



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:13 am BST

PDB ID : 2VZ9
Title : Crystal Structure of Mammalian Fatty Acid Synthase in complex with NADP
Authors : Maier, T.; Leibundgut, M.; Ban, N.
Deposited on : 2008-07-31
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

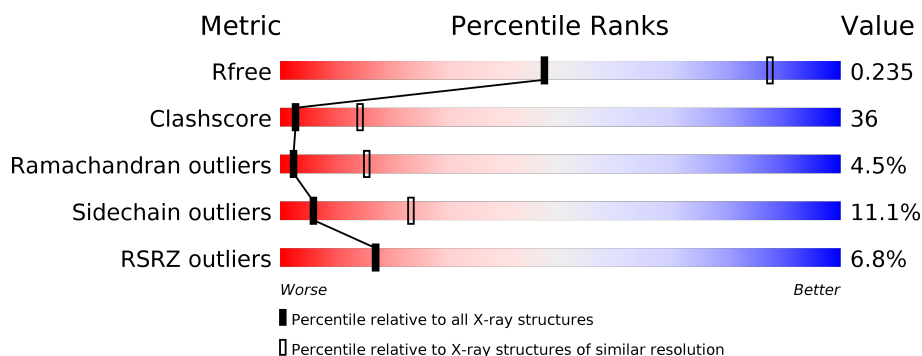
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2512	<div> <div>5%</div> <div>38%</div> <div>38%</div> <div>7%</div> <div>17%</div> </div>
1	B	2512	<div> <div>6%</div> <div>36%</div> <div>40%</div> <div>7%</div> <div>17%</div> </div>

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 31949 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called FATTY ACID SYNTHASE.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	834	ILE	UNK	conflict	UNP A5YV76
B	834	ILE	UNK	conflict	UNP A5YV76

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



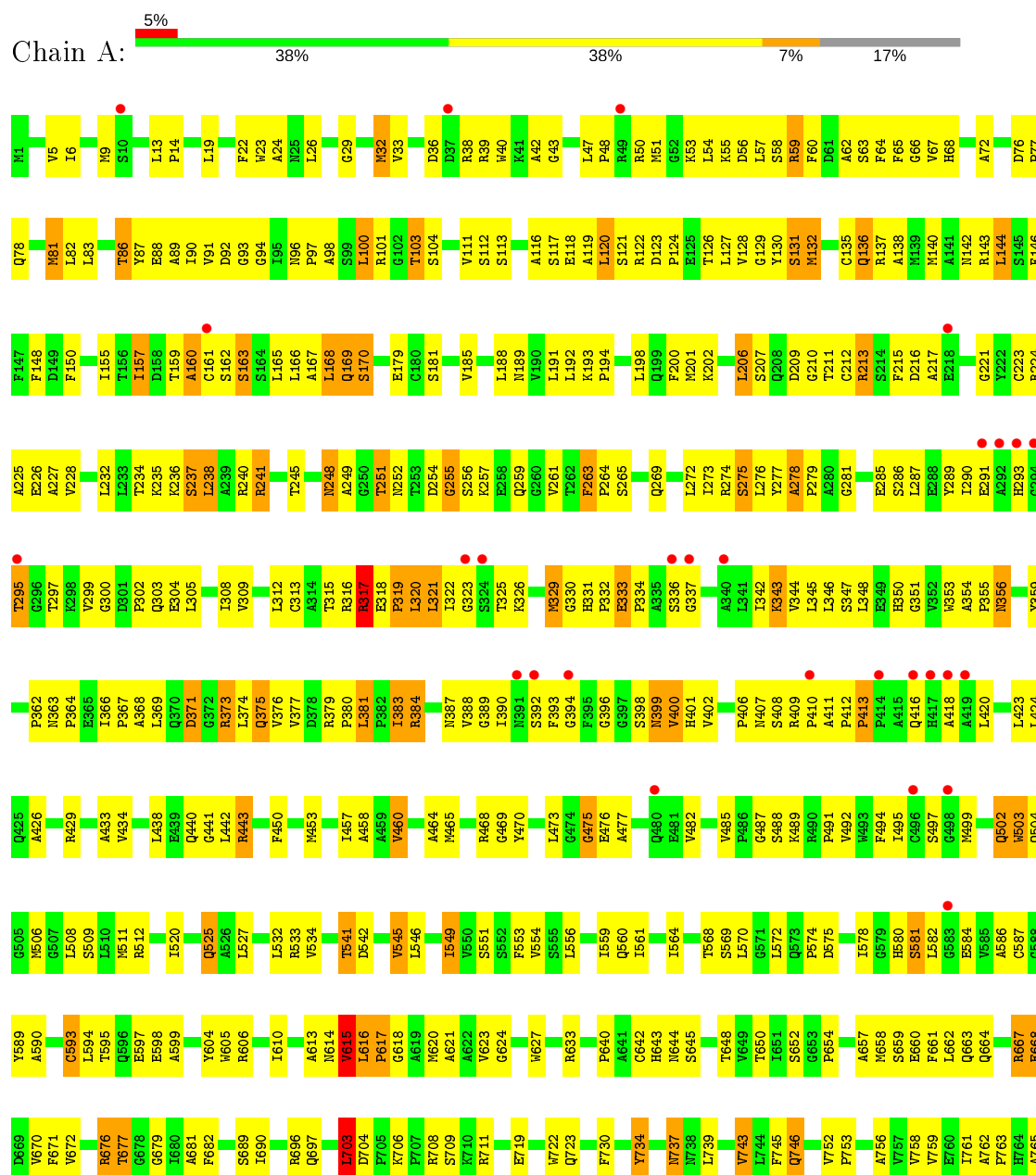
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

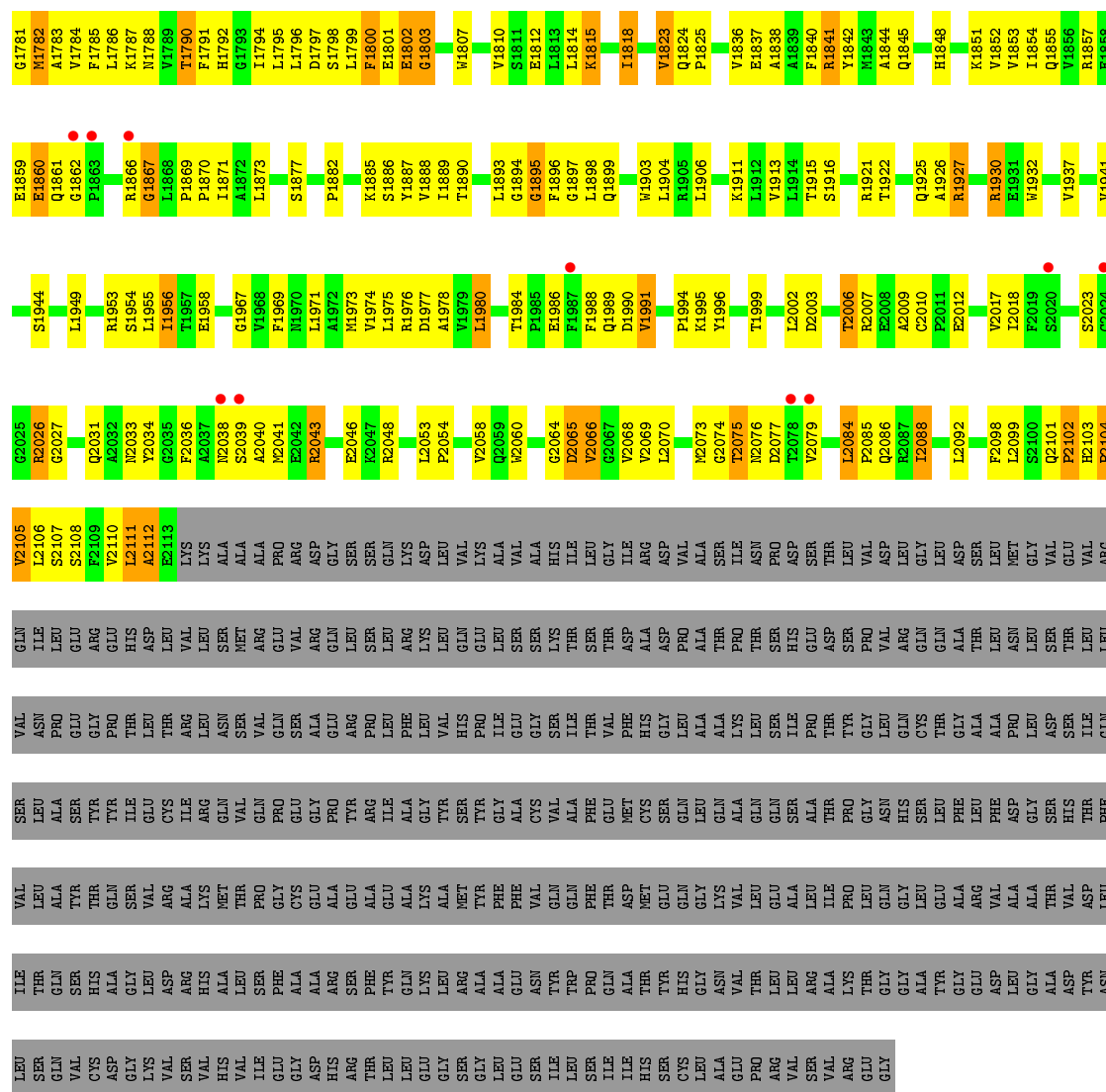
3 Residue-property plots [i](#)

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.

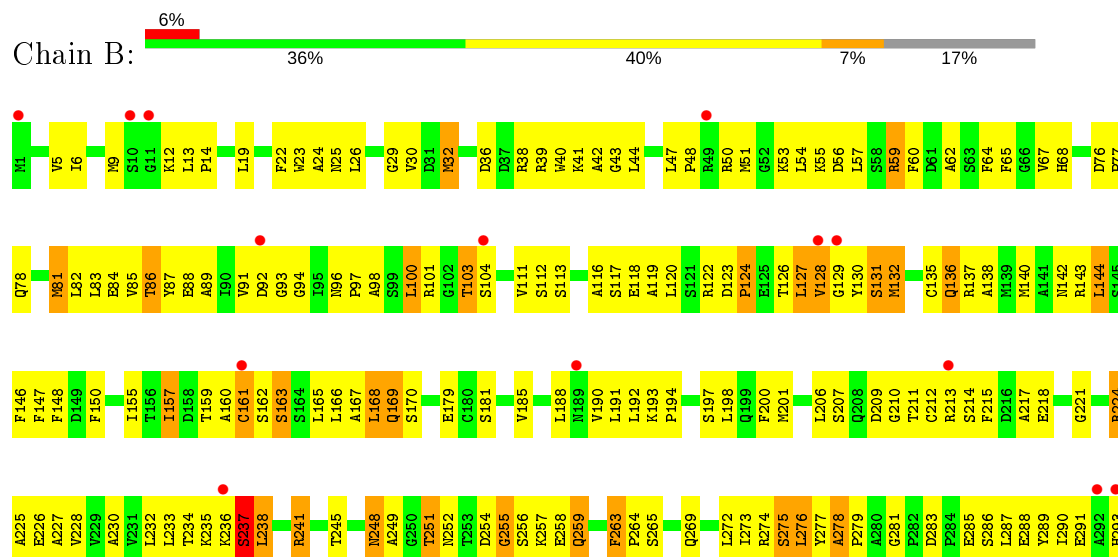
• Molecule 1: FATTY ACID SYNTHASE



WORLDWIDE
PDB
PROTEIN DATA BANK



• Molecule 1: FATTY ACID SYNTHASE



D1251	Q1189	H1124	P1051	A975	L894	P817	Y734	T850	I578	W503	L423	T381	Q294
G1252	L1190	V1125	F1051	V976	L895	P818	W737	I651	G579	Q504	L424	P362	T295
Q1253	Q1191	E1126	F1054	D977	M896	W819	W738	G552	H580	G505	Q425	I363	G296
L1254	L1192	S1127	F1055	P978	T398	E820	L739	G653	S581	M506	A426	P364	T297
V1255	N1193	G1128	T1055	A979	T399	F821	L739	P654	L582	G507	R429	E365	K298
S1256	G1194	D980	S1056	D980	L899	Q825	L743	Q655	G583	L508	R429	I366	V299
R1257	N1195	L1130	I1057	S981	A900	R825	W743	A656	E584	S509	R429	P367	Q300
	LEU	A1131		T982	L903	G826	L744	A657	A586	R512	A433	I367	Q301
	GLN	G1132	D1060	A983	L903	T827	F745	W658	A586		V434	A366	P302
	LEU	N1133	V1061	E984	S904	P828	Q746	S659	Y589	R515	L438	L369	Q303
	E1199	N1133	V1062	F985	Q905		Q746	S659	Y589	R515	L438	Q370	E304
	E1199	N1133	T1063	R986	N906	S831	W752	E660	A590	R515	L438	D371	L305
	L1200	L1136	K1067	L987	L907	P832	P763	L662	C593	I520	E439	R373	
	G1201	Q1137	L1068	S988	T910	H833	A754	Q663	T595	L521	Q440	L374	I308
	Q1202	E1138	T1069	Q989	T911	R834	W755	Q664	L594	L442	Q441	Q375	V309
	V1203	E1139	V1070	R990	P911	R835	A756	L665	T595	D524	R443		
	L1204	L1142	T1071	D991	V912	N836	W759	K666	Q596	Q526			L312
	A1205	L1142	Q1072	V992	V913	H837	E760	E668	E597	A526	W453	R379	
	Q1206	L1146	D1073	Y993	F914	H838	W761	E668	E597	L527	L454	P380	
	E1207	A1147	D1074	X994	E915	S839	W761	D669	E598		W455	L381	T315
	R1208	Q1148	T1075	A941	D916	A841	A762	W670	W604	L530		R382	R316
	L1210	A1149	Q1076	L998	V917		P763	V672	W605	G531	A458	R383	R317
	L1211	L1150	Q1076	L998	V917		W764	K673	W605	L532	A459	R384	E318
	G1212	L1150	A1077	R999	I924	V644	A765	E674	R606	R533	V460	G386	P319
	D1213	K1163	A1078	G1000	L925	P845	L766	W675	Y608	V534	S461	G387	L321
	D1214	V1164		Y1001		S846	Q768	W676	C609	L537	P462	V388	L322
	L1215	ALA	V1081	D1002	T928	D849	L775	T677	I610	L538	W463	G389	G323
	GLN	GLN	V1082	Y1003	G929	F850	E776	E681	A464	L539	L454	I390	S324
	GLN	GLN	D1083	Y1003	V931		W777	A681	K611	S540	W465	I391	T325
	GLY	GLY	R1084	F1007	E934	C856	S778	P682	E612	T541	R468	G392	K326
	LEU	LEU	N1085	Q1008	V935		S778	H683	E614	D542	W469	P393	S327
	LEU	LEU	L1086	L1009	R936	V859		S684	W615	E544	W470	G394	R328
	MET	MET	M1087	L1010	L937	A860	L782	W685	M620	A544	G474	P395	R329
	VAL	VAL	T1088	L1011	L937	R861	P783	V685	A621	L546	G475	G397	G330
	VAL	VAL	V1089	L1011			L784	P686	G624	L546	E476	P332	H331
	PRO	PRO	D1014	D1014	S941	V866	W790	S689	L625	I549	A477	P334	E333
	GLY	GLY	L1015	E1016		S867		I690	L625	V550		A395	A395
	LEU	LEU	E1016		F944	P868	L793	A691	G627		E481	S336	S336
	ASP	ASP	R1019		E945			P692	W627			V402	G337
	GLY	GLY	L1019		V946	H873	L797					L403	
	ALA	ALA	L1022	Q1023	S947		W798	Q697	R633	S555		L404	
	ALA	ALA	L1022	Q1023		V876	S798	L698	C634	L556	V485	P405	I342
	PRO	PRO	W1028	W1028	L953	D877	W798	R699	P635	S557	P486	P406	K342
	ARG	ARG	V1029	V1029	I954	H878	W800	R699	P636	S558	Q487	M407	K343
	GLU	GLU	S1030	S1030		C879	G801		P636	I559	S488	M407	V344
	ALA	ALA	F1031	F1031	V959	I880	R802	L703	P636	Q560	K489	S408	L345
	PRO	PRO	E1110	E1110		D881	L803	G637	G637	I561	R490	R409	L346
	GLN	GLN	L1032	L1032	W662	G882	H804	S709	I638		P491	P410	S347
	GLN	GLN	D1033	D1033	E963	R883	L805	K710	V639	I564	V492	A411	L348
	ALA	ALA	A1034	A1034	S964	V884	L805	R711	P640		W493	P412	E349
	SER	SER	M1035	M1035	P965	L885	W808	E719	A641	T568	W493	P413	H350
	L1180	L1180	L1036	L1036	P966	F886	S809		C642	S569	I495	P414	G351
	P1181	P1181	E1117	H1037	P967	P887	W810	W722	H643	L570	C496	P415	V352
	L1183	L1183	K1118	M1038		G888	R811		H643	L570	C496	Q416	W353
	L1184	L1184	F1119	S1039	F970	T889	P812		N644	L572	S497	H417	A354
	V1245	V1245	G1120	I1040	D971	G890	R813	R728	S645	Q573	W499	A418	P355
	E1246	E1246	F1121	L1042	T972	T891	H814		K646	D647	A501	A419	I356
	V1316	V1316	T1122	A1042	R973	L892	L815	F730	D647	D575	G500	L420	P355
	G1317	G1317	P1123	P1043	A974	W893	F816		W649			P421	I356
	N1318	N1318										R422	H360

GLY	ALA	ILE	LEU	ALA	V2058	L1980	L1893	K1815	V1671	G1597	R1523	M1456	V1390	G1319
ALA	VAL	GLU	SER	VAL	G2059	E1981	G1894	I1818	L1672	M1598	Q1527	V1457	R1394	A1320
CYS	ALA	GLY	SER	ALA	G2060	T1984	G1895	I1818	L1673	L1599	T1528	M1458	R1394	A1321
VAL	ILE	THR	LYS	THR	T1984	HIS	G1896	V1822	H1674	E1602	E1529	C1459	S1395	A1322
PHE	THR	THR	THR	THR	P1985	P1985	F1897	V1823	G1675	F1603	H1530	R1460	F1396	T1323
GLU	GLY	VAL	THR	GLY	E1986	G1897	G1897	V1823	G1676	R1606	E1531	R1461	T1324	L1324
MET	GLY	PHE	ASP	ILE	F1987	F1988	Q1824	Q1824	S1677	F1603	A1531	K1462	G1398	G1325
HIS	ARG	HIS	ALA	ARG	F1988	V1988	P1825	P1825	G1678	R1606	F1532	E1463	S1399	D1326
CYS	ASP	ASP	ALA	ASP	V1991	V1991	R1833	R1833	G1679	R1606	V1533	P1464	V1400	P1327
LEU	ASP	ASP	PRO	VAL	L1903	L1903	G1894	G1894	R1680	R1611	N1534	G1465	F1402	A1330
GLN	VAL	GLY	PRO	VAL	L1904	L1904	R1905	R1905	G1681	R1612	V1535	G1466	F1402	A1330
LEU	ALA	ALA	ALA	ALA	R1905	R1905	G1906	G1906	G1682	V1613	L1403	H1467	V1331	V1331
GLN	THR	THR	THR	THR	L1906	L1906	A1837	A1837	A1684	M1614	C1404	G1468	G1332	G1332
ALA	ILE	ILE	PRO	ILE	A1838	A1838	A1839	A1839	A1684	G1615	A1405	I1469	N1333	N1333
LEU	SER	SER	THR	SER	A1839	A1839	F1840	F1840	I1685	M1616	Q1406	R1470	Q1406	M1334
LEU	PRO	PRO	THR	PRO	R1841	R1841	G1770	G1770	A1686	P1617	T1407	C1471	Q1407	Q1407
ILE	ASP	ASP	HIS	ASP	R1842	R1842	R1765	R1765	I1687	P1618	L1472	T1408	P1409	T1337
PRO	SER	SER	GLU	SER	V1942	V1942	R1766	R1766	V1695	L1622	S1543	L1473	P1409	L1338
THR	THR	THR	ASP	THR	R1943	R1943	L1767	L1767	V1696	I1623	I1544	V1474	Q1410	L1339
THR	THR	THR	SER	THR	A1844	A1844	E1768	E1768	F1696	A1624	R1546	S1475	D1411	E1340
GLY	VAL	VAL	PRO	VAL	Q1845	Q1845	I1769	I1769	T1697	T1624	W1545	M1476	S1412	G1342
ASP	ASP	ASP	VAL	ASP	G1846	G1846	G1770	G1770	T1699	T1624	S1549	L1477	P1413	F1343
GLN	GLY	GLY	GLN	GLY	K1847	K1847	K1771	K1771	V1699	T1624	A1554	T1480	L1416	L1344
THR	THR	THR	GLN	THR	H1848	H1848	L1774	L1774	F1699	L1628	L1555	A1481	S1417	L1345
LEU	ASP	ASP	ALA	ASP	K1851	K1851	S1775	S1775	T1697	L1628	L1555	L1346	V1418	L1346
ALA	THR	THR	THR	THR	V1852	V1852	M1776	M1776	H1631	A1632	P1556	P1484	E1419	H1347
ALA	THR	THR	THR	THR	G1923	G1923	H1777	H1777	A1632	A1632	A1557	E1485	D1420	T1348
THR	SER	SER	LEU	SER	Q1924	Q1924	H1778	H1778	V1699	T1633	S1558	M1486	T1421	L1349
LEU	LEU	LEU	GLY	LEU	A1926	A1926	H1778	H1778	T1699	T1633	C1559	H1487	S1422	L1350
LEU	GLY	GLY	LEU	GLY	R1927	R1927	Q1855	Q1855	E1703	V1636	Q1560	P1488	S1422	L1351
GLY	ASP	ASP	VAL	VAL	V1856	V1856	G1781	G1781	K1704	V1636	D1581	P1488	R1424	A1351
SER	THR	THR	THR	THR	R1857	R1857	M1782	M1782	R1705	V1636	D1581	P1488	R1424	G1382
HIS	THR	THR	THR	THR	E1858	E1858	A1783	A1783	R1706	T1639	L1562	L1493	W1425	H1383
THR	THR	THR	THR	THR	V1931	V1931	F1784	F1784	A1706	V1640	C1564	Q1494	V1426	P1354
THR	THR	THR	THR	THR	E1859	E1859	V1784	V1784	R1711	L1641	C1564	K1495	D1427	P1354
THR	THR	THR	THR	THR	I1860	I1860	F1785	F1785	F1712	L1642	S1566	V1496	S1428	G1360
THR	THR	THR	THR	THR	Q1861	Q1861	L1786	L1786	F1712	L1642	S1566	V1496	S1428	F1361
THR	THR	THR	THR	THR	G1862	G1862	K1787	K1787	F1712	L1642	S1566	V1496	S1428	L1362
THR	THR	THR	THR	THR	P1863	P1863	K1788	K1788	F1712	L1642	S1566	V1496	S1428	T1363
THR	THR	THR	THR	THR	A1864	A1864	V1789	V1789	C1719	E1644	Y1567	G1499	D1431	S1364
THR	THR	THR	THR	THR	P1865	P1865	F1790	F1790	F1720	S1647	T1569	D1500	D1432	P1365
THR	THR	THR	THR	THR	L1868	L1868	H1791	H1791	A1721	S1647	T1569	D1500	D1432	P1365
THR	THR	THR	THR	THR	P1869	P1869	H1792	H1792	M1722	V1648	L1570	M1503	L1433	P1365
THR	THR	THR	THR	THR	I1955	I1955	G1793	G1793	S1723	P1649	L1571	M1504	S1437	E1367
THR	THR	THR	THR	THR	L1956	L1956	L1794	L1794	D1725	P1649	N1572	N1504	S1437	Q1367
THR	THR	THR	THR	THR	I1957	I1957	L1795	L1795	D1725	P1649	N1572	N1504	S1437	Q1367
THR	THR	THR	THR	THR	I1871	I1871	L1796	L1796	T1726	Y1651	F1573	Y1506	R1439	G1368
THR	THR	THR	THR	THR	P1870	P1870	D1797	D1797	T1727	Y1651	F1573	Y1506	R1439	G1368
THR	THR	THR	THR	THR	L1873	L1873	L1797	L1797	S1727	T1653	R1574	R1507	P1440	G1369
THR	THR	THR	THR	THR	G1874	G1874	S1798	S1798	E1729	Y1656	M1577	D1508	V1441	H1371
THR	THR	THR	THR	THR	I1875	I1875	L1799	L1799	E1729	Y1657	A1579	G1509	V1441	H1371
THR	THR	THR	THR	THR	L1876	L1876	F1800	F1800	V1732	S1658	T1580	G1512	W1442	L1372
THR	THR	THR	THR	THR	S1877	S1877	E1801	E1801	R1734	Y1661	K1581	A1513	L1443	L1373
THR	THR	THR	THR	THR	P1882	P1882	E1802	E1802	R1734	R1662	L1583	F1514	W1443	L1373
THR	THR	THR	THR	THR	G1803	G1803	H1735	H1735	R1735	R1662	L1583	F1514	W1443	L1373
THR	THR	THR	THR	THR	Q1804	Q1804	G1804	G1804	T1736	G1663	S1584	R1515	S1449	S1374
THR	THR	THR	THR	THR	K1885	K1885	V1810	V1810	K1739	Y1665	P1585	H1516	T1450	S1374
THR	THR	THR	THR	THR	S1886	S1886	V1810	V1810	K1739	Y1665	P1585	H1516	T1450	S1374
THR	THR	THR	THR	THR	Y1887	Y1887	S1811	S1811	G1740	Q1666	S1587	F1517	G1452	S1386
THR	THR	THR	THR	THR	V1888	V1888	E1812	E1812	V1741	Q1666	S1587	F1517	G1452	S1386
THR	THR	THR	THR	THR	L1813	L1813	L1813	L1813	D1742	E1669	T1588	E1520	V1453	L1387
THR	THR	THR	THR	THR	T1890	T1890	L1814	L1814	L1743	S1670	D1596	Q1521	V1453	L1388
THR	THR	THR	THR	THR	V1979	V1979	L1814	L1814	L1743	S1670	D1596	Q1521	V1453	L1388
THR	THR	THR	THR	THR	V1979	V1979	L1814	L1814	L1743	S1670	D1596	Q1521	V1453	L1388

PHE	ALA
PHE	GLU
VAL	ASN
GLN	TYR
GLN	TRP
PHE	PRO
THR	GLN
ASP	ALA
MET	THR
GLU	TYR
GLN	HIS
GLY	CYS
LYS	LEU
VAL	ALA
LEU	GLU
GLU	PRO
ALA	ARG
LEU	VAL
ARG	SER
ILE	VAL
PRO	ARG
LEU	GLU
GLN	GLY
GLY	ALA
GLY	ALA
ALA	LEU
LEU	TYR
ALA	GLY
ARG	GLU
VAL	ASP
ALA	LEU
ALA	GLY
THR	LYS
VAL	VAL
ASP	SER
ASP	VAL
TYR	HIS
ASN	VAL
LEU	VAL
ILE	ILE
THR	SER
GLN	GLN
SER	VAL
HIS	CYS
ALA	ASP
GLY	GLY
LEU	LYS
ASP	VAL
ARG	SER
ARG	VAL
HIS	HIS
ARG	VAL
SER	ILE
THR	SER
PHE	THR
ALA	LEU
ALA	LEU
ALA	GLN
ALA	LYS
ALA	GLY
ALA	LEU
ALA	SER
ALA	ARG
ALA	GLY

LEU
GLU
SER
ILE
LEU
SER
ILE
ILE
HIS
SER
CYS
LEU
ALA
GLU
PRO
ARG
VAL
SER
VAL
ARG
GLU
GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.15Å 244.89Å 135.37Å 90.00° 101.84° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 29.97 – 3.34	Depositor EDS
% Data completeness (in resolution range)	84.1 (30.00-3.30) 90.2 (29.97-3.34)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.31Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.193 , 0.244 0.184 , 0.235	Depositor DCC
R_{free} test set	4016 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	117.6	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 87.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31949	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (2282) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:GLU:HB2	1:B:334:PRO:HD3	1.26	1.17
1:A:333:GLU:HB2	1:A:334:PRO:HD3	1.28	1.13
1:A:616:LEU:HD23	1:A:617:PRO:HD2	1.32	1.10
1:A:123:ASP:HB3	1:A:126:THR:HB	1.18	1.10
1:A:1477:LEU:HD11	1:A:2043:ARG:HD2	1.36	1.06
1:B:1662:ARG:HG2	1:B:1662:ARG:HH11	0.90	1.03
1:B:1216:LEU:HD12	1:B:1218:SER:H	1.20	1.03
1:A:343:LYS:HE3	1:A:354:ALA:HB3	1.40	1.03
1:A:1190:LEU:HD13	1:A:1206:GLN:HE21	1.23	1.02
1:A:112:SER:HB2	1:A:334:PRO:HG3	1.39	1.02
1:B:112:SER:HB2	1:B:334:PRO:HG3	1.38	1.02
1:A:384:ARG:HH11	1:A:384:ARG:HG3	1.22	1.02
1:B:384:ARG:HH11	1:B:384:ARG:HG3	1.20	1.02
1:B:278:ALA:HB3	1:B:279:PRO:HD3	1.40	1.01
1:A:165:LEU:HD23	1:A:400:VAL:HG22	1.42	1.00
1:B:643:HIS:HA	1:B:649:VAL:HG22	1.41	1.00
1:B:1616:MET:HB3	1:B:1800:PHE:CZ	1.97	0.99
1:A:278:ALA:HB3	1:A:279:PRO:HD3	1.44	0.99
1:B:1662:ARG:NH1	1:B:1662:ARG:HG2	1.65	0.98
1:B:1003:TYR:CZ	1:B:1037:HIS:HE1	1.82	0.97
1:B:1220:LEU:HB3	1:B:1257:ARG:HH22	1.30	0.96
1:A:1216:LEU:HD12	1:A:1218:SER:H	1.31	0.95
1:B:1653:THR:HG22	1:B:1810:VAL:HG12	1.48	0.94
1:A:166:LEU:HD12	1:A:251:THR:HG21	1.50	0.94
1:B:165:LEU:HD23	1:B:400:VAL:HG22	1.51	0.93
1:B:1418:VAL:HG13	1:B:1425:TRP:CE2	2.03	0.93
1:B:1184:LEU:H	1:B:1216:LEU:HD21	1.32	0.93
1:B:333:GLU:HB2	1:B:334:PRO:CD	1.99	0.92
1:B:166:LEU:HD12	1:B:251:THR:HG21	1.51	0.92
1:A:1624:THR:HG22	1:A:1857:ARG:HH21	1.35	0.92
1:A:1790:THR:HG22	1:B:1662:ARG:HH22	1.33	0.92
1:A:1003:TYR:CE2	1:A:1037:HIS:HE1	1.87	0.92
1:A:1528:THR:HG22	1:A:1530:HIS:H	1.35	0.91
1:B:1616:MET:HE2	1:B:1650:ILE:HD13	1.53	0.91
1:A:1003:TYR:CZ	1:A:1037:HIS:HE1	1.89	0.90
1:B:1662:ARG:HH11	1:B:1662:ARG:CG	1.82	0.90
1:A:1133:ASN:HD22	1:A:1136:LEU:HD12	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1182:ARG:HB3	1:A:1216:LEU:HB2	1.52	0.90
1:B:1003:TYR:CE2	1:B:1037:HIS:HE1	1.88	0.90
1:B:1628:LEU:HD13	1:B:1633:THR:HG21	1.54	0.90
1:A:443:ARG:HH11	1:A:443:ARG:HG3	1.38	0.88
1:A:1349:LEU:HD13	1:A:1359:VAL:HG21	1.56	0.88
1:A:126:THR:HG22	1:A:127:LEU:HG	1.56	0.88
1:A:1545:ARG:HH11	1:A:1545:ARG:HG3	1.38	0.87
1:B:1475:SER:HB3	1:B:1505:VAL:HG13	1.53	0.87
1:A:1082:VAL:HG22	1:A:1089:VAL:HG22	1.56	0.87
1:B:1208:ARG:HH11	1:B:1211:LEU:HD22	1.39	0.87
1:B:1838:ALA:HA	1:B:1841:ARG:HG3	1.57	0.87
1:A:333:GLU:HB2	1:A:334:PRO:CD	2.04	0.86
1:B:443:ARG:HH11	1:B:443:ARG:HG3	1.40	0.86
1:A:319:PRO:HD2	1:A:373:ARG:O	1.74	0.86
1:B:1232:THR:HA	1:B:1515:ARG:HH21	1.40	0.86
1:A:1222:ASP:HB3	1:A:1257:ARG:CZ	2.07	0.85
1:A:1838:ALA:HA	1:A:1841:ARG:HG3	1.58	0.85
1:B:1315:LEU:O	1:B:1344:LEU:HD13	1.76	0.85
1:A:123:ASP:CB	1:A:126:THR:HB	2.06	0.85
1:B:1569:THR:HG21	1:B:1622:LEU:HA	1.59	0.85
1:A:502:GLN:HG2	1:A:556:LEU:HD11	1.59	0.84
1:A:1893:LEU:HB3	1:A:1925:GLN:NE2	1.92	0.84
1:A:527:LEU:HD12	1:A:534:VAL:HG22	1.59	0.84
1:B:319:PRO:HD2	1:B:373:ARG:O	1.76	0.84
1:A:82:LEU:O	1:A:86:THR:HG23	1.78	0.84
1:B:782:ILE:HD12	1:B:803:LEU:HD23	1.60	0.84
1:B:1326:ASP:OD1	1:B:1327:PRO:HD2	1.76	0.84
1:B:527:LEU:HD12	1:B:534:VAL:HG22	1.56	0.84
1:A:1009:LEU:HD11	1:A:1030:SER:HB2	1.58	0.83
1:A:1124:HIS:CD2	1:A:1512:GLY:HA2	2.13	0.83
1:B:1651:VAL:HG13	1:B:1680:VAL:HA	1.60	0.83
1:B:87:TYR:O	1:B:91:VAL:HG22	1.77	0.83
1:A:1771:LYS:HE2	1:A:1795:LEU:HD22	1.61	0.83
1:A:1034:ALA:HA	1:A:1037:HIS:CD2	2.12	0.83
1:A:1662:ARG:HH11	1:A:1662:ARG:CG	1.91	0.83
1:A:782:ILE:HD12	1:A:803:LEU:HD23	1.61	0.83
1:A:976:VAL:HG22	1:A:977:ASP:H	1.44	0.82
1:B:1486:MET:O	1:B:1488:PRO:HD3	1.78	0.82
1:B:82:LEU:O	1:B:86:THR:HG23	1.78	0.82
1:A:1505:VAL:HG23	1:A:1513:ALA:HA	1.61	0.82
1:B:680:ILE:HG12	1:B:681:ALA:N	1.94	0.82

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1662:ARG:HH11	1:A:1662:ARG:HG2	1.57	0.68
1:B:1180:LEU:HD23	1:B:1189:GLN:HE22	1.58	0.68
1:B:1036:LEU:HD21	1:B:1096:PHE:HE1	1.58	0.68
1:B:54:LEU:HG	1:B:226:GLU:HG3	1.76	0.68
1:B:333:GLU:CB	1:B:334:PRO:HD3	2.15	0.68
1:A:1034:ALA:O	1:A:1037:HIS:HB2	1.93	0.68
1:A:502:GLN:HG2	1:A:556:LEU:CD1	2.22	0.68
1:B:1361:PHE:O	1:B:1362:LEU:HD12	1.94	0.68
1:B:1554:ALA:HB2	1:B:1882:PRO:HG3	1.76	0.68
1:B:1703:GLU:O	1:B:1706:ALA:HB3	1.94	0.68
1:B:615:VAL:HG22	1:B:686:PHE:HD2	1.57	0.68
1:A:941:SER:HB2	1:B:945:GLU:OE2	1.93	0.68
1:A:1146:LEU:HD13	1:A:1189:GLN:HG2	1.75	0.68
1:A:808:VAL:HG12	1:A:809:SER:N	2.08	0.68
1:B:420:LEU:HD11	1:B:512:ARG:HD2	1.76	0.68
1:B:1060:ASP:OD1	1:B:1062:VAL:HG23	1.93	0.68
1:B:159:THR:CG2	1:B:398:SER:HB3	2.22	0.68
1:B:502:GLN:CG	1:B:556:LEU:HD11	2.23	0.68
1:A:1705:ARG:HG2	1:A:1720:PHE:HD2	1.59	0.68
1:A:50:ARG:HD3	1:A:210:GLY:O	1.94	0.68
1:B:1214:ASP:HB3	1:B:1215:PRO:HD3	1.74	0.68
1:A:1252:GLY:HA2	1:A:1318:ASN:HD22	1.59	0.68
1:A:953:LEU:HD12	1:A:954:ILE:N	2.09	0.68
1:B:1363:THR:HG22	1:B:1363:THR:O	1.93	0.68
1:A:976:VAL:O	1:A:978:PRO:HD3	1.93	0.68
1:B:1472:VAL:HG13	1:B:1502:VAL:O	1.94	0.68
1:B:1477:LEU:HD11	1:B:2043:ARG:HD2	1.74	0.68
1:A:1732:VAL:O	1:A:1736:THR:HB	1.93	0.67
1:A:1778:HIS:O	1:B:1782:MET:HB2	1.94	0.67
1:A:1009:LEU:CD1	1:A:1030:SER:HB2	2.23	0.67
1:A:1302:ALA:O	1:A:1303:ASN:HB2	1.92	0.67
1:B:1003:TYR:CE2	1:B:1037:HIS:CE1	2.78	0.67
1:B:917:VAL:CG1	1:B:1054:PHE:HB2	2.24	0.67
1:B:159:THR:HG22	1:B:159:THR:O	1.94	0.67
1:B:550:VAL:HG23	1:B:611:LYS:HD3	1.75	0.67
1:A:1248:LEU:HB3	1:A:1321:LEU:HD23	1.76	0.67
1:B:752:VAL:HG11	1:B:775:LEU:HD21	1.76	0.67
1:B:1457:VAL:HG21	1:B:1473:LEU:HD22	1.77	0.67
1:A:1268:MET:HA	1:A:1268:MET:HE2	1.76	0.67
1:A:1275:THR:CG2	1:A:1299:TRP:HB2	2.24	0.67
1:B:1252:GLY:HA3	1:B:1318:ASN:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1554:ALA:O	1:B:1556:PRO:HD3	1.93	0.67
1:B:1454:VAL:HG13	1:B:1503:MET:CE	2.25	0.67
1:B:953:LEU:HD12	1:B:954:ILE:N	2.09	0.67
1:A:1234:LEU:HD22	1:A:1262:LEU:HD22	1.76	0.67
1:A:254:ASP:HB2	1:A:257:LYS:HE2	1.76	0.67
1:B:98:ALA:HA	1:B:101:ARG:HG3	1.77	0.67
1:B:47:LEU:HA	1:B:201:MET:HE1	1.76	0.67
1:B:502:GLN:HG2	1:B:556:LEU:CD1	2.24	0.67
1:A:1247:VAL:HG23	1:A:1315:LEU:HD11	1.75	0.67
1:A:1457:VAL:HG11	1:A:1473:LEU:HD22	1.76	0.67
1:B:1387:LEU:HD23	1:B:1406:GLN:HB3	1.76	0.67
1:B:1585:PRO:HB3	1:B:1598:MET:CE	2.25	0.67
1:A:157:ILE:HD11	1:A:167:ALA:HA	1.77	0.67
1:B:570:LEU:HB3	1:B:810:VAL:HB	1.77	0.67
1:B:1705:ARG:HG2	1:B:1720:PHE:HD2	1.60	0.67
1:A:1353:HIS:HB3	1:A:1354:PRO:HD2	1.77	0.66
1:A:2075:THR:HG22	1:A:2076:ASN:H	1.60	0.66
1:B:1887:TYR:CD2	1:B:1967:GLY:HA3	2.30	0.66
1:B:288:GLU:HG3	1:B:385:GLY:O	1.95	0.66
1:B:420:LEU:CD1	1:B:512:ARG:HD2	2.26	0.66
1:A:1703:GLU:O	1:A:1706:ALA:HB3	1.94	0.66
1:A:460:VAL:HG21	1:A:465:MET:HG3	1.78	0.66
1:B:1344:LEU:HD12	1:B:1346:LEU:HD21	1.77	0.66
1:B:1725:ASP:OD1	1:B:1726:THR:N	2.28	0.66
1:B:359:TYR:OH	1:B:362:PRO:HG3	1.95	0.66
1:A:1350:LEU:O	1:A:1356:GLY:HA3	1.95	0.66
1:B:217:ALA:HB2	1:B:364:PRO:HD3	1.78	0.66
1:B:581:SER:HB2	1:B:683:HIS:NE2	2.10	0.66
1:A:1350:LEU:HD22	1:A:1373:LEU:O	1.96	0.66
1:A:289:TYR:HB3	1:A:388:VAL:HG22	1.76	0.66
1:B:2006:THR:HG21	1:B:2048:ARG:HH22	1.60	0.66
1:A:2053:LEU:HD22	1:A:2054:PRO:HD2	1.76	0.66
1:B:2075:THR:HG22	1:B:2076:ASN:H	1.59	0.66
1:A:78:GLN:HB3	1:A:188:LEU:HD13	1.77	0.66
1:A:56:ASP:OD2	1:A:59:ARG:HD3	1.96	0.66
1:B:1409:PRO:HB2	1:B:1439:ARG:HH12	1.61	0.66
1:B:1653:THR:HG22	1:B:1810:VAL:CG1	2.25	0.66
1:B:289:TYR:HB3	1:B:388:VAL:HG22	1.78	0.66
1:B:499:MET:SD	1:B:502:GLN:NE2	2.68	0.66
1:A:1890:THR:HA	1:A:1915:THR:HB	1.76	0.66
1:A:77:PRO:O	1:A:81:MET:HG2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1036:LEU:CD2	1:B:1096:PHE:HE1	2.09	0.66
1:A:1486:MET:CE	1:A:1506:TYR:HB3	2.26	0.66
1:A:1533:VAL:CG1	1:A:1622:LEU:HB3	2.25	0.65
1:B:215:PHE:CD2	1:B:305:LEU:HD11	2.31	0.65
1:A:545:VAL:HG22	1:A:551:SER:CB	2.26	0.65
1:A:64:PHE:HB2	1:A:429:ARG:HH21	1.61	0.65
1:B:263:PHE:HE2	1:B:303:GLN:HE21	1.44	0.65
1:A:1183:LEU:HB3	1:A:1216:LEU:HD23	1.78	0.65
1:A:1357:GLU:O	1:A:1361:PHE:CD1	2.48	0.65
1:B:82:LEU:HG	1:B:144:LEU:HD13	1.78	0.65
1:A:1783:ALA:H	1:B:1777:ASN:HD22	1.44	0.65
1:A:1484:PRO:O	1:A:1485:GLU:HB2	1.97	0.65
1:A:165:LEU:HB2	1:A:337:GLY:HA3	1.78	0.65
1:A:503:TRP:CD1	1:A:787:LYS:HB2	2.32	0.65
1:B:1009:LEU:CD1	1:B:1030:SER:HB2	2.26	0.65
1:B:1674:HIS:CD2	1:B:1698:THR:OG1	2.50	0.65
1:A:1060:ASP:OD1	1:A:1062:VAL:HG23	1.95	0.65
1:A:98:ALA:HA	1:A:101:ARG:HG3	1.79	0.65
1:B:2064:GLY:O	1:B:2066:VAL:N	2.24	0.65
1:A:118:GLU:HG3	1:B:118:GLU:HG3	1.77	0.65
1:A:1483:ALA:N	1:A:1484:PRO:HD3	2.11	0.65
1:A:1888:VAL:HG22	1:A:1913:VAL:HB	1.78	0.65
1:A:254:ASP:CB	1:A:257:LYS:HE2	2.27	0.65
1:B:1207:GLU:O	1:B:1211:LEU:HB2	1.96	0.65
1:B:1566:VAL:HG12	1:B:1856:VAL:HG21	1.77	0.65
1:B:254:ASP:CB	1:B:257:LYS:HE2	2.27	0.65
1:B:368:ALA:N	1:B:371:ASP:HB3	2.11	0.65
1:B:443:ARG:HG3	1:B:443:ARG:NH1	2.08	0.65
1:A:1140:LEU:HD21	1:A:1354:PRO:HG2	1.77	0.65
1:B:1374:SER:HB2	1:B:1377:GLN:HG3	1.79	0.65
1:B:1975:LEU:HD22	1:B:1977:ASP:OD1	1.96	0.65
1:A:1208:ARG:HH11	1:A:1211:LEU:CD2	2.11	0.64
1:A:1926:ALA:O	1:A:1930:ARG:HB2	1.95	0.64
1:B:1603:PHE:HE2	1:B:1615:GLY:C	2.00	0.64
1:B:662:LEU:HD13	1:B:672:VAL:HG12	1.79	0.64
1:A:1476:ASN:HA	1:A:1486:MET:SD	2.37	0.64
1:A:1574:ARG:HD2	1:A:1588:ILE:HD11	1.79	0.64
1:A:366:ILE:HD11	1:A:369:LEU:HD11	1.78	0.64
1:B:1470:ARG:HG3	1:B:1470:ARG:O	1.97	0.64
1:A:1887:TYR:CD2	1:A:1967:GLY:HA3	2.31	0.64
1:B:1374:SER:O	1:B:1378:TRP:HD1	1.81	0.64

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1995:LYS:HB3	1:A:2041:MET:SD	2.41	0.61
1:B:1570:SER:HB3	1:B:1853:VAL:HG22	1.83	0.61
1:A:159:THR:O	1:A:159:THR:HG22	2.00	0.61
1:A:1802:GLU:O	1:A:1802:GLU:HG2	2.01	0.61
1:B:1216:LEU:CD1	1:B:1218:SER:H	2.04	0.61
1:B:1888:VAL:HG22	1:B:1913:VAL:HB	1.82	0.61
1:A:890:GLY:HA2	1:A:1029:VAL:HG13	1.83	0.60
1:A:1528:THR:CG2	1:A:1530:HIS:H	2.12	0.60
1:A:1585:PRO:HB3	1:A:1598:MET:CE	2.30	0.60
1:A:259:GLN:HB2	1:A:263:PHE:CD1	2.35	0.60
1:B:1200:LEU:O	1:B:1203:VAL:HG23	2.00	0.60
1:B:252:ASN:ND2	1:B:272:LEU:HB2	2.15	0.60
1:A:1316:VAL:HG13	1:A:1345:LEU:HB3	1.82	0.60
1:B:1694:ARG:HH11	1:B:1694:ARG:HG3	1.67	0.60
1:B:236:LYS:HG3	1:B:237:SER:H	1.64	0.60
1:B:295:THR:HG22	1:B:331:HIS:CD2	2.36	0.60
1:B:662:LEU:HD22	1:B:672:VAL:CG1	2.32	0.60
1:B:994:LYS:HA	1:B:997:ARG:NH1	2.16	0.60
1:B:1011:LEU:HD21	1:B:1023:GLN:HB2	1.83	0.60
1:B:117:SER:HB3	1:B:135:CYS:HB3	1.82	0.60
1:B:215:PHE:CE2	1:B:305:LEU:HD11	2.36	0.60
1:B:491:PRO:HD2	1:B:756:ALA:HA	1.83	0.60
1:A:671:PHE:HE2	1:A:773:ARG:NH2	1.95	0.60
1:A:1476:ASN:ND2	1:A:1486:MET:HE2	2.17	0.60
1:B:1429:LEU:HD11	1:B:1443:LEU:HD11	1.84	0.60
1:B:1736:THR:CG2	1:B:1740:GLY:H	2.14	0.60
1:B:1955:LEU:O	1:B:1958:GLU:HB2	2.01	0.60
1:B:861:VAL:CG2	1:B:934:GLU:HB3	2.31	0.60
1:A:861:VAL:CG2	1:A:934:GLU:HB3	2.32	0.60
1:B:442:LEU:HD23	1:B:473:LEU:HD22	1.84	0.60
1:B:64:PHE:HB2	1:B:429:ARG:HH21	1.65	0.60
1:A:1259:PRO:HB2	1:A:1292:LEU:HD22	1.83	0.60
1:B:1423:PHE:O	1:B:1985:PRO:HB3	2.02	0.60
1:B:1569:THR:CG2	1:B:1622:LEU:HD23	2.31	0.60
1:B:353:TRP:HH2	1:B:388:VAL:HG21	1.67	0.60
1:A:118:GLU:HG3	1:B:118:GLU:CG	2.32	0.60
1:A:1182:ARG:NH2	1:A:1217:LEU:HB3	2.17	0.60
1:A:207:SER:OG	1:A:209:ASP:HB3	2.02	0.60
1:B:1857:ARG:CZ	1:B:1871:ILE:HD11	2.31	0.60
1:B:123:ASP:O	1:B:127:LEU:HB3	2.01	0.60
1:B:1320:ALA:O	1:B:1321:LEU:HG	2.01	0.60

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1456:MET:CG	1:B:2036:PHE:HB2	2.32	0.59
1:B:1574:ARG:HD2	1:B:1588:ILE:HD11	1.85	0.59
1:A:117:SER:HB2	1:A:135:CYS:HB3	1.85	0.58
1:A:1496:VAL:HG21	1:A:1511:TRP:CH2	2.38	0.58
1:A:1514:PHE:O	1:A:1515:ARG:NH1	2.35	0.58
1:A:1955:LEU:O	1:A:1958:GLU:HB2	2.02	0.58
1:A:200:PHE:HB3	1:A:206:LEU:HD12	1.83	0.58
1:A:672:VAL:HG12	1:A:672:VAL:O	2.01	0.58
1:B:1351:ALA:HB3	1:B:1372:LEU:O	2.03	0.58
1:B:1361:PHE:CE2	1:B:1370:ARG:HD3	2.37	0.58
1:A:1711:ARG:HG2	1:A:1712:PHE:CE1	2.37	0.58
1:A:442:LEU:HD23	1:A:473:LEU:HD22	1.84	0.58
1:A:82:LEU:HG	1:A:144:LEU:CD1	2.33	0.58
1:A:859:VAL:HG13	1:A:936:ARG:HG2	1.84	0.58
1:B:1442:TRP:HB3	1:B:1444:MET:HE1	1.85	0.58
1:B:1603:PHE:CD2	1:B:1603:PHE:N	2.69	0.58
1:B:1711:ARG:HG2	1:B:1712:PHE:CE1	2.38	0.58
1:B:2070:LEU:HD11	1:B:2076:ASN:HD21	1.68	0.58
1:A:1204:LEU:HD11	1:A:1365:PRO:HG2	1.85	0.58
1:A:1533:VAL:HG12	1:A:1622:LEU:HB3	1.85	0.58
1:B:1303:ASN:H	1:B:1304:PRO:CD	2.16	0.58
1:B:1720:PHE:N	1:B:1720:PHE:CD1	2.70	0.58
1:A:1001:TYR:HB3	1:A:1003:TYR:CD1	2.37	0.58
1:A:1472:VAL:HG12	1:A:1473:LEU:N	2.17	0.58
1:B:251:THR:HB	1:B:399:ASN:O	2.03	0.58
1:B:290:ILE:HD13	1:B:308:ILE:HD13	1.85	0.58
1:B:423:LEU:HB2	1:B:797:LEU:HD22	1.84	0.58
1:A:1528:THR:HG22	1:A:1530:HIS:N	2.14	0.58
1:A:322:ILE:O	1:A:377:VAL:HG23	2.03	0.58
1:B:1338:LEU:HD13	1:B:1406:GLN:HG3	1.85	0.58
1:B:594:LEU:HD13	1:B:599:ALA:HA	1.84	0.58
1:B:1276:ASP:O	1:B:1299:TRP:N	2.36	0.58
1:B:1364:SER:N	1:B:1365:PRO:CD	2.67	0.58
1:B:1794:ILE:O	1:B:1795:LEU:HD23	2.03	0.58
1:B:254:ASP:HB2	1:B:257:LYS:HE2	1.84	0.58
1:B:426:ALA:HA	1:B:458:ALA:HB2	1.86	0.58
1:A:36:ASP:HB3	1:A:38:ARG:HG3	1.86	0.58
1:A:553:PHE:CD2	1:A:582:LEU:HD13	2.38	0.58
1:A:1457:VAL:HG21	1:A:1473:LEU:HB3	1.86	0.58
1:A:423:LEU:HD23	1:A:812:PRO:HG3	1.85	0.58
1:B:1995:LYS:HB3	1:B:2041:MET:SD	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:THR:HG22	1:B:235:LYS:O	2.03	0.58
1:A:1656:TYR:CD2	1:A:1687:ILE:HD13	2.39	0.58
1:A:1842:TYR:CE2	1:A:1848:HIS:HB3	2.39	0.58
1:A:188:LEU:HD22	1:A:228:VAL:HG12	1.85	0.58
1:A:200:PHE:CD2	1:B:132:MET:HE1	2.38	0.58
1:A:997:ARG:HA	1:A:1001:TYR:O	2.04	0.58
1:B:1824:GLN:HG3	1:B:1825:PRO:HD2	1.86	0.58
1:B:655:GLN:O	1:B:655:GLN:HG2	2.03	0.58
1:A:1275:THR:HG22	1:A:1299:TRP:HB2	1.85	0.58
1:A:586:ALA:O	1:A:589:TYR:HB3	2.03	0.58
1:B:1322:ALA:HB1	1:B:1371:HIS:CE1	2.39	0.58
1:B:1461:ARG:HG3	1:B:1461:ARG:O	2.04	0.58
1:B:640:PRO:HA	1:B:651:ILE:HG22	1.85	0.58
1:A:426:ALA:HA	1:A:458:ALA:HB2	1.85	0.57
1:B:1214:ASP:OD2	1:B:1321:LEU:HD21	2.04	0.57
1:B:1802:GLU:O	1:B:1804:GLY:N	2.37	0.57
1:A:856:CYS:CB	1:B:856:CYS:HG	2.16	0.57
1:B:982:THR:O	1:B:984:GLU:N	2.34	0.57
1:A:1735:HIS:CD2	1:A:1735:HIS:H	2.21	0.57
1:A:765:ALA:HB1	1:A:768:GLN:HG3	1.85	0.57
1:B:997:ARG:HA	1:B:1001:TYR:O	2.04	0.57
1:B:993:TYR:CZ	1:B:1008:GLN:HA	2.39	0.57
1:B:1222:ASP:HA	1:B:1226:LEU:CD1	2.34	0.57
1:B:1836:VAL:HG13	1:B:1854:ILE:CD1	2.33	0.57
1:B:111:VAL:CG2	1:B:188:LEU:HB2	2.33	0.57
1:B:48:PRO:HD3	1:B:201:MET:CE	2.34	0.57
1:A:1208:ARG:HA	1:A:1211:LEU:HB2	1.86	0.57
1:A:1273:THR:HA	1:A:1295:THR:O	2.02	0.57
1:A:331:HIS:CE1	1:A:333:GLU:HA	2.39	0.57
1:A:953:LEU:HD12	1:A:954:ILE:H	1.69	0.57
1:B:1220:LEU:CB	1:B:1257:ARG:HH22	2.10	0.57
1:B:662:LEU:HD22	1:B:672:VAL:HG11	1.86	0.57
1:A:1182:ARG:NE	1:A:1217:LEU:H	2.01	0.57
1:A:1137:GLN:NE2	1:A:1396:PHE:CE1	2.72	0.57
1:A:215:PHE:O	1:A:363:ASN:HB2	2.04	0.57
1:B:1208:ARG:HH11	1:B:1211:LEU:CD2	2.14	0.57
1:B:1353:HIS:NE2	1:B:1398:GLY:HA2	2.19	0.57
1:A:1345:LEU:HD12	1:A:1402:PHE:O	2.04	0.57
1:A:273:ILE:O	1:A:277:TYR:HD1	1.87	0.57
1:A:1476:ASN:HA	1:A:1486:MET:HE1	1.85	0.57
1:A:1528:THR:HG21	1:A:1552:HIS:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:THR:O	1:A:160:ALA:HB3	2.05	0.57
1:A:1824:GLN:HG3	1:A:1825:PRO:HD2	1.85	0.57
1:A:91:VAL:HG21	1:A:834:ILE:HD13	1.86	0.57
1:B:1762:GLN:NE2	1:B:1787:LYS:HA	2.19	0.57
1:B:38:ARG:HB2	1:B:53:LYS:HD2	1.87	0.57
1:A:1418:VAL:O	1:A:1418:VAL:HG12	2.04	0.57
1:A:1673:ILE:HD13	1:A:1684:ALA:CB	2.35	0.57
1:A:633:ARG:O	1:A:633:ARG:HG2	2.04	0.57
1:B:1209:PRO:O	1:B:1210:LEU:HG	2.05	0.57
1:A:1001:TYR:HB3	1:A:1003:TYR:CE1	2.39	0.57
1:A:305:LEU:HD23	1:A:308:ILE:HD12	1.85	0.57
1:A:643:HIS:O	1:A:745:PHE:HB3	2.05	0.57
1:B:1299:TRP:CZ2	1:B:1305:ALA:HA	2.40	0.57
1:B:51:MET:CE	1:B:191:LEU:HD13	2.35	0.57
1:A:1674:HIS:NE2	1:A:1756:SER:OG	2.37	0.57
1:A:1836:VAL:HG13	1:A:1854:ILE:CD1	2.35	0.57
1:B:100:LEU:O	1:B:103:THR:OG1	2.23	0.57
1:B:188:LEU:HD22	1:B:228:VAL:HG12	1.87	0.57
1:B:1954:SER:O	1:B:1958:GLU:HG3	2.05	0.57
1:B:2101:GLN:HG3	1:B:2102:PRO:CD	2.35	0.57
1:A:1489:SER:N	1:A:1493:LEU:HD22	2.19	0.56
1:A:1762:GLN:NE2	1:A:1787:LYS:HA	2.20	0.56
1:A:290:ILE:HD13	1:A:308:ILE:HD13	1.87	0.56
1:B:1405:ARG:HH22	1:B:1470:ARG:NH2	2.03	0.56
1:B:1409:PRO:HB2	1:B:1439:ARG:NH1	2.20	0.56
1:B:1647:SER:HA	1:B:1851:LYS:HG3	1.87	0.56
1:B:77:PRO:O	1:B:81:MET:HG2	2.04	0.56
1:A:248:ASN:ND2	1:A:249:ALA:H	2.03	0.56
1:A:627:TRP:CH2	1:A:640:PRO:HB2	2.40	0.56
1:B:1180:LEU:HD23	1:B:1189:GLN:NE2	2.19	0.56
1:B:1565:SER:HB2	1:B:1857:ARG:NH2	2.20	0.56
1:B:1567:TYR:CE1	1:B:1606:ARG:HG3	2.40	0.56
1:B:455:ASN:HB2	1:B:813:ASN:HD21	1.69	0.56
1:A:1528:THR:HG22	1:A:1529:GLU:N	2.19	0.56
1:A:1736:THR:CG2	1:A:1740:GLY:H	2.18	0.56
1:A:1768:GLU:OE1	1:A:1768:GLU:HA	2.05	0.56
1:A:1477:LEU:CD1	1:A:2043:ARG:HD2	2.23	0.56
1:A:343:LYS:CE	1:A:354:ALA:HB3	2.26	0.56
1:B:302:PRO:HA	1:B:366:ILE:HG21	1.85	0.56
1:A:1672:LEU:N	1:A:1741:VAL:HG11	2.19	0.56
1:A:2101:GLN:HG3	1:A:2102:PRO:CD	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LEU:HD23	1:A:381:LEU:HD12	1.86	0.56
1:B:1265:GLN:HE21	1:B:2026:ARG:HH11	1.54	0.56
1:B:1409:PRO:HG2	1:B:1439:ARG:HH12	1.70	0.56
1:B:1570:SER:OG	1:B:1602:GLU:HB3	2.05	0.56
1:B:623:VAL:HG12	1:B:624:GLY:N	2.19	0.56
1:B:627:TRP:HB2	1:B:643:HIS:CE1	2.40	0.56
1:A:1204:LEU:HD21	1:A:1365:PRO:CG	2.34	0.56
1:A:1442:TRP:HB3	1:A:1444:MET:HE1	1.88	0.56
1:A:564:ILE:HD13	1:A:590:ALA:HB2	1.87	0.56
1:B:440:GLN:HG3	1:B:833:HIS:CG	2.39	0.56
1:A:1252:GLY:N	1:A:1321:LEU:HD11	2.20	0.56
1:A:1529:GLU:O	1:A:1529:GLU:HG3	2.05	0.56
1:A:1664:ARG:NH1	1:B:1664:ARG:HD3	2.20	0.56
1:A:1265:GLN:HE21	1:A:2026:ARG:NH1	2.01	0.56
1:B:1183:LEU:HD22	1:B:1213:ASP:O	2.05	0.56
1:B:209:ASP:OD2	1:B:213:ARG:NE	2.38	0.56
1:B:81:MET:HG3	1:B:228:VAL:HG11	1.87	0.56
1:A:889:THR:HG21	1:A:1032:LEU:HB2	1.87	0.56
1:A:1289:LEU:HD22	1:A:1294:VAL:HB	1.86	0.56
1:A:1350:LEU:CD1	1:A:1375:GLN:HG2	2.35	0.56
1:A:1397:TYR:CE1	1:A:1399:SER:HB2	2.41	0.56
1:A:1657:TYR:CZ	1:A:1662:ARG:HD2	2.40	0.56
1:A:1794:ILE:O	1:A:1795:LEU:HD23	2.06	0.56
1:A:251:THR:HB	1:A:399:ASN:O	2.06	0.56
1:B:890:GLY:HA2	1:B:1029:VAL:HG13	1.88	0.56
1:B:1109:GLN:HB3	1:B:1111:HIS:CE1	2.40	0.56
1:B:1413:PRO:CB	1:B:1440:PRO:HB2	2.36	0.56
1:A:883:ARG:HH21	1:A:1107:ARG:HD3	1.71	0.56
1:A:1408:THR:HG23	1:A:1409:PRO:HD2	1.87	0.56
1:A:1851:LYS:HG3	1:A:1852:VAL:N	2.21	0.56
1:A:278:ALA:CB	1:A:279:PRO:CD	2.84	0.56
1:A:118:GLU:CD	1:B:118:GLU:HG3	2.26	0.56
1:B:1275:THR:CG2	1:B:1299:TRP:HB2	2.36	0.56
1:B:1373:LEU:N	1:B:1373:LEU:HD23	2.21	0.56
1:B:1539:GLY:HA2	1:B:1580:THR:O	2.06	0.56
1:B:248:ASN:ND2	1:B:249:ALA:H	2.04	0.56
1:B:572:LEU:HD12	1:B:810:VAL:CG1	2.35	0.56
1:A:1720:PHE:N	1:A:1720:PHE:HD1	2.04	0.56
1:B:1180:LEU:HB2	1:B:1181:PRO:HD3	1.88	0.56
1:B:468:ARG:HD3	1:B:485:VAL:HG21	1.88	0.56
1:A:594:LEU:HD13	1:A:599:ALA:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1237:MET:SD	1:B:1242:MET:HG3	2.46	0.56
1:B:207:SER:HB2	1:B:221:GLY:O	2.06	0.56
1:B:527:LEU:HD12	1:B:534:VAL:CG2	2.32	0.56
1:B:620:MET:CG	1:B:677:THR:HG21	2.35	0.56
1:A:1109:GLN:HB3	1:A:1111:HIS:CE1	2.41	0.56
1:A:1644:GLU:HB3	1:A:1825:PRO:HB3	1.87	0.56
1:A:1653:THR:HG22	1:A:1810:VAL:HG11	1.86	0.56
1:B:665:LEU:HB2	1:B:672:VAL:HG21	1.87	0.56
1:B:1133:ASN:ND2	1:B:1136:LEU:HD12	2.18	0.55
1:B:1275:THR:HG22	1:B:1299:TRP:HB2	1.87	0.55
1:B:1661:VAL:HG21	1:B:1810:VAL:HG22	1.87	0.55
1:B:982:THR:C	1:B:984:GLU:N	2.58	0.55
1:A:1628:LEU:HD13	1:A:1633:THR:HG21	1.88	0.55
1:A:1652:TYR:CD1	1:A:1823:VAL:HB	2.40	0.55
1:A:379:ARG:O	1:A:381:LEU:HG	2.06	0.55
1:A:581:SER:OG	1:A:582:LEU:N	2.37	0.55
1:A:633:ARG:NH2	1:A:668:GLU:OE1	2.39	0.55
1:B:1138:GLU:HG3	1:B:1142:LEU:HD12	1.88	0.55
1:A:132:MET:HE1	1:B:200:PHE:CD2	2.42	0.55
1:A:122:ARG:O	1:A:124:PRO:HD3	2.05	0.55
1:A:1456:MET:HG3	1:A:2036:PHE:HB2	1.88	0.55
1:A:1724:ARG:NH1	2:A:3001:NAP:C8A	2.70	0.55
1:A:1969:PHE:CD2	1:A:2017:VAL:HB	2.41	0.55
1:A:776:GLU:HB3	1:A:778:SER:OG	2.06	0.55
1:B:1611:ARG:HG2	1:B:1612:ARG:H	1.71	0.55
1:B:353:TRP:CH2	1:B:388:VAL:HG21	2.41	0.55
1:A:128:VAL:HG11	1:A:130:TYR:CZ	2.40	0.55
1:A:1390:VAL:HG22	1:A:1501:LEU:HD21	1.89	0.55
1:A:287:LEU:HA	1:A:387:ASN:O	2.07	0.55
1:A:1662:ARG:HG3	1:A:1662:ARG:HH11	1.68	0.55
1:A:1674:HIS:O	1:A:1675:SER:HB2	2.07	0.55
1:A:1606:ARG:HH21	1:A:1860:GLU:HG3	1.71	0.55
1:A:38:ARG:HB2	1:A:53:LYS:HD2	1.87	0.55
1:B:1124:HIS:CD2	1:B:1512:GLY:HA2	2.41	0.55
1:B:1671:VAL:CG2	1:B:1743:LEU:HB2	2.37	0.55
1:B:438:LEU:O	1:B:442:LEU:HG	2.06	0.55
1:A:1549:SER:O	1:A:1552:HIS:HB3	2.06	0.55
1:A:2075:THR:HG22	1:A:2076:ASN:N	2.22	0.55
1:B:1523:ARG:NH1	1:B:1545:ARG:HE	2.03	0.55
1:A:1231:ASP:HB3	1:A:1515:ARG:HD2	1.89	0.55
1:A:241:ARG:NH2	1:A:827:THR:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1374:SER:O	1:B:1378:TRP:CD1	2.60	0.55
1:B:1671:VAL:HG23	1:B:1743:LEU:HB2	1.88	0.55
1:B:1115:ILE:HD11	1:B:2111:LEU:HD12	1.88	0.55
1:B:1311:LYS:O	1:B:1312:ALA:HB2	2.07	0.55
1:B:1422:SER:HB3	1:B:1424:ARG:HG3	1.87	0.55
1:B:1514:PHE:O	1:B:1515:ARG:NH1	2.40	0.55
1:B:1652:TYR:CD1	1:B:1823:VAL:HB	2.41	0.55
1:A:1419:GLU:CD	1:A:1447:GLY:HA3	2.28	0.55
1:A:1720:PHE:N	1:A:1720:PHE:CD1	2.75	0.55
1:A:207:SER:HB2	1:A:221:GLY:O	2.06	0.55
1:A:293:HIS:O	1:A:326:LYS:HD2	2.06	0.55
1:B:1183:LEU:HB3	1:B:1216:LEU:HD23	1.89	0.55
1:B:128:VAL:HG11	1:B:130:TYR:CZ	2.41	0.55
1:B:1662:ARG:HD3	1:B:1794:ILE:HG12	1.88	0.55
1:A:1041:LEU:O	1:A:1041:LEU:HG	2.07	0.55
1:A:1842:TYR:HE2	1:A:1848:HIS:HB3	1.71	0.55
1:A:887:PRO:HB2	1:A:890:GLY:H	1.72	0.55
1:B:1001:TYR:HB3	1:B:1003:TYR:CD1	2.42	0.55
1:B:1222:ASP:HA	1:B:1226:LEU:HD11	1.89	0.55
1:B:1418:VAL:CG1	1:B:1425:TRP:CE2	2.86	0.55
1:B:1672:LEU:N	1:B:1741:VAL:HG11	2.22	0.55
1:B:162:SER:OG	1:B:163:SER:N	2.39	0.54
1:B:1735:HIS:CD2	1:B:1735:HIS:H	2.25	0.54
1:B:501:ALA:O	1:B:763:PRO:HG2	2.07	0.54
1:B:635:PRO:O	1:B:637:GLY:N	2.40	0.54
1:A:100:LEU:O	1:A:103:THR:OG1	2.24	0.54
1:A:1486:MET:HE3	1:A:1506:TYR:HB3	1.90	0.54
1:A:1614:MET:HG3	1:A:1649:PRO:CG	2.38	0.54
1:A:1769:ILE:HG23	2:A:3001:NAP:C2N	2.38	0.54
1:B:331:HIS:CE1	1:B:333:GLU:HA	2.42	0.54
1:B:610:ILE:HG21	1:B:680:ILE:HD12	1.90	0.54
1:A:353:TRP:NE1	1:A:383:ILE:HB	2.22	0.54
1:A:527:LEU:HD12	1:A:534:VAL:CG2	2.34	0.54
1:A:598:GLU:OE1	1:A:706:LYS:NZ	2.39	0.54
1:B:136:GLN:NE2	1:B:138:ALA:H	2.04	0.54
1:A:1301:PRO:HG2	1:A:1324:LEU:CD2	2.38	0.54
1:A:1354:PRO:O	1:A:1358:MET:HG3	2.06	0.54
1:A:1801:GLU:C	1:A:1803:GLY:H	2.10	0.54
1:B:1611:ARG:HG2	1:B:1612:ARG:N	2.22	0.54
1:A:1338:LEU:HB2	1:A:1406:GLN:HE21	1.72	0.54
1:A:1530:HIS:HB3	1:A:1549:SER:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ARG:NH1	1:A:384:ARG:HG3	2.03	0.54
1:A:87:TYR:CE2	1:A:97:PRO:HG2	2.43	0.54
1:B:1316:VAL:HG13	1:B:1345:LEU:HB3	1.90	0.54
1:B:379:ARG:O	1:B:381:LEU:HG	2.07	0.54
1:B:525:GLN:NE2	1:B:525:GLN:HA	2.23	0.54
1:B:745:PHE:CE2	1:B:767:LEU:HD13	2.43	0.54
1:A:1200:LEU:HA	1:A:1203:VAL:HB	1.88	0.54
1:A:1220:LEU:CB	1:A:1257:ARG:HH22	2.17	0.54
1:A:1771:LYS:O	1:A:1775:SER:HB2	2.08	0.54
1:A:333:GLU:CB	1:A:334:PRO:CD	2.84	0.54
1:A:580:HIS:O	1:A:581:SER:HB3	2.07	0.54
1:A:1734:ARG:C	1:A:1736:THR:H	2.10	0.54
1:A:1455:GLY:HA3	1:A:2039:SER:HB2	1.90	0.54
1:A:348:LEU:HD13	1:A:406:PRO:HB3	1.89	0.54
1:B:1533:VAL:HG21	1:B:1836:VAL:HG11	1.89	0.54
1:B:200:PHE:HB3	1:B:206:LEU:HG	1.90	0.54
1:B:293:HIS:O	1:B:326:LYS:HD2	2.08	0.54
1:B:36:ASP:HB3	1:B:38:ARG:HG3	1.90	0.54
1:B:348:LEU:HD13	1:B:406:PRO:HB3	1.89	0.54
1:B:543:GLU:OE1	1:B:543:GLU:HA	2.07	0.54
1:B:615:VAL:HG22	1:B:686:PHE:CD2	2.40	0.54
1:B:883:ARG:HE	1:B:1107:ARG:HD3	1.72	0.54
1:A:889:THR:CG2	1:A:1032:LEU:HB2	2.38	0.54
1:A:1338:LEU:HD13	1:A:1406:GLN:CG	2.37	0.54
1:B:1330:ALA:O	1:B:1334:MET:HG2	2.08	0.54
1:B:1429:LEU:HD11	1:B:1443:LEU:HD21	1.88	0.54
1:B:953:LEU:HD12	1:B:954:ILE:H	1.70	0.54
1:A:1315:LEU:O	1:A:1344:LEU:HD13	2.07	0.54
1:A:287:LEU:HD23	1:A:387:ASN:O	2.08	0.54
1:A:941:SER:N	1:B:945:GLU:OE2	2.41	0.54
1:B:127:LEU:HG	1:B:127:LEU:O	2.07	0.54
1:B:166:LEU:CD1	1:B:251:THR:HG21	2.31	0.54
1:B:606:ARG:NH1	1:B:739:LEU:HG	2.23	0.54
1:A:1147:ALA:HB2	1:A:1188:CYS:SG	2.48	0.54
1:A:1301:PRO:HG2	1:A:1324:LEU:HD23	1.89	0.54
1:A:1648:VAL:HB	1:A:1649:PRO:HD3	1.89	0.54
1:A:491:PRO:HD2	1:A:756:ALA:HA	1.90	0.54
1:B:1243:LYS:HA	1:B:1271:ASP:HB2	1.90	0.54
1:A:1011:LEU:HD21	1:A:1023:GLN:HB2	1.91	0.53
1:A:118:GLU:HG3	1:B:118:GLU:CD	2.29	0.53
1:A:1472:VAL:HG12	1:A:1473:LEU:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1569:THR:HG23	1:A:1602:GLU:O	2.07	0.53
1:A:1893:LEU:HB3	1:A:1925:GLN:HE21	1.72	0.53
1:A:275:SER:HB2	1:A:276:LEU:HD23	1.88	0.53
1:B:137:ARG:O	1:B:140:MET:HG2	2.08	0.53
1:B:2002:LEU:O	1:B:2006:THR:HB	2.08	0.53
1:A:1652:TYR:CE1	1:A:1823:VAL:HB	2.43	0.53
1:A:993:TYR:CZ	1:A:1008:GLN:HA	2.43	0.53
1:A:1222:ASP:HB3	1:A:1257:ARG:NH1	2.22	0.53
1:A:1476:ASN:HB3	1:A:1486:MET:SD	2.49	0.53
1:A:1476:ASN:HA	1:A:1486:MET:CE	2.38	0.53
1:A:1594:THR:OG1	1:A:1596:ASP:HB2	2.08	0.53
1:A:606:ARG:HH12	1:A:739:LEU:HG	1.72	0.53
1:B:1420:ASP:HB3	1:B:1425:TRP:HZ3	1.72	0.53
1:B:1454:VAL:HG13	1:B:1503:MET:HE1	1.90	0.53
1:B:1540:ASP:HB3	1:B:1542:SER:OG	2.09	0.53
1:B:371:ASP:O	1:B:371:ASP:CG	2.46	0.53
1:B:642:CYS:HB2	1:B:650:THR:HB	1.89	0.53
1:A:1139:GLU:OE1	1:A:1182:ARG:NH2	2.38	0.53
1:A:1227:LYS:HB2	1:A:1261:LEU:HD22	1.91	0.53
1:A:371:ASP:CG	1:A:371:ASP:O	2.46	0.53
1:A:1353:HIS:CD2	1:A:1398:GLY:HA2	2.44	0.53
1:A:1466:GLY:O	1:A:1469:ILE:HB	2.09	0.53
1:A:1567:TYR:CE1	1:A:1606:ARG:HG3	2.43	0.53
1:B:889:THR:HG21	1:B:1032:LEU:HB2	1.91	0.53
1:B:1349:LEU:O	1:B:1372:LEU:HD22	2.09	0.53
1:B:278:ALA:CB	1:B:279:PRO:CD	2.81	0.53
1:B:122:ARG:NH1	1:B:849:ASP:O	2.42	0.53
1:A:1569:THR:HG21	1:A:1622:LEU:CA	2.36	0.53
1:A:1746:ASN:ND2	1:A:1753:LEU:HD12	2.24	0.53
1:A:326:LYS:CE	1:A:336:SER:HB2	2.38	0.53
1:A:438:LEU:O	1:A:442:LEU:HG	2.09	0.53
1:B:1532:PHE:CD1	1:B:1532:PHE:C	2.81	0.53
1:B:2006:THR:O	1:B:2010:CYS:HB2	2.08	0.53
1:B:23:TRP:CZ2	1:B:350:HIS:HD2	2.26	0.53
1:A:1477:LEU:HB3	1:A:1507:ARG:HE	1.73	0.53
1:A:1585:PRO:HB3	1:A:1598:MET:HE3	1.91	0.53
1:A:234:THR:HG22	1:A:235:LYS:O	2.09	0.53
1:B:586:ALA:O	1:B:589:TYR:HB3	2.08	0.53
1:A:1986:GLU:HB3	1:A:1989:GLN:NE2	2.24	0.53
1:A:2018:ILE:HG12	1:A:2041:MET:HE2	1.91	0.53
1:A:1973:MET:SD	2:A:3002:NAP:H3D	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:GLU:O	1:A:985:PHE:CB	2.51	0.53
1:B:917:VAL:HG12	1:B:1054:PHE:HB2	1.90	0.53
1:B:1418:VAL:HG13	1:B:1425:TRP:NE1	2.23	0.53
1:B:1420:ASP:HB3	1:B:1425:TRP:CZ3	2.44	0.53
1:B:1719:CYS:C	1:B:1720:PHE:HD1	2.12	0.53
1:B:1995:LYS:HD3	1:B:2038:ASN:OD1	2.09	0.53
1:A:1254:LEU:HD13	1:A:1316:VAL:CG1	2.38	0.53
1:A:1477:LEU:CD1	1:A:1507:ARG:HH21	2.22	0.53
1:A:23:TRP:CZ2	1:A:350:HIS:HD2	2.26	0.53
1:B:1121:PHE:HB2	1:B:1514:PHE:CE2	2.44	0.53
1:B:1251:ASP:HB3	1:B:1321:LEU:CD2	2.39	0.53
1:B:1456:MET:HG3	1:B:2036:PHE:HD1	1.74	0.53
1:B:1768:GLU:HA	1:B:1768:GLU:OE1	2.08	0.53
1:B:39:ARG:NH1	1:B:226:GLU:OE2	2.41	0.53
1:B:287:LEU:HA	1:B:387:ASN:O	2.08	0.53
1:B:680:ILE:CG1	1:B:681:ALA:N	2.70	0.53
1:A:112:SER:O	1:A:137:ARG:NH2	2.42	0.53
1:A:570:LEU:HD21	1:A:815:LEU:HD21	1.91	0.53
1:B:972:THR:HG23	1:B:1081:VAL:HG21	1.90	0.53
1:B:1371:HIS:O	1:B:1371:HIS:CG	2.62	0.53
1:B:1656:TYR:CE1	1:B:1687:ILE:HD11	2.44	0.53
1:B:997:ARG:HH21	1:B:2070:LEU:HD12	1.73	0.53
1:A:1147:ALA:HB1	1:A:1358:MET:CE	2.39	0.52
1:A:6:ILE:HG21	1:A:345:LEU:CD1	2.38	0.52
1:B:1231:ASP:HB3	1:B:1515:ARG:CD	2.39	0.52
1:B:1677:SER:CB	1:B:1704:LYS:HD3	2.38	0.52
1:B:1863:PRO:O	1:B:1865:PRO:HD3	2.09	0.52
1:B:424:LEU:CD2	1:B:441:GLY:HA3	2.39	0.52
1:A:1183:LEU:HD13	1:A:1210:LEU:O	2.09	0.52
1:A:1395:SER:HB3	1:A:1399:SER:O	2.09	0.52
1:A:1443:LEU:O	1:A:1473:LEU:HA	2.08	0.52
1:A:162:SER:OG	1:A:163:SER:N	2.40	0.52
1:B:1842:TYR:CE2	1:B:1848:HIS:HB3	2.45	0.52
1:B:321:LEU:HD12	1:B:321:LEU:N	2.24	0.52
1:B:624:GLY:O	1:B:625:LEU:HD23	2.09	0.52
1:A:945:GLU:OE2	1:B:941:SER:N	2.42	0.52
1:A:1454:VAL:HG13	1:A:1503:MET:HE1	1.91	0.52
1:A:1560:GLN:C	1:A:1562:ARG:H	2.13	0.52
1:A:161:CYS:HB2	1:A:394:GLY:HA2	1.91	0.52
1:A:831:SER:N	1:A:832:PRO:CD	2.73	0.52
1:B:1343:PHE:O	1:B:1344:LEU:HD22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1456:MET:HG3	1:B:2036:PHE:CD1	2.45	0.52
1:B:808:VAL:HG12	1:B:809:SER:N	2.25	0.52
1:B:1451:SER:O	1:B:1453:VAL:N	2.43	0.52
1:B:1657:TYR:HA	1:B:1661:VAL:HG23	1.90	0.52
1:B:1766:PHE:CD2	1:B:1791:PHE:CE1	2.97	0.52
1:B:287:LEU:HD23	1:B:387:ASN:O	2.09	0.52
1:B:637:GLY:O	1:B:685:TYR:HE2	1.92	0.52
1:A:1424:ARG:O	1:A:1426:VAL:N	2.42	0.52
1:A:1602:GLU:OE2	1:A:1650:ILE:N	2.42	0.52
1:A:1719:CYS:C	1:A:1720:PHE:HD1	2.12	0.52
1:A:275:SER:C	1:A:276:LEU:HD23	2.30	0.52
1:A:91:VAL:HG21	1:A:834:ILE:CD1	2.40	0.52
1:B:1363:THR:CG2	1:B:1363:THR:O	2.58	0.52
1:A:1489:SER:HA	1:A:1493:LEU:HD22	1.91	0.52
1:A:734:TYR:CD2	1:A:734:TYR:C	2.83	0.52
1:B:1234:LEU:HD11	1:B:1268:MET:CE	2.40	0.52
1:B:1499:GLY:O	1:B:1500:ASP:HB3	2.09	0.52
1:B:1580:THR:HG22	1:B:1581:GLY:N	2.25	0.52
1:B:1656:TYR:CE2	1:B:1687:ILE:HD13	2.45	0.52
1:B:297:THR:HB	1:B:300:GLY:H	1.74	0.52
1:B:351:GLY:C	1:B:383:ILE:HG22	2.29	0.52
1:B:506:MET:HB3	1:B:559:ILE:HD11	1.90	0.52
1:B:670:VAL:O	1:B:672:VAL:HG23	2.10	0.52
1:A:1470:ARG:HG3	1:A:1470:ARG:O	2.10	0.52
1:A:1502:VAL:HG12	1:A:1503:MET:HG2	1.91	0.52
1:A:1456:MET:HG3	1:A:2036:PHE:HD1	1.75	0.52
1:A:228:VAL:HG23	1:A:228:VAL:O	2.08	0.52
1:A:297:THR:HG22	1:A:299:VAL:H	1.75	0.52
1:A:137:ARG:NH1	1:B:137:ARG:HD2	2.24	0.52
1:B:1555:LEU:CD2	1:B:1560:GLN:HE21	2.22	0.52
1:B:1670:SER:O	1:B:1742:ASP:HB2	2.10	0.52
1:B:2065:ASP:C	1:B:2070:LEU:HD12	2.30	0.52
1:A:1986:GLU:HG2	1:A:1989:GLN:OE1	2.09	0.52
1:A:2102:PRO:HD2	1:A:2103:HIS:CD2	2.45	0.52
1:A:504:GLN:HG3	1:A:546:LEU:HD11	1.92	0.52
1:A:98:ALA:O	1:A:101:ARG:HG3	2.10	0.52
1:B:1011:LEU:CD2	1:B:1023:GLN:HB2	2.40	0.52
1:B:1734:ARG:C	1:B:1736:THR:H	2.12	0.52
1:B:1771:LYS:O	1:B:1775:SER:HB2	2.09	0.52
1:B:275:SER:C	1:B:276:LEU:HD23	2.29	0.52
1:A:1300:ASP:O	1:A:1302:ALA:N	2.43	0.52

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:895:THR:HA	1:B:935:VAL:HG11	1.91	0.51
1:A:1673:ILE:HD13	1:A:1684:ALA:HB1	1.92	0.51
1:B:2102:PRO:HD2	1:B:2103:HIS:CD2	2.46	0.51
1:A:1766:PHE:CD2	1:A:1791:PHE:CE1	2.98	0.51
1:A:322:ILE:HG22	1:A:376:VAL:HA	1.92	0.51
1:B:1353:HIS:HB2	1:B:1354:PRO:CD	2.39	0.51
1:A:1420:ASP:HB3	1:A:1425:TRP:CZ3	2.46	0.51
1:A:143:ARG:NH1	1:A:143:ARG:HG2	2.25	0.51
1:A:1122:THR:HG21	1:A:1517:PHE:HZ	1.76	0.51
1:A:1556:PRO:O	1:A:1557:ALA:C	2.49	0.51
1:A:1866:ARG:O	1:A:1867:GLY:O	2.29	0.51
1:A:1954:SER:O	1:A:1958:GLU:HG3	2.09	0.51
1:A:469:GLY:HA2	1:A:805:LEU:HD21	1.93	0.51
1:B:433:ALA:HB2	1:B:835:LYS:O	2.10	0.51
1:B:876:VAL:HG12	1:B:876:VAL:O	2.11	0.51
1:A:1390:VAL:HG22	1:A:1501:LEU:CD2	2.41	0.51
1:B:1303:ASN:H	1:B:1304:PRO:HD3	1.74	0.51
1:B:515:ARG:HH22	1:B:817:PRO:HA	1.76	0.51
1:B:973:ARG:O	1:B:974:ALA:HB3	2.10	0.51
1:A:64:PHE:HB2	1:A:429:ARG:NH2	2.25	0.51
1:A:2002:LEU:O	1:A:2006:THR:HB	2.11	0.50
1:A:965:PRO:O	1:A:967:PRO:HD3	2.11	0.50
1:B:1382:PHE:HA	1:B:1387:LEU:HD12	1.93	0.50
1:B:1408:THR:H	1:B:1409:PRO:HD3	1.76	0.50
1:B:1624:THR:HG22	1:B:1857:ARG:HH21	1.74	0.50
1:B:1889:ILE:HG23	1:B:1969:PHE:HB2	1.93	0.50
1:B:1430:LYS:CE	1:B:1981:GLU:O	2.56	0.50
1:B:612:GLU:HG2	1:B:612:GLU:O	2.11	0.50
1:B:734:TYR:C	1:B:734:TYR:CD2	2.82	0.50
1:B:983:ALA:O	1:B:985:PHE:N	2.41	0.50
1:A:1338:LEU:HD22	1:A:1406:GLN:HE21	1.76	0.50
1:A:1487:HIS:NE2	1:A:1490:SER:HB2	2.26	0.50
1:A:2065:ASP:C	1:A:2070:LEU:HD12	2.32	0.50
1:B:1674:HIS:HE1	1:B:1756:SER:OG	1.94	0.50
1:B:168:LEU:HA	1:B:185:VAL:HG21	1.93	0.50
1:B:265:SER:O	1:B:269:GLN:HG3	2.11	0.50
1:A:1454:VAL:HG13	1:A:1503:MET:HE3	1.94	0.50
1:A:1886:SER:HA	1:A:1911:LYS:HB2	1.92	0.50
1:A:325:THR:OG1	1:A:343:LYS:HG2	2.11	0.50
1:B:1085:ASN:C	1:B:1086:LEU:HD23	2.31	0.50
1:B:1279:PRO:HG3	1:B:1298:GLN:HE22	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ILE:HG21	1:B:345:LEU:CD1	2.39	0.50
1:A:297:THR:HB	1:A:300:GLY:H	1.76	0.50
1:B:1001:TYR:HB3	1:B:1003:TYR:CE1	2.45	0.50
1:B:1363:THR:HG22	1:B:1367:GLN:HE21	1.76	0.50
1:B:248:ASN:HD22	1:B:249:ALA:H	1.59	0.50
1:B:564:ILE:HD13	1:B:590:ALA:HB2	1.91	0.50
1:A:1411:ASP:OD2	1:A:1439:ARG:HB2	2.12	0.50
1:A:1841:ARG:O	1:A:1844:ALA:HB3	2.12	0.50
1:B:1431:ASP:C	1:B:1433:LEU:H	2.14	0.50
1:B:143:ARG:CG	1:B:143:ARG:HH11	2.19	0.50
1:B:159:THR:O	1:B:160:ALA:HB3	2.12	0.50
1:B:1833:ARG:NH2	1:B:1872:ALA:O	2.45	0.50
1:A:1651:VAL:HG12	1:A:1683:ALA:HB2	1.94	0.50
1:A:289:TYR:HE2	1:A:291:GLU:CA	2.25	0.50
1:B:1894:GLY:O	1:B:1896:PHE:N	2.45	0.50
1:B:275:SER:HB2	1:B:276:LEU:HD23	1.93	0.50
1:B:866:VAL:HG13	1:B:866:VAL:O	2.12	0.50
1:A:878:HIS:HB2	1:A:1007:PHE:HE1	1.75	0.50
1:A:128:VAL:HG11	1:A:130:TYR:CE2	2.46	0.50
1:A:1896:PHE:HB2	2:A:3002:NAP:O2N	2.12	0.50
1:B:1422:SER:CB	1:B:1424:ARG:HG3	2.42	0.50
1:B:903:LEU:O	1:B:905:GLN:HG3	2.12	0.50
1:A:1556:PRO:O	1:A:1558:SER:N	2.45	0.50
1:A:1857:ARG:CG	1:A:1871:ILE:HD11	2.40	0.50
1:A:112:SER:CB	1:A:334:PRO:CG	2.85	0.50
1:A:662:LEU:C	1:A:664:GLN:N	2.63	0.50
1:B:1001:TYR:CD2	1:B:1003:TYR:HE1	2.30	0.50
1:B:1657:TYR:CZ	1:B:1662:ARG:HD2	2.47	0.50
1:B:1886:SER:HA	1:B:1911:LYS:HB2	1.93	0.50
1:B:276:LEU:O	1:B:281:GLY:HA3	2.12	0.50
1:B:440:GLN:HG3	1:B:833:HIS:CD2	2.47	0.50
1:A:1568:TYR:CE2	1:A:1855:GLN:HB2	2.47	0.50
1:A:1734:ARG:O	1:A:1736:THR:N	2.42	0.50
1:A:1735:HIS:N	1:A:1735:HIS:CD2	2.79	0.50
1:A:23:TRP:CZ2	1:A:350:HIS:CD2	3.00	0.50
1:A:286:SER:HB2	1:A:387:ASN:HD22	1.77	0.50
1:A:72:ALA:HB3	1:A:842:TRP:CZ3	2.47	0.50
1:B:1041:LEU:HG	1:B:1041:LEU:O	2.12	0.50
1:B:51:MET:HE2	1:B:191:LEU:HD13	1.93	0.50
1:A:1086:LEU:HB2	1:A:1088:THR:HG23	1.94	0.49
1:A:1343:PHE:O	1:A:1344:LEU:HD22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:ASP:HB3	1:A:1425:TRP:HZ3	1.77	0.49
1:A:1894:GLY:O	1:A:1896:PHE:N	2.45	0.49
1:A:5:VAL:HG12	1:A:245:THR:HA	1.94	0.49
1:A:895:THR:HA	1:A:935:VAL:HG11	1.92	0.49
1:B:100:LEU:O	1:B:101:ARG:C	2.50	0.49
1:B:1416:LEU:HD21	1:B:1425:TRP:HB2	1.93	0.49
1:B:1652:TYR:CE1	1:B:1823:VAL:HB	2.47	0.49
1:B:1734:ARG:O	1:B:1736:THR:N	2.43	0.49
1:B:9:MET:HE3	1:B:345:LEU:HD12	1.94	0.49
1:A:1303:ASN:HA	1:A:1333:ASN:HB2	1.94	0.49
1:A:1470:ARG:O	1:A:1472:VAL:HG23	2.12	0.49
1:A:1504:ASN:HB3	1:A:1511:TRP:HZ3	1.77	0.49
1:A:1528:THR:HG23	1:A:1552:HIS:ND1	2.28	0.49
1:A:1746:ASN:HD21	1:A:1753:LEU:HD12	1.77	0.49
1:A:1785:PHE:HB2	1:B:1774:LEU:CD2	2.43	0.49
1:A:475:GLY:C	1:A:477:ALA:H	2.15	0.49
1:A:59:ARG:HD2	1:A:59:ARG:N	2.26	0.49
1:B:1285:ALA:HB1	1:B:1289:LEU:HG	1.94	0.49
1:B:1458:ASN:O	1:B:2027:GLY:HA3	2.13	0.49
1:B:495:ILE:CD1	1:B:578:ILE:HB	2.41	0.49
1:A:1672:LEU:HD12	1:A:1696:PHE:O	2.11	0.49
1:A:276:LEU:N	1:A:276:LEU:HD23	2.27	0.49
1:A:278:ALA:HB3	1:A:279:PRO:CD	2.29	0.49
1:A:309:VAL:CG2	1:A:374:LEU:HD11	2.42	0.49
1:A:983:ALA:O	1:A:984:GLU:HB3	2.11	0.49
1:B:112:SER:CB	1:B:334:PRO:CG	2.85	0.49
1:B:1568:TYR:CE2	1:B:1855:GLN:HB2	2.47	0.49
1:B:272:LEU:O	1:B:276:LEU:HG	2.12	0.49
1:A:1055:THR:HB	1:A:1097:LEU:O	2.13	0.49
1:A:1889:ILE:HG23	1:A:1969:PHE:HB2	1.93	0.49
1:A:2103:HIS:H	1:A:2103:HIS:CD2	2.30	0.49
1:A:166:LEU:CD1	1:A:251:THR:HG21	2.32	0.49
1:B:967:PRO:HB3	1:B:1063:THR:OG1	2.13	0.49
1:B:1232:THR:HA	1:B:1515:ARG:NH2	2.20	0.49
1:B:1885:LYS:HE2	1:B:2012:GLU:HB3	1.95	0.49
1:B:2103:HIS:H	1:B:2103:HIS:CD2	2.29	0.49
1:B:2086:GLN:HG2	1:B:2110:VAL:HG23	1.93	0.49
1:B:228:VAL:O	1:B:228:VAL:HG23	2.11	0.49
1:B:309:VAL:HG22	1:B:374:LEU:HD21	1.94	0.49
1:B:59:ARG:N	1:B:59:ARG:HD2	2.28	0.49
1:A:1234:LEU:HD21	1:A:1268:MET:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1451:SER:O	1:A:1453:VAL:N	2.45	0.49
1:A:1476:ASN:HD22	1:A:1486:MET:CE	2.25	0.49
1:A:1520:GLU:O	1:A:1522:ASP:N	2.44	0.49
1:A:1626:VAL:HG13	1:A:1627:LEU:N	2.27	0.49
1:A:1885:LYS:HE2	1:A:2012:GLU:HB3	1.94	0.49
1:B:972:THR:HG23	1:B:1081:VAL:CG2	2.42	0.49
1:B:1364:SER:OG	1:B:1370:ARG:HG2	2.12	0.49
1:B:1418:VAL:HG13	1:B:1425:TRP:CD2	2.46	0.49
1:B:143:ARG:HG2	1:B:143:ARG:NH1	2.21	0.49
1:B:1476:ASN:N	1:B:1476:ASN:OD1	2.44	0.49
1:B:1123:PRO:HB3	1:B:1510:ALA:HB1	1.94	0.49
1:B:1555:LEU:HD11	1:B:1563:LEU:HD22	1.92	0.49
1:B:1863:PRO:O	1:B:1865:PRO:CD	2.61	0.49
1:B:2076:ASN:HA	1:B:2085:PRO:HG2	1.94	0.49
1:B:389:GLY:O	1:B:390:ILE:HG13	2.12	0.49
1:A:1001:TYR:CD2	1:A:1003:TYR:HE1	2.29	0.49
1:A:384:ARG:NH1	1:A:384:ARG:CG	2.66	0.49
1:A:734:TYR:HD2	1:A:734:TYR:C	2.15	0.49
1:A:497:SER:OG	1:A:767:LEU:HG	2.13	0.49
1:B:1150:LEU:HB2	1:B:1192:LEU:HD21	1.94	0.49
1:B:1603:PHE:H	1:B:1603:PHE:HD2	1.59	0.49
1:B:305:LEU:O	1:B:309:VAL:HG23	2.13	0.49
1:A:1454:VAL:HA	1:A:1473:LEU:HD13	1.95	0.49
1:B:1395:SER:HB3	1:B:1399:SER:O	2.13	0.49
1:B:1569:THR:HG21	1:B:1622:LEU:CA	2.38	0.49
1:A:1338:LEU:CB	1:A:1406:GLN:HE21	2.26	0.49
1:A:1339:LYS:O	1:A:1340:GLU:HB2	2.12	0.49
1:A:1378:TRP:O	1:A:1382:PHE:CD1	2.65	0.49
1:A:1528:THR:HG22	1:A:1529:GLU:H	1.78	0.49
1:B:1694:ARG:HH11	1:B:1694:ARG:CG	2.26	0.49
1:B:581:SER:OG	1:B:582:LEU:N	2.45	0.49
1:B:765:ALA:HB1	1:B:768:GLN:HG2	1.95	0.49
1:A:1451:SER:O	1:A:1452:GLY:C	2.51	0.49
1:A:1433:LEU:HD21	1:A:1465:GLY:HA3	1.95	0.49
1:A:1476:ASN:N	1:A:1476:ASN:ND2	2.60	0.49
1:A:1545:ARG:CG	1:A:1545:ARG:NH1	2.69	0.49
1:A:495:ILE:CD1	1:A:578:ILE:HB	2.42	0.49
1:A:975:ALA:O	1:A:976:VAL:HB	2.12	0.49
1:B:1236:ASN:ND2	1:B:1502:VAL:H	2.11	0.49
1:B:1453:VAL:HG12	1:B:1457:VAL:HG23	1.95	0.49
1:B:1842:TYR:HE2	1:B:1848:HIS:HB3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1969:PHE:CD2	1:B:2017:VAL:HB	2.48	0.49
1:B:1117:GLU:HB2	1:B:2107:SER:HB2	1.94	0.49
1:B:506:MET:HE2	1:B:559:ILE:CD1	2.42	0.49
1:B:491:PRO:HA	1:B:575:ASP:OD2	2.13	0.49
1:B:734:TYR:C	1:B:734:TYR:HD2	2.16	0.49
1:A:1140:LEU:HD22	1:A:1140:LEU:O	2.12	0.49
1:A:2086:GLN:HG2	1:A:2110:VAL:HG23	1.94	0.49
1:A:408:SER:O	1:A:409:ARG:HB2	2.12	0.49
1:B:1086:LEU:N	1:B:1086:LEU:HD23	2.28	0.49
1:B:1647:SER:HB2	1:B:1851:LYS:HG3	1.95	0.49
1:A:1989:GLN:HG2	1:A:1990:ASP:N	2.28	0.48
1:A:997:ARG:HH21	1:A:2070:LEU:HD12	1.78	0.48
1:A:988:SER:O	1:A:989:GLN:C	2.51	0.48
1:B:1247:VAL:HG23	1:B:1315:LEU:HD11	1.95	0.48
1:B:1642:LEU:HG	1:B:1859:GLU:OE2	2.12	0.48
1:B:1736:THR:HG23	1:B:1740:GLY:H	1.78	0.48
1:B:91:VAL:HG21	1:B:834:ILE:HD13	1.93	0.48
1:B:896:TRP:CD2	1:B:907:LEU:HD11	2.48	0.48
1:A:1214:ASP:O	1:A:1216:LEU:N	2.41	0.48
1:A:137:ARG:O	1:A:140:MET:HG2	2.13	0.48
1:A:2006:THR:O	1:A:2010:CYS:HB2	2.13	0.48
1:A:846:SER:O	1:A:849:ASP:HB2	2.13	0.48
1:B:1252:GLY:HA2	1:B:1318:ASN:HD22	1.78	0.48
1:B:1413:PRO:HB3	1:B:1440:PRO:HB2	1.94	0.48
1:B:475:GLY:C	1:B:477:ALA:H	2.17	0.48
1:B:610:ILE:CG2	1:B:680:ILE:HD12	2.43	0.48
1:A:856:CYS:HB2	1:B:856:CYS:HG	1.77	0.48
1:B:896:TRP:CG	1:B:907:LEU:HD11	2.49	0.48
1:B:970:PHE:O	1:B:1067:LYS:NZ	2.45	0.48
1:A:1429:LEU:HD21	1:A:1443:LEU:HD21	1.95	0.48
1:A:276:LEU:O	1:A:281:GLY:HA3	2.12	0.48
1:A:2068:VAL:N	2:A:3002:NAP:O1N	2.46	0.48
1:A:506:MET:HB3	1:A:559:ILE:HD11	1.93	0.48
1:B:112:SER:O	1:B:137:ARG:NH2	2.46	0.48
1:B:143:ARG:NH1	1:B:143:ARG:CG	2.76	0.48
1:B:1504:ASN:HB3	1:B:1511:TRP:HZ3	1.77	0.48
1:A:1489:SER:CA	1:A:1493:LEU:HD22	2.43	0.48
1:A:1666:GLN:O	1:A:1669:GLU:HG3	2.13	0.48
1:A:903:LEU:O	1:A:904:SER:HB3	2.13	0.48
1:B:98:ALA:O	1:B:101:ARG:HG3	2.13	0.48
1:B:1476:ASN:C	1:B:1477:LEU:HD23	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1841:ARG:O	1:B:1844:ALA:HB3	2.14	0.48
1:B:662:LEU:HD13	1:B:672:VAL:CG1	2.43	0.48
1:B:988:SER:O	1:B:989:GLN:C	2.47	0.48
1:A:1416:LEU:HD21	1:A:1425:TRP:HB2	1.94	0.48
1:A:148:PHE:HB3	1:A:150:PHE:CE1	2.49	0.48
1:A:353:TRP:CE2	1:A:383:ILE:HB	2.49	0.48
1:B:1123:PRO:HA	1:B:1512:GLY:HA3	1.96	0.48
1:B:1246:GLU:CD	1:B:1254:LEU:HB2	2.34	0.48
1:B:1729:GLU:OE1	1:B:1758:ARG:HD2	2.13	0.48
1:B:191:LEU:O	1:B:192:LEU:HD23	2.13	0.48
1:B:342:ILE:O	1:B:346:LEU:HG	2.13	0.48
1:B:497:SER:HB2	1:B:762:ALA:HB2	1.94	0.48
1:B:87:TYR:CE2	1:B:97:PRO:HG2	2.48	0.48
1:A:136:GLN:NE2	1:A:138:ALA:H	2.06	0.48
1:A:1240:PRO:HD2	1:A:1462:LYS:HE3	1.95	0.48
1:A:1694:ARG:HH11	1:A:1694:ARG:CG	2.26	0.48
1:A:290:ILE:HG23	1:A:322:ILE:HG13	1.95	0.48
1:A:642:CYS:HA	1:A:743:VAL:HG23	1.95	0.48
1:B:12:LYS:HD2	1:B:81:MET:CE	2.44	0.48
1:B:1240:PRO:HD2	1:B:1462:LYS:HE3	1.96	0.48
1:B:1672:LEU:HD12	1:B:1696:PHE:O	2.14	0.48
1:B:1697:THR:CG2	1:B:1698:THR:N	2.76	0.48
1:B:2046:GLU:HG2	1:B:2104:PRO:HG2	1.95	0.48
1:A:917:VAL:HG12	1:A:1054:PHE:HB2	1.93	0.48
1:A:1147:ALA:O	1:A:1358:MET:HE1	2.14	0.48
1:A:1483:ALA:N	1:A:1484:PRO:CD	2.76	0.48
1:A:1624:THR:HG22	1:A:1857:ARG:NH2	2.16	0.48
1:A:1671:VAL:HG13	1:A:1673:ILE:HG13	1.94	0.48
1:A:39:ARG:NH1	1:A:226:GLU:OE2	2.47	0.48
1:A:506:MET:HE2	1:A:559:ILE:HD12	1.96	0.48
1:A:645:SER:OG	1:A:648:THR:N	2.47	0.48
1:A:450:PHE:CE2	1:A:828:PRO:HB2	2.49	0.48
1:B:1220:LEU:HB3	1:B:1257:ARG:NH2	2.14	0.48
1:A:236:LYS:C	1:A:238:LEU:H	2.17	0.48
1:A:236:LYS:O	1:A:238:LEU:N	2.42	0.48
1:A:342:ILE:O	1:A:346:LEU:HG	2.13	0.48
1:A:438:LEU:N	1:A:438:LEU:HD23	2.28	0.48
1:A:662:LEU:O	1:A:663:GLN:C	2.52	0.48
1:B:128:VAL:HG11	1:B:130:TYR:OH	2.14	0.48
1:B:1390:VAL:HG13	1:B:1501:LEU:HD22	1.95	0.48
1:B:1567:TYR:C	1:B:1856:VAL:HG23	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1904:LEU:HA	1:B:1904:LEU:HD23	1.56	0.48
1:B:289:TYR:HE2	1:B:291:GLU:CA	2.26	0.48
1:B:434:VAL:O	1:B:438:LEU:HG	2.14	0.48
1:B:572:LEU:C	1:B:572:LEU:HD23	2.34	0.48
1:A:1252:GLY:CA	1:A:1318:ASN:HD22	2.25	0.48
1:A:226:GLU:O	1:A:227:ALA:HB2	2.14	0.48
1:B:23:TRP:CZ2	1:B:350:HIS:CD2	3.00	0.48
1:B:64:PHE:HB2	1:B:429:ARG:NH2	2.29	0.48
1:B:981:SER:HA	1:B:986:ARG:NH2	2.29	0.48
1:A:100:LEU:O	1:A:101:ARG:C	2.52	0.48
1:A:103:THR:HG22	1:A:104:SER:H	1.77	0.48
1:A:1235:GLU:OE2	1:A:1515:ARG:NH1	2.47	0.48
1:A:1299:TRP:NE1	1:A:1306:PRO:HD2	2.25	0.48
1:A:1580:THR:HG22	1:A:1581:GLY:N	2.29	0.48
1:A:225:ALA:O	1:A:332:PRO:HA	2.14	0.48
1:A:937:LEU:HA	1:A:937:LEU:HD12	1.69	0.48
1:B:1069:TYR:CD1	1:B:1077:ALA:O	2.67	0.48
1:B:1636:VAL:HG22	1:B:1636:VAL:O	2.13	0.48
1:B:2023:SER:O	1:B:2027:GLY:HA2	2.14	0.48
1:A:1085:ASN:C	1:A:1086:LEU:HD23	2.34	0.47
1:A:1265:GLN:HG2	1:A:1266:PRO:HD2	1.94	0.47
1:A:1121:PHE:CE2	1:A:1507:ARG:HB2	2.49	0.47
1:A:1762:GLN:O	1:A:1763:HIS:HB2	2.12	0.47
1:A:1995:LYS:HD3	1:A:2038:ASN:OD1	2.13	0.47
1:A:642:CYS:SG	1:A:743:VAL:CG2	3.02	0.47
1:A:661:PHE:O	1:A:661:PHE:CG	2.67	0.47
1:A:886:PHE:HA	1:A:887:PRO:HD3	1.63	0.47
1:B:1578:LEU:C	1:B:1580:THR:H	2.16	0.47
1:B:2003:ASP:O	1:B:2007:ARG:HG3	2.14	0.47
1:A:146:PHE:O	1:B:256:SER:HB3	2.13	0.47
1:B:297:THR:HG22	1:B:299:VAL:H	1.79	0.47
1:B:883:ARG:HH21	1:B:1107:ARG:HD3	1.79	0.47
1:B:887:PRO:HB2	1:B:890:GLY:H	1.79	0.47
1:B:993:TYR:OH	1:B:1010:VAL:HG23	2.14	0.47
1:A:993:TYR:OH	1:A:1010:VAL:HG23	2.14	0.47
1:A:1446:VAL:HA	1:A:1476:ASN:OD1	2.14	0.47
1:A:1476:ASN:HD22	1:A:1486:MET:HE2	1.79	0.47
1:A:1786:LEU:C	1:A:1788:ASN:H	2.17	0.47
1:A:2076:ASN:HA	1:A:2085:PRO:HG2	1.96	0.47
1:A:645:SER:C	1:A:746:GLN:HG3	2.35	0.47
1:B:1071:LEU:HD12	1:B:1075:THR:OG1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1363:THR:HG22	1:B:1367:GLN:NE2	2.29	0.47
1:B:1442:TRP:CB	1:B:1444:MET:HE1	2.43	0.47
1:B:1915:THR:CG2	2:B:3002:NAP:H2A	2.43	0.47
1:B:506:MET:CE	1:B:559:ILE:HD12	2.44	0.47
1:B:606:ARG:O	1:B:610:ILE:HG13	2.13	0.47
1:A:330:GLY:O	1:A:332:PRO:HD3	2.13	0.47
1:A:605:TRP:O	1:A:606:ARG:C	2.53	0.47
1:A:856:CYS:HB2	1:B:856:CYS:SG	2.53	0.47
1:B:1183:LEU:HB3	1:B:1216:LEU:CD2	2.44	0.47
1:B:1327:PRO:O	1:B:1331:VAL:HG23	2.14	0.47
1:B:1228:ALA:HB2	1:B:1517:PHE:CZ	2.49	0.47
1:B:211:THR:HG22	1:B:212:CYS:N	2.28	0.47
1:A:1289:LEU:HD22	1:A:1294:VAL:CB	2.44	0.47
1:A:1616:MET:HB3	1:A:1800:PHE:CE2	2.49	0.47
1:A:2046:GLU:HG2	1:A:2104:PRO:HG2	1.95	0.47
1:A:533:ARG:HB2	1:A:533:ARG:HH11	1.79	0.47
1:A:620:MET:SD	1:A:677:THR:HG21	2.54	0.47
1:A:896:TRP:CG	1:A:907:LEU:HD11	2.49	0.47
1:A:1067:LYS:HB3	1:A:1092:GLY:HA2	1.95	0.47
1:A:1299:TRP:CH2	1:A:1333:ASN:CG	2.88	0.47
1:B:1153:LYS:HD3	1:B:1195:ASN:HD22	1.79	0.47
1:B:1221:LEU:O	1:B:1226:LEU:HD21	2.14	0.47
1:B:1338:LEU:HD22	1:B:1406:GLN:HG3	1.96	0.47
1:B:1477:LEU:HB3	1:B:1507:ARG:HE	1.79	0.47
1:B:1735:HIS:N	1:B:1735:HIS:CD2	2.83	0.47
1:B:1814:LEU:O	1:B:1818:ILE:HG13	2.15	0.47
1:B:1769:ILE:HG23	2:B:3001:NAP:C2N	2.45	0.47
1:B:299:VAL:O	1:B:302:PRO:HD2	2.13	0.47
1:A:1619:ALA:O	1:A:1620:GLU:HB2	2.15	0.47
1:A:277:TYR:CZ	1:A:287:LEU:HD11	2.49	0.47
1:A:433:ALA:HB2	1:A:835:LYS:O	2.15	0.47
1:B:1022:LEU:HD13	1:B:1034:ALA:HB3	1.97	0.47
1:B:1574:ARG:HD2	1:B:1588:ILE:CD1	2.45	0.47
1:B:333:GLU:O	1:B:336:SER:HB3	2.14	0.47
1:B:873:HIS:O	1:B:876:VAL:HG23	2.14	0.47
1:A:1223:ALA:O	1:A:1225:ALA:N	2.48	0.47
1:A:1473:LEU:HD23	1:A:1502:VAL:O	2.15	0.47
1:A:1578:LEU:C	1:A:1580:THR:H	2.17	0.47
1:A:504:GLN:HG3	1:A:546:LEU:CD1	2.45	0.47
1:B:1276:ASP:OD2	1:B:1281:ALA:HB3	2.14	0.47
1:B:1469:ILE:CG2	1:B:1469:ILE:O	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1585:PRO:HB3	1:B:1598:MET:HE1	1.96	0.47
1:A:1774:LEU:CD2	1:B:1785:PHE:HB2	2.45	0.47
1:B:331:HIS:C	1:B:333:GLU:H	2.18	0.47
1:B:709:SER:OG	1:B:711:ARG:HB2	2.14	0.47
1:A:1182:ARG:CB	1:A:1216:LEU:HB2	2.33	0.47
1:A:782:ILE:HG22	1:A:783:PRO:O	2.14	0.47
1:A:941:SER:CB	1:B:945:GLU:OE2	2.63	0.47
1:A:970:PHE:O	1:A:1067:LYS:HE2	2.15	0.47
1:B:1781:GLY:O	1:B:1784:VAL:HG23	2.15	0.47
1:B:274:ARG:O	1:B:276:LEU:N	2.47	0.47
1:B:330:GLY:O	1:B:332:PRO:HD3	2.14	0.47
1:B:633:ARG:HG2	1:B:633:ARG:O	2.14	0.47
1:A:1670:SER:OG	1:A:1741:VAL:HA	2.15	0.47
1:A:491:PRO:HA	1:A:575:ASP:OD2	2.15	0.47
1:A:420:LEU:HD11	1:A:512:ARG:HB3	1.96	0.47
1:A:64:PHE:HB2	1:A:429:ARG:HE	1.80	0.47
1:B:285:GLU:HG3	1:B:315:THR:OG1	2.15	0.47
1:A:1071:LEU:HD12	1:A:1075:THR:OG1	2.15	0.47
1:A:1680:VAL:N	2:A:3001:NAP:O1N	2.32	0.47
1:A:36:ASP:CB	1:A:38:ARG:HG3	2.45	0.47
1:A:424:LEU:CD2	1:A:441:GLY:HA3	2.45	0.47
1:A:912:VAL:HG22	1:A:913:VAL:N	2.29	0.47
1:B:1277:ARG:NH2	1:B:1323:THR:O	2.47	0.47
1:B:1338:LEU:HD13	1:B:1406:GLN:HG2	1.95	0.47
1:B:1762:GLN:O	1:B:1763:HIS:HB2	2.14	0.47
1:B:1766:PHE:O	1:B:1792:HIS:HB2	2.14	0.47
1:B:289:TYR:OH	1:B:323:GLY:HA3	2.13	0.47
1:B:644:ASN:HB2	1:B:648:THR:O	2.14	0.47
1:A:1433:LEU:HD11	1:A:1465:GLY:O	2.15	0.47
1:A:1476:ASN:CB	1:A:1486:MET:SD	3.03	0.47
1:A:1653:THR:HG22	1:A:1810:VAL:HG12	1.96	0.47
1:A:561:ILE:HG23	1:A:589:TYR:CE2	2.50	0.47
1:A:88:GLU:HB3	1:A:831:SER:HB2	1.97	0.47
1:B:1257:ARG:O	1:B:1260:ALA:HB3	2.15	0.47
1:B:1504:ASN:HB3	1:B:1511:TRP:CZ3	2.50	0.47
1:B:831:SER:N	1:B:832:PRO:CD	2.77	0.47
1:A:1348:THR:HG23	1:A:1372:LEU:HD22	1.97	0.46
1:A:1387:LEU:HD22	1:A:1404:CYS:HB3	1.96	0.46
1:A:1473:LEU:HD21	1:A:1503:MET:SD	2.55	0.46
1:A:1485:GLU:HG2	1:A:1506:TYR:OH	2.15	0.46
1:A:2017:VAL:HG21	1:A:2099:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2099:LEU:HD23	1:A:2099:LEU:HA	1.70	0.46
1:A:289:TYR:HE2	1:A:291:GLU:HA	1.80	0.46
1:A:765:ALA:HB1	1:A:768:GLN:HG2	1.96	0.46
1:A:91:VAL:CG2	1:A:834:ILE:CD1	2.94	0.46
1:B:1515:ARG:HD3	1:B:1515:ARG:HA	1.56	0.46
1:B:226:GLU:O	1:B:227:ALA:HB2	2.14	0.46
1:B:286:SER:HB2	1:B:387:ASN:HD22	1.79	0.46
1:B:556:LEU:O	1:B:560:GLN:HG3	2.15	0.46
1:B:980:ASP:CG	1:B:982:THR:HG22	2.35	0.46
1:A:1133:ASN:ND2	1:A:1136:LEU:HD12	2.17	0.46
1:A:1183:LEU:N	1:A:1216:LEU:HD22	2.29	0.46
1:A:1299:TRP:HE1	1:A:1306:PRO:CD	2.25	0.46
1:A:1420:ASP:CB	1:A:1425:TRP:HZ3	2.28	0.46
1:A:168:LEU:O	1:A:168:LEU:HG	2.14	0.46
1:A:331:HIS:C	1:A:333:GLU:H	2.18	0.46
1:A:509:SER:O	1:A:512:ARG:HG3	2.14	0.46
1:A:59:ARG:HG3	1:A:838:HIS:HB3	1.96	0.46
1:A:837:ASP:OD1	1:A:839:SER:HB3	2.16	0.46
1:B:1014:ASP:OD1	1:B:1015:LEU:N	2.49	0.46
1:B:1662:ARG:NH1	1:B:1662:ARG:CG	2.50	0.46
1:B:168:LEU:HG	1:B:168:LEU:O	2.14	0.46
1:B:1857:ARG:CZ	1:B:1871:ILE:CD1	2.93	0.46
1:B:297:THR:HB	1:B:300:GLY:N	2.31	0.46
1:A:1136:LEU:HD21	1:A:1217:LEU:HG	1.97	0.46
1:A:188:LEU:CD2	1:A:228:VAL:HG12	2.44	0.46
1:A:48:PRO:HD3	1:A:201:MET:HE3	1.97	0.46
1:B:1216:LEU:CD1	1:B:1217:LEU:N	2.78	0.46
1:B:1239:SER:C	1:B:1241:LYS:H	2.19	0.46
1:B:1444:MET:HE2	1:B:1444:MET:HB3	1.81	0.46
1:B:1568:TYR:HE2	1:B:1855:GLN:HB2	1.79	0.46
1:B:1762:GLN:HB3	1:B:1763:HIS:CD2	2.50	0.46
1:B:2069:VAL:HG12	1:B:2070:LEU:HD23	1.97	0.46
1:B:305:LEU:HD22	1:B:322:ILE:HD13	1.96	0.46
1:B:509:SER:O	1:B:512:ARG:HG3	2.15	0.46
1:A:1086:LEU:N	1:A:1086:LEU:HD23	2.31	0.46
1:A:1486:MET:HE1	1:A:1506:TYR:HB3	1.98	0.46
1:A:1798:SER:O	1:A:1802:GLU:OE1	2.33	0.46
1:A:1568:TYR:HE2	1:A:1855:GLN:HB2	1.80	0.46
1:A:248:ASN:HD22	1:A:249:ALA:H	1.61	0.46
1:A:1573:PHE:HD2	2:A:3001:NAP:HO3N	1.61	0.46
1:A:925:LEU:CD2	1:A:931:VAL:HG21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:SER:CB	1:B:135:CYS:HB3	2.44	0.46
1:B:1420:ASP:CB	1:B:1425:TRP:HZ3	2.28	0.46
1:B:1603:PHE:CE2	1:B:1615:GLY:C	2.85	0.46
1:B:1669:GLU:HG2	1:B:1742:ASP:OD2	2.15	0.46
1:B:209:ASP:CG	1:B:213:ARG:HH21	2.18	0.46
1:B:309:VAL:CG2	1:B:374:LEU:HD11	2.45	0.46
1:A:1347:HIS:HD1	1:A:1401:LEU:HD13	1.81	0.46
1:A:1439:ARG:O	1:A:1470:ARG:HB3	2.15	0.46
1:B:1460:LEU:O	1:B:1462:LYS:N	2.49	0.46
1:B:506:MET:HB3	1:B:559:ILE:CD1	2.46	0.46
1:B:934:GLU:CG	1:B:947:SER:HB2	2.46	0.46
1:A:1246:GLU:CD	1:A:1254:LEU:HB2	2.36	0.46
1:A:1466:GLY:HA2	1:A:1469:ILE:CG1	2.46	0.46
1:A:1122:THR:HG1	1:A:1517:PHE:HE1	1.60	0.46
1:A:1657:TYR:HA	1:A:1661:VAL:HG23	1.98	0.46
1:A:1671:VAL:HG23	1:A:1743:LEU:HD13	1.98	0.46
1:A:494:PHE:CD1	1:A:574:PRO:HB3	2.50	0.46
1:A:900:ALA:HB1	1:A:905:GLN:O	2.16	0.46
1:A:934:GLU:CG	1:A:947:SER:HB2	2.46	0.46
1:A:976:VAL:HG13	1:A:977:ASP:N	2.30	0.46
1:B:1697:THR:HG23	1:B:1698:THR:N	2.30	0.46
1:B:1452:GLY:O	1:B:2036:PHE:CD1	2.68	0.46
1:B:161:CYS:HB2	1:B:394:GLY:HA2	1.97	0.46
1:B:533:ARG:HB2	1:B:533:ARG:HH11	1.81	0.46
1:B:532:LEU:HD22	1:B:604:TYR:CE1	2.51	0.46
1:B:643:HIS:CD2	1:B:746:GLN:HB3	2.50	0.46
1:B:887:PRO:O	1:B:888:GLY:C	2.54	0.46
1:B:912:VAL:HG22	1:B:913:VAL:N	2.31	0.46
1:A:1064:HIS:O	1:A:1065:ARG:C	2.54	0.46
1:A:142:ASN:ND2	1:B:396:GLY:HA3	2.30	0.46
1:A:1894:GLY:O	1:A:1895:GLY:C	2.53	0.46
1:A:440:GLN:HG3	1:A:833:HIS:CG	2.50	0.46
1:A:62:ALA:O	1:A:67:VAL:HG22	2.16	0.46
1:B:1036:LEU:CD2	1:B:1096:PHE:CE1	2.94	0.46
1:B:119:ALA:HB2	1:B:850:PHE:CE2	2.51	0.46
1:B:1311:LYS:O	1:B:1312:ALA:CB	2.63	0.46
1:B:1245:VAL:HB	1:B:1315:LEU:HD13	1.97	0.46
1:B:1531:ALA:HA	1:B:1549:SER:H	1.81	0.46
1:B:1556:PRO:O	1:B:1558:SER:N	2.49	0.46
1:B:1647:SER:CB	1:B:1851:LYS:HG3	2.46	0.46
1:B:2075:THR:CG2	1:B:2076:ASN:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:LEU:N	1:B:438:LEU:HD23	2.30	0.46
1:A:1416:LEU:HD23	1:A:1429:LEU:CD2	2.45	0.46
1:A:1554:ALA:CB	1:A:1882:PRO:HB3	2.46	0.46
1:A:1724:ARG:HH12	2:A:3001:NAP:C8A	2.27	0.46
1:A:2058:VAL:HG11	1:A:2060:TRP:CE2	2.51	0.46
1:B:1289:LEU:HD22	1:B:1294:VAL:HB	1.96	0.46
1:B:1567:TYR:O	1:B:1856:VAL:HG23	2.16	0.46
1:B:384:ARG:NH1	1:B:384:ARG:CG	2.65	0.46
1:B:886:PHE:HA	1:B:887:PRO:HD3	1.64	0.46
1:A:1975:LEU:HD22	1:A:1977:ASP:OD1	2.16	0.46
1:A:556:LEU:O	1:A:560:GLN:HG3	2.15	0.46
1:B:1361:PHE:CZ	1:B:1370:ARG:HD3	2.51	0.46
1:B:1577:MET:CE	1:B:1582:LYS:HD3	2.46	0.46
1:A:1208:ARG:H	1:A:1209:PRO:CD	2.29	0.46
1:A:1669:GLU:O	1:A:1693:CYS:HB3	2.16	0.46
1:A:1904:LEU:HD23	1:A:1904:LEU:HA	1.58	0.46
1:A:2043:ARG:HD3	1:A:2043:ARG:HA	1.61	0.46
1:A:506:MET:HB3	1:A:506:MET:HE2	1.85	0.46
1:A:533:ARG:HB2	1:A:533:ARG:NH1	2.31	0.46
1:A:578:ILE:CG2	1:A:745:PHE:HE1	2.29	0.46
1:A:9:MET:HE3	1:A:345:LEU:HD12	1.98	0.46
1:B:127:LEU:HD12	1:B:127:LEU:C	2.36	0.46
1:B:2099:LEU:HA	1:B:2099:LEU:HD23	1.71	0.46
1:B:2017:VAL:HG21	1:B:2099:LEU:HD21	1.97	0.46
1:B:209:ASP:CG	1:B:213:ARG:NH2	2.70	0.46
1:B:737:ASN:C	1:B:737:ASN:ND2	2.70	0.46
1:A:1338:LEU:HG	1:A:1339:LYS:N	2.31	0.45
1:A:1360:GLY:CA	1:A:1369:GLY:O	2.64	0.45
1:A:1818:ILE:HG12	1:A:1823:VAL:CG1	2.47	0.45
1:A:240:ARG:HG2	1:A:821:PHE:CD2	2.51	0.45
1:A:356:ASN:HA	1:A:356:ASN:HD22	1.50	0.45
1:A:426:ALA:HA	1:A:458:ALA:CB	2.46	0.45
1:B:103:THR:HG22	1:B:104:SER:H	1.81	0.45
1:B:1360:GLY:O	1:B:1364:SER:OG	2.25	0.45
1:B:1690:SER:HB3	1:B:1822:VAL:HG13	1.98	0.45
1:B:201:MET:HA	1:B:206:LEU:HB2	1.97	0.45
1:B:23:TRP:O	1:B:24:ALA:C	2.54	0.45
1:B:468:ARG:HG2	1:B:804:HIS:NE2	2.31	0.45
1:B:530:LEU:HD13	1:B:604:TYR:CE2	2.51	0.45
1:A:1330:ALA:O	1:A:1334:MET:HG2	2.16	0.45
1:A:1371:HIS:O	1:A:1371:HIS:CD2	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1424:ARG:C	1:A:1426:VAL:N	2.70	0.45
1:A:1115:ILE:HD11	1:A:2111:LEU:HG	1.99	0.45
1:A:737:ASN:HD22	1:A:737:ASN:C	2.17	0.45
1:A:984:GLU:HG2	1:A:986:ARG:NE	2.27	0.45
1:B:1086:LEU:HB2	1:B:1088:THR:HG23	1.99	0.45
1:B:1130:LEU:HD22	1:B:1133:ASN:HD21	1.80	0.45
1:B:1261:LEU:O	1:B:1264:THR:HB	2.16	0.45
1:B:1351:ALA:HB2	1:B:1372:LEU:HB3	1.96	0.45
1:B:1370:ARG:O	1:B:1371:HIS:HB3	2.16	0.45
1:B:1405:ARG:NH1	1:B:1500:ASP:OD1	2.49	0.45
1:B:1674:HIS:CE1	1:B:1756:SER:OG	2.68	0.45
1:A:1785:PHE:HB2	1:B:1774:LEU:HD22	1.98	0.45
1:B:1647:SER:CA	1:B:1851:LYS:HG3	2.46	0.45
1:A:1130:LEU:O	1:A:1131:ALA:CB	2.65	0.45
1:A:1338:LEU:HD13	1:A:1406:GLN:HG3	1.97	0.45
1:A:1606:ARG:HH21	1:A:1860:GLU:CG	2.29	0.45
1:A:1618:PRO:O	1:A:1619:ALA:HB2	2.17	0.45
1:A:277:TYR:O	1:A:278:ALA:C	2.54	0.45
1:A:336:SER:OG	1:A:337:GLY:N	2.49	0.45
1:A:470:TYR:C	1:A:470:TYR:CD1	2.90	0.45
1:A:593:CYS:SG	1:A:708:ARG:HA	2.57	0.45
1:B:122:ARG:HG3	1:B:123:ASP:H	1.80	0.45
1:B:1418:VAL:HG12	1:B:1418:VAL:O	2.15	0.45
1:B:1413:PRO:CA	1:B:1440:PRO:HB2	2.47	0.45
1:B:1442:TRP:CD2	1:B:1472:VAL:HB	2.51	0.45
1:B:1473:LEU:HD23	1:B:1473:LEU:N	2.32	0.45
1:B:1746:ASN:ND2	1:B:1753:LEU:HD12	2.32	0.45
1:B:1837:GLU:O	1:B:1840:PHE:HB2	2.16	0.45
1:B:367:PRO:C	1:B:369:LEU:H	2.20	0.45
1:A:1345:LEU:O	1:A:1346:LEU:HD23	2.17	0.45
1:A:1470:ARG:O	1:A:1470:ARG:CG	2.65	0.45
1:A:1585:PRO:O	1:A:1595:ARG:NH1	2.49	0.45
1:A:169:GLN:HE21	1:A:169:GLN:C	2.19	0.45
1:A:621:ALA:O	1:A:650:THR:HA	2.15	0.45
1:A:892:LEU:HD22	1:A:1057:ILE:HD12	1.98	0.45
1:B:1216:LEU:HD12	1:B:1217:LEU:N	2.31	0.45
1:B:1282:LEU:HD21	1:B:1296:GLN:CB	2.41	0.45
1:B:1616:MET:C	1:B:1800:PHE:HZ	2.20	0.45
1:B:399:ASN:ND2	1:B:399:ASN:N	2.63	0.45
1:B:581:SER:CB	1:B:683:HIS:NE2	2.78	0.45
1:B:925:LEU:CD2	1:B:931:VAL:HG21	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1237:MET:SD	1:A:1242:MET:HG3	2.56	0.45
1:A:762:ALA:HB1	1:A:763:PRO:HD2	1.99	0.45
1:B:136:GLN:NE2	1:B:138:ALA:N	2.64	0.45
1:B:1572:ASN:OD1	1:B:1851:LYS:NZ	2.49	0.45
1:B:1894:GLY:O	1:B:1895:GLY:C	2.54	0.45
1:B:51:MET:HE1	1:B:191:LEU:HD13	1.98	0.45
1:B:40:TRP:CZ3	1:B:194:PRO:HA	2.51	0.45
1:B:19:LEU:HA	1:B:19:LEU:HD23	1.76	0.45
1:B:289:TYR:HH	1:B:323:GLY:HA3	1.82	0.45
1:B:605:TRP:O	1:B:606:ARG:C	2.55	0.45
1:B:62:ALA:O	1:B:67:VAL:HG22	2.17	0.45
1:A:1251:ASP:HB2	1:A:1321:LEU:HG	1.97	0.45
1:A:1369:GLY:C	1:A:1371:HIS:H	2.20	0.45
1:A:1408:THR:CG2	1:A:1409:PRO:HD2	2.46	0.45
1:A:1766:PHE:O	1:A:1792:HIS:HB2	2.17	0.45
1:A:475:GLY:O	1:A:477:ALA:N	2.48	0.45
1:A:549:ILE:HG13	1:A:553:PHE:CE1	2.52	0.45
1:B:1351:ALA:HB2	1:B:1372:LEU:CB	2.47	0.45
1:B:1454:VAL:HA	1:B:1473:LEU:HD13	1.98	0.45
1:B:1538:ARG:NH2	1:B:1585:PRO:HG2	2.32	0.45
1:B:1631:HIS:CD2	1:B:1803:GLY:HA3	2.51	0.45
1:A:1662:ARG:HH12	1:B:1790:THR:CG2	2.29	0.45
1:B:234:THR:HG22	1:B:235:LYS:N	2.31	0.45
1:B:782:ILE:CD1	1:B:803:LEU:HD23	2.40	0.45
1:A:1236:ASN:HA	1:A:1502:VAL:HG21	1.98	0.45
1:A:1118:LYS:HB3	1:A:1519:LEU:HD13	1.99	0.45
1:A:23:TRP:O	1:A:24:ALA:C	2.54	0.45
1:A:297:THR:HB	1:A:300:GLY:N	2.32	0.45
1:B:1339:LYS:O	1:B:1340:GLU:HB2	2.17	0.45
1:B:1338:LEU:CB	1:B:1406:GLN:HE21	2.29	0.45
1:B:1627:LEU:HD22	1:B:1627:LEU:HA	1.67	0.45
1:B:1801:GLU:C	1:B:1803:GLY:H	2.20	0.45
1:B:258:GLU:H	1:B:259:GLN:NE2	2.15	0.45
1:B:403:ILE:C	1:B:404:LEU:HD23	2.37	0.45
1:B:561:ILE:HG23	1:B:589:TYR:CE2	2.51	0.45
1:A:1350:LEU:HD13	1:A:1374:SER:HA	1.99	0.45
1:A:157:ILE:HD11	1:A:167:ALA:CA	2.44	0.45
1:A:305:LEU:O	1:A:309:VAL:HG23	2.16	0.45
1:A:572:LEU:C	1:A:572:LEU:HD23	2.37	0.45
1:A:642:CYS:HB2	1:A:650:THR:HB	1.99	0.45
1:A:759:VAL:HG23	1:A:759:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1067:LYS:HB3	1:B:1092:GLY:HA2	1.98	0.45
1:B:1326:ASP:HA	1:B:1327:PRO:HD2	1.70	0.45
1:B:1419:GLU:CD	1:B:1447:GLY:HA3	2.37	0.45
1:B:1674:HIS:HD2	1:B:1698:THR:OG1	1.97	0.45
1:B:1786:LEU:C	1:B:1788:ASN:H	2.20	0.45
1:B:1800:PHE:C	1:B:1800:PHE:CD2	2.90	0.45
1:B:2104:PRO:HD2	1:B:2105:VAL:H	1.82	0.45
1:A:1272:TYR:HB3	1:A:1294:VAL:HG22	1.99	0.45
1:A:1387:LEU:HD23	1:A:1406:GLN:HB3	1.98	0.45
1:A:136:GLN:NE2	1:A:138:ALA:N	2.65	0.45
1:A:168:LEU:HA	1:A:185:VAL:HG21	1.98	0.45
1:A:737:ASN:ND2	1:A:737:ASN:C	2.69	0.45
1:A:873:HIS:O	1:A:876:VAL:HG23	2.16	0.45
1:A:984:GLU:HG2	1:A:986:ARG:HG3	1.99	0.45
1:B:1387:LEU:HD22	1:B:1404:CYS:HB3	1.98	0.45
1:B:1424:ARG:O	1:B:1426:VAL:N	2.49	0.45
1:B:1560:GLN:HA	1:B:1563:LEU:HB2	1.98	0.45
1:B:1812:GLU:HA	1:B:1815:LYS:HB2	1.97	0.45
1:B:426:ALA:HA	1:B:458:ALA:CB	2.46	0.45
1:A:1385:ALA:O	1:A:1386:SER:HB2	2.16	0.45
1:A:363:ASN:HA	1:A:364:PRO:HD3	1.81	0.45
1:A:768:GLN:CD	1:A:783:PRO:HG3	2.36	0.45
1:A:58:SER:HB3	1:A:844:VAL:CG2	2.47	0.45
1:B:1412:SER:HA	1:B:1413:PRO:HD3	1.61	0.45
1:B:903:LEU:O	1:B:904:SER:HB3	2.17	0.45
1:A:1111:HIS:O	1:A:1112:LEU:HD23	2.17	0.44
1:A:1147:ALA:HB1	1:A:1358:MET:HE2	2.00	0.44
1:A:1515:ARG:HD3	1:A:1515:ARG:HA	1.62	0.44
1:A:1535:VAL:HG12	1:A:1537:SER:H	1.82	0.44
1:A:2003:ASP:O	1:A:2007:ARG:HG3	2.17	0.44
1:A:606:ARG:O	1:A:610:ILE:HG13	2.18	0.44
1:A:94:GLY:HA3	1:A:453:MET:HG2	1.97	0.44
1:A:970:PHE:O	1:A:1067:LYS:NZ	2.48	0.44
1:B:1028:TRP:O	1:B:1032:LEU:HB2	2.17	0.44
1:B:1000:GLY:HA2	1:B:1106:ARG:NH2	2.32	0.44
1:B:1221:LEU:HG	1:B:1221:LEU:O	2.17	0.44
1:B:2018:ILE:HG12	1:B:2041:MET:HE2	1.99	0.44
1:B:506:MET:HE2	1:B:559:ILE:HD12	1.99	0.44
1:B:542:ASP:O	1:B:545:VAL:HG12	2.17	0.44
1:A:1255:TYR:HA	1:A:1272:TYR:CE2	2.52	0.44
1:A:1373:LEU:HD22	1:A:1377:GLN:OE1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1411:ASP:HB2	1:A:1440:PRO:HD3	2.00	0.44
1:A:1473:LEU:HD23	1:A:1473:LEU:N	2.32	0.44
1:A:1698:THR:HA	1:A:1721:ALA:O	2.17	0.44
1:A:1857:ARG:HH11	1:A:1869:PRO:HG2	1.82	0.44
1:A:2084:LEU:HD12	1:A:2112:ALA:HA	1.99	0.44
1:A:211:THR:HG22	1:A:212:CYS:N	2.32	0.44
1:A:366:ILE:CG1	1:A:366:ILE:O	2.65	0.44
1:A:396:GLY:HA3	1:B:142:ASN:ND2	2.31	0.44
1:B:1472:VAL:HG12	1:B:1473:LEU:N	2.32	0.44
1:B:1898:LEU:HA	1:B:1898:LEU:HD23	1.78	0.44
1:B:2053:LEU:CD2	1:B:2054:PRO:HD2	2.47	0.44
1:B:206:LEU:HA	1:B:206:LEU:HD23	1.70	0.44
1:B:512:ARG:NH1	1:B:793:LEU:HD23	2.33	0.44
1:B:534:VAL:HG13	1:B:554:VAL:HG12	1.99	0.44
1:B:668:GLU:O	1:B:669:ASP:CB	2.60	0.44
1:A:903:LEU:O	1:A:905:GLN:HG3	2.18	0.44
1:B:123:ASP:HA	1:B:124:PRO:HD3	1.70	0.44
1:B:1662:ARG:NH1	1:B:1792:HIS:ND1	2.66	0.44
1:A:1413:PRO:HA	1:A:1440:PRO:O	2.18	0.44
1:A:1472:VAL:HG13	1:A:1502:VAL:O	2.16	0.44
1:A:261:VAL:HG22	1:B:146:PHE:CD1	2.53	0.44
1:A:654:PRO:HB2	1:A:657:ALA:HB3	1.99	0.44
1:B:169:GLN:C	1:B:169:GLN:HE21	2.21	0.44
1:B:254:ASP:O	1:B:255:GLY:O	2.36	0.44
1:B:642:CYS:O	1:B:649:VAL:HG13	2.18	0.44
1:A:1361:PHE:CZ	1:A:1370:ARG:NE	2.85	0.44
1:A:1574:ARG:O	1:A:1578:LEU:HG	2.18	0.44
1:A:1814:LEU:O	1:A:1818:ILE:HG13	2.17	0.44
1:A:1973:MET:O	1:A:1973:MET:HG3	2.18	0.44
1:A:252:ASN:HD21	1:A:272:LEU:HB2	1.80	0.44
1:A:285:GLU:HG3	1:A:315:THR:OG1	2.17	0.44
1:B:1036:LEU:HD13	1:B:1051:PRO:HG3	1.99	0.44
1:B:1265:GLN:HE21	1:B:2026:ARG:NH1	2.16	0.44
1:B:1251:ASP:CB	1:B:1321:LEU:HD22	2.47	0.44
1:B:1345:LEU:HD12	1:B:1402:PHE:O	2.17	0.44
1:B:148:PHE:HB3	1:B:150:PHE:CE1	2.53	0.44
1:B:161:CYS:HB3	1:B:331:HIS:HE1	1.82	0.44
1:B:994:LYS:HE2	1:B:1924:TYR:CE2	2.52	0.44
1:A:1011:LEU:CD2	1:A:1023:GLN:HB2	2.47	0.44
1:A:103:THR:HG22	1:A:104:SER:N	2.32	0.44
1:A:1234:LEU:HD13	1:A:1242:MET:SD	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1234:LEU:HD22	1:A:1262:LEU:CD2	2.46	0.44
1:A:136:GLN:HE22	1:A:138:ALA:N	2.09	0.44
1:A:1673:ILE:CD1	1:A:1684:ALA:HB1	2.48	0.44
1:A:169:GLN:HE21	1:A:170:SER:N	2.15	0.44
1:A:1812:GLU:HA	1:A:1815:LYS:HB2	1.99	0.44
1:A:22:PHE:CE2	1:A:26:LEU:HD11	2.53	0.44
1:B:1389:LEU:HD23	1:B:1389:LEU:HA	1.76	0.44
1:B:1424:ARG:C	1:B:1426:VAL:N	2.71	0.44
1:B:1472:VAL:HG12	1:B:1473:LEU:H	1.82	0.44
1:B:1535:VAL:HG12	1:B:1535:VAL:O	2.18	0.44
1:B:1538:ARG:CZ	1:B:1585:PRO:HG2	2.47	0.44
1:B:1656:TYR:CD1	1:B:1687:ILE:HD11	2.53	0.44
1:B:165:LEU:HD22	1:B:392:SER:HB2	1.98	0.44
1:B:2031:GLN:HB3	1:B:2034:TYR:HB3	1.99	0.44
1:B:55:LYS:HB3	1:B:55:LYS:HE2	1.77	0.44
1:B:699:ARG:O	1:B:703:LEU:HD23	2.18	0.44
1:B:784:LEU:HA	1:B:784:LEU:HD23	1.73	0.44
1:A:132:MET:HE1	1:B:200:PHE:HE2	1.77	0.44
1:A:1488:PRO:O	1:A:1489:SER:HB2	2.17	0.44
1:A:1390:VAL:HG13	1:A:1501:LEU:HD22	1.99	0.44
1:A:1726:THR:CG2	1:A:1726:THR:O	2.66	0.44
1:A:191:LEU:O	1:A:192:LEU:HD23	2.18	0.44
1:A:1941:VAL:HG12	1:A:1941:VAL:O	2.16	0.44
1:A:40:TRP:CZ3	1:A:194:PRO:HA	2.52	0.44
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.81	0.44
1:A:752:VAL:HG11	1:A:775:LEU:HD21	2.00	0.44
1:A:801:GLY:O	1:A:804:HIS:HB3	2.17	0.44
1:B:1137:GLN:HG2	1:B:1396:PHE:CZ	2.53	0.44
1:B:1733:LEU:HD23	1:B:1733:LEU:HA	1.84	0.44
1:B:78:GLN:HE21	1:B:190:VAL:H	1.65	0.44
1:B:1897:GLY:HA2	1:B:1971:LEU:HD12	2.00	0.44
1:B:64:PHE:HB2	1:B:429:ARG:HE	1.82	0.44
1:B:737:ASN:C	1:B:737:ASN:HD22	2.18	0.44
1:B:497:SER:HB2	1:B:762:ALA:CB	2.47	0.44
1:A:1476:ASN:HD22	1:A:1476:ASN:N	2.15	0.44
1:A:1476:ASN:ND2	1:A:1486:MET:CE	2.81	0.44
1:A:1837:GLU:O	1:A:1840:PHE:HB2	2.18	0.44
1:A:440:GLN:HG3	1:A:833:HIS:CD2	2.53	0.44
1:A:844:VAL:O	1:A:845:PRO:C	2.56	0.44
1:B:1444:MET:HB2	1:B:1474:VAL:HB	2.00	0.44
1:B:159:THR:HG22	1:B:398:SER:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1656:TYR:CD2	1:B:1687:ILE:HD13	2.53	0.44
1:B:1996:TYR:C	1:B:1996:TYR:CD2	2.91	0.44
1:B:368:ALA:HB1	1:B:374:LEU:HG	2.00	0.44
1:A:83:LEU:HD23	1:A:144:LEU:HD12	1.99	0.44
1:A:1456:MET:HG3	1:A:2036:PHE:CD1	2.53	0.44
1:A:1651:VAL:HG13	1:A:1679:GLY:C	2.38	0.44
1:A:896:TRP:CD2	1:A:907:LEU:HD11	2.53	0.44
1:B:1187:ALA:HB2	1:B:1210:LEU:HD13	1.99	0.44
1:B:1360:GLY:O	1:B:1364:SER:CB	2.66	0.44
1:B:1449:SER:HB3	1:B:2047:LYS:NZ	2.33	0.44
1:B:1532:PHE:HA	1:B:1546:TRP:HZ3	1.83	0.44
1:B:1941:VAL:HG12	1:B:1941:VAL:O	2.16	0.44
1:A:1243:LYS:HA	1:A:1271:ASP:HB2	2.00	0.43
1:A:1774:LEU:HD22	1:B:1785:PHE:HB2	1.99	0.43
1:A:399:ASN:H	1:A:399:ASN:ND2	2.16	0.43
1:A:584:GLU:O	1:A:587:CYS:HB2	2.18	0.43
1:B:1477:LEU:HD12	1:B:1507:ARG:HH21	1.82	0.43
1:B:336:SER:OG	1:B:337:GLY:N	2.51	0.43
1:B:276:LEU:HD12	1:B:401:HIS:HB3	2.00	0.43
1:B:506:MET:HB3	1:B:506:MET:HE2	1.89	0.43
1:B:643:HIS:CD2	1:B:746:GLN:CB	3.02	0.43
1:B:642:CYS:HA	1:B:743:VAL:HG23	2.00	0.43
1:A:1231:ASP:O	1:A:1232:THR:C	2.56	0.43
1:A:1418:VAL:HG21	1:A:1443:LEU:HD13	2.00	0.43
1:A:1442:TRP:CB	1:A:1444:MET:HE1	2.48	0.43
1:A:1616:MET:HB3	1:A:1800:PHE:HE2	1.83	0.43
1:A:287:LEU:HD13	1:A:312:LEU:HD13	2.00	0.43
1:A:316:ARG:O	1:A:317:ARG:O	2.35	0.43
1:A:389:GLY:O	1:A:390:ILE:HG13	2.18	0.43
1:A:159:THR:HG22	1:A:398:SER:HB3	2.00	0.43
1:A:784:LEU:HD23	1:A:784:LEU:HA	1.73	0.43
1:B:157:ILE:HD11	1:B:167:ALA:CA	2.46	0.43
1:B:801:GLY:O	1:B:804:HIS:HB3	2.17	0.43
1:B:837:ASP:OD1	1:B:839:SER:HB3	2.18	0.43
1:B:883:ARG:HG3	1:B:1107:ARG:CZ	2.48	0.43
1:B:982:THR:HG23	1:B:983:ALA:N	2.28	0.43
1:A:1038:MET:HE3	1:A:1041:LEU:HD23	1.99	0.43
1:A:128:VAL:HG12	1:A:129:GLY:H	1.83	0.43
1:A:1389:LEU:HA	1:A:1389:LEU:HD23	1.76	0.43
1:A:1418:VAL:HG13	1:A:1425:TRP:CZ2	2.52	0.43
1:A:1460:LEU:HD11	1:A:1980:LEU:CD1	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1657:TYR:CZ	1:A:1662:ARG:CD	3.00	0.43
1:A:1810:VAL:HG12	1:A:1810:VAL:O	2.18	0.43
1:A:2023:SER:O	1:A:2027:GLY:HA2	2.17	0.43
1:A:2066:VAL:HG22	1:A:2088:ILE:CD1	2.48	0.43
1:A:411:ALA:HA	1:A:412:PRO:HD3	1.83	0.43
1:A:613:ALA:O	1:A:615:VAL:N	2.51	0.43
1:B:1598:MET:O	1:B:1599:LEU:HD23	2.18	0.43
1:B:1666:GLN:O	1:B:1669:GLU:HB2	2.18	0.43
1:B:1671:VAL:HG23	1:B:1743:LEU:HD13	2.00	0.43
1:B:5:VAL:HG12	1:B:245:THR:HA	2.00	0.43
1:B:277:TYR:O	1:B:278:ALA:C	2.56	0.43
1:B:680:ILE:HG12	1:B:681:ALA:H	1.76	0.43
1:B:739:LEU:HD23	1:B:739:LEU:HA	1.78	0.43
1:B:761:ILE:HG22	1:B:761:ILE:O	2.18	0.43
1:A:1069:TYR:CD1	1:A:1077:ALA:O	2.71	0.43
1:A:1614:MET:HG3	1:A:1649:PRO:HG3	1.99	0.43
1:A:1662:ARG:HH12	1:B:1790:THR:HG21	1.84	0.43
1:A:1769:ILE:HG23	2:A:3001:NAP:H2N	2.01	0.43
1:A:19:LEU:HA	1:A:19:LEU:HD23	1.76	0.43
1:A:272:LEU:O	1:A:276:LEU:HG	2.18	0.43
1:A:333:GLU:O	1:A:336:SER:HB3	2.18	0.43
1:A:399:ASN:H	1:A:399:ASN:HD22	1.65	0.43
1:B:1133:ASN:HB2	1:B:1136:LEU:HB2	2.00	0.43
1:B:1443:LEU:O	1:B:1473:LEU:HA	2.19	0.43
1:B:1845:GLN:HB2	1:B:1847:LYS:HG3	2.00	0.43
1:B:2058:VAL:HG22	1:B:2098:PHE:HD2	1.83	0.43
1:B:289:TYR:HE2	1:B:291:GLU:HA	1.83	0.43
1:B:264:PRO:HG2	1:B:300:GLY:HA2	1.99	0.43
1:B:762:ALA:HB1	1:B:763:PRO:HD2	1.99	0.43
1:B:998:LEU:HD23	1:B:998:LEU:HA	1.87	0.43
1:A:1216:LEU:HD11	1:A:1218:SER:HB3	2.00	0.43
1:A:1252:GLY:HA3	1:A:1318:ASN:CB	2.43	0.43
1:A:1413:PRO:HA	1:A:1440:PRO:HB2	1.99	0.43
1:A:1472:VAL:CG1	1:A:1473:LEU:N	2.82	0.43
1:A:1236:ASN:ND2	1:A:1502:VAL:H	2.16	0.43
1:A:1568:TYR:HB2	1:A:1604:SER:OG	2.18	0.43
1:A:1651:VAL:HG12	1:A:1683:ALA:CB	2.48	0.43
1:A:854:SER:OG	1:A:855:SER:N	2.52	0.43
1:A:899:LEU:O	1:A:899:LEU:HD12	2.18	0.43
1:B:1183:LEU:CD1	1:B:1210:LEU:HB3	2.44	0.43
1:B:1405:ARG:HH22	1:B:1470:ARG:HH22	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1413:PRO:HA	1:B:1440:PRO:O	2.17	0.43
1:B:1538:ARG:NH2	1:B:1585:PRO:CG	2.82	0.43
1:B:594:LEU:HA	1:B:594:LEU:HD23	1.70	0.43
1:B:615:VAL:CG2	1:B:686:PHE:HD2	2.27	0.43
1:B:65:PHE:CE2	1:B:83:LEU:HB3	2.54	0.43
1:A:1001:TYR:CD2	1:A:1003:TYR:CE1	3.06	0.43
1:A:1559:CYS:O	1:A:1562:ARG:HB2	2.18	0.43
1:A:1818:ILE:HG12	1:A:1823:VAL:HG11	2.01	0.43
1:A:1841:ARG:O	1:A:1845:GLN:HG3	2.19	0.43
1:B:1424:ARG:C	1:B:1426:VAL:H	2.21	0.43
1:B:1896:PHE:HB2	2:B:3002:NAP:O2N	2.19	0.43
1:B:409:ARG:HA	1:B:410:PRO:HD3	1.67	0.43
1:B:455:ASN:HB2	1:B:813:ASN:ND2	2.34	0.43
1:B:782:ILE:HG22	1:B:783:PRO:O	2.19	0.43
1:B:765:ALA:HB2	1:B:783:PRO:HB3	2.00	0.43
1:B:768:GLN:CD	1:B:783:PRO:HG3	2.39	0.43
1:A:1036:LEU:HD13	1:A:1051:PRO:HG3	2.00	0.43
1:A:1184:LEU:HD23	1:A:1184:LEU:HA	1.81	0.43
1:A:1552:HIS:CG	1:A:1552:HIS:O	2.71	0.43
1:A:1796:LEU:HA	1:A:1796:LEU:HD12	1.88	0.43
1:A:2058:VAL:HG22	1:A:2098:PHE:HD2	1.83	0.43
1:A:504:GLN:N	1:A:546:LEU:HD11	2.34	0.43
1:A:594:LEU:HA	1:A:594:LEU:HD23	1.69	0.43
1:A:67:VAL:O	1:A:67:VAL:HG23	2.19	0.43
1:A:703:LEU:HG	1:A:703:LEU:O	2.19	0.43
1:A:981:SER:HA	1:A:986:ARG:NH2	2.34	0.43
1:B:103:THR:HG22	1:B:104:SER:N	2.33	0.43
1:B:1554:ALA:HB2	1:B:1882:PRO:CG	2.46	0.43
1:B:159:THR:CG2	1:B:398:SER:CB	2.94	0.43
1:B:1617:VAL:HG13	1:B:1618:PRO:HD2	2.01	0.43
1:B:1562:ARG:HB3	1:B:1627:LEU:HD13	1.99	0.43
1:B:1973:MET:HG3	1:B:1973:MET:O	2.19	0.43
1:B:321:LEU:HD23	1:B:381:LEU:CD1	2.49	0.43
1:B:508:LEU:HD23	1:B:508:LEU:HA	1.85	0.43
1:B:532:LEU:HD22	1:B:604:TYR:HE1	1.84	0.43
1:B:494:PHE:CD1	1:B:574:PRO:HB3	2.53	0.43
1:B:844:VAL:O	1:B:846:SER:N	2.52	0.43
1:B:988:SER:O	1:B:991:ASP:N	2.52	0.43
1:A:1015:LEU:HD23	1:A:1015:LEU:HA	1.76	0.43
1:A:1014:ASP:OD1	1:A:1015:LEU:N	2.51	0.43
1:A:1068:LEU:CD1	1:A:1078:ALA:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1119:PHE:HD1	1:A:1516:HIS:CD2	2.36	0.43
1:A:1312:ALA:O	1:A:1339:LYS:HB2	2.19	0.43
1:A:1956:ILE:HA	1:A:1956:ILE:HD12	1.84	0.43
1:A:494:PHE:CZ	1:A:574:PRO:HG3	2.54	0.43
1:B:1231:ASP:O	1:B:1234:LEU:N	2.50	0.43
1:B:1480:THR:HG22	1:B:1481:SER:H	1.83	0.43
1:B:1893:LEU:HB3	1:B:1925:GLN:HE21	1.79	0.43
1:B:2075:THR:CG2	1:B:2076:ASN:N	2.82	0.43
1:B:608:TYR:O	1:B:611:LYS:N	2.51	0.43
1:B:915:GLU:O	1:B:916:ASP:HB2	2.18	0.43
1:A:1653:THR:HG21	1:A:1807:TRP:CH2	2.53	0.43
1:A:202:LYS:HB2	1:B:129:GLY:HA3	2.01	0.43
1:A:876:VAL:O	1:A:876:VAL:HG12	2.19	0.43
1:A:90:ILE:HG12	1:A:232:LEU:HD22	2.00	0.43
1:B:1501:LEU:H	1:B:1501:LEU:HG	1.52	0.43
1:B:1544:ILE:HD12	1:B:1837:GLU:HA	2.00	0.43
1:B:1857:ARG:NE	1:B:1871:ILE:HD11	2.34	0.43
1:B:193:LYS:HG3	1:B:193:LYS:O	2.19	0.43
1:B:193:LYS:HA	1:B:194:PRO:HD3	1.87	0.43
1:B:2043:ARG:NH1	1:B:2046:GLU:OE1	2.51	0.43
1:B:521:LEU:O	1:B:524:ASP:HB2	2.19	0.43
1:A:2086:GLN:NE2	1:A:2108:SER:OG	2.49	0.43
1:A:254:ASP:HB3	1:A:257:LYS:HE2	2.00	0.43
1:B:1231:ASP:O	1:B:1232:THR:C	2.58	0.43
1:B:1288:LYS:O	1:B:1291:GLN:HG2	2.19	0.43
1:A:1405:ARG:HH22	1:A:1470:ARG:NH2	2.16	0.42
1:A:1894:GLY:O	1:A:1897:GLY:N	2.53	0.42
1:A:1974:VAL:O	1:A:1991:VAL:HG22	2.19	0.42
1:A:1996:TYR:CD2	1:A:1996:TYR:C	2.92	0.42
1:A:434:VAL:O	1:A:438:LEU:HG	2.19	0.42
1:A:624:GLY:HA3	1:A:671:PHE:HB3	2.01	0.42
1:A:652:SER:OG	1:A:681:ALA:HB1	2.19	0.42
1:A:808:VAL:CG1	1:A:809:SER:N	2.77	0.42
1:B:1068:LEU:CD1	1:B:1078:ALA:HB2	2.49	0.42
1:B:1459:CYS:CB	1:B:2032:ALA:HA	2.49	0.42
1:B:1119:PHE:CZ	1:B:1514:PHE:HB3	2.53	0.42
1:B:2105:VAL:O	1:B:2106:LEU:HD23	2.19	0.42
1:B:36:ASP:CB	1:B:38:ARG:HG3	2.49	0.42
1:A:1733:LEU:HD23	1:A:1733:LEU:HA	1.77	0.42
1:A:1735:HIS:HD2	1:A:1735:HIS:H	1.64	0.42
1:A:1932:TRP:O	1:A:1937:VAL:HB	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASP:HB3	1:A:38:ARG:CG	2.49	0.42
1:A:578:ILE:HG22	1:A:745:PHE:HE1	1.84	0.42
1:B:1220:LEU:HD21	1:B:1318:ASN:HD21	1.83	0.42
1:B:136:GLN:HE22	1:B:138:ALA:N	2.09	0.42
1:B:1453:VAL:O	1:B:1456:MET:N	2.53	0.42
1:B:1944:SER:HB2	1:B:1958:GLU:OE2	2.19	0.42
1:B:1975:LEU:HD21	1:B:2034:TYR:CD1	2.54	0.42
1:B:22:PHE:CE2	1:B:26:LEU:HD11	2.54	0.42
1:B:363:ASN:HA	1:B:364:PRO:HD3	1.80	0.42
1:B:423:LEU:HD23	1:B:812:PRO:HG3	2.00	0.42
1:B:900:ALA:HB1	1:B:905:GLN:O	2.19	0.42
1:A:1073:ASP:O	1:A:1074:THR:CG2	2.62	0.42
1:A:1221:LEU:HG	1:A:1221:LEU:O	2.20	0.42
1:A:1424:ARG:C	1:A:1426:VAL:H	2.22	0.42
1:A:1435:ASP:CG	1:A:1438:SER:HB3	2.40	0.42
1:A:1466:GLY:HA2	1:A:1469:ILE:HG13	2.01	0.42
1:A:1603:PHE:N	1:A:1603:PHE:CD2	2.87	0.42
1:A:1729:GLU:OE1	1:A:1758:ARG:HD2	2.19	0.42
1:A:265:SER:O	1:A:269:GLN:HG3	2.20	0.42
1:B:970:PHE:O	1:B:1067:LYS:HE2	2.19	0.42
1:B:972:THR:CG2	1:B:1081:VAL:HG21	2.49	0.42
1:B:1918:SER:HB3	1:B:1921:ARG:HD3	2.01	0.42
1:A:1565:SER:O	1:A:1605:GLY:HA3	2.19	0.42
1:A:1697:THR:CG2	1:A:1698:THR:N	2.81	0.42
1:A:1791:PHE:CD2	1:A:1791:PHE:C	2.92	0.42
1:A:234:THR:HG22	1:A:235:LYS:N	2.35	0.42
1:A:351:GLY:C	1:A:383:ILE:HG22	2.40	0.42
1:A:532:LEU:HD22	1:A:604:TYR:CE1	2.55	0.42
1:A:76:ASP:CG	1:A:116:ALA:HB3	2.40	0.42
1:B:1733:LEU:O	1:B:1736:THR:HG22	2.19	0.42
1:B:2066:VAL:HG22	1:B:2088:ILE:CD1	2.50	0.42
1:B:213:ARG:HD3	1:B:218:GLU:O	2.19	0.42
1:B:67:VAL:O	1:B:68:HIS:C	2.57	0.42
1:B:82:LEU:HA	1:B:85:VAL:HG22	2.02	0.42
1:B:89:ALA:O	1:B:92:ASP:HB3	2.19	0.42
1:A:98:ALA:CA	1:A:101:ARG:HG3	2.48	0.42
1:A:143:ARG:NH1	1:A:143:ARG:CG	2.83	0.42
1:A:1617:VAL:O	1:A:1617:VAL:HG12	2.19	0.42
1:A:65:PHE:CE2	1:A:83:LEU:HB3	2.54	0.42
1:A:851:PRO:HB2	1:B:122:ARG:HA	2.01	0.42
1:B:1253:GLN:HB3	1:B:1255:TYR:CE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1378:TRP:O	1:B:1382:PHE:CD1	2.73	0.42
1:B:1555:LEU:HD12	1:B:1559:CYS:SG	2.59	0.42
1:B:2053:LEU:HA	1:B:2053:LEU:HD23	1.72	0.42
1:B:276:LEU:CD1	1:B:401:HIS:HB3	2.50	0.42
1:B:525:GLN:CA	1:B:525:GLN:NE2	2.82	0.42
1:A:1246:GLU:HG3	1:A:1316:VAL:HB	2.00	0.42
1:A:1976:ARG:HB2	1:A:2033:ASN:HD21	1.85	0.42
1:A:47:LEU:HD21	1:A:198:LEU:HA	2.01	0.42
1:A:739:LEU:HA	1:A:739:LEU:HD23	1.76	0.42
1:B:1312:ALA:HB3	1:B:1337:THR:O	2.20	0.42
1:B:1533:VAL:N	1:B:1546:TRP:CZ3	2.88	0.42
1:B:1860:GLU:HB2	1:B:1865:PRO:HG2	2.01	0.42
1:B:540:SER:OG	1:B:545:VAL:HG21	2.20	0.42
1:B:550:VAL:CG2	1:B:611:LYS:HD3	2.48	0.42
1:A:1584:SER:C	1:A:1586:ASP:H	2.23	0.42
1:A:2105:VAL:O	1:A:2106:LEU:HD23	2.18	0.42
1:A:275:SER:CB	1:A:276:LEU:HD23	2.49	0.42
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.74	0.42
1:A:494:PHE:CE2	1:A:574:PRO:HG3	2.54	0.42
1:A:623:VAL:HA	1:A:671:PHE:O	2.19	0.42
1:A:945:GLU:OE2	1:B:941:SER:CB	2.67	0.42
1:B:1009:LEU:HD22	1:B:1023:GLN:O	2.20	0.42
1:B:128:VAL:O	1:B:131:SER:OG	2.34	0.42
1:B:1685:ILE:O	1:B:1686:ALA:C	2.58	0.42
1:B:454:LEU:HA	1:B:454:LEU:HD23	1.80	0.42
1:B:876:VAL:HA	1:B:884:VAL:HG11	2.01	0.42
1:A:1184:LEU:H	1:A:1216:LEU:CD2	2.33	0.42
1:A:1222:ASP:HA	1:A:1226:LEU:CD1	2.49	0.42
1:A:290:ILE:HG23	1:A:290:ILE:O	2.18	0.42
1:A:276:LEU:HD12	1:A:401:HIS:HB3	2.02	0.42
1:A:542:ASP:OD1	1:A:542:ASP:C	2.58	0.42
1:B:1073:ASP:O	1:B:1074:THR:CG2	2.61	0.42
1:B:1429:LEU:HD21	1:B:1443:LEU:HD21	2.00	0.42
1:B:1496:VAL:HG21	1:B:1511:TRP:CH2	2.55	0.42
1:B:1473:LEU:HD11	1:B:1503:MET:SD	2.60	0.42
1:B:1540:ASP:C	1:B:1542:SER:H	2.21	0.42
1:B:1565:SER:HB2	1:B:1857:ARG:CZ	2.50	0.42
1:B:1671:VAL:HG23	1:B:1743:LEU:CD1	2.49	0.42
1:B:185:VAL:O	1:B:230:ALA:HA	2.19	0.42
1:B:412:PRO:HA	1:B:413:PRO:HD3	1.89	0.42
1:B:892:LEU:HD22	1:B:1057:ILE:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1228:ALA:HB2	1:A:1517:PHE:CE2	2.55	0.42
1:A:1476:ASN:CA	1:A:1486:MET:SD	3.07	0.42
1:A:1477:LEU:HD12	1:A:1507:ARG:HH21	1.83	0.42
1:A:1522:ASP:O	1:A:1524:PRO:HD3	2.20	0.42
1:A:1697:THR:HG23	1:A:1698:THR:N	2.34	0.42
1:A:1739:LYS:O	1:A:1761:ALA:HB2	2.19	0.42
1:A:2104:PRO:HD2	1:A:2105:VAL:H	1.84	0.42
1:A:299:VAL:O	1:A:302:PRO:HD2	2.19	0.42
1:A:189:ASN:HB2	1:A:334:PRO:HD2	2.02	0.42
1:A:506:MET:HB3	1:A:559:ILE:CD1	2.49	0.42
1:A:506:MET:CE	1:A:559:ILE:HD12	2.49	0.42
1:A:677:THR:HG22	1:A:682:PHE:CE2	2.55	0.42
1:A:761:ILE:O	1:A:761:ILE:HG22	2.19	0.42
1:B:1147:ALA:C	1:B:1149:ALA:H	2.23	0.42
1:B:1243:LYS:HD3	1:B:1311:LYS:HB3	2.01	0.42
1:B:1312:ALA:O	1:B:1339:LYS:HB2	2.20	0.42
1:B:1454:VAL:HG13	1:B:1503:MET:HE3	2.02	0.42
1:B:1238:ALA:HB2	1:B:1468:ARG:HD3	2.02	0.42
1:B:47:LEU:HD21	1:B:198:LEU:HA	2.01	0.42
1:B:23:TRP:NE1	1:B:350:HIS:CD2	2.87	0.42
1:B:470:TYR:C	1:B:470:TYR:CD1	2.92	0.42
1:B:638:ILE:HD11	1:B:657:ALA:O	2.20	0.42
1:B:491:PRO:HG2	1:B:753:PRO:HG2	2.02	0.42
1:A:1121:PHE:HE1	1:A:1512:GLY:O	2.03	0.42
1:A:1316:VAL:HA	1:A:1345:LEU:O	2.20	0.42
1:A:1124:HIS:NE2	1:A:1512:GLY:HA2	2.35	0.42
1:A:1897:GLY:HA2	1:A:1971:LEU:HD12	2.02	0.42
1:B:1015:LEU:HA	1:B:1015:LEU:HD23	1.74	0.42
1:B:1244:VAL:HB	1:B:1272:TYR:HD1	1.84	0.42
1:B:1390:VAL:HG22	1:B:1501:LEU:HD21	2.02	0.42
1:B:1556:PRO:C	1:B:1558:SER:H	2.23	0.42
1:B:1578:LEU:C	1:B:1580:THR:N	2.73	0.42
1:B:1538:ARG:NH1	1:B:1585:PRO:HG2	2.35	0.42
1:B:327:SER:OG	1:B:356:ASN:ND2	2.53	0.42
1:B:550:VAL:CG2	1:B:608:TYR:HA	2.50	0.42
1:B:759:VAL:O	1:B:759:VAL:HG23	2.20	0.42
1:B:84:GLU:O	1:B:88:GLU:HG3	2.20	0.42
1:A:1302:ALA:O	1:A:1303:ASN:CB	2.65	0.41
1:A:1469:ILE:CG2	1:A:1469:ILE:O	2.68	0.41
1:A:1504:ASN:HB3	1:A:1511:TRP:CZ3	2.54	0.41
1:A:1859:GLU:CG	1:A:1860:GLU:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2031:GLN:HB3	1:A:2034:TYR:HB3	2.01	0.41
1:B:1068:LEU:HD13	1:B:1078:ALA:HB2	2.01	0.41
1:B:1251:ASP:HB3	1:B:1321:LEU:HD22	2.01	0.41
1:B:1350:LEU:HD23	1:B:1350:LEU:N	2.34	0.41
1:B:1442:TRP:HB3	1:B:1444:MET:CE	2.50	0.41
1:B:1563:LEU:HA	1:B:1563:LEU:HD12	1.88	0.41
1:B:1799:LEU:O	1:B:1801:GLU:N	2.54	0.41
1:B:1922:THR:H	1:B:1922:THR:HG1	1.64	0.41
1:B:1115:ILE:HD11	1:B:2111:LEU:CD1	2.49	0.41
1:B:355:PRO:CG	1:B:380:PRO:HG3	2.50	0.41
1:B:362:PRO:HB3	1:B:369:LEU:HB3	2.02	0.41
1:B:47:LEU:HA	1:B:48:PRO:HD3	1.85	0.41
1:A:1235:GLU:OE2	1:A:1515:ARG:CZ	2.68	0.41
1:A:120:LEU:HA	1:A:127:LEU:HD13	2.02	0.41
1:A:1419:GLU:OE2	1:A:1447:GLY:HA3	2.20	0.41
1:A:1949:LEU:HD21	1:A:1953:ARG:NH2	2.35	0.41
1:A:2043:ARG:NH1	1:A:2046:GLU:OE1	2.53	0.41
1:A:264:PRO:HG2	1:A:300:GLY:HA2	2.03	0.41
1:A:274:ARG:O	1:A:276:LEU:N	2.53	0.41
1:A:67:VAL:O	1:A:68:HIS:C	2.58	0.41
1:B:1394:ARG:HA	1:B:1400:VAL:HG22	2.02	0.41
1:B:1746:ASN:HD21	1:B:1753:LEU:HD12	1.85	0.41
1:B:283:ASP:C	1:B:285:GLU:H	2.22	0.41
1:B:94:GLY:HA3	1:B:453:MET:HG2	2.01	0.41
1:B:819:VAL:O	1:B:821:PHE:N	2.53	0.41
1:A:1252:GLY:N	1:A:1321:LEU:HD21	2.35	0.41
1:A:1578:LEU:C	1:A:1580:THR:N	2.74	0.41
1:A:1644:GLU:HB3	1:A:1825:PRO:CG	2.50	0.41
1:A:1616:MET:HE2	1:A:1650:ILE:HD13	2.01	0.41
1:A:91:VAL:O	1:A:457:ILE:HD11	2.20	0.41
1:A:765:ALA:HB2	1:A:783:PRO:HB3	2.02	0.41
1:A:874:TYR:CD1	1:A:1006:PHE:CE2	3.08	0.41
1:A:89:ALA:O	1:A:92:ASP:HB3	2.21	0.41
1:A:915:GLU:O	1:A:916:ASP:HB2	2.20	0.41
1:B:98:ALA:CA	1:B:101:ARG:HG3	2.47	0.41
1:B:1477:LEU:CD1	1:B:1507:ARG:HH21	2.33	0.41
1:B:147:PHE:C	1:B:147:PHE:CD2	2.94	0.41
1:B:2058:VAL:HG11	1:B:2060:TRP:CE2	2.54	0.41
1:B:350:HIS:O	1:B:352:VAL:HG12	2.21	0.41
1:B:366:ILE:O	1:B:366:ILE:CG1	2.68	0.41
1:A:1068:LEU:HD13	1:A:1078:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1432:ILE:O	1:A:1432:ILE:HG22	2.21	0.41
1:A:1435:ASP:OD2	1:A:1438:SER:HB3	2.20	0.41
1:A:14:PRO:HB2	1:A:32:MET:HB2	2.03	0.41
1:A:1530:HIS:CB	1:A:1549:SER:HB3	2.51	0.41
1:A:1678:GLY:O	1:A:1682:GLN:HG3	2.20	0.41
1:A:256:SER:HB3	1:B:146:PHE:O	2.19	0.41
1:A:313:CYS:HA	1:A:315:THR:HG22	2.03	0.41
1:A:33:VAL:HG13	1:A:51:MET:C	2.39	0.41
1:A:377:VAL:HG13	1:A:381:LEU:CD1	2.50	0.41
1:A:495:ILE:HG12	1:A:758:VAL:HG13	2.01	0.41
1:B:1220:LEU:CD2	1:B:1318:ASN:HD21	2.33	0.41
1:B:1305:ALA:HA	1:B:1306:PRO:HD2	1.83	0.41
1:B:1448:CYS:C	1:B:1450:THR:H	2.24	0.41
1:B:1433:LEU:HD11	1:B:1465:GLY:O	2.20	0.41
1:B:40:TRP:CH2	1:B:51:MET:HE3	2.56	0.41
1:B:595:THR:OG1	1:B:598:GLU:HG3	2.20	0.41
1:B:83:LEU:HD23	1:B:83:LEU:HA	1.89	0.41
1:A:1147:ALA:HB1	1:A:1358:MET:HE1	2.02	0.41
1:B:1473:LEU:HG	1:B:1503:MET:HA	2.02	0.41
1:B:1506:TYR:OH	1:B:1509:GLY:HA2	2.21	0.41
1:B:1698:THR:HB	1:B:1723:SER:HB3	2.01	0.41
1:B:2018:ILE:HG21	1:B:2041:MET:HB3	2.03	0.41
1:B:188:LEU:CD2	1:B:228:VAL:HG12	2.49	0.41
1:B:988:SER:H	1:B:991:ASP:HB2	1.85	0.41
1:B:9:MET:HE1	1:B:345:LEU:HB2	2.01	0.41
1:A:1442:TRP:HB3	1:A:1444:MET:CE	2.51	0.41
1:A:1680:VAL:CG1	1:A:1681:GLY:N	2.84	0.41
1:A:355:PRO:CG	1:A:380:PRO:HG3	2.51	0.41
1:A:564:ILE:HG12	1:A:761:ILE:HD13	2.03	0.41
1:A:644:ASN:HB3	1:A:770:VAL:CG1	2.51	0.41
1:A:719:GLU:HA	1:A:722:TRP:NE1	2.36	0.41
1:A:782:ILE:CD1	1:A:803:LEU:HD23	2.41	0.41
1:B:1146:LEU:HD22	1:B:1192:LEU:HD12	2.02	0.41
1:B:1818:ILE:HG12	1:B:1823:VAL:CG1	2.51	0.41
1:B:1932:TRP:O	1:B:1937:VAL:HB	2.21	0.41
1:B:1984:THR:C	1:B:1986:GLU:H	2.22	0.41
1:B:290:ILE:O	1:B:290:ILE:HG23	2.21	0.41
1:B:41:LYS:HD2	1:B:44:LEU:HD22	2.02	0.41
1:B:475:GLY:O	1:B:477:ALA:N	2.51	0.41
1:B:719:GLU:HA	1:B:722:TRP:NE1	2.35	0.41
1:B:581:SER:HA	1:B:738:ASN:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:VAL:O	1:A:131:SER:OG	2.39	0.41
1:A:1422:SER:O	1:A:1423:PHE:CB	2.68	0.41
1:A:1898:LEU:HA	1:A:1898:LEU:HD23	1.72	0.41
1:A:40:TRP:CE3	1:A:194:PRO:HG3	2.56	0.41
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.76	0.41
1:A:36:ASP:C	1:A:38:ARG:H	2.24	0.41
1:A:502:GLN:OE1	1:A:676:ARG:HD3	2.21	0.41
1:A:719:GLU:HA	1:A:722:TRP:CE2	2.55	0.41
1:A:831:SER:N	1:A:832:PRO:HD3	2.35	0.41
1:B:132:MET:HE3	1:B:132:MET:HB3	1.65	0.41
1:B:14:PRO:HB2	1:B:32:MET:HB2	2.02	0.41
1:B:1554:ALA:HB3	1:B:1882:PRO:HB3	2.02	0.41
1:B:2022:VAL:HG13	1:B:2026:ARG:HG2	2.03	0.41
1:B:291:GLU:OE2	1:B:325:THR:N	2.53	0.41
1:B:48:PRO:HD3	1:B:201:MET:HE3	2.02	0.41
1:B:827:THR:HA	1:B:828:PRO:HD3	1.96	0.41
1:A:1004:GLY:O	1:A:1008:GLN:HG3	2.20	0.41
1:A:1124:HIS:CD2	1:A:1511:TRP:O	2.73	0.41
1:A:1614:MET:HG2	1:A:1614:MET:O	2.19	0.41
1:A:165:LEU:HD23	1:A:400:VAL:CG2	2.30	0.41
1:A:1762:GLN:HB3	1:A:1763:HIS:CD2	2.55	0.41
1:A:997:ARG:HE	1:A:2070:LEU:CD1	2.34	0.41
1:A:305:LEU:CD2	1:A:308:ILE:HD12	2.51	0.41
1:A:63:SER:O	1:A:66:GLY:N	2.49	0.41
1:A:618:GLY:N	1:A:679:GLY:O	2.50	0.41
1:A:96:ASN:ND2	1:A:98:ALA:HB3	2.36	0.41
1:A:976:VAL:CG2	1:A:977:ASP:H	2.23	0.41
1:B:1127:SER:HA	1:B:1394:ARG:HB3	2.02	0.41
1:B:1214:ASP:HB3	1:B:1215:PRO:CD	2.47	0.41
1:B:169:GLN:HG3	1:B:249:ALA:HB1	2.02	0.41
1:B:1541:LEU:CD1	1:B:1840:PHE:HB3	2.44	0.41
1:B:197:SER:OG	1:B:224:ARG:HD3	2.21	0.41
1:A:132:MET:CE	1:B:200:PHE:CE2	2.96	0.41
1:B:533:ARG:HB2	1:B:533:ARG:NH1	2.35	0.41
1:A:1001:TYR:HD2	1:A:1003:TYR:CE1	2.39	0.41
1:A:1022:LEU:O	1:A:1077:ALA:HB1	2.20	0.41
1:A:1307:GLY:C	1:A:1309:LEU:H	2.24	0.41
1:A:1321:LEU:HA	1:A:1321:LEU:HD12	1.90	0.41
1:A:1654:THR:HG21	2:A:3001:NAP:C4N	2.51	0.41
1:A:1921:ARG:HB2	1:A:1921:ARG:HE	1.47	0.41
1:A:193:LYS:HG3	1:A:193:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ARG:HA	1:A:410:PRO:HD3	1.68	0.41
1:A:412:PRO:HA	1:A:413:PRO:HD3	1.89	0.41
1:B:1214:ASP:CG	1:B:1321:LEU:HD21	2.40	0.41
1:B:1540:ASP:C	1:B:1542:SER:N	2.73	0.41
1:B:1569:THR:HG23	1:B:1602:GLU:O	2.20	0.41
1:B:1695:VAL:HG12	1:B:1696:PHE:N	2.36	0.41
1:B:305:LEU:HA	1:B:305:LEU:HD23	1.79	0.41
1:B:40:TRP:HB2	1:B:41:LYS:H	1.66	0.41
1:B:59:ARG:HE	1:B:841:ALA:HB2	1.86	0.41
1:B:898:THR:HG22	1:B:937:LEU:HD22	2.02	0.41
1:A:1214:ASP:C	1:A:1216:LEU:N	2.74	0.41
1:A:1535:VAL:CG1	1:A:1537:SER:H	2.34	0.41
1:A:1569:THR:CG2	1:A:1622:LEU:HD23	2.51	0.41
1:A:1765:ARG:CD	1:A:1765:ARG:N	2.84	0.41
1:A:1893:LEU:CB	1:A:1925:GLN:NE2	2.75	0.41
1:A:193:LYS:HA	1:A:194:PRO:HD3	1.88	0.41
1:A:511:MET:HE2	1:A:511:MET:HB2	1.81	0.41
1:A:81:MET:HG2	1:A:81:MET:H	1.72	0.41
1:B:132:MET:HG2	1:B:136:GLN:HB2	2.02	0.41
1:B:1999:THR:HG23	1:B:2018:ILE:HD11	2.02	0.41
1:B:214:SER:HB3	1:B:327:SER:HB3	2.03	0.41
1:B:25:ASN:CB	1:B:32:MET:SD	3.09	0.41
1:B:399:ASN:H	1:B:399:ASN:HD22	1.69	0.41
1:B:610:ILE:HA	1:B:690:ILE:HD13	2.02	0.41
1:A:119:ALA:HB2	1:A:850:PHE:CE2	2.56	0.41
1:A:1216:LEU:HG	1:A:1219:GLY:H	1.86	0.41
1:A:1338:LEU:HD22	1:A:1406:GLN:HG3	2.03	0.41
1:A:200:PHE:CE2	1:B:132:MET:CE	2.98	0.41
1:A:545:VAL:HG22	1:A:551:SER:HB3	2.02	0.41
1:A:92:ASP:O	1:A:241:ARG:NH1	2.52	0.41
1:B:128:VAL:HG12	1:B:130:TYR:CE2	2.56	0.41
1:B:1651:VAL:HG12	1:B:1683:ALA:CB	2.51	0.41
1:B:1868:LEU:HA	1:B:1869:PRO:HD3	1.76	0.41
1:B:1999:THR:OG1	1:B:2041:MET:HG2	2.20	0.41
1:B:2043:ARG:HA	1:B:2043:ARG:HD3	1.61	0.41
1:B:2086:GLN:NE2	1:B:2108:SER:OG	2.50	0.41
1:B:287:LEU:HD13	1:B:312:LEU:HD13	2.02	0.41
1:B:494:PHE:CZ	1:B:574:PRO:HG3	2.56	0.41
1:B:737:ASN:O	1:B:737:ASN:ND2	2.52	0.41
1:B:12:LYS:HD2	1:B:81:MET:HE2	2.03	0.41
1:B:59:ARG:HH21	1:B:841:ALA:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1371:HIS:O	1:A:1372:LEU:HD23	2.20	0.40
1:A:1496:VAL:HG21	1:A:1511:TRP:CZ3	2.57	0.40
1:A:1734:ARG:C	1:A:1736:THR:N	2.75	0.40
1:A:1733:LEU:O	1:A:1736:THR:HG22	2.20	0.40
1:A:1653:THR:CG2	1:A:1810:VAL:HG12	2.52	0.40
1:A:1999:THR:HG23	1:A:2018:ILE:HD11	2.03	0.40
1:A:2069:VAL:HG12	1:A:2070:LEU:HD23	2.03	0.40
1:A:429:ARG:HA	1:A:429:ARG:HD2	1.98	0.40
1:A:534:VAL:HG13	1:A:554:VAL:HG12	2.04	0.40
1:A:898:THR:HG22	1:A:937:LEU:HD22	2.02	0.40
1:B:1001:TYR:CD2	1:B:1003:TYR:CE1	3.08	0.40
1:B:1227:LYS:O	1:B:1231:ASP:HB2	2.21	0.40
1:B:1698:THR:HA	1:B:1721:ALA:O	2.20	0.40
1:B:82:LEU:HD22	1:B:188:LEU:HD11	2.03	0.40
1:B:2072:THR:HB	1:B:2073:MET:H	1.69	0.40
1:B:236:LYS:C	1:B:238:LEU:H	2.24	0.40
1:B:288:GLU:CD	1:B:385:GLY:H	2.24	0.40
1:B:411:ALA:HA	1:B:412:PRO:HD3	1.85	0.40
1:B:416:GLN:C	1:B:418:ALA:H	2.25	0.40
1:B:570:LEU:HD11	1:B:800:VAL:HG22	2.03	0.40
1:B:76:ASP:CG	1:B:116:ALA:HB3	2.41	0.40
1:B:96:ASN:HD21	1:B:98:ALA:HB3	1.85	0.40
1:A:1345:LEU:HD12	1:A:1345:LEU:HA	1.93	0.40
1:A:254:ASP:O	1:A:255:GLY:O	2.39	0.40
1:A:289:TYR:HH	1:A:323:GLY:HA3	1.84	0.40
1:A:473:LEU:N	1:A:473:LEU:HD23	2.36	0.40
1:B:1001:TYR:HD2	1:B:1003:TYR:CE1	2.39	0.40
1:B:1038:MET:HE3	1:B:1041:LEU:HD23	2.03	0.40
1:B:1153:LYS:CD	1:B:1195:ASN:HD22	2.35	0.40
1:B:1247:VAL:CG1	1:B:1301:PRO:HG3	2.45	0.40
1:B:1322:ALA:HB1	1:B:1371:HIS:HE1	1.83	0.40
1:B:1236:ASN:HD21	1:B:1502:VAL:H	1.69	0.40
1:B:1858:GLU:HG3	1:B:1859:GLU:N	2.37	0.40
1:B:317:ARG:O	1:B:319:PRO:HD3	2.21	0.40
1:B:623:VAL:CG1	1:B:624:GLY:N	2.84	0.40
1:A:368:ALA:HB1	1:A:374:LEU:HG	2.03	0.40
1:A:416:GLN:C	1:A:418:ALA:H	2.24	0.40
1:B:232:LEU:HD12	1:B:233:LEU:N	2.36	0.40
1:B:274:ARG:C	1:B:276:LEU:N	2.75	0.40
1:B:719:GLU:HA	1:B:722:TRP:CE2	2.56	0.40
1:B:944:PHE:CD1	1:B:944:PHE:C	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:979:ALA:O	1:B:980:ASP:O	2.40	0.40
1:A:1223:ALA:CB	1:A:1224:PRO:HD2	2.39	0.40
1:A:1472:VAL:CG1	1:A:1473:LEU:H	2.33	0.40
1:A:368:ALA:CA	1:A:371:ASP:HB3	2.51	0.40
1:A:98:ALA:HA	1:A:101:ARG:CG	2.50	0.40
1:B:879:CYS:O	1:B:1002:ASP:HB2	2.21	0.40
1:B:1185:ALA:O	1:B:1189:GLN:HG3	2.22	0.40
1:B:1279:PRO:HG3	1:B:1298:GLN:NE2	2.35	0.40
1:B:1343:PHE:CE2	1:B:1405:ARG:HD2	2.57	0.40
1:B:1443:LEU:C	1:B:1444:MET:HE3	2.41	0.40
1:B:1818:ILE:HG12	1:B:1823:VAL:HG11	2.03	0.40
1:B:1894:GLY:O	1:B:1897:GLY:N	2.54	0.40
1:B:316:ARG:O	1:B:317:ARG:O	2.40	0.40
1:B:30:VAL:O	1:B:32:MET:HG2	2.21	0.40
1:B:461:SER:HA	1:B:462:PRO:HD3	1.84	0.40
1:A:1486:MET:HE3	1:A:1506:TYR:CB	2.50	0.40
1:A:1657:TYR:CZ	1:A:1799:LEU:HD11	2.57	0.40
1:A:165:LEU:HD22	1:A:392:SER:HB2	2.03	0.40
1:A:1976:ARG:HB2	1:A:2033:ASN:ND2	2.36	0.40
2:A:3001:NAP:H52A	2:A:3001:NAP:H52N	2.03	0.40
1:A:375:GLN:O	1:A:376:VAL:C	2.59	0.40
1:B:1453:VAL:O	1:B:1454:VAL:C	2.59	0.40
1:B:1493:LEU:HD23	1:B:1494:GLN:HE21	1.87	0.40
1:B:159:THR:CG2	1:B:159:THR:O	2.65	0.40
1:B:1612:ARG:CG	1:B:1642:LEU:HD21	2.51	0.40
1:B:1726:THR:CG2	1:B:1726:THR:O	2.69	0.40
1:B:1796:LEU:HA	1:B:1796:LEU:HD12	1.89	0.40
1:B:166:LEU:HB2	1:B:400:VAL:HG11	2.04	0.40
1:B:47:LEU:HD22	1:B:197:SER:HB3	2.04	0.40
1:B:537:LEU:HA	1:B:537:LEU:HD23	1.74	0.40
1:B:980:ASP:HB2	1:B:981:SER:H	1.44	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	2075/2512 (83%)	1683 (81%)	296 (14%)	96 (5%)	2	15
1	B	2080/2512 (83%)	1713 (82%)	276 (13%)	91 (4%)	2	16
All	All	4155/5024 (83%)	3396 (82%)	572 (14%)	187 (4%)	2	15

All (187) Ramachandran outliers are listed below:

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

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

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

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

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Mol	Chain	Res	Type
1	B	654	PRO
1	B	977	ASP
1	B	1181	PRO
1	B	1304	PRO
1	B	1692	GLY
1	B	1734	ARG
1	B	2009	ALA
1	A	29	GLY
1	A	845	PRO
1	A	1215	PRO
1	B	1408	THR
1	A	1240	PRO
1	A	1870	PRO
1	B	29	GLY
1	B	1240	PRO
1	B	2104	PRO
1	A	1306	PRO
1	A	1464	PRO
1	A	1651	VAL
1	A	1692	GLY
1	A	2104	PRO
1	B	1770	GLY
1	A	2074	GLY
1	B	692	PRO
1	B	1342	GLY
1	A	868	PRO
1	A	1145	GLY
1	B	352	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1717/2072 (83%)	1522 (89%)	195 (11%)	5	22
1	B	1722/2072 (83%)	1534 (89%)	188 (11%)	6	24
All	All	3439/4144 (83%)	3056 (89%)	383 (11%)	6	23

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAP	B	3002	-	45,52,52	1.37	4 (8%)	56,80,80	1.23	4 (7%)
2	NAP	B	3001	-	45,52,52	1.32	3 (6%)	56,80,80	1.41	5 (8%)
2	NAP	A	3002	-	45,52,52	1.24	3 (6%)	56,80,80	1.14	3 (5%)
2	NAP	A	3001	-	45,52,52	1.38	3 (6%)	56,80,80	1.22	3 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	B	3002	-	-	8/31/67/67	0/5/5/5
2	NAP	B	3001	-	-	2/31/67/67	0/5/5/5
2	NAP	A	3002	-	-	8/31/67/67	0/5/5/5
2	NAP	A	3001	-	-	11/31/67/67	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3002	NAP	C2N-N1N	5.09	1.41	1.35
2	A	3001	NAP	C2A-N3A	5.03	1.40	1.32
2	B	3001	NAP	C2N-N1N	4.97	1.41	1.35
2	A	3002	NAP	C2N-N1N	4.68	1.40	1.35
2	B	3002	NAP	C2A-N3A	4.46	1.39	1.32
2	A	3001	NAP	C2N-N1N	4.40	1.40	1.35
2	B	3001	NAP	C2A-N3A	4.17	1.38	1.32
2	A	3002	NAP	C2A-N3A	3.83	1.38	1.32
2	A	3001	NAP	C2A-N1A	3.20	1.39	1.33
2	B	3001	NAP	C2A-N1A	3.16	1.39	1.33
2	B	3002	NAP	C6N-N1N	2.35	1.41	1.35
2	A	3002	NAP	C2A-N1A	2.18	1.38	1.33
2	B	3002	NAP	C2A-N1A	2.12	1.37	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	NAP	N3A-C2A-N1A	-5.95	119.37	128.68
2	A	3002	NAP	N3A-C2A-N1A	-5.42	120.20	128.68
2	B	3001	NAP	N3A-C2A-N1A	-5.30	120.39	128.68
2	B	3002	NAP	N3A-C2A-N1A	-5.02	120.84	128.68
2	B	3001	NAP	C3N-C7N-N7N	-4.36	112.52	117.75
2	B	3002	NAP	C6N-N1N-C2N	-3.29	118.97	121.97
2	B	3001	NAP	O7N-C7N-C3N	2.76	122.93	119.63
2	B	3001	NAP	PN-O3-PA	-2.55	124.08	132.83
2	A	3001	NAP	C3B-C2B-C1B	2.38	107.36	102.89
2	A	3002	NAP	C3D-C2D-C1D	2.36	104.53	100.98
2	B	3002	NAP	C3N-C7N-N7N	-2.33	114.95	117.75
2	B	3001	NAP	C5D-C4D-C3D	-2.17	107.03	115.18
2	B	3002	NAP	C3D-C2D-C1D	2.17	104.25	100.98
2	A	3002	NAP	C3N-C7N-N7N	-2.12	115.21	117.75
2	A	3001	NAP	O2B-C2B-C1B	-2.03	102.80	110.10

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3002	NAP	C3B-C4B-C5B-O5B
2	B	3002	NAP	C3B-C2B-O2B-P2B
2	A	3002	NAP	C5B-O5B-PA-O3
2	A	3002	NAP	C3B-C4B-C5B-O5B
2	A	3002	NAP	O4D-C4D-C5D-O5D
2	A	3001	NAP	C5B-O5B-PA-O3
2	A	3001	NAP	C2B-O2B-P2B-O2X
2	A	3001	NAP	O4D-C1D-N1N-C6N
2	B	3002	NAP	O4D-C4D-C5D-O5D
2	A	3002	NAP	C3D-C4D-C5D-O5D
2	A	3001	NAP	O4B-C4B-C5B-O5B
2	B	3002	NAP	O4B-C4B-C5B-O5B
2	A	3002	NAP	O4B-C4B-C5B-O5B
2	B	3002	NAP	C3D-C4D-C5D-O5D
2	A	3001	NAP	C3B-C4B-C5B-O5B
2	B	3001	NAP	O4B-C4B-C5B-O5B
2	B	3002	NAP	PA-O3-PN-O5D
2	A	3001	NAP	C2B-O2B-P2B-O1X
2	B	3001	NAP	C4B-C5B-O5B-PA
2	A	3002	NAP	C5B-O5B-PA-O2A
2	A	3001	NAP	C5B-O5B-PA-O1A

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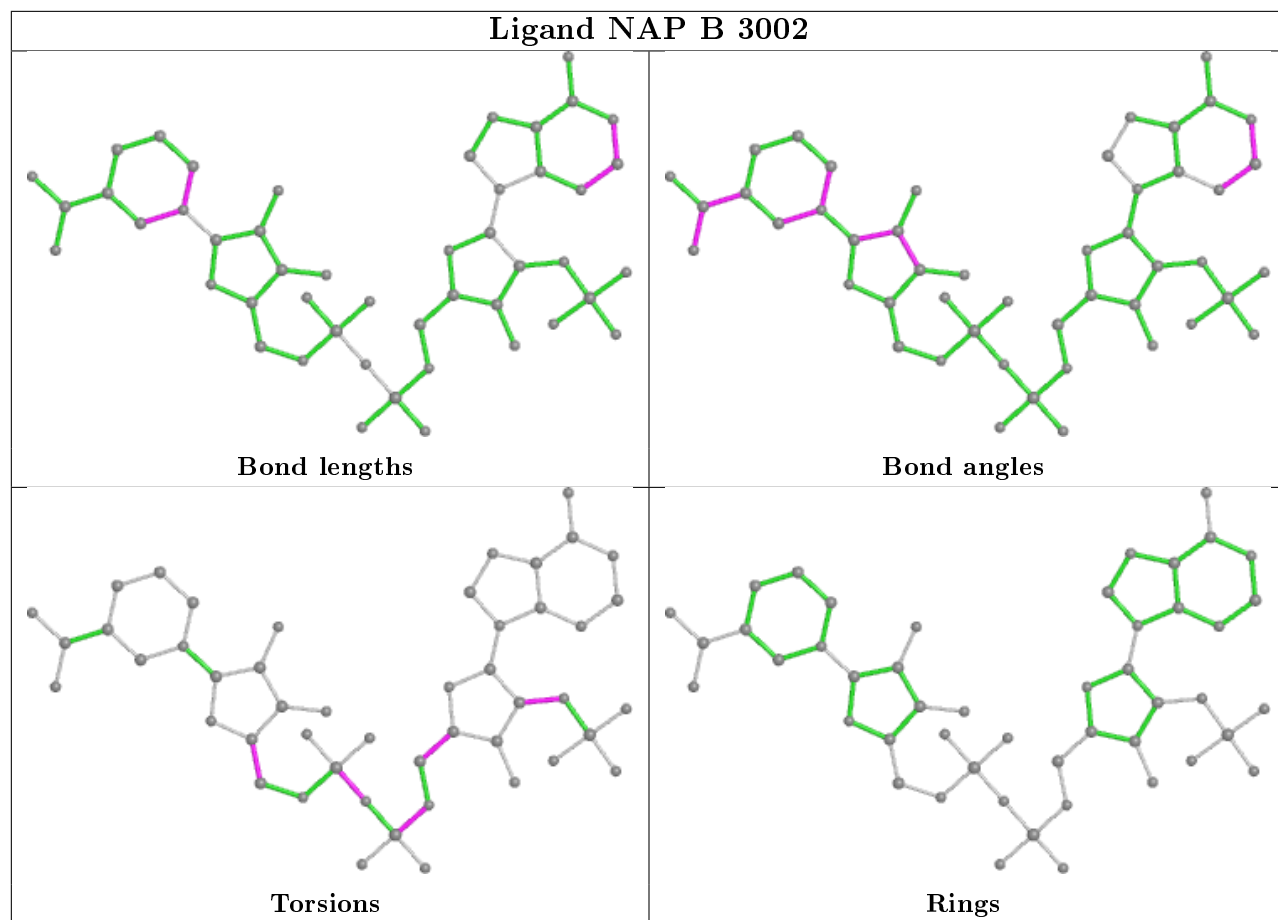
Mol	Chain	Res	Type	Atoms
2	A	3001	NAP	C5B-O5B-PA-O2A
2	B	3002	NAP	C1B-C2B-O2B-P2B
2	A	3001	NAP	PA-O3-PN-O2N
2	A	3002	NAP	PN-O3-PA-O1A
2	B	3002	NAP	C5B-O5B-PA-O3
2	A	3001	NAP	PA-O3-PN-O1N
2	A	3001	NAP	C5D-O5D-PN-O1N
2	A	3002	NAP	C4B-C5B-O5B-PA

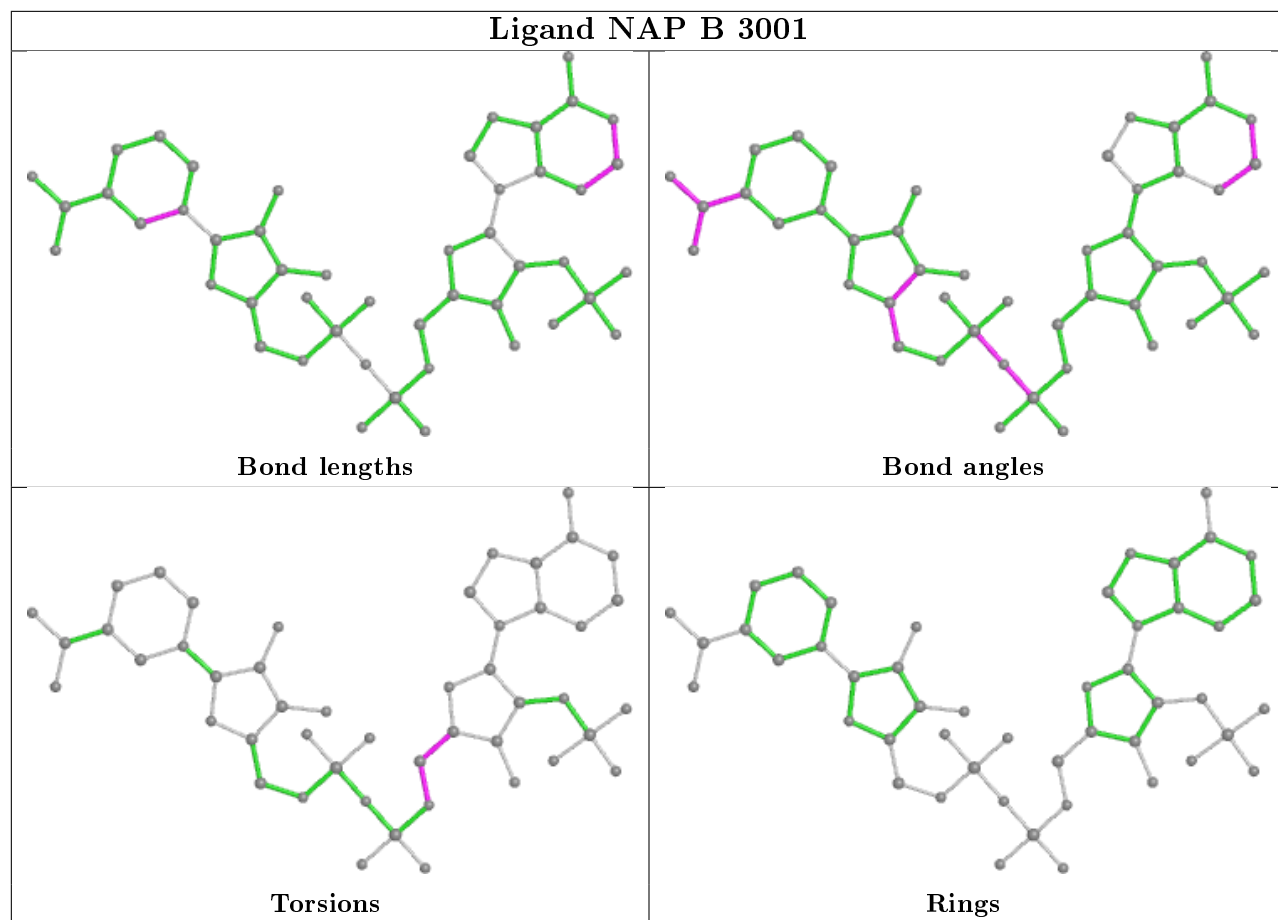
There are no ring outliers.

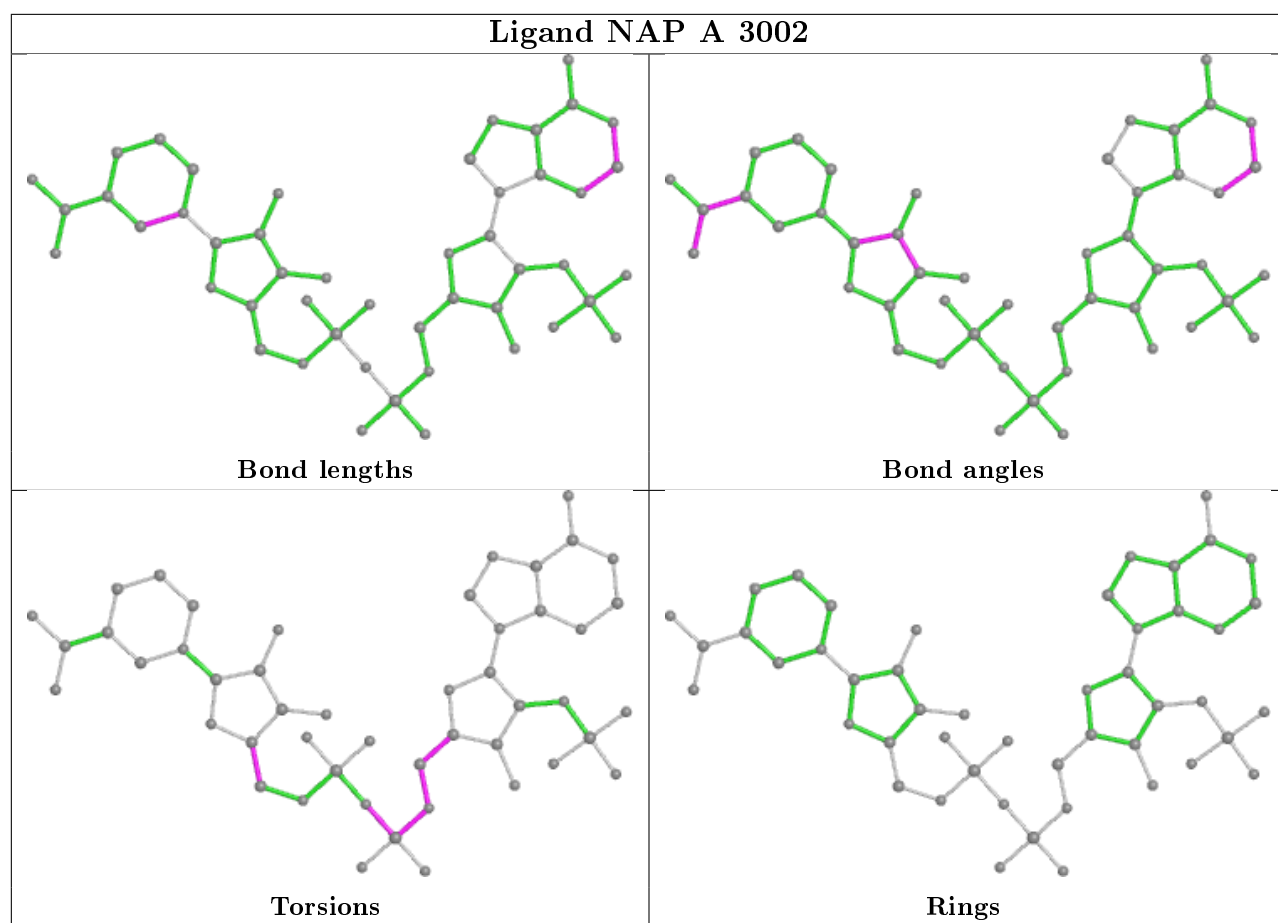
4 monomers are involved in 15 short contacts:

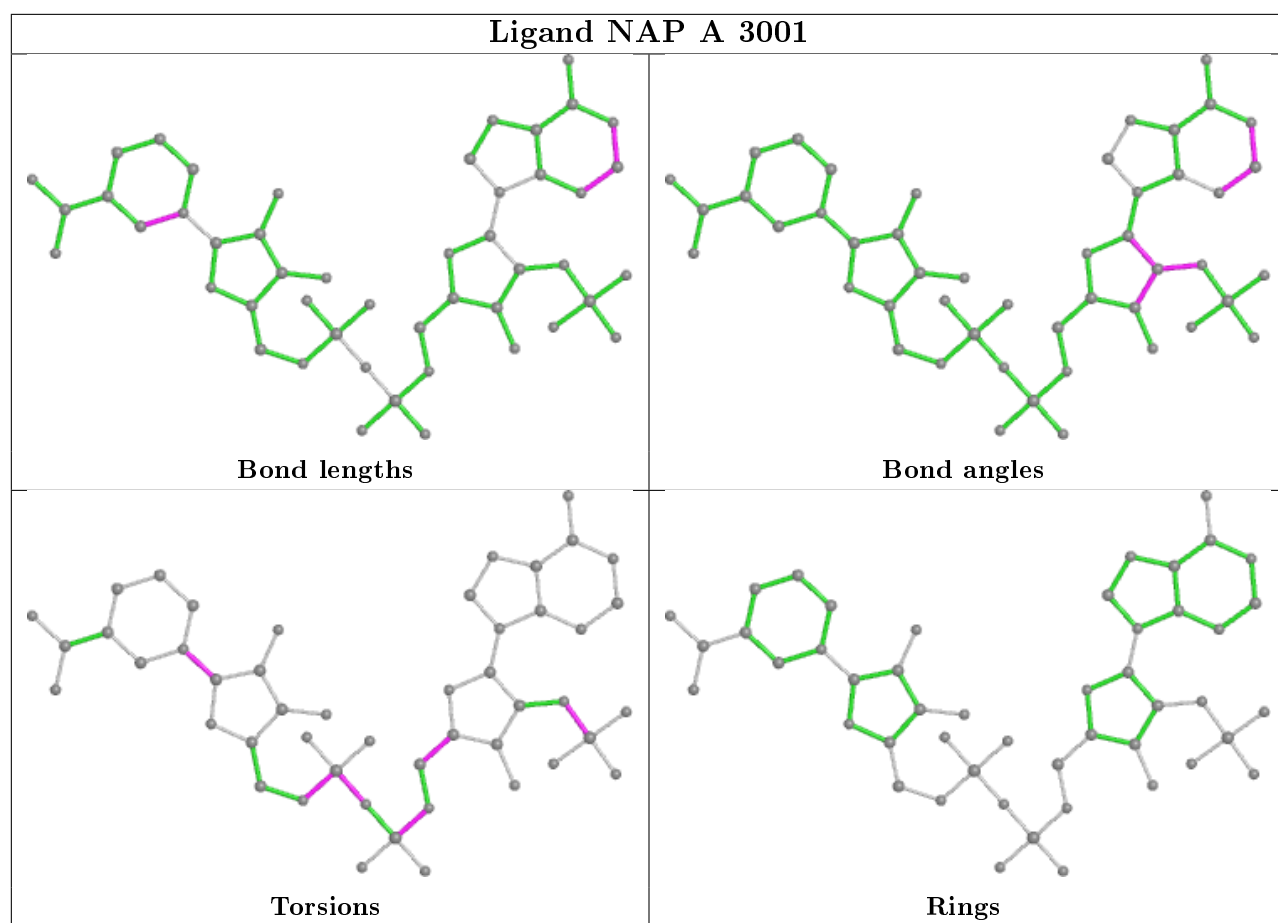
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3002	NAP	2	0
2	B	3001	NAP	1	0
2	A	3002	NAP	4	0
2	A	3001	NAP	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	2081/2512 (82%)	0.04	129 (6%)	20 20	73, 131, 230, 299	0
1	B	2086/2512 (83%)	0.22	155 (7%)	14 14	72, 166, 228, 299	0
All	All	4167/5024 (82%)	0.13	284 (6%)	17 17	72, 145, 229, 299	0

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	416	GLN	9.6
1	A	977	ASP	9.3
1	A	976	VAL	9.0
1	A	1297	GLY	7.1
1	B	672	VAL	6.8
1	A	1188	CYS	6.7
1	A	1406	GLN	6.5
1	A	975	ALA	6.3
1	B	667	ARG	6.2
1	A	1189	GLN	6.2
1	B	665	LEU	6.0
1	B	1191	GLN	5.9
1	B	496	CYS	5.9
1	B	1486	MET	5.8
1	A	978	PRO	5.7
1	B	581	SER	5.6
1	B	415	ALA	5.6
1	B	1863	PRO	5.6
1	A	1190	LEU	5.4
1	B	419	ALA	5.3
1	B	498	GLY	5.3
1	A	1181	PRO	5.2
1	A	1202	GLN	5.2
1	B	671	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	417	HIS	5.1
1	A	1205	ALA	5.1
1	B	579	GLY	5.0
1	A	1212	CYS	5.0
1	B	663	GLN	4.9
1	B	580	HIS	4.7
1	B	673	LYS	4.7
1	B	654	PRO	4.7
1	A	979	ALA	4.7
1	B	583	GLY	4.6
1	B	653	GLY	4.6
1	A	1287	ALA	4.6
1	B	10	SER	4.5
1	B	1408	THR	4.5
1	B	364	PRO	4.4
1	B	414	PRO	4.4
1	A	1204	LEU	4.4
1	A	2039	SER	4.3
1	B	497	SER	4.2
1	A	1318	ASN	4.2
1	A	1407	GLN	4.1
1	A	336	SER	4.1
1	A	1180	LEU	4.1
1	B	622	ALA	4.0
1	A	1195	ASN	4.0
1	B	1147	ALA	4.0
1	A	1308	SER	4.0
1	B	1407	GLN	4.0
1	A	1485	GLU	3.9
1	B	49	ARG	3.9
1	A	1187	ALA	3.9
1	B	392	SER	3.9
1	B	161	CYS	3.8
1	A	416	GLN	3.8
1	B	1193	ASN	3.8
1	B	790	ARG	3.7
1	B	1439	ARG	3.7
1	A	1367	GLN	3.7
1	B	1195	ASN	3.7
1	B	658	MET	3.7
1	A	980	ASP	3.7
1	B	476	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	1458	ASN	3.6
1	A	1192	LEU	3.6
1	B	315	THR	3.6
1	A	1408	THR	3.6
1	B	1455	GLY	3.6
1	A	2024	CYS	3.5
1	B	11	GLY	3.5
1	B	674	GLU	3.5
1	A	1311	LYS	3.5
1	B	1570	SER	3.5
1	B	1148	GLN	3.5
1	A	1296	GLN	3.4
1	A	414	PRO	3.4
1	A	392	SER	3.4
1	A	323	GLY	3.4
1	B	2024	CYS	3.4
1	B	1149	ALA	3.4
1	B	1368	GLY	3.4
1	B	669	ASP	3.4
1	B	128	VAL	3.4
1	B	670	VAL	3.4
1	B	488	SER	3.4
1	B	557	THR	3.4
1	A	1033	ASP	3.4
1	A	1486	MET	3.4
1	A	1191	GLN	3.3
1	B	1199	GLU	3.3
1	B	1485	GLU	3.3
1	B	2039	SER	3.3
1	A	1193	ASN	3.2
1	A	496	CYS	3.2
1	B	1189	GLN	3.2
1	B	975	ALA	3.2
1	B	676	ARG	3.2
1	B	539	LEU	3.2
1	B	1204	LEU	3.2
1	B	2021	SER	3.1
1	B	560	GLN	3.1
1	B	293	HIS	3.1
1	B	831	SER	3.1
1	A	293	HIS	3.1
1	B	623	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	418	ALA	3.1
1	A	1452	GLY	3.1
1	B	1201	GLY	3.1
1	A	2038	ASN	3.1
1	B	1437	SER	3.1
1	B	1468	ARG	3.1
1	A	1987	PHE	3.0
1	B	1297	GLY	3.0
1	A	1583	LEU	3.0
1	B	410	PRO	3.0
1	A	1206	GLN	3.0
1	B	1202	GLN	3.0
1	A	1468	ARG	3.0
1	B	409	ARG	3.0
1	A	1455	GLY	3.0
1	B	2114	LYS	3.0
1	B	189	ASN	2.9
1	A	1380	SER	2.9
1	B	1190	LEU	2.9
1	B	336	SER	2.9
1	B	2023	SER	2.9
1	B	418	ALA	2.9
1	B	929	GLY	2.9
1	B	2025	GLY	2.9
1	A	1481	SER	2.8
1	B	1681	GLY	2.8
1	B	1409	PRO	2.8
1	B	1467	HIS	2.8
1	B	324	SER	2.8
1	A	1434	ALA	2.8
1	B	1406	GLN	2.8
1	A	292	ALA	2.8
1	A	324	SER	2.8
1	B	1203	VAL	2.8
1	B	1572	ASN	2.8
1	A	1291	GLN	2.8
1	B	1	MET	2.7
1	B	558	SER	2.7
1	A	1203	VAL	2.7
1	A	1305	ALA	2.7
1	A	1207	GLU	2.7
1	A	1290	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	49	ARG	2.7
1	A	1307	GLY	2.7
1	A	1317	CYS	2.7
1	A	1587	SER	2.7
1	A	1863	PRO	2.7
1	B	1527	GLN	2.7
1	A	1482	PRO	2.7
1	B	413	PRO	2.7
1	B	104	SER	2.6
1	A	583	GLY	2.6
1	A	1484	PRO	2.6
1	B	316	ARG	2.6
1	B	1602	GLU	2.6
1	A	1208	ARG	2.6
1	A	1288	LYS	2.6
1	B	337	GLY	2.6
1	B	624	GLY	2.6
1	A	1201	GLY	2.6
1	B	1861	GLN	2.6
1	A	1282	LEU	2.6
1	A	1480	THR	2.6
1	B	1319	CYS	2.5
1	B	1208	ARG	2.5
1	A	161	CYS	2.5
1	B	660	GLU	2.5
1	B	1206	GLN	2.5
1	A	294	GLY	2.5
1	B	1296	GLN	2.5
1	B	928	THR	2.5
1	B	1194	GLY	2.5
1	B	722	TRP	2.5
1	A	1483	ALA	2.5
1	B	1487	HIS	2.5
1	B	213	ARG	2.5
1	A	1527	GLN	2.5
1	B	1340	GLU	2.5
1	B	584	GLU	2.4
1	B	868	PRO	2.4
1	B	1503	MET	2.4
1	A	340	ALA	2.4
1	B	762	ALA	2.4
1	A	295	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1194	GLY	2.4
1	A	1146	LEU	2.4
1	A	1458	ASN	2.4
1	A	1510	ALA	2.4
1	B	755	HIS	2.4
1	A	1437	SER	2.4
1	A	984	GLU	2.4
1	B	2078	THR	2.4
1	A	2020	SER	2.4
1	A	1336	ALA	2.4
1	A	1507	ARG	2.4
1	B	332	PRO	2.4
1	B	621	ALA	2.4
1	A	337	GLY	2.3
1	A	1681	GLY	2.3
1	B	489	LYS	2.3
1	A	2078	THR	2.3
1	A	1586	ASP	2.3
1	A	1136	LEU	2.3
1	B	360	HIS	2.3
1	B	543	GLU	2.3
1	A	10	SER	2.3
1	B	1875	GLY	2.3
1	B	1286	GLN	2.3
1	A	974	ALA	2.3
1	A	498	GLY	2.3
1	A	1509	GLY	2.3
1	A	1371	HIS	2.3
1	A	417	HIS	2.3
1	B	906	ASN	2.3
1	A	1135	ALA	2.3
1	A	1347	HIS	2.3
1	A	391	ASN	2.2
1	A	1409	PRO	2.2
1	B	412	PRO	2.2
1	B	1318	ASN	2.2
1	A	1467	HIS	2.2
1	A	1866	ARG	2.2
1	A	1209	PRO	2.2
1	B	1862	GLY	2.2
1	A	291	GLU	2.2
1	B	1452	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1410	GLN	2.2
1	A	1679	GLY	2.2
1	B	330	GLY	2.2
1	B	2027	GLY	2.2
1	A	1284	ALA	2.2
1	B	1235	GLU	2.2
1	B	664	GLN	2.2
1	A	928	THR	2.2
1	B	2111	LEU	2.2
1	A	1479	SER	2.2
1	B	422	ARG	2.2
1	B	888	GLY	2.2
1	B	1146	LEU	2.1
1	B	1312	ALA	2.1
1	A	37	ASP	2.1
1	B	92	ASP	2.1
1	A	1337	THR	2.1
1	A	480	GLN	2.1
1	A	1525	GLU	2.1
1	A	1354	PRO	2.1
1	A	1071	LEU	2.1
1	B	292	ALA	2.1
1	A	1319	CYS	2.1
1	B	499	MET	2.1
1	A	1862	GLY	2.1
1	B	728	ARG	2.1
1	B	1970	ASN	2.1
1	A	1451	SER	2.1
1	B	646	LYS	2.1
1	B	1111	HIS	2.1
1	B	1347	HIS	2.1
1	B	391	ASN	2.1
1	A	410	PRO	2.1
1	B	236	LYS	2.1
1	A	2079	VAL	2.1
1	B	1205	ALA	2.1
1	A	394	GLY	2.1
1	B	1456	MET	2.1
1	B	1459	CYS	2.0
1	A	889	THR	2.0
1	A	1398	GLY	2.0
1	B	353	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	419	ALA	2.0
1	B	889	THR	2.0
1	A	1375	GLN	2.0
1	A	1540	ASP	2.0
1	B	129	GLY	2.0
1	B	2035	GLY	2.0
1	B	1484	PRO	2.0
1	A	218	GLU	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](#)

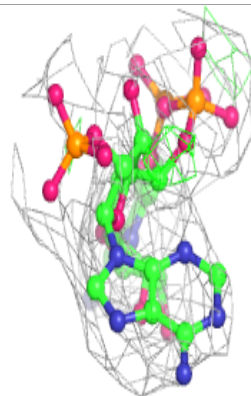
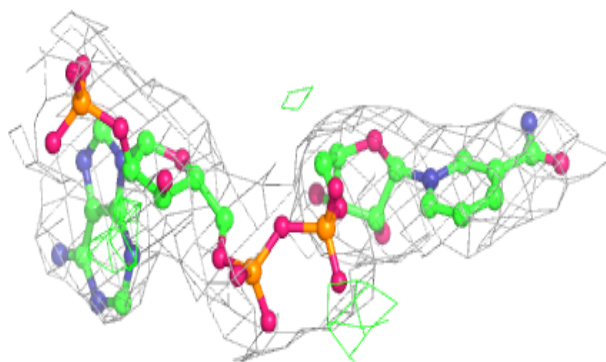
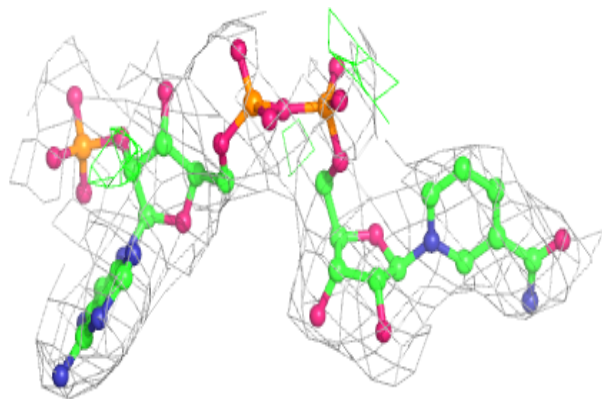
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAP	A	3001	48/48	0.90	0.32	100,122,179,189	0
2	NAP	B	3001	48/48	0.92	0.26	99,123,160,163	0
2	NAP	A	3002	48/48	0.95	0.20	96,135,161,194	0
2	NAP	B	3002	48/48	0.95	0.18	99,122,153,198	0

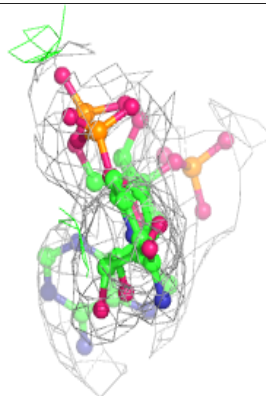
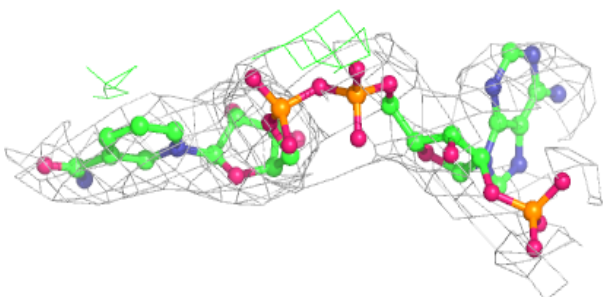
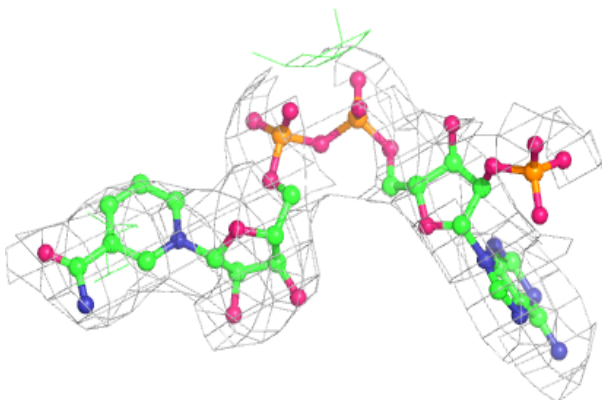
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAP A 3001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

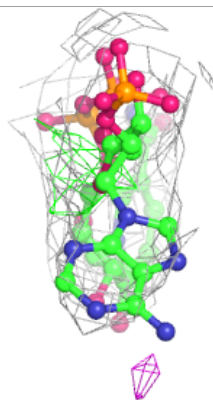
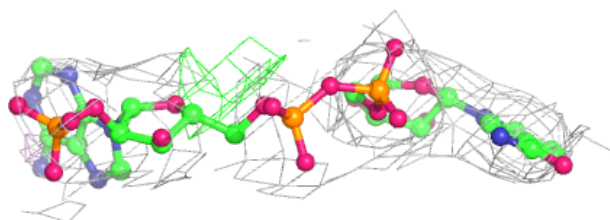
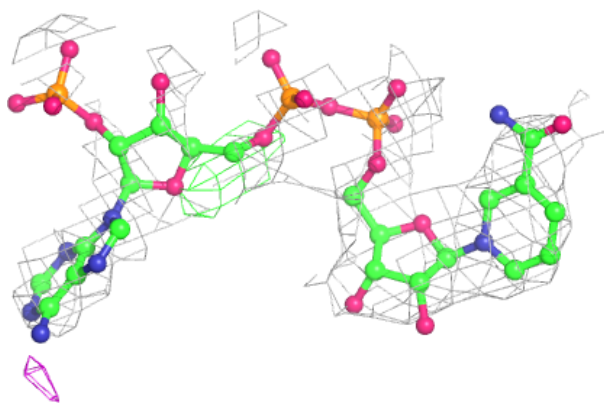
**Electron density around NAP B 3001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

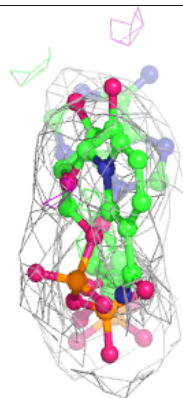
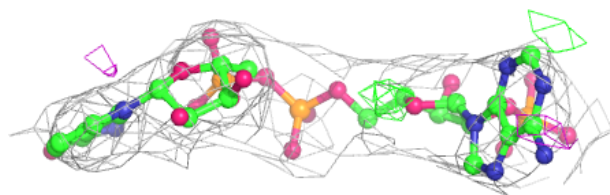
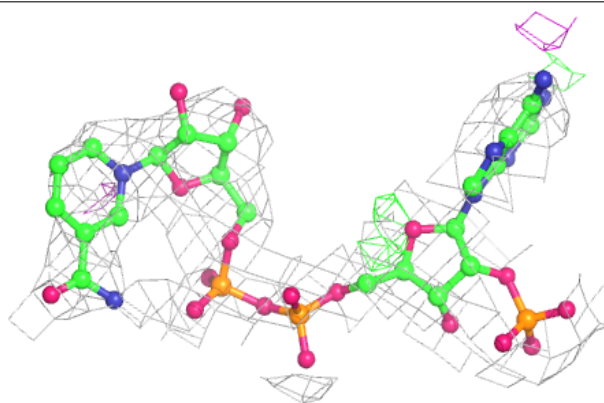


Electron density around NAP A 3002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAP B 3002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.