



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:52 PM UTC

PDB ID : 3CWG / pdb_00003cwg
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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

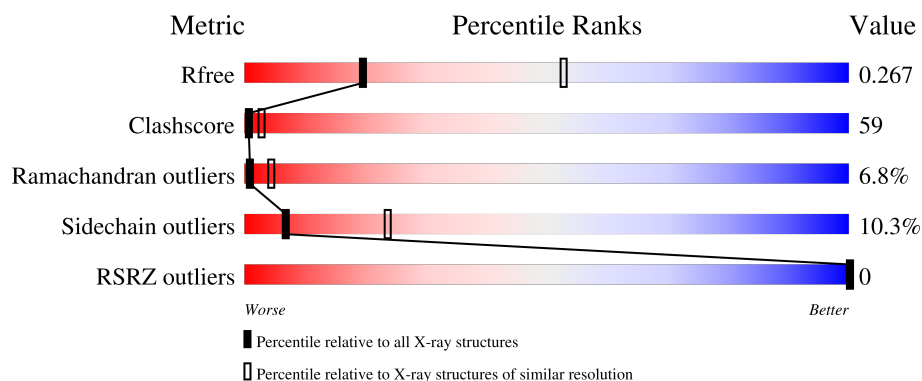
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (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	 21% 54% 14% • 11%
1	B	562	 24% 52% 13% • 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			

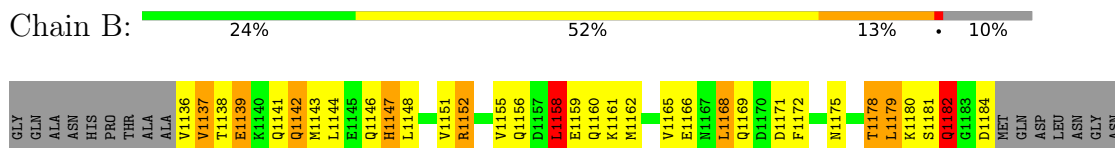
3 Residue-property plots

These plots are drawn for all protein, RNA, 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



N1646	ASN	L1585	Q1524	V1461	T1391	C1328	L1258	ASN
NET	M1686	L1525	L1526	V1462	M1396	M1329	C1259	GLN
SER	F1587	T1527	T1527	V1463	E1397	P1330	L1260	SER
F1650	I1589	L1528	L1529	N1466	E1398	M1331	D1261	V1195
A1651	S1590	E1529	A1530	I1467	E1398	H1332	R1262	T1196
E1652	K1591	E1530	K1531	C1468	SER		L1263	R1197
E1592	E1592	K1531	L1532	Q1469	ASN	R1335	Q1198	Q1198
R1593	R1593	L1532	L1532	Q1469	M1401	P1336	K1199	K1199
M1655	E1594	L1533	L1533	M1470	G1402	L1337	M1200	M1200
G1656	R1595	G1534	G1534	N1471	S1403	V1338	Q1201	Q1201
Y1657	A1596	P1535	P1535	N1472	L1404	I1339	Q1202	Q1202
K1658	I1597	G1536	G1536	A1473		K1340	L1203	L1203
ILE	L1598	V1537	V1537	A1474	K1409	T1341	A1271	A1271
NET	S1599	M1538	M1538	A1475	H1410	G1342	E1272	E1272
ASP	T1600	Y1539	Y1539	I1476	L1411	V1343	S1273	S1273
ALA	K1601	S1540	S1540	I1477	T1412	Q1344	Q1274	Q1274
T1663	P1602	G1541	G1541	L1478	L1413	F1345	L1275	L1275
N1664	P1603	C1542	C1542	N1479	R1414	T1346	Q1276	Q1276
L1665	G1604	Q1543	Q1543	Y1480	E1415		T1208	T1208
L1666	T1605	L1544	L1544	N1481		V1349	R1278	R1278
V1667	F1606			M1482	C1418	R1350	Q1279	Q1279
P1669	L1607	A1547	A1547	L1483	GLY	L1351	Q1280	Q1280
L1670	L1608	K1548	K1548	L1484	ASN	L1352	R1213	R1213
R1671	R1609	F1549	F1549	N1485	GLY	V1353	R1214	R1214
Y1672	F1610	C1550	C1550	P1487	GLY	K1354	R1215	R1215
L1673	E1611	E1552	E1552	K1488	ARG	F1355	V1218	V1218
Y1674	S1613	K1556	K1556		ALA	P1356	S1219	S1219
P1675	S1614	M1554	M1554	F1492	ASN	I1357	E1220	E1220
D1676	K1615	E1555	E1555	T1493	CYS	N1358	L1224	L1224
L1677	E1616	G1556	G1556	K1495	ALA	V1360	L1225	L1225
P1678	G1617	K1557	K1557	K1496	SER	Q1361	M1228	M1228
K1679	G1618	F1558	F1558	P1497	LEU	L1362	E1229	E1229
E1680	V1619	F1559	F1559	T1498	I1431	K1365	E1230	E1230
E1681	T1620	S1560	S1560	G1499	T1433	V1366	V1231	V1231
A1682	F1621	F1561	F1561	T1500		C1367	T1234	T1234
F1683	T1622	W1562	W1562	W1501	H1437	I1368	L1235	L1235
G1684	W1623	V1563	V1563	D1502	L1438	D1369	T1236	T1236
K1685	VAL	W1564	W1564	Q1503	I1439	K1370	D1237	D1237
Y1686	GLU	L1565	L1565	V1504	T1440	ASP	M1304	M1304
C1687	LYS	D1566	D1566	A1505	F1441	SER	E1238	E1238
R1688	ASP	N1567	N1567	E1506	E1442	GLY	E1239	E1239
	ILE	I1568	I1568	V1507	T1443	ASP	L1240	L1240
	SER	I1569	I1569	L1508	E1444	VAL	A1241	A1241
	GLY	D1570	D1570	S1509	V1445	ALA	D1242	D1242
	K1631	L1571	L1571	W1510	Y1446	ALA	E1311	E1311
	T1632	Q1633	Q1633	Q1511	H1447	LEU	K1244	K1244
	Q1633	K1573	K1573	F1512	Q1448	R1379	R1245	R1245
	I1634	K1574	K1574	S1513	G1449	G1380	R1246	R1246
	Q1635	Y1575	Y1575	S1514	L1450	S1381	Q1247	Q1247
	S1636	L1576	L1576	T1515	K1451	R1382	Q1248	Q1248
	V1637	L1577	L1577	T1516	I1452	F1383	M1317	M1317
	E1638	A1578	A1578	K1517	D1453	K1384	I1249	I1249
		L1579	L1579	R1518	L1454	N1385	A1250	A1250
		W1580	W1580	Q1519	E1455	I1386	C1251	C1251
	K1642	N1581	N1581	L1520		L1387	I1252	I1252
	Q1643	E1582	E1582	S1521	S1458	T1388	P1255	P1255
	Q1644	G1583	G1583	I1522	L1459	T1389	P1256	P1256
	L1645	Y1584	Y1584	E1523	P1460	N1390	P1327	P1327

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 30.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	91.2 (30.00-3.05) 91.2 (30.00-3.05)	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 (8.81%)	wwPDB-VP
Wilson B-factor (Å ²)	71.6	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.367 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.57	0/4159	1.11	31/5608 (0.6%)
1	B	0.57	0/4210	1.11	31/5675 (0.5%)
All	All	0.57	0/8369	1.11	62/11283 (0.5%)

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1432	VAL	N-CA-C	11.37	122.30	110.36
1	B	1288	GLN	N-CA-C	-9.16	101.88	112.87
1	B	1598	LEU	N-CA-C	-8.94	101.20	112.90
1	A	288	GLN	N-CA-C	-8.81	102.30	112.87
1	B	1171	ASP	N-CA-C	-7.63	102.90	111.07
1	A	663	THR	N-CA-C	-7.60	104.91	112.97
1	A	142	GLN	N-CA-C	-7.50	102.70	111.03
1	A	681	GLU	N-CA-C	-7.50	103.92	113.23
1	B	1142	GLN	N-CA-C	-7.41	102.81	111.03
1	A	171	ASP	N-CA-C	-7.38	103.17	111.14
1	A	432	VAL	N-CA-C	7.20	117.30	110.74
1	B	1199	LYS	N-CA-C	-7.09	104.27	114.12
1	A	527	THR	N-CA-C	-7.06	104.54	113.01
1	B	1527	THR	N-CA-C	-7.00	104.61	113.01
1	B	1494	THR	N-CA-C	-6.95	104.68	113.01
1	A	494	THR	N-CA-C	-6.92	104.71	113.01
1	B	1213	MET	N-CA-C	-6.73	103.56	111.03
1	A	140	LYS	N-CA-C	-6.58	103.94	112.23
1	A	578	ALA	N-CA-C	-6.52	105.19	113.01
1	B	1606	PHE	N-CA-C	6.47	119.01	109.24
1	A	606	PHE	N-CA-C	6.46	118.99	109.24
1	A	213	MET	N-CA-C	-6.37	103.96	111.03
1	B	1586	MET	N-CA-C	-6.36	104.78	112.54
1	B	1578	ALA	N-CA-C	-6.29	105.46	113.01
1	B	1673	LEU	N-CA-C	-6.26	102.71	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	LEU	N-CA-C	-6.20	102.78	110.41
1	A	247	GLN	N-CA-C	-6.15	103.31	111.24
1	A	586	MET	N-CA-C	-6.04	105.17	112.54
1	B	1335	ARG	CA-C-N	6.02	126.52	120.14
1	B	1335	ARG	C-N-CA	6.02	126.52	120.14
1	B	1681	GLU	N-CA-C	-5.88	106.11	113.28
1	B	1200	MET	N-CA-C	-5.81	106.32	113.41
1	A	335	ARG	CA-C-N	5.77	126.26	120.14
1	A	335	ARG	C-N-CA	5.77	126.26	120.14
1	B	1247	GLN	N-CA-C	-5.66	103.94	111.24
1	A	303	PRO	N-CA-C	-5.65	105.68	113.53
1	B	1276	GLN	N-CA-C	-5.64	105.50	112.90
1	A	517	LYS	N-CA-C	-5.64	106.29	112.72
1	A	158	LEU	N-CA-C	-5.64	105.13	111.28
1	A	179	LEU	N-CA-C	-5.62	106.19	113.16
1	B	1635	GLN	N-CA-C	5.57	117.30	107.61
1	B	1303	PRO	N-CA-C	-5.55	105.82	113.53
1	A	534	GLY	CA-C-N	5.46	125.89	119.99
1	A	534	GLY	C-N-CA	5.46	125.89	119.99
1	B	1241	ALA	N-CA-C	-5.44	104.74	111.33
1	B	1517	LYS	N-CA-C	-5.42	106.54	112.72
1	A	148	LEU	N-CA-C	5.37	117.14	111.28
1	A	241	ALA	N-CA-C	-5.37	104.84	111.33
1	B	1152	ARG	N-CA-C	-5.35	105.56	111.71
1	A	152	ARG	N-CA-C	-5.32	105.59	111.71
1	B	1139	GLU	N-CA-C	-5.30	106.95	113.41
1	B	1280	GLN	N-CA-C	-5.29	104.43	112.04
1	B	1158	LEU	N-CA-C	-5.27	105.53	111.28
1	A	276	GLN	N-CA-C	-5.17	105.26	112.45
1	B	1179	LEU	N-CA-C	-5.12	106.81	113.16
1	A	342	GLY	N-CA-C	-5.10	108.30	114.92
1	B	1342	GLY	N-CA-C	-5.09	108.30	114.92
1	B	1534	GLY	CA-C-N	5.06	125.85	120.13
1	B	1534	GLY	C-N-CA	5.06	125.85	120.13
1	A	415	GLU	N-CA-C	5.04	117.18	109.07
1	A	280	GLN	N-CA-C	-5.04	104.79	112.04
1	A	362	LEU	N-CA-C	5.01	116.58	108.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4082	0	4139	508	0
1	B	4133	0	4195	484	1
All	All	8215	0	8334	979	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 59.

All (979) 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
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:B:1201:GLN:HA	1:B:1204:GLU:CD	1.97	0.89
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLN:HA	1:A:204:GLU:CD	1.97	0.89
1:B:1162:MET:HE2	1:B:1283:LYS:HB3	1.54	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:A:246:ARG:HG2	1:A:258:ILE:HG22	1.59	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:1531:LYS:HZ1	1:B:1612:GLU:HB3	1.43	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
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:A:531:LYS:HZ1	1:A:612:GLU:HB3	1.48	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:1195:VAL:HG11	1:B:1200:MET:HE2	1.66	0.78
1:B:1607:LEU:O	1:B:1608:LEU:HG	1.82	0.78
1:B:1539:TYR:HA	1:B:1542:CYS:SG	2.22	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:162:MET:HE2	1:A:283:LYS:HB3	1.66	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: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
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:A:287:LEU:C	1:A:289:GLN:H	1.95	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:A:644:GLN:C	1:A:646:ASN:H	1.97	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:1287:LEU:C	1:B:1289:GLN:H	1.95	0.73
1:B:1597:ILE:HA	1:B:1674:TYR:HE1	1.53	0.73
1:B:1598:LEU:HD22	1:B:1623:TRP:C	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1631:LYS:O	1:B:1632:THR:C	2.34	0.71
1:B:1644:GLN:C	1:B:1646:ASN:H	1.98	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:B:1583:GLY:C	1:B:1585:ILE:H	1.99	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:583:GLY:C	1:A:585:ILE:H	2.01	0.69
1:A:596:ALA:HB1	1:B:1535:PRO:HB2	1.74	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:B:1329:MET:HE2	1:B:1338:VAL:O	1.94	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:329:MET:HE2	1:A:338:VAL:O	1.93	0.68
1:A:493:PHE:HA	1:A:496:PRO:HG3	1.75	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:B:1582:GLU:CD	1:B:1582:GLU:H	2.02	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
1:A:582:GLU:CD	1:A:582:GLU:H	2.03	0.67
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:A:331:MET:HA	1:A:331:MET:HE2	1.77	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: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:1331:MET:HE2	1:B:1331:MET:HA	1.76	0.66
1:A:172:PHE:N	1:A:206:MET:HE1	2.10	0.66
1:A:338:VAL:HG11	1:A:470:MET:HE3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1287:LEU:C	1:B:1289:GLN:N	2.53	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:A:287:LEU:C	1:A:289:GLN:N	2.54	0.66
1:A:631:LYS:O	1:A:632:THR:C	2.39	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: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:498:ILE:HD12	1:A:545:THR:HG22	1.78	0.65
1:A:288:GLN:CD	1:A:302:ARG:HH21	2.05	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:A:338:VAL:HG11	1:A:470:MET:CE	2.26	0.64
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: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
1:A:379:ARG:HH11	1:A:380:GLY:H	1.45	0.64
1:A:597:ILE:C	1:A:600:THR:HG22	2.22	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:A:633:GLN:HG3	1:A:634:ILE:N	2.12	0.63
1:B:1263:LEU:O	1:B:1267:ILE:HG13	1.98	0.63
1:A:304:MET:HA	1:A:304:MET:HE2	1.81	0.63
1:B:1460:PRO:HD3	1:B:1487:PRO:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:330:PRO:O	1:A:331:MET:HE2	2.00	0.62
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: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:1304:MET:HE2	1:B:1304:MET:HA	1.81	0.62
1:B:1320:ALA:CB	1:B:1353:VAL:HG23	2.29	0.62
1:B:1396:MET:HE2	1:B:1402:GLY:O	1.99	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:1633:GLN:C	1:B:1634:ILE:HD12	2.25	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:1195:VAL:CG1	1:B:1200:MET:HE2	2.29	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:B:1288:GLN:CD	1:B:1302:ARG:HH21	2.08	0.61
1:A:245:ARG:HE	1:A:249:ILE:HD11	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:304:MET:CE	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:A:575:TYR:C	1:A:576:ILE:HD12	2.26	0.60
1:B:1138:THR:HG23	1:B:1141:GLN:NE2	2.16	0.60
1:B:1330:PRO:O	1:B:1331:MET:HE2	2.01	0.60
1:B:1338:VAL:HG11	1:B:1470:MET:HE3	1.82	0.60
1:A:517:LYS:H	1:A:517:LYS:CD	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: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:A:659:ILE:O	1:A:660:MET:C	2.46	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:288:GLN:NE2	1:A:299:VAL:HA	2.18	0.59
1:B:1482:MET:HE3	1:B:1503:GLN:NE2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:168:LEU:HD23	1:A:213:MET:HE2	1.85	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:1162:MET:HE2	1:B:1283:LYS:CB	2.29	0.58
1:B:1195:VAL:CB	1:B:1200:MET:HE2	2.33	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:A:482:MET:HE3	1:A:503:GLN:NE2	2.18	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:A:248:GLN:HE21	1:A:481:ASN:HA	1.69	0.57
1:A:396:MET:HE2	1:A:402:GLY:O	2.05	0.57
1:A:441:PHE:C	1:A:442:GLU:HG3	2.30	0.57
1:B:1156:GLN:O	1:B:1159:GLU:HB3	2.05	0.57
1:B:1201:GLN:C	1:B:1203:LEU:H	2.12	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:B:1354:LYS:HG2	1:B:1396:MET:HE3	1.86	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:144:LEU:C	1:A:146:GLN:N	2.63	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: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:1379:ARG:C	1:B:1381:SER:H	2.14	0.56
1:B:1674:TYR:HB3	1:B:1675:PRO:HD3	1.87	0.56
1:B:1142:GLN:HB2	1:B:1143:MET:HE2	1.88	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: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:201:GLN:C	1:A:203:LEU:H	2.14	0.55
1:A:594:GLU:HG3	1:A:607:LEU:CD2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:530:GLU:C	1:A:532:LEU:H	2.15	0.55
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:A:634:ILE:C	1:A:635:GLN:HG3	2.32	0.55
1:B:1144:LEU:C	1:B:1146:GLN:N	2.62	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:B:1335:ARG:HD2	1:B:1470:MET:HE2	1.88	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:A:531:LYS:NZ	1:A:612:GLU:HB3	2.21	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:1441:PHE:C	1:B:1442:GLU:HG3	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1554:MET:O	1:B:1555:ALA:C	2.51	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
1:A:567:ASN:O	1:A:571:LEU:HB2	2.08	0.54
1:B:1622:THR:C	1:B:1623:TRP:HD1	2.16	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:A:644:GLN:C	1:A:646:ASN:N	2.65	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:1386:ILE:C	1:B:1387:LEU:HD23	2.34	0.53
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:B:1644:GLN:C	1:B:1646:ASN:N	2.67	0.53
1:A:357:GLU:CD	1:A:357:GLU:H	2.17	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:674:TYR:O	1:A:675:PRO:C	2.51	0.53
1:A:142:GLN:HB2	1:A:143:MET:HE2	1.90	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:A:673:LEU:O	1:A:674:TYR:C	2.52	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:658:LYS:C	1:A:659:ILE:HG13	2.34	0.53
1:A:623:TRP:CD1	1:A:635:GLN:O	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:554:MET:O	1:A:555:ALA:C	2.52	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:1477:ILE:HG22	1:B:1478:LEU:N	2.24	0.52
1:B:1530:GLU:C	1:B:1532:LEU:H	2.16	0.52
1:A:559:PHE:CD2	1:A:564:TRP:HB2	2.45	0.52
1:B:1673:LEU:O	1:B:1674:TYR:C	2.53	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:B:1583:GLY:C	1:B:1585:ILE:N	2.68	0.52
1:A:146:GLN:O	1:A:147:HIS:C	2.52	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:1357:GLU:CD	1:B:1357:GLU:H	2.17	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:386:ILE:C	1:A:387:LEU:HD23	2.34	0.51
1:A:658:LYS:CE	1:A:669:PRO:HD3	2.40	0.51
1:B:1580:TRP:CD1	1:B:1580:TRP:C	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LEU:HD11	1:A:445:VAL:HG22	1.92	0.51
1:A:447:HIS:C	1:A:449:GLY:N	2.66	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:A:656:GLY:O	1:A:657:TYR:C	2.53	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:1550:CYS:HB3	1:B:1562:TRP:CB	2.40	0.51
1:A:144:LEU:C	1:A:146:GLN:H	2.18	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
1:B:1475:ALA:HB2	1:B:1562:TRP:HE1	1.75	0.51
1:A:473:ALA:C	1:A:475:ALA:N	2.65	0.51
1:A:662:ALA:C	1:A:664:ASN:H	2.18	0.51
1:A:669:PRO:O	1:A:670:LEU:C	2.54	0.51
1:B:1493:PHE:C	1:B:1496:PRO:HD3	2.36	0.51
1:B:1674:TYR:O	1:B:1675:PRO:C	2.52	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:A:592:GLU:C	1:A:592:GLU:OE1	2.54	0.51
1:B:1669:PRO:O	1:B:1670:LEU:C	2.54	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:171:ASP:HB2	1:A:206:MET:HE1	1.93	0.50
1:A:176:TYR:HA	1:A:203:LEU:HD21	1.93	0.50
1:A:205:GLN:C	1:A:207:LEU:N	2.68	0.50
1:B:1144:LEU:C	1:B:1146:GLN:H	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:SER:O	1:A:525:LEU:HB2	2.12	0.50
1:B:1473:ALA:C	1:B:1475:ALA:N	2.66	0.50
1:B:1592:GLU:C	1:B:1592:GLU:OE1	2.54	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:B:1600:THR:HG23	1:B:1601:LYS:HG2	1.93	0.50
1:B:1656:GLY:O	1:B:1657:TYR:C	2.55	0.50
1:B:1447:HIS:C	1:B:1449:GLY:N	2.66	0.50
1:A:473:ALA:O	1:A:476:SER:N	2.45	0.50
1:A:493:PHE:C	1:A:496:PRO:HD3	2.37	0.50
1:B:1654:ILE:HG22	1:B:1654:ILE:O	2.11	0.50
1:A:584:TYR:O	1:A:608:LEU:HD12	2.12	0.50
1:B:1622:THR:C	1:B:1623:TRP:CD1	2.90	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:1476:SER:HB3	1:B:1493:PHE:CE2	2.47	0.49
1:B:1582:GLU:CD	1:B:1582:GLU:N	2.68	0.49
1:B:1146:GLN:O	1:B:1147:HIS:C	2.54	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:1182:GLN:C	1:B:1184:ASP:H	2.21	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
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:A:285:GLU:O	1:A:289:GLN:HG3	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1344:GLN:CG	1:B:1410:HIS:HA	2.43	0.49
1:A:526:THR:C	1:A:528:LEU:N	2.71	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: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:582:GLU:CD	1:A:582:GLU:N	2.68	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: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:162:MET:HE2	1:A:283:LYS:CB	2.41	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:447:HIS:O	1:A:448:GLN:C	2.56	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: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:583:GLY:C	1:A:585:ILE:N	2.70	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:1512:PHE:O	1:B:1516:THR:OG1	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1582:GLU:N	1:B:1582:GLU:OE2	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:1205:GLN:C	1:B:1207:LEU:N	2.70	0.47
1:B:1493:PHE:O	1:B:1496:PRO:HD3	2.13	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:432:VAL:C	1:A:434:GLU:H	2.22	0.47
1:B:1623:TRP:NE1	1:B:1635:GLN:O	2.48	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:A:580:TRP:CD1	1:A:580:TRP:C	2.91	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:A:585:ILE:HD13	1:A:608:LEU:HD13	1.96	0.47
1:B:1447:HIS:O	1:B:1448:GLN:C	2.58	0.47
1:B:1592:GLU:C	1:B:1594:GLU:N	2.72	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:252:ILE:HG23	1:A:481:ASN:ND2	2.27	0.47
1:A:592:GLU:C	1:A:594:GLU:N	2.73	0.47
1:A:595:ARG:O	1:A:597:ILE:N	2.42	0.47
1:A:414:ARG:HG2	1:A:415:GLU:N	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1622:THR:CG2	1:B:1634:ILE:HG23	2.44	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: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:1526:THR:C	1:B:1528:LEU:N	2.72	0.46
1:B:1656:GLY:O	1:B:1658:LYS:HE3	2.15	0.46
1:A:201:GLN:HA	1:A:204:GLU:CG	2.46	0.46
1:A:205:GLN:O	1:A:206:MET:C	2.59	0.46
1:B:1152:ARG:O	1:B:1156:GLN:HG2	2.15	0.46
1:B:1379:ARG:HD3	1:B:1379:ARG:C	2.41	0.46
1:B:1540:SER:C	1:B:1542:CYS:H	2.23	0.46
1:A:161:LYS:NZ	1:A:216:SER:OG	2.48	0.46
1:A:671:VAL:HG12	1:A:679:LYS:NZ	2.31	0.46
1:A:172:PHE:CD2	1:A:172:PHE:C	2.94	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:1530:GLU:C	1:B:1532:LEU:N	2.74	0.46
1:B:1671:VAL:HG12	1:B:1679:LYS:HZ3	1.81	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
1:A:602:PRO:O	1:A:603:PRO:C	2.59	0.46
1:B:1607:LEU:HB3	1:B:1608:LEU:H	1.56	0.46
1:A:252:ILE:HG21	1:A:478:LEU:HA	1.98	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:309:ILE:HD13	1:A:309:ILE:C	2.40	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:A:288:GLN:NE2	1:A:298:ILE:HG22	2.31	0.45
1:B:1172:PHE:C	1:B:1172:PHE:CD2	2.95	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:A:284:LEU:C	1:A:286:GLU:H	2.24	0.45
1:A:358:LEU:O	1:A:361:GLN:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:335:ARG:HD2	1:A:470:MET:HE2	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
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:1172:PHE:N	1:B:1206:MET:HE1	2.32	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:A:526:THR:C	1:A:528:LEU:H	2.23	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:329:MET:HE3	1:A:332:HIS:HB2	1.99	0.45
1:A:590:SER:O	1:A:591:LYS:C	2.60	0.45
1:B:1287:LEU:N	1:B:1287:LEU:HD12	2.32	0.45
1:B:1329:MET:HE3	1:B:1332:HIS:HB2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:SER:HB3	1:A:614:SER:HG	1.82	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:1590:SER:O	1:B:1591:LYS:C	2.60	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: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:431:ILE:O	1:A:435:GLU:HB2	2.16	0.44
1:A:577:LEU:C	1:A:579:LEU:H	2.26	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:1205:GLN:O	1:B:1206:MET:C	2.60	0.44
1:B:1442:GLU:HG2	1:B:1455:GLU:HB2	1.99	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
1:A:660:MET:HG3	1:A:666:LEU:HD12	1.99	0.44
1:B:1602:PRO:O	1:B:1603:PRO:C	2.61	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:A:540:SER:C	1:A:542:CYS:H	2.24	0.44
1:A:577:LEU:C	1:A:579:LEU:N	2.75	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:1201:GLN:C	1:B:1203:LEU:N	2.76	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: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:459:LEU:O	1:A:460:PRO:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:1590:SER:C	1:B:1592:GLU:N	2.75	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: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
1:B:1168:LEU:HD23	1:B:1213:MET:HE2	2.00	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:B:1595:ARG:C	1:B:1597:ILE:H	2.27	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:530:GLU:C	1:A:532:LEU:N	2.73	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:B:1526:THR:C	1:B:1528:LEU:H	2.25	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:590:SER:C	1:A:592:GLU:N	2.75	0.43
1:B:1284:LEU:C	1:B:1286:GLU:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1634:ILE:C	1:B:1635:GLN:HG3	2.43	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:643:GLN:O	1:A:646:ASN:HB2	2.19	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
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:482:MET:HE3	1:A:503:GLN:HE21	1.84	0.42
1:A:531:LYS:NZ	1:A:557:LYS:HE2	2.33	0.42
1:B:1459:LEU:O	1:B:1460:PRO:C	2.62	0.42
1:B:1482:MET:HE3	1:B:1503:GLN:HE21	1.82	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:1160:GLN:O	1:B:1161:LYS:C	2.62	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:201:GLN:C	1:A:203:LEU:N	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:473:ALA:O	1:A:474:TRP:C	2.63	0.42
1:B:1162:MET:HE2	1:B:1283:LYS:CG	2.49	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: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:1598:LEU:HD13	1:B:1623:TRP:HA	2.02	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:480:TYR:CD1	1:A:480:TYR:C	2.98	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:A:154:ARG:HB2	1:A:224:LEU:HD13	2.02	0.41
1:A:160:GLN:O	1:A:161:LYS:C	2.64	0.41
1:A:245:ARG:HD3	1:A:485:ASN:HB3	2.02	0.41
1:A:394:MET:HE2	1:A:405:SER:HA	2.02	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:260:LEU:HB2	1:A:350:ARG:NH2	2.35	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: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:245:ARG:HH11	1:A:485:ASN:HB3	1.85	0.41
1:A:501:TRP:O	1:A:502:ASP:C	2.63	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:151:VAL:HG11	1:A:228:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1252:ILE:HG23	1:B:1481:ASN:ND2	2.34	0.41
1:B:1501:TRP:O	1:B:1502:ASP:C	2.63	0.41
1:B:1577:LEU:C	1:B:1579:LEU:N	2.77	0.41
1:B:1670:LEU:HD22	1:B:1670:LEU:N	2.11	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:B:1181:SER:O	1:B:1182:GLN:HB3	2.20	0.41
1:A:280:GLN:HE21	1:A:280:GLN:CA	2.13	0.41
1:A:401:ASN:O	1:A:401:ASN:CG	2.63	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: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: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:B:1504:VAL:C	1:B:1508:LEU:HD12	2.45	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:1172:PHE:HB2	1:B:1206:MET:HE2	2.02	0.40
1:B:1196:THR:CB	1:B:1199:LYS:HB2	2.49	0.40
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:A:595:ARG:C	1:A:597:ILE:H	2.28	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:651:ALA:O	1:A:655:MET:HG2	2.21	0.40
1:A:652:GLU:C	1:A:654:ILE:N	2.77	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:B:1681:GLU:N	1:B:1681:GLU:CD	2.80	0.40
1:A:144:LEU:HD12	1:A:144:LEU:HA	1.94	0.40
1:A:504:VAL:C	1:A:508:LEU:HD12	2.46	0.40
1:B:1496:PRO:HA	1:B:1497:PRO:HD3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:TRP:CZ2	1:A:260:LEU:HD21	2.56	0.40
1:A:305:LEU:O	1:A:306:GLU:C	2.64	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:A:680:GLU:C	1:A:684:GLY:H	2.30	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	5
1	B	491/562 (87%)	362 (74%)	95 (19%)	34 (7%)	1	4
All	All	976/1124 (87%)	724 (74%)	186 (19%)	66 (7%)	1	4

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	PRO
1	A	368	ILE

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	411 (90%)	47 (10%)	7	24
1	B	464/505 (92%)	416 (90%)	48 (10%)	7	24
All	All	922/1010 (91%)	827 (90%)	95 (10%)	7	24

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	LEU

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Mol	Chain	Res	Type
1	A	168	LEU
1	A	178	THR
1	A	203	LEU
1	A	204	GLU
1	A	218	VAL
1	A	225	LEU
1	A	229	GLU
1	A	235	LEU
1	A	267	ILE
1	A	275	LEU
1	A	280	GLN
1	A	287	LEU
1	A	304	MET
1	A	306	GLU
1	A	309	ILE
1	A	350	ARG
1	A	351	LEU
1	A	397	GLU
1	A	409	LYS
1	A	413	LEU
1	A	452	ILE
1	A	453	ASP
1	A	503	GLN
1	A	513	SER
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	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
1	A	633	GLN
1	A	637	VAL
1	A	652	GLU
1	A	653	ILE

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Mol	Chain	Res	Type
1	A	659	ILE
1	A	670	LEU
1	A	686	TYR
1	A	688	ARG
1	B	1137	VAL
1	B	1158	LEU
1	B	1168	LEU
1	B	1178	THR
1	B	1182	GLN
1	B	1203	LEU
1	B	1204	GLU
1	B	1218	VAL
1	B	1225	LEU
1	B	1229	GLU
1	B	1235	LEU
1	B	1275	LEU
1	B	1280	GLN
1	B	1287	LEU
1	B	1304	MET
1	B	1306	GLU
1	B	1349	VAL
1	B	1350	ARG
1	B	1351	LEU
1	B	1397	GLU
1	B	1409	LYS
1	B	1413	LEU
1	B	1431	ILE
1	B	1452	ILE
1	B	1453	ASP
1	B	1477	ILE
1	B	1503	GLN
1	B	1513	SER
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	1575	TYR
1	B	1580	TRP
1	B	1582	GLU

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Mol	Chain	Res	Type
1	B	1586	MET
1	B	1592	GLU
1	B	1597	ILE
1	B	1621	PHE
1	B	1623	TRP
1	B	1637	VAL
1	B	1652	GLU
1	B	1670	LEU
1	B	1686	TYR
1	B	1688	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	248	GLN
1	A	279	GLN
1	A	280	GLN
1	A	300	GLN
1	A	332	HIS
1	A	385	ASN
1	A	437	HIS
1	A	466	ASN
1	A	472	ASN
1	A	481	ASN
1	A	503	GLN
1	A	538	ASN
1	A	644	GLN
1	B	1141	GLN
1	B	1167	ASN
1	B	1248	GLN
1	B	1279	GLN
1	B	1280	GLN
1	B	1300	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

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Mol	Chain	Res	Type
1	B	1538	ASN
1	B	1553	ASN
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 oligosaccharides 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%)	-1.45	0 100 100	43, 92, 127, 139	0
1	B	507/562 (90%)	-1.37	0 100 100	36, 101, 131, 143	0
All	All	1008/1124 (89%)	-1.41	0 100 100	36, 97, 130, 143	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.