	0.44
1:B:512:ARG:NH1	1:B:793:LEU:HD23	2.33	0.44
1:B:668:GLU:O	1:B:669:ASP:CB	2.60	0.44
1:B:2053:LEU:CD2	1:B:2054:PRO:HD2	2.47	0.44
1:A:1373:LEU:HD22	1:A:1377:GLN:OE1	2.16	0.44
1:A:366:ILE:CG1	1:A:366:ILE:O	2.65	0.44
1:A:1255:TYR:HA	1:A:1272:TYR:CE2	2.52	0.44
1:A:396:GLY:HA3	1:B:142:ASN:ND2	2.31	0.44
1:A:2084:LEU:HD12	1:A:2112:ALA:HA	1.99	0.44
1:A:211:THR:HG22	1:A:212:CYS:N	2.32	0.44
1:A:1698:THR:HA	1:A:1721:ALA:O	2.17	0.44
1:B:1898:LEU:HA	1:B:1898:LEU:HD23	1.78	0.44
1:B:1662:ARG:NH1	1:B:1792:HIS:ND1	2.66	0.44
1:B:123:ASP:HA	1:B:124:PRO:HD3	1.70	0.44
1:A:903:LEU:O	1:A:905:GLN:HG3	2.18	0.44
1:B:642:CYS:O	1:B:649:VAL:HG13	2.18	0.44
1:A:1413:PRO:HA	1:A:1440:PRO:O	2.18	0.44
1:A:1472:VAL:HG13	1:A:1502:VAL:O	2.16	0.44
1:B:254:ASP:O	1:B:255:GLY:O	2.36	0.44
1:B:169:GLN:C	1:B:169:GLN:HE21	2.21	0.44
1:A:261:VAL:HG22	1:B:146:PHE:CD1	2.53	0.44
1:A:654:PRO:HB2	1:A:657:ALA:HB3	1.99	0.44
1:B:161:CYS:HB3	1:B:331:HIS:HE1	1.82	0.44
1:B:994:LYS:HE2	1:B:1924:TYR:CE2	2.52	0.44
1:A:1361:PHE:CZ	1:A:1370:ARG:NE	2.85	0.44
1:B:1345:LEU:HD12	1:B:1402:PHE:O	2.17	0.44
1:B:1036:LEU:HD13	1:B:1051:PRO:HG3	1.99	0.44
1:B:1251:ASP:CB	1:B:1321:LEU:HD22	2.47	0.44
1:A:1973:MET:O	1:A:1973:MET:HG3	2.18	0.44
1:A:1574:ARG:O	1:A:1578:LEU:HG	2.18	0.44
1:A:1814:LEU:O	1:A:1818:ILE:HG13	2.17	0.44
1:B:1265:GLN:HE21	1:B:2026:ARG:NH1	2.16	0.44
1:A:252:ASN:HD21	1:A:272:LEU:HB2	1.80	0.44
1:B:148:PHE:HB3	1:B:150:PHE:CE1	2.53	0.44
1:A:285:GLU:HG3	1:A:315:THR:OG1	2.17	0.44
1:B:165:LEU:HD22	1:B:392:SER:HB2	1.98	0.44
1:B:1472:VAL:HG12	1:B:1473:LEU:H	1.82	0.44
1:A:136:GLN:HE22	1:A:138:ALA:N	2.09	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1234:LEU:HD13	1:A:1242:MET:SD	2.58	0.44
1:A:1234:LEU:HD22	1:A:1262:LEU:CD2	2.46	0.44
1:B:1538:ARG:CZ	1:B:1585:PRO:HG2	2.47	0.44
1:A:103:THR:HG22	1:A:104:SER:N	2.32	0.44
1:B:2031:GLN:HB3	1:B:2034:TYR:HB3	1.99	0.44
1:B:1424:ARG:C	1:B:1426:VAL:N	2.71	0.44
1:A:1673:ILE:CD1	1:A:1684:ALA:HB1	2.48	0.44
1:A:1011:LEU:CD2	1:A:1023:GLN:HB2	2.47	0.44
1:B:1656:TYR:CD1	1:B:1687:ILE:HD11	2.53	0.44
1:A:169:GLN:HE21	1:A:170:SER:N	2.15	0.44
1:B:699:ARG:O	1:B:703:LEU:HD23	2.18	0.44
1:A:22:PHE:CE2	1:A:26:LEU:HD11	2.53	0.44
1:A:1812:GLU:HA	1:A:1815:LYS:HB2	1.99	0.44
1:B:784:LEU:HD23	1:B:784:LEU:HA	1.73	0.44
1:B:1535:VAL:HG12	1:B:1535:VAL:O	2.18	0.44
1:B:1389:LEU:HD23	1:B:1389:LEU:HA	1.76	0.44
1:B:55:LYS:HB3	1:B:55:LYS:HE2	1.77	0.44
1:B:78:GLN:HE21	1:B:190:VAL:H	1.65	0.44
1:A:132:MET:HE1	1:B:200:PHE:HE2	1.77	0.44
1:A:1726:THR:CG2	1:A:1726:THR:O	2.66	0.44
1:B:1733:LEU:HA	1:B:1733:LEU:HD23	1.84	0.44
1:A:1488:PRO:O	1:A:1489:SER:HB2	2.17	0.44
1:A:191:LEU:O	1:A:192:LEU:HD23	2.18	0.44
1:B:64:PHE:HB2	1:B:429:ARG:HE	1.82	0.44
1:B:1897:GLY:HA2	1:B:1971:LEU:HD12	2.00	0.44
1:A:1390:VAL:HG13	1:A:1501:LEU:HD22	1.99	0.44
1:B:497:SER:HB2	1:B:762:ALA:CB	2.47	0.44
1:B:737:ASN:C	1:B:737:ASN:HD22	2.18	0.44
1:B:1137:GLN:HG2	1:B:1396:PHE:CZ	2.53	0.44
1:A:801:GLY:O	1:A:804:HIS:HB3	2.17	0.44
1:A:40:TRP:CZ3	1:A:194:PRO:HA	2.52	0.44
1:A:752:VAL:HG11	1:A:775:LEU:HD21	2.00	0.44
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.81	0.44
1:A:1941:VAL:HG12	1:A:1941:VAL:O	2.16	0.44
1:A:1476:ASN:HD22	1:A:1476:ASN:N	2.15	0.44
1:A:1476:ASN:ND2	1:A:1486:MET:CE	2.81	0.44
1:B:1444:MET:HB2	1:B:1474:VAL:HB	2.00	0.44
1:B:368:ALA:HB1	1:B:374:LEU:HG	2.00	0.44
1:B:1996:TYR:C	1:B:1996:TYR:CD2	2.91	0.44
1:B:159:THR:HG22	1:B:398:SER:HB3	1.98	0.44
1:B:1656:TYR:CD2	1:B:1687:ILE:HD13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:GLN:HG3	1:A:833:HIS:CD2	2.53	0.44
1:A:844:VAL:O	1:A:845:PRO:C	2.56	0.44
1:A:1837:GLU:O	1:A:1840:PHE:HB2	2.18	0.44
1:B:1187:ALA:HB2	1:B:1210:LEU:HD13	1.99	0.44
1:B:1532:PHE:HA	1:B:1546:TRP:HZ3	1.83	0.44
1:A:83:LEU:HD23	1:A:144:LEU:HD12	1.99	0.44
1:B:1360:GLY:O	1:B:1364:SER:CB	2.66	0.44
1:A:1456:MET:HG3	1:A:2036:PHE:CD1	2.53	0.44
1:A:1651:VAL:HG13	1:A:1679:GLY:C	2.38	0.44
1:A:896:TRP:CD2	1:A:907:LEU:HD11	2.53	0.44
1:B:1941:VAL:HG12	1:B:1941:VAL:O	2.16	0.44
1:B:1449:SER:HB3	1:B:2047:LYS:NZ	2.33	0.44
1:B:336:SER:OG	1:B:337:GLY:N	2.51	0.43
1:B:642:CYS:HA	1:B:743:VAL:HG23	2.00	0.43
1:B:643:HIS:CD2	1:B:746:GLN:CB	3.02	0.43
1:A:399:ASN:H	1:A:399:ASN:ND2	2.16	0.43
1:B:1477:LEU:HD12	1:B:1507:ARG:HH21	1.82	0.43
1:B:276:LEU:HD12	1:B:401:HIS:HB3	2.00	0.43
1:B:506:MET:HE2	1:B:506:MET:HB3	1.89	0.43
1:A:1774:LEU:HD22	1:B:1785:PHE:HB2	1.99	0.43
1:A:1243:LYS:HA	1:A:1271:ASP:HB2	2.00	0.43
1:A:584:GLU:O	1:A:587:CYS:HB2	2.18	0.43
1:B:157:ILE:HD11	1:B:167:ALA:CA	2.46	0.43
1:A:287:LEU:HD13	1:A:312:LEU:HD13	2.00	0.43
1:A:1418:VAL:HG21	1:A:1443:LEU:HD13	2.00	0.43
1:A:1616:MET:HB3	1:A:1800:PHE:HE2	1.83	0.43
1:B:883:ARG:HG3	1:B:1107:ARG:CZ	2.48	0.43
1:B:982:THR:HG23	1:B:983:ALA:N	2.28	0.43
1:A:159:THR:HG22	1:A:398:SER:HB3	2.00	0.43
1:A:1231:ASP:O	1:A:1232:THR:C	2.56	0.43
1:A:1442:TRP:CB	1:A:1444:MET:HE1	2.48	0.43
1:B:801:GLY:O	1:B:804:HIS:HB3	2.17	0.43
1:A:389:GLY:O	1:A:390:ILE:HG13	2.18	0.43
1:B:837:ASP:OD1	1:B:839:SER:HB3	2.18	0.43
1:A:784:LEU:HD23	1:A:784:LEU:HA	1.73	0.43
1:A:316:ARG:O	1:A:317:ARG:O	2.35	0.43
1:B:277:TYR:O	1:B:278:ALA:C	2.56	0.43
1:A:1657:TYR:CZ	1:A:1662:ARG:CD	3.00	0.43
1:A:1810:VAL:HG12	1:A:1810:VAL:O	2.18	0.43
1:B:680:ILE:HG12	1:B:681:ALA:H	1.76	0.43
1:B:739:LEU:HD23	1:B:739:LEU:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1418:VAL:HG13	1:A:1425:TRP:CZ2	2.52	0.43
1:A:1460:LEU:HD11	1:A:1980:LEU:CD1	2.42	0.43
1:A:2066:VAL:HG22	1:A:2088:ILE:CD1	2.48	0.43
1:B:1598:MET:O	1:B:1599:LEU:HD23	2.18	0.43
1:A:128:VAL:HG12	1:A:129:GLY:H	1.83	0.43
1:B:1671:VAL:HG23	1:B:1743:LEU:HD13	2.00	0.43
1:A:1038:MET:HE3	1:A:1041:LEU:HD23	1.99	0.43
1:B:1666:GLN:O	1:B:1669:GLU:HB2	2.18	0.43
1:A:411:ALA:HA	1:A:412:PRO:HD3	1.83	0.43
1:A:613:ALA:O	1:A:615:VAL:N	2.51	0.43
1:A:2023:SER:O	1:A:2027:GLY:HA2	2.17	0.43
1:B:5:VAL:HG12	1:B:245:THR:HA	2.00	0.43
1:B:761:ILE:HG22	1:B:761:ILE:O	2.18	0.43
1:A:1389:LEU:HA	1:A:1389:LEU:HD23	1.76	0.43
1:A:333:GLU:O	1:A:336:SER:HB3	2.18	0.43
1:A:399:ASN:H	1:A:399:ASN:HD22	1.65	0.43
1:B:1443:LEU:O	1:B:1473:LEU:HA	2.19	0.43
1:A:1614:MET:HG3	1:A:1649:PRO:HG3	1.99	0.43
1:A:1662:ARG:HH12	1:B:1790:THR:HG21	1.84	0.43
1:A:19:LEU:HA	1:A:19:LEU:HD23	1.76	0.43
1:B:1133:ASN:HB2	1:B:1136:LEU:HB2	2.00	0.43
1:B:289:TYR:HE2	1:B:291:GLU:HA	1.83	0.43
1:A:272:LEU:O	1:A:276:LEU:HG	2.18	0.43
1:B:2058:VAL:HG22	1:B:2098:PHE:HD2	1.83	0.43
1:B:264:PRO:HG2	1:B:300:GLY:HA2	1.99	0.43
1:A:1769:ILE:HG23	2:A:3001:NAP:H2N	2.01	0.43
1:B:762:ALA:HB1	1:B:763:PRO:HD2	1.99	0.43
1:B:1845:GLN:HB2	1:B:1847:LYS:HG3	2.00	0.43
1:A:1069:TYR:CD1	1:A:1077:ALA:O	2.71	0.43
1:B:998:LEU:HD23	1:B:998:LEU:HA	1.87	0.43
1:B:1183:LEU:CD1	1:B:1210:LEU:HB3	2.44	0.43
1:A:1216:LEU:HD11	1:A:1218:SER:HB3	2.00	0.43
1:B:1405:ARG:HH22	1:B:1470:ARG:HH22	1.66	0.43
1:A:1252:GLY:HA3	1:A:1318:ASN:CB	2.43	0.43
1:A:1413:PRO:HA	1:A:1440:PRO:HB2	1.99	0.43
1:A:1472:VAL:CG1	1:A:1473:LEU:N	2.82	0.43
1:A:1236:ASN:ND2	1:A:1502:VAL:H	2.16	0.43
1:B:1413:PRO:HA	1:B:1440:PRO:O	2.17	0.43
1:A:854:SER:OG	1:A:855:SER:N	2.52	0.43
1:B:615:VAL:CG2	1:B:686:PHE:HD2	2.27	0.43
1:B:1538:ARG:NH2	1:B:1585:PRO:CG	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:LEU:HA	1:B:594:LEU:HD23	1.70	0.43
1:A:1651:VAL:HG12	1:A:1683:ALA:CB	2.48	0.43
1:A:1568:TYR:HB2	1:A:1604:SER:OG	2.18	0.43
1:A:899:LEU:O	1:A:899:LEU:HD12	2.18	0.43
1:B:65:PHE:CE2	1:B:83:LEU:HB3	2.54	0.43
1:A:1001:TYR:CD2	1:A:1003:TYR:CE1	3.06	0.43
1:A:1841:ARG:O	1:A:1845:GLN:HG3	2.19	0.43
1:B:782:ILE:HG22	1:B:783:PRO:O	2.19	0.43
1:B:765:ALA:HB2	1:B:783:PRO:HB3	2.00	0.43
1:B:768:GLN:CD	1:B:783:PRO:HG3	2.39	0.43
1:A:1818:ILE:HG12	1:A:1823:VAL:HG11	2.01	0.43
1:B:1896:PHE:HB2	2:B:3002:NAP:O2N	2.19	0.43
1:B:1424:ARG:C	1:B:1426:VAL:H	2.21	0.43
1:B:455:ASN:HB2	1:B:813:ASN:ND2	2.34	0.43
1:A:1559:CYS:O	1:A:1562:ARG:HB2	2.18	0.43
1:B:409:ARG:HA	1:B:410:PRO:HD3	1.67	0.43
1:A:1184:LEU:HD23	1:A:1184:LEU:HA	1.81	0.43
1:A:1552:HIS:CG	1:A:1552:HIS:O	2.71	0.43
1:B:532:LEU:HD22	1:B:604:TYR:HE1	1.84	0.43
1:A:981:SER:HA	1:A:986:ARG:NH2	2.34	0.43
1:A:504:GLN:N	1:A:546:LEU:HD11	2.34	0.43
1:A:1036:LEU:HD13	1:A:1051:PRO:HG3	2.00	0.43
1:B:1554:ALA:HB2	1:B:1882:PRO:CG	2.46	0.43
1:B:159:THR:CG2	1:B:398:SER:CB	2.94	0.43
1:B:103:THR:HG22	1:B:104:SER:N	2.33	0.43
1:A:2058:VAL:HG22	1:A:2098:PHE:HD2	1.83	0.43
1:B:1617:VAL:HG13	1:B:1618:PRO:HD2	2.01	0.43
1:A:594:LEU:HA	1:A:594:LEU:HD23	1.69	0.43
1:B:321:LEU:HD23	1:B:381:LEU:CD1	2.49	0.43
1:B:988:SER:O	1:B:991:ASP:N	2.52	0.43
1:A:67:VAL:O	1:A:67:VAL:HG23	2.19	0.43
1:B:1562:ARG:HB3	1:B:1627:LEU:HD13	1.99	0.43
1:B:844:VAL:O	1:B:846:SER:N	2.52	0.43
1:B:494:PHE:CD1	1:B:574:PRO:HB3	2.53	0.43
1:A:1796:LEU:HA	1:A:1796:LEU:HD12	1.88	0.43
1:B:508:LEU:HD23	1:B:508:LEU:HA	1.85	0.43
1:A:703:LEU:HG	1:A:703:LEU:O	2.19	0.43
1:B:1973:MET:HG3	1:B:1973:MET:O	2.19	0.43
1:A:1119:PHE:HD1	1:A:1516:HIS:CD2	2.36	0.43
1:B:2075:THR:CG2	1:B:2076:ASN:N	2.82	0.43
1:B:1231:ASP:O	1:B:1234:LEU:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1893:LEU:HB3	1:B:1925:GLN:HE21	1.79	0.43
1:B:608:TYR:O	1:B:611:LYS:N	2.51	0.43
1:A:1312:ALA:O	1:A:1339:LYS:HB2	2.19	0.43
1:A:494:PHE:CZ	1:A:574:PRO:HG3	2.54	0.43
1:A:1068:LEU:CD1	1:A:1078:ALA:HB2	2.49	0.43
1:B:1480:THR:HG22	1:B:1481:SER:H	1.83	0.43
1:B:915:GLU:O	1:B:916:ASP:HB2	2.18	0.43
1:A:1015:LEU:HD23	1:A:1015:LEU:HA	1.76	0.43
1:A:1014:ASP:OD1	1:A:1015:LEU:N	2.51	0.43
1:A:1956:ILE:HA	1:A:1956:ILE:HD12	1.84	0.43
1:B:2043:ARG:NH1	1:B:2046:GLU:OE1	2.51	0.43
1:A:1653:THR:HG21	1:A:1807:TRP:CH2	2.53	0.43
1:B:1544:ILE:HD12	1:B:1837:GLU:HA	2.00	0.43
1:B:1857:ARG:NE	1:B:1871:ILE:HD11	2.34	0.43
1:B:193:LYS:HG3	1:B:193:LYS:O	2.19	0.43
1:B:193:LYS:HA	1:B:194:PRO:HD3	1.87	0.43
1:B:1501:LEU:H	1:B:1501:LEU:HG	1.52	0.43
1:A:876:VAL:HG12	1:A:876:VAL:O	2.19	0.43
1:A:90:ILE:HG12	1:A:232:LEU:HD22	2.00	0.43
1:B:521:LEU:O	1:B:524:ASP:HB2	2.19	0.43
1:A:202:LYS:HB2	1:B:129:GLY:HA3	2.01	0.43
1:B:1231:ASP:O	1:B:1232:THR:C	2.58	0.43
1:A:254:ASP:HB3	1:A:257:LYS:HE2	2.00	0.43
1:A:2086:GLN:NE2	1:A:2108:SER:OG	2.49	0.43
1:B:1288:LYS:O	1:B:1291:GLN:HG2	2.19	0.43
1:B:1119:PHE:CZ	1:B:1514:PHE:HB3	2.53	0.42
1:B:2105:VAL:O	1:B:2106:LEU:HD23	2.19	0.42
1:A:624:GLY:HA3	1:A:671:PHE:HB3	2.01	0.42
1:A:1405:ARG:HH22	1:A:1470:ARG:NH2	2.16	0.42
1:A:1996:TYR:CD2	1:A:1996:TYR:C	2.92	0.42
1:A:1974:VAL:O	1:A:1991:VAL:HG22	2.19	0.42
1:A:808:VAL:CG1	1:A:809:SER:N	2.77	0.42
1:A:1894:GLY:O	1:A:1897:GLY:N	2.53	0.42
1:A:434:VAL:O	1:A:438:LEU:HG	2.19	0.42
1:B:36:ASP:CB	1:B:38:ARG:HG3	2.49	0.42
1:B:1068:LEU:CD1	1:B:1078:ALA:HB2	2.49	0.42
1:B:1459:CYS:CB	1:B:2032:ALA:HA	2.49	0.42
1:A:652:SER:OG	1:A:681:ALA:HB1	2.19	0.42
1:B:1220:LEU:HD21	1:B:1318:ASN:HD21	1.83	0.42
1:B:1453:VAL:O	1:B:1456:MET:N	2.53	0.42
1:A:578:ILE:HG22	1:A:745:PHE:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:GLN:HE22	1:B:138:ALA:N	2.09	0.42
1:A:1733:LEU:HD23	1:A:1733:LEU:HA	1.77	0.42
1:B:363:ASN:HA	1:B:364:PRO:HD3	1.80	0.42
1:B:1975:LEU:HD21	1:B:2034:TYR:CD1	2.54	0.42
1:B:1944:SER:HB2	1:B:1958:GLU:OE2	2.19	0.42
1:B:423:LEU:HD23	1:B:812:PRO:HG3	2.00	0.42
1:A:36:ASP:HB3	1:A:38:ARG:CG	2.49	0.42
1:A:1735:HIS:HD2	1:A:1735:HIS:H	1.64	0.42
1:B:900:ALA:HB1	1:B:905:GLN:O	2.19	0.42
1:B:22:PHE:CE2	1:B:26:LEU:HD11	2.54	0.42
1:A:1932:TRP:O	1:A:1937:VAL:HB	2.18	0.42
1:A:1073:ASP:O	1:A:1074:THR:CG2	2.62	0.42
1:A:1424:ARG:C	1:A:1426:VAL:H	2.22	0.42
1:A:1466:GLY:HA2	1:A:1469:ILE:HG13	2.01	0.42
1:B:972:THR:CG2	1:B:1081:VAL:HG21	2.49	0.42
1:B:970:PHE:O	1:B:1067:LYS:HE2	2.19	0.42
1:A:1435:ASP:CG	1:A:1438:SER:HB3	2.40	0.42
1:A:265:SER:O	1:A:269:GLN:HG3	2.20	0.42
1:A:1729:GLU:OE1	1:A:1758:ARG:HD2	2.19	0.42
1:B:1918:SER:HB3	1:B:1921:ARG:HD3	2.01	0.42
1:A:1221:LEU:O	1:A:1221:LEU:HG	2.20	0.42
1:A:1603:PHE:CD2	1:A:1603:PHE:N	2.87	0.42
1:A:532:LEU:HD22	1:A:604:TYR:CE1	2.55	0.42
1:B:82:LEU:HA	1:B:85:VAL:HG22	2.02	0.42
1:B:1733:LEU:O	1:B:1736:THR:HG22	2.19	0.42
1:B:2066:VAL:HG22	1:B:2088:ILE:CD1	2.50	0.42
1:A:1791:PHE:CD2	1:A:1791:PHE:C	2.92	0.42
1:B:213:ARG:HD3	1:B:218:GLU:O	2.19	0.42
1:A:351:GLY:C	1:A:383:ILE:HG22	2.40	0.42
1:A:234:THR:HG22	1:A:235:LYS:N	2.35	0.42
1:B:67:VAL:O	1:B:68:HIS:C	2.57	0.42
1:A:1697:THR:CG2	1:A:1698:THR:N	2.81	0.42
1:B:89:ALA:O	1:B:92:ASP:HB3	2.19	0.42
1:A:1565:SER:O	1:A:1605:GLY:HA3	2.19	0.42
1:A:76:ASP:CG	1:A:116:ALA:HB3	2.40	0.42
1:A:65:PHE:CE2	1:A:83:LEU:HB3	2.54	0.42
1:A:143:ARG:NH1	1:A:143:ARG:CG	2.83	0.42
1:B:2053:LEU:HA	1:B:2053:LEU:HD23	1.72	0.42
1:B:1378:TRP:O	1:B:1382:PHE:CD1	2.73	0.42
1:A:98:ALA:CA	1:A:101:ARG:HG3	2.48	0.42
1:B:276:LEU:CD1	1:B:401:HIS:HB3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:851:PRO:HB2	1:B:122:ARG:HA	2.01	0.42
1:B:525:GLN:CA	1:B:525:GLN:NE2	2.82	0.42
1:B:1555:LEU:HD12	1:B:1559:CYS:SG	2.59	0.42
1:B:1253:GLN:HB3	1:B:1255:TYR:CE2	2.53	0.42
1:A:1617:VAL:O	1:A:1617:VAL:HG12	2.19	0.42
1:B:1533:VAL:N	1:B:1546:TRP:CZ3	2.88	0.42
1:A:739:LEU:HA	1:A:739:LEU:HD23	1.76	0.42
1:A:1246:GLU:HG3	1:A:1316:VAL:HB	2.00	0.42
1:A:1976:ARG:HB2	1:A:2033:ASN:HD21	1.85	0.42
1:A:47:LEU:HD21	1:A:198:LEU:HA	2.01	0.42
1:B:550:VAL:CG2	1:B:611:LYS:HD3	2.48	0.42
1:B:1312:ALA:HB3	1:B:1337:THR:O	2.20	0.42
1:B:1860:GLU:HB2	1:B:1865:PRO:HG2	2.01	0.42
1:B:540:SER:OG	1:B:545:VAL:HG21	2.20	0.42
1:A:2105:VAL:O	1:A:2106:LEU:HD23	2.18	0.42
1:B:1009:LEU:HD22	1:B:1023:GLN:O	2.20	0.42
1:A:623:VAL:HA	1:A:671:PHE:O	2.19	0.42
1:A:945:GLU:OE2	1:B:941:SER:CB	2.67	0.42
1:A:275:SER:CB	1:A:276:LEU:HD23	2.49	0.42
1:B:128:VAL:O	1:B:131:SER:OG	2.34	0.42
1:B:876:VAL:HA	1:B:884:VAL:HG11	2.01	0.42
1:A:494:PHE:CE2	1:A:574:PRO:HG3	2.54	0.42
1:B:1685:ILE:O	1:B:1686:ALA:C	2.58	0.42
1:A:1584:SER:C	1:A:1586:ASP:H	2.23	0.42
1:B:454:LEU:HA	1:B:454:LEU:HD23	1.80	0.42
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.74	0.42
1:A:1184:LEU:H	1:A:1216:LEU:CD2	2.33	0.42
1:B:1429:LEU:HD21	1:B:1443:LEU:HD21	2.00	0.42
1:B:1473:LEU:HD11	1:B:1503:MET:SD	2.60	0.42
1:A:290:ILE:HG23	1:A:290:ILE:O	2.18	0.42
1:A:1222:ASP:HA	1:A:1226:LEU:CD1	2.49	0.42
1:B:1073:ASP:O	1:B:1074:THR:CG2	2.61	0.42
1:B:185:VAL:O	1:B:230:ALA:HA	2.19	0.42
1:B:1565:SER:HB2	1:B:1857:ARG:CZ	2.50	0.42
1:A:276:LEU:HD12	1:A:401:HIS:HB3	2.02	0.42
1:B:1671:VAL:HG23	1:B:1743:LEU:CD1	2.49	0.42
1:B:1540:ASP:C	1:B:1542:SER:H	2.21	0.42
1:B:1496:VAL:HG21	1:B:1511:TRP:CH2	2.55	0.42
1:B:412:PRO:HA	1:B:413:PRO:HD3	1.89	0.42
1:B:892:LEU:HD22	1:B:1057:ILE:HD12	2.00	0.42
1:A:542:ASP:OD1	1:A:542:ASP:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASN:HB2	1:A:334:PRO:HD2	2.02	0.42
1:A:1476:ASN:CA	1:A:1486:MET:SD	3.07	0.42
1:A:1477:LEU:HD12	1:A:1507:ARG:HH21	1.83	0.42
1:A:2104:PRO:HD2	1:A:2105:VAL:H	1.84	0.42
1:B:1454:VAL:HG13	1:B:1503:MET:HE3	2.02	0.42
1:B:47:LEU:HD21	1:B:198:LEU:HA	2.01	0.42
1:B:23:TRP:NE1	1:B:350:HIS:CD2	2.87	0.42
1:A:1739:LYS:O	1:A:1761:ALA:HB2	2.19	0.42
1:A:299:VAL:O	1:A:302:PRO:HD2	2.19	0.42
1:B:491:PRO:HG2	1:B:753:PRO:HG2	2.02	0.42
1:A:761:ILE:O	1:A:761:ILE:HG22	2.19	0.42
1:B:1243:LYS:HD3	1:B:1311:LYS:HB3	2.01	0.42
1:B:1312:ALA:O	1:B:1339:LYS:HB2	2.20	0.42
1:A:506:MET:CE	1:A:559:ILE:HD12	2.49	0.42
1:A:506:MET:HB3	1:A:559:ILE:CD1	2.49	0.42
1:A:1228:ALA:HB2	1:A:1517:PHE:CE2	2.55	0.42
1:A:1522:ASP:O	1:A:1524:PRO:HD3	2.20	0.42
1:A:677:THR:HG22	1:A:682:PHE:CE2	2.55	0.42
1:A:1697:THR:HG23	1:A:1698:THR:N	2.34	0.42
1:B:1238:ALA:HB2	1:B:1468:ARG:HD3	2.02	0.42
1:B:1147:ALA:C	1:B:1149:ALA:H	2.23	0.42
1:B:638:ILE:HD11	1:B:657:ALA:O	2.20	0.42
1:B:470:TYR:C	1:B:470:TYR:CD1	2.92	0.42
1:A:1124:HIS:NE2	1:A:1512:GLY:HA2	2.35	0.42
1:A:1121:PHE:HE1	1:A:1512:GLY:O	2.03	0.42
1:A:1316:VAL:HA	1:A:1345:LEU:O	2.20	0.42
1:B:1556:PRO:C	1:B:1558:SER:H	2.23	0.42
1:B:550:VAL:CG2	1:B:608:TYR:HA	2.50	0.42
1:B:1538:ARG:NH1	1:B:1585:PRO:HG2	2.35	0.42
1:A:1897:GLY:HA2	1:A:1971:LEU:HD12	2.02	0.42
1:B:1578:LEU:C	1:B:1580:THR:N	2.73	0.42
1:B:327:SER:OG	1:B:356:ASN:ND2	2.53	0.42
1:B:1390:VAL:HG22	1:B:1501:LEU:HD21	2.02	0.42
1:B:1015:LEU:HD23	1:B:1015:LEU:HA	1.74	0.42
1:B:84:GLU:O	1:B:88:GLU:HG3	2.20	0.42
1:B:1244:VAL:HB	1:B:1272:TYR:HD1	1.84	0.42
1:B:759:VAL:HG23	1:B:759:VAL:O	2.20	0.42
1:A:1504:ASN:HB3	1:A:1511:TRP:CZ3	2.54	0.41
1:B:1442:TRP:HB3	1:B:1444:MET:CE	2.50	0.41
1:B:47:LEU:HA	1:B:48:PRO:HD3	1.85	0.41
1:A:1302:ALA:O	1:A:1303:ASN:CB	2.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1251:ASP:HB3	1:B:1321:LEU:HD22	2.01	0.41
1:B:362:PRO:HB3	1:B:369:LEU:HB3	2.02	0.41
1:B:1799:LEU:O	1:B:1801:GLU:N	2.54	0.41
1:A:1859:GLU:CG	1:A:1860:GLU:H	2.33	0.41
1:B:1115:ILE:HD11	1:B:2111:LEU:CD1	2.49	0.41
1:A:1469:ILE:CG2	1:A:1469:ILE:O	2.68	0.41
1:B:1563:LEU:HA	1:B:1563:LEU:HD12	1.88	0.41
1:B:1068:LEU:HD13	1:B:1078:ALA:HB2	2.01	0.41
1:B:355:PRO:CG	1:B:380:PRO:HG3	2.50	0.41
1:A:2031:GLN:HB3	1:A:2034:TYR:HB3	2.01	0.41
1:B:1350:LEU:HD23	1:B:1350:LEU:N	2.34	0.41
1:B:1922:THR:H	1:B:1922:THR:HG1	1.64	0.41
1:A:120:LEU:HA	1:A:127:LEU:HD13	2.02	0.41
1:A:2043:ARG:NH1	1:A:2046:GLU:OE1	2.53	0.41
1:A:264:PRO:HG2	1:A:300:GLY:HA2	2.03	0.41
1:A:274:ARG:O	1:A:276:LEU:N	2.53	0.41
1:A:1235:GLU:OE2	1:A:1515:ARG:CZ	2.68	0.41
1:A:1419:GLU:OE2	1:A:1447:GLY:HA3	2.20	0.41
1:B:283:ASP:C	1:B:285:GLU:H	2.22	0.41
1:A:67:VAL:O	1:A:68:HIS:C	2.58	0.41
1:B:1746:ASN:HD21	1:B:1753:LEU:HD12	1.85	0.41
1:B:94:GLY:HA3	1:B:453:MET:HG2	2.01	0.41
1:A:1949:LEU:HD21	1:A:1953:ARG:NH2	2.35	0.41
1:B:819:VAL:O	1:B:821:PHE:N	2.53	0.41
1:B:1394:ARG:HA	1:B:1400:VAL:HG22	2.02	0.41
1:B:1477:LEU:CD1	1:B:1507:ARG:HH21	2.33	0.41
1:A:765:ALA:HB2	1:A:783:PRO:HB3	2.02	0.41
1:A:1252:GLY:N	1:A:1321:LEU:HD21	2.35	0.41
1:B:350:HIS:O	1:B:352:VAL:HG12	2.21	0.41
1:A:1616:MET:HE2	1:A:1650:ILE:HD13	2.01	0.41
1:A:91:VAL:O	1:A:457:ILE:HD11	2.20	0.41
1:B:98:ALA:CA	1:B:101:ARG:HG3	2.47	0.41
1:A:1578:LEU:C	1:A:1580:THR:N	2.74	0.41
1:A:89:ALA:O	1:A:92:ASP:HB3	2.21	0.41
1:B:2058:VAL:HG11	1:B:2060:TRP:CE2	2.54	0.41
1:A:1644:GLU:HB3	1:A:1825:PRO:CG	2.50	0.41
1:B:366:ILE:CG1	1:B:366:ILE:O	2.68	0.41
1:A:915:GLU:O	1:A:916:ASP:HB2	2.20	0.41
1:A:874:TYR:CD1	1:A:1006:PHE:CE2	3.08	0.41
1:B:147:PHE:C	1:B:147:PHE:CD2	2.94	0.41
1:B:1220:LEU:CD2	1:B:1318:ASN:HD21	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1530:HIS:CB	1:A:1549:SER:HB3	2.51	0.41
1:A:377:VAL:HG13	1:A:381:LEU:CD1	2.50	0.41
1:B:1305:ALA:HA	1:B:1306:PRO:HD2	1.83	0.41
1:A:495:ILE:HG12	1:A:758:VAL:HG13	2.01	0.41
1:A:1432:ILE:HG22	1:A:1432:ILE:O	2.21	0.41
1:A:14:PRO:HB2	1:A:32:MET:HB2	2.03	0.41
1:A:33:VAL:HG13	1:A:51:MET:C	2.39	0.41
1:B:1433:LEU:HD11	1:B:1465:GLY:O	2.20	0.41
1:B:40:TRP:CH2	1:B:51:MET:HE3	2.56	0.41
1:A:256:SER:HB3	1:B:146:PHE:O	2.19	0.41
1:A:313:CYS:HA	1:A:315:THR:HG22	2.03	0.41
1:B:83:LEU:HD23	1:B:83:LEU:HA	1.89	0.41
1:A:1068:LEU:HD13	1:A:1078:ALA:HB2	2.01	0.41
1:A:1435:ASP:OD2	1:A:1438:SER:HB3	2.20	0.41
1:B:595:THR:OG1	1:B:598:GLU:HG3	2.20	0.41
1:B:1448:CYS:C	1:B:1450:THR:H	2.24	0.41
1:A:1678:GLY:O	1:A:1682:GLN:HG3	2.20	0.41
1:B:1473:LEU:HG	1:B:1503:MET:HA	2.02	0.41
1:B:188:LEU:CD2	1:B:228:VAL:HG12	2.49	0.41
1:B:9:MET:HE1	1:B:345:LEU:HB2	2.01	0.41
1:A:1147:ALA:HB1	1:A:1358:MET:HE1	2.02	0.41
1:B:1698:THR:HB	1:B:1723:SER:HB3	2.01	0.41
1:B:2018:ILE:HG21	1:B:2041:MET:HB3	2.03	0.41
1:B:988:SER:H	1:B:991:ASP:HB2	1.85	0.41
1:B:1506:TYR:OH	1:B:1509:GLY:HA2	2.21	0.41
1:B:290:ILE:O	1:B:290:ILE:HG23	2.21	0.41
1:A:782:ILE:CD1	1:A:803:LEU:HD23	2.41	0.41
1:B:1146:LEU:HD22	1:B:1192:LEU:HD12	2.02	0.41
1:B:581:SER:HA	1:B:738:ASN:HD21	1.85	0.41
1:B:1818:ILE:HG12	1:B:1823:VAL:CG1	2.51	0.41
1:A:644:ASN:HB3	1:A:770:VAL:CG1	2.51	0.41
1:B:41:LYS:HD2	1:B:44:LEU:HD22	2.02	0.41
1:A:1442:TRP:HB3	1:A:1444:MET:CE	2.51	0.41
1:A:564:ILE:HG12	1:A:761:ILE:HD13	2.03	0.41
1:A:1680:VAL:CG1	1:A:1681:GLY:N	2.84	0.41
1:B:475:GLY:O	1:B:477:ALA:N	2.51	0.41
1:B:1984:THR:C	1:B:1986:GLU:H	2.22	0.41
1:A:719:GLU:HA	1:A:722:TRP:NE1	2.36	0.41
1:B:719:GLU:HA	1:B:722:TRP:NE1	2.35	0.41
1:B:1932:TRP:O	1:B:1937:VAL:HB	2.21	0.41
1:A:355:PRO:CG	1:A:380:PRO:HG3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.76	0.41
1:A:502:GLN:OE1	1:A:676:ARG:HD3	2.21	0.41
1:B:48:PRO:HD3	1:B:201:MET:HE3	2.02	0.41
1:B:132:MET:HE3	1:B:132:MET:HB3	1.65	0.41
1:B:291:GLU:OE2	1:B:325:THR:N	2.53	0.41
1:B:14:PRO:HB2	1:B:32:MET:HB2	2.02	0.41
1:B:1554:ALA:HB3	1:B:1882:PRO:HB3	2.02	0.41
1:B:2022:VAL:HG13	1:B:2026:ARG:HG2	2.03	0.41
1:A:1422:SER:O	1:A:1423:PHE:CB	2.68	0.41
1:A:36:ASP:C	1:A:38:ARG:H	2.24	0.41
1:A:128:VAL:O	1:A:131:SER:OG	2.39	0.41
1:A:831:SER:N	1:A:832:PRO:HD3	2.35	0.41
1:A:40:TRP:CE3	1:A:194:PRO:HG3	2.56	0.41
1:A:719:GLU:HA	1:A:722:TRP:CE2	2.55	0.41
1:B:827:THR:HA	1:B:828:PRO:HD3	1.96	0.41
1:A:1898:LEU:HA	1:A:1898:LEU:HD23	1.72	0.41
1:A:165:LEU:HD23	1:A:400:VAL:CG2	2.30	0.41
1:A:1124:HIS:CD2	1:A:1511:TRP:O	2.73	0.41
1:A:997:ARG:HE	1:A:2070:LEU:CD1	2.34	0.41
1:A:305:LEU:CD2	1:A:308:ILE:HD12	2.51	0.41
1:A:1614:MET:HG2	1:A:1614:MET:O	2.19	0.41
1:A:976:VAL:CG2	1:A:977:ASP:H	2.23	0.41
1:B:197:SER:OG	1:B:224:ARG:HD3	2.21	0.41
1:A:132:MET:CE	1:B:200:PHE:CE2	2.96	0.41
1:B:1541:LEU:CD1	1:B:1840:PHE:HB3	2.44	0.41
1:B:1214:ASP:HB3	1:B:1215:PRO:CD	2.47	0.41
1:A:96:ASN:ND2	1:A:98:ALA:HB3	2.36	0.41
1:A:1762:GLN:HB3	1:A:1763:HIS:CD2	2.55	0.41
1:B:169:GLN:HG3	1:B:249:ALA:HB1	2.02	0.41
1:A:1004:GLY:O	1:A:1008:GLN:HG3	2.20	0.41
1:B:533:ARG:HB2	1:B:533:ARG:NH1	2.35	0.41
1:B:1127:SER:HA	1:B:1394:ARG:HB3	2.02	0.41
1:A:63:SER:O	1:A:66:GLY:N	2.49	0.41
1:A:618:GLY:N	1:A:679:GLY:O	2.50	0.41
1:B:399:ASN:HD22	1:B:399:ASN:H	1.69	0.41
1:A:1214:ASP:C	1:A:1216:LEU:N	2.74	0.41
1:A:1001:TYR:HD2	1:A:1003:TYR:CE1	2.39	0.41
1:B:1569:THR:HG23	1:B:1602:GLU:O	2.20	0.41
1:A:1893:LEU:CB	1:A:1925:GLN:NE2	2.75	0.41
1:B:305:LEU:HA	1:B:305:LEU:HD23	1.79	0.41
1:B:610:ILE:HA	1:B:690:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1321:LEU:HA	1:A:1321:LEU:HD12	1.90	0.41
1:B:132:MET:HG2	1:B:136:GLN:HB2	2.02	0.41
1:A:1569:THR:CG2	1:A:1622:LEU:HD23	2.51	0.41
1:A:81:MET:HG2	1:A:81:MET:H	1.72	0.41
1:B:25:ASN:CB	1:B:32:MET:SD	3.09	0.41
1:B:1214:ASP:CG	1:B:1321:LEU:HD21	2.40	0.41
1:B:59:ARG:HE	1:B:841:ALA:HB2	1.86	0.41
1:A:1307:GLY:C	1:A:1309:LEU:H	2.24	0.41
1:B:1999:THR:HG23	1:B:2018:ILE:HD11	2.02	0.41
1:B:40:TRP:HB2	1:B:41:LYS:H	1.66	0.41
1:A:1654:THR:HG21	2:A:3001:NAP:C4N	2.51	0.41
1:B:1695:VAL:HG12	1:B:1696:PHE:N	2.36	0.41
1:B:1540:ASP:C	1:B:1542:SER:N	2.73	0.41
1:B:214:SER:HB3	1:B:327:SER:HB3	2.03	0.41
1:A:409:ARG:HA	1:A:410:PRO:HD3	1.68	0.41
1:A:1535:VAL:CG1	1:A:1537:SER:H	2.34	0.41
1:A:193:LYS:HG3	1:A:193:LYS:O	2.21	0.41
1:A:193:LYS:HA	1:A:194:PRO:HD3	1.88	0.41
1:A:412:PRO:HA	1:A:413:PRO:HD3	1.89	0.41
1:A:1022:LEU:O	1:A:1077:ALA:HB1	2.20	0.41
1:B:898:THR:HG22	1:B:937:LEU:HD22	2.02	0.41
1:A:1921:ARG:HB2	1:A:1921:ARG:HE	1.47	0.41
1:A:511:MET:HB2	1:A:511:MET:HE2	1.81	0.41
1:A:1765:ARG:CD	1:A:1765:ARG:N	2.84	0.41
1:A:1216:LEU:HG	1:A:1219:GLY:H	1.86	0.41
1:B:2043:ARG:HA	1:B:2043:ARG:HD3	1.61	0.41
1:B:1651:VAL:HG12	1:B:1683:ALA:CB	2.51	0.41
1:B:12:LYS:HD2	1:B:81:MET:HE2	2.03	0.41
1:A:200:PHE:CE2	1:B:132:MET:CE	2.98	0.41
1:A:545:VAL:HG22	1:A:551:SER:HB3	2.02	0.41
1:A:92:ASP:O	1:A:241:ARG:NH1	2.52	0.41
1:B:59:ARG:HH21	1:B:841:ALA:HB2	1.86	0.41
1:B:1999:THR:OG1	1:B:2041:MET:HG2	2.20	0.41
1:B:128:VAL:HG12	1:B:130:TYR:CE2	2.56	0.41
1:A:1338:LEU:HD22	1:A:1406:GLN:HG3	2.03	0.41
1:B:287:LEU:HD13	1:B:312:LEU:HD13	2.02	0.41
1:B:2086:GLN:NE2	1:B:2108:SER:OG	2.50	0.41
1:B:737:ASN:O	1:B:737:ASN:ND2	2.52	0.41
1:B:494:PHE:CZ	1:B:574:PRO:HG3	2.56	0.41
1:B:1868:LEU:HA	1:B:1869:PRO:HD3	1.76	0.41
1:A:119:ALA:HB2	1:A:850:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1496:VAL:HG21	1:A:1511:TRP:CZ3	2.57	0.40
1:B:1001:TYR:CD2	1:B:1003:TYR:CE1	3.08	0.40
1:A:2069:VAL:HG12	1:A:2070:LEU:HD23	2.03	0.40
1:B:1227:LYS:O	1:B:1231:ASP:HB2	2.21	0.40
1:A:534:VAL:HG13	1:A:554:VAL:HG12	2.04	0.40
1:A:1653:THR:CG2	1:A:1810:VAL:HG12	2.52	0.40
1:B:82:LEU:HD22	1:B:188:LEU:HD11	2.03	0.40
1:B:416:GLN:C	1:B:418:ALA:H	2.25	0.40
1:A:1734:ARG:C	1:A:1736:THR:N	2.75	0.40
1:A:1733:LEU:O	1:A:1736:THR:HG22	2.20	0.40
1:B:96:ASN:HD21	1:B:98:ALA:HB3	1.85	0.40
1:B:570:LEU:HD11	1:B:800:VAL:HG22	2.03	0.40
1:B:288:GLU:CD	1:B:385:GLY:H	2.24	0.40
1:A:429:ARG:HA	1:A:429:ARG:HD2	1.98	0.40
1:B:1698:THR:HA	1:B:1721:ALA:O	2.20	0.40
1:A:1999:THR:HG23	1:A:2018:ILE:HD11	2.03	0.40
1:B:236:LYS:C	1:B:238:LEU:H	2.24	0.40
1:A:898:THR:HG22	1:A:937:LEU:HD22	2.02	0.40
1:A:1371:HIS:O	1:A:1372:LEU:HD23	2.20	0.40
1:B:411:ALA:HA	1:B:412:PRO:HD3	1.85	0.40
1:B:2072:THR:HB	1:B:2073:MET:H	1.69	0.40
1:B:76:ASP:CG	1:B:116:ALA:HB3	2.41	0.40
1:B:1001:TYR:HD2	1:B:1003:TYR:CE1	2.39	0.40
1:B:1236:ASN:HD21	1:B:1502:VAL:H	1.69	0.40
1:B:1247:VAL:CG1	1:B:1301:PRO:HG3	2.45	0.40
1:B:317:ARG:O	1:B:319:PRO:HD3	2.21	0.40
1:B:1858:GLU:HG3	1:B:1859:GLU:N	2.37	0.40
1:B:1322:ALA:HB1	1:B:1371:HIS:HE1	1.83	0.40
1:A:1345:LEU:HD12	1:A:1345:LEU:HA	1.93	0.40
1:A:254:ASP:O	1:A:255:GLY:O	2.39	0.40
1:A:289:TYR:HH	1:A:323:GLY:HA3	1.84	0.40
1:A:473:LEU:N	1:A:473:LEU:HD23	2.36	0.40
1:B:623:VAL:CG1	1:B:624:GLY:N	2.84	0.40
1:B:1038:MET:HE3	1:B:1041:LEU:HD23	2.03	0.40
1:B:1153:LYS:CD	1:B:1195:ASN:HD22	2.35	0.40
1:A:368:ALA:HB1	1:A:374:LEU:HG	2.03	0.40
1:B:944:PHE:CD1	1:B:944:PHE:C	2.94	0.40
1:A:416:GLN:C	1:A:418:ALA:H	2.24	0.40
1:B:979:ALA:O	1:B:980:ASP:O	2.40	0.40
1:B:274:ARG:C	1:B:276:LEU:N	2.75	0.40
1:B:719:GLU:HA	1:B:722:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LEU:HD12	1:B:233:LEU:N	2.36	0.40
1:B:1443:LEU:C	1:B:1444:MET:HE3	2.41	0.40
1:A:368:ALA:CA	1:A:371:ASP:HB3	2.51	0.40
1:B:1343:PHE:CE2	1:B:1405:ARG:HD2	2.57	0.40
1:B:316:ARG:O	1:B:317:ARG:O	2.40	0.40
1:A:1472:VAL:CG1	1:A:1473:LEU:H	2.33	0.40
1:B:30:VAL:O	1:B:32:MET:HG2	2.21	0.40
1:A:1223:ALA:CB	1:A:1224:PRO:HD2	2.39	0.40
1:B:1185:ALA:O	1:B:1189:GLN:HG3	2.22	0.40
1:A:98:ALA:HA	1:A:101:ARG:CG	2.50	0.40
1:B:1818:ILE:HG12	1:B:1823:VAL:HG11	2.03	0.40
1:B:1894:GLY:O	1:B:1897:GLY:N	2.54	0.40
1:B:1279:PRO:HG3	1:B:1298:GLN:NE2	2.35	0.40
1:B:461:SER:HA	1:B:462:PRO:HD3	1.84	0.40
1:B:879:CYS:O	1:B:1002:ASP:HB2	2.21	0.40
1:A:165:LEU:HD22	1:A:392:SER:HB2	2.03	0.40
1:B:166:LEU:HB2	1:B:400:VAL:HG11	2.04	0.40
1:A:1486:MET:HE3	1:A:1506:TYR:CB	2.50	0.40
1:B:1453:VAL:O	1:B:1454:VAL:C	2.59	0.40
1:A:375:GLN:O	1:A:376:VAL:C	2.59	0.40
1:A:1657:TYR:CZ	1:A:1799:LEU:HD11	2.57	0.40
1:B:1612:ARG:CG	1:B:1642:LEU:HD21	2.51	0.40
1:B:47:LEU:HD22	1:B:197:SER:HB3	2.04	0.40
1:A:1976:ARG:HB2	1:A:2033:ASN:ND2	2.36	0.40
1:B:980:ASP:HB2	1:B:981:SER:H	1.44	0.40
1:B:1726:THR:CG2	1:B:1726:THR:O	2.69	0.40
1:B:159:THR:CG2	1:B:159:THR:O	2.65	0.40
2:A:3001:NAP:H52A	2:A:3001:NAP:H52N	2.03	0.40
1:B:1493:LEU:HD23	1:B:1494:GLN:HE21	1.87	0.40
1:B:1796:LEU:HA	1:B:1796:LEU:HD12	1.89	0.40
1:B:537:LEU:HA	1:B:537:LEU:HD23	1.74	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	2075/2512 (83%)	1683 (81%)	296 (14%)	96 (5%)	3	21
1	B	2080/2512 (83%)	1713 (82%)	276 (13%)	91 (4%)	3	22
All	All	4155/5024 (83%)	3396 (82%)	572 (14%)	187 (4%)	3	21

All (187) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	ALA
1	A	317	ARG
1	A	333	GLU
1	A	614	ASN
1	A	854	SER
1	A	976	VAL
1	A	985	PHE
1	A	1150	LEU
1	A	1224	PRO
1	A	1303	ASN
1	A	1436	ALA
1	A	1438	SER
1	A	1485	GLU
1	A	1611	ARG
1	A	1750	GLU
1	A	1802	GLU
1	A	1803	GLY
1	A	1895	GLY
1	A	2065	ASP
1	A	2073	MET
1	B	278	ALA
1	B	317	ARG
1	B	333	GLU
1	B	370	GLN
1	B	636	PRO
1	B	669	ASP
1	B	820	GLU
1	B	973	ARG
1	B	980	ASP
1	B	984	GLU
1	B	1224	PRO
1	B	1452	GLY
1	B	1521	GLN

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Mol	Chain	Res	Type
1	B	1596	ASP
1	B	1750	GLU
1	B	1800	PHE
1	B	1803	GLY
1	B	1864	ALA
1	B	1895	GLY
1	B	2065	ASP
1	A	163	SER
1	A	255	GLY
1	A	413	PRO
1	A	475	GLY
1	A	541	THR
1	A	615	VAL
1	A	853	GLY
1	A	1362	LEU
1	A	1425	TRP
1	A	1452	GLY
1	A	1557	ALA
1	A	1596	ASP
1	A	1622	LEU
1	A	1862	GLY
1	A	1867	GLY
1	B	163	SER
1	B	255	GLY
1	B	475	GLY
1	B	488	SER
1	B	881	ASP
1	B	983	ALA
1	B	1182	ARG
1	B	1321	LEU
1	B	1354	PRO
1	B	1371	HIS
1	B	1461	ARG
1	B	1679	GLY
1	B	1861	GLN
1	B	1862	GLY
1	A	42	ALA
1	A	43	GLY
1	A	216	ASP
1	A	237	SER
1	A	238	LEU
1	A	275	SER

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Mol	Chain	Res	Type
1	A	318	GLU
1	A	476	GLU
1	A	487	GLY
1	A	488	SER
1	A	581	SER
1	A	984	GLU
1	A	1014	ASP
1	A	1301	PRO
1	A	1327	PRO
1	A	1409	PRO
1	A	1423	PHE
1	A	1467	HIS
1	A	1538	ARG
1	A	1678	GLY
1	A	1735	HIS
1	A	1861	GLN
1	B	42	ALA
1	B	43	GLY
1	B	161	CYS
1	B	238	LEU
1	B	275	SER
1	B	318	GLU
1	B	413	PRO
1	B	476	GLU
1	B	614	ASN
1	B	1301	PRO
1	B	1425	TRP
1	B	1437	SER
1	B	1467	HIS
1	B	1557	ALA
1	B	1649	PRO
1	B	1735	HIS
1	B	1979	VAL
1	A	160	ALA
1	A	213	ARG
1	A	367	PRO
1	A	373	ARG
1	A	617	PRO
1	A	1056	SER
1	A	1308	SER
1	A	1311	LYS
1	A	1461	ARG

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Mol	Chain	Res	Type
1	A	1558	SER
1	A	1587	SER
1	A	1649	PRO
1	A	2066	VAL
1	A	2112	ALA
1	B	367	PRO
1	B	487	GLY
1	B	503	TRP
1	B	845	PRO
1	B	978	PRO
1	B	1293	HIS
1	B	1312	ALA
1	B	1432	ILE
1	B	1587	SER
1	B	1863	PRO
1	B	2066	VAL
1	B	2102	PRO
1	A	319	PRO
1	A	503	TRP
1	A	667	ARG
1	A	881	ASP
1	A	1073	ASP
1	A	1978	ALA
1	A	2009	ALA
1	A	2102	PRO
1	B	60	PHE
1	B	319	PRO
1	B	373	ARG
1	B	753	PRO
1	B	974	ALA
1	B	1014	ASP
1	B	1302	ALA
1	B	1327	PRO
1	B	1423	PHE
1	B	1676	GLY
1	A	60	PHE
1	A	753	PRO
1	A	1208	ARG
1	A	1310	GLY
1	B	124	PRO
1	B	237	SER
1	B	637	GLY

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Mol	Chain	Res	Type
1	B	654	PRO
1	B	977	ASP
1	B	1181	PRO
1	B	1304	PRO
1	B	1692	GLY
1	B	1734	ARG
1	B	2009	ALA
1	A	29	GLY
1	A	845	PRO
1	A	1215	PRO
1	B	1408	THR
1	A	1240	PRO
1	A	1870	PRO
1	B	29	GLY
1	B	1240	PRO
1	B	2104	PRO
1	A	1306	PRO
1	A	1464	PRO
1	A	1651	VAL
1	A	1692	GLY
1	A	2104	PRO
1	B	1770	GLY
1	A	2074	GLY
1	B	692	PRO
1	B	1342	GLY
1	A	868	PRO
1	A	1145	GLY
1	B	352	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	1717/2072 (83%)	1522 (89%)	195 (11%)	7	29
1	B	1722/2072 (83%)	1534 (89%)	188 (11%)	8	32
All	All	3439/4144 (83%)	3056 (89%)	383 (11%)	8	31

All (383) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	MET
1	A	59	ARG
1	A	81	MET
1	A	86	THR
1	A	100	LEU
1	A	103	THR
1	A	113	SER
1	A	120	LEU
1	A	121	SER
1	A	131	SER
1	A	132	MET
1	A	136	GLN
1	A	144	LEU
1	A	157	ILE
1	A	168	LEU
1	A	169	GLN
1	A	170	SER
1	A	179	GLU
1	A	181	SER
1	A	206	LEU
1	A	213	ARG
1	A	223	CYS
1	A	224	ARG
1	A	237	SER
1	A	241	ARG
1	A	248	ASN
1	A	251	THR
1	A	263	PHE
1	A	295	THR
1	A	317	ARG
1	A	320	LEU
1	A	329	MET
1	A	343	LYS
1	A	347	SER
1	A	356	ASN
1	A	371	ASP
1	A	375	GLN
1	A	381	LEU
1	A	383	ILE
1	A	384	ARG
1	A	399	ASN
1	A	400	VAL

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Mol	Chain	Res	Type
1	A	402	VAL
1	A	407	ASN
1	A	443	ARG
1	A	460	VAL
1	A	482	VAL
1	A	489	LYS
1	A	492	VAL
1	A	502	GLN
1	A	520	ILE
1	A	525	GLN
1	A	545	VAL
1	A	549	ILE
1	A	568	THR
1	A	569	SER
1	A	593	CYS
1	A	595	THR
1	A	597	GLU
1	A	615	VAL
1	A	616	LEU
1	A	658	MET
1	A	659	SER
1	A	660	GLU
1	A	668	GLU
1	A	670	VAL
1	A	676	ARG
1	A	677	THR
1	A	689	SER
1	A	696	ARG
1	A	697	GLN
1	A	703	LEU
1	A	704	ASP
1	A	723	GLN
1	A	730	PHE
1	A	734	TYR
1	A	737	ASN
1	A	743	VAL
1	A	746	GLN
1	A	776	GLU
1	A	778	SER
1	A	798	SER
1	A	825	ARG
1	A	846	SER

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Mol	Chain	Res	Type
1	A	858	SER
1	A	866	VAL
1	A	894	LEU
1	A	910	THR
1	A	931	VAL
1	A	937	LEU
1	A	947	SER
1	A	953	LEU
1	A	959	VAL
1	A	980	ASP
1	A	981	SER
1	A	985	PHE
1	A	1011	LEU
1	A	1019	ARG
1	A	1038	MET
1	A	1039	SER
1	A	1062	VAL
1	A	1063	THR
1	A	1068	LEU
1	A	1069	TYR
1	A	1072	GLN
1	A	1084	ARG
1	A	1087	ASN
1	A	1088	THR
1	A	1101	SER
1	A	1107	ARG
1	A	1112	LEU
1	A	1122	THR
1	A	1140	LEU
1	A	1216	LEU
1	A	1265	GLN
1	A	1268	MET
1	A	1275	THR
1	A	1276	ASP
1	A	1290	GLU
1	A	1299	TRP
1	A	1319	CYS
1	A	1324	LEU
1	A	1333	ASN
1	A	1346	LEU
1	A	1350	LEU
1	A	1374	SER

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Mol	Chain	Res	Type
1	A	1421	THR
1	A	1444	MET
1	A	1449	SER
1	A	1473	LEU
1	A	1476	ASN
1	A	1480	THR
1	A	1481	SER
1	A	1505	VAL
1	A	1537	SER
1	A	1545	ARG
1	A	1551	LEU
1	A	1561	ASP
1	A	1573	PHE
1	A	1574	ARG
1	A	1583	LEU
1	A	1587	SER
1	A	1596	ASP
1	A	1601	MET
1	A	1614	MET
1	A	1617	VAL
1	A	1629	LEU
1	A	1636	VAL
1	A	1639	THR
1	A	1653	THR
1	A	1662	ARG
1	A	1671	VAL
1	A	1697	THR
1	A	1699	VAL
1	A	1720	PHE
1	A	1726	THR
1	A	1736	THR
1	A	1756	SER
1	A	1760	LEU
1	A	1765	ARG
1	A	1766	PHE
1	A	1768	GLU
1	A	1782	MET
1	A	1790	THR
1	A	1797	ASP
1	A	1800	PHE
1	A	1815	LYS
1	A	1818	ILE

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Mol	Chain	Res	Type
1	A	1823	VAL
1	A	1841	ARG
1	A	1860	GLU
1	A	1873	LEU
1	A	1877	SER
1	A	1899	GLN
1	A	1906	LEU
1	A	1916	SER
1	A	1922	THR
1	A	1927	ARG
1	A	1930	ARG
1	A	1944	SER
1	A	1956	ILE
1	A	1980	LEU
1	A	1984	THR
1	A	1988	PHE
1	A	1991	VAL
1	A	2006	THR
1	A	2026	ARG
1	A	2043	ARG
1	A	2075	THR
1	A	2079	VAL
1	A	2084	LEU
1	A	2088	ILE
1	A	2105	VAL
1	A	2107	SER
1	A	2111	LEU
1	B	32	MET
1	B	59	ARG
1	B	81	MET
1	B	86	THR
1	B	100	LEU
1	B	103	THR
1	B	113	SER
1	B	120	LEU
1	B	126	THR
1	B	127	LEU
1	B	128	VAL
1	B	131	SER
1	B	132	MET
1	B	136	GLN
1	B	144	LEU

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Mol	Chain	Res	Type
1	B	157	ILE
1	B	168	LEU
1	B	169	GLN
1	B	170	SER
1	B	179	GLU
1	B	181	SER
1	B	224	ARG
1	B	237	SER
1	B	241	ARG
1	B	248	ASN
1	B	251	THR
1	B	259	GLN
1	B	263	PHE
1	B	276	LEU
1	B	295	THR
1	B	317	ARG
1	B	320	LEU
1	B	329	MET
1	B	343	LYS
1	B	347	SER
1	B	352	VAL
1	B	356	ASN
1	B	371	ASP
1	B	375	GLN
1	B	381	LEU
1	B	383	ILE
1	B	384	ARG
1	B	398	SER
1	B	399	ASN
1	B	400	VAL
1	B	402	VAL
1	B	407	ASN
1	B	443	ARG
1	B	460	VAL
1	B	489	LYS
1	B	492	VAL
1	B	502	GLN
1	B	504	GLN
1	B	520	ILE
1	B	525	GLN
1	B	549	ILE
1	B	568	THR

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Mol	Chain	Res	Type
1	B	569	SER
1	B	593	CYS
1	B	597	GLU
1	B	615	VAL
1	B	664	GLN
1	B	675	VAL
1	B	680	ILE
1	B	689	SER
1	B	697	GLN
1	B	730	PHE
1	B	734	TYR
1	B	737	ASN
1	B	743	VAL
1	B	746	GLN
1	B	798	SER
1	B	819	VAL
1	B	821	PHE
1	B	825	ARG
1	B	856	CYS
1	B	866	VAL
1	B	894	LEU
1	B	910	THR
1	B	931	VAL
1	B	937	LEU
1	B	947	SER
1	B	959	VAL
1	B	972	THR
1	B	980	ASP
1	B	982	THR
1	B	985	PHE
1	B	1011	LEU
1	B	1019	ARG
1	B	1038	MET
1	B	1039	SER
1	B	1062	VAL
1	B	1063	THR
1	B	1068	LEU
1	B	1069	TYR
1	B	1072	GLN
1	B	1084	ARG
1	B	1087	ASN
1	B	1088	THR

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Mol	Chain	Res	Type
1	B	1101	SER
1	B	1102	SER
1	B	1107	ARG
1	B	1122	THR
1	B	1184	LEU
1	B	1216	LEU
1	B	1264	THR
1	B	1275	THR
1	B	1299	TRP
1	B	1321	LEU
1	B	1333	ASN
1	B	1346	LEU
1	B	1373	LEU
1	B	1386	SER
1	B	1421	THR
1	B	1433	LEU
1	B	1443	LEU
1	B	1444	MET
1	B	1449	SER
1	B	1456	MET
1	B	1473	LEU
1	B	1476	ASN
1	B	1477	LEU
1	B	1480	THR
1	B	1481	SER
1	B	1505	VAL
1	B	1528	THR
1	B	1532	PHE
1	B	1543	SER
1	B	1549	SER
1	B	1573	PHE
1	B	1574	ARG
1	B	1583	LEU
1	B	1587	SER
1	B	1603	PHE
1	B	1612	ARG
1	B	1614	MET
1	B	1627	LEU
1	B	1636	VAL
1	B	1639	THR
1	B	1653	THR
1	B	1662	ARG

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Mol	Chain	Res	Type
1	B	1666	GLN
1	B	1671	VAL
1	B	1694	ARG
1	B	1697	THR
1	B	1699	VAL
1	B	1720	PHE
1	B	1726	THR
1	B	1736	THR
1	B	1756	SER
1	B	1760	LEU
1	B	1765	ARG
1	B	1768	GLU
1	B	1782	MET
1	B	1789	VAL
1	B	1790	THR
1	B	1797	ASP
1	B	1818	ILE
1	B	1823	VAL
1	B	1841	ARG
1	B	1856	VAL
1	B	1857	ARG
1	B	1860	GLU
1	B	1868	LEU
1	B	1871	ILE
1	B	1873	LEU
1	B	1877	SER
1	B	1899	GLN
1	B	1906	LEU
1	B	1916	SER
1	B	1922	THR
1	B	1927	ARG
1	B	1930	ARG
1	B	1944	SER
1	B	1956	ILE
1	B	1974	VAL
1	B	1979	VAL
1	B	1984	THR
1	B	1988	PHE
1	B	1991	VAL
1	B	2006	THR
1	B	2026	ARG
1	B	2043	ARG

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Mol	Chain	Res	Type
1	B	2079	VAL
1	B	2084	LEU
1	B	2088	ILE
1	B	2105	VAL
1	B	2107	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	136	GLN
1	A	142	ASN
1	A	169	GLN
1	A	199	GLN
1	A	248	ASN
1	A	259	GLN
1	A	306	ASN
1	A	350	HIS
1	A	356	ASN
1	A	387	ASN
1	A	399	ASN
1	A	425	GLN
1	A	440	GLN
1	A	525	GLN
1	A	560	GLN
1	A	643	HIS
1	A	644	ASN
1	A	697	GLN
1	A	737	ASN
1	A	833	HIS
1	A	1023	GLN
1	A	1037	HIS
1	A	1111	HIS
1	A	1124	HIS
1	A	1133	ASN
1	A	1191	GLN
1	A	1206	GLN
1	A	1236	ASN
1	A	1265	GLN
1	A	1298	GLN
1	A	1318	ASN
1	A	1353	HIS

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Mol	Chain	Res	Type
1	A	1406	GLN
1	A	1407	GLN
1	A	1467	HIS
1	A	1476	ASN
1	A	1504	ASN
1	A	1516	HIS
1	A	1735	HIS
1	A	1763	HIS
1	A	1777	ASN
1	A	1855	GLN
1	A	2028	ASN
1	A	2076	ASN
1	A	2086	GLN
1	A	2103	HIS
1	B	25	ASN
1	B	136	GLN
1	B	142	ASN
1	B	199	GLN
1	B	248	ASN
1	B	259	GLN
1	B	306	ASN
1	B	350	HIS
1	B	356	ASN
1	B	387	ASN
1	B	399	ASN
1	B	425	GLN
1	B	440	GLN
1	B	504	GLN
1	B	525	GLN
1	B	560	GLN
1	B	614	ASN
1	B	643	HIS
1	B	697	GLN
1	B	723	GLN
1	B	737	ASN
1	B	738	ASN
1	B	746	GLN
1	B	833	HIS
1	B	1023	GLN
1	B	1037	HIS
1	B	1111	HIS
1	B	1124	HIS

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Mol	Chain	Res	Type
1	B	1133	ASN
1	B	1189	GLN
1	B	1195	ASN
1	B	1236	ASN
1	B	1265	GLN
1	B	1293	HIS
1	B	1298	GLN
1	B	1318	ASN
1	B	1347	HIS
1	B	1407	GLN
1	B	1494	GLN
1	B	1530	HIS
1	B	1560	GLN
1	B	1674	HIS
1	B	1735	HIS
1	B	1763	HIS
1	B	1777	ASN
1	B	1855	GLN
1	B	1983	GLN
1	B	2028	ASN
1	B	2076	ASN
1	B	2086	GLN
1	B	2103	HIS

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	NAP	A	3001	-	42,52,52	1.16	2 (4%)	54,80,80	1.97	4 (7%)
2	NAP	A	3002	-	42,52,52	0.99	2 (4%)	54,80,80	1.77	3 (5%)
2	NAP	B	3001	-	42,52,52	1.05	2 (4%)	54,80,80	1.97	6 (11%)
2	NAP	B	3002	-	42,52,52	1.09	3 (7%)	54,80,80	1.91	6 (11%)

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	NAP	A	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	A	3002	-	-	0/27/67/67	0/5/5/5
2	NAP	B	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	B	3002	-	-	0/27/67/67	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3002	NAP	C2A-N1A	2.08	1.37	1.33
2	B	3002	NAP	C6N-N1N	2.12	1.41	1.35
2	A	3002	NAP	C2A-N1A	2.13	1.38	1.33
2	B	3001	NAP	C2A-N1A	3.10	1.39	1.33
2	A	3001	NAP	C2A-N1A	3.13	1.39	1.33
2	A	3002	NAP	C2A-N3A	3.43	1.38	1.32
2	B	3001	NAP	C2A-N3A	3.74	1.38	1.32
2	B	3002	NAP	C2A-N3A	4.01	1.39	1.32
2	A	3001	NAP	C2A-N3A	4.53	1.40	1.32

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	NAP	N3A-C2A-N1A	-12.43	119.37	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3002	NAP	N3A-C2A-N1A	-11.35	120.20	128.89
2	B	3001	NAP	N3A-C2A-N1A	-11.11	120.39	128.89
2	B	3002	NAP	N3A-C2A-N1A	-10.52	120.84	128.89
2	B	3002	NAP	C4B-O4B-C1B	-5.34	103.85	109.72
2	B	3001	NAP	C3N-C7N-N7N	-4.84	112.52	117.82
2	B	3001	NAP	PN-O3-PA	-3.08	124.08	132.73
2	B	3002	NAP	C3N-C7N-N7N	-2.62	114.95	117.82
2	A	3002	NAP	C3N-C7N-N7N	-2.38	115.21	117.82
2	B	3002	NAP	C4A-C5A-N7A	-2.06	107.58	109.48
2	B	3001	NAP	C5D-C4D-C3D	-2.06	107.03	115.21
2	A	3001	NAP	C3N-C7N-N7N	-2.01	115.62	117.82
2	B	3002	NAP	O4D-C1D-N1N	2.02	110.35	108.13
2	A	3002	NAP	O4B-C1B-N9A	2.08	112.46	108.10
2	A	3001	NAP	C4D-O4D-C1D	2.09	112.02	109.72
2	B	3001	NAP	O4B-C1B-N9A	2.32	112.96	108.10
2	A	3001	NAP	C3B-C2B-C1B	2.39	107.36	102.73
2	B	3001	NAP	O7N-C7N-C3N	3.07	122.93	119.59
2	B	3002	NAP	O4B-C1B-N9A	3.55	115.52	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	NAP	8	0
2	A	3002	NAP	4	0
2	B	3001	NAP	1	0
2	B	3002	NAP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	2081/2512 (82%)	0.06	132 (6%)	23 19	73, 131, 230, 299	0
1	B	2086/2512 (83%)	0.25	165 (7%)	15 12	72, 166, 228, 299	0
All	All	4167/5024 (82%)	0.15	297 (7%)	19 15	72, 145, 229, 299	0

All (297) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	416	GLN	9.8
1	A	977	ASP	9.6
1	A	976	VAL	9.4
1	A	1188	CYS	7.0
1	A	1297	GLY	7.0
1	B	672	VAL	7.0
1	A	1406	GLN	6.7
1	A	1189	GLN	6.4
1	B	667	ARG	6.4
1	A	975	ALA	6.3
1	B	665	LEU	6.2
1	B	1191	GLN	6.1
1	B	496	CYS	6.1
1	A	978	PRO	5.9
1	B	1486	MET	5.9
1	B	581	SER	5.8
1	A	1190	LEU	5.7
1	B	1863	PRO	5.7
1	B	415	ALA	5.6
1	B	498	GLY	5.5
1	B	419	ALA	5.4
1	A	1181	PRO	5.3
1	B	417	HIS	5.3
1	B	671	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	1205	ALA	5.2
1	A	1202	GLN	5.2
1	B	579	GLY	5.1
1	A	1212	CYS	5.1
1	B	663	GLN	5.0
1	B	654	PRO	4.9
1	B	673	LYS	4.9
1	A	979	ALA	4.8
1	B	580	HIS	4.8
1	B	583	GLY	4.8
1	B	10	SER	4.7
1	B	653	GLY	4.7
1	A	1287	ALA	4.7
1	B	1408	THR	4.6
1	B	364	PRO	4.5
1	B	414	PRO	4.5
1	A	1204	LEU	4.5
1	A	2039	SER	4.4
1	B	497	SER	4.4
1	A	1318	ASN	4.3
1	A	336	SER	4.2
1	A	1407	GLN	4.2
1	A	1308	SER	4.2
1	A	1195	ASN	4.2
1	B	622	ALA	4.1
1	A	1180	LEU	4.1
1	A	1485	GLU	4.1
1	B	1147	ALA	4.1
1	B	49	ARG	4.1
1	A	1187	ALA	4.1
1	B	1407	GLN	4.0
1	B	392	SER	4.0
1	B	161	CYS	4.0
1	A	416	GLN	3.9
1	B	1439	ARG	3.9
1	B	790	ARG	3.9
1	B	1193	ASN	3.8
1	B	658	MET	3.8
1	B	1195	ASN	3.8
1	A	1367	GLN	3.8
1	B	476	GLU	3.8
1	A	414	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	1192	LEU	3.7
1	B	1458	ASN	3.7
1	A	980	ASP	3.7
1	B	1455	GLY	3.7
1	B	315	THR	3.7
1	A	2024	CYS	3.7
1	B	11	GLY	3.7
1	B	1570	SER	3.6
1	A	1408	THR	3.6
1	B	674	GLU	3.6
1	A	323	GLY	3.6
1	B	2024	CYS	3.6
1	A	392	SER	3.6
1	A	1311	LYS	3.6
1	B	1148	GLN	3.6
1	A	1486	MET	3.5
1	A	1296	GLN	3.5
1	B	128	VAL	3.5
1	B	1368	GLY	3.5
1	B	1149	ALA	3.5
1	B	670	VAL	3.5
1	B	557	THR	3.5
1	B	488	SER	3.5
1	B	669	ASP	3.4
1	A	1191	GLN	3.4
1	B	1199	GLU	3.4
1	A	1033	ASP	3.4
1	B	676	ARG	3.4
1	B	1485	GLU	3.4
1	A	1193	ASN	3.4
1	A	496	CYS	3.4
1	B	2039	SER	3.3
1	B	539	LEU	3.3
1	B	1189	GLN	3.3
1	B	560	GLN	3.2
1	B	2021	SER	3.2
1	B	975	ALA	3.2
1	A	418	ALA	3.2
1	A	1452	GLY	3.2
1	A	293	HIS	3.2
1	B	293	HIS	3.2
1	B	831	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	1468	ARG	3.2
1	B	1204	LEU	3.2
1	B	1201	GLY	3.2
1	A	1206	GLN	3.2
1	A	2038	ASN	3.2
1	B	623	VAL	3.1
1	B	1437	SER	3.1
1	B	1297	GLY	3.1
1	B	1202	GLN	3.1
1	A	1455	GLY	3.1
1	A	1468	ARG	3.1
1	A	1987	PHE	3.1
1	B	409	ARG	3.1
1	B	410	PRO	3.1
1	A	1583	LEU	3.1
1	B	929	GLY	3.0
1	B	189	ASN	3.0
1	B	2114	LYS	3.0
1	A	1380	SER	3.0
1	B	418	ALA	3.0
1	B	336	SER	3.0
1	B	1190	LEU	3.0
1	B	2023	SER	2.9
1	B	2025	GLY	2.9
1	B	1406	GLN	2.9
1	B	1681	GLY	2.9
1	B	1409	PRO	2.9
1	B	324	SER	2.9
1	B	1572	ASN	2.9
1	A	1481	SER	2.9
1	A	324	SER	2.9
1	A	1290	GLU	2.9
1	A	292	ALA	2.9
1	A	1587	SER	2.9
1	B	1203	VAL	2.9
1	A	1291	GLN	2.9
1	A	1307	GLY	2.9
1	A	1317	CYS	2.8
1	A	1203	VAL	2.8
1	B	558	SER	2.8
1	B	1	MET	2.8
1	A	1434	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1207	GLU	2.8
1	A	1305	ALA	2.8
1	A	49	ARG	2.8
1	A	1482	PRO	2.8
1	B	413	PRO	2.8
1	B	1467	HIS	2.7
1	A	1863	PRO	2.7
1	B	1527	GLN	2.7
1	B	316	ARG	2.7
1	A	1288	LYS	2.7
1	A	1484	PRO	2.7
1	A	583	GLY	2.7
1	B	104	SER	2.7
1	B	1602	GLU	2.7
1	A	1201	GLY	2.7
1	A	1282	LEU	2.7
1	B	660	GLU	2.7
1	B	337	GLY	2.7
1	A	1208	ARG	2.7
1	B	1861	GLN	2.7
1	A	1480	THR	2.7
1	B	928	THR	2.6
1	B	1208	ARG	2.6
1	A	161	CYS	2.6
1	A	294	GLY	2.6
1	B	624	GLY	2.6
1	B	1319	CYS	2.6
1	A	1527	GLN	2.6
1	B	722	TRP	2.6
1	B	1296	GLN	2.6
1	A	1483	ALA	2.6
1	B	1194	GLY	2.6
1	B	1206	GLN	2.6
1	B	1340	GLU	2.6
1	B	213	ARG	2.5
1	A	295	THR	2.5
1	B	1503	MET	2.5
1	A	1194	GLY	2.5
1	B	584	GLU	2.5
1	B	1487	HIS	2.5
1	A	2020	SER	2.5
1	B	868	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	340	ALA	2.5
1	A	1146	LEU	2.5
1	A	1681	GLY	2.5
1	B	332	PRO	2.5
1	B	755	HIS	2.5
1	A	337	GLY	2.4
1	B	2078	THR	2.4
1	A	1437	SER	2.4
1	A	2078	THR	2.4
1	A	1458	ASN	2.4
1	A	984	GLU	2.4
1	A	1136	LEU	2.4
1	B	762	ALA	2.4
1	A	1507	ARG	2.4
1	A	1510	ALA	2.4
1	B	489	LYS	2.4
1	B	543	GLU	2.4
1	A	1371	HIS	2.4
1	A	1586	ASP	2.4
1	B	621	ALA	2.4
1	B	1875	GLY	2.4
1	B	360	HIS	2.4
1	A	498	GLY	2.4
1	A	10	SER	2.4
1	B	422	ARG	2.4
1	A	417	HIS	2.3
1	A	1336	ALA	2.3
1	A	1135	ALA	2.3
1	A	1866	ARG	2.3
1	A	1509	GLY	2.3
1	A	974	ALA	2.3
1	A	1347	HIS	2.3
1	B	1286	GLN	2.3
1	A	391	ASN	2.3
1	B	906	ASN	2.3
1	A	1209	PRO	2.3
1	B	330	GLY	2.3
1	B	2027	GLY	2.3
1	B	1452	GLY	2.3
1	B	1862	GLY	2.3
1	A	291	GLU	2.3
1	B	1318	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1409	PRO	2.3
1	A	1467	HIS	2.3
1	B	1146	LEU	2.3
1	B	2111	LEU	2.3
1	A	1479	SER	2.3
1	B	412	PRO	2.2
1	B	1312	ALA	2.2
1	A	928	THR	2.2
1	A	1319	CYS	2.2
1	B	1235	GLU	2.2
1	A	1679	GLY	2.2
1	A	37	ASP	2.2
1	A	1354	PRO	2.2
1	B	499	MET	2.2
1	A	1284	ALA	2.2
1	B	92	ASP	2.2
1	B	664	GLN	2.2
1	B	728	ARG	2.2
1	B	888	GLY	2.2
1	A	1071	LEU	2.2
1	A	2079	VAL	2.2
1	B	1410	GLN	2.2
1	B	292	ALA	2.2
1	A	1451	SER	2.2
1	A	1862	GLY	2.2
1	B	353	TRP	2.2
1	B	1456	MET	2.2
1	A	410	PRO	2.2
1	A	1398	GLY	2.2
1	A	480	GLN	2.2
1	B	1459	CYS	2.2
1	B	236	LYS	2.1
1	B	646	LYS	2.1
1	A	1337	THR	2.1
1	A	1525	GLU	2.1
1	B	1347	HIS	2.1
1	B	1970	ASN	2.1
1	A	889	THR	2.1
1	B	391	ASN	2.1
1	B	1111	HIS	2.1
1	A	394	GLY	2.1
1	B	889	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1205	ALA	2.1
1	B	129	GLY	2.1
1	B	710	LYS	2.1
1	A	419	ALA	2.1
1	B	1110	GLU	2.1
1	B	2035	GLY	2.1
1	B	1200	LEU	2.1
1	A	326	LYS	2.1
1	A	218	GLU	2.1
1	B	1484	PRO	2.1
1	A	1375	GLN	2.1
1	A	1540	ASP	2.1
1	B	661	PHE	2.1
1	B	587	CYS	2.0
1	A	1387	LEU	2.0
1	B	320	LEU	2.0
1	B	2	GLU	2.0
1	B	662	LEU	2.0
1	A	2040	ALA	2.0
1	B	41	LYS	2.0
1	B	1440	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAP	A	3001	48/48	0.90	0.32	0.86	100,122,179,189	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAP	B	3001	48/48	0.92	0.26	0.12	99,123,160,163	0
2	NAP	A	3002	48/48	0.95	0.20	-0.36	96,135,161,194	0
2	NAP	B	3002	48/48	0.95	0.18	-0.51	99,122,153,198	0

6.5 Other polymers

There are no such residues in this entry.