



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:40 am GMT

PDB ID : 2VZ8
Title : CRYSTAL STRUCTURE OF MAMMALIAN FATTY ACID SYNTHASE
Authors : Maier, T.; Leibundgut, M.; Ban, N.
Deposited on : 2008-07-31
Resolution : 3.22 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

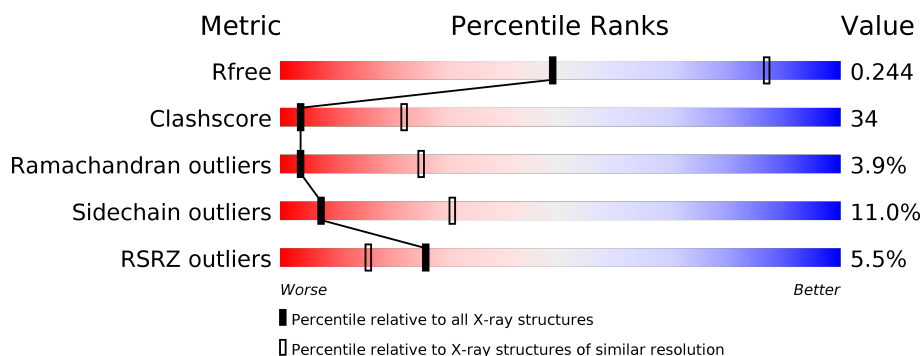
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 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}	100719	1036 (3.24-3.20)
Clashscore	112137	1161 (3.24-3.20)
Ramachandran outliers	110173	1140 (3.24-3.20)
Sidechain outliers	110143	1139 (3.24-3.20)
RSRZ outliers	101464	1040 (3.24-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	2512	<div> <div>3%</div> <div>35% 36% 6% 22%</div> </div>
1	B	2512	<div> <div>5%</div> <div>36% 37% 6% 20%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30281 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FATTY ACID SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1962	Total	C	N	O	S	0	0	0
			14977	9466	2630	2803	78			
1	B	2004	Total	C	N	O	S	0	0	0
			15304	9671	2684	2869	80			

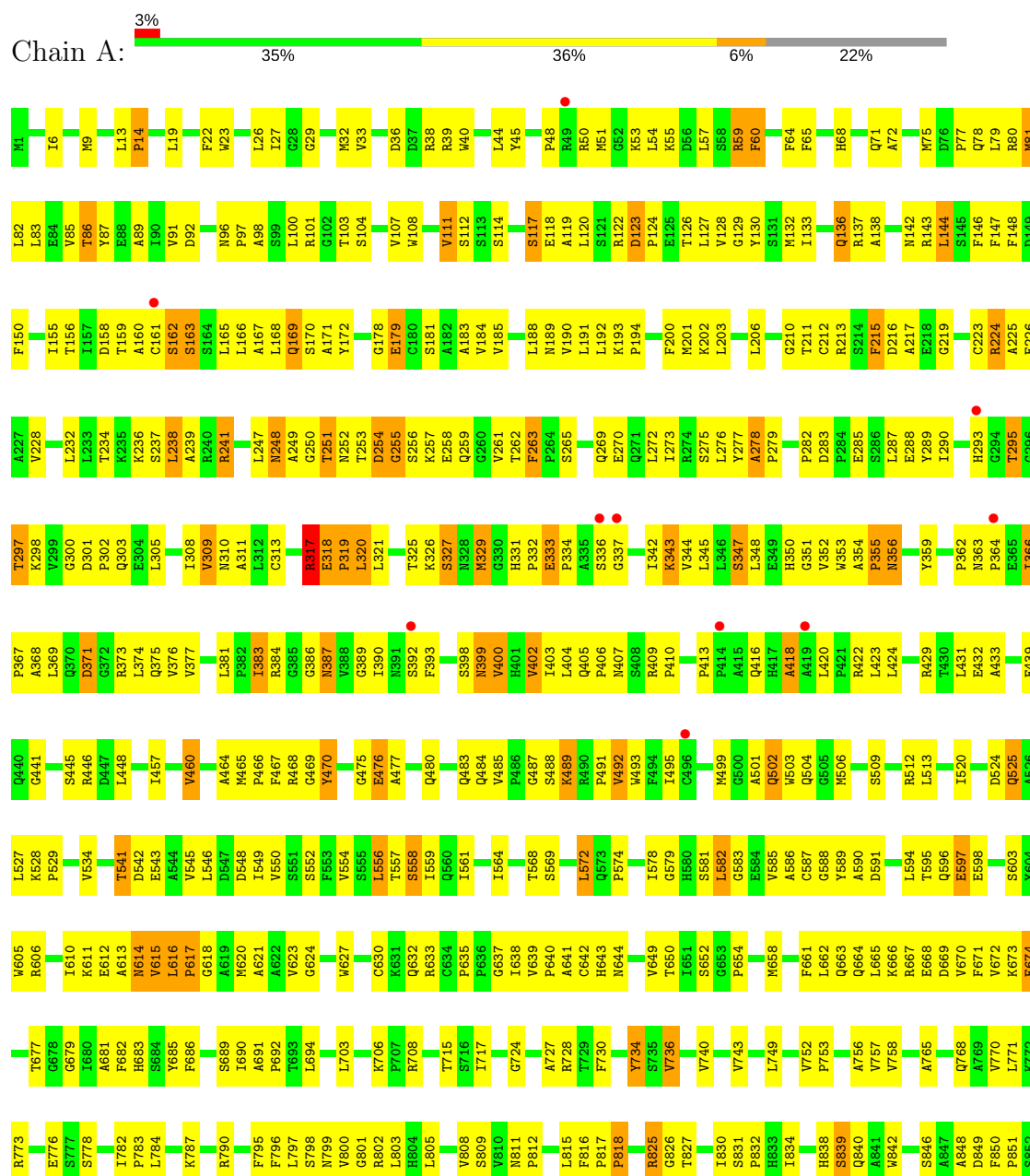
There are 2 discrepancies between the modelled and reference sequences:

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

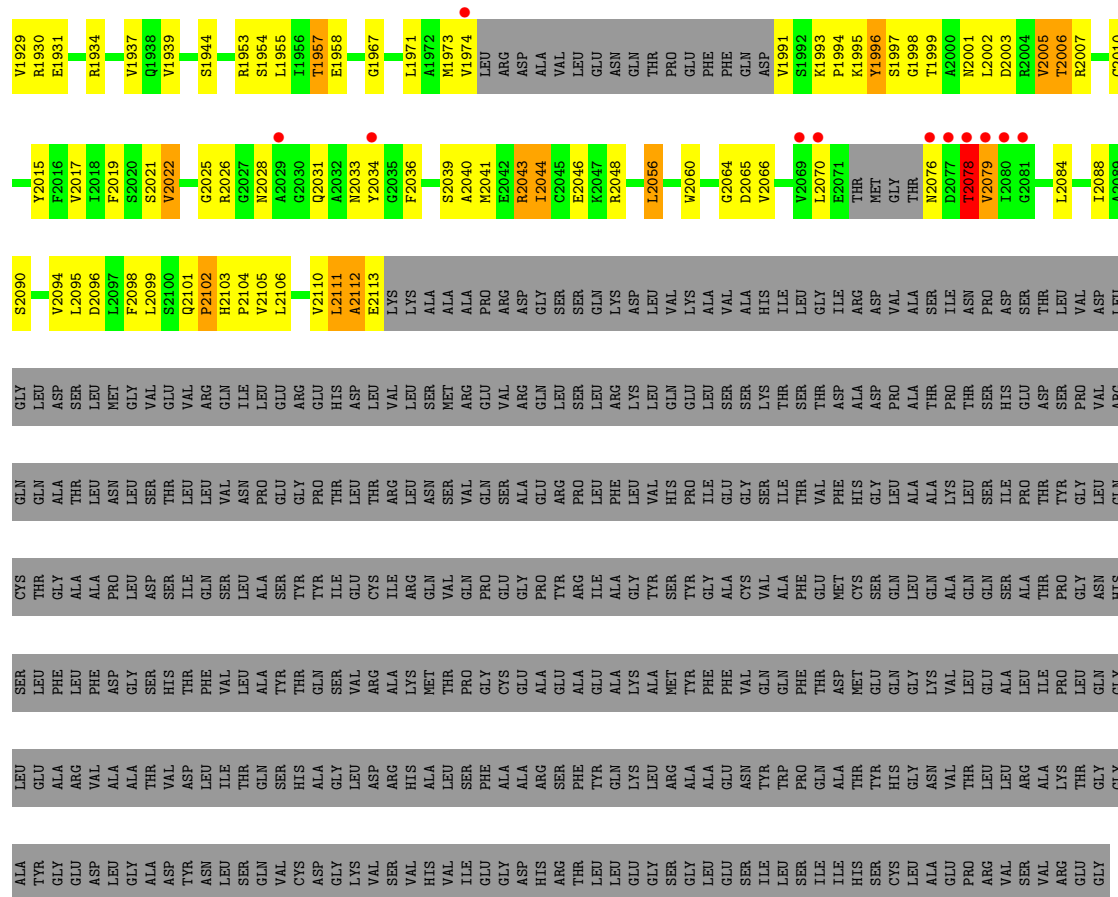
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

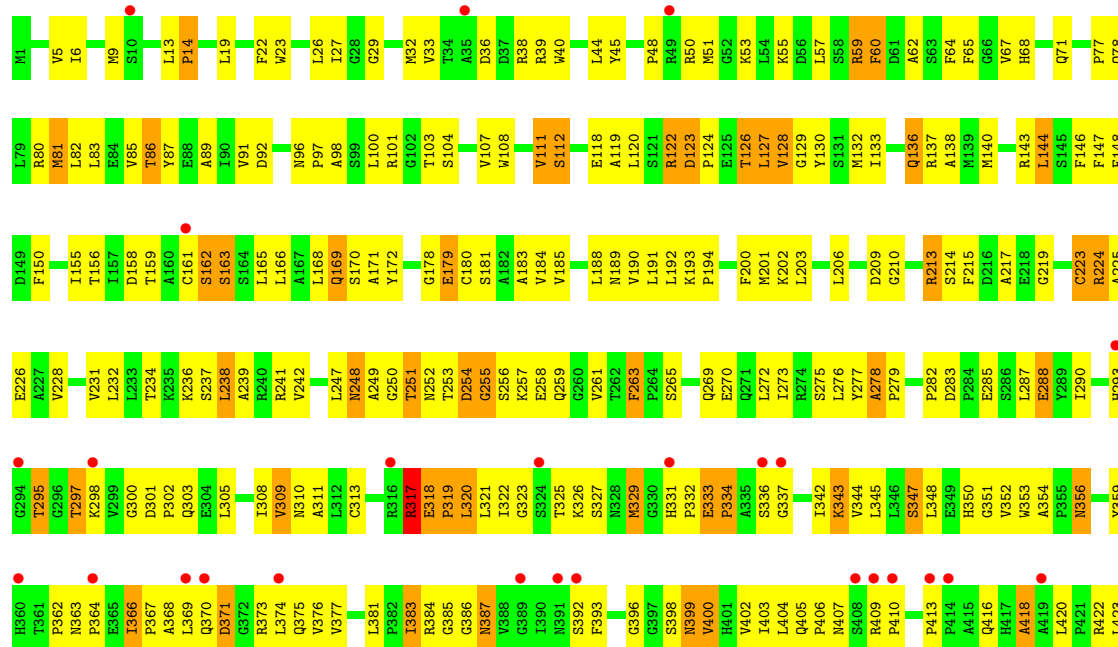
• Molecule 1: FATTY ACID SYNTHASE



V1853	L1769	L1689	V1617	S1542	L1477	L1416	GLY	L1292	A1223	VAL	G1098	S941	G853
L1854	G1770	G1692	P1618	S1543	T1480	S1417	HIS	H1293	P1224	VAL	S1101	F944	S854
L1855	D1773	C1693	A1619	I1544	E1419	V1418	PRO	V1294	A1225	PRO	S1102	F945	S855
L1857	L1774	P1694	E1620	R1545	S1481	V1295	LEU	T1296	L1226	GLY	L1226	V946	C856
L1858			G1621		P1482	T1420	GLY	G1297	K1227	LEU	A1103	S947	S857
L1859	N1777	V1695	L1622	S1549	A1483	T1421	GLY	Q1298	A1228	ASP	V1104	D948	S858
E1860	H1778	F1696	A1623	H1552	P1484	S1422	MET	Q1298	C1229	GLY	P1105	S949	
L1861	A1779	T1697	T1624	Y1553	E1485	F1423	VAL	D1299	V1230	ALA	R1106		V861
G1862	L1780	T1698	S1625	Y1553	E1486	R1424	GLY	D1300	T1231	GLN	R1107		V862
L1863	G1781		V1626	A1554	H1487	P1425	PHE	P1301	T1232	ALA	Q1108		V863
A1864		E1703	L1627	L1555	P1488	V1426	LEU	A1302	A1233	PRO	Q1109		
P1865	M1782	K1704	L1628	P1556	S1489	D1427	THR	N1303	L1234	ARG	H1110		V866
	M1783	S1705	L1629	A1557	S1490	S1428	SER	P1304	L1235	GLY	E1111		
	V1784	A1706	Q1630	S1558	S1491	L1429	PRO	A1305	N1236	ALA	L1112		S870
P1869	F1785			C1559	E1492	K1430	GLY	P1306	M1237	PRO	K1113		P871
P1870	L1786		T1633	Q1560	L1493	D1431	GLN	SER	A1238	GLN	S1039		E962
L1871						I1432	GLY	LEU	S1239	GLN	P1114		E963
L1872	N1788		V1636	L1563	L1497	L1433	GLY	LEU	P1240	SER	L1115		V874
L1873	V1789		P1637	C1564		A1434	ARG	GLY	K1241	LEU	F1117		V875
L1874	F1720		S1638		D1500	D1435	HIS	LYS	M1242	PRO	H1118		V876
	N1722		O1639	Y1567	L1501	A1436	LEU	A1312	K1243	ARG	L1119		V877
	S1723		W1640	Y1568	V1502	S1437	LEU	D1313	V1244	LEU	T1122		R883
	G1724			T1569	M1503	S1438	SER	L1314	V1245	LEU	H1124		
	D1725		E1644	S1570	N1504	R1439	GLN	L1315		ALA	P1123		P887
	S1727			L1571	V1505	P1440		V1316	L1248	ALA	H1125		
	F1728		S1647	N1572	Y1506	V1441		G1317	A1249	ALA	V1126		G888
	E1729		P1648	F1573	R1507	W1442		N1318	D1250	CYS	E1126		G889
			V1649	R1574	D1508	L1443		C1319	D1251	GLN			T890
	F1732		T1650	T1575	G1509	M1444		A1320	Q1252	GLN	H1129		L894
	L1733		V1651	V1576	A1445	A1445		LEU	Q1253	GLN	L1130		T895
	G1734		Y1652	V1576	V1446	V1446		ALA	L1254	LEU	L1134		H896
	H1735		L1653	T1580	G1512	G1447		THR	Y1255	ASN	N1133		
	T1736			G1581	A1513	C1448		LEU	S1256	GLY	T1134		
			Y1656	K1582	F1514	S1449	ASP	GLY	I1257	ASN	A1135		
			Y1657	L1583	H1516	L1387	GLY	ASP	I1258	LEU			L899
			V1660	S1584	H1517	T1450	PRO	ALA	P1259	GLN	GLY		A902
			V1661	P1585	F1517	G1452	ALA	VAL	A1260	LEU	GLU		L903
			R1662			V1453	ALA	ALA	L1261	GLY	GLU		S904
				W1592		V1454	VAL	VAL	L1262	LEU			Q905
			Q1666	L1593		G1455	VAL	GLY		GLY	D1073		R906
			P1667	E1594		M1456	GLY	ASN	V1267	GLN	T1074		L907
			E1668	R1595		V1457	ASN	MET	M1268	VAL	ARG		V913
			S1670	C1597			G1398	ALA	D1269	LEU	D995		F914
			V1671	M1598		L1460	S1399	ALA		ALA			E915
			L1672			K1461	V1400	ALA	Y1272	GLU	L998		D916
			L1673			E1462	L1401	THR	T1273	ARG	Y1001		V917
			L1674	E1602		P1464	F1402	LEU	A1274	PRO	D1002		
			S1675	E1529		G1465	L1403	LYS	T1275	LEU	Y1003		
				H1530		G1465	C1404	GLY	D1276	LEU	D1086		L925
				A1531		G1466	R1405		R1277	LEU	N1087		
			G1676	F1532		R1467	Q1406	G1341	N1278	CYS	THR		T930
			S1677	V1533		R1468	Q1407	F1342	P1279	ASP	LYS		V931
			G1678	M1534		I1469	T1408	L1344	A1285	ASP	VAL		Q1008
			G1679	G1610		R1470	P1409	L1345	Q1286	PRO	ALA		E934
			V1680	R1611		C1471	L1346	L1346	A1287	GLN	ALA		V935
			G1681	R1612		V1472	Q1410	L1347	K1288	GLN	L1010		R936
			Q1682	S1537		V1473	D1411	H1347	L1289	GLY	L1011		L937
				R1538		V1474	S1412	T1348	L1289	LEU	D1014		L938
				G1539		V1475	P1413	L1349	L1289	LEU	L1015		E939
				M1614		S1475	V1414	LEU	L1220	LEU	L1016		A940
				M1616		N1476	F1415	ALA	D1222	MET			



Molecule 1: FATTY ACID SYNTHASE







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.32Å 244.70Å 135.25Å 90.00° 101.65° 90.00°	Depositor
Resolution (Å)	29.50 – 3.22 29.50 – 3.22	Depositor EDS
% Data completeness (in resolution range)	94.8 (29.50-3.22) 97.6 (29.50-3.22)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.24Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.217 , 0.259 0.202 , 0.244	Depositor DCC
R_{free} test set	4841 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	95.2	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 73.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30281	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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	0.45	1/15302 (0.0%)	0.63	0/20792
1	B	0.41	0/15634	0.60	1/21243 (0.0%)
All	All	0.43	1/30936 (0.0%)	0.61	1/42035 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1759	CYS	CB-SG	-5.79	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1694	ARG	NE-CZ-NH1	6.90	123.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	14977	0	14938	1049	0
1	B	15304	0	15266	1083	0
All	All	30281	0	30204	2085	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (2085) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1694:ARG:HH11	1:B:1694:ARG:HG3	1.17	1.10
1:B:1303:ASN:H	1:B:1304:PRO:HD3	1.25	1.02
1:A:1473:LEU:HD21	1:A:1503:MET:HG2	1.36	1.02
1:A:165:LEU:HD23	1:A:400:VAL:HG22	1.37	1.02
1:B:1456:MET:HG2	1:B:2036:PHE:HB2	1.41	1.01
1:A:1736:THR:HG23	1:A:1739:LYS:H	1.26	1.00
1:B:1003:TYR:CZ	1:B:1037:HIS:HE1	1.79	1.00
1:A:1539:GLY:HA2	1:A:1580:THR:O	1.62	0.99
1:A:333:GLU:HB2	1:A:334:PRO:HD3	1.42	0.98
1:A:642:CYS:HB2	1:A:650:THR:HB	1.42	0.98
1:A:118:GLU:HG3	1:B:118:GLU:HG3	1.43	0.98
1:B:1338:LEU:HD13	1:B:1406:GLN:HE21	1.27	0.98
1:B:1387:LEU:HD22	1:B:1404:CYS:HB3	1.43	0.98
1:B:1651:VAL:HG13	1:B:1680:VAL:HA	1.45	0.97
1:B:1348:THR:HG22	1:B:1349:LEU:H	1.27	0.97
1:A:1003:TYR:CZ	1:A:1037:HIS:HE1	1.83	0.97
1:A:368:ALA:H	1:A:371:ASP:HB3	1.31	0.96
1:B:1418:VAL:HG13	1:B:1425:TRP:CZ2	1.99	0.96
1:B:165:LEU:HD23	1:B:400:VAL:HG22	1.43	0.96
1:B:333:GLU:HB2	1:B:334:PRO:HD3	1.44	0.96
1:B:1457:VAL:HG21	1:B:1473:LEU:HD22	1.47	0.95
1:B:368:ALA:H	1:B:371:ASP:HB3	1.31	0.95
1:B:1473:LEU:HD21	1:B:1503:MET:HG2	1.49	0.95
1:B:1299:TRP:HZ3	1:B:1301:PRO:HA	1.29	0.95
1:B:1335:ALA:HA	1:B:1406:GLN:HE22	1.30	0.94
1:B:1330:ALA:O	1:B:1334:MET:HG2	1.67	0.93
1:B:616:LEU:HB2	1:B:686:PHE:HE2	1.30	0.93
1:B:1565:SER:HB2	1:B:1857:ARG:NH2	1.84	0.93
1:B:1312:ALA:HB2	1:B:1337:THR:HG22	1.48	0.91
1:B:1736:THR:HG23	1:B:1739:LYS:H	1.33	0.91
1:A:1115:ILE:HD11	1:A:2111:LEU:HG	1.51	0.91
1:A:1457:VAL:HG21	1:A:1473:LEU:HD22	1.51	0.90
1:A:1418:VAL:HG13	1:A:1425:TRP:CZ2	2.06	0.90
1:B:1662:ARG:HH11	1:B:1662:ARG:CG	1.82	0.90
1:B:662:LEU:HD22	1:B:672:VAL:HG11	1.54	0.89
1:B:1446:VAL:HA	1:B:1476:ASN:ND2	1.87	0.89
1:A:82:LEU:O	1:A:86:THR:HG23	1.74	0.88
1:B:50:ARG:HD3	1:B:210:GLY:O	1.74	0.88
1:B:1446:VAL:HA	1:B:1476:ASN:HD21	1.37	0.88
1:A:1644:GLU:HB3	1:A:1825:PRO:HB3	1.52	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:VAL:HG22	1:A:977:ASP:H	1.38	0.88
1:B:384:ARG:HH11	1:B:384:ARG:HG3	1.38	0.88
1:A:1662:ARG:HH11	1:A:1662:ARG:CG	1.87	0.88
1:B:616:LEU:HB2	1:B:686:PHE:CE2	2.09	0.87
1:B:82:LEU:O	1:B:86:THR:HG23	1.75	0.87
1:B:1299:TRP:CZ3	1:B:1301:PRO:HA	2.09	0.87
1:A:1348:THR:HG22	1:A:1349:LEU:H	1.37	0.87
1:A:384:ARG:HH11	1:A:384:ARG:HG3	1.39	0.87
1:A:1477:LEU:HD11	1:A:2043:ARG:HD2	1.56	0.86
1:A:1545:ARG:HH11	1:A:1545:ARG:HG3	1.39	0.86
1:A:1662:ARG:HG3	1:A:1662:ARG:HH11	1.40	0.86
1:A:50:ARG:HD3	1:A:210:GLY:O	1.75	0.86
1:B:64:PHE:HB2	1:B:429:ARG:HH21	1.40	0.86
1:A:861:VAL:HG22	1:A:934:GLU:HB3	1.58	0.85
1:B:643:HIS:HA	1:B:649:VAL:HG22	1.59	0.84
1:B:1530:HIS:HB2	1:B:1552:HIS:HB2	1.60	0.84
1:A:64:PHE:HB2	1:A:429:ARG:HH21	1.41	0.83
1:A:96:ASN:HD21	1:A:98:ALA:HB3	1.41	0.83
1:B:1312:ALA:CB	1:B:1337:THR:HG22	2.08	0.83
1:B:112:SER:CB	1:B:334:PRO:HG3	2.09	0.83
1:A:112:SER:HB2	1:A:334:PRO:HG3	1.59	0.83
1:A:944:PHE:CD2	1:A:959:VAL:HG22	2.14	0.83
1:A:1245:VAL:HG13	1:A:1273:THR:HB	1.57	0.83
1:B:1082:VAL:HG22	1:B:1089:VAL:HG22	1.61	0.83
1:A:1082:VAL:HG22	1:A:1089:VAL:HG22	1.60	0.83
1:A:616:LEU:HD23	1:A:617:PRO:HD2	1.58	0.83
1:A:1289:LEU:HD22	1:A:1294:VAL:HB	1.60	0.83
1:A:1528:THR:HG22	1:A:1530:HIS:H	1.43	0.83
1:A:319:PRO:HD2	1:A:373:ARG:O	1.78	0.83
1:A:112:SER:CB	1:A:334:PRO:HG3	2.07	0.83
1:B:96:ASN:HD21	1:B:98:ALA:HB3	1.42	0.82
1:A:468:ARG:HD3	1:A:485:VAL:HG21	1.59	0.82
1:A:663:GLN:O	1:A:667:ARG:HD2	1.79	0.82
1:A:123:ASP:HB3	1:A:126:THR:HB	1.62	0.82
1:B:1732:VAL:O	1:B:1736:THR:HB	1.78	0.82
1:B:319:PRO:HD2	1:B:373:ARG:O	1.79	0.82
1:B:944:PHE:CD2	1:B:959:VAL:HG22	2.15	0.82
1:B:982:THR:HG23	1:B:983:ALA:H	1.45	0.82
1:B:1416:LEU:HD21	1:B:1425:TRP:HB2	1.59	0.82
1:B:112:SER:HB2	1:B:334:PRO:HG3	1.60	0.81
1:A:1222:ASP:HB3	1:A:1257:ARG:CZ	2.09	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1285:ALA:HB1	1:A:1289:LEU:HG	1.61	0.81
1:A:1341:GLY:HA2	1:A:1406:GLN:O	1.80	0.81
1:A:278:ALA:HB3	1:A:279:PRO:HD3	1.63	0.81
1:A:1616:MET:HE3	1:A:1650:ILE:HA	1.62	0.81
1:A:333:GLU:HB2	1:A:334:PRO:CD	2.09	0.81
1:B:980:ASP:HB2	1:B:982:THR:HG22	1.63	0.81
1:B:861:VAL:HG22	1:B:934:GLU:HB3	1.63	0.81
1:B:1662:ARG:HH11	1:B:1662:ARG:HG3	1.44	0.80
1:B:278:ALA:HB3	1:B:279:PRO:HD3	1.61	0.80
1:B:1003:TYR:CZ	1:B:1037:HIS:CE1	2.67	0.80
1:B:1222:ASP:HB3	1:B:1257:ARG:CZ	2.11	0.80
1:B:1456:MET:CG	1:B:2036:PHE:HB2	2.11	0.80
1:A:368:ALA:N	1:A:371:ASP:HB3	1.96	0.80
1:B:14:PRO:HG2	1:B:329:MET:HG3	1.64	0.79
1:A:215:PHE:CD2	1:A:305:LEU:HD11	2.18	0.79
1:A:416:GLN:O	1:A:420:LEU:HB2	1.82	0.79
1:B:1285:ALA:HB1	1:B:1289:LEU:HG	1.64	0.79
1:B:1303:ASN:N	1:B:1304:PRO:HD3	1.96	0.79
1:B:416:GLN:O	1:B:420:LEU:HB2	1.81	0.79
1:B:368:ALA:N	1:B:371:ASP:HB3	1.98	0.79
1:A:1735:HIS:CD2	1:A:1735:HIS:H	2.00	0.79
1:B:1545:ARG:HD2	1:B:1876:LEU:HD11	1.63	0.79
1:A:642:CYS:HB2	1:A:650:THR:CB	2.12	0.78
1:B:1245:VAL:HG13	1:B:1273:THR:HB	1.64	0.78
1:A:1003:TYR:CZ	1:A:1037:HIS:CE1	2.70	0.78
1:A:1034:ALA:HA	1:A:1037:HIS:CD2	2.19	0.78
1:A:118:GLU:HG3	1:B:118:GLU:CG	2.14	0.78
1:B:333:GLU:HB2	1:B:334:PRO:CD	2.12	0.78
1:A:856:CYS:SG	1:B:856:CYS:HB2	2.23	0.78
1:A:1466:GLY:HA2	1:A:1469:ILE:HG13	1.65	0.78
1:A:14:PRO:HG2	1:A:329:MET:HG3	1.64	0.78
1:B:1034:ALA:HA	1:B:1037:HIS:CD2	2.19	0.78
1:A:118:GLU:CG	1:B:118:GLU:HG3	2.13	0.78
1:B:1888:VAL:HG22	1:B:1913:VAL:HB	1.66	0.77
1:B:1407:GLN:CG	1:B:1409:PRO:HD2	2.14	0.77
1:A:1732:VAL:O	1:A:1736:THR:HB	1.82	0.77
1:A:903:LEU:HD22	1:A:905:GLN:NE2	1.99	0.77
1:B:1338:LEU:HD21	1:B:1341:GLY:HA2	1.64	0.77
1:A:1003:TYR:CE2	1:A:1037:HIS:HE1	2.02	0.77
1:A:1736:THR:CG2	1:A:1740:GLY:H	1.98	0.77
1:B:1641:THR:HG23	1:B:1644:GLU:OE1	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1736:THR:CG2	1:B:1740:GLY:H	1.98	0.76
1:A:1890:THR:HA	1:A:1915:THR:HB	1.66	0.76
1:B:1538:ARG:HH22	1:B:1585:PRO:HG2	1.50	0.76
1:B:254:ASP:HB3	1:B:257:LYS:HE2	1.67	0.76
1:A:627:TRP:HB2	1:A:643:HIS:CD2	2.21	0.76
1:B:297:THR:HB	1:B:300:GLY:H	1.51	0.76
1:B:1259:PRO:HB2	1:B:1292:LEU:HD22	1.68	0.76
1:B:1407:GLN:HG3	1:B:1409:PRO:HD2	1.66	0.76
1:B:1735:HIS:CD2	1:B:1735:HIS:H	2.02	0.76
1:B:1890:THR:HA	1:B:1915:THR:HB	1.66	0.76
1:A:278:ALA:CB	1:A:279:PRO:HD3	2.16	0.76
1:B:278:ALA:CB	1:B:279:PRO:HD3	2.16	0.76
1:B:642:CYS:HB2	1:B:650:THR:HB	1.66	0.76
1:B:903:LEU:HD22	1:B:905:GLN:NE2	2.01	0.76
1:B:1003:TYR:CE2	1:B:1037:HIS:HE1	2.03	0.76
1:B:1289:LEU:HD22	1:B:1294:VAL:HB	1.69	0.75
1:B:506:MET:HE3	1:B:559:ILE:HD12	1.68	0.75
1:A:502:GLN:HG3	1:A:556:LEU:HD11	1.67	0.75
1:B:1674:HIS:CD2	1:B:1698:THR:HG21	2.22	0.75
1:B:1477:LEU:HD11	1:B:2043:ARG:HD2	1.68	0.75
1:B:1541:LEU:HD22	1:B:1544:ILE:HD11	1.68	0.75
1:A:200:PHE:HB3	1:A:206:LEU:HG	1.67	0.75
1:B:1533:VAL:CG1	1:B:1622:LEU:HB3	2.17	0.75
1:A:297:THR:HB	1:A:300:GLY:H	1.52	0.75
1:A:217:ALA:HB2	1:A:364:PRO:HD3	1.69	0.74
1:A:1222:ASP:HB3	1:A:1257:ARG:NH1	2.03	0.74
1:A:1130:LEU:HD11	1:A:1221:LEU:HD13	1.69	0.74
1:A:938:LEU:HB3	1:B:945:GLU:OE1	1.86	0.74
1:B:1618:PRO:HD3	1:B:1629:LEU:HD11	1.68	0.74
1:A:36:ASP:HB3	1:A:38:ARG:HG3	1.69	0.74
1:B:1418:VAL:HG13	1:B:1425:TRP:CE2	2.22	0.74
1:A:1387:LEU:HD22	1:A:1404:CYS:HB3	1.70	0.73
1:A:1736:THR:HG23	1:A:1739:LYS:N	2.01	0.73
1:A:581:SER:HB2	1:A:683:HIS:NE2	2.03	0.73
1:B:1227:LYS:HB2	1:B:1261:LEU:HD22	1.69	0.73
1:B:622:ALA:HA	1:B:650:THR:HA	1.69	0.73
1:A:1445:ALA:O	1:A:1476:ASN:ND2	2.20	0.73
1:A:1818:ILE:HA	1:A:1823:VAL:HG13	1.68	0.73
1:B:44:LEU:HG	1:B:45:TYR:CE1	2.24	0.73
1:A:1227:LYS:HB2	1:A:1261:LEU:HD22	1.71	0.73
1:A:1612:ARG:O	1:A:1636:VAL:HG12	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1953:ARG:HG2	1:A:2005:VAL:HG13	1.70	0.73
1:B:1533:VAL:HG12	1:B:1622:LEU:HB3	1.70	0.73
1:B:1694:ARG:HH11	1:B:1694:ARG:CG	2.01	0.73
1:B:682:PHE:HB3	1:B:683:HIS:CD2	2.24	0.73
1:B:1338:LEU:HD13	1:B:1406:GLN:NE2	2.03	0.73
1:B:1818:ILE:HA	1:B:1823:VAL:HG13	1.71	0.73
1:A:333:GLU:CB	1:A:334:PRO:HD3	2.17	0.72
1:B:1439:ARG:HB3	1:B:1440:PRO:HD3	1.71	0.72
1:A:1859:GLU:HG2	1:A:1860:GLU:N	2.04	0.72
1:B:123:ASP:O	1:B:127:LEU:HB3	1.89	0.72
1:B:1327:PRO:O	1:B:1381:LEU:HD21	1.90	0.72
1:A:1678:GLY:O	1:A:1682:GLN:HG3	1.89	0.72
1:B:1345:LEU:HD12	1:B:1402:PHE:O	1.89	0.72
1:A:1824:GLN:HG3	1:A:1825:PRO:HD2	1.70	0.72
1:A:1234:LEU:HD22	1:A:1262:LEU:HD22	1.72	0.72
1:A:82:LEU:HD22	1:A:188:LEU:HD11	1.72	0.72
1:B:82:LEU:HD22	1:B:188:LEU:HD11	1.71	0.72
1:A:1299:TRP:HE1	1:A:1306:PRO:HD2	1.53	0.72
1:B:265:SER:O	1:B:269:GLN:HG3	1.90	0.72
1:A:137:ARG:HD2	1:B:137:ARG:NH1	2.05	0.72
1:B:668:GLU:O	1:B:669:ASP:HB2	1.90	0.71
1:B:1222:ASP:HB3	1:B:1257:ARG:NH1	2.04	0.71
1:B:1408:THR:N	1:B:1409:PRO:HD3	2.05	0.71
1:A:633:ARG:NH2	1:A:668:GLU:OE1	2.23	0.71
1:B:1953:ARG:HG2	1:B:2005:VAL:HG13	1.70	0.71
1:A:1419:GLU:CD	1:A:1447:GLY:HA3	2.10	0.71
1:B:36:ASP:HB3	1:B:38:ARG:HG3	1.72	0.71
1:A:1418:VAL:HG13	1:A:1425:TRP:CE2	2.25	0.71
1:B:502:GLN:HG3	1:B:556:LEU:HD11	1.70	0.71
1:A:2105:VAL:O	1:A:2106:LEU:HD23	1.91	0.71
1:B:1926:ALA:O	1:B:1930:ARG:HB2	1.90	0.71
1:A:1472:VAL:HG12	1:A:1473:LEU:H	1.56	0.71
1:A:1569:THR:HG21	1:A:1622:LEU:HA	1.72	0.71
1:A:1576:VAL:HG21	1:A:1843:MET:HG2	1.71	0.71
1:A:1535:VAL:HG12	1:A:1537:SER:H	1.55	0.71
1:A:87:TYR:CE2	1:A:97:PRO:HG2	2.26	0.71
1:A:1888:VAL:HG22	1:A:1913:VAL:HB	1.70	0.70
1:A:44:LEU:HG	1:A:45:TYR:CE1	2.26	0.70
1:B:627:TRP:HB2	1:B:643:HIS:CE1	2.27	0.70
1:B:1234:LEU:HD22	1:B:1262:LEU:HD22	1.73	0.70
1:B:23:TRP:HA	1:B:26:LEU:HD12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1669:GLU:O	1:A:1693:CYS:HB3	1.91	0.70
1:B:575:ASP:O	1:B:711:ARG:HG2	1.91	0.70
1:B:1670:SER:O	1:B:1742:ASP:HB2	1.91	0.70
1:A:944:PHE:HD2	1:A:959:VAL:HG22	1.55	0.70
1:B:1254:LEU:HD21	1:B:1318:ASN:HB2	1.72	0.70
1:B:136:GLN:HE21	1:B:136:GLN:C	1.95	0.70
1:A:1887:TYR:HD2	1:A:1967:GLY:HA3	1.57	0.70
1:B:1477:LEU:CD1	1:B:2043:ARG:HD2	2.21	0.70
1:A:1991:VAL:O	1:A:1994:PRO:HD2	1.91	0.70
1:A:254:ASP:HB3	1:A:257:LYS:HE2	1.72	0.70
1:B:1975:LEU:HD22	1:B:1977:ASP:OD2	1.91	0.70
1:B:641:ALA:HB1	1:B:683:HIS:HB2	1.74	0.70
1:A:77:PRO:O	1:A:81:MET:HG2	1.91	0.69
1:B:944:PHE:HD2	1:B:959:VAL:HG22	1.55	0.69
1:A:1735:HIS:HD2	1:A:1735:HIS:H	1.40	0.69
1:B:1335:ALA:HA	1:B:1406:GLN:NE2	2.07	0.69
1:B:1671:VAL:HG23	1:B:1743:LEU:HB2	1.73	0.69
1:B:1338:LEU:CD1	1:B:1406:GLN:HE21	2.05	0.69
1:B:1651:VAL:CG1	1:B:1680:VAL:HA	2.19	0.69
1:B:87:TYR:O	1:B:91:VAL:HG22	1.92	0.69
1:A:610:ILE:HG12	1:A:690:ILE:HG21	1.74	0.69
1:A:917:VAL:HG13	1:A:1054:PHE:HB2	1.74	0.69
1:B:1887:TYR:HD2	1:B:1967:GLY:HA3	1.56	0.69
1:A:2015:TYR:CD2	1:A:2099:LEU:HD22	2.28	0.69
1:B:1288:LYS:O	1:B:1291:GLN:HG2	1.92	0.69
1:B:1736:THR:HG23	1:B:1739:LYS:N	2.07	0.69
1:A:136:GLN:C	1:A:136:GLN:HE21	1.96	0.69
1:B:1382:PHE:HB3	1:B:1387:LEU:HB2	1.73	0.69
1:A:504:GLN:HA	1:A:541:THR:HG21	1.75	0.68
1:B:1653:THR:HG22	1:B:1810:VAL:HG12	1.73	0.68
1:B:87:TYR:CE2	1:B:97:PRO:HG2	2.28	0.68
1:A:111:VAL:CG2	1:A:188:LEU:HB2	2.23	0.68
1:A:1477:LEU:CD1	1:A:2043:ARG:HD2	2.22	0.68
1:A:252:ASN:ND2	1:A:272:LEU:HB2	2.07	0.68
1:B:917:VAL:HG13	1:B:1054:PHE:HB2	1.75	0.68
1:B:1303:ASN:O	1:B:1333:ASN:HB2	1.93	0.68
1:B:627:TRP:HB2	1:B:643:HIS:ND1	2.08	0.68
1:A:2070:LEU:HD21	1:A:2076:ASN:N	2.08	0.68
1:A:23:TRP:HA	1:A:26:LEU:HD12	1.75	0.68
1:A:1348:THR:HG21	1:A:1378:TRP:CZ2	2.29	0.68
1:A:1126:GLU:HB3	1:A:1129:CYS:SG	2.34	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1254:LEU:HD13	1:A:1316:VAL:HG12	1.75	0.68
1:A:506:MET:HE3	1:A:559:ILE:HD12	1.74	0.68
1:B:333:GLU:CB	1:B:334:PRO:HD3	2.22	0.68
1:A:1489:SER:H	1:A:1493:LEU:HD22	1.58	0.68
1:A:1606:ARG:HH21	1:A:1860:GLU:HG3	1.59	0.68
1:B:1227:LYS:HE3	1:B:1231:ASP:OD2	1.94	0.68
1:B:1460:LEU:HD13	1:B:2032:ALA:CB	2.23	0.68
1:A:1416:LEU:HD21	1:A:1425:TRP:HB2	1.76	0.67
1:B:1576:VAL:HG21	1:B:1843:MET:HG2	1.76	0.67
1:B:1477:LEU:O	1:B:1507:ARG:HG2	1.94	0.67
1:A:1651:VAL:HG12	1:A:1680:VAL:HA	1.77	0.67
1:A:1735:HIS:N	1:A:1735:HIS:CD2	2.61	0.67
1:B:1035:MET:HE3	1:B:1089:VAL:HG12	1.77	0.67
1:B:1139:GLU:CD	1:B:1218:SER:HB2	2.14	0.67
1:B:2015:TYR:CD2	1:B:2099:LEU:HD22	2.30	0.67
1:A:460:VAL:HG21	1:A:465:MET:HG3	1.76	0.67
1:B:1814:LEU:O	1:B:1818:ILE:HG13	1.94	0.67
1:B:111:VAL:CG2	1:B:188:LEU:HB2	2.25	0.67
1:B:635:PRO:HD2	1:B:638:ILE:HB	1.77	0.67
1:B:1430:LYS:HE3	1:B:1981:GLU:HA	1.75	0.67
1:A:614:ASN:O	1:A:615:VAL:O	2.13	0.67
1:B:1279:PRO:HG3	1:B:1298:GLN:NE2	2.10	0.67
1:B:1341:GLY:HA3	1:B:1407:GLN:HA	1.76	0.67
1:B:1954:SER:O	1:B:1958:GLU:HG3	1.95	0.67
1:B:288:GLU:OE1	1:B:383:ILE:HG13	1.95	0.67
1:B:1666:GLN:O	1:B:1669:GLU:HB2	1.95	0.67
1:B:1735:HIS:N	1:B:1735:HIS:CD2	2.62	0.67
1:B:643:HIS:CD2	1:B:746:GLN:HB3	2.30	0.67
1:A:277:TYR:CE2	1:A:287:LEU:HD11	2.30	0.67
1:A:1226:LEU:HD23	1:A:1401:LEU:HD21	1.77	0.67
1:A:581:SER:HB2	1:A:683:HIS:CE1	2.30	0.67
1:B:1126:GLU:HB3	1:B:1129:CYS:SG	2.35	0.67
1:B:1433:LEU:HD21	1:B:1465:GLY:HA3	1.77	0.67
1:B:1824:GLN:HG3	1:B:1825:PRO:HD2	1.76	0.67
1:B:1991:VAL:O	1:B:1994:PRO:HD2	1.95	0.67
1:B:1538:ARG:HH22	1:B:1585:PRO:CG	2.08	0.66
1:A:1285:ALA:O	1:A:1289:LEU:N	2.27	0.66
1:A:1618:PRO:HD3	1:A:1629:LEU:HD11	1.77	0.66
1:A:1814:LEU:O	1:A:1818:ILE:HG13	1.95	0.66
1:A:2098:PHE:CE2	1:A:2106:LEU:HB2	2.30	0.66
1:B:252:ASN:ND2	1:B:272:LEU:HB2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:SER:O	1:A:269:GLN:HG3	1.95	0.66
1:A:976:VAL:O	1:A:978:PRO:HD3	1.94	0.66
1:B:1034:ALA:O	1:B:1037:HIS:HB2	1.95	0.66
1:A:1564:CYS:CB	1:A:1628:LEU:HD21	2.25	0.66
1:B:98:ALA:HA	1:B:101:ARG:HG3	1.78	0.66
1:B:1671:VAL:CG2	1:B:1743:LEU:HB2	2.25	0.66
1:A:1644:GLU:HB3	1:A:1825:PRO:CB	2.24	0.66
1:A:503:TRP:CD1	1:A:787:LYS:HB2	2.31	0.66
1:B:1395:SER:HB3	1:B:1399:SER:O	1.95	0.66
1:B:1673:ILE:O	1:B:1697:THR:HA	1.95	0.66
1:B:1694:ARG:NH1	1:B:1694:ARG:HG3	1.95	0.66
1:A:1470:ARG:O	1:A:1472:VAL:HG23	1.96	0.66
1:B:680:ILE:HG12	1:B:681:ALA:N	2.11	0.66
1:B:620:MET:SD	1:B:682:PHE:HB2	2.35	0.66
1:A:1411:ASP:HB2	1:A:1440:PRO:HD3	1.76	0.66
1:A:1857:ARG:HH11	1:A:1869:PRO:HB3	1.61	0.66
1:B:1244:VAL:HB	1:B:1272:TYR:HD1	1.61	0.66
1:B:1244:VAL:HG13	1:B:1314:LEU:HD23	1.77	0.66
1:A:1252:GLY:HA3	1:A:1318:ASN:HB3	1.77	0.66
1:A:168:LEU:HB2	1:A:185:VAL:HG11	1.77	0.66
1:A:254:ASP:CB	1:A:257:LYS:HE2	2.26	0.66
1:B:123:ASP:CB	1:B:126:THR:HB	2.25	0.66
1:A:87:TYR:O	1:A:91:VAL:HG22	1.96	0.65
1:B:59:ARG:HG3	1:B:838:HIS:HB3	1.78	0.65
1:A:1653:THR:HG22	1:A:1796:LEU:HD21	1.78	0.65
1:A:1974:VAL:HG22	1:A:1994:PRO:HG2	1.77	0.65
1:B:1095:LEU:HD12	1:B:1095:LEU:C	2.17	0.65
1:B:2003:ASP:O	1:B:2007:ARG:HG3	1.95	0.65
1:B:982:THR:C	1:B:984:GLU:H	2.00	0.65
1:A:2003:ASP:O	1:A:2007:ARG:HG3	1.96	0.65
1:B:496:CYS:O	1:B:583:GLY:HA3	1.96	0.65
1:B:645:SER:HB3	1:B:770:VAL:HG13	1.77	0.65
1:A:1035:MET:HE3	1:A:1089:VAL:HG12	1.78	0.65
1:B:1247:VAL:HG11	1:B:1301:PRO:HG3	1.76	0.65
1:A:1268:MET:HA	1:A:1268:MET:HE2	1.79	0.65
1:A:1439:ARG:HB3	1:A:1440:PRO:HD3	1.79	0.65
1:A:502:GLN:HB2	1:A:546:LEU:HD22	1.78	0.65
1:B:1282:LEU:HD21	1:B:1296:GLN:HB2	1.78	0.65
1:B:1486:MET:O	1:B:1488:PRO:HD3	1.97	0.65
1:B:2070:LEU:HD21	1:B:2076:ASN:N	2.11	0.65
1:A:889:THR:HG21	1:A:1032:LEU:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1244:VAL:HG13	1:A:1314:LEU:HD23	1.79	0.65
1:A:399:ASN:H	1:A:399:ASN:HD22	1.43	0.65
1:B:1220:LEU:HB3	1:B:1257:ARG:HH22	1.61	0.65
1:B:1279:PRO:HG3	1:B:1298:GLN:HE22	1.61	0.65
1:B:1528:THR:HG22	1:B:1530:HIS:H	1.61	0.65
1:A:1628:LEU:HD13	1:A:1633:THR:HG21	1.79	0.65
1:B:1569:THR:HG21	1:B:1622:LEU:HA	1.79	0.65
1:B:1736:THR:HG23	1:B:1740:GLY:H	1.61	0.65
1:A:1838:ALA:HA	1:A:1841:ARG:HG3	1.77	0.64
1:A:2102:PRO:HD2	1:A:2103:HIS:HD2	1.63	0.64
1:B:1532:PHE:HD2	1:B:1549:SER:HA	1.61	0.64
1:B:2105:VAL:O	1:B:2106:LEU:HD23	1.97	0.64
1:B:615:VAL:HG22	1:B:686:PHE:HD2	1.63	0.64
1:A:1395:SER:HB3	1:A:1399:SER:O	1.97	0.64
1:A:325:THR:OG1	1:A:343:LYS:HG2	1.97	0.64
1:A:302:PRO:HA	1:A:366:ILE:HG21	1.79	0.64
1:A:44:LEU:HG	1:A:45:TYR:CD1	2.32	0.64
1:B:1408:THR:N	1:B:1409:PRO:CD	2.61	0.64
1:B:1433:LEU:HD11	1:B:1465:GLY:O	1.97	0.64
1:B:1466:GLY:HA2	1:B:1469:ILE:HG13	1.77	0.64
1:B:64:PHE:HB2	1:B:429:ARG:NH2	2.11	0.64
1:B:217:ALA:HB2	1:B:364:PRO:HD3	1.79	0.64
1:A:1001:TYR:HB3	1:A:1003:TYR:CE1	2.32	0.64
1:A:1227:LYS:HE3	1:A:1231:ASP:OD2	1.98	0.64
1:B:1472:VAL:HG12	1:B:1473:LEU:H	1.62	0.64
1:B:660:GLU:HG2	1:B:663:GLN:NE2	2.12	0.64
1:B:736:VAL:O	1:B:740:VAL:HG23	1.98	0.64
1:A:1532:PHE:CE1	1:A:1597:CYS:HB3	2.32	0.64
1:A:1594:THR:OG1	1:A:1596:ASP:HB2	1.98	0.64
1:B:2102:PRO:HD2	1:B:2103:HIS:HD2	1.62	0.64
1:B:64:PHE:CE2	1:B:464:ALA:HB1	2.32	0.64
1:A:1220:LEU:HB3	1:A:1257:ARG:HH22	1.63	0.64
1:A:1859:GLU:HG2	1:A:1860:GLU:H	1.59	0.64
1:A:2002:LEU:O	1:A:2006:THR:HB	1.97	0.64
1:A:59:ARG:HG3	1:A:838:HIS:HB3	1.79	0.64
1:B:1348:THR:HG22	1:B:1349:LEU:N	2.06	0.64
1:B:1449:SER:O	1:B:1477:LEU:HD22	1.98	0.64
1:B:168:LEU:HB2	1:B:185:VAL:HG11	1.78	0.64
1:B:127:LEU:HG	1:B:127:LEU:O	1.97	0.64
1:B:1285:ALA:O	1:B:1289:LEU:N	2.29	0.64
1:A:137:ARG:NH1	1:B:137:ARG:HD2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:LEU:HB3	1:B:810:VAL:HB	1.78	0.64
1:A:1564:CYS:SG	1:A:1628:LEU:HD21	2.38	0.64
1:B:2002:LEU:O	1:B:2006:THR:HB	1.97	0.64
1:B:302:PRO:HA	1:B:366:ILE:HG21	1.80	0.64
1:A:132:MET:HE1	1:B:200:PHE:CE2	2.33	0.64
1:B:2098:PHE:CE2	1:B:2106:LEU:HB2	2.33	0.64
1:B:319:PRO:HB2	1:B:320:LEU:HD23	1.79	0.64
1:B:1836:VAL:HG13	1:B:1854:ILE:CD1	2.28	0.63
1:A:1411:ASP:O	1:A:1413:PRO:HD3	1.98	0.63
1:A:1926:ALA:O	1:A:1930:ARG:HB2	1.98	0.63
1:B:1991:VAL:HG21	1:B:2033:ASN:ND2	2.13	0.63
1:A:1442:TRP:CZ2	1:A:1497:LEU:HD23	2.32	0.63
1:A:112:SER:HB3	1:A:334:PRO:HG3	1.79	0.63
1:B:44:LEU:HG	1:B:45:TYR:CD1	2.33	0.63
1:A:1746:ASN:HD21	1:A:1753:LEU:HD12	1.62	0.63
1:A:736:VAL:O	1:A:740:VAL:HG23	1.99	0.63
1:A:984:GLU:O	1:A:985:PHE:HB2	1.96	0.63
1:B:1303:ASN:N	1:B:1304:PRO:CD	2.61	0.63
1:B:159:THR:HB	1:B:162:SER:OG	1.99	0.63
1:B:351:GLY:C	1:B:383:ILE:HG22	2.19	0.63
1:B:1475:SER:HB3	1:B:1505:VAL:HG13	1.81	0.63
1:B:1735:HIS:HD2	1:B:1735:HIS:H	1.43	0.63
1:B:9:MET:HE3	1:B:345:LEU:HD12	1.80	0.63
1:A:1954:SER:O	1:A:1958:GLU:HG3	1.97	0.63
1:A:501:ALA:HB3	1:A:556:LEU:HD21	1.80	0.63
1:B:1139:GLU:OE2	1:B:1218:SER:HB2	1.99	0.63
1:A:1472:VAL:HG12	1:A:1473:LEU:N	2.13	0.63
1:B:1460:LEU:HD13	1:B:2032:ALA:HB2	1.81	0.63
1:B:254:ASP:CB	1:B:257:LYS:HE2	2.28	0.63
1:B:853:GLY:O	1:B:854:SER:HB3	1.97	0.63
1:B:1268:MET:HA	1:B:1268:MET:HE2	1.79	0.62
1:B:460:VAL:HG21	1:B:465:MET:HG3	1.79	0.62
1:A:1302:ALA:O	1:A:1303:ASN:HB2	1.97	0.62
1:A:1486:MET:HE1	1:A:1506:TYR:HB3	1.81	0.62
1:A:1616:MET:HB3	1:A:1800:PHE:CZ	2.33	0.62
1:B:2006:THR:HG21	1:B:2048:ARG:HH22	1.62	0.62
1:A:1545:ARG:HG3	1:A:1545:ARG:NH1	2.12	0.62
1:A:399:ASN:N	1:A:399:ASN:ND2	2.46	0.62
1:A:641:ALA:HB1	1:A:683:HIS:HB2	1.81	0.62
1:B:1433:LEU:HD13	1:B:1469:ILE:HD11	1.79	0.62
1:B:251:THR:HB	1:B:399:ASN:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:SER:O	1:A:583:GLY:N	2.33	0.62
1:B:1857:ARG:NH1	1:B:1871:ILE:HD11	2.15	0.62
1:B:200:PHE:HB3	1:B:206:LEU:HG	1.81	0.62
1:B:325:THR:OG1	1:B:343:LYS:HG2	1.99	0.62
1:B:643:HIS:HD2	1:B:746:GLN:HB3	1.65	0.62
1:A:1484:PRO:O	1:A:1485:GLU:HB2	2.00	0.62
1:A:1762:GLN:HG2	1:A:1787:LYS:O	1.99	0.62
1:B:1857:ARG:CZ	1:B:1871:ILE:HD11	2.30	0.62
1:B:1917:ARG:HH12	1:B:1974:VAL:HG12	1.63	0.62
1:B:399:ASN:HD22	1:B:399:ASN:H	1.47	0.62
1:B:77:PRO:O	1:B:81:MET:HG2	1.99	0.62
1:A:159:THR:HB	1:A:162:SER:OG	1.99	0.62
1:A:1734:ARG:O	1:A:1736:THR:N	2.32	0.62
1:A:319:PRO:HB2	1:A:320:LEU:HD23	1.82	0.62
1:A:542:ASP:O	1:A:545:VAL:HG12	1.99	0.62
1:B:752:VAL:HG11	1:B:775:LEU:HD21	1.81	0.62
1:A:1009:LEU:HD13	1:A:1023:GLN:O	2.00	0.62
1:A:542:ASP:H	1:A:545:VAL:HG12	1.63	0.62
1:B:9:MET:HE1	1:B:345:LEU:HB2	1.82	0.62
1:A:1429:LEU:HD11	1:A:1443:LEU:HD11	1.80	0.62
1:A:1836:VAL:HG13	1:A:1854:ILE:CD1	2.29	0.62
1:A:251:THR:HB	1:A:399:ASN:O	2.00	0.62
1:B:1454:VAL:HG13	1:B:1503:MET:HE1	1.80	0.62
1:B:570:LEU:HD13	1:B:800:VAL:HG13	1.82	0.62
1:B:972:THR:HG22	1:B:1081:VAL:CG2	2.29	0.62
1:B:420:LEU:HD11	1:B:512:ARG:HB3	1.82	0.62
1:A:874:TYR:HB2	1:A:1006:PHE:CD2	2.34	0.62
1:A:353:TRP:NE1	1:A:383:ILE:HB	2.14	0.62
1:A:817:PRO:O	1:A:818:PRO:O	2.18	0.62
1:B:1001:TYR:HB3	1:B:1003:TYR:CE1	2.35	0.62
1:B:1139:GLU:OE2	1:B:1216:LEU:HD12	1.99	0.62
1:B:1335:ALA:CA	1:B:1406:GLN:HE22	2.09	0.62
1:A:123:ASP:HB3	1:A:126:THR:CB	2.28	0.61
1:A:23:TRP:CE2	1:A:350:HIS:CD2	2.88	0.61
1:A:808:VAL:HG12	1:A:809:SER:N	2.15	0.61
1:A:976:VAL:HG13	1:A:977:ASP:N	2.14	0.61
1:B:112:SER:HB3	1:B:334:PRO:HG3	1.82	0.61
1:B:1580:THR:HG22	1:B:1581:GLY:N	2.14	0.61
1:A:1095:LEU:HD12	1:A:1095:LEU:C	2.20	0.61
1:A:317:ARG:O	1:A:319:PRO:HD3	1.99	0.61
1:A:1420:ASP:O	1:A:1425:TRP:CH2	2.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:THR:HG22	1:B:104:SER:N	2.15	0.61
1:B:277:TYR:CE2	1:B:287:LEU:HD11	2.34	0.61
1:B:331:HIS:CE1	1:B:333:GLU:HA	2.35	0.61
1:A:1124:HIS:CD2	1:A:1512:GLY:HA2	2.35	0.61
1:A:1765:ARG:HG3	1:A:1790:THR:HG23	1.83	0.61
1:A:384:ARG:HH11	1:A:384:ARG:CG	2.13	0.61
1:B:1768:GLU:HA	1:B:1768:GLU:OE1	2.00	0.61
1:B:1974:VAL:HG22	1:B:1994:PRO:HG2	1.81	0.61
1:A:1454:VAL:HG13	1:A:1503:MET:HE1	1.82	0.61
1:A:331:HIS:CE1	1:A:333:GLU:HA	2.35	0.61
1:B:889:THR:HG21	1:B:1032:LEU:HB2	1.80	0.61
1:B:347:SER:HB2	1:B:352:VAL:O	2.00	0.61
1:A:1466:GLY:HA2	1:A:1469:ILE:CG1	2.29	0.61
1:A:368:ALA:CA	1:A:371:ASP:HB3	2.31	0.61
1:B:1838:ALA:HA	1:B:1841:ARG:HG3	1.80	0.61
1:B:248:ASN:ND2	1:B:249:ALA:H	1.98	0.61
1:B:1703:GLU:O	1:B:1706:ALA:HB3	2.01	0.61
1:B:1647:SER:HA	1:B:1851:LYS:HG3	1.81	0.61
1:B:322:ILE:CD1	1:B:374:LEU:HD13	2.31	0.61
1:B:416:GLN:HG3	1:B:422:ARG:HH21	1.65	0.61
1:A:2078:THR:O	1:A:2079:VAL:HG13	2.01	0.61
1:B:89:ALA:O	1:B:92:ASP:HB3	2.01	0.61
1:A:366:ILE:O	1:A:366:ILE:HG12	2.00	0.61
1:A:416:GLN:HG3	1:A:422:ARG:HH21	1.64	0.61
1:B:1455:GLY:HA3	1:B:2039:SER:HB2	1.82	0.61
1:B:1841:ARG:O	1:B:1844:ALA:HB3	2.00	0.61
1:A:64:PHE:CE2	1:A:464:ALA:HB1	2.36	0.61
1:A:913:VAL:HG23	1:A:962:TRP:HB2	1.83	0.61
1:A:1343:PHE:O	1:A:1344:LEU:HD22	2.01	0.60
1:A:1746:ASN:ND2	1:A:1753:LEU:HD12	2.16	0.60
1:A:98:ALA:HA	1:A:101:ARG:HG3	1.82	0.60
1:B:1442:TRP:CZ2	1:B:1497:LEU:HD23	2.36	0.60
1:A:1248:LEU:HD21	1:A:1277:ARG:HE	1.66	0.60
1:B:1408:THR:H	1:B:1409:PRO:HD3	1.65	0.60
1:B:403:ILE:O	1:B:404:LEU:HD23	2.00	0.60
1:B:981:SER:HA	1:B:984:GLU:HG3	1.82	0.60
1:A:1656:TYR:CD2	1:A:1687:ILE:HD13	2.35	0.60
1:B:1035:MET:SD	1:B:1091:ALA:HB3	2.42	0.60
1:B:123:ASP:HB3	1:B:126:THR:HB	1.81	0.60
1:B:1299:TRP:CZ2	1:B:1304:PRO:O	2.54	0.60
1:B:327:SER:OG	1:B:356:ASN:ND2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1439:ARG:O	1:A:1470:ARG:HB3	2.01	0.60
1:A:2006:THR:HG21	1:A:2048:ARG:HH22	1.66	0.60
1:A:247:LEU:HD11	1:A:405:GLN:HB2	1.82	0.60
1:B:215:PHE:CD2	1:B:305:LEU:HD11	2.37	0.60
1:B:501:ALA:HB3	1:B:556:LEU:HD21	1.83	0.60
1:A:665:LEU:HD22	1:A:670:VAL:HB	1.83	0.60
1:B:1073:ASP:O	1:B:1074:THR:HG22	2.02	0.60
1:A:45:TYR:HE2	1:B:124:PRO:HB2	1.66	0.60
1:B:1429:LEU:HD11	1:B:1443:LEU:HD11	1.82	0.60
1:B:1652:TYR:CD1	1:B:1823:VAL:HB	2.37	0.60
1:A:1575:ASP:HA	1:A:1599:LEU:HD23	1.83	0.60
1:A:368:ALA:HA	1:A:371:ASP:HB3	1.82	0.60
1:B:112:SER:HB2	1:B:334:PRO:CG	2.32	0.60
1:B:1119:PHE:CE1	1:B:1516:HIS:CE1	2.89	0.60
1:A:1279:PRO:HG3	1:A:1298:GLN:NE2	2.16	0.60
1:A:143:ARG:HG2	1:A:143:ARG:HH11	1.67	0.60
1:B:1580:THR:HG22	1:B:1582:LYS:N	2.16	0.60
1:B:1672:LEU:HD12	1:B:1696:PHE:O	2.02	0.60
1:B:2078:THR:O	1:B:2079:VAL:HG13	2.01	0.60
1:B:359:TYR:OH	1:B:362:PRO:HG3	2.02	0.60
1:B:468:ARG:HD3	1:B:485:VAL:HG21	1.83	0.60
1:A:586:ALA:O	1:A:589:TYR:HB3	2.02	0.60
1:A:1038:MET:HA	1:A:1038:MET:CE	2.32	0.60
1:A:883:ARG:HH21	1:A:1107:ARG:HD3	1.67	0.60
1:A:1549:SER:O	1:A:1552:HIS:HB3	2.01	0.60
1:A:582:LEU:O	1:A:585:VAL:HG23	2.01	0.60
1:A:595:THR:HB	1:A:598:GLU:H	1.66	0.60
1:A:670:VAL:HG12	1:A:671:PHE:N	2.16	0.60
1:B:1657:TYR:HA	1:B:1661:VAL:CG2	2.32	0.60
1:B:343:LYS:HE3	1:B:354:ALA:HB3	1.84	0.60
1:B:654:PRO:O	1:B:658:MET:HB2	2.01	0.60
1:A:1086:LEU:N	1:A:1086:LEU:HD23	2.17	0.60
1:A:36:ASP:CB	1:A:38:ARG:HG3	2.32	0.60
1:B:1396:PHE:CE2	1:B:1397:TYR:HD2	2.20	0.60
1:B:1466:GLY:HA2	1:B:1469:ILE:CG1	2.32	0.59
1:B:14:PRO:HD3	1:B:226:GLU:O	2.02	0.59
1:B:1625:SER:O	1:B:1626:VAL:HG23	2.02	0.59
1:B:646:LYS:HG2	1:B:746:GLN:HE21	1.67	0.59
1:A:1580:THR:HG22	1:A:1582:LYS:N	2.17	0.59
1:A:327:SER:OG	1:A:356:ASN:ND2	2.35	0.59
1:B:1035:MET:HE3	1:B:1089:VAL:CG1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ARG:HH11	1:B:384:ARG:CG	2.12	0.59
1:A:166:LEU:HD12	1:A:251:THR:HG21	1.83	0.59
1:B:1662:ARG:NH1	1:B:1662:ARG:CG	2.49	0.59
1:A:1857:ARG:NH1	1:A:1869:PRO:CB	2.66	0.59
1:B:1657:TYR:HA	1:B:1661:VAL:HG23	1.84	0.59
1:B:662:LEU:HD22	1:B:672:VAL:CG1	2.29	0.59
1:A:1475:SER:O	1:A:1486:MET:HE1	2.01	0.59
1:A:1703:GLU:O	1:A:1706:ALA:HB3	2.02	0.59
1:B:1097:LEU:HD12	1:B:1098:GLY:N	2.17	0.59
1:B:1765:ARG:HG3	1:B:1790:THR:HG23	1.85	0.59
1:A:1774:LEU:HD22	1:B:1785:PHE:HB2	1.85	0.59
1:B:143:ARG:HG2	1:B:143:ARG:HH11	1.68	0.59
1:B:366:ILE:HG12	1:B:366:ILE:O	2.02	0.59
1:B:322:ILE:HD12	1:B:374:LEU:HD13	1.85	0.59
1:B:630:CYS:HB3	1:B:640:PRO:HG3	1.85	0.59
1:A:1736:THR:HG23	1:A:1740:GLY:H	1.66	0.59
1:A:9:MET:HE3	1:A:345:LEU:HD12	1.85	0.59
1:B:1662:ARG:HG2	1:B:1662:ARG:HH11	1.67	0.59
1:A:1034:ALA:O	1:A:1037:HIS:HB2	2.02	0.59
1:A:1397:TYR:CE1	1:A:1399:SER:HB2	2.37	0.59
1:A:615:VAL:HG22	1:A:616:LEU:H	1.68	0.59
1:B:1003:TYR:CE1	1:B:1037:HIS:CE1	2.90	0.59
1:B:2101:GLN:HG3	1:B:2102:PRO:CD	2.33	0.59
1:B:317:ARG:O	1:B:319:PRO:HD3	2.02	0.59
1:B:288:GLU:HG3	1:B:385:GLY:O	2.02	0.59
1:B:399:ASN:N	1:B:399:ASN:ND2	2.51	0.59
1:A:1118:LYS:HD2	1:A:2103:HIS:CE1	2.38	0.59
1:B:1454:VAL:HG13	1:B:1503:MET:CE	2.33	0.59
1:B:646:LYS:HG2	1:B:746:GLN:NE2	2.18	0.59
1:B:128:VAL:HG11	1:B:130:TYR:CZ	2.37	0.59
1:A:200:PHE:CE2	1:B:132:MET:HE1	2.38	0.59
1:A:1785:PHE:HB2	1:B:1774:LEU:HD22	1.83	0.59
1:A:1248:LEU:CD2	1:A:1277:ARG:HE	2.16	0.58
1:A:1580:THR:HG22	1:A:1581:GLY:N	2.17	0.58
1:A:165:LEU:HB2	1:A:337:GLY:HA3	1.85	0.58
1:B:878:HIS:HB2	1:B:1007:PHE:CE1	2.38	0.58
1:B:13:LEU:HB3	1:B:14:PRO:HD2	1.84	0.58
1:A:1122:THR:HG1	1:A:1517:PHE:HE1	1.49	0.58
1:A:1528:THR:HG22	1:A:1530:HIS:N	2.15	0.58
1:A:64:PHE:HB2	1:A:429:ARG:NH2	2.13	0.58
1:B:1472:VAL:HG12	1:B:1473:LEU:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1539:GLY:HA2	1:B:1580:THR:O	2.02	0.58
1:B:165:LEU:HB2	1:B:337:GLY:HA3	1.85	0.58
1:B:1736:THR:O	1:B:1739:LYS:HB2	2.03	0.58
1:B:527:LEU:HD12	1:B:534:VAL:HG22	1.85	0.58
1:B:680:ILE:HG12	1:B:681:ALA:H	1.67	0.58
1:A:1073:ASP:O	1:A:1074:THR:HG22	2.03	0.58
1:B:68:HIS:HB3	1:B:71:GLN:HG3	1.85	0.58
1:B:1007:PHE:HE2	1:B:1030:SER:HA	1.67	0.58
1:B:1299:TRP:HE1	1:B:1306:PRO:HD2	1.68	0.58
1:B:612:GLU:HG2	1:B:612:GLU:O	2.04	0.58
1:A:1236:ASN:HA	1:A:1502:VAL:HG21	1.86	0.58
1:A:1991:VAL:HG21	1:A:2033:ASN:ND2	2.18	0.58
1:A:23:TRP:CE2	1:A:350:HIS:HD2	2.22	0.58
1:A:466:PRO:HG2	1:A:467:PHE:HD1	1.68	0.58
1:B:1694:ARG:CG	1:B:1694:ARG:NH1	2.65	0.58
1:A:917:VAL:CG1	1:A:1054:PHE:HB2	2.34	0.58
1:B:1662:ARG:NH2	1:B:1793:GLY:O	2.36	0.58
1:B:1674:HIS:CD2	1:B:1698:THR:CG2	2.87	0.58
1:B:297:THR:HB	1:B:300:GLY:N	2.19	0.58
1:A:1248:LEU:HD21	1:A:1277:ARG:HH21	1.69	0.58
1:A:1122:THR:HG21	1:A:1517:PHE:HZ	1.68	0.58
1:A:595:THR:CG2	1:A:597:GLU:HG2	2.33	0.58
1:B:1300:ASP:O	1:B:1302:ALA:N	2.36	0.58
1:A:155:ILE:HD11	1:B:166:LEU:HD11	1.85	0.58
1:B:1860:GLU:HB2	1:B:1865:PRO:HG2	1.84	0.58
1:A:321:LEU:HD23	1:A:381:LEU:HD13	1.86	0.58
1:B:386:GLY:O	1:B:387:ASN:HB2	2.03	0.58
1:A:1299:TRP:NE1	1:A:1306:PRO:HD2	2.19	0.58
1:B:1003:TYR:CE1	1:B:1037:HIS:HE1	2.21	0.58
1:B:23:TRP:CE2	1:B:350:HIS:CD2	2.92	0.58
1:A:1068:LEU:HD12	1:A:1077:ALA:O	2.04	0.57
1:A:112:SER:HB2	1:A:334:PRO:CG	2.31	0.57
1:A:13:LEU:HB3	1:A:14:PRO:HD2	1.85	0.57
1:A:1580:THR:HG22	1:A:1582:LYS:H	1.69	0.57
1:B:1241:LYS:O	1:B:1241:LYS:HG3	2.03	0.57
1:A:103:THR:HG22	1:A:104:SER:N	2.19	0.57
1:B:1277:ARG:HD3	1:B:1300:ASP:OD2	2.04	0.57
1:A:945:GLU:OE1	1:B:938:LEU:HB3	2.03	0.57
1:A:1953:ARG:HG2	1:A:2005:VAL:CG1	2.33	0.57
1:B:889:THR:CG2	1:B:1032:LEU:HB2	2.34	0.57
1:B:1138:GLU:HG3	1:B:1138:GLU:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1456:MET:HG3	1:B:2036:PHE:HD1	1.70	0.57
1:B:1762:GLN:HG2	1:B:1787:LYS:O	2.05	0.57
1:A:1007:PHE:HE2	1:A:1030:SER:HA	1.70	0.57
1:A:1616:MET:HE2	1:A:1650:ILE:HD13	1.87	0.57
1:A:1917:ARG:HH12	1:A:1974:VAL:HG12	1.69	0.57
1:A:333:GLU:CB	1:A:334:PRO:CD	2.79	0.57
1:A:476:GLU:HB2	1:A:790:ARG:HH12	1.68	0.57
1:A:883:ARG:HE	1:A:1107:ARG:HD3	1.69	0.57
1:B:1953:ARG:HG2	1:B:2005:VAL:CG1	2.34	0.57
1:B:234:THR:HG21	1:B:239:ALA:HB2	1.84	0.57
1:A:1647:SER:O	1:A:1651:VAL:HG21	2.04	0.57
1:A:1736:THR:O	1:A:1739:LYS:HB2	2.04	0.57
1:B:1097:LEU:HD12	1:B:1097:LEU:C	2.24	0.57
1:B:1616:MET:HB3	1:B:1800:PHE:CZ	2.39	0.57
1:B:492:VAL:HG11	1:B:572:LEU:HD21	1.87	0.57
1:B:883:ARG:HH21	1:B:1107:ARG:HD3	1.68	0.57
1:B:91:VAL:O	1:B:457:ILE:HD11	2.04	0.57
1:A:1734:ARG:C	1:A:1736:THR:H	2.08	0.57
1:A:1773:ASP:OD1	1:A:1778:HIS:HD2	1.88	0.57
1:A:1841:ARG:O	1:A:1844:ALA:HB3	2.03	0.57
1:B:1538:ARG:HH12	1:B:1585:PRO:CG	2.17	0.57
1:B:234:THR:CG2	1:B:239:ALA:HB2	2.34	0.57
1:B:257:LYS:HD3	1:B:263:PHE:O	2.04	0.57
1:A:1672:LEU:HD12	1:A:1696:PHE:O	2.04	0.57
1:A:393:PHE:CD1	1:A:399:ASN:HB3	2.40	0.57
1:A:652:SER:OG	1:A:681:ALA:HB1	2.04	0.57
1:B:1996:TYR:C	1:B:1996:TYR:CD2	2.78	0.57
1:B:368:ALA:CA	1:B:371:ASP:HB3	2.34	0.57
1:A:889:THR:CG2	1:A:1032:LEU:HB2	2.35	0.57
1:A:1448:CYS:C	1:A:1450:THR:H	2.08	0.57
1:A:1653:THR:CG2	1:A:1796:LEU:HD21	2.35	0.57
1:A:293:HIS:O	1:A:326:LYS:HD2	2.04	0.57
1:A:403:ILE:O	1:A:404:LEU:HD23	2.04	0.57
1:A:638:ILE:O	1:A:638:ILE:HG22	2.05	0.57
1:B:123:ASP:HB3	1:B:126:THR:CB	2.34	0.57
1:B:1720:PHE:HD1	1:B:1720:PHE:N	2.01	0.57
1:B:466:PRO:HG2	1:B:467:PHE:HD1	1.70	0.57
1:A:1657:TYR:CZ	1:A:1799:LEU:HD11	2.40	0.57
1:A:399:ASN:H	1:A:399:ASN:ND2	2.00	0.57
1:B:1277:ARG:HD3	1:B:1300:ASP:CG	2.24	0.57
1:B:22:PHE:CD2	1:B:26:LEU:HD11	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LEU:HD11	1:B:405:GLN:HB2	1.85	0.57
1:B:799:ASN:HA	1:B:802:ARG:HG3	1.86	0.57
1:A:1485:GLU:HB3	1:A:1506:TYR:OH	2.05	0.57
1:B:1320:ALA:HA	1:B:1349:LEU:HD11	1.85	0.57
1:B:1580:THR:HG22	1:B:1582:LYS:H	1.70	0.57
1:B:1565:SER:HB2	1:B:1857:ARG:HH22	1.63	0.57
1:B:362:PRO:HB3	1:B:369:LEU:HB3	1.87	0.57
1:B:913:VAL:HG23	1:B:962:TRP:HB2	1.86	0.57
1:A:14:PRO:HD3	1:A:226:GLU:O	2.04	0.56
1:A:343:LYS:HG3	1:A:344:VAL:N	2.19	0.56
1:A:371:ASP:CG	1:A:371:ASP:O	2.43	0.56
1:B:1651:VAL:HG23	1:B:1851:LYS:HZ1	1.70	0.56
1:A:1457:VAL:CG2	1:A:1473:LEU:HD22	2.32	0.56
1:A:148:PHE:HB3	1:A:150:PHE:CZ	2.40	0.56
1:A:309:VAL:HG12	1:A:313:CYS:HB2	1.87	0.56
1:A:527:LEU:HD12	1:A:534:VAL:HG22	1.86	0.56
1:B:980:ASP:CB	1:B:982:THR:HG22	2.33	0.56
1:A:1279:PRO:HG3	1:A:1298:GLN:HE22	1.70	0.56
1:A:1425:TRP:HA	1:A:1428:SER:HB2	1.87	0.56
1:A:492:VAL:HG11	1:A:572:LEU:HD21	1.88	0.56
1:A:615:VAL:HG22	1:A:616:LEU:N	2.20	0.56
1:B:166:LEU:HD12	1:B:251:THR:HG21	1.87	0.56
1:A:19:LEU:HD11	1:A:342:ILE:HD13	1.87	0.56
1:B:970:PHE:O	1:B:1067:LYS:HE2	2.05	0.56
1:A:1545:ARG:CG	1:A:1545:ARG:HH11	2.17	0.56
1:A:248:ASN:ND2	1:A:249:ALA:H	2.03	0.56
1:B:506:MET:HE3	1:B:559:ILE:CD1	2.36	0.56
1:B:903:LEU:O	1:B:905:GLN:HG3	2.05	0.56
1:A:1486:MET:CE	1:A:1506:TYR:HB3	2.35	0.56
1:B:326:LYS:HE3	1:B:336:SER:HB2	1.87	0.56
1:B:642:CYS:HA	1:B:743:VAL:HG22	1.86	0.56
1:A:1299:TRP:HE1	1:A:1305:ALA:HA	1.71	0.56
1:A:1765:ARG:HD3	1:A:1765:ARG:N	2.21	0.56
1:A:68:HIS:HB3	1:A:71:GLN:HG3	1.88	0.56
1:B:1222:ASP:HA	1:B:1226:LEU:CD1	2.35	0.56
1:B:1373:LEU:N	1:B:1373:LEU:HD23	2.20	0.56
1:B:1662:ARG:NH1	1:B:1662:ARG:HG2	2.18	0.56
1:A:1348:THR:HG22	1:A:1349:LEU:N	2.14	0.56
1:B:1407:GLN:HG2	1:B:1409:PRO:HD2	1.83	0.56
1:B:1422:SER:O	1:B:1423:PHE:HB2	2.06	0.56
1:B:1423:PHE:CD1	1:B:1989:GLN:HB3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1514:PHE:O	1:B:1515:ARG:NH1	2.39	0.56
1:B:1765:ARG:HD3	1:B:1765:ARG:N	2.21	0.56
1:B:278:ALA:CB	1:B:279:PRO:CD	2.83	0.56
1:A:1244:VAL:HB	1:A:1272:TYR:HD1	1.69	0.56
1:A:1662:ARG:NH1	1:A:1792:HIS:ND1	2.54	0.56
1:A:1720:PHE:N	1:A:1720:PHE:CD1	2.74	0.56
1:B:993:TYR:CZ	1:B:1008:GLN:HA	2.40	0.56
1:B:309:VAL:HG12	1:B:313:CYS:HB2	1.88	0.56
1:B:19:LEU:HD11	1:B:342:ILE:HD13	1.88	0.56
1:A:89:ALA:O	1:A:92:ASP:HB3	2.05	0.56
1:B:1451:SER:O	1:B:2036:PHE:CE1	2.59	0.56
1:B:1656:TYR:O	1:B:1661:VAL:HG23	2.06	0.56
1:B:1720:PHE:N	1:B:1720:PHE:CD1	2.71	0.56
1:B:1669:GLU:HG2	1:B:1742:ASP:OD2	2.06	0.56
1:A:799:ASN:HA	1:A:802:ARG:HG3	1.88	0.56
1:A:903:LEU:O	1:A:905:GLN:HG3	2.06	0.56
1:A:1275:THR:CG2	1:A:1299:TRP:HB2	2.36	0.55
1:A:1720:PHE:N	1:A:1720:PHE:HD1	2.04	0.55
1:A:1996:TYR:CD2	1:A:1996:TYR:C	2.79	0.55
1:A:9:MET:HE1	1:A:345:LEU:HB2	1.88	0.55
1:B:1746:ASN:HD21	1:B:1753:LEU:HD12	1.71	0.55
1:B:424:LEU:CD2	1:B:441:GLY:HA3	2.36	0.55
1:A:1570:SER:OG	1:A:1602:GLU:HB3	2.07	0.55
1:A:257:LYS:HD3	1:A:263:PHE:O	2.05	0.55
1:A:670:VAL:HG12	1:A:671:PHE:H	1.72	0.55
1:B:1007:PHE:CE2	1:B:1030:SER:HA	2.41	0.55
1:B:1038:MET:HA	1:B:1038:MET:CE	2.36	0.55
1:B:22:PHE:CE2	1:B:26:LEU:HD11	2.40	0.55
1:A:1569:THR:HG23	1:A:1602:GLU:O	2.06	0.55
1:B:1893:LEU:HB3	1:B:1925:GLN:NE2	2.20	0.55
1:B:371:ASP:O	1:B:371:ASP:CG	2.43	0.55
1:A:36:ASP:HB3	1:A:38:ARG:CG	2.37	0.55
1:B:1996:TYR:CD1	1:B:2040:ALA:HB1	2.41	0.55
1:B:278:ALA:HB3	1:B:279:PRO:CD	2.34	0.55
1:B:36:ASP:CB	1:B:38:ARG:HG3	2.35	0.55
1:B:621:ALA:CB	1:B:662:LEU:HD11	2.36	0.55
1:A:1003:TYR:CE1	1:A:1037:HIS:CE1	2.94	0.55
1:A:1418:VAL:HG13	1:A:1425:TRP:CH2	2.42	0.55
1:A:1484:PRO:O	1:A:1485:GLU:CB	2.53	0.55
1:A:1674:HIS:ND1	1:A:1698:THR:HG21	2.21	0.55
1:A:1777:ASN:HD22	1:B:1783:ALA:H	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1996:TYR:CD1	1:A:2040:ALA:HB1	2.41	0.55
1:B:1736:THR:HG21	1:B:1740:GLY:H	1.72	0.55
1:B:2103:HIS:H	1:B:2103:HIS:CD2	2.23	0.55
1:A:1097:LEU:HD12	1:A:1098:GLY:N	2.22	0.55
1:A:1443:LEU:O	1:A:1473:LEU:HA	2.06	0.55
1:A:1563:LEU:HD12	1:A:1564:CYS:H	1.72	0.55
1:B:1414:VAL:HG11	1:B:1432:ILE:HD13	1.89	0.55
1:B:1470:ARG:HG3	1:B:1470:ARG:O	2.05	0.55
1:A:1616:MET:HB3	1:A:1800:PHE:HZ	1.72	0.55
1:A:1768:GLU:OE1	1:A:1768:GLU:HA	2.06	0.55
1:A:81:MET:HG3	1:A:228:VAL:HG11	1.89	0.55
1:A:22:PHE:CD2	1:A:26:LEU:HD11	2.41	0.55
1:A:386:GLY:O	1:A:387:ASN:HB2	2.05	0.55
1:B:1299:TRP:CH2	1:B:1333:ASN:ND2	2.75	0.55
1:B:1473:LEU:HG	1:B:1503:MET:HA	1.88	0.55
1:B:1560:GLN:HA	1:B:1563:LEU:HB3	1.87	0.55
1:A:1470:ARG:HG3	1:A:1470:ARG:O	2.07	0.55
1:A:1482:PRO:C	1:A:1484:PRO:HD3	2.26	0.55
1:A:1530:HIS:HB2	1:A:1552:HIS:HB2	1.87	0.55
1:A:429:ARG:HH11	1:A:429:ARG:HB3	1.70	0.55
1:A:146:PHE:O	1:B:256:SER:HB3	2.07	0.55
1:A:1857:ARG:HH11	1:A:1869:PRO:CB	2.19	0.55
1:A:111:VAL:HG22	1:A:188:LEU:HB2	1.88	0.55
1:A:40:TRP:CH2	1:A:194:PRO:HA	2.42	0.55
1:A:297:THR:HB	1:A:300:GLY:N	2.20	0.55
1:B:98:ALA:O	1:B:101:ARG:HG3	2.07	0.55
1:B:23:TRP:CE2	1:B:350:HIS:HD2	2.25	0.55
1:B:82:LEU:HD13	1:B:188:LEU:HD21	1.88	0.55
1:B:1416:LEU:HD23	1:B:1429:LEU:HG	1.88	0.55
1:B:1448:CYS:C	1:B:1450:THR:H	2.11	0.55
1:B:393:PHE:CD1	1:B:399:ASN:HB3	2.42	0.55
1:B:644:ASN:HB2	1:B:648:THR:O	2.06	0.55
1:B:615:VAL:HG22	1:B:686:PHE:CD2	2.42	0.55
1:A:1035:MET:SD	1:A:1091:ALA:HB3	2.47	0.54
1:A:1097:LEU:HD12	1:A:1097:LEU:C	2.27	0.54
1:A:1300:ASP:O	1:A:1302:ALA:N	2.38	0.54
1:A:1476:ASN:HA	1:A:1486:MET:SD	2.47	0.54
1:A:878:HIS:HB2	1:A:1007:PHE:CE1	2.42	0.54
1:B:1570:SER:OG	1:B:1602:GLU:HB3	2.07	0.54
1:B:1917:ARG:NH1	1:B:1974:VAL:HG12	2.23	0.54
1:A:166:LEU:HD23	1:A:166:LEU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1766:PHE:CD2	1:A:1791:PHE:CE1	2.95	0.54
1:B:1223:ALA:HB1	1:B:1224:PRO:HD2	1.89	0.54
1:B:1227:LYS:HE2	1:B:1516:HIS:O	2.07	0.54
1:B:1766:PHE:CD2	1:B:1791:PHE:CE1	2.96	0.54
1:A:1783:ALA:H	1:B:1777:ASN:HD22	1.54	0.54
1:B:40:TRP:CH2	1:B:194:PRO:HA	2.42	0.54
1:B:420:LEU:HD11	1:B:512:ARG:HD2	1.89	0.54
1:A:1115:ILE:CD1	1:A:2111:LEU:HG	2.31	0.54
1:A:278:ALA:CB	1:A:279:PRO:CD	2.84	0.54
1:A:506:MET:HE3	1:A:559:ILE:CD1	2.37	0.54
1:B:917:VAL:CG1	1:B:1054:PHE:HB2	2.37	0.54
1:B:1051:PRO:HA	1:B:1101:SER:HB3	1.90	0.54
1:B:1802:GLU:O	1:B:1804:GLY:N	2.39	0.54
1:B:228:VAL:O	1:B:228:VAL:HG23	2.07	0.54
1:A:1801:GLU:O	1:A:1803:GLY:N	2.41	0.54
1:A:1996:TYR:HD1	1:A:2040:ALA:HB1	1.72	0.54
1:B:1563:LEU:HD12	1:B:1564:CYS:H	1.72	0.54
1:B:1734:ARG:O	1:B:1736:THR:N	2.40	0.54
1:B:293:HIS:O	1:B:326:LYS:HD2	2.06	0.54
1:B:420:LEU:HD11	1:B:512:ARG:CB	2.37	0.54
1:A:1222:ASP:HA	1:A:1226:LEU:CD1	2.38	0.54
1:A:1857:ARG:CG	1:A:1871:ILE:HD11	2.38	0.54
1:A:2101:GLN:HG3	1:A:2102:PRO:CD	2.38	0.54
1:B:1472:VAL:HG13	1:B:1502:VAL:O	2.08	0.54
1:B:1470:ARG:O	1:B:1472:VAL:HG23	2.07	0.54
1:A:1606:ARG:NH2	1:A:1860:GLU:HG3	2.20	0.54
1:A:1698:THR:OG1	1:A:1723:SER:HB3	2.06	0.54
1:A:1973:MET:HB3	1:A:1995:LYS:HE3	1.89	0.54
1:A:215:PHE:HD2	1:A:305:LEU:HD11	1.68	0.54
1:A:940:ALA:HB3	1:B:945:GLU:OE2	2.07	0.54
1:B:1422:SER:HB2	1:B:1424:ARG:HG3	1.90	0.54
1:B:1570:SER:HB3	1:B:1853:VAL:HG22	1.89	0.54
1:A:353:TRP:CZ2	1:A:383:ILE:HD12	2.43	0.54
1:B:1229:CYS:HB3	1:B:1403:LEU:HD22	1.90	0.54
1:B:343:LYS:HG3	1:B:344:VAL:N	2.22	0.54
1:A:1769:ILE:HG22	1:A:1770:GLY:N	2.22	0.54
1:A:1996:TYR:HD2	1:A:1997:SER:N	2.06	0.54
1:A:2019:PHE:CD1	1:A:2060:TRP:NE1	2.76	0.54
1:A:2102:PRO:HD2	1:A:2103:HIS:CD2	2.42	0.54
1:A:359:TYR:OH	1:A:362:PRO:HG3	2.08	0.54
1:A:1003:TYR:CE1	1:A:1037:HIS:HE1	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1446:VAL:HA	1:A:1476:ASN:ND2	2.23	0.54
1:A:1893:LEU:HB3	1:A:1925:GLN:NE2	2.22	0.54
1:A:856:CYS:SG	1:B:856:CYS:CB	2.96	0.54
1:A:851:PRO:CB	1:B:122:ARG:HB3	2.37	0.54
1:A:228:VAL:HG23	1:A:228:VAL:O	2.08	0.54
1:A:295:THR:HG22	1:A:331:HIS:HD2	1.72	0.54
1:B:1656:TYR:CE2	1:B:1687:ILE:HD13	2.43	0.54
1:B:1773:ASP:OD1	1:B:1778:HIS:HD2	1.91	0.54
1:B:96:ASN:ND2	1:B:98:ALA:HB3	2.19	0.54
1:A:1035:MET:HE3	1:A:1089:VAL:CG1	2.38	0.53
1:A:1408:THR:HB	1:A:1439:ARG:HH12	1.72	0.53
1:A:162:SER:OG	1:A:163:SER:N	2.41	0.53
1:A:48:PRO:HD3	1:A:201:MET:HE3	1.89	0.53
1:A:278:ALA:HB3	1:A:279:PRO:CD	2.35	0.53
1:A:502:GLN:HG3	1:A:556:LEU:CD1	2.35	0.53
1:B:1068:LEU:HD12	1:B:1077:ALA:O	2.08	0.53
1:B:123:ASP:HB3	1:B:126:THR:OG1	2.09	0.53
1:B:148:PHE:HB3	1:B:150:PHE:CZ	2.43	0.53
1:B:1538:ARG:NH2	1:B:1585:PRO:HG2	2.21	0.53
1:B:1996:TYR:HD2	1:B:1997:SER:N	2.06	0.53
1:B:642:CYS:HA	1:B:743:VAL:CG2	2.37	0.53
1:A:1275:THR:HG21	1:A:1299:TRP:HB2	1.90	0.53
1:A:1748:LEU:O	1:A:1749:ALA:O	2.26	0.53
1:A:22:PHE:CE2	1:A:26:LEU:HD11	2.43	0.53
1:A:685:TYR:CD1	1:A:686:PHE:N	2.76	0.53
1:B:120:LEU:HD21	1:B:845:PRO:HG3	1.89	0.53
1:B:1394:ARG:HA	1:B:1400:VAL:HG22	1.88	0.53
1:B:254:ASP:O	1:B:255:GLY:O	2.27	0.53
1:B:368:ALA:HA	1:B:371:ASP:HB3	1.90	0.53
1:B:621:ALA:HB2	1:B:662:LEU:HD11	1.90	0.53
1:B:691:ALA:HB3	1:B:692:PRO:HD3	1.91	0.53
1:A:234:THR:CG2	1:A:239:ALA:HB2	2.38	0.53
1:A:351:GLY:C	1:A:383:ILE:HG22	2.28	0.53
1:B:1333:ASN:ND2	1:B:1334:MET:SD	2.82	0.53
1:B:1618:PRO:CD	1:B:1629:LEU:HD11	2.38	0.53
1:B:201:MET:HA	1:B:206:LEU:HB2	1.89	0.53
1:B:586:ALA:O	1:B:589:TYR:HB3	2.07	0.53
1:B:623:VAL:HG12	1:B:624:GLY:N	2.23	0.53
1:B:874:TYR:HB2	1:B:1006:PHE:CD2	2.43	0.53
1:A:945:GLU:OE2	1:B:940:ALA:HB3	2.09	0.53
1:A:1315:LEU:HB3	1:A:1344:LEU:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1394:ARG:HA	1:A:1400:VAL:HG22	1.90	0.53
1:B:1248:LEU:HD21	1:B:1277:ARG:HE	1.74	0.53
1:B:1390:VAL:HG13	1:B:1501:LEU:HD21	1.89	0.53
1:B:2101:GLN:HG3	1:B:2102:PRO:HD2	1.89	0.53
1:B:209:ASP:OD2	1:B:213:ARG:NE	2.42	0.53
1:B:432:GLU:HG3	1:B:433:ALA:N	2.24	0.53
1:A:100:LEU:O	1:A:103:THR:OG1	2.24	0.53
1:A:2006:THR:O	1:A:2010:CYS:HB2	2.08	0.53
1:B:1418:VAL:HG13	1:B:1425:TRP:CH2	2.41	0.53
1:B:301:ASP:HB2	1:B:302:PRO:HD3	1.90	0.53
1:B:159:THR:CG2	1:B:398:SER:HB3	2.39	0.53
1:A:1656:TYR:HD2	1:A:1660:VAL:HG21	1.72	0.53
1:A:234:THR:HG21	1:A:239:ALA:HB2	1.89	0.53
1:A:275:SER:C	1:A:276:LEU:HD23	2.29	0.53
1:A:542:ASP:H	1:A:545:VAL:CG1	2.22	0.53
1:B:972:THR:CG2	1:B:1081:VAL:HG23	2.38	0.53
1:B:495:ILE:CD1	1:B:578:ILE:HB	2.39	0.53
1:A:165:LEU:HD23	1:A:400:VAL:CG2	2.25	0.53
1:A:2103:HIS:HB2	1:A:2106:LEU:HD21	1.90	0.53
1:B:1338:LEU:CD1	1:B:1406:GLN:HG3	2.38	0.53
1:B:963:GLU:HA	1:B:963:GLU:OE1	2.09	0.53
1:A:423:LEU:HD23	1:A:812:PRO:HG3	1.89	0.53
1:A:91:VAL:O	1:A:457:ILE:HD11	2.09	0.53
1:A:963:GLU:O	1:A:965:PRO:HD3	2.09	0.53
1:A:963:GLU:HA	1:A:963:GLU:OE1	2.09	0.53
1:B:1136:LEU:HD21	1:B:1218:SER:HA	1.89	0.53
1:B:1418:VAL:HG12	1:B:1418:VAL:O	2.08	0.53
1:B:1607:ASP:OD1	1:B:1611:ARG:HB3	2.09	0.53
1:B:214:SER:HB3	1:B:327:SER:HB3	1.91	0.53
1:B:963:GLU:O	1:B:965:PRO:HD3	2.08	0.53
1:A:1416:LEU:HD11	1:A:1425:TRP:HB3	1.90	0.53
1:A:254:ASP:O	1:A:255:GLY:O	2.26	0.53
1:A:252:ASN:HD21	1:A:272:LEU:HB2	1.74	0.53
1:A:542:ASP:N	1:A:545:VAL:HG12	2.23	0.53
1:A:887:PRO:HB2	1:A:890:GLY:H	1.73	0.53
1:B:1469:ILE:HG22	1:B:1471:CYS:SG	2.49	0.53
1:A:1252:GLY:CA	1:A:1318:ASN:HD22	2.22	0.53
1:A:1348:THR:HG21	1:A:1378:TRP:HZ2	1.70	0.53
1:A:1640:TRP:CZ2	1:A:1825:PRO:HD3	2.44	0.53
1:B:1413:PRO:HA	1:B:1440:PRO:HB2	1.91	0.53
1:B:1461:ARG:HG3	1:B:1461:ARG:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1669:GLU:O	1:B:1693:CYS:HB3	2.09	0.53
1:B:1734:ARG:C	1:B:1736:THR:H	2.11	0.53
1:B:1554:ALA:CB	1:B:1882:PRO:HB3	2.39	0.53
1:B:765:ALA:HB1	1:B:768:GLN:HG2	1.89	0.53
1:A:856:CYS:SG	1:B:856:CYS:SG	3.06	0.52
1:B:1996:TYR:HD1	1:B:2040:ALA:HB1	1.74	0.52
1:A:98:ALA:O	1:A:101:ARG:HG3	2.08	0.52
1:B:1276:ASP:O	1:B:1298:GLN:HA	2.09	0.52
1:B:1874:THR:HG22	1:B:1874:THR:O	2.09	0.52
1:A:132:MET:HE1	1:B:200:PHE:HE2	1.73	0.52
1:A:1648:VAL:HB	1:A:1649:PRO:HD3	1.91	0.52
1:A:159:THR:CG2	1:A:398:SER:HB3	2.40	0.52
1:A:429:ARG:NH1	1:A:429:ARG:HB3	2.23	0.52
1:A:91:VAL:HG21	1:A:834:ILE:HD13	1.92	0.52
1:B:1121:PHE:HE1	1:B:1512:GLY:C	2.13	0.52
1:B:2019:PHE:CD1	1:B:2060:TRP:NE1	2.78	0.52
1:A:1051:PRO:HA	1:A:1101:SER:HB3	1.90	0.52
1:A:1418:VAL:O	1:A:1418:VAL:HG12	2.09	0.52
1:A:2103:HIS:H	1:A:2103:HIS:CD2	2.27	0.52
1:B:165:LEU:HD22	1:B:392:SER:HB2	1.91	0.52
1:B:219:GLY:O	1:B:298:LYS:HB2	2.09	0.52
1:B:429:ARG:HB3	1:B:429:ARG:HH11	1.73	0.52
1:B:502:GLN:HG3	1:B:556:LEU:CD1	2.37	0.52
1:B:638:ILE:HD11	1:B:657:ALA:O	2.09	0.52
1:B:765:ALA:HB2	1:B:783:PRO:HB3	1.91	0.52
1:A:1252:GLY:HA2	1:A:1318:ASN:HD22	1.73	0.52
1:A:1553:TYR:CD1	1:A:1880:PHE:HB2	2.45	0.52
1:A:166:LEU:HD11	1:B:155:ILE:HD11	1.90	0.52
1:A:39:ARG:NH1	1:A:57:LEU:HD22	2.24	0.52
1:B:1009:LEU:HD13	1:B:1023:GLN:O	2.10	0.52
1:B:1855:GLN:NE2	1:B:1858:GLU:HA	2.24	0.52
1:A:1616:MET:CE	1:A:1650:ILE:HD13	2.40	0.52
1:B:1338:LEU:HG	1:B:1342:GLY:H	1.75	0.52
1:B:166:LEU:O	1:B:166:LEU:HD23	2.09	0.52
1:B:2103:HIS:HB2	1:B:2106:LEU:HD21	1.90	0.52
1:B:275:SER:C	1:B:276:LEU:HD23	2.30	0.52
1:B:506:MET:HB3	1:B:559:ILE:CD1	2.39	0.52
1:B:564:ILE:HD13	1:B:590:ALA:HB2	1.92	0.52
1:A:1221:LEU:HG	1:A:1221:LEU:O	2.10	0.52
1:A:1677:SER:HB2	1:A:1704:LYS:HE2	1.92	0.52
1:A:1917:ARG:NH1	1:A:1974:VAL:HG12	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:PHE:O	1:A:800:VAL:HG23	2.09	0.52
1:B:1973:MET:HB3	1:B:1995:LYS:HE3	1.91	0.52
1:B:2006:THR:CG2	1:B:2048:ARG:HH22	2.22	0.52
1:B:2019:PHE:CE1	1:B:2060:TRP:NE1	2.77	0.52
1:B:808:VAL:HG12	1:B:809:SER:N	2.25	0.52
1:A:1003:TYR:CE2	1:A:1037:HIS:CE1	2.92	0.52
1:A:1007:PHE:CE2	1:A:1030:SER:HA	2.44	0.52
1:A:112:SER:O	1:A:137:ARG:NH2	2.43	0.52
1:A:1736:THR:HG21	1:A:1740:GLY:H	1.71	0.52
1:A:424:LEU:CD2	1:A:441:GLY:HA3	2.40	0.52
1:A:691:ALA:HB3	1:A:692:PRO:HD3	1.91	0.52
1:A:765:ALA:HB1	1:A:768:GLN:HG2	1.92	0.52
1:B:1568:TYR:CZ	1:B:1643:GLU:HG3	2.45	0.52
1:B:1585:PRO:HB3	1:B:1598:MET:HE1	1.92	0.52
1:A:1001:TYR:HB3	1:A:1003:TYR:CD1	2.44	0.52
1:A:993:TYR:CZ	1:A:1008:GLN:HA	2.45	0.52
1:A:1241:LYS:HG3	1:A:1241:LYS:O	2.10	0.52
1:B:100:LEU:O	1:B:103:THR:OG1	2.20	0.52
1:B:1222:ASP:HA	1:B:1226:LEU:HD11	1.92	0.52
1:B:1255:TYR:O	1:B:1292:LEU:HD13	2.10	0.52
1:B:1416:LEU:HD11	1:B:1425:TRP:HB3	1.92	0.52
1:B:1698:THR:OG1	1:B:1723:SER:HB3	2.09	0.52
1:A:1899:GLN:HG2	1:A:2088:ILE:HG21	1.92	0.52
1:B:1748:LEU:O	1:B:1749:ALA:O	2.28	0.52
1:A:1302:ALA:O	1:A:1304:PRO:HD3	2.10	0.51
1:A:1524:PRO:O	1:A:1877:SER:HB2	2.10	0.51
1:A:326:LYS:HE3	1:A:336:SER:HB2	1.91	0.51
1:B:269:GLN:O	1:B:273:ILE:HG13	2.08	0.51
1:B:665:LEU:HD22	1:B:670:VAL:HG21	1.92	0.51
1:A:1422:SER:HB2	1:A:1424:ARG:HG3	1.92	0.51
1:A:831:SER:OG	1:A:832:PRO:HD3	2.10	0.51
1:A:851:PRO:HB2	1:B:122:ARG:HB3	1.90	0.51
1:B:1466:GLY:O	1:B:1469:ILE:HB	2.10	0.51
1:B:1593:LEU:HD23	1:B:1594:THR:HG22	1.92	0.51
1:B:191:LEU:HD22	1:B:224:ARG:CZ	2.40	0.51
1:B:2102:PRO:HD2	1:B:2103:HIS:CD2	2.42	0.51
1:B:399:ASN:ND2	1:B:399:ASN:H	2.07	0.51
1:B:429:ARG:HB3	1:B:429:ARG:NH1	2.26	0.51
1:B:724:GLY:O	1:B:728:ARG:HB2	2.10	0.51
1:B:914:PHE:O	1:B:915:GLU:HG3	2.09	0.51
1:A:1456:MET:HG2	1:A:2036:PHE:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1119:PHE:CE1	1:A:1516:HIS:CE1	2.98	0.51
1:A:130:TYR:HA	1:B:203:LEU:HD21	1.92	0.51
1:B:506:MET:HE1	1:B:555:SER:HB3	1.92	0.51
1:A:1674:HIS:CE1	1:A:1698:THR:HG21	2.45	0.51
1:A:1570:SER:HB3	1:A:1853:VAL:HG22	1.92	0.51
1:A:2101:GLN:HG3	1:A:2102:PRO:HD2	1.93	0.51
1:A:416:GLN:C	1:A:418:ALA:H	2.13	0.51
1:A:765:ALA:HB2	1:A:783:PRO:HB3	1.92	0.51
1:B:1227:LYS:HB2	1:B:1261:LEU:CD2	2.39	0.51
1:B:1275:THR:CG2	1:B:1299:TRP:HB2	2.39	0.51
1:B:2070:LEU:HD11	1:B:2076:ASN:ND2	2.26	0.51
1:B:169:GLN:OE1	1:B:250:GLY:HA2	2.10	0.51
1:A:1289:LEU:HD22	1:A:1294:VAL:CB	2.36	0.51
1:A:1461:ARG:NH1	1:A:1502:VAL:HG22	2.26	0.51
1:A:1662:ARG:NH1	1:A:1662:ARG:CG	2.55	0.51
1:A:605:TRP:O	1:A:606:ARG:C	2.49	0.51
1:A:662:LEU:O	1:A:666:LYS:HG2	2.09	0.51
1:B:1302:ALA:HB3	1:B:1304:PRO:HD3	1.92	0.51
1:B:1460:LEU:HD12	1:B:1463:GLU:OE1	2.11	0.51
1:B:1677:SER:HB2	1:B:1704:LYS:HE2	1.93	0.51
1:B:1746:ASN:ND2	1:B:1753:LEU:HD12	2.25	0.51
1:B:333:GLU:CB	1:B:334:PRO:CD	2.84	0.51
1:B:887:PRO:HB2	1:B:890:GLY:H	1.76	0.51
1:A:1528:THR:HG21	1:A:1530:HIS:O	2.11	0.51
1:A:1763:HIS:HA	1:A:1788:ASN:O	2.10	0.51
1:A:82:LEU:HD13	1:A:188:LEU:HD21	1.91	0.51
1:A:976:VAL:CG2	1:A:977:ASP:H	2.17	0.51
1:A:1526:LYS:HD3	1:A:1552:HIS:NE2	2.25	0.51
1:B:1276:ASP:OD2	1:B:1281:ALA:HB3	2.11	0.51
1:B:1501:LEU:HB2	1:B:1504:ASN:OD1	2.10	0.51
1:B:1544:ILE:HD12	1:B:1837:GLU:HA	1.92	0.51
1:B:81:MET:HG3	1:B:228:VAL:HG11	1.92	0.51
1:A:1639:THR:O	1:A:1640:TRP:HD1	1.93	0.51
1:A:2019:PHE:CE1	1:A:2060:TRP:NE1	2.79	0.51
1:B:1001:TYR:CE2	1:B:1040:ILE:HD13	2.46	0.51
1:B:1418:VAL:HG22	1:B:1425:TRP:CD2	2.45	0.51
1:B:1470:ARG:O	1:B:1470:ARG:CG	2.58	0.51
1:B:1585:PRO:HB3	1:B:1598:MET:CE	2.41	0.51
1:B:183:ALA:O	1:B:232:LEU:HD12	2.11	0.51
1:A:122:ARG:HG3	1:A:123:ASP:H	1.76	0.51
1:A:1411:ASP:HB2	1:A:1440:PRO:CD	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:MET:HE3	1:A:682:PHE:O	2.11	0.51
1:A:941:SER:N	1:B:945:GLU:OE2	2.44	0.51
1:B:111:VAL:HG22	1:B:188:LEU:HB2	1.93	0.51
1:B:2006:THR:O	1:B:2010:CYS:HB2	2.11	0.51
1:B:321:LEU:HD12	1:B:321:LEU:H	1.75	0.51
1:B:625:LEU:HD22	1:B:629:GLU:OE1	2.11	0.51
1:B:982:THR:HG23	1:B:983:ALA:N	2.19	0.51
1:B:1473:LEU:HD21	1:B:1503:MET:CG	2.32	0.51
1:B:416:GLN:C	1:B:418:ALA:H	2.15	0.51
1:A:45:TYR:CE2	1:B:124:PRO:HB2	2.45	0.50
1:A:970:PHE:O	1:A:1067:LYS:HE2	2.10	0.50
1:B:1439:ARG:O	1:B:1470:ARG:HB3	2.11	0.50
1:B:1457:VAL:CG2	1:B:1473:LEU:HD22	2.33	0.50
1:B:1554:ALA:HB2	1:B:1882:PRO:HG3	1.93	0.50
1:B:248:ASN:HD22	1:B:249:ALA:H	1.56	0.50
1:A:1223:ALA:HB1	1:A:1224:PRO:HD2	1.93	0.50
1:A:321:LEU:CD2	1:A:381:LEU:HD13	2.41	0.50
1:B:1560:GLN:HA	1:B:1563:LEU:CB	2.41	0.50
1:B:1651:VAL:HG23	1:B:1851:LYS:NZ	2.26	0.50
1:B:416:GLN:NE2	1:B:422:ARG:HH22	2.09	0.50
1:B:642:CYS:O	1:B:649:VAL:HG13	2.11	0.50
1:B:883:ARG:HE	1:B:1107:ARG:HD3	1.76	0.50
1:A:1314:LEU:HG	1:A:1315:LEU:N	2.25	0.50
1:A:1470:ARG:HD3	1:A:1472:VAL:CG2	2.41	0.50
1:A:1723:SER:C	1:A:1725:ASP:H	2.15	0.50
1:A:1800:PHE:C	1:A:1800:PHE:HD2	2.15	0.50
1:A:1861:GLN:O	1:A:1865:PRO:HG3	2.11	0.50
1:A:165:LEU:HD22	1:A:392:SER:HB2	1.93	0.50
1:B:1674:HIS:HE1	1:B:1756:SER:OG	1.94	0.50
1:B:36:ASP:HB3	1:B:38:ARG:CG	2.40	0.50
1:A:1606:ARG:HH21	1:A:1860:GLU:CG	2.23	0.50
1:B:309:VAL:HG22	1:B:374:LEU:HD11	1.94	0.50
1:B:972:THR:HG22	1:B:1081:VAL:HG21	1.92	0.50
1:A:1422:SER:O	1:A:1423:PHE:HB2	2.11	0.50
1:A:1996:TYR:HD1	1:A:2040:ALA:CB	2.24	0.50
1:A:776:GLU:HB3	1:A:778:SER:OG	2.12	0.50
1:B:1333:ASN:C	1:B:1335:ALA:H	2.14	0.50
1:B:925:LEU:HD22	1:B:931:VAL:HG21	1.94	0.50
1:B:995:ASP:O	1:B:998:LEU:HB2	2.10	0.50
1:A:1038:MET:HE2	1:A:1038:MET:HA	1.92	0.50
1:A:495:ILE:CD1	1:A:578:ILE:HB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ARG:HD2	1:A:59:ARG:N	2.26	0.50
1:B:225:ALA:O	1:B:332:PRO:HA	2.12	0.50
1:B:9:MET:HE1	1:B:342:ILE:HA	1.93	0.50
1:B:579:GLY:O	1:B:715:THR:HG21	2.11	0.50
1:A:1657:TYR:CZ	1:A:1662:ARG:HD2	2.47	0.50
1:A:169:GLN:HE21	1:A:169:GLN:C	2.15	0.50
1:A:191:LEU:HD22	1:A:224:ARG:NH1	2.27	0.50
1:A:256:SER:HB3	1:B:146:PHE:O	2.12	0.50
1:A:269:GLN:O	1:A:273:ILE:HG13	2.11	0.50
1:A:287:LEU:HA	1:A:387:ASN:O	2.12	0.50
1:A:384:ARG:NH1	1:A:384:ARG:HG3	2.17	0.50
1:B:1024:TRP:HB2	1:B:1068:LEU:HD11	1.94	0.50
1:B:420:LEU:HG	1:B:793:LEU:HD21	1.94	0.50
1:A:1064:HIS:HB2	1:A:1093:GLY:HA3	1.94	0.50
1:A:1241:LYS:HA	1:A:1269:ASP:HB3	1.93	0.50
1:A:1800:PHE:C	1:A:1800:PHE:CD2	2.85	0.50
1:A:290:ILE:HD13	1:A:308:ILE:HD13	1.94	0.50
1:A:241:ARG:NH2	1:A:827:THR:O	2.45	0.50
1:A:946:VAL:O	1:A:954:ILE:HB	2.12	0.50
1:A:96:ASN:ND2	1:A:98:ALA:HB3	2.18	0.50
1:B:136:GLN:NE2	1:B:138:ALA:H	2.10	0.50
1:B:1981:GLU:HG3	1:B:1982:ASN:OD1	2.12	0.50
1:B:2001:ASN:O	1:B:2005:VAL:HG23	2.10	0.50
1:B:965:PRO:O	1:B:967:PRO:HD3	2.12	0.50
1:A:1229:CYS:HB3	1:A:1403:LEU:HD22	1.94	0.50
1:A:621:ALA:O	1:A:650:THR:HG23	2.12	0.50
1:B:9:MET:HE2	1:B:342:ILE:HG12	1.94	0.50
1:A:301:ASP:HB2	1:A:302:PRO:HD3	1.94	0.49
1:A:838:HIS:O	1:A:839:SER:C	2.50	0.49
1:B:366:ILE:HD11	1:B:369:LEU:HD11	1.94	0.49
1:B:638:ILE:HG22	1:B:638:ILE:O	2.11	0.49
1:A:1461:ARG:HG3	1:A:1461:ARG:O	2.12	0.49
1:A:2006:THR:CG2	1:A:2048:ARG:HH22	2.25	0.49
1:A:9:MET:HE1	1:A:342:ILE:HA	1.93	0.49
1:A:668:GLU:O	1:A:669:ASP:HB3	2.11	0.49
1:A:734:TYR:CD2	1:A:734:TYR:C	2.86	0.49
1:B:1459:CYS:CB	1:B:2032:ALA:HA	2.43	0.49
1:B:1858:GLU:HG3	1:B:1859:GLU:N	2.26	0.49
1:A:1533:VAL:HG23	1:A:1545:ARG:O	2.12	0.49
1:B:1429:LEU:CD1	1:B:1443:LEU:HD11	2.42	0.49
1:B:295:THR:HG22	1:B:331:HIS:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:LEU:HD13	1:B:406:PRO:HB3	1.94	0.49
1:B:706:LYS:N	1:B:706:LYS:HD2	2.27	0.49
1:B:866:VAL:HG13	1:B:876:VAL:HG22	1.95	0.49
1:A:1130:LEU:HD22	1:A:1133:ASN:ND2	2.28	0.49
1:A:2017:VAL:HG21	1:A:2099:LEU:HD21	1.93	0.49
1:A:554:VAL:O	1:A:558:SER:HB2	2.13	0.49
1:A:853:GLY:O	1:A:854:SER:HB2	2.12	0.49
1:B:1312:ALA:HB1	1:B:1337:THR:O	2.12	0.49
1:B:1423:PHE:O	1:B:1985:PRO:HB3	2.12	0.49
1:B:554:VAL:O	1:B:558:SER:HB2	2.12	0.49
1:B:82:LEU:HG	1:B:144:LEU:CD1	2.42	0.49
1:A:1483:ALA:N	1:A:1484:PRO:HD3	2.27	0.49
1:A:1780:LEU:HD12	1:A:1781:GLY:H	1.78	0.49
1:A:1874:THR:HG22	1:A:1874:THR:O	2.11	0.49
1:B:1328:ALA:HB2	1:B:1381:LEU:HD11	1.94	0.49
1:B:1887:TYR:CD2	1:B:1967:GLY:HA3	2.44	0.49
1:B:527:LEU:HD12	1:B:534:VAL:CG2	2.43	0.49
1:A:595:THR:HG21	1:A:597:GLU:HG2	1.94	0.49
1:B:60:PHE:CD2	1:B:80:ARG:HD3	2.48	0.49
1:A:1345:LEU:O	1:A:1346:LEU:HD23	2.13	0.49
1:A:1390:VAL:HG13	1:A:1501:LEU:CD2	2.42	0.49
1:A:1766:PHE:HD2	1:A:1791:PHE:CE1	2.30	0.49
1:A:309:VAL:HG22	1:A:374:LEU:HD11	1.95	0.49
1:A:416:GLN:NE2	1:A:422:ARG:HH22	2.10	0.49
1:B:1032:LEU:O	1:B:1035:MET:HB2	2.13	0.49
1:B:1106:ARG:O	1:B:1108:PRO:HD3	2.13	0.49
1:B:831:SER:OG	1:B:832:PRO:HD3	2.13	0.49
1:A:1415:PHE:CD2	1:A:1444:MET:HE1	2.48	0.49
1:A:475:GLY:C	1:A:477:ALA:H	2.15	0.49
1:B:1460:LEU:HD11	1:B:1980:LEU:HD13	1.95	0.49
1:B:1882:PRO:HG2	1:B:1885:LYS:HD2	1.95	0.49
1:B:1974:VAL:O	1:B:1974:VAL:HG23	2.13	0.49
1:A:1050:LEU:O	1:A:1101:SER:CB	2.60	0.49
1:A:236:LYS:C	1:A:238:LEU:H	2.16	0.49
1:A:635:PRO:HD3	1:A:661:PHE:CE2	2.48	0.49
1:B:1244:VAL:HB	1:B:1272:TYR:CD1	2.43	0.49
1:B:1532:PHE:CD2	1:B:1549:SER:HA	2.45	0.49
1:B:491:PRO:HD2	1:B:756:ALA:HA	1.95	0.49
1:B:838:HIS:O	1:B:839:SER:C	2.51	0.49
1:B:913:VAL:HG22	1:B:1058:ARG:HG2	1.95	0.49
1:A:1245:VAL:HG13	1:A:1273:THR:CB	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLN:NE2	1:A:138:ALA:H	2.10	0.49
1:A:527:LEU:HD12	1:A:534:VAL:CG2	2.43	0.49
1:B:1430:LYS:HE3	1:B:1981:GLU:CA	2.42	0.49
1:A:156:THR:OG1	1:B:158:ASP:O	2.31	0.49
1:B:1603:PHE:CD2	1:B:1603:PHE:N	2.80	0.49
1:B:305:LEU:O	1:B:309:VAL:HG23	2.13	0.49
1:B:384:ARG:NH1	1:B:384:ARG:CG	2.74	0.49
1:B:717:ILE:HD13	1:B:727:ALA:HB2	1.95	0.49
1:A:1602:GLU:CD	1:A:1650:ILE:HG12	2.34	0.48
1:A:348:LEU:HD13	1:A:406:PRO:HB3	1.95	0.48
1:A:1085:ASN:C	1:A:1086:LEU:HD23	2.33	0.48
1:A:1405:ARG:HH22	1:A:1470:ARG:NH2	2.11	0.48
1:A:1470:ARG:O	1:A:1470:ARG:CG	2.61	0.48
1:A:1541:LEU:HD23	1:A:1541:LEU:N	2.29	0.48
1:A:1528:THR:HG23	1:A:1552:HIS:ND1	2.28	0.48
1:A:1593:LEU:HD23	1:A:1594:THR:HG22	1.95	0.48
1:A:1666:GLN:HG2	1:A:1667:PRO:HD2	1.94	0.48
1:A:359:TYR:OH	1:A:369:LEU:HD22	2.12	0.48
1:A:82:LEU:HG	1:A:144:LEU:CD1	2.44	0.48
1:B:1086:LEU:N	1:B:1086:LEU:HD23	2.27	0.48
1:B:1551:LEU:HD21	1:B:1627:LEU:HD21	1.95	0.48
1:B:1653:THR:HG22	1:B:1810:VAL:CG1	2.40	0.48
1:B:78:GLN:HB3	1:B:188:LEU:HD13	1.95	0.48
1:B:1996:TYR:HD1	1:B:2040:ALA:CB	2.25	0.48
1:B:287:LEU:HA	1:B:387:ASN:O	2.13	0.48
1:A:130:TYR:CA	1:B:203:LEU:HD21	2.43	0.48
1:A:1523:ARG:HH12	1:A:1536:LEU:HD12	1.78	0.48
1:A:1452:GLY:HA2	1:A:2039:SER:HB3	1.96	0.48
1:A:377:VAL:HG13	1:A:381:LEU:CD1	2.44	0.48
1:A:782:ILE:CD1	1:A:803:LEU:HD23	2.43	0.48
1:B:111:VAL:HG23	1:B:188:LEU:HB2	1.94	0.48
1:B:1428:SER:O	1:B:1432:ILE:HG13	2.13	0.48
1:B:1672:LEU:HB3	1:B:1744:VAL:HG22	1.95	0.48
1:B:1899:GLN:HG2	1:B:2088:ILE:HG21	1.94	0.48
1:B:290:ILE:HD13	1:B:308:ILE:HD13	1.96	0.48
1:A:1670:SER:O	1:A:1742:ASP:HB2	2.13	0.48
1:A:2056:LEU:HA	1:A:2104:PRO:O	2.13	0.48
1:B:1083:ASP:O	1:B:1086:LEU:N	2.46	0.48
1:B:191:LEU:HD22	1:B:224:ARG:NH1	2.29	0.48
1:B:236:LYS:HG3	1:B:237:SER:N	2.27	0.48
1:B:39:ARG:NH1	1:B:57:LEU:HD22	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:SER:OG	1:B:582:LEU:N	2.42	0.48
1:A:1024:TRP:HB2	1:A:1068:LEU:HD11	1.96	0.48
1:A:1418:VAL:HG22	1:A:1425:TRP:CD2	2.49	0.48
1:A:1666:GLN:O	1:A:1669:GLU:HB2	2.13	0.48
1:A:469:GLY:HA2	1:A:805:LEU:HD21	1.94	0.48
1:A:902:ALA:HB1	1:A:939:GLU:OE2	2.14	0.48
1:A:913:VAL:HG22	1:A:1058:ARG:HG2	1.95	0.48
1:A:914:PHE:O	1:A:915:GLU:HG3	2.14	0.48
1:B:1001:TYR:HB3	1:B:1003:TYR:CD1	2.48	0.48
1:A:856:CYS:HB3	1:B:856:CYS:SG	2.54	0.48
1:A:1507:ARG:HH22	1:A:2046:GLU:CD	2.16	0.48
1:A:2070:LEU:HD11	1:A:2076:ASN:ND2	2.28	0.48
1:A:215:PHE:O	1:A:363:ASN:HB2	2.14	0.48
1:A:541:THR:HA	1:A:545:VAL:HG11	1.95	0.48
1:A:856:CYS:C	1:A:858:SER:H	2.17	0.48
1:B:133:ILE:HD12	1:B:143:ARG:HH21	1.79	0.48
1:B:782:ILE:CD1	1:B:803:LEU:HD23	2.43	0.48
1:A:1519:LEU:HD12	1:A:1520:GLU:H	1.78	0.48
1:A:183:ALA:O	1:A:232:LEU:HD12	2.14	0.48
1:A:261:VAL:HG22	1:B:146:PHE:CE1	2.48	0.48
1:A:612:GLU:C	1:A:614:ASN:N	2.67	0.48
1:B:2098:PHE:CD2	1:B:2106:LEU:HD12	2.48	0.48
1:B:504:GLN:N	1:B:546:LEU:HD11	2.28	0.48
1:B:988:SER:O	1:B:991:ASP:N	2.47	0.48
1:A:1432:ILE:HG22	1:A:1432:ILE:O	2.14	0.48
1:A:225:ALA:O	1:A:332:PRO:HA	2.13	0.48
1:A:475:GLY:O	1:A:477:ALA:N	2.45	0.48
1:A:861:VAL:HG22	1:A:934:GLU:CB	2.39	0.48
1:B:1302:ALA:HB3	1:B:1304:PRO:CD	2.44	0.48
1:B:1442:TRP:CZ3	1:B:1472:VAL:HG11	2.48	0.48
1:B:1898:LEU:HA	1:B:1898:LEU:HD23	1.70	0.48
1:A:1457:VAL:HG11	1:A:1473:LEU:HD22	1.96	0.48
1:A:564:ILE:HD13	1:A:590:ALA:HB2	1.95	0.48
1:A:612:GLU:C	1:A:614:ASN:H	2.16	0.48
1:B:1882:PRO:HD2	1:B:1887:TYR:OH	2.13	0.48
1:B:321:LEU:HD12	1:B:321:LEU:N	2.28	0.48
1:B:638:ILE:HD11	1:B:657:ALA:C	2.34	0.48
1:B:902:ALA:HB1	1:B:939:GLU:OE2	2.13	0.48
1:A:1016:GLU:HA	1:A:1043:PRO:HG3	1.96	0.48
1:A:1106:ARG:O	1:A:1108:PRO:HD3	2.13	0.48
1:A:1315:LEU:HB3	1:A:1344:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1536:LEU:HB2	1:A:1543:SER:HB3	1.95	0.48
1:A:1567:TYR:HA	1:A:1857:ARG:HB2	1.96	0.48
1:A:423:LEU:HB2	1:A:797:LEU:HD22	1.96	0.48
1:A:431:LEU:HD23	1:A:431:LEU:C	2.34	0.48
1:A:506:MET:HB3	1:A:559:ILE:CD1	2.44	0.48
1:A:642:CYS:CB	1:A:650:THR:HB	2.29	0.48
1:B:1038:MET:HE2	1:B:1038:MET:HA	1.96	0.48
1:B:1248:LEU:HD21	1:B:1277:ARG:HH21	1.79	0.48
1:B:1124:HIS:CD2	1:B:1512:GLY:HA2	2.48	0.48
1:B:1554:ALA:HB3	1:B:1882:PRO:HB3	1.96	0.48
1:B:1912:LEU:HB2	1:B:1939:VAL:HG22	1.96	0.48
1:B:81:MET:O	1:B:85:VAL:HG22	2.14	0.48
1:B:1995:LYS:HB3	1:B:2041:MET:SD	2.54	0.47
1:B:639:VAL:HG12	1:B:640:PRO:O	2.14	0.47
1:A:1476:ASN:O	1:A:1477:LEU:HD23	2.14	0.47
1:A:1647:SER:O	1:A:1651:VAL:CG2	2.61	0.47
1:A:1729:GLU:OE1	1:A:1758:ARG:HD2	2.14	0.47
1:A:1886:SER:HA	1:A:1911:LYS:HB2	1.95	0.47
1:B:1236:ASN:HA	1:B:1502:VAL:HG21	1.95	0.47
1:B:1554:ALA:C	1:B:1556:PRO:HD3	2.34	0.47
1:B:621:ALA:O	1:B:623:VAL:HG23	2.14	0.47
1:B:259:GLN:CD	1:B:259:GLN:H	2.18	0.47
1:A:1123:PRO:HB3	1:A:1510:ALA:HB1	1.95	0.47
1:A:499:MET:HE2	1:A:582:LEU:HD22	1.95	0.47
1:B:1656:TYR:CZ	1:B:1687:ILE:HD13	2.49	0.47
1:B:1800:PHE:CD2	1:B:1800:PHE:C	2.88	0.47
1:A:1556:PRO:O	1:A:1558:SER:N	2.47	0.47
1:A:1912:LEU:HB2	1:A:1939:VAL:HG22	1.95	0.47
1:A:2098:PHE:CD2	1:A:2106:LEU:HB2	2.48	0.47
1:B:1723:SER:C	1:B:1725:ASP:H	2.18	0.47
1:B:1800:PHE:HD2	1:B:1800:PHE:C	2.17	0.47
1:B:51:MET:HB2	1:B:53:LYS:HE3	1.95	0.47
1:B:557:THR:HG21	1:B:603:SER:OG	2.14	0.47
1:A:856:CYS:CB	1:B:856:CYS:HG	2.27	0.47
1:A:1544:ILE:O	1:A:1545:ARG:HG3	2.15	0.47
1:A:262:THR:O	1:A:262:THR:CG2	2.63	0.47
1:B:1486:MET:SD	1:B:1506:TYR:CD1	3.08	0.47
1:B:1983:GLN:HG2	1:B:1988:PHE:HE1	1.78	0.47
1:B:2022:VAL:CG1	1:B:2022:VAL:O	2.62	0.47
1:B:326:LYS:CE	1:B:336:SER:HB2	2.44	0.47
1:B:321:LEU:HD23	1:B:381:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:GLN:NE2	1:B:525:GLN:HA	2.30	0.47
1:B:972:THR:HG22	1:B:1081:VAL:HG23	1.97	0.47
1:B:982:THR:C	1:B:984:GLU:N	2.68	0.47
1:A:2001:ASN:O	1:A:2005:VAL:HG23	2.14	0.47
1:A:432:GLU:HG3	1:A:433:ALA:N	2.29	0.47
1:B:1003:TYR:CE2	1:B:1037:HIS:CE1	2.92	0.47
1:B:1050:LEU:O	1:B:1101:SER:CB	2.63	0.47
1:A:1774:LEU:O	1:B:1783:ALA:HB2	2.14	0.47
1:B:1981:GLU:C	1:B:1983:GLN:H	2.18	0.47
1:B:359:TYR:CD2	1:B:376:VAL:HG11	2.50	0.47
1:B:685:TYR:CD1	1:B:686:PHE:N	2.83	0.47
1:A:107:VAL:HG13	1:A:184:VAL:HB	1.96	0.47
1:A:111:VAL:HG23	1:A:188:LEU:HB2	1.97	0.47
1:A:503:TRP:CG	1:A:787:LYS:HB2	2.50	0.47
1:B:1418:VAL:HG22	1:B:1425:TRP:CG	2.50	0.47
1:B:2006:THR:HG21	1:B:2048:ARG:NH2	2.29	0.47
1:B:2017:VAL:HG21	1:B:2099:LEU:HD21	1.97	0.47
1:B:48:PRO:HD3	1:B:201:MET:HE3	1.97	0.47
1:A:1592:TRP:HB2	1:A:1595:ARG:HD3	1.97	0.47
1:A:618:GLY:N	1:A:679:GLY:O	2.47	0.47
1:A:838:HIS:O	1:A:840:GLN:N	2.48	0.47
1:B:128:VAL:CG1	1:B:130:TYR:CZ	2.98	0.47
1:B:59:ARG:N	1:B:59:ARG:HD2	2.29	0.47
1:B:670:VAL:HG12	1:B:671:PHE:H	1.79	0.47
1:B:796:PHE:O	1:B:800:VAL:HG23	2.14	0.47
1:A:1107:ARG:HG3	1:A:1107:ARG:O	2.15	0.47
1:A:1416:LEU:HD23	1:A:1429:LEU:HG	1.96	0.47
1:A:1636:VAL:HA	1:A:1637:PRO:HD3	1.73	0.47
1:A:1669:GLU:HG2	1:A:1742:ASP:CB	2.45	0.47
1:A:1794:ILE:C	1:A:1795:LEU:HD23	2.35	0.47
1:A:1711:ARG:HH22	1:A:1826:LEU:CD2	2.28	0.47
1:B:1236:ASN:CG	1:B:1502:VAL:HG23	2.36	0.47
1:B:1239:SER:C	1:B:1241:LYS:H	2.18	0.47
1:B:1411:ASP:HB2	1:B:1440:PRO:HG3	1.95	0.47
1:A:261:VAL:HG22	1:B:146:PHE:CZ	2.50	0.47
1:B:1656:TYR:CD2	1:B:1813:LEU:HB3	2.49	0.47
1:B:1685:ILE:HG22	1:B:1686:ALA:N	2.30	0.47
1:B:1725:ASP:OD2	1:B:1727:SER:HB3	2.15	0.47
1:B:1733:LEU:HA	1:B:1733:LEU:HD23	1.70	0.47
1:B:1894:GLY:O	1:B:1895:GLY:C	2.54	0.47
1:B:610:ILE:HA	1:B:690:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:LEU:HD11	1:A:1221:LEU:CD1	2.44	0.47
1:A:1248:LEU:HD21	1:A:1277:ARG:NH2	2.30	0.47
1:A:1553:TYR:O	1:A:1554:ALA:HB2	2.15	0.47
1:A:1748:LEU:HD23	1:A:1748:LEU:HA	1.69	0.47
1:A:866:VAL:HG13	1:A:876:VAL:HG22	1.97	0.47
1:A:976:VAL:HG22	1:A:977:ASP:N	2.18	0.47
1:B:1129:CYS:O	1:B:1130:LEU:HB2	2.14	0.47
1:B:1239:SER:OG	1:B:1241:LYS:HG2	2.15	0.47
1:B:1303:ASN:HA	1:B:1333:ASN:HB2	1.96	0.47
1:B:1443:LEU:O	1:B:1473:LEU:HA	2.15	0.47
1:B:1729:GLU:OE1	1:B:1758:ARG:HD2	2.15	0.47
1:B:983:ALA:O	1:B:985:PHE:N	2.43	0.47
1:A:1460:LEU:HD12	1:A:1463:GLU:OE1	2.15	0.46
1:A:2098:PHE:CD2	1:A:2106:LEU:HD12	2.50	0.46
1:A:65:PHE:CE2	1:A:83:LEU:HB3	2.49	0.46
1:B:1275:THR:HG21	1:B:1299:TRP:HB2	1.96	0.46
1:B:1390:VAL:HG13	1:B:1501:LEU:CD2	2.45	0.46
1:B:1415:PHE:HD2	1:B:1444:MET:HE1	1.79	0.46
1:B:776:GLU:HB3	1:B:778:SER:OG	2.15	0.46
1:A:111:VAL:HG21	1:A:188:LEU:HD12	1.98	0.46
1:A:92:ASP:HA	1:A:830:ILE:HB	1.97	0.46
1:A:118:GLU:CD	1:B:118:GLU:HG3	2.34	0.46
1:B:112:SER:O	1:B:137:ARG:NH2	2.48	0.46
1:B:1411:ASP:HB2	1:B:1440:PRO:CG	2.44	0.46
1:B:1794:ILE:C	1:B:1795:LEU:HD23	2.36	0.46
1:B:2031:GLN:HB3	1:B:2034:TYR:HB3	1.98	0.46
1:B:668:GLU:O	1:B:669:ASP:CB	2.62	0.46
1:A:1234:LEU:HD12	1:A:1234:LEU:O	2.16	0.46
1:A:1480:THR:HB	1:A:1482:PRO:HD2	1.97	0.46
1:A:1573:PHE:O	1:A:1576:VAL:HB	2.15	0.46
1:A:1999:THR:HG22	1:A:2044:ILE:HD12	1.98	0.46
1:A:269:GLN:OE1	1:A:393:PHE:CE2	2.68	0.46
1:A:249:ALA:HB2	1:A:402:VAL:HB	1.97	0.46
1:A:483:GLN:HG2	1:A:484:GLN:N	2.30	0.46
1:A:831:SER:N	1:A:832:PRO:CD	2.79	0.46
1:B:1616:MET:CE	1:B:1650:ILE:HD13	2.46	0.46
1:B:39:ARG:NH1	1:B:226:GLU:OE2	2.47	0.46
1:B:384:ARG:NH1	1:B:384:ARG:HG3	2.16	0.46
1:B:577:ILE:HG22	1:B:712:TRP:CD1	2.50	0.46
1:A:1226:LEU:CD2	1:A:1401:LEU:HD21	2.43	0.46
1:A:60:PHE:CD2	1:A:80:ARG:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1119:PHE:HB3	1:B:2105:VAL:HB	1.98	0.46
1:B:743:VAL:O	1:B:743:VAL:HG23	2.15	0.46
1:A:1231:ASP:O	1:A:1234:LEU:N	2.47	0.46
1:A:1414:VAL:HG11	1:A:1432:ILE:HD13	1.96	0.46
1:A:1556:PRO:O	1:A:1557:ALA:C	2.53	0.46
1:A:2098:PHE:CE2	1:A:2106:LEU:CB	2.98	0.46
1:A:749:LEU:HD11	1:A:771:LEU:HD23	1.96	0.46
1:A:925:LEU:HD22	1:A:931:VAL:HG21	1.97	0.46
1:B:1016:GLU:HA	1:B:1043:PRO:HG3	1.96	0.46
1:B:1220:LEU:HB3	1:B:1257:ARG:NH2	2.30	0.46
1:B:1786:LEU:C	1:B:1788:ASN:H	2.18	0.46
1:B:2098:PHE:CE2	1:B:2106:LEU:CB	2.98	0.46
1:B:359:TYR:CG	1:B:376:VAL:HG11	2.50	0.46
1:B:65:PHE:HA	1:B:147:PHE:CE1	2.50	0.46
1:A:1262:LEU:HB3	1:A:1268:MET:SD	2.56	0.46
1:A:1602:GLU:OE2	1:A:1650:ILE:N	2.49	0.46
1:A:416:GLN:C	1:A:418:ALA:N	2.69	0.46
1:B:107:VAL:HG13	1:B:184:VAL:HB	1.96	0.46
1:B:1443:LEU:HA	1:B:1443:LEU:HD23	1.78	0.46
1:B:1586:ASP:HA	1:B:1595:ARG:HH12	1.81	0.46
1:B:765:ALA:HB1	1:B:768:GLN:CG	2.46	0.46
1:A:1220:LEU:HB3	1:A:1257:ARG:NH2	2.31	0.46
1:A:1418:VAL:HG22	1:A:1425:TRP:CG	2.51	0.46
1:A:717:ILE:HD13	1:A:727:ALA:HB2	1.97	0.46
1:B:1254:LEU:HD13	1:B:1316:VAL:HG12	1.98	0.46
1:A:200:PHE:HE2	1:B:132:MET:HE1	1.80	0.46
1:B:1338:LEU:CD2	1:B:1406:GLN:HG3	2.46	0.46
1:B:1531:ALA:HA	1:B:1549:SER:H	1.81	0.46
1:B:1617:VAL:HG21	1:B:1626:VAL:CG1	2.46	0.46
1:B:1995:LYS:O	1:B:2041:MET:HE3	2.15	0.46
1:B:377:VAL:HG13	1:B:381:LEU:CD1	2.46	0.46
1:A:1415:PHE:HD2	1:A:1444:MET:HE1	1.81	0.46
1:A:1532:PHE:HE1	1:A:1597:CYS:HB3	1.81	0.46
1:A:1676:GLY:HA2	1:A:1681:GLY:HA3	1.98	0.46
1:A:1689:LEU:O	1:A:1692:GLY:HA2	2.16	0.46
1:A:1725:ASP:OD2	1:A:1727:SER:HB3	2.15	0.46
1:B:1239:SER:HA	1:B:1240:PRO:HD3	1.85	0.46
1:B:1651:VAL:HG13	1:B:1680:VAL:CA	2.31	0.46
1:B:166:LEU:HD23	1:B:166:LEU:C	2.36	0.46
1:B:657:ALA:O	1:B:661:PHE:HB2	2.16	0.46
1:A:856:CYS:HB3	1:B:856:CYS:HG	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1222:ASP:HA	1:A:1226:LEU:HD11	1.96	0.46
1:A:1347:HIS:HD2	1:A:1348:THR:O	1.99	0.46
1:A:1472:VAL:CG1	1:A:1473:LEU:H	2.25	0.46
1:A:1528:THR:CG2	1:A:1530:HIS:H	2.22	0.46
1:A:627:TRP:CZ3	1:A:640:PRO:HB2	2.50	0.46
1:A:706:LYS:HD2	1:A:706:LYS:N	2.31	0.46
1:B:1469:ILE:CG2	1:B:1469:ILE:O	2.64	0.46
1:A:1345:LEU:HD12	1:A:1402:PHE:O	2.16	0.46
1:A:1481:SER:N	1:A:1482:PRO:CD	2.79	0.46
1:A:203:LEU:HD21	1:B:130:TYR:HA	1.98	0.46
1:A:9:MET:HE2	1:A:342:ILE:HG12	1.97	0.46
1:B:81:MET:HG2	1:B:81:MET:H	1.62	0.46
1:A:1257:ARG:O	1:A:1260:ALA:HB3	2.17	0.45
1:A:2070:LEU:HD11	1:A:2076:ASN:CG	2.36	0.45
1:A:2084:LEU:HD12	1:A:2111:LEU:O	2.15	0.45
1:A:33:VAL:HB	1:A:50:ARG:NH1	2.32	0.45
1:A:491:PRO:HD2	1:A:756:ALA:HA	1.97	0.45
1:A:965:PRO:O	1:A:967:PRO:HD3	2.16	0.45
1:B:1338:LEU:HD22	1:B:1406:GLN:NE2	2.31	0.45
1:B:1432:ILE:O	1:B:1432:ILE:HG22	2.16	0.45
1:B:1931:GLU:O	1:B:1933:ARG:N	2.50	0.45
1:B:420:LEU:CD1	1:B:512:ARG:HD2	2.46	0.45
1:B:431:LEU:C	1:B:431:LEU:HD23	2.36	0.45
1:B:976:VAL:O	1:B:977:ASP:C	2.54	0.45
1:B:988:SER:O	1:B:989:GLN:C	2.54	0.45
1:A:1419:GLU:OE2	1:A:1447:GLY:HA3	2.15	0.45
1:A:1390:VAL:HG13	1:A:1501:LEU:HD21	1.98	0.45
1:A:65:PHE:HA	1:A:147:PHE:CE1	2.51	0.45
1:A:72:ALA:HB3	1:A:842:TRP:CZ3	2.51	0.45
1:A:856:CYS:O	1:A:858:SER:N	2.46	0.45
1:B:1064:HIS:HB2	1:B:1093:GLY:HA3	1.97	0.45
1:B:1420:ASP:O	1:B:1425:TRP:CH2	2.70	0.45
1:B:1603:PHE:HD2	1:B:1603:PHE:N	2.15	0.45
1:B:1754:GLN:OE1	1:B:1754:GLN:HA	2.16	0.45
1:B:1886:SER:HA	1:B:1911:LYS:HB2	1.97	0.45
1:B:236:LYS:C	1:B:238:LEU:H	2.20	0.45
1:B:269:GLN:OE1	1:B:393:PHE:CE2	2.69	0.45
1:B:460:VAL:CG2	1:B:465:MET:HG3	2.46	0.45
1:B:501:ALA:HA	1:B:766:LEU:HD11	1.98	0.45
1:A:1428:SER:O	1:A:1432:ILE:HG13	2.15	0.45
1:A:133:ILE:HD12	1:A:143:ARG:HH21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1476:ASN:HB3	1:A:1486:MET:SD	2.56	0.45
1:A:1953:ARG:O	1:A:1957:THR:HB	2.16	0.45
1:A:1112:LEU:HD22	1:A:2110:VAL:HG11	1.98	0.45
1:A:23:TRP:NE1	1:A:350:HIS:CD2	2.84	0.45
1:B:1418:VAL:HA	1:B:1425:TRP:CE3	2.51	0.45
1:B:1527:GLN:OE1	1:B:1872:ALA:HB1	2.15	0.45
1:A:142:ASN:HD22	1:B:396:GLY:HA3	1.81	0.45
1:B:635:PRO:O	1:B:637:GLY:N	2.50	0.45
1:B:979:ALA:HB1	1:B:983:ALA:HB3	1.98	0.45
1:A:1254:LEU:HD21	1:A:1318:ASN:HB2	1.98	0.45
1:A:1466:GLY:O	1:A:1469:ILE:HB	2.17	0.45
1:A:1124:HIS:NE2	1:A:1501:LEU:HD13	2.31	0.45
1:A:1624:THR:HG22	1:A:1857:ARG:HH21	1.82	0.45
1:A:1857:ARG:NH1	1:A:1869:PRO:HB3	2.30	0.45
1:A:557:THR:HG21	1:A:603:SER:OG	2.16	0.45
1:B:1095:LEU:HD12	1:B:1095:LEU:O	2.16	0.45
1:B:1456:MET:HE3	1:B:2032:ALA:O	2.16	0.45
1:B:1977:ASP:OD1	1:B:2031:GLN:HG2	2.15	0.45
1:B:65:PHE:CE2	1:B:83:LEU:HB3	2.51	0.45
1:A:1780:LEU:HD12	1:A:1781:GLY:N	2.32	0.45
1:A:1802:GLU:O	1:A:1802:GLU:HG2	2.17	0.45
1:A:618:GLY:O	1:A:679:GLY:O	2.34	0.45
1:A:963:GLU:C	1:A:965:PRO:HD3	2.37	0.45
1:B:1107:ARG:O	1:B:1107:ARG:HG3	2.17	0.45
1:B:159:THR:HB	1:B:162:SER:HG	1.81	0.45
1:B:1748:LEU:HD23	1:B:1748:LEU:HA	1.66	0.45
1:B:1953:ARG:HA	1:B:2005:VAL:HG11	1.98	0.45
1:B:1953:ARG:O	1:B:1957:THR:HB	2.16	0.45
1:B:1456:MET:CE	1:B:2032:ALA:HB1	2.46	0.45
1:B:623:VAL:HG13	1:B:672:VAL:HG22	1.97	0.45
1:A:1545:ARG:CG	1:A:1545:ARG:NH1	2.76	0.45
1:A:1629:LEU:O	1:A:1630:GLN:C	2.55	0.45
1:A:1694:ARG:NH2	1:A:1735:HIS:HB3	2.31	0.45
1:A:2022:VAL:CG1	1:A:2022:VAL:O	2.64	0.45
1:A:493:TRP:CD2	1:A:752:VAL:HG22	2.52	0.45
1:B:1248:LEU:CD2	1:B:1277:ARG:HE	2.30	0.45
1:B:1629:LEU:HB3	1:B:1631:HIS:CE1	2.51	0.45
1:B:1904:LEU:HA	1:B:1904:LEU:HD23	1.62	0.45
1:B:1931:GLU:O	1:B:1934:ARG:N	2.50	0.45
1:A:1231:ASP:O	1:A:1232:THR:C	2.55	0.45
1:A:1235:GLU:OE2	1:A:1515:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1786:LEU:HD23	1:A:1786:LEU:HA	1.73	0.45
1:A:1882:PRO:HD2	1:A:1887:TYR:OH	2.17	0.45
1:B:1541:LEU:HD13	1:B:1840:PHE:HB3	1.97	0.45
1:B:169:GLN:C	1:B:169:GLN:HE21	2.19	0.45
1:B:2098:PHE:CD2	1:B:2106:LEU:HB2	2.51	0.45
1:A:124:PRO:HB2	1:B:45:TYR:CE2	2.52	0.45
1:B:838:HIS:O	1:B:840:GLN:N	2.50	0.45
1:A:1095:LEU:HD12	1:A:1095:LEU:O	2.17	0.45
1:A:1599:LEU:O	1:A:1622:LEU:HD12	2.16	0.45
1:A:191:LEU:HD22	1:A:224:ARG:CZ	2.47	0.45
1:A:548:ASP:OD2	1:A:611:LYS:NZ	2.50	0.45
1:A:724:GLY:O	1:A:728:ARG:HB2	2.16	0.45
1:A:752:VAL:HA	1:A:753:PRO:HD3	1.87	0.45
1:A:995:ASP:O	1:A:998:LEU:HB2	2.16	0.45
1:B:1137:GLN:HG2	1:B:1396:PHE:CZ	2.52	0.45
1:B:1481:SER:N	1:B:1482:PRO:CD	2.80	0.45
1:B:1973:MET:CB	1:B:1995:LYS:HE3	2.46	0.45
1:B:2056:LEU:HA	1:B:2104:PRO:O	2.16	0.45
1:B:258:GLU:HB2	1:B:259:GLN:NE2	2.32	0.45
1:B:475:GLY:C	1:B:477:ALA:H	2.20	0.45
1:B:734:TYR:C	1:B:734:TYR:CD2	2.89	0.45
1:B:98:ALA:HA	1:B:101:ARG:CG	2.46	0.45
1:A:1001:TYR:CE2	1:A:1040:ILE:HD13	2.52	0.45
1:A:1259:PRO:HG2	1:A:1292:LEU:HD22	1.99	0.45
1:A:1248:LEU:HD21	1:A:1277:ARG:NE	2.30	0.45
1:A:1757:VAL:O	1:A:1760:LEU:HB2	2.17	0.45
1:A:1818:ILE:HG12	1:A:1823:VAL:CG1	2.46	0.45
1:B:1890:THR:O	1:B:1971:LEU:HB2	2.17	0.45
1:A:1474:VAL:HA	1:A:1504:ASN:O	2.17	0.45
1:A:1931:GLU:O	1:A:1934:ARG:N	2.50	0.45
1:A:2064:GLY:O	1:A:2066:VAL:N	2.50	0.45
1:A:217:ALA:HB2	1:A:363:ASN:HA	1.99	0.45
1:A:895:THR:HA	1:A:935:VAL:HG11	1.99	0.45
1:B:1343:PHE:HE2	1:B:1390:VAL:HG21	1.82	0.45
1:B:1123:PRO:O	1:B:1393:LYS:NZ	2.50	0.45
1:B:1449:SER:C	1:B:1477:LEU:HD22	2.37	0.45
1:B:1689:LEU:HD23	1:B:1689:LEU:HA	1.70	0.45
1:B:1567:TYR:O	1:B:1856:VAL:HG23	2.16	0.45
1:B:2036:PHE:CD2	1:B:2036:PHE:C	2.91	0.45
1:B:699:ARG:O	1:B:703:LEU:HD23	2.17	0.45
1:A:75:MET:SD	1:A:79:LEU:HD23	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:THR:CG2	1:B:104:SER:N	2.80	0.44
1:B:1541:LEU:O	1:B:1837:GLU:HG3	2.17	0.44
1:B:159:THR:HG22	1:B:398:SER:HB3	1.99	0.44
1:B:1567:TYR:CE1	1:B:1606:ARG:HG3	2.52	0.44
1:B:1678:GLY:O	1:B:1682:GLN:HG3	2.16	0.44
1:B:581:SER:HB2	1:B:683:HIS:NE2	2.32	0.44
1:A:1065:ARG:HD3	1:A:1065:ARG:HA	1.82	0.44
1:A:1262:LEU:O	1:A:1268:MET:HG3	2.17	0.44
1:A:1449:SER:O	1:A:1477:LEU:HD22	2.17	0.44
1:A:1473:LEU:HG	1:A:1503:MET:HA	2.00	0.44
1:A:158:ASP:O	1:B:156:THR:OG1	2.34	0.44
1:A:1781:GLY:O	1:A:1784:VAL:HG23	2.17	0.44
1:A:1971:LEU:HD21	1:A:2019:PHE:CD2	2.53	0.44
1:A:326:LYS:CE	1:A:336:SER:HB2	2.47	0.44
1:A:595:THR:HG22	1:A:597:GLU:HG2	1.98	0.44
1:A:627:TRP:CH2	1:A:640:PRO:HB2	2.52	0.44
1:A:620:MET:HE1	1:A:682:PHE:HB2	1.99	0.44
1:B:111:VAL:O	1:B:111:VAL:HG12	2.17	0.44
1:B:1251:ASP:O	1:B:1253:GLN:HG3	2.17	0.44
1:B:1442:TRP:CH2	1:B:1497:LEU:HD23	2.52	0.44
1:B:108:TRP:CD1	1:B:171:ALA:HB2	2.52	0.44
1:B:581:SER:HB2	1:B:683:HIS:CE1	2.52	0.44
1:B:647:ASP:OD1	1:B:647:ASP:N	2.50	0.44
1:A:118:GLU:HG3	1:B:118:GLU:CD	2.37	0.44
1:A:1617:VAL:HG12	1:A:1619:ALA:H	1.82	0.44
1:A:2043:ARG:HD3	1:A:2043:ARG:HA	1.69	0.44
1:A:2015:TYR:HD2	1:A:2099:LEU:HD22	1.78	0.44
1:A:643:HIS:HA	1:A:649:VAL:HG22	1.99	0.44
1:B:1245:VAL:O	1:B:1315:LEU:HD12	2.16	0.44
1:B:1818:ILE:HG12	1:B:1823:VAL:CG1	2.48	0.44
1:B:1893:LEU:HB3	1:B:1925:GLN:CD	2.38	0.44
1:B:2111:LEU:HA	1:B:2111:LEU:HD23	1.83	0.44
1:B:321:LEU:H	1:B:321:LEU:CD1	2.31	0.44
1:A:1250:GLY:N	1:A:1276:ASP:OD2	2.50	0.44
1:A:1476:ASN:HA	1:A:1486:MET:CE	2.47	0.44
1:A:166:LEU:C	1:A:166:LEU:HD23	2.38	0.44
1:A:409:ARG:HA	1:A:410:PRO:HD3	1.73	0.44
1:A:850:PHE:HB3	1:A:851:PRO:HD2	2.00	0.44
1:B:1567:TYR:C	1:B:1856:VAL:HG23	2.37	0.44
1:B:831:SER:N	1:B:832:PRO:CD	2.80	0.44
1:A:1112:LEU:O	1:A:1114:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1456:MET:CG	1:A:2036:PHE:HB2	2.46	0.44
1:A:305:LEU:O	1:A:309:VAL:HG23	2.17	0.44
1:B:13:LEU:HD13	1:B:22:PHE:CD1	2.53	0.44
1:B:189:ASN:HB2	1:B:334:PRO:HD2	1.98	0.44
1:B:605:TRP:O	1:B:606:ARG:C	2.56	0.44
1:B:62:ALA:HB1	1:B:67:VAL:HG23	2.00	0.44
1:B:907:LEU:HA	1:B:907:LEU:HD12	1.87	0.44
1:A:1487:HIS:O	1:A:1487:HIS:CD2	2.71	0.44
1:A:1487:HIS:HA	1:A:1488:PRO:HD3	1.80	0.44
1:A:1515:ARG:HD3	1:A:1515:ARG:HA	1.55	0.44
1:A:1571:LEU:O	1:A:1851:LYS:HD2	2.17	0.44
1:A:1995:LYS:O	1:A:2041:MET:HE3	2.17	0.44
1:A:6:ILE:HG21	1:A:345:LEU:HD11	2.00	0.44
1:A:815:LEU:HB2	1:A:816:PHE:CD1	2.53	0.44
1:A:81:MET:O	1:A:85:VAL:HG22	2.18	0.44
1:B:1445:ALA:O	1:B:1476:ASN:ND2	2.51	0.44
1:B:1768:GLU:CA	1:B:1768:GLU:OE1	2.64	0.44
1:B:1986:GLU:HA	1:B:1989:GLN:HG2	2.00	0.44
1:B:2070:LEU:HD11	1:B:2076:ASN:CG	2.37	0.44
1:B:2103:HIS:HA	1:B:2104:PRO:HD3	1.78	0.44
1:B:582:LEU:O	1:B:585:VAL:HG23	2.18	0.44
1:B:9:MET:CE	1:B:342:ILE:HA	2.48	0.44
1:A:1052:THR:HG22	1:A:1053:ARG:HG3	1.98	0.44
1:A:1249:ALA:N	1:A:1276:ASP:OD1	2.40	0.44
1:A:1290:GLU:HG2	1:A:1291:GLN:N	2.33	0.44
1:A:1973:MET:CB	1:A:1995:LYS:HE3	2.47	0.44
1:A:2036:PHE:C	1:A:2036:PHE:CD2	2.90	0.44
1:A:2066:VAL:HG22	1:A:2088:ILE:HD12	2.00	0.44
1:A:213:ARG:HG3	1:A:213:ARG:HH11	1.81	0.44
1:A:309:VAL:HG13	1:A:313:CYS:SG	2.58	0.44
1:A:309:VAL:C	1:A:311:ALA:H	2.21	0.44
1:B:1221:LEU:O	1:B:1221:LEU:HG	2.18	0.44
1:B:1766:PHE:HD2	1:B:1791:PHE:CE1	2.36	0.44
1:B:1993:LYS:N	1:B:1994:PRO:CD	2.81	0.44
1:B:353:TRP:CZ2	1:B:383:ILE:HD12	2.53	0.44
1:B:963:GLU:C	1:B:965:PRO:HD3	2.38	0.44
1:A:1657:TYR:CE1	1:A:1799:LEU:HD11	2.53	0.44
1:A:190:VAL:HG12	1:A:192:LEU:HG	2.00	0.44
1:A:359:TYR:CG	1:A:376:VAL:HG11	2.53	0.44
1:A:587:CYS:O	1:A:591:ASP:N	2.50	0.44
1:B:1416:LEU:CD2	1:B:1429:LEU:HG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1475:SER:HB3	1:B:1505:VAL:CG1	2.47	0.44
1:B:19:LEU:HA	1:B:19:LEU:HD23	1.70	0.44
1:B:895:THR:HA	1:B:935:VAL:HG11	2.00	0.44
1:A:120:LEU:C	1:A:127:LEU:HD13	2.38	0.44
1:A:1231:ASP:HB3	1:A:1515:ARG:HD2	2.00	0.44
1:A:169:GLN:OE1	1:A:250:GLY:HA2	2.17	0.44
1:A:1754:GLN:HA	1:A:1754:GLN:OE1	2.17	0.44
1:A:1762:GLN:O	1:A:1763:HIS:HB2	2.18	0.44
1:A:1818:ILE:HG12	1:A:1823:VAL:HG11	1.99	0.44
1:A:1882:PRO:HA	1:A:1883:PRO:HD3	1.85	0.44
1:A:189:ASN:O	1:A:226:GLU:HB2	2.17	0.44
1:A:1955:LEU:O	1:A:1958:GLU:HB2	2.17	0.44
1:A:259:GLN:H	1:A:259:GLN:CD	2.20	0.44
1:A:27:ILE:C	1:A:29:GLY:H	2.20	0.44
1:A:331:HIS:HE1	1:A:333:GLU:HA	1.83	0.44
1:A:499:MET:HG3	1:A:502:GLN:NE2	2.32	0.44
1:A:642:CYS:HA	1:A:743:VAL:CG2	2.48	0.44
1:A:889:THR:CG2	1:A:1032:LEU:CB	2.96	0.44
1:B:1971:LEU:HD21	1:B:2019:PHE:CD2	2.52	0.44
1:B:587:CYS:O	1:B:591:ASP:N	2.51	0.44
1:A:1216:LEU:HD13	1:A:1217:LEU:H	1.83	0.43
1:A:123:ASP:CB	1:A:126:THR:HB	2.42	0.43
1:A:1953:ARG:HA	1:A:2005:VAL:HG11	1.99	0.43
1:A:159:THR:HG22	1:A:398:SER:HB3	2.00	0.43
1:A:984:GLU:O	1:A:985:PHE:CB	2.64	0.43
1:B:1338:LEU:HD13	1:B:1406:GLN:CG	2.48	0.43
1:B:143:ARG:HG2	1:B:143:ARG:NH1	2.33	0.43
1:B:1466:GLY:HA2	1:B:1469:ILE:CD1	2.48	0.43
1:B:190:VAL:HG12	1:B:192:LEU:HG	1.99	0.43
1:B:1118:LYS:HD2	1:B:2103:HIS:ND1	2.33	0.43
1:B:23:TRP:NE1	1:B:350:HIS:CD2	2.86	0.43
1:B:91:VAL:HG21	1:B:834:ILE:HD13	1.99	0.43
1:B:914:PHE:HB2	1:B:1057:ILE:HB	2.00	0.43
1:B:925:LEU:CD2	1:B:931:VAL:HG21	2.48	0.43
1:A:143:ARG:NH1	1:A:143:ARG:HG2	2.31	0.43
1:A:1609:SER:C	1:A:1611:ARG:H	2.21	0.43
1:A:1887:TYR:CD2	1:A:1967:GLY:HA3	2.46	0.43
1:A:470:TYR:C	1:A:470:TYR:CD1	2.90	0.43
1:A:525:GLN:HA	1:A:525:GLN:NE2	2.32	0.43
1:A:579:GLY:O	1:A:715:THR:HG21	2.19	0.43
1:B:1553:TYR:O	1:B:1554:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:PRO:HG3	1:B:363:ASN:ND2	2.33	0.43
1:B:416:GLN:C	1:B:418:ALA:N	2.70	0.43
1:A:1483:ALA:HB1	1:A:1508:ASP:HA	2.01	0.43
1:A:1786:LEU:C	1:A:1788:ASN:H	2.21	0.43
1:A:1857:ARG:NH1	1:A:1869:PRO:HB2	2.33	0.43
1:A:1995:LYS:HB3	1:A:2041:MET:SD	2.58	0.43
1:B:1769:ILE:HG22	1:B:1770:GLY:N	2.32	0.43
1:B:2043:ARG:HA	1:B:2043:ARG:HD3	1.71	0.43
1:B:948:ASP:OD1	1:B:948:ASP:C	2.57	0.43
1:A:1036:LEU:O	1:A:1037:HIS:C	2.57	0.43
1:A:1299:TRP:NE1	1:A:1304:PRO:O	2.51	0.43
1:A:1238:ALA:O	1:A:1462:LYS:HG3	2.17	0.43
1:A:1442:TRP:CH2	1:A:1497:LEU:HD23	2.54	0.43
1:A:1619:ALA:O	1:A:1620:GLU:HB2	2.18	0.43
1:A:1624:THR:HG22	1:A:1857:ARG:NH2	2.33	0.43
1:A:1993:LYS:H	1:A:1994:PRO:CD	2.32	0.43
1:A:343:LYS:HE3	1:A:354:ALA:HB3	2.00	0.43
1:A:366:ILE:CG1	1:A:366:ILE:O	2.66	0.43
1:A:542:ASP:OD1	1:A:542:ASP:C	2.56	0.43
1:A:639:VAL:HG12	1:A:640:PRO:O	2.18	0.43
1:A:811:ASN:HA	1:A:812:PRO:HD3	1.82	0.43
1:A:830:ILE:O	1:A:831:SER:C	2.56	0.43
1:A:856:CYS:C	1:A:858:SER:N	2.72	0.43
1:B:627:TRP:CZ3	1:B:640:PRO:HB2	2.53	0.43
1:A:1049:TYR:CZ	1:A:1103:VAL:HG23	2.54	0.43
1:A:1469:ILE:CG2	1:A:1469:ILE:O	2.66	0.43
1:A:1662:ARG:NH1	1:A:1662:ARG:HG2	2.33	0.43
1:A:2006:THR:HG21	1:A:2048:ARG:NH2	2.32	0.43
1:A:870:SER:HA	1:A:871:PRO:HD3	1.88	0.43
1:B:98:ALA:CA	1:B:101:ARG:HG3	2.47	0.43
1:B:1234:LEU:HD21	1:B:1268:MET:HE3	2.01	0.43
1:B:1569:THR:HG23	1:B:1602:GLU:O	2.19	0.43
1:B:1648:VAL:HB	1:B:1649:PRO:HD3	1.99	0.43
1:B:1675:SER:O	1:B:1681:GLY:HA3	2.19	0.43
1:B:185:VAL:HB	1:B:231:VAL:HG23	2.00	0.43
1:B:259:GLN:CD	1:B:259:GLN:N	2.72	0.43
1:A:1118:LYS:HA	1:A:2106:LEU:HD22	2.01	0.43
1:A:1864:ALA:HA	1:A:1865:PRO:HD3	1.82	0.43
1:A:1882:PRO:HG2	1:A:1885:LYS:HD2	2.01	0.43
1:A:1929:VAL:HG13	1:A:1939:VAL:HG11	1.99	0.43
1:A:336:SER:OG	1:A:337:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.62	0.43
1:B:1112:LEU:O	1:B:1114:PRO:HD3	2.17	0.43
1:B:228:VAL:CG2	1:B:228:VAL:O	2.67	0.43
1:B:23:TRP:CE2	1:B:27:ILE:HG12	2.53	0.43
1:B:290:ILE:CG2	1:B:322:ILE:HG12	2.49	0.43
1:B:637:GLY:O	1:B:685:TYR:HE2	2.00	0.43
1:B:946:VAL:O	1:B:954:ILE:HB	2.18	0.43
1:B:982:THR:O	1:B:984:GLU:N	2.49	0.43
1:A:1251:ASP:O	1:A:1253:GLN:HG3	2.19	0.43
1:A:1476:ASN:CB	1:A:1486:MET:SD	3.06	0.43
1:A:1757:VAL:HG11	1:A:1784:VAL:HG21	2.01	0.43
1:A:78:GLN:HB3	1:A:188:LEU:HD13	2.01	0.43
1:A:51:MET:HB2	1:A:53:LYS:HE3	2.01	0.43
1:A:782:ILE:HA	1:A:783:PRO:HD3	1.88	0.43
1:B:1333:ASN:C	1:B:1335:ALA:N	2.72	0.43
1:B:14:PRO:HA	1:B:53:LYS:O	2.19	0.43
1:B:1995:LYS:HA	1:B:2041:MET:HE3	2.01	0.43
1:B:283:ASP:C	1:B:285:GLU:H	2.22	0.43
1:B:161:CYS:HB3	1:B:331:HIS:CE1	2.53	0.43
1:B:654:PRO:HG3	1:B:685:TYR:OH	2.18	0.43
1:B:6:ILE:HG21	1:B:345:LEU:HD11	2.01	0.43
1:B:752:VAL:HA	1:B:753:PRO:HD3	1.89	0.43
1:A:1083:ASP:O	1:A:1086:LEU:N	2.51	0.43
1:A:108:TRP:CD1	1:A:171:ALA:HB2	2.54	0.43
1:A:2031:GLN:HB3	1:A:2034:TYR:HB3	1.99	0.43
1:A:23:TRP:CH2	1:A:347:SER:HA	2.54	0.43
1:A:524:ASP:OD1	1:A:534:VAL:N	2.52	0.43
1:B:137:ARG:O	1:B:140:MET:HG2	2.19	0.43
1:B:1984:THR:C	1:B:1986:GLU:H	2.22	0.43
1:A:129:GLY:HA3	1:B:202:LYS:HB2	2.00	0.43
1:B:2066:VAL:HG22	1:B:2088:ILE:HD12	2.00	0.43
1:B:252:ASN:N	1:B:272:LEU:HD13	2.33	0.43
1:B:363:ASN:HA	1:B:364:PRO:HD3	1.81	0.43
1:B:499:MET:HG3	1:B:502:GLN:NE2	2.34	0.43
1:B:416:GLN:OE1	1:B:817:PRO:HG2	2.18	0.43
1:A:1235:GLU:HG2	1:A:1235:GLU:H	1.58	0.43
1:A:1390:VAL:HG22	1:A:1501:LEU:HD21	2.00	0.43
1:A:206:LEU:HA	1:A:206:LEU:HD23	1.64	0.43
1:B:1389:LEU:HD23	1:B:1389:LEU:HA	1.83	0.43
1:B:1137:GLN:NE2	1:B:1396:PHE:CE1	2.86	0.43
1:B:161:CYS:HB3	1:B:331:HIS:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:VAL:C	1:B:311:ALA:H	2.22	0.43
1:B:953:LEU:HD12	1:B:954:ILE:N	2.34	0.43
1:A:1345:LEU:HD13	1:A:1403:LEU:HD13	2.01	0.43
1:A:1842:TYR:CE2	1:A:1848:HIS:HB3	2.53	0.43
1:A:217:ALA:C	1:A:219:GLY:H	2.21	0.43
1:A:295:THR:HG22	1:A:331:HIS:CD2	2.53	0.43
1:A:548:ASP:OD1	1:A:550:VAL:N	2.50	0.43
1:A:863:LYS:HB3	1:A:930:THR:HG21	2.01	0.43
1:B:1477:LEU:HD11	1:B:2043:ARG:CD	2.43	0.43
1:B:1515:ARG:HD3	1:B:1515:ARG:HA	1.30	0.43
1:B:1555:LEU:HA	1:B:1555:LEU:HD12	1.93	0.43
1:B:1525:GLU:OE1	1:B:1874:THR:HG23	2.19	0.43
1:B:1921:ARG:HB2	1:B:1921:ARG:HE	1.65	0.43
1:B:200:PHE:HB3	1:B:206:LEU:CG	2.48	0.43
1:B:23:TRP:CZ2	1:B:27:ILE:HG12	2.54	0.43
1:B:470:TYR:C	1:B:470:TYR:CD1	2.92	0.43
1:A:1420:ASP:O	1:A:1425:TRP:CZ3	2.71	0.42
1:A:1657:TYR:CZ	1:A:1662:ARG:CD	3.02	0.42
1:A:1815:LYS:O	1:A:1819:GLN:HG3	2.18	0.42
1:A:248:ASN:HD22	1:A:249:ALA:H	1.65	0.42
1:A:262:THR:O	1:A:262:THR:HG22	2.18	0.42
1:A:662:LEU:C	1:A:664:GLN:N	2.71	0.42
1:B:1085:ASN:C	1:B:1086:LEU:HD23	2.40	0.42
1:B:1469:ILE:CG2	1:B:1471:CYS:SG	3.07	0.42
1:B:1119:PHE:CZ	1:B:1514:PHE:HB3	2.54	0.42
1:B:1536:LEU:HG	1:B:1543:SER:O	2.19	0.42
1:B:1780:LEU:HD12	1:B:1781:GLY:H	1.83	0.42
1:B:1955:LEU:O	1:B:1958:GLU:HB2	2.19	0.42
1:B:259:GLN:HB2	1:B:263:PHE:CD1	2.54	0.42
1:B:497:SER:HB2	1:B:762:ALA:HB2	2.00	0.42
1:A:1032:LEU:O	1:A:1035:MET:HB2	2.19	0.42
1:A:119:ALA:HB2	1:A:850:PHE:CE2	2.53	0.42
1:A:1468:ARG:HA	1:A:1468:ARG:HD3	1.85	0.42
1:A:1661:VAL:HG21	1:A:1810:VAL:HG22	2.01	0.42
1:A:470:TYR:CD2	1:A:801:GLY:HA3	2.55	0.42
1:B:111:VAL:HG21	1:B:188:LEU:HD12	2.01	0.42
1:B:1468:ARG:HD3	1:B:1468:ARG:HA	1.71	0.42
1:B:1477:LEU:O	1:B:1507:ARG:CG	2.67	0.42
1:B:178:GLY:O	1:B:179:GLU:C	2.58	0.42
1:B:1818:ILE:HG12	1:B:1823:VAL:HG11	2.00	0.42
1:B:1977:ASP:O	1:B:1978:ALA:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:863:LYS:HB3	1:B:930:THR:HG21	2.01	0.42
1:A:1090:VAL:HG22	1:A:1095:LEU:HB2	2.02	0.42
1:A:1894:GLY:O	1:A:1895:GLY:C	2.57	0.42
1:A:1896:PHE:CE2	1:A:2019:PHE:CE1	3.07	0.42
1:A:2041:MET:HA	1:A:2044:ILE:HG13	2.02	0.42
1:A:708:ARG:HD3	1:A:727:ALA:O	2.19	0.42
1:A:743:VAL:O	1:A:743:VAL:HG23	2.20	0.42
1:A:808:VAL:HG12	1:A:809:SER:H	1.84	0.42
1:B:1315:LEU:HD23	1:B:1344:LEU:HD11	2.00	0.42
1:B:1636:VAL:HG22	1:B:1636:VAL:O	2.19	0.42
1:B:1786:LEU:HD23	1:B:1786:LEU:HA	1.82	0.42
1:B:475:GLY:O	1:B:477:ALA:N	2.51	0.42
1:B:557:THR:HA	1:B:560:GLN:HE21	1.84	0.42
1:A:1411:ASP:OD2	1:A:1439:ARG:HB2	2.19	0.42
1:A:1598:MET:O	1:A:1598:MET:HG2	2.20	0.42
1:A:202:LYS:HB2	1:B:129:GLY:HA3	2.02	0.42
1:A:2095:LEU:CD1	1:A:2099:LEU:HG	2.49	0.42
1:A:39:ARG:NH1	1:A:226:GLU:OE2	2.51	0.42
1:A:48:PRO:HD3	1:A:201:MET:CE	2.50	0.42
1:B:972:THR:CG2	1:B:1081:VAL:CG2	2.96	0.42
1:B:1551:LEU:HD21	1:B:1627:LEU:CD2	2.48	0.42
1:B:1676:GLY:O	1:B:1682:GLN:HG2	2.20	0.42
1:B:1993:LYS:H	1:B:1994:PRO:CD	2.31	0.42
1:B:27:ILE:C	1:B:29:GLY:H	2.21	0.42
1:A:1585:PRO:HB3	1:A:1598:MET:CE	2.49	0.42
1:A:1787:LYS:HB2	1:A:1789:VAL:HG23	2.01	0.42
1:A:289:TYR:CD2	1:A:289:TYR:C	2.93	0.42
1:A:321:LEU:HD12	1:A:321:LEU:H	1.84	0.42
1:A:347:SER:HB2	1:A:352:VAL:O	2.19	0.42
1:A:606:ARG:HA	1:A:694:LEU:HD11	2.00	0.42
1:A:925:LEU:CD2	1:A:931:VAL:HG21	2.49	0.42
1:A:988:SER:O	1:A:989:GLN:C	2.56	0.42
1:B:1670:SER:OG	1:B:1741:VAL:HA	2.19	0.42
1:B:1757:VAL:O	1:B:1760:LEU:HB2	2.19	0.42
1:B:40:TRP:CZ3	1:B:194:PRO:HA	2.55	0.42
1:B:263:PHE:HE2	1:B:303:GLN:HE21	1.66	0.42
1:B:40:TRP:HB3	1:B:847:ALA:CB	2.49	0.42
1:B:895:THR:O	1:B:898:THR:HB	2.20	0.42
1:A:1245:VAL:HB	1:A:1315:LEU:CD1	2.49	0.42
1:A:1433:LEU:HD11	1:A:1465:GLY:C	2.40	0.42
1:A:1656:TYR:O	1:A:1657:TYR:C	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1734:ARG:C	1:A:1736:THR:N	2.72	0.42
1:A:1996:TYR:CD2	1:A:1997:SER:N	2.85	0.42
1:A:1119:PHE:HB3	1:A:2105:VAL:HB	2.01	0.42
1:A:211:THR:HG22	1:A:212:CYS:N	2.34	0.42
1:A:321:LEU:HD23	1:A:381:LEU:CD1	2.48	0.42
1:A:189:ASN:HB2	1:A:334:PRO:HD2	1.99	0.42
1:A:765:ALA:HB1	1:A:768:GLN:CG	2.49	0.42
1:A:644:ASN:HB3	1:A:770:VAL:HG11	2.01	0.42
1:B:1222:ASP:N	1:B:1222:ASP:OD1	2.49	0.42
1:B:165:LEU:HD23	1:B:400:VAL:CG2	2.31	0.42
1:B:1815:LYS:O	1:B:1819:GLN:HG3	2.20	0.42
1:B:2049:ARG:HD2	1:B:2049:ARG:HA	1.84	0.42
1:B:367:PRO:O	1:B:368:ALA:HB3	2.20	0.42
1:B:462:PRO:HA	1:B:465:MET:O	2.19	0.42
1:B:55:LYS:HB3	1:B:55:LYS:HE2	1.69	0.42
1:B:423:LEU:HB2	1:B:797:LEU:HD22	2.01	0.42
1:B:82:LEU:HG	1:B:144:LEU:HD13	2.02	0.42
1:A:1240:PRO:HB3	1:A:1267:VAL:O	2.20	0.42
1:A:1603:PHE:HZ	1:A:1628:LEU:HD22	1.84	0.42
1:A:1637:PRO:O	1:A:1639:THR:N	2.52	0.42
1:A:163:SER:O	1:A:167:ALA:N	2.47	0.42
1:A:228:VAL:CG2	1:A:228:VAL:O	2.67	0.42
1:A:257:LYS:NZ	1:A:261:VAL:O	2.51	0.42
1:A:27:ILE:HD13	1:A:27:ILE:HA	1.81	0.42
1:A:353:TRP:O	1:A:355:PRO:HD3	2.19	0.42
1:A:98:ALA:HA	1:A:101:ARG:CG	2.49	0.42
1:B:1382:PHE:HA	1:B:1387:LEU:HD12	2.01	0.42
1:B:1711:ARG:HG2	1:B:1712:PHE:CE1	2.55	0.42
1:B:305:LEU:HD22	1:B:322:ILE:CD1	2.50	0.42
1:A:1239:SER:C	1:A:1241:LYS:H	2.23	0.42
1:A:1514:PHE:O	1:A:1515:ARG:NH1	2.53	0.42
1:A:1879:THR:HG1	1:A:1903:TRP:HH2	1.65	0.42
1:A:672:VAL:HG12	1:A:672:VAL:O	2.18	0.42
1:A:620:MET:CE	1:A:682:PHE:O	2.66	0.42
1:A:948:ASP:OD1	1:A:948:ASP:C	2.58	0.42
1:B:193:LYS:HA	1:B:194:PRO:HD3	1.85	0.42
1:B:5:VAL:HG21	1:B:242:VAL:HG22	2.01	0.42
1:B:409:ARG:HA	1:B:410:PRO:HD3	1.74	0.42
1:B:416:GLN:HE21	1:B:448:LEU:CD1	2.33	0.42
1:B:876:VAL:HG12	1:B:876:VAL:O	2.20	0.42
1:A:1451:SER:O	1:A:2036:PHE:CE1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:CD1	1:A:251:THR:HG21	2.49	0.42
1:A:283:ASP:C	1:A:285:GLU:H	2.23	0.42
1:A:302:PRO:HA	1:A:366:ILE:CG2	2.49	0.42
1:A:384:ARG:NH1	1:A:384:ARG:CG	2.75	0.42
1:A:595:THR:HG22	1:A:596:GLN:N	2.35	0.42
1:A:495:ILE:HG12	1:A:758:VAL:HG13	2.02	0.42
1:A:795:PHE:CE1	1:A:799:ASN:ND2	2.86	0.42
1:A:899:LEU:HA	1:A:899:LEU:HD12	1.82	0.42
1:B:1763:HIS:HA	1:B:1788:ASN:O	2.20	0.42
1:B:1801:GLU:O	1:B:1803:GLY:N	2.53	0.42
1:B:1941:VAL:HG12	1:B:1941:VAL:O	2.18	0.42
1:B:527:LEU:HD11	1:B:554:VAL:HG11	2.01	0.42
1:A:1116:LEU:HD22	1:A:2098:PHE:CE1	2.55	0.42
1:A:114:SER:O	1:A:117:SER:HB3	2.19	0.42
1:A:1123:PRO:HA	1:A:1512:GLY:HA3	2.01	0.42
1:A:1557:ALA:O	1:A:1560:GLN:HB3	2.20	0.42
1:A:178:GLY:O	1:A:179:GLU:C	2.57	0.42
1:A:1862:GLY:O	1:A:1863:PRO:C	2.59	0.42
1:A:19:LEU:HA	1:A:19:LEU:HD23	1.68	0.42
1:A:420:LEU:HD11	1:A:512:ARG:HB3	2.01	0.42
1:B:1038:MET:CE	1:B:1041:LEU:HD23	2.50	0.42
1:B:1234:LEU:HD12	1:B:1234:LEU:O	2.19	0.42
1:B:1303:ASN:OD1	1:B:1332:GLY:HA3	2.19	0.42
1:B:1671:VAL:HG23	1:B:1743:LEU:HD13	2.02	0.42
1:B:1757:VAL:HG11	1:B:1784:VAL:HG21	2.01	0.42
1:B:270:GLU:HG3	1:B:311:ALA:HB2	2.01	0.42
1:A:1480:THR:CG2	1:A:1482:PRO:HD2	2.50	0.41
1:A:253:THR:O	1:A:254:ASP:C	2.59	0.41
1:A:503:TRP:HB3	1:A:787:LYS:HD2	2.02	0.41
1:B:1303:ASN:C	1:B:1333:ASN:HB2	2.41	0.41
1:B:147:PHE:C	1:B:147:PHE:CD2	2.93	0.41
1:B:1537:SER:H	1:B:1543:SER:HB2	1.85	0.41
1:B:2064:GLY:O	1:B:2066:VAL:N	2.53	0.41
1:B:119:ALA:HB2	1:B:850:PHE:CZ	2.55	0.41
1:A:1656:TYR:CE2	1:A:1687:ILE:HD13	2.55	0.41
1:A:1873:LEU:HD22	1:A:1874:THR:N	2.34	0.41
1:A:1993:LYS:N	1:A:1994:PRO:CD	2.82	0.41
1:A:254:ASP:HB2	1:A:257:LYS:HE2	2.02	0.41
1:A:366:ILE:HD11	1:A:369:LEU:HD11	2.01	0.41
1:A:359:TYR:CD2	1:A:376:VAL:HG11	2.55	0.41
1:A:630:CYS:C	1:A:632:GLN:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:GLU:HB3	1:A:778:SER:H	1.84	0.41
1:A:9:MET:CE	1:A:342:ILE:HA	2.50	0.41
1:B:128:VAL:HG12	1:B:130:TYR:CE2	2.54	0.41
1:B:1966:GLY:HA2	1:B:2013:LEU:HA	2.02	0.41
1:B:979:ALA:O	1:B:980:ASP:C	2.58	0.41
1:A:118:GLU:OE2	1:B:118:GLU:HG3	2.20	0.41
1:A:1272:TYR:HB3	1:A:1294:VAL:HG22	2.01	0.41
1:A:1413:PRO:HA	1:A:1440:PRO:O	2.21	0.41
1:A:111:VAL:CG2	1:A:188:LEU:HD12	2.50	0.41
1:A:894:LEU:HD12	1:A:894:LEU:HA	1.81	0.41
1:B:1060:ASP:OD1	1:B:1062:VAL:HG23	2.20	0.41
1:B:1049:TYR:CZ	1:B:1103:VAL:HG23	2.55	0.41
1:B:1241:LYS:HA	1:B:1269:ASP:HB3	2.02	0.41
1:B:1996:TYR:CD2	1:B:1997:SER:N	2.85	0.41
1:B:273:ILE:O	1:B:277:TYR:HD1	2.01	0.41
1:B:322:ILE:HD11	1:B:374:LEU:HD13	2.01	0.41
1:B:830:ILE:O	1:B:831:SER:C	2.59	0.41
1:A:1242:MET:HG3	1:A:1313:ASP:HB3	2.02	0.41
1:A:1442:TRP:CZ3	1:A:1472:VAL:HG11	2.55	0.41
1:A:40:TRP:CZ3	1:A:194:PRO:HA	2.55	0.41
1:A:23:TRP:CE2	1:A:27:ILE:HG12	2.55	0.41
1:A:259:GLN:N	1:A:259:GLN:CD	2.74	0.41
1:A:302:PRO:HG3	1:A:363:ASN:ND2	2.35	0.41
1:A:367:PRO:O	1:A:368:ALA:HB3	2.20	0.41
1:A:795:PHE:O	1:A:798:SER:HB2	2.20	0.41
1:A:896:TRP:CG	1:A:907:LEU:HD11	2.56	0.41
1:B:1405:ARG:HH22	1:B:1470:ARG:NH2	2.19	0.41
1:B:162:SER:OG	1:B:163:SER:N	2.50	0.41
1:B:1766:PHE:O	1:B:1792:HIS:HB2	2.20	0.41
1:B:889:THR:CG2	1:B:1032:LEU:CB	2.98	0.41
1:B:894:LEU:HA	1:B:894:LEU:HD12	1.83	0.41
1:A:1296:GLN:H	1:A:1296:GLN:HG2	1.64	0.41
1:A:1277:ARG:HD3	1:A:1300:ASP:OD2	2.19	0.41
1:A:13:LEU:HD13	1:A:22:PHE:CD1	2.55	0.41
1:A:489:LYS:HE2	1:A:489:LYS:HB3	1.77	0.41
1:A:954:ILE:HD13	1:A:954:ILE:HA	1.91	0.41
1:B:1519:LEU:HD12	1:B:1520:GLU:H	1.85	0.41
1:B:1706:ALA:O	1:B:1707:TYR:C	2.59	0.41
1:B:1712:PHE:HA	1:B:1713:PRO:HD3	1.84	0.41
1:B:1879:THR:HG1	1:B:1903:TRP:HH2	1.67	0.41
1:B:1115:ILE:HD11	1:B:2111:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:VAL:HG11	1:B:223:CYS:SG	2.60	0.41
1:B:423:LEU:HD23	1:B:812:PRO:HG3	2.02	0.41
1:A:111:VAL:HG12	1:A:111:VAL:O	2.20	0.41
1:A:1568:TYR:CE2	1:A:1855:GLN:HB2	2.56	0.41
1:A:1921:ARG:HB2	1:A:1921:ARG:HE	1.67	0.41
1:A:1998:GLY:O	1:A:2002:LEU:HD12	2.20	0.41
1:A:257:LYS:HG3	1:A:257:LYS:H	1.68	0.41
1:A:527:LEU:HD11	1:A:554:VAL:HG11	2.02	0.41
1:A:749:LEU:HA	1:A:749:LEU:HD23	1.88	0.41
1:A:469:GLY:CA	1:A:805:LEU:HD21	2.51	0.41
1:B:1122:THR:HA	1:B:1123:PRO:HD3	1.92	0.41
1:B:178:GLY:O	1:B:180:CYS:N	2.53	0.41
1:B:1836:VAL:HG13	1:B:1854:ILE:HD13	2.03	0.41
1:B:13:LEU:HB2	1:B:22:PHE:CD1	2.55	0.41
1:A:1216:LEU:O	1:A:1220:LEU:HD12	2.21	0.41
1:A:1234:LEU:CD2	1:A:1262:LEU:HD22	2.48	0.41
1:A:1671:VAL:HG23	1:A:1743:LEU:HB2	2.02	0.41
1:A:1669:GLU:CG	1:A:1742:ASP:OD2	2.69	0.41
1:A:252:ASN:N	1:A:272:LEU:HD13	2.36	0.41
1:A:258:GLU:HB2	1:A:259:GLN:NE2	2.36	0.41
1:A:263:PHE:HE2	1:A:303:GLN:HE21	1.68	0.41
1:A:460:VAL:CG2	1:A:465:MET:HG3	2.46	0.41
1:A:513:LEU:HA	1:A:513:LEU:HD23	1.79	0.41
1:A:561:ILE:HG23	1:A:589:TYR:CE2	2.56	0.41
1:A:953:LEU:HD12	1:A:954:ILE:N	2.35	0.41
1:B:1538:ARG:HH12	1:B:1585:PRO:HG2	1.86	0.41
1:B:1617:VAL:N	1:B:1800:PHE:HZ	2.19	0.41
1:B:257:LYS:NZ	1:B:261:VAL:O	2.49	0.41
1:B:322:ILE:CG2	1:B:323:GLY:N	2.83	0.41
1:B:744:LEU:HA	1:B:747:GLU:OE1	2.21	0.41
1:A:1011:LEU:HA	1:A:1011:LEU:HD12	1.85	0.41
1:A:1096:PHE:CD2	1:A:1096:PHE:N	2.89	0.41
1:A:147:PHE:CD2	1:A:147:PHE:C	2.94	0.41
1:A:1789:VAL:CG1	1:A:1790:THR:N	2.83	0.41
1:A:2112:ALA:O	1:A:2113:GLU:HG2	2.21	0.41
1:A:288:GLU:OE2	1:A:383:ILE:HG13	2.21	0.41
1:A:541:THR:O	1:A:542:ASP:HB3	2.20	0.41
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.68	0.41
1:A:623:VAL:HA	1:A:671:PHE:O	2.21	0.41
1:A:637:GLY:O	1:A:654:PRO:HD2	2.20	0.41
1:A:857:SER:O	1:A:902:ALA:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1315:LEU:O	1:B:1344:LEU:HD13	2.21	0.41
1:B:1433:LEU:HD12	1:B:1433:LEU:HA	1.79	0.41
1:B:214:SER:O	1:B:301:ASP:OD2	2.38	0.41
1:B:513:LEU:HA	1:B:513:LEU:HD23	1.77	0.41
1:B:581:SER:HA	1:B:738:ASN:HD21	1.85	0.41
1:B:635:PRO:O	1:B:636:PRO:C	2.59	0.41
1:B:980:ASP:OD1	1:B:980:ASP:N	2.53	0.41
1:A:1669:GLU:HG2	1:A:1742:ASP:OD2	2.21	0.41
1:A:1893:LEU:HB3	1:A:1925:GLN:CD	2.41	0.41
1:A:193:LYS:HA	1:A:194:PRO:HD3	1.86	0.41
1:A:300:GLY:O	1:A:301:ASP:C	2.59	0.41
1:A:64:PHE:CB	1:A:429:ARG:HH21	2.23	0.41
1:A:528:LYS:HB3	1:A:529:PRO:HD3	2.03	0.41
1:B:1243:LYS:HA	1:B:1271:ASP:HB2	2.02	0.41
1:B:1312:ALA:HB1	1:B:1337:THR:HG22	2.00	0.41
1:B:1343:PHE:CZ	1:B:1405:ARG:HD2	2.56	0.41
1:B:1457:VAL:HG11	1:B:1473:LEU:HD22	2.02	0.41
1:B:1567:TYR:HA	1:B:1857:ARG:HG3	2.02	0.41
1:B:1755:ALA:HA	1:B:1758:ARG:NH1	2.36	0.41
1:B:2006:THR:CG2	1:B:2048:ARG:HH12	2.34	0.41
1:B:333:GLU:O	1:B:336:SER:HB3	2.21	0.41
1:B:453:MET:HE2	1:B:453:MET:HB3	1.89	0.41
1:B:561:ILE:HG23	1:B:589:TYR:CE2	2.56	0.41
1:B:704:ASP:O	1:B:706:LYS:HD2	2.20	0.41
1:B:795:PHE:CE1	1:B:799:ASN:ND2	2.87	0.41
1:A:1583:LEU:HD23	1:A:1583:LEU:HA	1.88	0.41
1:A:389:GLY:O	1:A:390:ILE:HG13	2.21	0.41
1:A:416:GLN:HE21	1:A:448:LEU:CD1	2.34	0.41
1:A:598:GLU:OE1	1:A:706:LYS:NZ	2.48	0.41
1:A:624:GLY:H	1:A:671:PHE:HB3	1.86	0.41
1:A:639:VAL:HG12	1:A:640:PRO:HD2	2.02	0.41
1:B:1429:LEU:HD11	1:B:1443:LEU:HD21	2.03	0.41
1:B:1842:TYR:CE2	1:B:1848:HIS:HB3	2.56	0.41
1:B:1998:GLY:O	1:B:2002:LEU:HD12	2.20	0.41
1:B:277:TYR:HB3	1:B:278:ALA:H	1.58	0.41
1:B:494:PHE:O	1:B:495:ILE:HD13	2.20	0.41
1:B:33:VAL:HB	1:B:50:ARG:NH1	2.34	0.41
1:A:1408:THR:HG22	1:A:1409:PRO:HD2	2.03	0.41
1:A:1480:THR:HG22	1:A:1482:PRO:HD2	2.02	0.41
1:A:1766:PHE:O	1:A:1792:HIS:HB2	2.21	0.41
1:A:674:GLU:HG2	1:A:674:GLU:H	1.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:LEU:HD12	1:A:907:LEU:HA	1.88	0.41
1:B:1257:ARG:O	1:B:1260:ALA:HB3	2.21	0.41
1:B:1951:GLY:O	1:B:1954:SER:HB2	2.20	0.41
1:B:1991:VAL:HG21	1:B:2033:ASN:HD22	1.84	0.41
1:B:429:ARG:HD2	1:B:429:ARG:HA	1.91	0.41
1:B:634:CYS:HA	1:B:635:PRO:HD3	1.89	0.41
1:B:6:ILE:HG21	1:B:345:LEU:CD1	2.51	0.41
1:A:1243:LYS:HD2	1:A:1312:ALA:N	2.37	0.40
1:A:1240:PRO:HD2	1:A:1462:LYS:HZ1	1.87	0.40
1:A:1514:PHE:O	1:A:1515:ARG:HD3	2.21	0.40
1:A:1689:LEU:O	1:A:1692:GLY:N	2.48	0.40
1:A:1857:ARG:HG3	1:A:1871:ILE:HD11	2.03	0.40
1:A:1974:VAL:HG23	1:A:1974:VAL:O	2.21	0.40
1:A:270:GLU:HG3	1:A:311:ALA:HB2	2.03	0.40
1:B:1139:GLU:OE2	1:B:1216:LEU:CD1	2.68	0.40
1:B:1453:VAL:HG12	1:B:1457:VAL:HG23	2.03	0.40
1:B:1456:MET:HE2	1:B:1460:LEU:HD22	2.02	0.40
1:B:1473:LEU:CG	1:B:1503:MET:HA	2.51	0.40
1:B:1643:GLU:O	1:B:1644:GLU:C	2.60	0.40
1:B:1741:VAL:CG1	1:B:1742:ASP:N	2.84	0.40
1:B:1780:LEU:HD12	1:B:1781:GLY:N	2.36	0.40
1:B:1931:GLU:OE1	1:B:1931:GLU:HA	2.21	0.40
1:B:253:THR:O	1:B:254:ASP:C	2.59	0.40
1:B:295:THR:HG22	1:B:331:HIS:CD2	2.55	0.40
1:B:366:ILE:CG1	1:B:366:ILE:O	2.68	0.40
1:A:1315:LEU:HB3	1:A:1344:LEU:HD11	2.02	0.40
1:A:1433:LEU:HD21	1:A:1465:GLY:HA3	2.03	0.40
1:A:23:TRP:CZ2	1:A:27:ILE:HG12	2.57	0.40
1:A:305:LEU:HD23	1:A:308:ILE:HD12	2.03	0.40
1:A:161:CYS:HB3	1:A:331:HIS:CE1	2.56	0.40
1:A:612:GLU:O	1:A:614:ASN:N	2.54	0.40
1:A:734:TYR:CD2	1:A:734:TYR:O	2.74	0.40
1:A:82:LEU:HG	1:A:144:LEU:HD13	2.02	0.40
1:B:122:ARG:O	1:B:123:ASP:C	2.58	0.40
1:B:1118:LYS:N	1:B:1517:PHE:O	2.47	0.40
1:B:1659:LEU:HD23	1:B:1767:LEU:CD1	2.51	0.40
1:B:641:ALA:HB1	1:B:683:HIS:CB	2.49	0.40
1:A:1118:LYS:HD2	1:A:2103:HIS:ND1	2.35	0.40
1:A:1347:HIS:CD2	1:A:1348:THR:O	2.74	0.40
1:A:1674:HIS:ND1	1:A:1698:THR:CG2	2.83	0.40
1:A:2090:SER:O	1:A:2094:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLY:O	1:A:298:LYS:HB2	2.20	0.40
1:A:429:ARG:HA	1:A:429:ARG:HD2	1.94	0.40
1:A:784:LEU:HD23	1:A:784:LEU:HA	1.68	0.40
1:A:81:MET:HG2	1:A:81:MET:H	1.62	0.40
1:B:1573:PHE:O	1:B:1576:VAL:HB	2.21	0.40
1:B:1636:VAL:HG23	1:B:1640:TRP:HB2	2.03	0.40
1:B:1863:PRO:O	1:B:1865:PRO:HD3	2.21	0.40
1:B:2041:MET:HA	1:B:2044:ILE:HG13	2.03	0.40
1:B:420:LEU:HD12	1:B:512:ARG:HH11	1.86	0.40
1:B:490:ARG:HA	1:B:491:PRO:HD3	1.96	0.40
1:B:623:VAL:CG1	1:B:624:GLY:N	2.85	0.40
1:B:654:PRO:O	1:B:658:MET:CB	2.68	0.40
1:B:588:GLY:HA3	1:B:730:PHE:CE1	2.57	0.40
1:A:1238:ALA:HB1	1:A:1467:HIS:CD2	2.56	0.40
1:A:159:THR:O	1:A:160:ALA:HB3	2.21	0.40
1:A:1733:LEU:HD23	1:A:1733:LEU:HA	1.68	0.40
1:A:588:GLY:O	1:A:594:LEU:HB2	2.21	0.40
1:A:666:LYS:O	1:A:668:GLU:N	2.55	0.40
1:A:654:PRO:HD3	1:A:686:PHE:HE1	1.86	0.40
1:A:825:ARG:HG2	1:A:826:GLY:N	2.36	0.40
1:B:1122:THR:HG1	1:B:1517:PHE:HE1	1.68	0.40
1:B:1314:LEU:HG	1:B:1315:LEU:N	2.36	0.40
1:B:1456:MET:CE	1:B:1460:LEU:HD22	2.52	0.40
1:B:1617:VAL:HG21	1:B:1626:VAL:HG11	2.04	0.40
1:B:1553:TYR:O	1:B:1882:PRO:HG3	2.21	0.40
1:B:2017:VAL:HG12	1:B:2018:ILE:N	2.37	0.40
1:B:189:ASN:O	1:B:226:GLU:HB2	2.21	0.40
1:B:252:ASN:HD21	1:B:272:LEU:HB2	1.81	0.40
1:B:300:GLY:O	1:B:301:ASP:C	2.59	0.40
1:B:876:VAL:HA	1:B:884:VAL:HG11	2.03	0.40
1:A:273:ILE:O	1:A:277:TYR:HD1	2.05	0.40
1:A:509:SER:O	1:A:512:ARG:HG3	2.22	0.40
1:B:1726:THR:CG2	1:B:1726:THR:O	2.70	0.40
1:B:2022:VAL:HG13	1:B:2026:ARG:HG2	2.04	0.40
1:B:912:VAL:HG22	1:B:913:VAL:N	2.36	0.40
1:B:971:ASP:OD1	1:B:973:ARG:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1948/2512 (78%)	1586 (81%)	282 (14%)	80 (4%)	3	24
1	B	1992/2512 (79%)	1622 (81%)	296 (15%)	74 (4%)	4	26
All	All	3940/5024 (78%)	3208 (81%)	578 (15%)	154 (4%)	3	25

All (154) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	GLU
1	A	255	GLY
1	A	278	ALA
1	A	333	GLU
1	A	413	PRO
1	A	418	ALA
1	A	582	LEU
1	A	615	VAL
1	A	818	PRO
1	A	839	SER
1	A	976	VAL
1	A	1224	PRO
1	A	1303	ASN
1	A	1485	GLU
1	A	1611	ARG
1	A	1638	SER
1	A	1749	ALA
1	A	1802	GLU
1	A	1862	GLY
1	B	179	GLU
1	B	255	GLY
1	B	278	ALA
1	B	333	GLU
1	B	418	ALA
1	B	636	PRO

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Mol	Chain	Res	Type
1	B	669	ASP
1	B	839	SER
1	B	978	PRO
1	B	980	ASP
1	B	1224	PRO
1	B	1749	ALA
1	B	1800	PHE
1	B	1862	GLY
1	A	163	SER
1	A	282	PRO
1	A	318	GLU
1	A	387	ASN
1	A	476	GLU
1	A	488	SER
1	A	984	GLU
1	A	985	PHE
1	A	1056	SER
1	A	1301	PRO
1	A	1593	LEU
1	A	1735	HIS
1	A	1801	GLU
1	A	1870	PRO
1	A	2025	GLY
1	A	2079	VAL
1	A	2112	ALA
1	B	163	SER
1	B	282	PRO
1	B	318	GLU
1	B	370	GLN
1	B	387	ASN
1	B	413	PRO
1	B	476	GLU
1	B	856	CYS
1	B	974	ALA
1	B	983	ALA
1	B	984	GLU
1	B	1225	ALA
1	B	1301	PRO
1	B	1302	ALA
1	B	1593	LEU
1	B	1735	HIS
1	B	1802	GLU

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Mol	Chain	Res	Type
1	B	1858	GLU
1	B	2025	GLY
1	B	2079	VAL
1	A	216	ASP
1	A	254	ASP
1	A	310	ASN
1	A	317	ARG
1	A	319	PRO
1	A	613	ALA
1	A	854	SER
1	A	1014	ASP
1	A	1110	GLU
1	A	1225	ALA
1	A	1596	ASP
1	A	1649	PRO
1	A	1706	ALA
1	A	2021	SER
1	B	213	ARG
1	B	254	ASP
1	B	317	ARG
1	B	319	PRO
1	B	488	SER
1	B	820	GLU
1	B	1056	SER
1	B	1560	GLN
1	B	1596	ASP
1	B	1706	ALA
1	B	1863	PRO
1	B	2065	ASP
1	A	14	PRO
1	A	237	SER
1	A	238	LEU
1	A	445	SER
1	A	848	ALA
1	A	857	SER
1	A	1389	LEU
1	A	1409	PRO
1	A	1557	ALA
1	A	1734	ARG
1	A	1800	PHE
1	A	1835	LYS
1	A	2065	ASP

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Mol	Chain	Res	Type
1	A	2078	THR
1	B	14	PRO
1	B	60	PHE
1	B	162	SER
1	B	238	LEU
1	B	310	ASN
1	B	445	SER
1	B	1014	ASP
1	B	1110	GLU
1	B	1449	SER
1	B	1464	PRO
1	B	1491	SER
1	B	1548	CYS
1	B	1734	ARG
1	B	1932	TRP
1	B	1982	ASN
1	B	2021	SER
1	B	2078	THR
1	B	2102	PRO
1	A	60	PHE
1	A	162	SER
1	A	215	PHE
1	A	617	PRO
1	A	1464	PRO
1	A	1471	CYS
1	A	1597	CYS
1	A	1692	GLY
1	A	1865	PRO
1	A	2056	LEU
1	A	2102	PRO
1	B	1835	LYS
1	B	1978	ALA
1	B	1979	VAL
1	B	2056	LEU
1	A	1500	ASP
1	B	635	PRO
1	B	1467	HIS
1	A	487	GLY
1	A	853	GLY
1	B	1303	ASN
1	B	1409	PRO
1	B	487	GLY

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Mol	Chain	Res	Type
1	A	355	PRO
1	A	1240	PRO
1	B	1408	THR

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	1624/2072 (78%)	1450 (89%)	174 (11%)	8	32
1	B	1660/2072 (80%)	1473 (89%)	187 (11%)	7	29
All	All	3284/4144 (79%)	2923 (89%)	361 (11%)	7	31

All (361) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	MET
1	A	59	ARG
1	A	81	MET
1	A	86	THR
1	A	111	VAL
1	A	117	SER
1	A	123	ASP
1	A	128	VAL
1	A	136	GLN
1	A	144	LEU
1	A	169	GLN
1	A	170	SER
1	A	172	TYR
1	A	181	SER
1	A	223	CYS
1	A	224	ARG
1	A	241	ARG
1	A	248	ASN
1	A	251	THR
1	A	263	PHE

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Mol	Chain	Res	Type
1	A	295	THR
1	A	297	THR
1	A	309	VAL
1	A	317	ARG
1	A	318	GLU
1	A	320	LEU
1	A	327	SER
1	A	329	MET
1	A	343	LYS
1	A	347	SER
1	A	356	ASN
1	A	366	ILE
1	A	371	ASP
1	A	375	GLN
1	A	383	ILE
1	A	399	ASN
1	A	400	VAL
1	A	402	VAL
1	A	407	ASN
1	A	439	GLU
1	A	446	ARG
1	A	460	VAL
1	A	470	TYR
1	A	480	GLN
1	A	489	LYS
1	A	492	VAL
1	A	502	GLN
1	A	520	ILE
1	A	525	GLN
1	A	541	THR
1	A	543	GLU
1	A	549	ILE
1	A	552	SER
1	A	556	LEU
1	A	558	SER
1	A	568	THR
1	A	569	SER
1	A	572	LEU
1	A	574	PRO
1	A	597	GLU
1	A	614	ASN
1	A	616	LEU

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Mol	Chain	Res	Type
1	A	658	MET
1	A	673	LYS
1	A	674	GLU
1	A	677	THR
1	A	689	SER
1	A	703	LEU
1	A	730	PHE
1	A	734	TYR
1	A	736	VAL
1	A	757	VAL
1	A	773	ARG
1	A	825	ARG
1	A	846	SER
1	A	849	ASP
1	A	857	SER
1	A	866	VAL
1	A	894	LEU
1	A	917	VAL
1	A	931	VAL
1	A	937	LEU
1	A	941	SER
1	A	947	SER
1	A	949	SER
1	A	953	LEU
1	A	959	VAL
1	A	972	THR
1	A	1011	LEU
1	A	1026	ASP
1	A	1038	MET
1	A	1052	THR
1	A	1055	THR
1	A	1068	LEU
1	A	1069	TYR
1	A	1070	THR
1	A	1074	THR
1	A	1084	ARG
1	A	1087	ASN
1	A	1088	THR
1	A	1095	LEU
1	A	1097	LEU
1	A	1101	SER
1	A	1105	PRO

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Mol	Chain	Res	Type
1	A	1107	ARG
1	A	1112	LEU
1	A	1122	THR
1	A	1216	LEU
1	A	1267	VAL
1	A	1275	THR
1	A	1299	TRP
1	A	1346	LEU
1	A	1376	ASP
1	A	1408	THR
1	A	1421	THR
1	A	1428	SER
1	A	1456	MET
1	A	1460	LEU
1	A	1468	ARG
1	A	1473	LEU
1	A	1476	ASN
1	A	1480	THR
1	A	1481	SER
1	A	1491	SER
1	A	1505	VAL
1	A	1525	GLU
1	A	1527	GLN
1	A	1541	LEU
1	A	1542	SER
1	A	1573	PHE
1	A	1583	LEU
1	A	1596	ASP
1	A	1597	CYS
1	A	1614	MET
1	A	1626	VAL
1	A	1638	SER
1	A	1639	THR
1	A	1651	VAL
1	A	1660	VAL
1	A	1662	ARG
1	A	1669	GLU
1	A	1697	THR
1	A	1698	THR
1	A	1722	ASN
1	A	1735	HIS
1	A	1736	THR

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Mol	Chain	Res	Type
1	A	1760	LEU
1	A	1762	GLN
1	A	1768	GLU
1	A	1790	THR
1	A	1800	PHE
1	A	1823	VAL
1	A	1841	ARG
1	A	1843	MET
1	A	1860	GLU
1	A	1861	GLN
1	A	1873	LEU
1	A	1877	SER
1	A	1922	THR
1	A	1927	ARG
1	A	1937	VAL
1	A	1944	SER
1	A	1957	THR
1	A	1996	TYR
1	A	2005	VAL
1	A	2006	THR
1	A	2022	VAL
1	A	2026	ARG
1	A	2028	ASN
1	A	2043	ARG
1	A	2044	ILE
1	A	2078	THR
1	A	2096	ASP
1	A	2111	LEU
1	B	32	MET
1	B	59	ARG
1	B	81	MET
1	B	86	THR
1	B	111	VAL
1	B	112	SER
1	B	122	ARG
1	B	123	ASP
1	B	126	THR
1	B	127	LEU
1	B	128	VAL
1	B	136	GLN
1	B	144	LEU
1	B	169	GLN

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Mol	Chain	Res	Type
1	B	170	SER
1	B	172	TYR
1	B	181	SER
1	B	223	CYS
1	B	224	ARG
1	B	241	ARG
1	B	248	ASN
1	B	251	THR
1	B	263	PHE
1	B	288	GLU
1	B	295	THR
1	B	297	THR
1	B	309	VAL
1	B	317	ARG
1	B	318	GLU
1	B	320	LEU
1	B	329	MET
1	B	334	PRO
1	B	343	LYS
1	B	347	SER
1	B	356	ASN
1	B	366	ILE
1	B	371	ASP
1	B	375	GLN
1	B	383	ILE
1	B	399	ASN
1	B	400	VAL
1	B	402	VAL
1	B	407	ASN
1	B	439	GLU
1	B	446	ARG
1	B	460	VAL
1	B	489	LYS
1	B	492	VAL
1	B	502	GLN
1	B	520	ILE
1	B	545	VAL
1	B	549	ILE
1	B	552	SER
1	B	556	LEU
1	B	558	SER
1	B	568	THR

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Mol	Chain	Res	Type
1	B	569	SER
1	B	572	LEU
1	B	574	PRO
1	B	615	VAL
1	B	635	PRO
1	B	664	GLN
1	B	670	VAL
1	B	675	VAL
1	B	676	ARG
1	B	689	SER
1	B	730	PHE
1	B	734	TYR
1	B	736	VAL
1	B	757	VAL
1	B	821	PHE
1	B	825	ARG
1	B	846	SER
1	B	866	VAL
1	B	894	LEU
1	B	917	VAL
1	B	931	VAL
1	B	937	LEU
1	B	941	SER
1	B	947	SER
1	B	949	SER
1	B	959	VAL
1	B	964	SER
1	B	971	ASP
1	B	972	THR
1	B	976	VAL
1	B	980	ASP
1	B	982	THR
1	B	1011	LEU
1	B	1026	ASP
1	B	1038	MET
1	B	1052	THR
1	B	1055	THR
1	B	1068	LEU
1	B	1069	TYR
1	B	1070	THR
1	B	1074	THR
1	B	1084	ARG

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Mol	Chain	Res	Type
1	B	1087	ASN
1	B	1088	THR
1	B	1095	LEU
1	B	1097	LEU
1	B	1101	SER
1	B	1107	ARG
1	B	1122	THR
1	B	1216	LEU
1	B	1218	SER
1	B	1235	GLU
1	B	1267	VAL
1	B	1275	THR
1	B	1299	TRP
1	B	1337	THR
1	B	1340	GLU
1	B	1346	LEU
1	B	1373	LEU
1	B	1395	SER
1	B	1421	THR
1	B	1428	SER
1	B	1456	MET
1	B	1460	LEU
1	B	1473	LEU
1	B	1480	THR
1	B	1481	SER
1	B	1486	MET
1	B	1487	HIS
1	B	1505	VAL
1	B	1515	ARG
1	B	1525	GLU
1	B	1528	THR
1	B	1548	CYS
1	B	1551	LEU
1	B	1558	SER
1	B	1573	PHE
1	B	1583	LEU
1	B	1595	ARG
1	B	1597	CYS
1	B	1598	MET
1	B	1603	PHE
1	B	1612	ARG
1	B	1614	MET

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Mol	Chain	Res	Type
1	B	1636	VAL
1	B	1639	THR
1	B	1653	THR
1	B	1661	VAL
1	B	1662	ARG
1	B	1669	GLU
1	B	1671	VAL
1	B	1687	ILE
1	B	1694	ARG
1	B	1697	THR
1	B	1698	THR
1	B	1722	ASN
1	B	1735	HIS
1	B	1736	THR
1	B	1760	LEU
1	B	1762	GLN
1	B	1768	GLU
1	B	1790	THR
1	B	1800	PHE
1	B	1823	VAL
1	B	1841	ARG
1	B	1843	MET
1	B	1856	VAL
1	B	1860	GLU
1	B	1868	LEU
1	B	1873	LEU
1	B	1877	SER
1	B	1904	LEU
1	B	1922	THR
1	B	1927	ARG
1	B	1937	VAL
1	B	1940	LEU
1	B	1944	SER
1	B	1957	THR
1	B	1979	VAL
1	B	1982	ASN
1	B	1988	PHE
1	B	1996	TYR
1	B	2005	VAL
1	B	2006	THR
1	B	2022	VAL
1	B	2026	ARG

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Mol	Chain	Res	Type
1	B	2028	ASN
1	B	2043	ARG
1	B	2044	ILE
1	B	2078	THR
1	B	2096	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	96	ASN
1	A	136	GLN
1	A	248	ASN
1	A	306	ASN
1	A	350	HIS
1	A	356	ASN
1	A	399	ASN
1	A	425	GLN
1	A	444	HIS
1	A	525	GLN
1	A	560	GLN
1	A	632	GLN
1	A	644	ASN
1	A	697	GLN
1	A	737	ASN
1	A	833	HIS
1	A	1023	GLN
1	A	1037	HIS
1	A	1111	HIS
1	A	1133	ASN
1	A	1298	GLN
1	A	1318	ASN
1	A	1388	HIS
1	A	1467	HIS
1	A	1487	HIS
1	A	1735	HIS
1	A	1777	ASN
1	A	1778	HIS
1	A	1855	GLN
1	A	2076	ASN
1	A	2086	GLN
1	A	2103	HIS

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Mol	Chain	Res	Type
1	B	25	ASN
1	B	96	ASN
1	B	136	GLN
1	B	199	GLN
1	B	248	ASN
1	B	306	ASN
1	B	350	HIS
1	B	356	ASN
1	B	399	ASN
1	B	425	GLN
1	B	502	GLN
1	B	525	GLN
1	B	560	GLN
1	B	632	GLN
1	B	643	HIS
1	B	663	GLN
1	B	697	GLN
1	B	737	ASN
1	B	738	ASN
1	B	833	HIS
1	B	1023	GLN
1	B	1037	HIS
1	B	1111	HIS
1	B	1133	ASN
1	B	1298	GLN
1	B	1333	ASN
1	B	1406	GLN
1	B	1458	ASN
1	B	1467	HIS
1	B	1674	HIS
1	B	1735	HIS
1	B	1777	ASN
1	B	1778	HIS
1	B	1855	GLN
1	B	2076	ASN
1	B	2086	GLN
1	B	2103	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1962/2512 (78%)	-0.12	86 (4%)	35	23	63, 118, 226, 276	0
1	B	2004/2512 (79%)	0.09	132 (6%)	19	12	54, 158, 230, 276	0
All	All	3966/5024 (78%)	-0.01	218 (5%)	26	16	54, 136, 229, 276	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	581	SER	7.8
1	B	496	CYS	7.4
1	B	579	GLY	7.4
1	A	1297	GLY	7.3
1	B	498	GLY	7.1
1	B	672	VAL	7.0
1	A	1387	LEU	6.5
1	A	1406	GLN	6.2
1	B	580	HIS	6.1
1	B	2078	THR	5.9
1	B	497	SER	5.8
1	B	671	PHE	5.3
1	B	583	GLY	5.3
1	A	2078	THR	5.2
1	B	1863	PRO	5.1
1	A	1398	GLY	5.0
1	A	1415	PHE	4.9
1	A	1407	GLN	4.9
1	A	1386	SER	4.9
1	B	703	LEU	4.7
1	A	2079	VAL	4.6
1	A	1486	MET	4.6
1	A	1441	VAL	4.6
1	B	2069	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	674	GLU	4.3
1	B	622	ALA	4.2
1	B	2076	ASN	4.2
1	B	410	PRO	4.2
1	B	392	SER	4.1
1	A	419	ALA	4.1
1	B	673	LYS	4.0
1	A	1269	ASP	4.0
1	B	667	ARG	3.9
1	B	2080	ILE	3.9
1	B	1140	LEU	3.9
1	A	982	THR	3.8
1	A	2029	ALA	3.8
1	B	1286	GLN	3.8
1	B	1136	LEU	3.7
1	B	1296	GLN	3.7
1	A	414	PRO	3.7
1	B	1486	MET	3.7
1	B	10	SER	3.7
1	A	336	SER	3.6
1	B	1437	SER	3.6
1	B	1297	GLY	3.6
1	B	414	PRO	3.6
1	B	1384	GLY	3.6
1	B	928	THR	3.6
1	A	1442	TRP	3.6
1	A	1468	ARG	3.5
1	A	983	ALA	3.5
1	A	1385	ALA	3.5
1	B	1276	ASP	3.5
1	A	1135	ALA	3.5
1	A	1464	PRO	3.5
1	A	2080	ILE	3.4
1	B	717	ILE	3.4
1	B	617	PRO	3.4
1	B	670	VAL	3.4
1	B	2068	VAL	3.4
1	A	1296	GLN	3.4
1	A	1384	GLY	3.4
1	B	161	CYS	3.3
1	B	391	ASN	3.3
1	B	1439	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	1437	SER	3.3
1	B	669	ASP	3.3
1	B	1869	PRO	3.3
1	B	413	PRO	3.2
1	A	981	SER	3.2
1	B	1143	CYS	3.2
1	A	1465	GLY	3.2
1	B	1441	VAL	3.2
1	B	2079	VAL	3.1
1	A	2081	GLY	3.1
1	A	293	HIS	3.1
1	B	408	SER	3.0
1	B	646	LYS	3.0
1	B	1340	GLU	3.0
1	A	1510	ALA	3.0
1	B	1523	ARG	3.0
1	B	1864	ALA	3.0
1	B	293	HIS	3.0
1	B	2077	ASP	3.0
1	A	1382	PHE	3.0
1	B	1275	THR	3.0
1	B	1458	ASN	3.0
1	B	560	GLN	2.9
1	A	1388	HIS	2.9
1	B	1876	LEU	2.9
1	A	1509	GLY	2.9
1	B	1455	GLY	2.9
1	A	1305	ALA	2.9
1	B	661	PHE	2.9
1	B	316	ARG	2.9
1	A	364	PRO	2.9
1	B	336	SER	2.8
1	B	666	LYS	2.8
1	B	653	GLY	2.8
1	A	392	SER	2.8
1	B	624	GLY	2.8
1	B	1987	PHE	2.7
1	B	324	SER	2.7
1	B	2071	GLU	2.7
1	A	1482	PRO	2.7
1	B	298	LYS	2.7
1	A	2077	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	978	PRO	2.7
1	B	658	MET	2.7
1	A	975	ALA	2.7
1	A	2034	TYR	2.7
1	B	665	LEU	2.7
1	A	1426	VAL	2.6
1	B	1979	VAL	2.6
1	B	664	GLN	2.6
1	A	2070	LEU	2.6
1	B	488	SER	2.6
1	A	976	VAL	2.6
1	A	1349	LEU	2.6
1	A	1430	LYS	2.6
1	B	1280	GLN	2.6
1	A	49	ARG	2.6
1	A	1429	LEU	2.6
1	A	1134	THR	2.5
1	B	625	LEU	2.5
1	A	2069	VAL	2.5
1	A	980	ASP	2.5
1	B	1586	ASP	2.5
1	A	2076	ASN	2.5
1	B	337	GLY	2.5
1	B	762	ALA	2.5
1	B	2070	LEU	2.5
1	A	496	CYS	2.5
1	A	1484	PRO	2.5
1	B	647	ASP	2.5
1	B	539	LEU	2.4
1	B	1981	GLU	2.4
1	A	1491	SER	2.4
1	A	1436	ALA	2.4
1	B	1231	ASP	2.4
1	B	499	MET	2.4
1	B	1243	LYS	2.4
1	A	1348	THR	2.4
1	A	1487	HIS	2.4
1	A	1974	VAL	2.4
1	B	541	THR	2.4
1	B	644	ASN	2.4
1	B	663	GLN	2.4
1	B	1412	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	419	ALA	2.4
1	B	1468	ARG	2.4
1	B	360	HIS	2.4
1	B	1284	ALA	2.4
1	A	1467	HIS	2.4
1	A	1286	GLN	2.3
1	A	1304	PRO	2.3
1	B	1484	PRO	2.3
1	B	790	ARG	2.3
1	B	369	LEU	2.3
1	B	1978	ALA	2.3
1	A	1300	ASP	2.3
1	B	721	GLN	2.3
1	A	1255	TYR	2.3
1	A	1287	ALA	2.3
1	A	1513	ALA	2.3
1	B	495	ILE	2.3
1	B	389	GLY	2.3
1	A	1383	ALA	2.3
1	B	1320	ALA	2.3
1	B	1141	GLN	2.3
1	A	1278	ASN	2.2
1	B	1327	PRO	2.2
1	B	294	GLY	2.2
1	A	1306	PRO	2.2
1	B	1408	THR	2.2
1	A	1298	GLN	2.2
1	B	364	PRO	2.2
1	B	1570	SER	2.2
1	B	654	PRO	2.2
1	A	1397	TYR	2.2
1	B	621	ALA	2.2
1	B	374	LEU	2.2
1	B	35	ALA	2.2
1	A	977	ASP	2.2
1	B	409	ARG	2.2
1	B	1313	ASP	2.2
1	B	1485	GLU	2.2
1	A	161	CYS	2.2
1	A	1408	THR	2.2
1	A	337	GLY	2.2
1	B	975	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1291	GLN	2.2
1	A	1033	ASP	2.2
1	B	1294	VAL	2.2
1	A	1434	ALA	2.1
1	B	660	GLU	2.1
1	B	1976	ARG	2.1
1	B	1339	LYS	2.1
1	B	49	ARG	2.1
1	B	1587	SER	2.1
1	B	722	TRP	2.1
1	B	1602	GLU	2.1
1	B	331	HIS	2.1
1	B	370	GLN	2.1
1	B	2082	GLY	2.1
1	A	1238	ALA	2.1
1	A	1341	GLY	2.1
1	B	483	GLN	2.1
1	A	1235	GLU	2.1
1	A	1240	PRO	2.1
1	A	1681	GLY	2.1
1	A	1377	GLN	2.0
1	B	1557	ALA	2.0
1	B	788	ASP	2.0
1	B	1584	SER	2.0
1	B	557	THR	2.0
1	B	634	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.