



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:59 AM GMT

PDB ID : 3CWG
Title : Unphosphorylated mouse STAT3 core fragment
Authors : Ren, Z.; Mao, X.; Mertens, C.; Krishnaraj, R.; Qin, J.; Mandal, P.K.; Romanowshi, M.J.; McMurray, J.S.
Deposited on : 2008-04-21
Resolution : 3.05 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

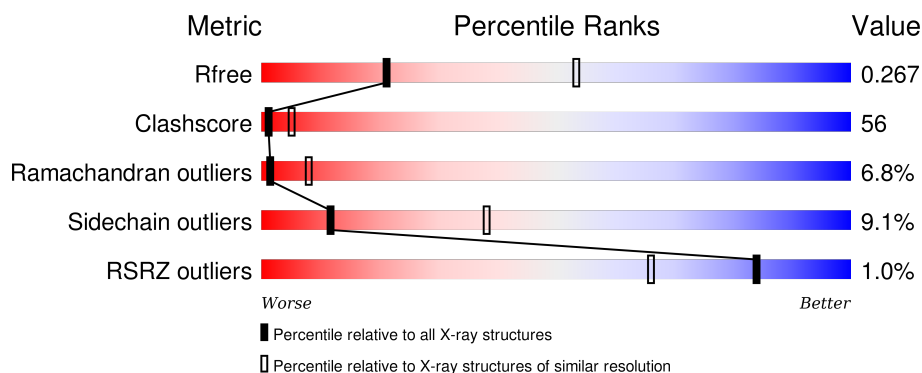
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

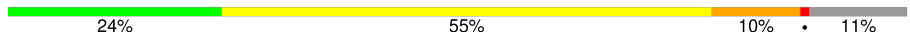

The reported resolution of this entry is 3.05 Å.

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	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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	562	 24% 55% 10% • 11%
1	B	562	 27% 53% 9% • 10%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8215 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.

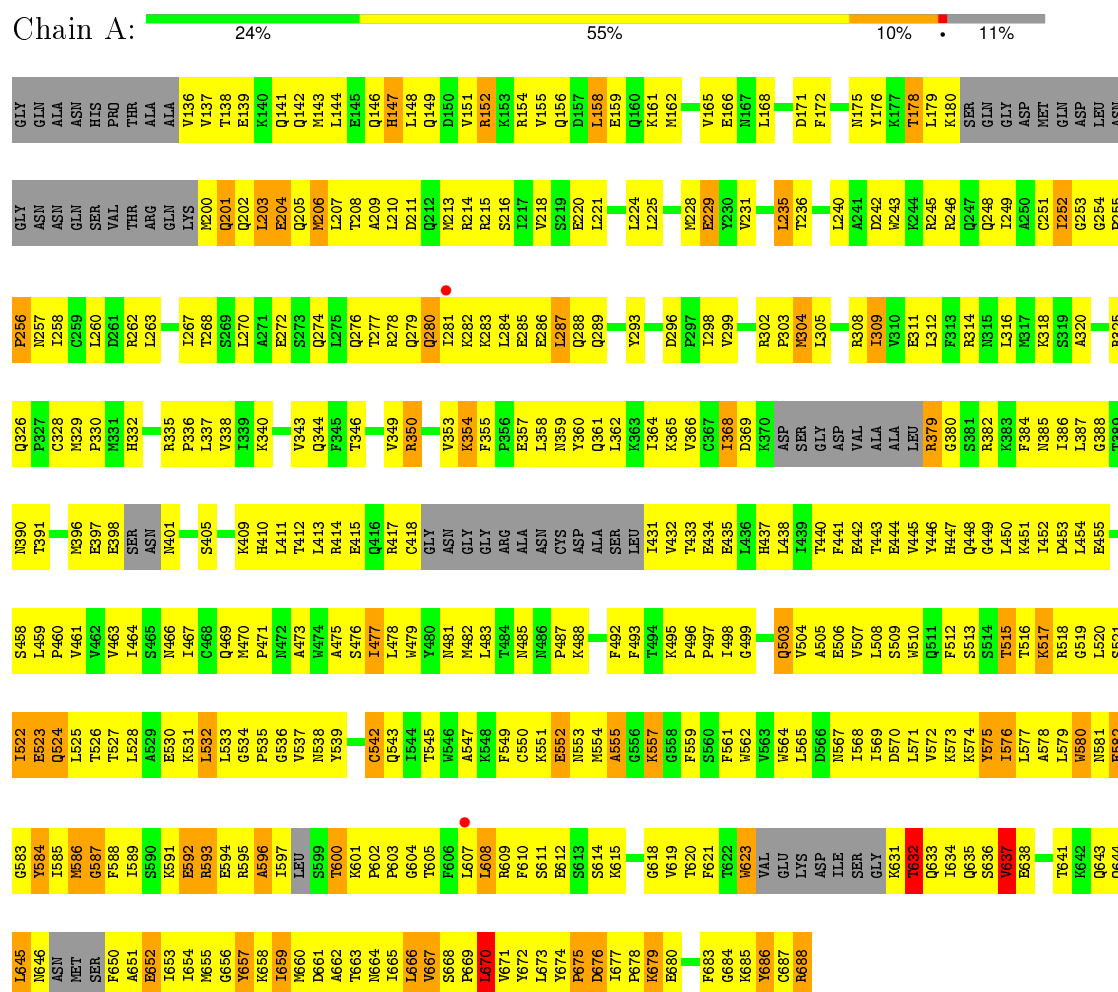
- Molecule 1 is a protein called Signal transducer and activator of transcription 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			4082	2615	692	748	27			
1	B	507	Total	C	N	O	S	0	0	0
			4133	2645	704	758	26			

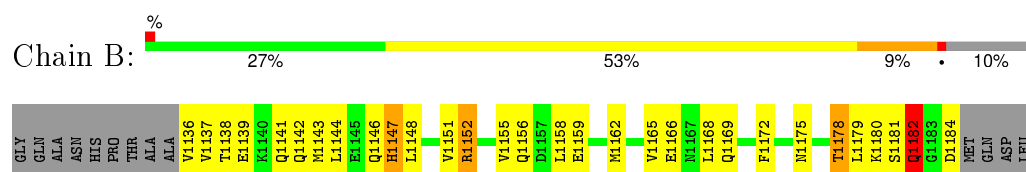
3 Residue-property plots

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: Signal transducer and activator of transcription 3



• Molecule 1: Signal transducer and activator of transcription 3



G1656	R1595	G1534	M1470	H1401	H1332	L1260	SER
Y1657	A1596	P1535	P1471	L1404	R1335	D1261	L1260
K1658	I1597	G1536	M1472	L1404	P1336	L1262	V1195
ILE	L1598	V1537	A1473	K1409	L1337	L1263	T1196
MET	S1599	M1538	W1474	H1410	L1338	I1267	R1197
ASP	T1600	Y1539	A1475	K1411	I1339	T1268	Q1198
ALA	K1601	S1540	S1476	T1412	K1340	M1200	K1199
T1663	P1602	G1541	I1477	T1413	L1340	Q1201	M1200
N1664	P1603	C1542	L1478	R1414	V1343	Q1202	Q1201
I1665	G1604	Q1543	W1479	R1415	Q1344	L1270	L1203
L1666	T1605	I1544	Y1480	E1415	E1272	E1272	E1204
V1667	F1606	M1481	M1481	C1418	F1345	S1273	Q1205
S1668	L1607	M1482	L1483	GLY	T1346	Q1274	M1206
P1669	L1608	T1484	L1483	ASN	R1350	L1275	M1206
L1670	F1609	F1549	T1484	GLY	R1350	Q1276	L1207
V1671	F1610	C1550	M1485	GLY	V1353	T1277	T1208
Y1672	S1611	K1551	M1486	GLY	Y1353	R1278	A1209
L1673	E1612	E1552	P1487	ARG	K1354	Q1279	L1210
Y1674	S1613	M1553	K1488	ALA	F1355	Q1280	D1211
P1675	S1614	M1554	F1492	ASN	P1356	L1281	Q1212
D1676	A1555	M1555	F1493	CYS	E1357	K1282	M1213
I1677	G1556	K1557	T1494	ASP	L1358	L1283	M1214
P1678	G1617	K1557	T1494	ALA	M1359	L1284	R1215
K1679	G1618	G1558	K1495	ASP	Y1360	E1285	
E1680	V1619	F1559	P1496	SER	Q1361	E1286	V1218
E1681	T1620	S1560	P1497	LEU	Q1361	L1287	S1219
A1682	F1621	F1561	I1498	I1431	L1362	E1288	E1220
F1683	W1622	W1562	G1499	T1433	K1365	Q1288	L1224
G1684	W1623	W1563	Q1503	H1437	V1366	Q1289	L1225
K1685	VAL	V1564	H1437	H1437	C1367	Y1293	
GLY	GLY	L1565	L1438	L1438	I1368		M1228
LYS	LYS	D1566	L1439	L1439	D1369	D1296	E1229
ASP	ASP	M1567	T1440	T1440	K1370	P1297	E1230
ILE	ILE	I1568	F1441	F1441	ASP	I1298	Y1231
SER	SER	I1569	E1442	E1442	SER	V1299	
GLY	GLY	D1570	T1443	T1443	GLY	T1234	T1234
K1631	K1631	L1571	E1444	E1444	ASP	L1235	L1235
T1632	T1632	V1572	V1445	V1445	VAL	T1236	T1236
Q1633	Q1633	K1573	H1446	H1446	ALA	D1237	D1237
I1634	I1634	K1574	H1447	H1447	ALA	E1238	E1238
Q1635	Q1635	Y1575	S1514	S1514	LEU	R1308	L1240
S1636	S1636	I1576	T1515	T1515	R1379	E1308	L1240
V1637	V1637	L1577	T1516	T1516	G1380	E1311	A1241
E1638	E1638	A1578	K1517	K1517	S1381	L1312	D1242
		L1579	A1518	A1518	A1382	W1243	W1243
T1641	T1641	W1580	G1519	G1519	K1383	R1244	R1244
K1642	K1642	M1581	L1520	L1520	F1384	R1245	R1245
Q1643	Q1643	E1582	S1521	S1521	M1385	R1246	R1246
Q1644	Q1644	G1583	I1522	I1522	T1386	Q1247	Q1247
L1645	L1645	Y1584	E1523	E1523	L1387	Q1248	Q1248
N1646	N1646	I1585	Q1524	Q1524	S1319	I1249	I1249
ASN	ASN	M1586	L1525	L1525	A1320	A1250	A1250
MET	MET	G1587	T1526	T1526	M1390	C1251	C1251
SER	SER	F1588	T1527	T1527	T1391	I1252	I1252
F1650	F1650	I1589	L1528	L1528	M1396	Q1326	Q1326
A1651	A1651	S1590	A1529	A1529	P1397	C1328	C1328
E1652	E1652	K1591	E1530	E1530	E1397	M1257	M1257
I1653	I1653	E1592	K1531	K1531	E1398	P1330	P1330
L1654	L1654	R1593	L1532	L1532	SER	M1331	M1331
M1655	M1655	E1594	L1533	L1533	ASN		C1259

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	254.78Å 254.78Å 123.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.05 29.70 – 3.02	Depositor EDS
% Data completeness (in resolution range)	91.2 (30.00-3.05) 90.1 (29.70-3.02)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.269 0.245 , 0.267	Depositor DCC
R_{free} test set	7413 reflections (10.20%)	DCC
Wilson B-factor (Å ²)	71.6	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.2	EDS
Estimated twinning fraction	0.367 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 84177 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8215	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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](#)

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	0.47	0/4159	0.71	0/5608
1	B	0.47	0/4210	0.70	0/5675
All	All	0.47	0/8369	0.70	0/11283

There are no bond length outliers.

There are no bond angle outliers.

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	4082	0	4139	481	0
1	B	4133	0	4195	461	1
All	All	8215	0	8334	929	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 56.

All (929) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:MET:HA	1:A:666:LEU:HA	1.37	1.07
1:B:1597:ILE:HG13	1:B:1598:LEU:H	1.22	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:PHE:HA	1:A:653:ILE:HD13	1.39	1.04
1:B:1605:THR:HG22	1:B:1672:TYR:HB2	1.42	1.01
1:A:547:ALA:HA	1:A:551:LYS:HB3	1.43	1.00
1:A:517:LYS:HD2	1:A:517:LYS:H	1.28	0.99
1:B:1547:ALA:HA	1:B:1551:LYS:HB3	1.41	0.98
1:B:1470:MET:HB3	1:B:1471:PRO:HD3	1.46	0.98
1:A:535:PRO:HB2	1:B:1596:ALA:HB1	1.43	0.98
1:B:1137:VAL:HG22	1:B:1262:ARG:HH22	1.27	0.97
1:B:1670:LEU:H	1:B:1670:LEU:HD22	1.27	0.97
1:B:1576:ILE:HA	1:B:1579:LEU:HD13	1.45	0.97
1:B:1517:LYS:HD2	1:B:1517:LYS:H	1.30	0.95
1:A:670:LEU:HD22	1:A:670:LEU:H	1.26	0.95
1:A:470:MET:HB3	1:A:471:PRO:HD3	1.46	0.95
1:A:221:LEU:HD13	1:A:281:ILE:HD13	1.47	0.95
1:B:1595:ARG:NH1	1:B:1634:ILE:HD13	1.82	0.94
1:A:576:ILE:HA	1:A:579:LEU:HD13	1.47	0.94
1:B:1280:GLN:HE21	1:B:1280:GLN:HA	1.34	0.93
1:A:280:GLN:HE21	1:A:280:GLN:HA	1.34	0.92
1:A:137:VAL:HG22	1:A:262:ARG:HH22	1.33	0.92
1:A:537:VAL:HG11	1:B:1523:GLU:HG2	1.53	0.89
1:B:1595:ARG:HH11	1:B:1634:ILE:HD13	1.34	0.89
1:A:235:LEU:HD13	1:A:267:ILE:HD13	1.52	0.89
1:A:605:THR:HG22	1:A:672:TYR:HB2	1.55	0.88
1:B:1598:LEU:HD11	1:B:1604:GLY:H	1.37	0.88
1:B:1379:ARG:HD3	1:B:1380:GLY:N	1.89	0.88
1:A:512:PHE:HB2	1:A:519:GLY:HA2	1.58	0.85
1:B:1201:GLN:HA	1:B:1204:GLU:CD	1.97	0.85
1:A:246:ARG:HG2	1:A:258:ILE:HG22	1.59	0.84
1:A:201:GLN:HA	1:A:204:GLU:CD	1.97	0.84
1:B:1512:PHE:HB2	1:B:1519:GLY:HA2	1.60	0.84
1:A:591:LYS:HE2	1:A:609:ARG:NH2	1.93	0.83
1:B:1633:GLN:HG2	1:B:1634:ILE:N	1.93	0.83
1:B:1633:GLN:CG	1:B:1634:ILE:N	2.38	0.83
1:A:658:LYS:O	1:A:667:VAL:HG23	1.80	0.82
1:A:314:ARG:HA	1:A:452:ILE:HD11	1.59	0.82
1:B:1597:ILE:HG13	1:B:1598:LEU:N	1.92	0.82
1:B:1229:GLU:HG3	1:B:1312:LEU:HD21	1.61	0.82
1:A:535:PRO:CB	1:B:1596:ALA:HB1	2.10	0.82
1:A:139:GLU:HA	1:A:142:GLN:HG2	1.62	0.81
1:A:663:THR:O	1:A:665:ILE:HG12	1.80	0.81
1:A:138:THR:HG23	1:A:141:GLN:NE2	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1346:THR:HG22	1:B:1409:LYS:HA	1.61	0.81
1:B:1246:ARG:HG2	1:B:1258:ILE:HG22	1.61	0.81
1:A:229:GLU:HG3	1:A:312:LEU:HD21	1.61	0.80
1:B:1601:LYS:HB3	1:B:1602:PRO:HD2	1.64	0.80
1:A:603:PRO:HB3	1:A:632:THR:HG21	1.63	0.80
1:B:1314:ARG:HA	1:B:1452:ILE:HD11	1.64	0.80
1:B:1379:ARG:HH11	1:B:1380:GLY:H	1.29	0.80
1:B:1565:LEU:HA	1:B:1568:ILE:CD1	2.11	0.80
1:A:670:LEU:CD2	1:A:670:LEU:H	1.94	0.80
1:A:601:LYS:HB3	1:A:602:PRO:HD2	1.64	0.79
1:A:660:MET:HB2	1:A:666:LEU:HG	1.63	0.79
1:B:1565:LEU:HA	1:B:1568:ILE:HD12	1.64	0.79
1:B:1670:LEU:H	1:B:1670:LEU:CD2	1.95	0.79
1:B:1195:VAL:HG12	1:B:1196:THR:H	1.47	0.79
1:A:539:TYR:HA	1:A:542:CYS:SG	2.23	0.78
1:A:607:LEU:O	1:A:608:LEU:HG	1.84	0.78
1:B:1498:ILE:HG21	1:B:1543:GLN:HB3	1.65	0.78
1:B:1607:LEU:O	1:B:1608:LEU:HG	1.82	0.78
1:A:338:VAL:HG11	1:A:470:MET:HE3	1.64	0.78
1:B:1539:TYR:HA	1:B:1542:CYS:SG	2.22	0.78
1:A:604:GLY:O	1:A:670:LEU:HB3	1.83	0.78
1:B:1278:ARG:HD3	1:B:1448:GLN:OE1	1.84	0.78
1:B:1633:GLN:HG3	1:B:1634:ILE:H	1.49	0.77
1:A:498:ILE:HG21	1:A:543:GLN:HB3	1.66	0.77
1:B:1547:ALA:HA	1:B:1551:LYS:CB	2.14	0.77
1:A:547:ALA:HA	1:A:551:LYS:CB	2.15	0.77
1:B:1685:LYS:HE3	1:B:1686:TYR:CE1	2.20	0.77
1:A:325:ARG:NH1	1:A:325:ARG:HB3	2.00	0.76
1:B:1605:THR:HG22	1:B:1672:TYR:CB	2.14	0.76
1:A:346:THR:HG22	1:A:409:LYS:HA	1.66	0.76
1:B:1198:GLN:HG3	1:B:1201:GLN:OE1	1.84	0.76
1:B:1633:GLN:CG	1:B:1634:ILE:H	1.96	0.76
1:A:221:LEU:HD13	1:A:281:ILE:CD1	2.16	0.76
1:B:1338:VAL:HG11	1:B:1470:MET:HE3	1.68	0.76
1:A:568:ILE:O	1:A:572:VAL:HG23	1.86	0.76
1:B:1296:ASP:O	1:B:1299:VAL:HG22	1.86	0.75
1:B:1139:GLU:HA	1:B:1142:GLN:HG2	1.67	0.75
1:B:1658:LYS:HA	1:B:1658:LYS:HE2	1.69	0.75
1:A:536:GLY:O	1:B:1593:ARG:NH2	2.19	0.75
1:A:296:ASP:O	1:A:299:VAL:HG22	1.87	0.75
1:A:658:LYS:HA	1:A:658:LYS:HE2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1365:LYS:HG3	1:B:1391:THR:HG22	1.69	0.74
1:B:1325:ARG:HB3	1:B:1325:ARG:NH1	2.01	0.74
1:B:1568:ILE:O	1:B:1572:VAL:HG23	1.86	0.74
1:A:325:ARG:HH11	1:A:325:ARG:HB3	1.52	0.74
1:A:573:LYS:HA	1:A:577:LEU:HD13	1.68	0.74
1:A:268:THR:O	1:A:272:GLU:HG3	1.87	0.74
1:B:1268:THR:O	1:B:1272:GLU:HG3	1.88	0.74
1:A:522:ILE:H	1:A:522:ILE:HD13	1.51	0.73
1:B:1179:LEU:HD12	1:B:1182:GLN:OE1	1.88	0.73
1:B:1573:LYS:HA	1:B:1577:LEU:HD13	1.69	0.73
1:A:654:ILE:HG21	1:A:683:PHE:CE1	2.23	0.73
1:B:1597:ILE:HA	1:B:1674:TYR:HE1	1.53	0.73
1:A:344:GLN:HG2	1:A:410:HIS:HA	1.71	0.72
1:A:623:TRP:CH2	1:A:659:ILE:HD13	2.25	0.72
1:B:1475:ALA:HB2	1:B:1562:TRP:CD1	2.25	0.72
1:A:475:ALA:HB2	1:A:562:TRP:CD1	2.24	0.72
1:B:1325:ARG:HB3	1:B:1325:ARG:HH11	1.53	0.71
1:B:1641:THR:HG23	1:B:1644:GLN:HE21	1.55	0.71
1:A:504:VAL:HG12	1:A:508:LEU:HD11	1.73	0.71
1:B:1355:PHE:HB2	1:B:1358:LEU:HD12	1.73	0.71
1:A:503:GLN:O	1:A:507:VAL:HG23	1.90	0.71
1:A:641:THR:HG23	1:A:644:GLN:HE21	1.55	0.71
1:B:1148:LEU:HD12	1:B:1231:VAL:HG11	1.73	0.71
1:A:661:ASP:HB2	1:A:667:VAL:HG13	1.71	0.71
1:B:1576:ILE:CA	1:B:1579:LEU:HD13	2.20	0.71
1:B:1619:VAL:HG23	1:B:1650:PHE:CE1	2.26	0.71
1:A:475:ALA:HB2	1:A:562:TRP:NE1	2.06	0.71
1:B:1332:HIS:CE1	1:B:1467:ILE:HD11	2.26	0.70
1:B:1475:ALA:HB2	1:B:1562:TRP:NE1	2.06	0.70
1:B:1151:VAL:O	1:B:1155:VAL:HG23	1.91	0.70
1:B:1483:LEU:HD13	1:B:1497:PRO:HB2	1.73	0.70
1:A:547:ALA:HB1	1:A:552:GLU:OE1	1.92	0.70
1:B:1152:ARG:HH22	1:B:1272:GLU:HB2	1.56	0.70
1:A:248:GLN:HE22	1:A:485:ASN:HA	1.55	0.70
1:A:576:ILE:CA	1:A:579:LEU:HD13	2.21	0.70
1:A:252:ILE:CG2	1:A:481:ASN:HD22	2.05	0.70
1:A:162:MET:O	1:A:166:GLU:HG3	1.92	0.70
1:A:604:GLY:HA2	1:A:670:LEU:HD12	1.72	0.70
1:B:1530:GLU:HG3	1:B:1534:GLY:O	1.91	0.70
1:A:637:VAL:HG13	1:A:638:GLU:N	2.07	0.70
1:B:1162:MET:O	1:B:1166:GLU:HG3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:GLU:HG3	1:A:534:GLY:O	1.92	0.70
1:B:1504:VAL:HG12	1:B:1508:LEU:HD11	1.73	0.70
1:B:1283:LYS:HA	1:B:1286:GLU:HG3	1.74	0.70
1:B:1685:LYS:HE3	1:B:1686:TYR:HE1	1.57	0.70
1:A:483:LEU:HD13	1:A:497:PRO:HB2	1.74	0.70
1:A:288:GLN:OE1	1:A:302:ARG:NH2	2.23	0.69
1:B:1386:ILE:O	1:B:1387:LEU:HD23	1.92	0.69
1:B:1531:LYS:HZ1	1:B:1612:GLU:HB3	1.57	0.69
1:B:1470:MET:CB	1:B:1471:PRO:HD3	2.22	0.69
1:B:1498:ILE:HD12	1:B:1498:ILE:H	1.56	0.69
1:B:1288:GLN:OE1	1:B:1302:ARG:NH2	2.25	0.69
1:A:287:LEU:C	1:A:289:GLN:H	1.95	0.69
1:B:1503:GLN:O	1:B:1507:VAL:HG23	1.92	0.69
1:B:1547:ALA:HB1	1:B:1552:GLU:OE1	1.91	0.69
1:A:252:ILE:HB	1:A:478:LEU:HD23	1.74	0.69
1:B:1637:VAL:HG13	1:B:1638:GLU:N	2.07	0.69
1:A:151:VAL:O	1:A:155:VAL:HG23	1.93	0.69
1:B:1531:LYS:NZ	1:B:1612:GLU:HB3	2.08	0.69
1:A:379:ARG:HD3	1:A:380:GLY:N	2.07	0.69
1:B:1287:LEU:C	1:B:1289:GLN:H	1.95	0.69
1:B:1554:MET:HB2	1:B:1557:LYS:HB2	1.75	0.69
1:A:386:ILE:HG22	1:A:411:LEU:HD22	1.74	0.69
1:A:596:ALA:HB1	1:B:1535:PRO:HB2	1.74	0.69
1:A:535:PRO:HG3	1:B:1600:THR:HB	1.75	0.69
1:A:644:GLN:C	1:A:646:ASN:H	1.97	0.68
1:B:1337:LEU:HA	1:B:1461:VAL:HG22	1.74	0.68
1:A:386:ILE:O	1:A:387:LEU:HD23	1.93	0.68
1:B:1598:LEU:HD22	1:B:1623:TRP:C	2.14	0.68
1:A:493:PHE:HA	1:A:496:PRO:HG3	1.75	0.68
1:B:1493:PHE:HA	1:B:1496:PRO:HG3	1.75	0.68
1:A:596:ALA:HB1	1:B:1535:PRO:CB	2.24	0.68
1:A:470:MET:CB	1:A:471:PRO:HD3	2.22	0.68
1:A:355:PHE:HB2	1:A:358:LEU:HD12	1.76	0.68
1:B:1137:VAL:HG22	1:B:1262:ARG:NH2	2.07	0.68
1:A:446:TYR:HA	1:A:450:LEU:O	1.94	0.68
1:B:1583:GLY:O	1:B:1585:ILE:N	2.27	0.67
1:A:337:LEU:HA	1:A:461:VAL:HG22	1.76	0.67
1:A:211:ASP:O	1:A:215:ARG:HG3	1.94	0.67
1:A:573:LYS:O	1:A:577:LEU:HD22	1.94	0.67
1:A:593:ARG:NH2	1:B:1536:GLY:O	2.26	0.67
1:B:1532:LEU:HD12	1:B:1561:PHE:CE2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1517:LYS:N	1:B:1517:LYS:HD2	2.08	0.67
1:B:1573:LYS:O	1:B:1577:LEU:HD22	1.94	0.67
1:A:417:ARG:HG2	1:A:418:CYS:H	1.59	0.67
1:B:1644:GLN:C	1:B:1646:ASN:H	1.98	0.66
1:B:1631:LYS:O	1:B:1632:THR:C	2.34	0.66
1:B:1284:LEU:HD22	1:B:1298:ILE:CD1	2.26	0.66
1:A:554:MET:HB2	1:A:557:LYS:HB2	1.76	0.66
1:B:1564:TRP:CD2	1:B:1568:ILE:HD11	2.30	0.66
1:B:1196:THR:HB	1:B:1199:LYS:HB2	1.78	0.66
1:B:1267:ILE:HG23	1:B:1316:LEU:HD11	1.78	0.66
1:A:283:LYS:HA	1:A:286:GLU:HG3	1.76	0.66
1:B:1288:GLN:HE21	1:B:1298:ILE:HG22	1.61	0.66
1:B:1211:ASP:O	1:B:1215:ARG:HG3	1.95	0.66
1:B:1675:PRO:HB2	1:B:1677:ILE:HG13	1.77	0.66
1:A:532:LEU:HD12	1:A:561:PHE:CE2	2.30	0.66
1:B:1591:LYS:HE2	1:B:1609:ARG:NH2	2.10	0.66
1:A:515:THR:HG21	1:A:573:LYS:HG3	1.78	0.66
1:B:1446:TYR:HA	1:B:1450:LEU:O	1.96	0.66
1:B:1444:GLU:OE1	1:B:1451:LYS:HE3	1.95	0.66
1:B:1583:GLY:C	1:B:1585:ILE:H	1.99	0.66
1:B:1252:ILE:CG2	1:B:1481:ASN:HD22	2.09	0.66
1:A:479:TRP:HD1	1:A:492:PHE:HE1	1.44	0.65
1:B:1252:ILE:HB	1:B:1478:LEU:HD23	1.77	0.65
1:A:523:GLU:HG2	1:B:1537:VAL:HG11	1.78	0.65
1:A:686:TYR:H	1:A:686:TYR:HD2	1.44	0.65
1:A:633:GLN:HG3	1:A:634:ILE:N	2.12	0.65
1:A:498:ILE:HD12	1:A:545:THR:HG22	1.78	0.65
1:B:1344:GLN:HG2	1:B:1410:HIS:HA	1.77	0.65
1:A:611:SER:HB3	1:A:614:SER:OG	1.97	0.65
1:A:267:ILE:HG23	1:A:316:LEU:HD11	1.78	0.65
1:A:309:ILE:O	1:A:309:ILE:HD13	1.97	0.65
1:B:1515:THR:HG21	1:B:1573:LYS:HG3	1.77	0.65
1:A:246:ARG:HG2	1:A:258:ILE:CG2	2.27	0.65
1:A:444:GLU:OE1	1:A:451:LYS:HE3	1.96	0.65
1:B:1248:GLN:HE22	1:B:1485:ASN:HA	1.61	0.64
1:A:657:TYR:CE2	1:A:659:ILE:HG12	2.33	0.64
1:A:517:LYS:HD2	1:A:517:LYS:N	2.06	0.64
1:A:512:PHE:HB3	1:A:518:ARG:O	1.97	0.64
1:A:338:VAL:HG11	1:A:470:MET:CE	2.26	0.64
1:A:460:PRO:HD3	1:A:487:PRO:O	1.98	0.64
1:A:583:GLY:C	1:A:585:ILE:H	2.01	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ILE:HG23	1:A:481:ASN:HD22	1.62	0.64
1:A:379:ARG:HH11	1:A:380:GLY:H	1.45	0.64
1:B:1479:TRP:HD1	1:B:1492:PHE:HE1	1.45	0.64
1:A:675:PRO:HB2	1:A:677:ILE:HG13	1.79	0.64
1:B:1609:ARG:HH11	1:B:1620:THR:HG21	1.63	0.64
1:B:1263:LEU:O	1:B:1267:ILE:HG13	1.98	0.63
1:B:1460:PRO:HD3	1:B:1487:PRO:O	1.98	0.63
1:B:1582:GLU:CD	1:B:1582:GLU:H	2.02	0.63
1:A:609:ARG:HH11	1:A:620:THR:HG21	1.64	0.63
1:B:1288:GLN:HB2	1:B:1298:ILE:HG21	1.80	0.63
1:A:623:TRP:CB	1:A:670:LEU:HG	2.29	0.63
1:B:1335:ARG:HG3	1:B:1470:MET:SD	2.38	0.63
1:A:583:GLY:O	1:A:585:ILE:N	2.29	0.62
1:B:1493:PHE:HD1	1:B:1496:PRO:HG3	1.63	0.62
1:A:650:PHE:CA	1:A:653:ILE:HD13	2.23	0.62
1:A:288:GLN:HB2	1:A:298:ILE:HG21	1.82	0.62
1:A:148:LEU:HD12	1:A:231:VAL:HG11	1.81	0.62
1:B:1512:PHE:HB3	1:B:1518:ARG:O	1.99	0.62
1:A:582:GLU:CD	1:A:582:GLU:H	2.03	0.62
1:B:1686:TYR:N	1:B:1686:TYR:CD1	2.68	0.62
1:A:493:PHE:HD1	1:A:496:PRO:HG3	1.64	0.62
1:B:1320:ALA:CB	1:B:1353:VAL:HG23	2.29	0.62
1:A:597:ILE:HD11	1:A:634:ILE:HD12	1.80	0.62
1:A:143:MET:O	1:A:146:GLN:HB3	2.00	0.62
1:A:602:PRO:HG2	1:A:605:THR:HG23	1.82	0.62
1:A:210:LEU:O	1:A:214:ARG:HG3	2.00	0.62
1:B:1368:ILE:CG2	1:B:1386:ILE:HG13	2.30	0.62
1:B:1672:TYR:HA	1:B:1677:ILE:O	2.00	0.62
1:A:576:ILE:CD1	1:A:645:LEU:HD13	2.30	0.62
1:A:320:ALA:CB	1:A:353:VAL:HG23	2.30	0.62
1:A:537:VAL:CG1	1:B:1523:GLU:HG2	2.27	0.61
1:B:1246:ARG:HG2	1:B:1258:ILE:CG2	2.28	0.61
1:A:235:LEU:HD13	1:A:267:ILE:CD1	2.25	0.61
1:B:1287:LEU:C	1:B:1289:GLN:N	2.53	0.61
1:A:654:ILE:HG21	1:A:683:PHE:CD1	2.36	0.61
1:A:571:LEU:O	1:A:575:TYR:O	2.18	0.61
1:B:1143:MET:O	1:B:1146:GLN:HB3	1.99	0.61
1:A:445:VAL:HB	1:A:452:ILE:HG22	1.82	0.61
1:A:531:LYS:HZ1	1:A:612:GLU:HB3	1.65	0.61
1:A:270:LEU:O	1:A:274:GLN:HG3	2.01	0.61
1:A:631:LYS:O	1:A:632:THR:C	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1651:ALA:HB3	1:B:1688:ARG:HH22	1.66	0.61
1:A:287:LEU:C	1:A:289:GLN:N	2.54	0.61
1:A:245:ARG:HE	1:A:249:ILE:HD11	1.66	0.61
1:B:1595:ARG:O	1:B:1599:SER:HB2	2.01	0.61
1:B:1195:VAL:HG21	1:B:1200:MET:CE	2.31	0.61
1:B:1611:SER:HB3	1:B:1614:SER:OG	2.01	0.61
1:B:1602:PRO:HG2	1:B:1605:THR:HG23	1.81	0.61
1:B:1283:LYS:O	1:B:1287:LEU:HD13	2.01	0.61
1:A:576:ILE:HD11	1:A:645:LEU:HD13	1.83	0.60
1:B:1210:LEU:O	1:B:1214:ARG:HG3	2.01	0.60
1:A:288:GLN:HE21	1:A:298:ILE:HG22	1.64	0.60
1:A:304:MET:HA	1:A:304:MET:CE	2.29	0.60
1:B:1138:THR:HG23	1:B:1141:GLN:NE2	2.16	0.60
1:A:517:LYS:CD	1:A:517:LYS:H	2.05	0.60
1:A:288:GLN:CD	1:A:302:ARG:HH21	2.05	0.60
1:B:1523:GLU:HG3	1:B:1524:GLN:N	2.17	0.60
1:A:597:ILE:HD11	1:A:634:ILE:CD1	2.30	0.60
1:B:1605:THR:HA	1:B:1672:TYR:O	2.02	0.60
1:B:1565:LEU:HA	1:B:1568:ILE:CG1	2.32	0.60
1:A:549:PHE:O	1:A:561:PHE:HB3	2.02	0.60
1:B:1248:GLN:O	1:B:1251:CYS:HB2	2.01	0.60
1:B:1571:LEU:O	1:B:1575:TYR:O	2.19	0.60
1:A:550:CYS:HB3	1:A:562:TRP:HB3	1.83	0.60
1:B:1598:LEU:HD23	1:B:1632:THR:HG22	1.84	0.59
1:A:137:VAL:CG2	1:A:262:ARG:HH22	2.13	0.59
1:B:1384:PHE:O	1:B:1385:ASN:ND2	2.34	0.59
1:B:1270:LEU:O	1:B:1274:GLN:HG3	2.02	0.59
1:A:672:TYR:HA	1:A:677:ILE:O	2.01	0.59
1:B:1155:VAL:O	1:B:1159:GLU:HB2	2.01	0.59
1:A:512:PHE:CB	1:A:519:GLY:HA2	2.31	0.59
1:A:171:ASP:HB2	1:A:206:MET:HE1	1.84	0.59
1:B:1550:CYS:HB3	1:B:1562:TRP:HB3	1.83	0.59
1:A:314:ARG:O	1:A:318:LYS:HG3	2.02	0.59
1:B:1528:LEU:HA	1:B:1531:LYS:HB2	1.84	0.59
1:B:1304:MET:HA	1:B:1304:MET:CE	2.31	0.59
1:B:1603:PRO:HB3	1:B:1632:THR:HG21	1.84	0.59
1:B:1668:SER:HB2	1:B:1669:PRO:HD2	1.84	0.59
1:B:1282:LYS:O	1:B:1286:GLU:HG2	2.02	0.59
1:A:155:VAL:O	1:A:159:GLU:HB2	2.03	0.59
1:B:1445:VAL:HB	1:B:1452:ILE:HG22	1.84	0.59
1:A:597:ILE:C	1:A:600:THR:HG22	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PHE:HB2	1:A:206:MET:HE2	1.84	0.59
1:A:288:GLN:NE2	1:A:299:VAL:HA	2.18	0.59
1:A:523:GLU:HG3	1:A:524:GLN:N	2.18	0.59
1:B:1622:THR:HG22	1:B:1623:TRP:N	2.18	0.59
1:B:1136:VAL:HG22	1:B:1137:VAL:H	1.67	0.59
1:B:1412:THR:HG22	1:B:1413:LEU:N	2.18	0.59
1:B:1179:LEU:HD22	1:B:1199:LYS:O	2.03	0.59
1:A:668:SER:HB2	1:A:669:PRO:HD2	1.84	0.58
1:A:412:THR:HG22	1:A:413:LEU:N	2.17	0.58
1:B:1338:VAL:HG11	1:B:1470:MET:CE	2.34	0.58
1:A:152:ARG:HH22	1:A:272:GLU:HB2	1.69	0.58
1:A:384:PHE:O	1:A:385:ASN:ND2	2.37	0.58
1:B:1245:ARG:HE	1:B:1249:ILE:HD11	1.69	0.58
1:A:576:ILE:O	1:A:576:ILE:HG22	2.03	0.58
1:B:1314:ARG:O	1:B:1318:LYS:HG3	2.04	0.58
1:B:1236:THR:O	1:B:1240:LEU:HB3	2.02	0.58
1:A:528:LEU:HA	1:A:531:LYS:HB2	1.84	0.58
1:A:283:LYS:O	1:A:287:LEU:HD13	2.02	0.58
1:A:547:ALA:CA	1:A:551:LYS:HB3	2.28	0.58
1:B:1441:PHE:O	1:B:1442:GLU:HG3	2.04	0.58
1:A:565:LEU:HA	1:A:568:ILE:CG1	2.33	0.58
1:A:686:TYR:N	1:A:686:TYR:CD2	2.71	0.58
1:B:1654:ILE:HG21	1:B:1683:PHE:CD1	2.39	0.57
1:B:1637:VAL:HG22	1:B:1638:GLU:H	1.69	0.57
1:B:1248:GLN:HE21	1:B:1481:ASN:HA	1.69	0.57
1:A:591:LYS:O	1:A:594:GLU:HB3	2.03	0.57
1:A:282:LYS:O	1:A:286:GLU:HG2	2.05	0.57
1:B:1564:TRP:O	1:B:1568:ILE:HG13	2.04	0.57
1:B:1549:PHE:O	1:B:1561:PHE:HB3	2.03	0.57
1:B:1598:LEU:HD22	1:B:1623:TRP:O	2.03	0.57
1:B:1258:ILE:HD12	1:B:1258:ILE:O	2.04	0.57
1:B:1510:TRP:HA	1:B:1513:SER:OG	2.04	0.57
1:A:437:HIS:HD2	1:A:463:VAL:HG23	1.69	0.57
1:A:674:TYR:HB3	1:A:675:PRO:HD3	1.85	0.57
1:B:1633:GLN:C	1:B:1634:ILE:HD12	2.25	0.57
1:B:1576:ILE:HG22	1:B:1576:ILE:O	2.05	0.57
1:B:1288:GLN:NE2	1:B:1299:VAL:HA	2.20	0.57
1:A:354:LYS:HG2	1:A:396:MET:CE	2.33	0.57
1:A:248:GLN:HE21	1:A:481:ASN:HA	1.69	0.57
1:B:1156:GLN:O	1:B:1159:GLU:HB3	2.05	0.57
1:B:1559:PHE:CE2	1:B:1564:TRP:HB2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1498:ILE:HG22	1:B:1499:GLY:H	1.70	0.57
1:B:1591:LYS:O	1:B:1594:GLU:HB3	2.04	0.56
1:A:498:ILE:HG22	1:A:499:GLY:H	1.70	0.56
1:A:248:GLN:O	1:A:251:CYS:HB2	2.04	0.56
1:A:510:TRP:HA	1:A:513:SER:OG	2.04	0.56
1:A:658:LYS:NZ	1:A:668:SER:HA	2.20	0.56
1:B:1547:ALA:CA	1:B:1551:LYS:HB3	2.26	0.56
1:A:623:TRP:CD1	1:A:623:TRP:N	2.73	0.56
1:B:1517:LYS:CD	1:B:1517:LYS:H	2.05	0.56
1:A:258:ILE:HD12	1:A:258:ILE:O	2.04	0.56
1:B:1318:LYS:HA	1:B:1454:LEU:CD2	2.35	0.56
1:B:1288:GLN:CD	1:B:1302:ARG:HH21	2.08	0.56
1:A:653:ILE:N	1:A:653:ILE:HD12	2.21	0.56
1:B:1284:LEU:HD22	1:B:1298:ILE:HD11	1.87	0.56
1:B:1284:LEU:HD22	1:B:1298:ILE:HD12	1.87	0.56
1:A:565:LEU:HA	1:A:568:ILE:HG12	1.87	0.56
1:A:527:THR:HG21	1:A:589:ILE:HA	1.88	0.56
1:B:1437:HIS:HD2	1:B:1463:VAL:HG23	1.69	0.56
1:B:1337:LEU:CA	1:B:1461:VAL:HG22	2.35	0.56
1:A:664:ASN:O	1:A:665:ILE:HD13	2.06	0.56
1:A:653:ILE:HD12	1:A:653:ILE:H	1.71	0.56
1:B:1641:THR:CG2	1:B:1644:GLN:HE21	2.19	0.56
1:A:311:GLU:HA	1:A:311:GLU:OE1	2.06	0.56
1:A:441:PHE:O	1:A:442:GLU:HG3	2.05	0.56
1:B:1674:TYR:HB3	1:B:1675:PRO:HD3	1.87	0.56
1:B:1215:ARG:HH11	1:B:1215:ARG:HG2	1.70	0.56
1:B:1575:TYR:O	1:B:1576:ILE:HB	2.06	0.56
1:A:575:TYR:C	1:A:576:ILE:HD12	2.26	0.56
1:B:1252:ILE:HG23	1:B:1481:ASN:HD22	1.70	0.56
1:B:1498:ILE:CG2	1:B:1543:GLN:HB3	2.35	0.56
1:A:221:LEU:HD22	1:A:281:ILE:HD11	1.88	0.55
1:B:1215:ARG:NH1	1:B:1215:ARG:HG2	2.21	0.55
1:B:1584:TYR:O	1:B:1608:LEU:HD12	2.06	0.55
1:A:575:TYR:O	1:A:576:ILE:HB	2.06	0.55
1:B:1512:PHE:CB	1:B:1519:GLY:HA2	2.34	0.55
1:A:559:PHE:CE2	1:A:564:TRP:HB2	2.41	0.55
1:A:531:LYS:NZ	1:A:612:GLU:HB3	2.21	0.55
1:B:1311:GLU:HA	1:B:1311:GLU:OE1	2.06	0.55
1:A:594:GLU:HG3	1:A:607:LEU:CD2	2.36	0.55
1:A:368:ILE:HG21	1:A:385:ASN:HA	1.89	0.55
1:A:349:VAL:O	1:A:405:SER:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1623:TRP:CD1	1:B:1623:TRP:N	2.75	0.55
1:A:137:VAL:HG22	1:A:262:ARG:NH2	2.12	0.55
1:A:344:GLN:CG	1:A:410:HIS:HA	2.35	0.55
1:A:644:GLN:O	1:A:646:ASN:N	2.39	0.55
1:A:637:VAL:HG22	1:A:638:GLU:H	1.71	0.55
1:A:215:ARG:HG2	1:A:215:ARG:NH1	2.22	0.55
1:B:1527:THR:HG21	1:B:1589:ILE:HA	1.88	0.55
1:A:236:THR:O	1:A:240:LEU:HB3	2.05	0.55
1:A:564:TRP:O	1:A:568:ILE:HG12	2.06	0.55
1:B:1567:ASN:O	1:B:1571:LEU:HB2	2.07	0.55
1:A:279:GLN:NE2	1:A:282:LYS:HD2	2.22	0.55
1:A:365:LYS:HG3	1:A:391:THR:HG22	1.89	0.55
1:B:1669:PRO:HG2	1:B:1679:LYS:HE3	1.89	0.55
1:B:1279:GLN:NE2	1:B:1282:LYS:HD2	2.22	0.55
1:B:1686:TYR:N	1:B:1686:TYR:HD1	2.04	0.55
1:A:522:ILE:N	1:A:522:ILE:HD13	2.20	0.55
1:A:669:PRO:HG2	1:A:679:LYS:HE3	1.88	0.55
1:B:1195:VAL:HG12	1:B:1196:THR:N	2.19	0.55
1:A:659:ILE:O	1:A:660:MET:C	2.46	0.55
1:B:1365:LYS:HG3	1:B:1391:THR:CG2	2.37	0.54
1:B:1368:ILE:HG21	1:B:1386:ILE:HG13	1.89	0.54
1:A:175:ASN:O	1:A:178:THR:HG22	2.06	0.54
1:A:641:THR:CG2	1:A:644:GLN:HE21	2.19	0.54
1:B:1224:LEU:O	1:B:1228:MET:HG3	2.07	0.54
1:B:1644:GLN:O	1:B:1646:ASN:N	2.40	0.54
1:A:215:ARG:HG2	1:A:215:ARG:HH11	1.72	0.54
1:B:1479:TRP:HD1	1:B:1492:PHE:CE1	2.25	0.54
1:A:179:LEU:HD21	1:A:200:MET:HA	1.89	0.54
1:B:1314:ARG:HG3	1:B:1452:ILE:HD11	1.90	0.54
1:B:1610:PHE:HA	1:B:1618:GLY:O	2.06	0.54
1:A:414:ARG:HG2	1:A:415:GLU:H	1.73	0.54
1:A:260:LEU:HB2	1:A:350:ARG:HH21	1.73	0.54
1:B:1195:VAL:HG11	1:B:1200:MET:HE1	1.90	0.54
1:B:1594:GLU:HG3	1:B:1607:LEU:HD22	1.89	0.54
1:B:1337:LEU:O	1:B:1461:VAL:HG13	2.06	0.54
1:B:1325:ARG:NH1	1:B:1325:ARG:CB	2.70	0.54
1:A:337:LEU:O	1:A:461:VAL:HG13	2.07	0.54
1:A:337:LEU:CA	1:A:461:VAL:HG22	2.37	0.54
1:B:1565:LEU:HA	1:B:1568:ILE:HG13	1.89	0.54
1:A:559:PHE:HB3	1:A:615:LYS:HE3	1.90	0.54
1:A:567:ASN:O	1:A:571:LEU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:THR:CG2	1:A:413:LEU:N	2.71	0.54
1:B:1632:THR:HG22	1:B:1632:THR:O	2.08	0.54
1:B:1148:LEU:CD1	1:B:1231:VAL:HG11	2.37	0.54
1:A:621:PHE:O	1:A:636:SER:HA	2.08	0.54
1:A:398:GLU:O	1:A:401:ASN:N	2.41	0.54
1:B:1498:ILE:N	1:B:1498:ILE:HD12	2.23	0.53
1:B:1504:VAL:HG12	1:B:1508:LEU:CD1	2.38	0.53
1:B:1414:ARG:HG2	1:B:1415:GLU:H	1.74	0.53
1:A:488:LYS:HG3	1:A:488:LYS:O	2.09	0.53
1:B:1597:ILE:CG1	1:B:1598:LEU:N	2.68	0.53
1:B:1564:TRP:CE2	1:B:1568:ILE:HD11	2.43	0.53
1:A:325:ARG:NH1	1:A:325:ARG:CB	2.69	0.53
1:A:650:PHE:CD2	1:A:654:ILE:HD11	2.43	0.53
1:A:335:ARG:HG3	1:A:470:MET:SD	2.49	0.53
1:A:156:GLN:O	1:A:159:GLU:HB3	2.08	0.53
1:A:623:TRP:CE3	1:A:670:LEU:HD21	2.44	0.53
1:A:504:VAL:HG12	1:A:508:LEU:CD1	2.38	0.53
1:A:477:ILE:HG22	1:A:478:LEU:N	2.24	0.53
1:B:1396:MET:HG3	1:B:1404:LEU:HD23	1.91	0.53
1:B:1175:ASN:O	1:B:1178:THR:HG22	2.08	0.53
1:B:1619:VAL:O	1:B:1619:VAL:HG23	2.09	0.53
1:A:158:LEU:HG	1:A:220:GLU:OE1	2.09	0.53
1:A:287:LEU:N	1:A:287:LEU:CD1	2.72	0.53
1:A:505:ALA:HB1	1:A:525:LEU:HD21	1.90	0.53
1:A:623:TRP:CD1	1:A:635:GLN:O	2.62	0.53
1:A:660:MET:HB2	1:A:666:LEU:CG	2.38	0.53
1:B:1557:LYS:H	1:B:1557:LYS:HD2	1.74	0.53
1:A:685:LYS:HE3	1:A:686:TYR:HE2	1.74	0.53
1:B:1412:THR:CG2	1:B:1413:LEU:N	2.71	0.53
1:B:1431:ILE:N	1:B:1431:ILE:HD13	2.24	0.53
1:A:594:GLU:HG3	1:A:607:LEU:HD22	1.90	0.52
1:A:658:LYS:HZ3	1:A:668:SER:HA	1.73	0.52
1:A:619:VAL:O	1:A:619:VAL:HG23	2.08	0.52
1:B:1505:ALA:HB1	1:B:1525:LEU:HD21	1.91	0.52
1:B:1687:CYS:HA	1:B:1688:ARG:HH21	1.74	0.52
1:A:248:GLN:NE2	1:A:485:ASN:HA	2.23	0.52
1:B:1260:LEU:HB2	1:B:1350:ARG:HH21	1.74	0.52
1:A:621:PHE:CZ	1:A:637:VAL:HG11	2.43	0.52
1:B:1678:PRO:O	1:B:1680:GLU:N	2.40	0.52
1:A:670:LEU:N	1:A:670:LEU:CD2	2.68	0.52
1:A:610:PHE:HA	1:A:618:GLY:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1379:ARG:NH1	1:B:1380:GLY:H	2.02	0.52
1:B:1559:PHE:CD2	1:B:1564:TRP:HB2	2.44	0.52
1:A:659:ILE:O	1:A:667:VAL:CG2	2.57	0.52
1:A:441:PHE:C	1:A:442:GLU:HG3	2.30	0.52
1:A:633:GLN:CG	1:A:634:ILE:N	2.72	0.52
1:B:1201:GLN:C	1:B:1203:LEU:H	2.12	0.52
1:A:364:ILE:HD13	1:A:443:THR:HG21	1.92	0.52
1:B:1195:VAL:HB	1:B:1200:MET:HE2	1.92	0.52
1:B:1477:ILE:HG22	1:B:1478:LEU:N	2.24	0.52
1:A:559:PHE:CD2	1:A:564:TRP:HB2	2.45	0.52
1:A:557:LYS:HD2	1:A:557:LYS:H	1.75	0.52
1:A:340:LYS:HB3	1:A:343:VAL:HG21	1.91	0.52
1:A:633:GLN:HG3	1:A:634:ILE:H	1.74	0.52
1:A:386:ILE:CG2	1:A:411:LEU:HD22	2.38	0.52
1:A:366:VAL:HA	1:A:440:THR:O	2.09	0.52
1:A:600:THR:HG23	1:A:601:LYS:HG2	1.92	0.51
1:B:1594:GLU:HG3	1:B:1607:LEU:CD2	2.39	0.51
1:B:1571:LEU:HD11	1:B:1576:ILE:HD12	1.91	0.51
1:A:438:LEU:HD21	1:A:460:PRO:HG3	1.91	0.51
1:A:658:LYS:CE	1:A:669:PRO:HD3	2.40	0.51
1:B:1609:ARG:NH1	1:B:1620:THR:HG21	2.25	0.51
1:B:1521:SER:O	1:B:1525:LEU:HB2	2.10	0.51
1:A:362:LEU:HD11	1:A:445:VAL:HG22	1.92	0.51
1:A:475:ALA:HB2	1:A:562:TRP:HE1	1.76	0.51
1:A:479:TRP:HD1	1:A:492:PHE:CE1	2.25	0.51
1:B:1438:LEU:HD21	1:B:1460:PRO:HG3	1.93	0.51
1:A:654:ILE:HG22	1:A:654:ILE:O	2.10	0.51
1:A:476:SER:HB3	1:A:493:PHE:CE2	2.46	0.51
1:B:1493:PHE:CD1	1:B:1496:PRO:HG3	2.45	0.51
1:A:671:VAL:HG12	1:A:679:LYS:HZ3	1.75	0.51
1:B:1379:ARG:C	1:B:1381:SER:H	2.14	0.51
1:A:498:ILE:CG2	1:A:543:GLN:HB3	2.36	0.51
1:B:1550:CYS:HB3	1:B:1562:TRP:CB	2.40	0.51
1:B:1340:LYS:HB3	1:B:1343:VAL:HG21	1.92	0.51
1:A:609:ARG:NH1	1:A:620:THR:HG21	2.26	0.51
1:A:605:THR:HA	1:A:671:VAL:O	2.11	0.51
1:A:517:LYS:CD	1:A:517:LYS:N	2.71	0.51
1:A:512:PHE:CZ	1:A:569:ILE:HD13	2.45	0.51
1:A:172:PHE:HD1	1:A:206:MET:HB3	1.75	0.51
1:A:302:ARG:N	1:A:303:PRO:CD	2.74	0.51
1:B:1475:ALA:HB2	1:B:1562:TRP:HE1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:C	1:A:146:GLN:N	2.63	0.51
1:A:288:GLN:CG	1:A:299:VAL:HG12	2.41	0.51
1:A:493:PHE:O	1:A:496:PRO:HD3	2.11	0.51
1:B:1332:HIS:HB3	1:B:1335:ARG:HB2	1.92	0.51
1:B:1276:GLN:O	1:B:1280:GLN:HG2	2.11	0.51
1:B:1287:LEU:CD1	1:B:1287:LEU:N	2.73	0.51
1:B:1604:GLY:O	1:B:1670:LEU:HB3	2.11	0.50
1:A:176:TYR:HA	1:A:203:LEU:HD21	1.93	0.50
1:A:332:HIS:HB3	1:A:335:ARG:HB2	1.92	0.50
1:A:521:SER:O	1:A:525:LEU:HB2	2.12	0.50
1:B:1520:LEU:HB2	1:B:1525:LEU:HD13	1.93	0.50
1:B:1252:ILE:HG21	1:B:1481:ASN:HD22	1.77	0.50
1:A:634:ILE:C	1:A:635:GLN:HG3	2.32	0.50
1:B:1600:THR:HG23	1:B:1601:LYS:HG2	1.93	0.50
1:A:332:HIS:CE1	1:A:467:ILE:HD11	2.47	0.50
1:B:1144:LEU:C	1:B:1146:GLN:N	2.62	0.50
1:B:1654:ILE:HG22	1:B:1654:ILE:O	2.11	0.50
1:A:473:ALA:O	1:A:476:SER:N	2.45	0.50
1:A:584:TYR:O	1:A:608:LEU:HD12	2.12	0.50
1:B:1670:LEU:N	1:B:1670:LEU:CD2	2.69	0.50
1:A:473:ALA:C	1:A:475:ALA:N	2.65	0.50
1:B:1594:GLU:O	1:B:1597:ILE:HG12	2.12	0.50
1:A:280:GLN:NE2	1:A:280:GLN:HA	2.16	0.50
1:B:1302:ARG:N	1:B:1303:PRO:CD	2.74	0.50
1:A:148:LEU:CD1	1:A:231:VAL:HG11	2.42	0.50
1:A:288:GLN:NE2	1:A:302:ARG:HH21	2.09	0.50
1:A:550:CYS:HB3	1:A:562:TRP:CB	2.41	0.50
1:B:1586:MET:O	1:B:1588:PHE:N	2.45	0.50
1:A:585:ILE:HG22	1:A:587:GLY:N	2.27	0.49
1:A:573:LYS:CA	1:A:577:LEU:HD13	2.41	0.49
1:B:1285:GLU:O	1:B:1289:GLN:HG3	2.12	0.49
1:B:1476:SER:HB3	1:B:1493:PHE:CE2	2.47	0.49
1:B:1441:PHE:C	1:B:1442:GLU:HG3	2.30	0.49
1:A:530:GLU:C	1:A:532:LEU:H	2.15	0.49
1:A:605:THR:HG22	1:A:672:TYR:CB	2.35	0.49
1:A:201:GLN:C	1:A:203:LEU:H	2.14	0.49
1:A:493:PHE:CD1	1:A:496:PRO:HG3	2.47	0.49
1:B:1488:LYS:O	1:B:1488:LYS:HG3	2.12	0.49
1:B:1576:ILE:HA	1:B:1579:LEU:CD1	2.31	0.49
1:A:209:ALA:O	1:A:213:MET:HG2	2.13	0.49
1:B:1622:THR:C	1:B:1623:TRP:HD1	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1606:PHE:HZ	1:B:1679:LYS:HB3	1.78	0.49
1:B:1573:LYS:CA	1:B:1577:LEU:HD13	2.40	0.49
1:B:1550:CYS:CB	1:B:1562:TRP:HB3	2.42	0.49
1:B:1554:MET:O	1:B:1555:ALA:C	2.51	0.49
1:A:591:LYS:HE2	1:A:609:ARG:HH22	1.72	0.49
1:A:657:TYR:CZ	1:A:659:ILE:HG12	2.48	0.49
1:B:1288:GLN:CG	1:B:1299:VAL:HG12	2.43	0.49
1:A:285:GLU:O	1:A:289:GLN:HG3	2.12	0.49
1:A:482:MET:HE3	1:A:483:LEU:CD2	2.43	0.49
1:B:1344:GLN:CG	1:B:1410:HIS:HA	2.43	0.49
1:B:1601:LYS:HE3	1:B:1674:TYR:CE2	2.48	0.49
1:A:678:PRO:O	1:A:680:GLU:N	2.41	0.49
1:B:1604:GLY:HA2	1:B:1670:LEU:HB3	1.94	0.49
1:A:576:ILE:HA	1:A:579:LEU:CD1	2.32	0.49
1:B:1280:GLN:NE2	1:B:1280:GLN:HA	2.16	0.49
1:A:276:GLN:O	1:A:280:GLN:HG2	2.13	0.49
1:B:1386:ILE:C	1:B:1387:LEU:HD23	2.34	0.49
1:A:179:LEU:CD2	1:A:200:MET:HA	2.43	0.49
1:A:504:VAL:O	1:A:508:LEU:HD12	2.12	0.49
1:B:1504:VAL:O	1:B:1508:LEU:HD12	2.13	0.49
1:A:328:CYS:SG	1:A:336:PRO:HA	2.52	0.49
1:B:1600:THR:HG23	1:B:1601:LYS:N	2.28	0.48
1:B:1328:CYS:SG	1:B:1336:PRO:HA	2.53	0.48
1:B:1346:THR:CG2	1:B:1409:LYS:HA	2.38	0.48
1:A:325:ARG:CZ	1:A:325:ARG:CB	2.91	0.48
1:A:357:GLU:CD	1:A:357:GLU:H	2.17	0.48
1:A:224:LEU:O	1:A:228:MET:HG3	2.12	0.48
1:A:600:THR:HG23	1:A:601:LYS:H	1.78	0.48
1:A:520:LEU:HB2	1:A:525:LEU:HD13	1.94	0.48
1:A:674:TYR:O	1:A:675:PRO:C	2.51	0.48
1:B:1178:THR:O	1:B:1182:GLN:HG2	2.13	0.48
1:B:1293:TYR:CE1	1:B:1296:ASP:HA	2.48	0.48
1:A:550:CYS:CB	1:A:562:TRP:HB3	2.43	0.48
1:B:1439:ILE:N	1:B:1439:ILE:HD12	2.28	0.48
1:A:654:ILE:HD13	1:A:683:PHE:HE1	1.78	0.48
1:A:498:ILE:HG22	1:A:499:GLY:N	2.28	0.48
1:B:1473:ALA:O	1:B:1476:SER:N	2.47	0.48
1:B:1665:ILE:O	1:B:1667:VAL:N	2.46	0.48
1:A:634:ILE:HG22	1:A:635:GLN:N	2.28	0.48
1:A:658:LYS:C	1:A:659:ILE:HG13	2.34	0.48
1:A:673:LEU:O	1:A:674:TYR:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1136:VAL:HG22	1:B:1137:VAL:N	2.28	0.48
1:A:586:MET:O	1:A:588:PHE:N	2.47	0.48
1:A:364:ILE:HD13	1:A:443:THR:CG2	2.44	0.48
1:A:665:ILE:O	1:A:667:VAL:N	2.47	0.48
1:B:1498:ILE:HG22	1:B:1499:GLY:N	2.28	0.48
1:B:1616:GLU:O	1:B:1642:LYS:HE3	2.14	0.48
1:B:1585:ILE:HG22	1:B:1587:GLY:N	2.28	0.48
1:B:1622:THR:HG23	1:B:1634:ILE:HG23	1.95	0.48
1:B:1622:THR:CG2	1:B:1623:TRP:N	2.77	0.48
1:A:600:THR:HG23	1:A:601:LYS:N	2.29	0.48
1:B:1517:LYS:N	1:B:1517:LYS:CD	2.73	0.48
1:A:139:GLU:HA	1:A:142:GLN:CG	2.37	0.48
1:B:1179:LEU:HD11	1:B:1195:VAL:HG12	1.96	0.48
1:A:659:ILE:O	1:A:667:VAL:HG22	2.14	0.48
1:B:1195:VAL:CB	1:B:1200:MET:HE2	2.44	0.48
1:B:1582:GLU:OE2	1:B:1582:GLU:N	2.38	0.48
1:A:634:ILE:CG2	1:A:635:GLN:N	2.76	0.47
1:B:1493:PHE:O	1:B:1496:PRO:HD3	2.13	0.47
1:B:1530:GLU:C	1:B:1532:LEU:H	2.16	0.47
1:A:379:ARG:HH11	1:A:380:GLY:N	2.12	0.47
1:A:688:ARG:H	1:A:688:ARG:HE	1.62	0.47
1:B:1600:THR:HG23	1:B:1601:LYS:H	1.78	0.47
1:B:1201:GLN:O	1:B:1203:LEU:N	2.39	0.47
1:B:1532:LEU:HD12	1:B:1561:PHE:HE2	1.79	0.47
1:A:554:MET:O	1:A:555:ALA:C	2.52	0.47
1:A:326:GLN:OE1	1:A:458:SER:HB2	2.14	0.47
1:B:1623:TRP:NE1	1:B:1635:GLN:O	2.48	0.47
1:B:1673:LEU:O	1:B:1674:TYR:C	2.53	0.47
1:B:1671:VAL:HG12	1:B:1679:LYS:HZ3	1.80	0.47
1:A:204:GLU:HG3	1:A:204:GLU:H	1.40	0.47
1:A:318:LYS:HA	1:A:454:LEU:CD2	2.44	0.47
1:B:1565:LEU:CD1	1:B:1568:ILE:HD12	2.45	0.47
1:B:1674:TYR:O	1:B:1675:PRO:C	2.52	0.47
1:A:243:TRP:NE1	1:A:258:ILE:HB	2.29	0.47
1:B:1243:TRP:NE1	1:B:1258:ILE:HB	2.30	0.47
1:B:1288:GLN:HG3	1:B:1299:VAL:HG12	1.97	0.47
1:B:1288:GLN:NE2	1:B:1302:ARG:HH21	2.13	0.47
1:A:278:ARG:HD3	1:A:448:GLN:OE1	2.15	0.47
1:B:1172:PHE:HD1	1:B:1206:MET:HB3	1.80	0.47
1:A:585:ILE:HD13	1:A:608:LEU:HD13	1.96	0.47
1:A:146:GLN:O	1:A:147:HIS:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1357:GLU:H	1:B:1357:GLU:CD	2.17	0.47
1:A:136:VAL:HG22	1:A:137:VAL:H	1.80	0.47
1:A:288:GLN:HG3	1:A:299:VAL:HG12	1.97	0.47
1:A:252:ILE:HG21	1:A:481:ASN:HD22	1.77	0.47
1:A:386:ILE:C	1:A:387:LEU:HD23	2.34	0.47
1:B:1580:TRP:C	1:B:1580:TRP:CD1	2.88	0.47
1:A:595:ARG:O	1:A:597:ILE:N	2.42	0.47
1:B:1447:HIS:C	1:B:1449:GLY:N	2.66	0.47
1:A:252:ILE:HG23	1:A:481:ASN:ND2	2.27	0.47
1:A:656:GLY:O	1:A:657:TYR:C	2.53	0.46
1:B:1622:THR:CG2	1:B:1634:ILE:HG23	2.44	0.46
1:B:1246:ARG:HD2	1:B:1257:ASN:O	2.16	0.46
1:B:1296:ASP:HB3	1:B:1299:VAL:HG22	1.97	0.46
1:A:414:ARG:HG2	1:A:415:GLU:N	2.30	0.46
1:B:1566:ASP:HA	1:B:1569:ILE:HD12	1.97	0.46
1:A:592:GLU:OE1	1:A:592:GLU:C	2.54	0.46
1:B:1325:ARG:CZ	1:B:1325:ARG:CB	2.93	0.46
1:A:662:ALA:C	1:A:664:ASN:H	2.18	0.46
1:B:1583:GLY:C	1:B:1585:ILE:N	2.68	0.46
1:A:152:ARG:O	1:A:156:GLN:HG2	2.15	0.46
1:B:1201:GLN:HA	1:B:1204:GLU:CG	2.45	0.46
1:B:1443:THR:O	1:B:1454:LEU:HB2	2.15	0.46
1:B:1656:GLY:O	1:B:1658:LYS:HE3	2.15	0.46
1:A:447:HIS:C	1:A:449:GLY:N	2.66	0.46
1:B:1482:MET:HE3	1:B:1483:LEU:CD2	2.45	0.46
1:B:1644:GLN:C	1:B:1646:ASN:N	2.67	0.46
1:B:1152:ARG:O	1:B:1156:GLN:HG2	2.15	0.46
1:A:201:GLN:HA	1:A:204:GLU:CG	2.46	0.46
1:A:144:LEU:C	1:A:146:GLN:H	2.18	0.46
1:A:669:PRO:O	1:A:670:LEU:C	2.54	0.46
1:A:671:VAL:HG12	1:A:679:LYS:NZ	2.31	0.46
1:B:1493:PHE:C	1:B:1496:PRO:HD3	2.36	0.46
1:A:161:LYS:NZ	1:A:216:SER:OG	2.48	0.46
1:B:1669:PRO:O	1:B:1670:LEU:C	2.54	0.46
1:A:246:ARG:HD2	1:A:257:ASN:O	2.16	0.46
1:A:293:TYR:CE1	1:A:296:ASP:HA	2.50	0.46
1:A:296:ASP:HB3	1:A:299:VAL:HG22	1.97	0.46
1:B:1144:LEU:C	1:B:1146:GLN:H	2.17	0.46
1:B:1607:LEU:HB3	1:B:1608:LEU:H	1.56	0.46
1:A:530:GLU:OE2	1:B:1593:ARG:NH1	2.41	0.46
1:B:1473:ALA:C	1:B:1475:ALA:N	2.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:PHE:CD1	1:A:441:PHE:N	2.84	0.46
1:A:433:THR:CG2	1:A:469:GLN:HB3	2.46	0.46
1:A:653:ILE:CD1	1:A:653:ILE:H	2.28	0.46
1:A:205:GLN:C	1:A:207:LEU:N	2.68	0.46
1:A:252:ILE:HG21	1:A:478:LEU:HA	1.98	0.46
1:A:582:GLU:CD	1:A:582:GLU:N	2.68	0.46
1:B:1158:LEU:HG	1:B:1220:GLU:OE1	2.16	0.46
1:B:1589:ILE:HD13	1:B:1607:LEU:HD21	1.98	0.46
1:A:417:ARG:HG2	1:A:418:CYS:N	2.27	0.46
1:B:1414:ARG:HG2	1:B:1415:GLU:N	2.30	0.46
1:A:607:LEU:HB3	1:A:608:LEU:H	1.58	0.46
1:B:1592:GLU:OE1	1:B:1592:GLU:C	2.54	0.46
1:A:214:ARG:CZ	1:A:298:ILE:HD12	2.46	0.46
1:B:1366:VAL:HA	1:B:1440:THR:O	2.15	0.46
1:B:1656:GLY:O	1:B:1657:TYR:C	2.55	0.45
1:A:288:GLN:NE2	1:A:298:ILE:HG22	2.31	0.45
1:B:1330:PRO:HD2	1:B:1344:GLN:O	2.16	0.45
1:B:1209:ALA:O	1:B:1213:MET:HG2	2.16	0.45
1:B:1318:LYS:HA	1:B:1454:LEU:HD22	1.98	0.45
1:B:1162:MET:O	1:B:1165:VAL:HG12	2.16	0.45
1:B:1686:TYR:O	1:B:1688:ARG:NH2	2.50	0.45
1:A:358:LEU:O	1:A:361:GLN:HB3	2.17	0.45
1:B:1605:THR:HA	1:B:1671:VAL:O	2.17	0.45
1:A:329:MET:HE1	1:A:338:VAL:O	2.16	0.45
1:A:201:GLN:O	1:A:204:GLU:HG3	2.16	0.45
1:B:1288:GLN:NE2	1:B:1298:ILE:HG22	2.29	0.45
1:B:1611:SER:N	1:B:1618:GLY:O	2.43	0.45
1:A:287:LEU:N	1:A:287:LEU:HD12	2.31	0.45
1:A:493:PHE:C	1:A:496:PRO:HD3	2.37	0.45
1:B:1326:GLN:OE1	1:B:1458:SER:HB2	2.17	0.45
1:B:1433:THR:CG2	1:B:1469:GLN:HB3	2.46	0.45
1:B:1585:ILE:HD13	1:B:1608:LEU:HD13	1.98	0.45
1:B:1279:GLN:OE1	1:B:1448:GLN:NE2	2.49	0.45
1:A:447:HIS:O	1:A:449:GLY:N	2.50	0.45
1:B:1358:LEU:O	1:B:1361:GLN:HB3	2.15	0.45
1:A:531:LYS:HZ1	1:A:557:LYS:HE2	1.82	0.45
1:A:610:PHE:CD1	1:A:619:VAL:HG12	2.52	0.45
1:B:1201:GLN:O	1:B:1204:GLU:HG3	2.16	0.45
1:B:1652:GLU:OE1	1:B:1652:GLU:HA	2.16	0.45
1:A:443:THR:O	1:A:454:LEU:HB2	2.16	0.45
1:B:1362:LEU:HD11	1:B:1445:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1139:GLU:HA	1:B:1142:GLN:CG	2.43	0.45
1:A:532:LEU:HD12	1:A:561:PHE:HE2	1.79	0.45
1:A:596:ALA:HB1	1:B:1535:PRO:HB3	1.97	0.45
1:A:459:LEU:HD23	1:A:459:LEU:HA	1.84	0.45
1:B:1521:SER:OG	1:B:1524:GLN:HG2	2.16	0.45
1:A:283:LYS:HA	1:A:286:GLU:CG	2.47	0.45
1:A:330:PRO:HD2	1:A:344:GLN:O	2.16	0.45
1:B:1336:PRO:O	1:B:1337:LEU:HB2	2.16	0.45
1:B:1470:MET:CB	1:B:1471:PRO:CD	2.94	0.45
1:A:243:TRP:HE1	1:A:258:ILE:HB	1.82	0.45
1:A:201:GLN:O	1:A:203:LEU:N	2.41	0.45
1:A:382:ARG:HB2	1:A:384:PHE:HE1	1.82	0.45
1:A:384:PHE:CD1	1:A:384:PHE:N	2.85	0.45
1:B:1287:LEU:HD12	1:B:1287:LEU:N	2.32	0.45
1:B:1503:GLN:HG3	1:B:1503:GLN:H	1.49	0.45
1:B:1146:GLN:O	1:B:1147:HIS:C	2.54	0.45
1:B:1172:PHE:HB2	1:B:1206:MET:HE2	1.99	0.45
1:A:660:MET:CG	1:A:666:LEU:HD12	2.47	0.45
1:B:1597:ILE:HD11	1:B:1622:THR:HG22	1.97	0.45
1:A:442:GLU:HG2	1:A:455:GLU:HB2	1.99	0.45
1:B:1622:THR:C	1:B:1623:TRP:CD1	2.90	0.44
1:A:470:MET:HB3	1:A:471:PRO:CD	2.33	0.44
1:A:277:THR:O	1:A:281:ILE:HG12	2.16	0.44
1:B:1182:GLN:C	1:B:1184:ASP:H	2.21	0.44
1:A:521:SER:OG	1:A:524:GLN:HG2	2.16	0.44
1:A:611:SER:N	1:A:618:GLY:O	2.43	0.44
1:B:1578:ALA:O	1:B:1581:ASN:HB2	2.17	0.44
1:B:1523:GLU:CG	1:B:1524:GLN:N	2.80	0.44
1:B:1447:HIS:O	1:B:1449:GLY:N	2.50	0.44
1:B:1582:GLU:CD	1:B:1582:GLU:N	2.68	0.44
1:A:272:GLU:O	1:A:276:GLN:HG3	2.17	0.44
1:A:409:LYS:HB2	1:A:409:LYS:HZ2	1.82	0.44
1:B:1442:GLU:HG2	1:B:1455:GLU:HB2	1.99	0.44
1:A:340:LYS:HE3	1:A:343:VAL:CG2	2.48	0.44
1:A:680:GLU:O	1:A:684:GLY:HA3	2.17	0.44
1:A:652:GLU:OE1	1:A:652:GLU:HA	2.17	0.44
1:A:431:ILE:O	1:A:435:GLU:HB2	2.16	0.44
1:A:658:LYS:HE2	1:A:668:SER:HA	2.00	0.44
1:A:656:GLY:O	1:A:658:LYS:HE3	2.18	0.44
1:A:660:MET:HG3	1:A:666:LEU:HD12	1.99	0.44
1:B:1650:PHE:O	1:B:1654:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1643:GLN:O	1:B:1646:ASN:HB2	2.18	0.44
1:A:482:MET:HE3	1:A:483:LEU:HD21	1.98	0.44
1:A:526:THR:C	1:A:528:LEU:N	2.71	0.44
1:A:285:GLU:HA	1:A:288:GLN:HB2	2.00	0.44
1:A:503:GLN:H	1:A:503:GLN:HG3	1.47	0.44
1:A:162:MET:O	1:A:165:VAL:HG12	2.17	0.44
1:B:1652:GLU:OE2	1:B:1688:ARG:NE	2.50	0.44
1:B:1610:PHE:CD1	1:B:1619:VAL:HG12	2.53	0.44
1:B:1685:LYS:HB2	1:B:1686:TYR:CD1	2.52	0.44
1:B:1531:LYS:NZ	1:B:1557:LYS:HE2	2.33	0.44
1:A:336:PRO:O	1:A:337:LEU:HB2	2.18	0.44
1:B:1205:GLN:C	1:B:1207:LEU:N	2.70	0.44
1:B:1589:ILE:HG23	1:B:1589:ILE:O	2.17	0.44
1:B:1671:VAL:HG12	1:B:1679:LYS:HG2	2.00	0.44
1:B:1335:ARG:HB3	1:B:1470:MET:HE1	2.00	0.44
1:B:1162:MET:CE	1:B:1283:LYS:HB3	2.47	0.44
1:A:214:ARG:NH2	1:A:287:LEU:HB3	2.33	0.44
1:A:589:ILE:HG23	1:A:589:ILE:O	2.17	0.44
1:A:671:VAL:HG12	1:A:679:LYS:HG2	2.00	0.44
1:B:1592:GLU:O	1:B:1594:GLU:N	2.51	0.44
1:B:1272:GLU:O	1:B:1276:GLN:HG3	2.18	0.44
1:B:1382:ARG:HB2	1:B:1384:PHE:HE1	1.82	0.44
1:A:583:GLY:C	1:A:585:ILE:N	2.70	0.43
1:B:1243:TRP:HE1	1:B:1258:ILE:HB	1.83	0.43
1:A:225:LEU:CD2	1:A:308:ARG:HB3	2.48	0.43
1:B:1663:THR:O	1:B:1665:ILE:HG13	2.17	0.43
1:A:256:PRO:HB2	1:A:257:ASN:H	1.66	0.43
1:B:1284:LEU:HD23	1:B:1284:LEU:HA	1.83	0.43
1:B:1441:PHE:N	1:B:1441:PHE:CD1	2.85	0.43
1:A:340:LYS:O	1:A:343:VAL:HG23	2.18	0.43
1:B:1533:LEU:HD21	1:B:1544:ILE:HG12	1.99	0.43
1:B:1576:ILE:HA	1:B:1579:LEU:HB2	1.99	0.43
1:B:1255:PRO:HA	1:B:1256:PRO:HD2	1.82	0.43
1:A:447:HIS:O	1:A:448:GLN:C	2.56	0.43
1:B:1340:LYS:O	1:B:1343:VAL:HG23	2.19	0.43
1:B:1214:ARG:NH2	1:B:1287:LEU:HB3	2.33	0.43
1:B:1651:ALA:HB3	1:B:1688:ARG:NH2	2.31	0.43
1:A:279:GLN:HE21	1:A:282:LYS:HD2	1.82	0.43
1:B:1531:LYS:HZ1	1:B:1557:LYS:HE2	1.84	0.43
1:A:578:ALA:O	1:A:581:ASN:HB2	2.18	0.43
1:B:1592:GLU:C	1:B:1594:GLU:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1651:ALA:O	1:B:1655:MET:HG2	2.18	0.43
1:B:1681:GLU:O	1:B:1685:LYS:CE	2.66	0.43
1:A:361:GLN:HG2	1:A:361:GLN:O	2.19	0.43
1:A:650:PHE:CE2	1:A:654:ILE:HD11	2.52	0.43
1:A:364:ILE:CD1	1:A:443:THR:HG21	2.49	0.43
1:B:1384:PHE:N	1:B:1384:PHE:CD1	2.86	0.43
1:A:523:GLU:CG	1:A:524:GLN:N	2.81	0.43
1:A:685:LYS:HE3	1:A:686:TYR:CE2	2.52	0.43
1:B:1225:LEU:CD2	1:B:1308:ARG:HB3	2.48	0.43
1:A:592:GLU:O	1:A:594:GLU:N	2.51	0.43
1:A:619:VAL:HG23	1:A:650:PHE:CE1	2.53	0.43
1:A:205:GLN:O	1:A:207:LEU:N	2.51	0.43
1:A:308:ARG:O	1:A:311:GLU:HB3	2.18	0.43
1:A:136:VAL:HG22	1:A:137:VAL:N	2.34	0.43
1:A:470:MET:CB	1:A:471:PRO:CD	2.95	0.43
1:A:432:VAL:C	1:A:434:GLU:H	2.22	0.43
1:B:1623:TRP:CB	1:B:1670:LEU:HG	2.49	0.42
1:B:1201:GLN:HA	1:B:1204:GLU:OE1	2.19	0.42
1:A:205:GLN:O	1:A:208:THR:N	2.51	0.42
1:A:288:GLN:HE22	1:A:302:ARG:HH21	1.67	0.42
1:A:253:GLY:O	1:A:510:TRP:HB3	2.19	0.42
1:B:1671:VAL:HG12	1:B:1679:LYS:NZ	2.33	0.42
1:A:512:PHE:O	1:A:516:THR:OG1	2.29	0.42
1:A:621:PHE:CZ	1:A:637:VAL:CG1	3.03	0.42
1:B:1340:LYS:HE3	1:B:1343:VAL:CG2	2.48	0.42
1:B:1205:GLN:O	1:B:1208:THR:N	2.52	0.42
1:A:623:TRP:NE1	1:A:635:GLN:O	2.53	0.42
1:B:1466:ASN:ND2	1:B:1467:ILE:H	2.18	0.42
1:A:575:TYR:CB	1:A:576:ILE:HD12	2.49	0.42
1:A:283:LYS:HA	1:A:283:LYS:HD2	1.83	0.42
1:B:1359:ASN:O	1:B:1360:TYR:HB2	2.19	0.42
1:A:655:MET:HG3	1:A:687:CYS:SG	2.59	0.42
1:A:576:ILE:HA	1:A:579:LEU:HB2	2.00	0.42
1:A:285:GLU:HB2	1:A:302:ARG:HD3	2.01	0.42
1:A:515:THR:HG21	1:A:573:LYS:CG	2.49	0.42
1:B:1515:THR:HG21	1:B:1573:LYS:CG	2.48	0.42
1:B:1482:MET:HE3	1:B:1483:LEU:HD21	2.01	0.42
1:A:643:GLN:O	1:A:646:ASN:HB2	2.19	0.42
1:A:580:TRP:CD1	1:A:580:TRP:C	2.91	0.42
1:A:221:LEU:CD1	1:A:281:ILE:HD13	2.33	0.42
1:A:592:GLU:C	1:A:594:GLU:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1609:ARG:HH11	1:B:1620:THR:CG2	2.32	0.42
1:B:1606:PHE:CZ	1:B:1679:LYS:HB3	2.55	0.42
1:A:263:LEU:O	1:A:267:ILE:CG1	2.68	0.42
1:B:1447:HIS:O	1:B:1448:GLN:C	2.58	0.42
1:A:206:MET:O	1:A:210:LEU:HG	2.19	0.42
1:A:531:LYS:NZ	1:A:557:LYS:HE2	2.33	0.42
1:A:254:GLY:HA2	1:A:510:TRP:CD2	2.55	0.42
1:A:388:GLY:O	1:A:390:ASN:N	2.53	0.42
1:A:654:ILE:HD13	1:A:683:PHE:CE1	2.54	0.42
1:A:445:VAL:HB	1:A:452:ILE:CG2	2.50	0.42
1:B:1256:PRO:HB2	1:B:1257:ASN:H	1.67	0.42
1:B:1196:THR:HG22	1:B:1197:ARG:N	2.34	0.42
1:A:382:ARG:HB2	1:A:384:PHE:CE1	2.55	0.42
1:B:1172:PHE:N	1:B:1206:MET:HE1	2.35	0.42
1:A:591:LYS:CE	1:A:609:ARG:NH2	2.77	0.42
1:A:658:LYS:CE	1:A:668:SER:HA	2.50	0.42
1:A:623:TRP:HB2	1:A:670:LEU:HG	2.01	0.42
1:B:1279:GLN:HE21	1:B:1282:LYS:HD2	1.83	0.42
1:A:409:LYS:CB	1:A:409:LYS:NZ	2.83	0.42
1:A:368:ILE:CD1	1:A:413:LEU:HD21	2.49	0.42
1:B:1331:MET:HE2	1:B:1331:MET:HA	2.02	0.42
1:A:281:ILE:HD12	1:A:305:LEU:HB3	2.02	0.42
1:B:1283:LYS:HA	1:B:1286:GLU:CG	2.45	0.42
1:A:530:GLU:C	1:A:532:LEU:N	2.73	0.42
1:B:1517:LYS:HE2	1:B:1581:ASN:OD1	2.20	0.42
1:B:1518:ARG:HG2	1:B:1519:GLY:O	2.19	0.42
1:B:1526:THR:C	1:B:1528:LEU:N	2.72	0.42
1:B:1205:GLN:O	1:B:1207:LEU:N	2.53	0.42
1:B:1598:LEU:HD13	1:B:1623:TRP:HA	2.02	0.41
1:B:1540:SER:C	1:B:1542:CYS:H	2.23	0.41
1:A:621:PHE:CE1	1:A:637:VAL:HB	2.54	0.41
1:B:1368:ILE:O	1:B:1369:ASP:HB2	2.20	0.41
1:B:1169:GLN:O	1:B:1169:GLN:HG2	2.20	0.41
1:A:180:LYS:O	1:A:180:LYS:HG2	2.20	0.41
1:B:1379:ARG:C	1:B:1379:ARG:HD3	2.41	0.41
1:A:246:ARG:NH1	1:A:258:ILE:HA	2.35	0.41
1:A:362:LEU:HD23	1:A:362:LEU:HA	1.77	0.41
1:A:205:GLN:O	1:A:206:MET:C	2.59	0.41
1:B:1180:LYS:O	1:B:1180:LYS:HG2	2.19	0.41
1:A:506:GLU:O	1:A:509:SER:HB3	2.20	0.41
1:B:1181:SER:O	1:B:1182:GLN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1283:LYS:HA	1:B:1283:LYS:HD2	1.85	0.41
1:A:245:ARG:HD3	1:A:485:ASN:HB3	2.02	0.41
1:B:1368:ILE:HG21	1:B:1385:ASN:HA	2.02	0.41
1:A:154:ARG:HB2	1:A:224:LEU:HD13	2.02	0.41
1:B:1601:LYS:HB3	1:B:1602:PRO:CD	2.43	0.41
1:A:335:ARG:HA	1:A:335:ARG:HD3	1.90	0.41
1:A:332:HIS:HE1	1:A:467:ILE:HD11	1.84	0.41
1:A:260:LEU:HB2	1:A:350:ARG:NH2	2.35	0.41
1:A:172:PHE:C	1:A:172:PHE:CD2	2.94	0.41
1:B:1530:GLU:C	1:B:1532:LEU:N	2.74	0.41
1:A:304:MET:HA	1:A:304:MET:HE1	2.02	0.41
1:A:602:PRO:O	1:A:603:PRO:C	2.59	0.41
1:A:146:GLN:O	1:A:149:GLN:N	2.52	0.41
1:A:340:LYS:HA	1:A:464:ILE:HG13	2.03	0.41
1:B:1409:LYS:NZ	1:B:1409:LYS:CB	2.84	0.41
1:A:245:ARG:HH11	1:A:485:ASN:HB3	1.85	0.41
1:B:1382:ARG:HB2	1:B:1384:PHE:CE1	2.55	0.41
1:B:1433:THR:HG21	1:B:1472:ASN:HB2	2.03	0.41
1:A:535:PRO:CG	1:B:1600:THR:HB	2.47	0.41
1:B:1670:LEU:N	1:B:1670:LEU:HD22	2.11	0.41
1:A:279:GLN:OE1	1:A:448:GLN:OE1	2.39	0.41
1:B:1252:ILE:HG23	1:B:1481:ASN:ND2	2.34	0.41
1:A:623:TRP:HH2	1:A:659:ILE:HG21	1.86	0.41
1:A:466:ASN:ND2	1:A:467:ILE:H	2.19	0.41
1:A:309:ILE:C	1:A:309:ILE:HD13	2.40	0.41
1:A:604:GLY:HA2	1:A:670:LEU:HB3	2.01	0.41
1:B:1677:ILE:HG13	1:B:1677:ILE:H	1.67	0.41
1:B:1470:MET:HB3	1:B:1471:PRO:CD	2.33	0.41
1:A:280:GLN:CA	1:A:280:GLN:HE21	2.13	0.41
1:B:1524:GLN:HE21	1:B:1524:GLN:HB3	1.59	0.41
1:B:1246:ARG:NH1	1:B:1258:ILE:HA	2.36	0.41
1:B:1285:GLU:HA	1:B:1288:GLN:HB2	2.02	0.41
1:A:284:LEU:C	1:A:286:GLU:H	2.24	0.41
1:A:522:ILE:CD1	1:A:522:ILE:H	2.13	0.41
1:B:1172:PHE:C	1:B:1172:PHE:CD2	2.95	0.41
1:B:1195:VAL:HG11	1:B:1200:MET:CE	2.51	0.41
1:B:1308:ARG:O	1:B:1311:GLU:HB3	2.21	0.41
1:B:1234:THR:O	1:B:1238:GLU:HB2	2.21	0.41
1:A:240:LEU:HD13	1:A:263:LEU:HD13	2.02	0.40
1:B:1243:TRP:CZ2	1:B:1260:LEU:HD21	2.56	0.40
1:B:1196:THR:CB	1:B:1199:LYS:HB2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1361:GLN:HG2	1:B:1361:GLN:O	2.20	0.40
1:A:337:LEU:HD22	1:A:461:VAL:HG23	2.03	0.40
1:B:1314:ARG:CA	1:B:1452:ILE:HD11	2.44	0.40
1:A:288:GLN:NE2	1:A:302:ARG:HE	2.20	0.40
1:B:1365:LYS:HA	1:B:1391:THR:HG22	2.01	0.40
1:B:1277:THR:O	1:B:1281:ILE:HG13	2.21	0.40
1:B:1388:GLY:O	1:B:1390:ASN:N	2.54	0.40
1:B:1459:LEU:HD23	1:B:1459:LEU:HA	1.84	0.40
1:A:359:ASN:O	1:A:360:TYR:HB2	2.21	0.40
1:B:1335:ARG:N	1:B:1336:PRO:CD	2.84	0.40
1:B:1576:ILE:HG23	1:B:1579:LEU:HB2	2.03	0.40
1:A:526:THR:C	1:A:528:LEU:H	2.23	0.40
1:B:1228:MET:HE1	1:B:1274:GLN:N	2.36	0.40
1:A:651:ALA:O	1:A:655:MET:HG2	2.21	0.40
1:B:1496:PRO:HA	1:B:1497:PRO:HD3	1.86	0.40
1:A:144:LEU:HA	1:A:144:LEU:HD12	1.94	0.40
1:A:592:GLU:O	1:A:595:ARG:N	2.53	0.40
1:A:671:VAL:CG1	1:A:679:LYS:NZ	2.84	0.40
1:B:1592:GLU:O	1:B:1595:ARG:N	2.53	0.40
1:B:1335:ARG:HA	1:B:1335:ARG:HD3	1.91	0.40
1:A:243:TRP:CZ2	1:A:260:LEU:HD21	2.56	0.40
1:A:533:LEU:HD13	1:A:542:CYS:HB3	2.04	0.40
1:B:1683:PHE:O	1:B:1687:CYS:SG	2.80	0.40
1:A:337:LEU:HD13	1:A:460:PRO:O	2.21	0.40
1:A:570:ASP:O	1:A:574:LYS:HB2	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1575:TYR:OH	1:B:1643:GLN:OE1[5_554]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/562 (86%)	362 (75%)	91 (19%)	32 (7%)	1	8
1	B	491/562 (87%)	362 (74%)	95 (19%)	34 (7%)	1	8
All	All	976/1124 (87%)	724 (74%)	186 (19%)	66 (7%)	1	8

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	PRO
1	A	368	ILE
1	A	555	ALA
1	A	557	LYS
1	A	667	VAL
1	A	676	ASP
1	A	679	LYS
1	B	1256	PRO
1	B	1555	ALA
1	B	1557	LYS
1	B	1584	TYR
1	B	1633	GLN
1	B	1664	ASN
1	B	1667	VAL
1	B	1676	ASP
1	B	1679	LYS
1	A	542	CYS
1	A	584	TYR
1	A	587	GLY
1	A	600	THR
1	A	632	THR
1	A	645	LEU
1	A	657	TYR
1	A	666	LEU
1	B	1182	GLN
1	B	1542	CYS
1	B	1587	GLY
1	B	1600	THR
1	B	1645	LEU
1	B	1657	TYR
1	B	1666	LEU
1	A	202	GLN
1	A	369	ASP

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Mol	Chain	Res	Type
1	A	593	ARG
1	A	670	LEU
1	B	1202	GLN
1	B	1593	ARG
1	B	1670	LEU
1	A	147	HIS
1	A	596	ALA
1	A	608	LEU
1	A	637	VAL
1	B	1147	HIS
1	B	1369	ASP
1	B	1608	LEU
1	B	1632	THR
1	B	1637	VAL
1	A	354	LYS
1	A	538	ASN
1	A	675	PRO
1	B	1354	LYS
1	B	1368	ILE
1	B	1538	ASN
1	B	1665	ILE
1	B	1675	PRO
1	A	206	MET
1	A	252	ILE
1	A	255	PRO
1	B	1252	ILE
1	B	1255	PRO
1	B	1495	LYS
1	A	495	LYS
1	A	576	ILE
1	B	1576	ILE
1	A	477	ILE
1	B	1477	ILE

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	458/505 (91%)	416 (91%)	42 (9%)	11	37
1	B	464/505 (92%)	422 (91%)	42 (9%)	12	38
All	All	922/1010 (91%)	838 (91%)	84 (9%)	12	38

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	ARG
1	A	158	LEU
1	A	168	LEU
1	A	178	THR
1	A	201	GLN
1	A	203	LEU
1	A	204	GLU
1	A	218	VAL
1	A	229	GLU
1	A	235	LEU
1	A	242	ASP
1	A	280	GLN
1	A	287	LEU
1	A	304	MET
1	A	309	ILE
1	A	350	ARG
1	A	379	ARG
1	A	397	GLU
1	A	453	ASP
1	A	503	GLN
1	A	515	THR
1	A	517	LYS
1	A	522	ILE
1	A	523	GLU
1	A	524	GLN
1	A	532	LEU
1	A	552	GLU
1	A	553	ASN
1	A	575	TYR
1	A	580	TRP
1	A	582	GLU
1	A	586	MET
1	A	592	GLU
1	A	623	TRP
1	A	632	THR

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Mol	Chain	Res	Type
1	A	637	VAL
1	A	652	GLU
1	A	659	ILE
1	A	670	LEU
1	A	676	ASP
1	A	686	TYR
1	A	688	ARG
1	B	1152	ARG
1	B	1168	LEU
1	B	1178	THR
1	B	1182	GLN
1	B	1201	GLN
1	B	1203	LEU
1	B	1204	GLU
1	B	1218	VAL
1	B	1229	GLU
1	B	1235	LEU
1	B	1242	ASP
1	B	1280	GLN
1	B	1287	LEU
1	B	1304	MET
1	B	1350	ARG
1	B	1379	ARG
1	B	1397	GLU
1	B	1431	ILE
1	B	1453	ASP
1	B	1503	GLN
1	B	1515	THR
1	B	1517	LYS
1	B	1522	ILE
1	B	1523	GLU
1	B	1524	GLN
1	B	1532	LEU
1	B	1552	GLU
1	B	1553	ASN
1	B	1575	TYR
1	B	1580	TRP
1	B	1582	GLU
1	B	1586	MET
1	B	1592	GLU
1	B	1597	ILE
1	B	1621	PHE

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Mol	Chain	Res	Type
1	B	1623	TRP
1	B	1637	VAL
1	B	1652	GLU
1	B	1670	LEU
1	B	1676	ASP
1	B	1686	TYR
1	B	1688	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	201	GLN
1	A	205	GLN
1	A	248	GLN
1	A	279	GLN
1	A	280	GLN
1	A	332	HIS
1	A	385	ASN
1	A	401	ASN
1	A	437	HIS
1	A	466	ASN
1	A	481	ASN
1	A	503	GLN
1	A	644	GLN
1	B	1167	ASN
1	B	1248	GLN
1	B	1279	GLN
1	B	1280	GLN
1	B	1332	HIS
1	B	1385	ASN
1	B	1390	ASN
1	B	1437	HIS
1	B	1466	ASN
1	B	1472	ASN
1	B	1481	ASN
1	B	1503	GLN
1	B	1644	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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	501/562 (89%)	0.12	2 (0%) 93 84	43, 92, 127, 139	0
1	B	507/562 (90%)	0.16	8 (1%) 74 52	36, 101, 131, 143	0
All	All	1008/1124 (89%)	0.14	10 (0%) 84 66	36, 97, 130, 143	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1199	LYS	3.4
1	B	1198	GLN	3.3
1	B	1667	VAL	3.1
1	A	607	LEU	2.4
1	B	1339	ILE	2.3
1	B	1607	LEU	2.2
1	B	1202	GLN	2.2
1	A	281	ILE	2.0
1	B	1669	PRO	2.0
1	B	1576	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.