



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 05:10 AM EDT

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

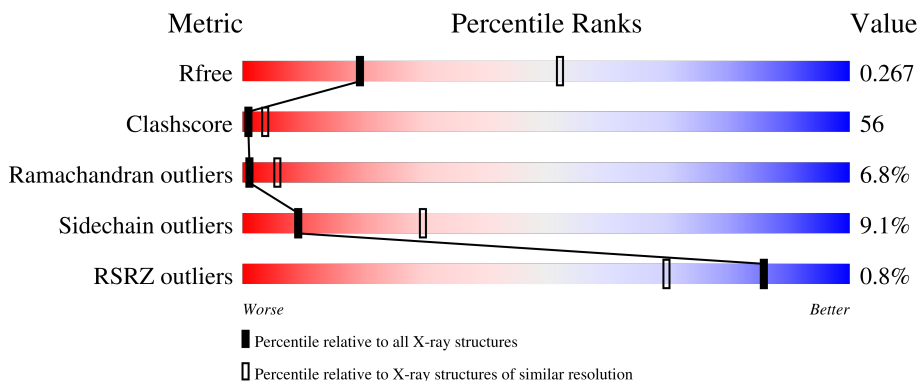
1 Overall quality at a glance

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}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	562	

2 Entry composition [i](#)

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.

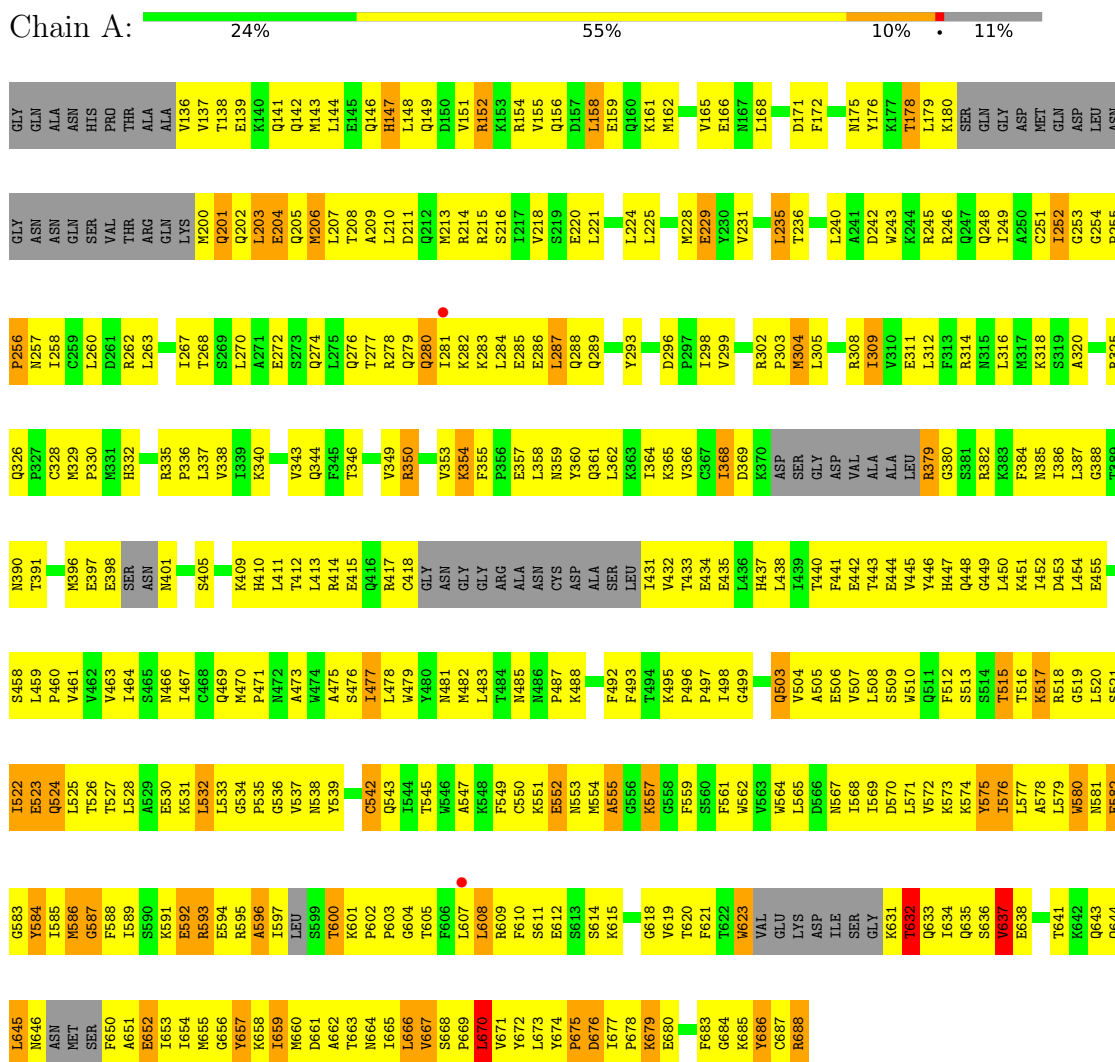
- Molecule 1 is a protein called Signal transducer and activator of transcription 3.

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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



G1856	R1595	G1534	M1470	W1401	H1332	L1260	SER	GLY
Y1657	A1596	P1535	P1471	L1404	R1335	D1261	V1195	GLN
K1658	I1597	G1536	M1472	A1473	P1336	R1262	T1196	ALA
ILE	L1598	V1537	A1473	K1409	L1337	L1263	R1197	ASN
MET	S1599	M1538	M1474	H1410	V1338	I1267	K1199	HIS
ASP	T1600	Y1539	A1475	L1411	H1339	T1268	K1199	PRO
ALA	K1601	S1540	S1476	L1412	K1340	S1269	M1200	THR
T1663	P1602	G1541	I1477	L1413	A1271	S1270	Q1201	ALA
M1664	P1603	C1542	L1478	L1413	V1343	L1270	Q1202	ALA
I1665	G1604	Q1543	M1479	E1414	E1272	A1271	L1203	V1136
L1666	T1605	I1544	Y1480	E1415	Q1344	E1272	E1204	V1137
V1667	F1606	M1481	M1481	C1418	F1345	S1273	T1138	T1138
S1668	L1607	M1482	M1482	GLY	T1346	Q1274	M1205	E1139
P1669	L1608	L1483	L1483	ASN	I1281	L1275	M1206	E1139
L1670	R1609	K1546	L1484	ASN	R1350	L1276	L1207	K1146
V1671	F1610	F1549	T1484	GLY	R1350	Q1276	T1208	Q1141
Y1672	F1610	C1550	M1485	GLY	V1353	T1277	A1209	Q1142
L1673	S1611	K1551	M1486	GLY	K1354	L1278	L1210	M1143
V1674	E1612	E1552	P1487	ARG	F1355	Q1280	D1211	M1144
P1675	S1613	M1553	K1488	ALA	F1356	I1281	Q1212	E1145
D1676	K1615	A1555	F1492	ASN	E1357	I1281	M1213	Q1146
I1677	E1616	G1556	F1493	CYS	L1358	K1282	R1214	H1147
P1678	G1617	K1557	T1494	ALA	M1359	K1283	R1215	L1148
K1679	G1618	G1558	P1495	LEU	Y1360	L1284	E1151	V1151
E1680	V1619	F1559	P1496	SER	Q1361	E1286	S1219	V1151
E1681	T1620	S1560	P1497	I1431	L1362	L1287	E1220	V1152
A1682	F1621	F1561	I1498	V1432	K1365	Q1288	V1155	V1155
F1683	T1622	W1562	G1499	T1433	V1366	Q1289	L1224	Q1156
G1684	W1623	V1563	G1499	H1437	C1367	Y1293	L1225	D1157
K1685	VAL	W1564	Q1503	I1437	I1368	D1296	M1228	L1158
V1686	GUJ	L1565	V1504	L1438	D1369	F1297	E1229	E1159
C1687	LYS	D1566	A1505	I1439	D1369	P1297	Y1230	M1162
R1688	ASP	M1567	E1506	I1440	K1370	F1297	V1231	M1162
	ILE	I1568	V1507	F1441	ASP	I1299	T1234	V1165
	SER	I1569	L1508	E1442	SER	V1299	L1234	E1166
	GLY	D1570	S1509	T1443	GLY	R1302	L1235	N1167
	K1631	L1571	M1510	E1444	ASP	P1303	L1236	L1168
	T1632	V1572	D1571	V1445	VAL	M1304	Q1169	Q1169
	Q1633	K1573	F1512	Y1446	ALA	R1308	E1238	F1172
	I1634	K1574	S1513	H1447	ALA	L1240	E1239	M1175
	Q1635	Y1575	T1514	Q1448	R1379	L1241	L1240	M1175
	S1636	L1576	T1515	G1449	LEU	A1241	A1241	M1175
	V1637	M1577	T1516	L1450	G1380	D1242	D1242	T1178
	E1638	A1578	K1517	K1451	S1381	W1243	W1243	L1179
		L1579	R1518	I1452	R1382	K1244	K1244	K1180
		W1580	G1519	D1453	K1383	R1245	R1245	K1180
		M1581	L1520	L1454	F1384	R1246	R1246	S1181
		E1582	S1521	E1455	M1385	Q1247	Q1247	Q1182
		G1583	I1522	S1458	I1386	I1248	I1248	C1183
		Y1584	E1523	L1459	L1387	L1249	L1249	D1184
		I1585	Q1524	L1459	G1388	A1320	A1250	MET
		M1586	L1525	P1460	T1389	R1325	C1251	GLN
		G1587	T1526	V1461	M1390	Q1326	ASP	ASP
		F1588	T1527	V1462	T1391	P1337	I1252	LEU
		I1589	L1528	V1463	M1396	C1328	ASN	ASN
		S1590	A1529	M1466	E1397	M1329	P1255	GLY
		K1591	E1530	I1467	E1397	C1328	P1256	GLY
		E1592	K1531	C1468	E1398	M1330	M1257	ASN
		R1593	L1532	L1533	E1398	P1330	I1258	ASN
		E1594	L1533	Q1469	ASN	L1331	C1259	GLN

4 Data and refinement statistics i

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)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.269 0.245 , 0.267	Depositor DCC
R_{free} test set	7413 reflections (8.81%)	wwPDB-VP
Wilson B-factor (Å ²)	71.6	Xtrriage
Anisotropy	0.491	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.367 for -h,-k,l	Xtrriage
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

Xtrriage'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, 0.333 respectively for untwinned datasets, and 0.375, 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:H	1:A:517:LYS:HD2	1.28	0.99
1:B:1470:MET:HB3	1:B:1471:PRO:HD3	1.46	0.98
1:B:1547:ALA:HA	1:B:1551:LYS:HB3	1.41	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:HD22	1:B:1670:LEU:H	1.27	0.97
1:B:1576:ILE:HA	1:B:1579:LEU:HD13	1.45	0.97
1:B:1517:LYS:H	1:B:1517:LYS:HD2	1.30	0.95
1:A:670:LEU:H	1:A:670:LEU:HD22	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:HA	1:B:1280:GLN:HE21	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:314:ARG:HA	1:A:452:ILE:HD11	1.59	0.82
1:A:658:LYS:O	1:A:667:VAL:HG23	1.80	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:138:THR:HG23	1:A:141:GLN:NE2	1.94	0.81
1:A:663:THR:O	1:A:665:ILE:HG12	1.80	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:H	1:A:670:LEU:CD2	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:1195:VAL:HG12	1:B:1196:THR:H	1.47	0.79
1:B:1670:LEU:H	1:B:1670:LEU:CD2	1.95	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:A:498:ILE:HG21	1:A:543:GLN:HB3	1.66	0.77
1:B:1633:GLN:HG3	1:B:1634:ILE:H	1.49	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:HB3	1:A:325:ARG:NH1	2.00	0.76
1:A:346:THR:HG22	1:A:409:LYS:HA	1.66	0.76
1:B:1605:THR:HG22	1:B:1672:TYR:CB	2.14	0.76
1:B:1198:GLN:HG3	1:B:1201:GLN:OE1	1.84	0.76
1:A:221:LEU:HD13	1:A:281:ILE:CD1	2.16	0.76
1:B:1633:GLN:CG	1:B:1634:ILE:H	1.96	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:HE2	1:B:1658:LYS:HA	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:1325:ARG:HB3	1:B:1325:ARG:NH1	2.01	0.74
1:B:1365:LYS:HG3	1:B:1391:THR:HG22	1.69	0.74
1:A:325:ARG:HB3	1:A:325:ARG:HH11	1.52	0.74
1:B:1568:ILE:O	1:B:1572:VAL:HG23	1.86	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:HD13	1:A:522:ILE:H	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:A:504:VAL:HG12	1:A:508:LEU:HD11	1.73	0.71
1:B:1641:THR:HG23	1:B:1644:GLN:HE21	1.55	0.71
1:A:503:GLN:O	1:A:507:VAL:HG23	1.90	0.71
1:B:1355:PHE:HB2	1:B:1358:LEU:HD12	1.73	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:475:ALA:HB2	1:A:562:TRP:NE1	2.06	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: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:A:248:GLN:HE22	1:A:485:ASN:HA	1.55	0.70
1:B:1152:ARG:HH22	1:B:1272:GLU:HB2	1.56	0.70
1:A:252:ILE:CG2	1:A:481:ASN:HD22	2.05	0.70
1:A:576:ILE:CA	1:A:579:LEU:HD13	2.21	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:A:637:VAL:HG13	1:A:638:GLU:N	2.07	0.70
1:B:1530:GLU:HG3	1:B:1534:GLY:O	1.91	0.70
1:A:530:GLU:HG3	1:A:534:GLY:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1162:MET:O	1:B:1166:GLU:HG3	1.92	0.70
1:B:1504:VAL:HG12	1:B:1508:LEU:HD11	1.73	0.70
1:A:483:LEU:HD13	1:A:497:PRO:HB2	1.74	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: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:A:287:LEU:C	1:A:289:GLN:H	1.95	0.69
1:B:1288:GLN:OE1	1:B:1302:ARG:NH2	2.25	0.69
1:B:1470:MET:CB	1:B:1471:PRO:HD3	2.22	0.69
1:B:1498:ILE:H	1:B:1498:ILE:HD12	1.56	0.69
1:B:1503:GLN:O	1:B:1507:VAL:HG23	1.92	0.69
1:A:252:ILE:HB	1:A:478:LEU:HD23	1.74	0.69
1:B:1547:ALA:HB1	1:B:1552:GLU:OE1	1.91	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: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: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: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:A:493:PHE:HA	1:A:496:PRO:HG3	1.75	0.68
1:B:1598:LEU:HD22	1:B:1623:TRP:C	2.14	0.68
1:A:596:ALA:HB1	1:B:1535:PRO:CB	2.24	0.68
1:B:1493:PHE:HA	1:B:1496:PRO:HG3	1.75	0.68
1:A:355:PHE:HB2	1:A:358:LEU:HD12	1.76	0.68
1:A:470:MET:CB	1:A:471:PRO:HD3	2.22	0.68
1:A:446:TYR:HA	1:A:450:LEU:O	1.94	0.68
1:B:1137:VAL:HG22	1:B:1262:ARG:NH2	2.07	0.68
1:A:211:ASP:O	1:A:215:ARG:HG3	1.94	0.67
1:A:337:LEU:HA	1:A:461:VAL:HG22	1.76	0.67
1:B:1583:GLY:O	1:B:1585:ILE:N	2.27	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:HD2	1:B:1517:LYS:N	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:A:554:MET:HB2	1:A:557:LYS:HB2	1.76	0.66
1:B:1284:LEU:HD22	1:B:1298:ILE:CD1	2.26	0.66
1:B:1631:LYS:O	1:B:1632:THR:C	2.34	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:B:1564:TRP:CD2	1:B:1568:ILE:HD11	2.30	0.66
1:A:283:LYS:HA	1:A:286:GLU:HG3	1.76	0.66
1:B:1211:ASP:O	1:B:1215:ARG:HG3	1.95	0.66
1:B:1288:GLN:HE21	1:B:1298:ILE:HG22	1.61	0.66
1:A:532:LEU:HD12	1:A:561:PHE:CE2	2.30	0.66
1:B:1675:PRO:HB2	1:B:1677:ILE:HG13	1.77	0.66
1:A:515:THR:HG21	1:A:573:LYS:HG3	1.78	0.66
1:B:1444:GLU:OE1	1:B:1451:LYS:HE3	1.95	0.66
1:B:1446:TYR:HA	1:B:1450:LEU:O	1.96	0.66
1:B:1591:LYS:HE2	1:B:1609:ARG:NH2	2.10	0.66
1:B:1252:ILE:CG2	1:B:1481:ASN:HD22	2.09	0.66
1:B:1583:GLY:C	1:B:1585:ILE:H	1.99	0.66
1:A:479:TRP:HD1	1:A:492:PHE:HE1	1.44	0.65
1:A:523:GLU:HG2	1:B:1537:VAL:HG11	1.78	0.65
1:B:1252:ILE:HB	1:B:1478:LEU:HD23	1.77	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:267:ILE:HG23	1:A:316:LEU:HD11	1.78	0.65
1:A:309:ILE:HD13	1:A:309:ILE:O	1.97	0.65
1:A:611:SER:HB3	1:A:614:SER:OG	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:512:PHE:HB3	1:A:518:ARG:O	1.97	0.64
1:A:517:LYS:HD2	1:A:517:LYS:N	2.06	0.64
1:A:657:TYR:CE2	1:A:659:ILE:HG12	2.33	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:252:ILE:HG23	1:A:481:ASN:HD22	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:GLY:C	1:A:585:ILE:H	2.01	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:148:LEU:HD12	1:A:231:VAL:HG11	1.81	0.62
1:A:288:GLN:HB2	1:A:298:ILE:HG21	1.82	0.62
1:A:650:PHE:CA	1:A:653:ILE:HD13	2.23	0.62
1:A:582:GLU:CD	1:A:582:GLU:H	2.03	0.62
1:B:1512:PHE:HB3	1:B:1518:ARG:O	1.99	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:B:1686:TYR:CD1	1:B:1686:TYR:N	2.68	0.62
1:A:143:MET:O	1:A:146:GLN:HB3	2.00	0.62
1:A:597:ILE:HD11	1:A:634:ILE:HD12	1.80	0.62
1:A:210:LEU:O	1:A:214:ARG:HG3	2.00	0.62
1:A:602:PRO:HG2	1:A:605:THR:HG23	1.82	0.62
1:B:1368:ILE:CG2	1:B:1386:ILE:HG13	2.30	0.62
1:A:320:ALA:CB	1:A:353:VAL:HG23	2.30	0.62
1:A:576:ILE:CD1	1:A:645:LEU:HD13	2.30	0.62
1:B:1672:TYR:HA	1:B:1677:ILE:O	2.00	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:571:LEU:O	1:A:575:TYR:O	2.18	0.61
1:A:654:ILE:HG21	1:A:683:PHE:CD1	2.36	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:270:LEU:O	1:A:274:GLN:HG3	2.01	0.61
1:A:531:LYS:HZ1	1:A:612:GLU:HB3	1.65	0.61
1:A:245:ARG:HE	1:A:249:ILE:HD11	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LEU:C	1:A:289:GLN:N	2.54	0.61
1:A:631:LYS:O	1:A:632:THR:C	2.39	0.61
1:B:1651:ALA:HB3	1:B:1688:ARG:HH22	1.66	0.61
1:B:1195:VAL:HG21	1:B:1200:MET:CE	2.31	0.61
1:B:1595:ARG:O	1:B:1599:SER:HB2	2.01	0.61
1:B:1611:SER:HB3	1:B:1614:SER:OG	2.01	0.61
1:B:1283:LYS:O	1:B:1287:LEU:HD13	2.01	0.61
1:B:1602:PRO:HG2	1:B:1605:THR:HG23	1.81	0.61
1:A:288:GLN:HE21	1:A:298:ILE:HG22	1.64	0.60
1:A:304:MET:CE	1:A:304:MET:HA	2.29	0.60
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:B:1138:THR:HG23	1:B:1141:GLN:NE2	2.16	0.60
1:A:517:LYS:H	1:A:517:LYS:CD	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:549:PHE:O	1:A:561:PHE:HB3	2.02	0.60
1:A:597:ILE:HD11	1:A:634:ILE:CD1	2.30	0.60
1:B:1248:GLN:O	1:B:1251:CYS:HB2	2.01	0.60
1:B:1565:LEU:HA	1:B:1568:ILE:CG1	2.32	0.60
1:B:1605:THR:HA	1:B:1672:TYR:O	2.02	0.60
1:A:550:CYS:HB3	1:A:562:TRP:HB3	1.83	0.60
1:B:1571:LEU:O	1:B:1575:TYR:O	2.19	0.60
1:A:137:VAL:CG2	1:A:262:ARG:HH22	2.13	0.59
1:B:1270:LEU:O	1:B:1274:GLN:HG3	2.02	0.59
1:B:1384:PHE:O	1:B:1385:ASN:ND2	2.34	0.59
1:B:1598:LEU:HD23	1:B:1632:THR:HG22	1.84	0.59
1:A:171:ASP:HB2	1:A:206:MET:HE1	1.84	0.59
1:A:512:PHE:CB	1:A:519:GLY:HA2	2.31	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: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:1304:MET:HA	1:B:1304:MET:CE	2.31	0.59
1:B:1528:LEU:HA	1:B:1531:LYS:HB2	1.84	0.59
1:B:1282:LYS:O	1:B:1286:GLU:HG2	2.02	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: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:172:PHE:HB2	1:A:206:MET:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLN:NE2	1:A:299:VAL:HA	2.18	0.59
1:A:597:ILE:C	1:A:600:THR:HG22	2.22	0.59
1:A:523:GLU:HG3	1:A:524:GLN:N	2.18	0.59
1:B:1136:VAL:HG22	1:B:1137:VAL:H	1.67	0.59
1:B:1622:THR:HG22	1:B:1623:TRP:N	2.18	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: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:B:1338:VAL:HG11	1:B:1470:MET:CE	2.34	0.58
1:A:576:ILE:HG22	1:A:576:ILE:O	2.03	0.58
1:B:1236:THR:O	1:B:1240:LEU:HB3	2.02	0.58
1:B:1314:ARG:O	1:B:1318:LYS:HG3	2.04	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:CD2	1:A:686:TYR:N	2.71	0.58
1:B:1637:VAL:HG22	1:B:1638:GLU:H	1.69	0.57
1:B:1654:ILE:HG21	1:B:1683:PHE:CD1	2.39	0.57
1:B:1248:GLN:HE21	1:B:1481:ASN:HA	1.69	0.57
1:A:282:LYS:O	1:A:286:GLU:HG2	2.05	0.57
1:A:591:LYS:O	1:A:594:GLU:HB3	2.03	0.57
1:B:1549:PHE:O	1:B:1561:PHE:HB3	2.03	0.57
1:B:1564:TRP:O	1:B:1568:ILE:HG13	2.04	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:B:1598:LEU:HD22	1:B:1623:TRP:O	2.03	0.57
1:A:437:HIS:HD2	1:A:463:VAL:HG23	1.69	0.57
1:A:354:LYS:HG2	1:A:396:MET:CE	2.33	0.57
1:A:674:TYR:HB3	1:A:675:PRO:HD3	1.85	0.57
1:B:1288:GLN:NE2	1:B:1299:VAL:HA	2.20	0.57
1:B:1576:ILE:O	1:B:1576:ILE:HG22	2.05	0.57
1:B:1633:GLN:C	1:B:1634:ILE:HD12	2.25	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:1498:ILE:HG22	1:B:1499:GLY:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1559:PHE:CE2	1:B:1564:TRP:HB2	2.40	0.57
1:B:1591:LYS:O	1:B:1594:GLU:HB3	2.04	0.56
1:A:248:GLN:O	1:A:251:CYS:HB2	2.04	0.56
1:A:498:ILE:HG22	1:A:499:GLY:H	1.70	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:258:ILE:O	1:A:258:ILE:HD12	2.04	0.56
1:A:623:TRP:CD1	1:A:623:TRP:N	2.73	0.56
1:B:1288:GLN:CD	1:B:1302:ARG:HH21	2.08	0.56
1:B:1318:LYS:HA	1:B:1454:LEU:CD2	2.35	0.56
1:B:1517:LYS:H	1:B:1517:LYS:CD	2.05	0.56
1:A:527:THR:HG21	1:A:589:ILE:HA	1.88	0.56
1:A:565:LEU:HA	1:A:568:ILE:HG12	1.87	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: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:311:GLU:OE1	1:A:311:GLU:HA	2.06	0.56
1:A:441:PHE:O	1:A:442:GLU:HG3	2.05	0.56
1:A:653:ILE:HD12	1:A:653:ILE:H	1.71	0.56
1:A:664:ASN:O	1:A:665:ILE:HD13	2.06	0.56
1:B:1641:THR:CG2	1:B:1644:GLN:HE21	2.19	0.56
1:B:1215:ARG:HG2	1:B:1215:ARG:HH11	1.70	0.56
1:B:1674:TYR:HB3	1:B:1675:PRO:HD3	1.87	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:1575:TYR:O	1:B:1576:ILE:HB	2.06	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:HG2	1:B:1215:ARG:NH1	2.21	0.55
1:A:531:LYS:NZ	1:A:612:GLU:HB3	2.21	0.55
1:A:559:PHE:CE2	1:A:564:TRP:HB2	2.41	0.55
1:A:575:TYR:O	1:A:576:ILE:HB	2.06	0.55
1:B:1311:GLU:HA	1:B:1311:GLU:OE1	2.06	0.55
1:B:1512:PHE:CB	1:B:1519:GLY:HA2	2.34	0.55
1:B:1584:TYR:O	1:B:1608:LEU:HD12	2.06	0.55
1:A:594:GLU:HG3	1:A:607:LEU:CD2	2.36	0.55
1:A:349:VAL:O	1:A:405:SER:HB2	2.06	0.55
1:A:368:ILE:HG21	1:A:385:ASN:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:VAL:HG22	1:A:262:ARG:NH2	2.12	0.55
1:A:215:ARG:NH1	1:A:215:ARG:HG2	2.22	0.55
1:A:344:GLN:CG	1:A:410:HIS:HA	2.35	0.55
1:A:637:VAL:HG22	1:A:638:GLU:H	1.71	0.55
1:A:644:GLN:O	1:A:646:ASN:N	2.39	0.55
1:B:1623:TRP:N	1:B:1623:TRP:CD1	2.75	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:1527:THR:HG21	1:B:1589:ILE:HA	1.88	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:1567:ASN:O	1:B:1571:LEU:HB2	2.07	0.55
1:A:522:ILE:HD13	1:A:522:ILE:N	2.20	0.55
1:B:1279:GLN:NE2	1:B:1282:LYS:HD2	2.22	0.55
1:B:1669:PRO:HG2	1:B:1679:LYS:HE3	1.89	0.55
1:B:1686:TYR:N	1:B:1686:TYR:HD1	2.04	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:A:175:ASN:O	1:A:178:THR:HG22	2.06	0.54
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: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:A:179:LEU:HD21	1:A:200:MET:HA	1.89	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:B:1644:GLN:O	1:B:1646:ASN:N	2.40	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: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:1325:ARG:NH1	1:B:1325:ARG:CB	2.70	0.54
1:B:1337:LEU:O	1:B:1461:VAL:HG13	2.06	0.54
1:B:1594:GLU:HG3	1:B:1607:LEU:HD22	1.89	0.54
1:A:559:PHE:HB3	1:A:615:LYS:HE3	1.90	0.54
1:B:1565:LEU:HA	1:B:1568:ILE:HG13	1.89	0.54
1:A:412:THR:CG2	1:A:413:LEU:N	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ASN:O	1:A:571:LEU:HB2	2.08	0.54
1:A:398:GLU:O	1:A:401:ASN:N	2.41	0.54
1:A:621:PHE:O	1:A:636:SER:HA	2.08	0.54
1:B:1148:LEU:CD1	1:B:1231:VAL:HG11	2.37	0.54
1:B:1632:THR:HG22	1:B:1632:THR:O	2.08	0.54
1:B:1414:ARG:HG2	1:B:1415:GLU:H	1.74	0.53
1:B:1498:ILE:HD12	1:B:1498:ILE:N	2.23	0.53
1:B:1504:VAL:HG12	1:B:1508:LEU:CD1	2.38	0.53
1:A:488:LYS:O	1:A:488:LYS:HG3	2.09	0.53
1:B:1564:TRP:CE2	1:B:1568:ILE:HD11	2.43	0.53
1:B:1597:ILE:CG1	1:B:1598:LEU:N	2.68	0.53
1:A:325:ARG:NH1	1:A:325:ARG:CB	2.69	0.53
1:A:156:GLN:O	1:A:159:GLU:HB3	2.08	0.53
1:A:335:ARG:HG3	1:A:470:MET:SD	2.49	0.53
1:A:650:PHE:CD2	1:A:654:ILE:HD11	2.43	0.53
1:A:477:ILE:HG22	1:A:478:LEU:N	2.24	0.53
1:A:504:VAL:HG12	1:A:508:LEU:CD1	2.38	0.53
1:A:623:TRP:CE3	1:A:670:LEU:HD21	2.44	0.53
1:B:1396:MET:HG3	1:B:1404:LEU:HD23	1.91	0.53
1:A:158:LEU:HG	1:A:220:GLU:OE1	2.09	0.53
1:B:1175:ASN:O	1:B:1178:THR:HG22	2.08	0.53
1:B:1619:VAL:HG23	1:B:1619:VAL:O	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: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:HD13	1:B:1431:ILE:N	2.24	0.53
1:B:1557:LYS:H	1:B:1557:LYS:HD2	1.74	0.53
1:A:248:GLN:NE2	1:A:485:ASN:HA	2.23	0.52
1:A:594:GLU:HG3	1:A:607:LEU:HD22	1.90	0.52
1:A:619:VAL:HG23	1:A:619:VAL:O	2.08	0.52
1:A:658:LYS:HZ3	1:A:668:SER:HA	1.73	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:621:PHE:CZ	1:A:637:VAL:HG11	2.43	0.52
1:B:1260:LEU:HB2	1:B:1350:ARG:HH21	1.74	0.52
1:B:1678:PRO:O	1:B:1680:GLU:N	2.40	0.52
1:A:610:PHE:HA	1:A:618:GLY:O	2.10	0.52
1:A:670:LEU:CD2	1:A:670:LEU:N	2.68	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:441:PHE:C	1:A:442:GLU:HG3	2.30	0.52
1:A:659:ILE:O	1:A:667:VAL:CG2	2.57	0.52
1:A:364:ILE:HD13	1:A:443:THR:HG21	1.92	0.52
1:A:633:GLN:CG	1:A:634:ILE:N	2.72	0.52
1:B:1195:VAL:HB	1:B:1200:MET:HE2	1.92	0.52
1:B:1201:GLN:C	1:B:1203:LEU:H	2.12	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:340:LYS:HB3	1:A:343:VAL:HG21	1.91	0.52
1:A:557:LYS:HD2	1:A:557:LYS:H	1.75	0.52
1:A:366:VAL:HA	1:A:440:THR:O	2.09	0.52
1:A:386:ILE:CG2	1:A:411:LEU:HD22	2.38	0.52
1:A:633:GLN:HG3	1:A:634:ILE:H	1.74	0.52
1:A:438:LEU:HD21	1:A:460:PRO:HG3	1.91	0.51
1:A:600:THR:HG23	1:A:601:LYS:HG2	1.92	0.51
1:B:1571:LEU:HD11	1:B:1576:ILE:HD12	1.91	0.51
1:B:1594:GLU:HG3	1:B:1607:LEU:CD2	2.39	0.51
1:A:658:LYS:CE	1:A:669:PRO:HD3	2.40	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:B:1521:SER:O	1:B:1525:LEU:HB2	2.10	0.51
1:B:1609:ARG:NH1	1:B:1620:THR:HG21	2.25	0.51
1:A:476:SER:HB3	1:A:493:PHE:CE2	2.46	0.51
1:A:654:ILE:HG22	1:A:654:ILE:O	2.10	0.51
1:B:1493:PHE:CD1	1:B:1496:PRO:HG3	2.45	0.51
1:A:498:ILE:CG2	1:A:543:GLN:HB3	2.36	0.51
1:A:671:VAL:HG12	1:A:679:LYS:HZ3	1.75	0.51
1:B:1340:LYS:HB3	1:B:1343:VAL:HG21	1.92	0.51
1:B:1379:ARG:C	1:B:1381:SER:H	2.14	0.51
1:B:1550:CYS:HB3	1:B:1562:TRP:CB	2.40	0.51
1:A:144:LEU:C	1:A:146:GLN:N	2.63	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:A:512:PHE:CZ	1:A:569:ILE:HD13	2.45	0.51
1:A:517:LYS:N	1:A:517:LYS:CD	2.71	0.51
1:A:605:THR:HA	1:A:671:VAL:O	2.11	0.51
1:A:609:ARG:NH1	1:A:620:THR:HG21	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1475:ALA:HB2	1:B:1562:TRP:HE1	1.75	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: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:1332:HIS:HB3	1:B:1335:ARG:HB2	1.92	0.51
1:A:176:TYR:HA	1:A:203:LEU:HD21	1.93	0.50
1:B:1604:GLY:O	1:B:1670:LEU:HB3	2.11	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:1252:ILE:HG21	1:B:1481:ASN:HD22	1.77	0.50
1:B:1520:LEU:HB2	1:B:1525:LEU:HD13	1.93	0.50
1:A:332:HIS:CE1	1:A:467:ILE:HD11	2.47	0.50
1:A:634:ILE:C	1:A:635:GLN:HG3	2.32	0.50
1:B:1144:LEU:C	1:B:1146:GLN:N	2.62	0.50
1:B:1600:THR:HG23	1:B:1601:LYS:HG2	1.93	0.50
1:A:473:ALA:O	1:A:476:SER:N	2.45	0.50
1:B:1654:ILE:HG22	1:B:1654:ILE:O	2.11	0.50
1:A:473:ALA:C	1:A:475:ALA:N	2.65	0.50
1:A:584:TYR:O	1:A:608:LEU:HD12	2.12	0.50
1:B:1670:LEU:CD2	1:B:1670:LEU:N	2.69	0.50
1:A:148:LEU:CD1	1:A:231:VAL:HG11	2.42	0.50
1:A:280:GLN:HA	1:A:280:GLN:NE2	2.16	0.50
1:B:1302:ARG:N	1:B:1303:PRO:CD	2.74	0.50
1:B:1594:GLU:O	1:B:1597:ILE:HG12	2.12	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:573:LYS:CA	1:A:577:LEU:HD13	2.41	0.49
1:A:585:ILE:HG22	1:A:587:GLY:N	2.27	0.49
1:B:1285:GLU:O	1:B:1289:GLN:HG3	2.12	0.49
1:B:1441:PHE:C	1:B:1442:GLU:HG3	2.30	0.49
1:B:1476:SER:HB3	1:B:1493:PHE:CE2	2.47	0.49
1:A:530:GLU:C	1:A:532:LEU:H	2.15	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:A:605:THR:HG22	1:A:672:TYR:CB	2.35	0.49
1:B:1488:LYS:HG3	1:B:1488:LYS:O	2.12	0.49
1:A:209:ALA:O	1:A:213:MET:HG2	2.13	0.49
1:B:1576:ILE:HA	1:B:1579:LEU:CD1	2.31	0.49
1:B:1550:CYS:CB	1:B:1562:TRP:HB3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1554:MET:O	1:B:1555:ALA:C	2.51	0.49
1:B:1573:LYS:CA	1:B:1577:LEU:HD13	2.40	0.49
1:B:1606:PHE:HZ	1:B:1679:LYS:HB3	1.78	0.49
1:B:1622:THR:C	1:B:1623:TRP:HD1	2.16	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: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:B:1344:GLN:CG	1:B:1410:HIS:HA	2.43	0.49
1:A:678:PRO:O	1:A:680:GLU:N	2.41	0.49
1:B:1601:LYS:HE3	1:B:1674:TYR:CE2	2.48	0.49
1:A:179:LEU:CD2	1:A:200:MET:HA	2.43	0.49
1:A:276:GLN:O	1:A:280:GLN:HG2	2.13	0.49
1:A:576:ILE:HA	1:A:579:LEU:CD1	2.32	0.49
1:B:1280:GLN:HA	1:B:1280:GLN:NE2	2.16	0.49
1:B:1386:ILE:C	1:B:1387:LEU:HD23	2.34	0.49
1:B:1604:GLY:HA2	1:B:1670:LEU:HB3	1.94	0.49
1:A:328:CYS:SG	1:A:336:PRO:HA	2.52	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:224:LEU:O	1:A:228:MET:HG3	2.12	0.48
1:A:325:ARG:CB	1:A:325:ARG:CZ	2.91	0.48
1:A:357:GLU:CD	1:A:357:GLU:H	2.17	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:B:1600:THR:HG23	1:B:1601:LYS:N	2.28	0.48
1:A:520:LEU:HB2	1:A:525:LEU:HD13	1.94	0.48
1:A:600:THR:HG23	1:A:601:LYS:H	1.78	0.48
1:A:550:CYS:CB	1:A:562:TRP:HB3	2.43	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:B:1439:ILE:N	1:B:1439:ILE:HD12	2.28	0.48
1:A:498:ILE:HG22	1:A:499:GLY:N	2.28	0.48
1:A:654:ILE:HD13	1:A:683:PHE:HE1	1.78	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:586:MET:O	1:A:588:PHE:N	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:LEU:O	1:A:674:TYR:C	2.52	0.48
1:B:1136:VAL:HG22	1:B:1137:VAL:N	2.28	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:139:GLU:HA	1:A:142:GLN:CG	2.37	0.48
1:A:600:THR:HG23	1:A:601:LYS:N	2.29	0.48
1:B:1179:LEU:HD11	1:B:1195:VAL:HG12	1.96	0.48
1:B:1517:LYS:N	1:B:1517:LYS:CD	2.73	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:379:ARG:HH11	1:A:380:GLY:N	2.12	0.47
1:A:634:ILE:CG2	1:A:635:GLN:N	2.76	0.47
1:A:688:ARG:H	1:A:688:ARG:HE	1.62	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: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:B:1600:THR:HG23	1:B:1601:LYS:H	1.78	0.47
1:A:326:GLN:OE1	1:A:458:SER:HB2	2.14	0.47
1:A:554:MET:O	1:A:555:ALA:C	2.52	0.47
1:B:1623:TRP:NE1	1:B:1635:GLN:O	2.48	0.47
1:B:1671:VAL:HG12	1:B:1679:LYS:HZ3	1.80	0.47
1:B:1673:LEU:O	1:B:1674:TYR:C	2.53	0.47
1:A:204:GLU:H	1:A:204:GLU:HG3	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:A:243:TRP:NE1	1:A:258:ILE:HB	2.29	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:B:1243:TRP:NE1	1:B:1258:ILE:HB	2.30	0.47
1:B:1288:GLN:NE2	1:B:1302:ARG:HH21	2.13	0.47
1:B:1288:GLN:HG3	1:B:1299:VAL:HG12	1.97	0.47
1:B:1674:TYR:O	1:B:1675:PRO:C	2.52	0.47
1:A:146:GLN:O	1:A:147:HIS:C	2.52	0.47
1:A:585:ILE:HD13	1:A:608:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1357:GLU:CD	1:B:1357:GLU:H	2.17	0.47
1:A:136:VAL:HG22	1:A:137:VAL:H	1.80	0.47
1:A:252:ILE:HG21	1:A:481:ASN:HD22	1.77	0.47
1:A:288:GLN:HG3	1:A:299:VAL:HG12	1.97	0.47
1:A:386:ILE:C	1:A:387:LEU:HD23	2.34	0.47
1:B:1580:TRP:CD1	1:B:1580:TRP:C	2.88	0.47
1:A:252:ILE:HG23	1:A:481:ASN:ND2	2.27	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:414:ARG:HG2	1:A:415:GLU:N	2.30	0.46
1:A:656:GLY:O	1:A:657:TYR:C	2.53	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:B:1566:ASP:HA	1:B:1569:ILE:HD12	1.97	0.46
1:B:1622:THR:CG2	1:B:1634:ILE:HG23	2.44	0.46
1:A:592:GLU:C	1:A:592:GLU:OE1	2.54	0.46
1:B:1325:ARG:CB	1:B:1325:ARG:CZ	2.93	0.46
1:A:152:ARG:O	1:A:156:GLN:HG2	2.15	0.46
1:A:447:HIS:C	1:A:449:GLY:N	2.66	0.46
1:A:662:ALA:C	1:A:664:ASN:H	2.18	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:1482:MET:HE3	1:B:1483:LEU:CD2	2.45	0.46
1:B:1583:GLY:C	1:B:1585:ILE:N	2.68	0.46
1:B:1644:GLN:C	1:B:1646:ASN:N	2.67	0.46
1:B:1656:GLY:O	1:B:1658:LYS:HE3	2.15	0.46
1:A:144:LEU:C	1:A:146:GLN:H	2.18	0.46
1:A:201:GLN:HA	1:A:204:GLU:CG	2.46	0.46
1:B:1152:ARG:O	1:B:1156:GLN:HG2	2.15	0.46
1:A:161:LYS:NZ	1:A:216:SER:OG	2.48	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: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:1669:PRO:O	1:B:1670:LEU:C	2.54	0.46
1:A:433:THR:CG2	1:A:469:GLN:HB3	2.46	0.46
1:A:441:PHE:N	1:A:441:PHE:CD1	2.84	0.46
1:A:530:GLU:OE2	1:B:1593:ARG:NH1	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1473:ALA:C	1:B:1475:ALA:N	2.66	0.46
1:B:1607:LEU:HB3	1:B:1608:LEU:H	1.56	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:A:653:ILE:H	1:A:653:ILE:CD1	2.28	0.46
1:B:1158:LEU:HG	1:B:1220:GLU:OE1	2.16	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:B:1589:ILE:HD13	1:B:1607:LEU:HD21	1.98	0.46
1:A:214:ARG:CZ	1:A:298:ILE:HD12	2.46	0.46
1:A:607:LEU:HB3	1:A:608:LEU:H	1.58	0.46
1:B:1366:VAL:HA	1:B:1440:THR:O	2.15	0.46
1:B:1592:GLU:C	1:B:1592:GLU:OE1	2.54	0.46
1:A:288:GLN:NE2	1:A:298:ILE:HG22	2.31	0.45
1:B:1209:ALA:O	1:B:1213:MET:HG2	2.16	0.45
1:B:1330:PRO:HD2	1:B:1344:GLN:O	2.16	0.45
1:B:1656:GLY:O	1:B:1657:TYR:C	2.55	0.45
1:A:358:LEU:O	1:A:361:GLN:HB3	2.17	0.45
1:B:1162:MET:O	1:B:1165:VAL:HG12	2.16	0.45
1:B:1318:LYS:HA	1:B:1454:LEU:HD22	1.98	0.45
1:B:1686:TYR:O	1:B:1688:ARG:NH2	2.50	0.45
1:A:201:GLN:O	1:A:204:GLU:HG3	2.16	0.45
1:A:287:LEU:N	1:A:287:LEU:HD12	2.31	0.45
1:A:329:MET:HE1	1:A:338:VAL:O	2.16	0.45
1:A:493:PHE:C	1:A:496:PRO:HD3	2.37	0.45
1:B:1288:GLN:NE2	1:B:1298:ILE:HG22	2.29	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:1605:THR:HA	1:B:1671:VAL:O	2.17	0.45
1:B:1611:SER:N	1:B:1618:GLY:O	2.43	0.45
1:A:447:HIS:O	1:A:449:GLY:N	2.50	0.45
1:A:531:LYS:HZ1	1:A:557:LYS:HE2	1.82	0.45
1:B:1279:GLN:OE1	1:B:1448:GLN:NE2	2.49	0.45
1:B:1358:LEU:O	1:B:1361:GLN:HB3	2.15	0.45
1:B:1585:ILE:HD13	1:B:1608:LEU:HD13	1.98	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:HA	1:B:1652:GLU:OE1	2.16	0.45
1:A:443:THR:O	1:A:454:LEU:HB2	2.16	0.45
1:A:459:LEU:HD23	1:A:459:LEU:HA	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1139:GLU:HA	1:B:1142:GLN:CG	2.43	0.45
1:B:1362:LEU:HD11	1:B:1445:VAL:HG22	1.98	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:1521:SER:OG	1:B:1524:GLN:HG2	2.16	0.45
1:A:201:GLN:O	1:A:203:LEU:N	2.41	0.45
1:A:243:TRP:HE1	1:A:258:ILE:HB	1.82	0.45
1:A:382:ARG:HB2	1:A:384:PHE:HE1	1.82	0.45
1:A:384:PHE:N	1:A:384:PHE:CD1	2.85	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: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:B:1287:LEU:N	1:B:1287:LEU:HD12	2.32	0.45
1:B:1503:GLN:H	1:B:1503:GLN:HG3	1.49	0.45
1:A:442:GLU:HG2	1:A:455:GLU:HB2	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:277:THR:O	1:A:281:ILE:HG12	2.16	0.44
1:A:470:MET:HB3	1:A:471:PRO:CD	2.33	0.44
1:A:521:SER:OG	1:A:524:GLN:HG2	2.16	0.44
1:B:1182:GLN:C	1:B:1184:ASP:H	2.21	0.44
1:B:1622:THR:C	1:B:1623:TRP:CD1	2.90	0.44
1:A:611:SER:N	1:A:618:GLY:O	2.43	0.44
1:B:1447:HIS:O	1:B:1449:GLY:N	2.50	0.44
1:B:1523:GLU:CG	1:B:1524:GLN:N	2.80	0.44
1:B:1578:ALA:O	1:B:1581:ASN:HB2	2.17	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:340:LYS:HE3	1:A:343:VAL:CG2	2.48	0.44
1:A:409:LYS:HZ2	1:A:409:LYS:HB2	1.82	0.44
1:A:431:ILE:O	1:A:435:GLU:HB2	2.16	0.44
1:A:652:GLU:OE1	1:A:652:GLU:HA	2.17	0.44
1:A:680:GLU:O	1:A:684:GLY:HA3	2.17	0.44
1:B:1442:GLU:HG2	1:B:1455:GLU:HB2	1.99	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:656:GLY:O	1:A:658:LYS:HE3	2.18	0.44
1:A:658:LYS:HE2	1:A:668:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:MET:HG3	1:A:666:LEU:HD12	1.99	0.44
1:B:1643:GLN:O	1:B:1646:ASN:HB2	2.18	0.44
1:B:1650:PHE:O	1:B:1654:ILE:HG12	2.18	0.44
1:A:162:MET:O	1:A:165:VAL:HG12	2.17	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:B:1652:GLU:OE2	1:B:1688:ARG:NE	2.50	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:1531:LYS:NZ	1:B:1557:LYS:HE2	2.33	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: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:B:1162:MET:CE	1:B:1283:LYS:HB3	2.47	0.44
1:B:1335:ARG:HB3	1:B:1470:MET:HE1	2.00	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:A:671:VAL:HG12	1:A:679:LYS:HG2	2.00	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:B:1592:GLU:O	1:B:1594:GLU:N	2.51	0.44
1:A:225:LEU:CD2	1:A:308:ARG:HB3	2.48	0.43
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: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:A:340:LYS:O	1:A:343:VAL:HG23	2.18	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:B:1533:LEU:HD21	1:B:1544:ILE:HG12	1.99	0.43
1:A:447:HIS:O	1:A:448:GLN:C	2.56	0.43
1:B:1255:PRO:HA	1:B:1256:PRO:HD2	1.82	0.43
1:B:1340:LYS:O	1:B:1343:VAL:HG23	2.19	0.43
1:B:1576:ILE:HA	1:B:1579:LEU:HB2	1.99	0.43
1:A:279:GLN:HE21	1:A:282:LYS:HD2	1.82	0.43
1:A:578:ALA:O	1:A:581:ASN:HB2	2.18	0.43
1:B:1214:ARG:NH2	1:B:1287:LEU:HB3	2.33	0.43
1:B:1531:LYS:HZ1	1:B:1557:LYS:HE2	1.84	0.43
1:B:1651:ALA:HB3	1:B:1688:ARG:NH2	2.31	0.43
1:A:361:GLN:O	1:A:361:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1592:GLU:C	1:B:1594:GLU:N	2.72	0.43
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:364:ILE:CD1	1:A:443:THR:HG21	2.49	0.43
1:A:650:PHE:CE2	1:A:654:ILE:HD11	2.52	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:B:1384:PHE:N	1:B:1384:PHE:CD1	2.86	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: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:136:VAL:HG22	1:A:137:VAL:N	2.34	0.43
1:A:432:VAL:C	1:A:434:GLU:H	2.22	0.43
1:A:470:MET:CB	1:A:471:PRO:CD	2.95	0.43
1:A:205:GLN:O	1:A:208:THR:N	2.51	0.42
1:A:253:GLY:O	1:A:510:TRP:HB3	2.19	0.42
1:A:288:GLN:HE22	1:A:302:ARG:HH21	1.67	0.42
1:B:1201:GLN:HA	1:B:1204:GLU:OE1	2.19	0.42
1:B:1623:TRP:CB	1:B:1670:LEU:HG	2.49	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:1205:GLN:O	1:B:1208:THR:N	2.52	0.42
1:B:1340:LYS:HE3	1:B:1343:VAL:CG2	2.48	0.42
1:B:1671:VAL:HG12	1:B:1679:LYS:NZ	2.33	0.42
1:A:283:LYS:HA	1:A:283:LYS:HD2	1.83	0.42
1:A:575:TYR:CB	1:A:576:ILE:HD12	2.49	0.42
1:A:623:TRP:NE1	1:A:635:GLN:O	2.53	0.42
1:A:655:MET:HG3	1:A:687:CYS:SG	2.59	0.42
1:B:1359:ASN:O	1:B:1360:TYR:HB2	2.19	0.42
1:B:1466:ASN:ND2	1:B:1467:ILE:H	2.18	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:A:576:ILE:HA	1:A:579:LEU:HB2	2.00	0.42
1:A:580:TRP:CD1	1:A:580:TRP:C	2.91	0.42
1:A:643:GLN:O	1:A:646:ASN:HB2	2.19	0.42
1:B:1482:MET:HE3	1:B:1483:LEU:HD21	2.01	0.42
1:B:1515:THR:HG21	1:B:1573:LYS:CG	2.48	0.42
1:A:221:LEU:CD1	1:A:281:ILE:HD13	2.33	0.42
1:A:206:MET:O	1:A:210:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLY:HA2	1:A:510:TRP:CD2	2.55	0.42
1:A:263:LEU:O	1:A:267:ILE:CG1	2.68	0.42
1:A:388:GLY:O	1:A:390:ASN:N	2.53	0.42
1:A:531:LYS:NZ	1:A:557:LYS:HE2	2.33	0.42
1:A:592:GLU:C	1:A:594:GLU:N	2.73	0.42
1:B:1447:HIS:O	1:B:1448:GLN:C	2.58	0.42
1:B:1606:PHE:CZ	1:B:1679:LYS:HB3	2.55	0.42
1:B:1609:ARG:HH11	1:B:1620:THR:CG2	2.32	0.42
1:A:382:ARG:HB2	1:A:384:PHE:CE1	2.55	0.42
1:A:445:VAL:HB	1:A:452:ILE:CG2	2.50	0.42
1:A:654:ILE:HD13	1:A:683:PHE:CE1	2.54	0.42
1:B:1172:PHE:N	1:B:1206:MET:HE1	2.35	0.42
1:B:1196:THR:HG22	1:B:1197:ARG:N	2.34	0.42
1:B:1256:PRO:HB2	1:B:1257:ASN:H	1.67	0.42
1:A:368:ILE:CD1	1:A:413:LEU:HD21	2.49	0.42
1:A:409:LYS:NZ	1:A:409:LYS:CB	2.83	0.42
1:A:591:LYS:CE	1:A:609:ARG:NH2	2.77	0.42
1:A:623:TRP:HB2	1:A:670:LEU:HG	2.01	0.42
1:A:658:LYS:CE	1:A:668:SER:HA	2.50	0.42
1:B:1279:GLN:HE21	1:B:1282:LYS:HD2	1.83	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:A:530:GLU:C	1:A:532:LEU:N	2.73	0.42
1:B:1283:LYS:HA	1:B:1286:GLU:CG	2.45	0.42
1:B:1205:GLN:O	1:B:1207:LEU:N	2.53	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:A:180:LYS:O	1:A:180:LYS:HG2	2.20	0.41
1:A:621:PHE:CE1	1:A:637:VAL:HB	2.54	0.41
1:B:1169:GLN:O	1:B:1169:GLN:HG2	2.20	0.41
1:B:1368:ILE:O	1:B:1369:ASP:HB2	2.20	0.41
1:B:1540:SER:C	1:B:1542:CYS:H	2.23	0.41
1:B:1598:LEU:HD13	1:B:1623:TRP:HA	2.02	0.41
1:A:205:GLN:O	1:A:206:MET:C	2.59	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:506:GLU:O	1:A:509:SER:HB3	2.20	0.41
1:B:1180:LYS:O	1:B:1180:LYS:HG2	2.19	0.41
1:B:1379:ARG:HD3	1:B:1379:ARG:C	2.41	0.41
1:A:154:ARG:HB2	1:A:224:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ARG:HD3	1:A:485:ASN:HB3	2.02	0.41
1:B:1181:SER:O	1:B:1182:GLN:HB3	2.20	0.41
1:B:1283:LYS:HA	1:B:1283:LYS:HD2	1.85	0.41
1:B:1368:ILE:HG21	1:B:1385:ASN:HA	2.02	0.41
1:A:172:PHE:CD2	1:A:172:PHE:C	2.94	0.41
1:A:260:LEU:HB2	1:A:350:ARG:NH2	2.35	0.41
1:A:304:MET:HA	1:A:304:MET:HE1	2.02	0.41
1:A:332:HIS:HE1	1:A:467:ILE:HD11	1.84	0.41
1:A:335:ARG:HD3	1:A:335:ARG:HA	1.90	0.41
1:B:1530:GLU:C	1:B:1532:LEU:N	2.74	0.41
1:B:1601:LYS:HB3	1:B:1602:PRO:CD	2.43	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:A:602:PRO:O	1:A:603:PRO:C	2.59	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:1409:LYS:NZ	1:B:1409:LYS:CB	2.84	0.41
1:B:1433:THR:HG21	1:B:1472:ASN:HB2	2.03	0.41
1:A:279:GLN:OE1	1:A:448:GLN:OE1	2.39	0.41
1:A:535:PRO:CG	1:B:1600:THR:HB	2.47	0.41
1:B:1252:ILE:HG23	1:B:1481:ASN:ND2	2.34	0.41
1:B:1670:LEU:HD22	1:B:1670:LEU:N	2.11	0.41
1:A:309:ILE:HD13	1:A:309:ILE:C	2.40	0.41
1:A:466:ASN:ND2	1:A:467:ILE:H	2.19	0.41
1:A:623:TRP:HH2	1:A:659:ILE:HG21	1.86	0.41
1:A:280:GLN:HE21	1:A:280:GLN:CA	2.13	0.41
1:A:284:LEU:C	1:A:286:GLU:H	2.24	0.41
1:A:522:ILE:H	1:A:522:ILE:CD1	2.13	0.41
1:A:604:GLY:HA2	1:A:670:LEU:HB3	2.01	0.41
1:B:1172:PHE:CD2	1:B:1172:PHE:C	2.95	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:B:1470:MET:HB3	1:B:1471:PRO:CD	2.33	0.41
1:B:1524:GLN:HE21	1:B:1524:GLN:HB3	1.59	0.41
1:B:1677:ILE:HG13	1:B:1677:ILE:H	1.67	0.41
1:B:1195:VAL:HG11	1:B:1200:MET:CE	2.51	0.41
1:B:1234:THR:O	1:B:1238:GLU:HB2	2.21	0.41
1:B:1308:ARG:O	1:B:1311:GLU:HB3	2.21	0.41
1:A:240:LEU:HD13	1:A:263:LEU:HD13	2.02	0.40
1:A:337:LEU:HD22	1:A:461:VAL:HG23	2.03	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:1243:TRP:CZ2	1:B:1260:LEU:HD21	2.56	0.40
1:B:1361:GLN:O	1:B:1361:GLN:HG2	2.20	0.40
1:A:288:GLN:NE2	1:A:302:ARG:HE	2.20	0.40
1:A:359:ASN:O	1:A:360:TYR:HB2	2.21	0.40
1:B:1277:THR:O	1:B:1281:ILE:HG13	2.21	0.40
1:B:1314:ARG:CA	1:B:1452:ILE:HD11	2.44	0.40
1:B:1365:LYS:HA	1:B:1391:THR:HG22	2.01	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:526:THR:C	1:A:528:LEU:H	2.23	0.40
1:A:651:ALA:O	1:A:655:MET:HG2	2.21	0.40
1:B:1228:MET:HE1	1:B:1274:GLN:N	2.36	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:144:LEU:HD12	1:A:144:LEU:HA	1.94	0.40
1:B:1496:PRO:HA	1:B:1497:PRO:HD3	1.86	0.40
1:A:243:TRP:CZ2	1:A:260:LEU:HD21	2.56	0.40
1:A:337:LEU:HD13	1:A:460:PRO:O	2.21	0.40
1:A:533:LEU:HD13	1:A:542:CYS:HB3	2.04	0.40
1:A:570:ASP:O	1:A:574:LYS:HB2	2.21	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:1335:ARG:HD3	1:B:1335:ARG:HA	1.91	0.40
1:B:1592:GLU:O	1:B:1595:ARG:N	2.53	0.40
1:B:1683:PHE:O	1:B:1687:CYS:SG	2.80	0.40

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

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

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	485/562 (86%)	362 (75%)	91 (19%)	32 (7%)	1	6
1	B	491/562 (87%)	362 (74%)	95 (19%)	34 (7%)	1	5
All	All	976/1124 (87%)	724 (74%)	186 (19%)	66 (7%)	1	6

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	458/505 (91%)	416 (91%)	42 (9%)	9	29
1	B	464/505 (92%)	422 (91%)	42 (9%)	9	30
All	All	922/1010 (91%)	838 (91%)	84 (9%)	9	30

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

Sometimes 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 monosaccharides 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%)	0.10	2 (0%) 92 82	43, 92, 127, 139	0
1	B	507/562 (90%)	0.14	6 (1%) 79 58	36, 101, 131, 143	0
All	All	1008/1124 (89%)	0.12	8 (0%) 86 70	36, 97, 130, 143	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1199	LYS	3.3
1	B	1198	GLN	3.3
1	B	1667	VAL	3.0
1	A	607	LEU	2.4
1	B	1339	ILE	2.2
1	B	1607	LEU	2.1
1	B	1202	GLN	2.1
1	A	281	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 monosaccharides 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.