



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:49 AM UTC

PDB ID : 2VZ9 / pdb_00002vz9
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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

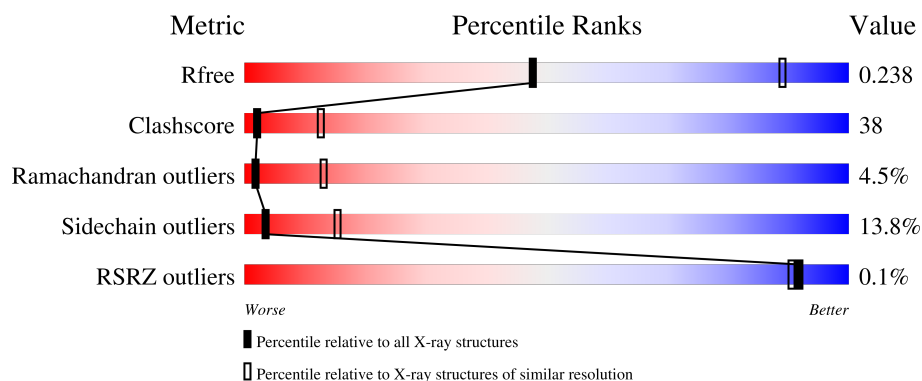
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	A	2512	
1	B	2512	

2 Entry composition [i](#)

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.

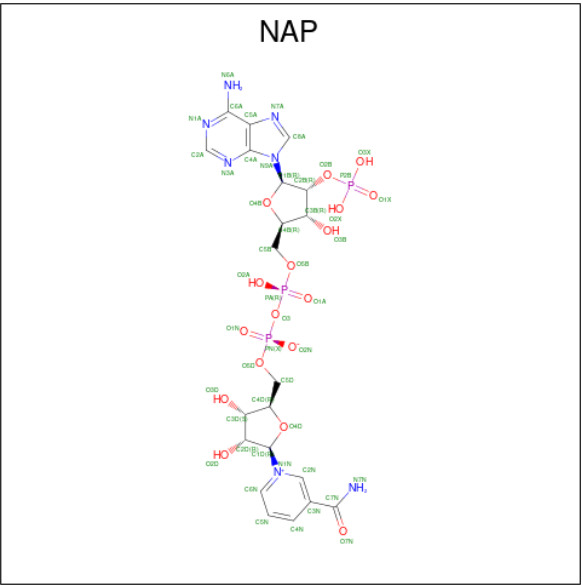
- Molecule 1 is a protein called FATTY ACID SYNTHASE.

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 (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



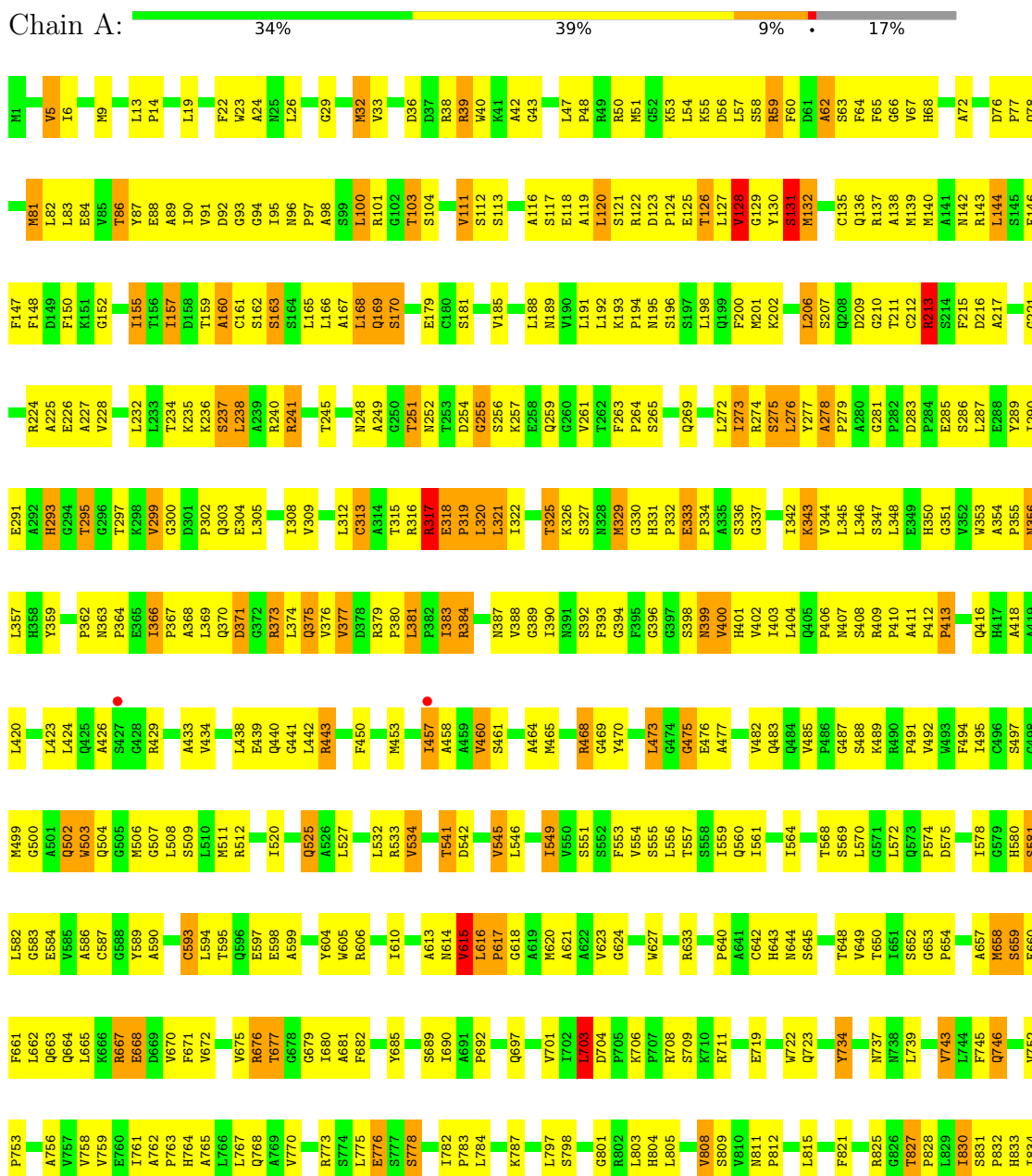
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: FATTY ACID SYNTHASE







Response	Percentage
Doing a good job	33%
Not doing a good job	41%
Don't know	9%
No answer	17%



V1453	H1388	G1319	D1251	A1187	V1125	T1055	A979	H896	F821	N738	I651	Q573	M499	A419
V1454	L1389	A1320	G1252	G1168	E1126	S1056	D980	A897	F825	L739	I654	P574	G500	L420
G1455	V1390	L1321	Q1253	Q1189	S1127	I1057	S981	T898	G825	V743	P654	D575	Q502	L423
M1456	A1322	L1190	L1254	L1190	G1128	T982	A983	L899	T827	L744	A656	Q655	Q504	L424
N1457	R1394	L1323	Y1255	Q1191	C1129	D1060	A984	A900	P828	F745	A657	Q504	Q504	Q425
N1458	L1395	L1324	S1256	L1192	L1130	P1061	E984	L903	T827	Q746	P658	S581	G506	A426
C1459	F1396	G1325	R1257		A1131	Y1062	F985	L904	L830		S659	L582	M506	R429
L1460	G1397	D1326		N1195	G1132	T1063	F986	S904	S831	V752	L662	A586	Q507	
G1398	L1327	L1328	A1260	LEU	N1133	H1064	L987	Q905	Q905	P753	L662	A586	L508	A433
L1461	A1328	A1329	L1261	GLN		Q1065	Q989	N906	P832		Q664	Y589	S509	V434
K1462	V1400	V1329	L1262	LEU	L1136	Q1066	Q989	Q988	H833	A756	Q664	L510	M511	L438
L1463	F1401	A1330	M1263	E1199	Q1137	K1067	G990	E908	R834		L665	A590	R512	
F1402	L1402	V1331	T1264	L1200	E1138	L1068	D991	E909	K835				M511	
L1403	L1403	G1332	Q1265		E1139	Y1069	Y992	T910	P836	V759			R512	
C1404	M1268	M1334		V1203	L1140	T1070	Y993	P911	D837	E760	E668	C593	L439	
R1405	L1269	L1334		L1204	Q1141	Y993	K994	P912	H838	I761	D669	L594	Q440	
Q1406	L1270	Q1206	L1270	Q1206	C1143	Q1072	Y913	V913	S839	A762	V670	T595	G441	
T1407	D1271	E1207	L1271	E1207	R1144	D1073	L998	F914	Q840	P763	F671	Q596	L442	
T1408	Y1272	R1208	Y1272	R1208	G1145	T1074	L999	E915	A841	H764	V672	E597	L443	
P1409	T1273	P1209	T1273	P1209	L1146	T1075	G999	D916	A765			E598	M453	
S1412	A1274	L1210	T1275	L1210	A1147	Q1076	Y1001	P845	P845	L767	T677	Y604	Q525	
P1413	L1211	L1211	A1077	A1077	Q1148	A1078	D1002	S846	S846	Q768	G678	W605	N455	
L1416	C1212	C1212	A1149	A1149	L1150	V1081	Y1003	L925		V770	G679	R606	L527	
S1417	D1214	D1214				V1082	F1007	V931	D849		I680	G607	L530	
V1418	P1215	P1215	K1153				Q1008		F850	L775	A681	Y608	G531	
E1419	L1216	L1216	V1154			M1085	Q1009	E934	C856	E776	F682	C609	L532	
D1420	L1217	L1217	ALA		ALA	L1086	Y935	V935			H683	T610	L532	
T1421	S1218	S1218	GLN		GLN	N1087	R936	R936	S777		S684	K611	S461	
S1422	G1219	G1219	GLN		GLN	T1088	L937	L937	S778		G685	E612	P462	
F1423	L1220	L1220	GLY		GLY	V1089	D1014	S941	I782		F686	A613	V463	
R1424	D1222	D1222	LEU		LEU	V1090	L1015	S941	P783		M687	M614	M465	
V1425	A1223	A1223	LYS		LYS	G1092	E1016	F944	L784		E688	V615	S540	
D1427	E1224	E1224	VAL		VAL	F1096	R1019	V946	L793		A691	A621	E543	
S1428	L1226	L1226	PRO		PRO	L1097	L1022	S947			P692	A622	G469	
L1429	H1293	H1293	GLY		GLY	S1101	Q1023		L797		Q697	V623	L473	
D1430	V1294	V1294	ASP		ASP	S1102	W1028	L953	S798		L698	G624	G474	
L1432	T1295	T1295	GLY		GLY	V1103	V1029	F954	V800		R699	L625	G475	
L1433	Q1296	Q1296	ALA		ALA	F1031	S1030	V959	Q801		K700	S626	E476	
G1434	G1297	G1297	ALA		ALA	R106	F1031		H802		V701	W627	V550	
A1435	Q1298	Q1298	GLN		GLN	R107	L1032	W962	L803		I702	R633	V554	
A1436	W1299	W1299	ALA		ALA	P1108	L1032	E963	H804		L703	C634	V554	
S1437	P1301	P1301	PRO		PRO	Q1109	D1033	S964				P635	S555	
S1438	L1371	L1371	ARG		ARG	E1110	A1034	S964				P636	L556	
R1439	A1302	A1302	GLU		GLU	H1111	M1035	P965				G637	T557	
P1440	M1303	M1303	ALA		ALA	L1111	L1036	D966				K710	S558	
L1441	P1304	P1304	PRO		PRO	I1115	H1037	P967				I638	S488	
W1442	A1305	A1305	GLN		GLN	L1116	M1038					V639	I559	
L1443	K1241	K1241	GLN		GLN	L1116	F970	P887				P640	Q560	
M1444	M1242	M1242	SER		SER	E1117	S1039	P887				A641	I561	
G1447	K1311	K1311	L1180		L1180	L1118	T1040	G888				W722	I564	
R1448	F1382	F1382	P1181		P1181	G1120	A1042	T889				H643	T568	
S1449	V1245	V1245	R1182		R1182	F1119	R973	G890				H644	S569	
F1450	E1246	E1246	L1183		L1183	F1121	P1043	A974				P817	L570	
S1451	V1247	V1247	L1184		L1184	T1122	A976					T648	G496	
G1452	C1317	C1317	A1185		A1185	P1123	D977	P883				V649	S497	
	N1318	N1318	A1186		A1186	H1124	P978	T895				T650	L572	

GLY	GLY	SER	ILE	THR	HIS	V2110	G2035	I1956	L1873	F1800	L1733	R1662	D1522
LYS	LYS	VAL	GLU	LEU	ASP	L2111	F2036	T1957	S1877	E1801	R1734	G1663	R1523
VAL	SER	ARG	ILE	THR	LEU	K2114	A2037	E1988	R1735	E1802	R1736	M1598	T1528
VAL	HIS	LYS	ARG	LEU	VAL	LYS	M2038	G1963	G1803	G1803	L1599	G1600	H1529
VAL	ALA	MET	GLN	ASN	SER	ALA	A2040	P1964	P1882	G1804	K1739	M1601	H1530
THR	THR	THR	VAL	SER	MET	ALA	M2041	P1964	K1885	V1810	G1740	M1601	A1531
PRO	PRO	PRO	GLN	VAL	ARG	ALA	E2042	G1967	Y1886	S1811	V1741	M1601	F1532
GLU	GLU	GLY	PRO	GLN	ARG	ALA	R2043	V1968	Y1887	E1812	G1742	F1603	S1543
ASP	ALA	CYS	GLU	SER	VAL	ARG	F1969	V1969	V1888	L1813	L1743	S1604	N1534
HIS	ASP	ALA	GLY	ALA	ARG	ASP	E2046	M1970	V1889	L1814	L1743	G1605	V1535
ARG	ALA	ALA	PRO	GLN	GLN	GLY	K2047	L1971	T1890	K1815	M1746	R1606	G1605
THR	THR	GLU	TYR	ARG	LEU	SER	R2048	L1971	T1890	K1816	M1746	R1606	R1538
GLU	GLU	ALA	ARG	PRO	SER	SER	V1974	V1974	L1893	G1817	G1676	R1611	G1539
LEU	LEU	GLU	ILE	LEU	SER	LEU	L1975	L1975	G1894	G1817	G1676	R1611	D1540
GLU	GLU	ALA	ILE	LEU	ARG	GLN	R1976	R1976	G1895	I1818	G1677	R1612	L1541
LYS	LYS	LYS	GLY	VAL	ARG	LYS	D1977	D1977	F1896	V1822	G1678	V1613	L1541
GLY	VAL	VAL	VAL	LEU	LYS	LEU	A1978	A1978	F1897	V1823	G1679	M1614	S1542
GLY	VAL	GLN	VAL	LEU	GLN	VAL	W2058	W2058	L1897	V1823	G1679	M1614	S1543
GLY	VAL	GLN	VAL	LEU	GLN	VAL	W2059	W2059	L1898	Q1824	W1757	M1616	T1544
GLY	VAL	GLN	VAL	LEU	GLN	VAL	W2060	W2060	Q1824	P1825	W1757	M1616	T1544
GLY	VAL	GLN	VAL	LEU	GLN	VAL	I2063	I2063	L1900	P1825	R1758	P1617	R1546
GLY	VAL	GLN	VAL	LEU	GLN	VAL	G2064	G2064	A1901	V1830	G1759	P1618	W1546
GLY	VAL	GLN	VAL	LEU	GLN	VAL	D2065	D2065	Q1902	V1830	G1759	P1618	W1546
GLY	VAL	GLN	VAL	LEU	GLN	VAL	V2066	V2066	W1903	R1833	Q1762	A1688	S1549
GLY	VAL	GLN	VAL	LEU	GLN	VAL	I2063	I2063	L1904	R1833	Q1762	A1688	L1551
GLY	VAL	GLN	VAL	LEU	GLN	VAL	G2074	G2074	R1905	V1836	G1764	L1689	A1554
GLY	VAL	GLN	VAL	LEU	GLN	VAL	L2070	L2070	L1906	E1837	R1766	P1690	L1555
GLY	VAL	GLN	VAL	LEU	GLN	VAL	E2071	E2071	Q1910	A1838	R1766	L1627	L1555
GLY	VAL	GLN	VAL	LEU	GLN	VAL	T2072	T2072	K1911	A1839	L1767	G1692	P1556
GLY	VAL	GLN	VAL	LEU	GLN	VAL	M2073	M2073	F1840	F1840	L1767	G1692	A1557
GLY	VAL	GLN	VAL	LEU	GLN	VAL	G2074	G2074	R1841	R1841	L1769	C1693	L1629
GLY	VAL	GLN	VAL	LEU	GLN	VAL	T2075	T2075	Y1842	Y1842	C1770	P1695	S1558
GLY	VAL	GLN	VAL	LEU	GLN	VAL	M2076	M2076	M1843	M1843	F1696	A1632	C1559
GLY	VAL	GLN	VAL	LEU	GLN	VAL	D2077	D2077	Q1845	Q1845	T1697	T1633	Q1560
GLY	VAL	GLN	VAL	LEU	GLN	VAL	T2078	T2078	S1916	S1916	T1698	W1634	D1561
GLY	VAL	GLN	VAL	LEU	GLN	VAL	V2079	V2079	R1917	R1846	L1774	L1563	R1562
GLY	VAL	GLN	VAL	LEU	GLN	VAL	L2084	L2084	S1918	K1847	S1775	C1564	C1564
GLY	VAL	GLN	VAL	LEU	GLN	VAL	P2085	P2085	R1921	H1848	E1703	S1565	S1565
GLY	VAL	GLN	VAL	LEU	GLN	VAL	Q2086	Q2086	T1922	K1851	R1704	V1566	V1566
GLY	VAL	GLN	VAL	LEU	GLN	VAL	R2087	R2087	G1923	V1852	R1705	Y1567	Y1567
GLY	VAL	GLN	VAL	LEU	GLN	VAL	L2088	L2088	Y1924	V1853	A1706	Y1568	Y1568
GLY	VAL	GLN	VAL	LEU	GLN	VAL	A2089	A2089	Q1925	T1854	G1781	T1569	T1569
GLY	VAL	GLN	VAL	LEU	GLN	VAL	L2092	L2092	A1926	Q1855	M1782	E1643	S1570
GLY	VAL	GLN	VAL	LEU	GLN	VAL	L2097	L2097	R1927	V1856	F1712	L1571	L1571
GLY	VAL	GLN	VAL	LEU	GLN	VAL	P2098	P2098	E1930	R1857	Q1714	N1572	N1572
GLY	VAL	GLN	VAL	LEU	GLN	VAL	L2099	L2099	E1931	E1858	F1786	F1573	R1574
GLY	VAL	GLN	VAL	LEU	GLN	VAL	S2100	S2100	E1931	E1858	L1786	S1647	S1647
GLY	VAL	GLN	VAL	LEU	GLN	VAL	Q2101	Q2101	W1932	E1860	C1719	V1648	V1648
GLY	VAL	GLN	VAL	LEU	GLN	VAL	P2102	P2102	V1937	E1860	F1720	P1649	P1649
GLY	VAL	GLN	VAL	LEU	GLN	VAL	H2103	H2103	Q1938	P1863	A1721	I1578	I1578
GLY	VAL	GLN	VAL	LEU	GLN	VAL	P2104	P2104	V1939	A1864	N1722	A1579	A1579
GLY	VAL	GLN	VAL	LEU	GLN	VAL	G2027	G2027	L1940	P1865	T1723	T1580	T1580
GLY	VAL	GLN	VAL	LEU	GLN	VAL	Q2031	Q2031	V1941	P1865	R1724	G1581	G1581
GLY	VAL	GLN	VAL	LEU	GLN	VAL	L2106	L2106	S1944	L1868	T1726	A1655	K1582
GLY	VAL	GLN	VAL	LEU	GLN	VAL	S2107	S2107	Q2031	P1869	T1727	Y1656	L1583
GLY	VAL	GLN	VAL	LEU	GLN	VAL	T2108	T2108	A2032	P1870	Y1657	S1584	S1584
GLY	VAL	GLN	VAL	LEU	GLN	VAL	F2109	F2109	S1954	T1871	F1728	P1585	P1585
GLY	VAL	GLN	VAL	LEU	GLN	VAL			S1954	T1871	E1729	D1586	D1586
GLY	VAL	GLN	VAL	LEU	GLN	VAL			L1955	A1872	V1732	V1660	V1660
GLY	VAL	GLN	VAL	LEU	GLN	VAL						V1661	L1588

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 30.00 – 3.34	Depositor EDS
% Data completeness (in resolution range)	84.1 (30.00-3.30) 90.1 (30.00-3.34)	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 0.187 , 0.238	Depositor DCC
R_{free} test set	4016 reflections (4.74%)	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)	0.31 , 104.6	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

5.1 Standard geometry

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	0.57	1/16199 (0.0%)	1.00	66/22016 (0.3%)
1	B	0.54	0/16240	0.98	56/22070 (0.3%)
All	All	0.56	1/32439 (0.0%)	0.99	122/44086 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1769	ILE	CA-CB	-5.20	1.47	1.54

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	886	PHE	CA-C-N	10.78	131.47	119.93
1	A	886	PHE	C-N-CA	10.78	131.47	119.93
1	B	886	PHE	CA-C-N	9.62	130.22	119.93
1	B	886	PHE	C-N-CA	9.62	130.22	119.93
1	B	1223	ALA	CA-C-N	8.75	130.78	119.84
1	B	1223	ALA	C-N-CA	8.75	130.78	119.84
1	B	1412	SER	CA-C-N	7.81	129.34	120.98
1	B	1412	SER	C-N-CA	7.81	129.34	120.98
1	B	1617	VAL	CA-C-N	7.70	127.25	119.24
1	B	1617	VAL	C-N-CA	7.70	127.25	119.24
1	B	1326	ASP	CA-C-N	7.49	129.20	119.84
1	B	1326	ASP	C-N-CA	7.49	129.20	119.84
1	A	703	LEU	N-CA-C	-7.25	97.08	108.90
1	A	1223	ALA	CA-C-N	7.22	128.86	119.84
1	A	1223	ALA	C-N-CA	7.22	128.86	119.84
1	B	1300	ASP	CA-C-N	7.20	128.83	119.84
1	B	1300	ASP	C-N-CA	7.20	128.83	119.84
1	B	867	SER	CA-C-N	7.18	128.82	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	867	SER	C-N-CA	7.18	128.82	119.84
1	B	1102	SER	N-CA-C	7.10	119.35	108.42
1	A	1617	VAL	CA-C-N	7.09	126.79	119.56
1	A	1617	VAL	C-N-CA	7.09	126.79	119.56
1	A	1326	ASP	CA-C-N	7.06	128.67	119.84
1	A	1326	ASP	C-N-CA	7.06	128.67	119.84
1	B	1660	VAL	N-CA-C	6.92	117.89	111.45
1	A	125	GLU	N-CA-C	-6.92	105.46	114.04
1	A	1102	SER	N-CA-C	6.90	119.04	108.42
1	A	867	SER	CA-C-N	6.88	128.44	119.84
1	A	867	SER	C-N-CA	6.88	128.44	119.84
1	A	321	LEU	N-CA-C	-6.79	101.11	110.35
1	B	1144	ARG	N-CA-C	-6.77	105.31	113.97
1	A	5	VAL	N-CA-C	6.72	118.39	108.45
1	A	925	LEU	CA-C-N	6.63	126.39	119.76
1	A	925	LEU	C-N-CA	6.63	126.39	119.76
1	B	1605	GLY	N-CA-C	6.61	118.92	110.20
1	A	653	GLY	CA-C-N	6.57	128.05	119.84
1	A	653	GLY	C-N-CA	6.57	128.05	119.84
1	B	5	VAL	N-CA-C	6.54	118.20	108.46
1	A	1869	PRO	CA-C-N	6.52	127.99	119.84
1	A	1869	PRO	C-N-CA	6.52	127.99	119.84
1	A	457	ILE	CB-CA-C	-6.51	103.64	111.97
1	B	925	LEU	CA-C-N	6.43	126.19	119.76
1	B	925	LEU	C-N-CA	6.43	126.19	119.76
1	B	856	CYS	N-CA-C	6.39	119.98	111.30
1	A	1661	VAL	CB-CA-C	-6.31	103.62	112.14
1	A	1490	SER	N-CA-C	6.29	113.94	108.78
1	A	870	SER	CA-C-N	6.18	126.63	119.47
1	A	870	SER	C-N-CA	6.18	126.63	119.47
1	A	500	GLY	N-CA-C	-6.17	106.56	115.27
1	A	811	ASN	CA-C-N	6.15	127.53	119.84
1	A	811	ASN	C-N-CA	6.15	127.53	119.84
1	B	457	ILE	CB-CA-C	-6.15	104.09	111.97
1	B	1521	GLN	N-CA-C	6.11	123.82	110.80
1	A	370	GLN	N-CA-C	-6.10	105.13	114.16
1	A	1987	PHE	N-CA-C	-6.08	104.76	111.82
1	B	313	CYS	N-CA-C	6.08	118.52	108.49
1	B	1824	GLN	CA-C-N	6.05	126.01	119.78
1	B	1824	GLN	C-N-CA	6.05	126.01	119.78
1	B	152	GLY	CA-C-N	6.04	127.39	119.84
1	B	152	GLY	C-N-CA	6.04	127.39	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1408	THR	CA-C-N	6.02	127.36	119.84
1	A	1408	THR	C-N-CA	6.02	127.36	119.84
1	A	827	THR	CA-C-N	6.00	127.33	119.84
1	A	827	THR	C-N-CA	6.00	127.33	119.84
1	B	870	SER	CA-C-N	5.99	126.42	119.47
1	B	870	SER	C-N-CA	5.99	126.42	119.47
1	A	128	VAL	CB-CA-C	-5.90	105.10	111.59
1	B	1648	VAL	N-CA-C	5.88	121.59	108.88
1	B	827	THR	CA-C-N	5.88	127.19	119.84
1	B	827	THR	C-N-CA	5.88	127.19	119.84
1	A	808	VAL	CB-CA-C	-5.86	104.89	111.45
1	A	62	ALA	N-CA-C	5.84	118.59	111.82
1	B	1055	THR	N-CA-C	-5.83	106.30	113.41
1	B	62	ALA	N-CA-C	5.82	118.58	111.82
1	A	313	CYS	N-CA-C	5.81	118.07	108.49
1	A	1830	VAL	N-CA-C	5.72	116.82	108.58
1	B	811	ASN	CA-C-N	5.71	126.98	119.84
1	B	811	ASN	C-N-CA	5.71	126.98	119.84
1	A	1213	ASP	N-CA-C	-5.68	105.48	113.20
1	A	483	GLN	N-CA-C	5.68	116.89	108.60
1	B	1270	LEU	N-CA-C	5.67	117.65	108.41
1	A	1824	GLN	CA-C-N	5.66	125.61	119.78
1	A	1824	GLN	C-N-CA	5.66	125.61	119.78
1	A	152	GLY	CA-C-N	5.66	126.92	119.84
1	A	152	GLY	C-N-CA	5.66	126.92	119.84
1	A	377	VAL	N-CA-C	5.65	112.26	106.21
1	B	1830	VAL	N-CA-C	5.64	116.71	108.58
1	A	1309	LEU	N-CA-C	-5.62	108.22	114.62
1	B	1268	MET	N-CA-C	5.62	117.93	109.23
1	A	963	GLU	N-CA-C	5.60	117.07	111.07
1	A	981	SER	N-CA-C	-5.60	102.19	110.48
1	B	1213	ASP	N-CA-C	-5.60	107.04	112.97
1	B	1736	THR	N-CA-C	-5.52	105.54	114.09
1	B	963	GLU	N-CA-C	5.48	116.94	111.07
1	A	1270	LEU	N-CA-C	5.45	117.29	108.41
1	B	1115	ILE	CB-CA-C	-5.41	105.39	111.23
1	B	1910	GLN	N-CA-C	-5.39	107.71	114.56
1	B	388	VAL	N-CA-C	5.39	116.35	108.53
1	A	1610	GLY	N-CA-C	-5.34	107.17	114.64
1	B	770	VAL	N-CA-C	5.30	115.51	110.42
1	B	377	VAL	N-CA-C	5.30	111.89	106.21
1	B	1212	CYS	N-CA-C	-5.29	106.84	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1186	ALA	N-CA-C	5.26	116.70	111.07
1	B	214	SER	N-CA-C	5.22	117.64	111.33
1	B	131	SER	N-CA-C	-5.20	105.68	112.23
1	A	299	VAL	CB-CA-C	-5.13	106.56	111.44
1	A	1300	ASP	CA-C-N	5.13	126.25	119.84
1	A	1300	ASP	C-N-CA	5.13	126.25	119.84
1	A	1490	SER	CA-C-O	5.12	120.91	117.94
1	A	1305	ALA	CA-C-N	5.12	126.24	119.84
1	A	1305	ALA	C-N-CA	5.12	126.24	119.84
1	B	678	GLY	N-CA-C	-5.11	106.69	115.08
1	A	131	SER	N-CA-C	-5.10	105.80	112.23
1	A	155	ILE	N-CA-C	5.10	115.08	108.35
1	A	1736	THR	N-CA-C	-5.09	106.19	114.09
1	A	1055	THR	N-CA-C	-5.07	107.27	113.50
1	B	1430	LYS	N-CA-C	-5.07	106.95	113.23
1	A	293	HIS	N-CA-C	-5.06	105.22	111.40
1	A	1490	SER	CB-CA-C	-5.05	109.79	117.07
1	B	500	GLY	N-CA-C	-5.05	108.64	115.21
1	A	1430	LYS	N-CA-C	-5.02	107.01	113.23
1	A	1648	VAL	N-CA-C	5.01	119.71	108.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15858	0	15834	1200	0
1	B	15899	0	15882	1249	0
2	A	96	0	50	12	0
2	B	96	0	50	4	0
All	All	31949	0	31816	2395	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 38.

All (2395) 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:B:1585:PRO:HB3	1:B:1598:MET:HE1	1.29	1.12
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:1616:MET:HE3	1:B:1650:ILE:HD13	1.35	1.06
1:A:1454:VAL:HG13	1:A:1503:MET:HE1	1.38	1.05
1:A:1585:PRO:HB3	1:A:1598:MET:HE1	1.36	1.04
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:HG2	1:B:1662:ARG:NH1	1.65	0.98
1:A:51:MET:HE2	1:A:191:LEU:HD13	1.44	0.97
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:506:MET:HE3	1:B:559:ILE:HD12	1.49	0.95
1:B:1653:THR:HG22	1:B:1810:VAL:HG12	1.48	0.94
1:B:1454:VAL:HG13	1:B:1503:MET:HE1	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:B:51:MET:HE2	1:B:191:LEU:HD13	1.51	0.92
1:A:1528:THR:HG22	1:A:1530:HIS:H	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:506:MET:HE3	1:A:559:ILE:HD12	1.54	0.89
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:527:LEU:HD12	1:A:534:VAL:HG22	1.59	0.84
1:A:1893:LEU:HB3	1:A:1925:GLN:NE2	1.92	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:A:1147:ALA:HB1	1:A:1358:MET:HE1	1.60	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:47:LEU:HA	1:A:201:MET:HE1	1.60	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:87:TYR:O	1:B:91:VAL:HG22	1.77	0.83
1:B:1651:VAL:HG13	1:B:1680:VAL:HA	1.60	0.83
1:A:1771:LYS:HE2	1:A:1795:LEU:HD22	1.61	0.83
1:A:782:ILE:HD12	1:A:803:LEU:HD23	1.61	0.83
1:A:1034:ALA:HA	1:A:1037:HIS:CD2	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1662:ARG:HH11	1:A:1662:ARG:CG	1.91	0.83
1:A:976:VAL:HG22	1:A:977:ASP:H	1.44	0.82
1:B:82:LEU:O	1:B:86:THR:HG23	1.78	0.82
1:B:1486:MET:O	1:B:1488:PRO:HD3	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
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: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:623:VAL:HG22	1:A:672:VAL:HG22	1.63	0.81
1:A:1418:VAL:HG13	1:A:1425:TRP:CE2	2.14	0.81
1:A:984:GLU:O	1:A:985:PHE:HB2	1.79	0.81
1:A:883:ARG:HH11	1:A:924:ILE:HD11	1.45	0.80
1:A:1428:SER:O	1:A:1432:ILE:HG13	1.82	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:944:PHE:CD2	1:B:959:VAL:HG22	2.17	0.80
1:B:1073:ASP:O	1:B:1074:THR:HG22	1.81	0.80
1:B:1282:LEU:HD21	1:B:1296:GLN:HB2	1.64	0.80
1:B:982:THR:C	1:B:984:GLU:H	1.90	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:278:ALA:CB	1:A:279:PRO:HD3	2.12	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:B:420:LEU:HD11	1:B:512:ARG:HB3	1.62	0.79
1:B:1771:LYS:HE2	1:B:1795:LEU:HD22	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:155:ILE:HD11	1:B:166:LEU:HD11	1.66	0.78
1:B:1299:TRP:HZ3	1:B:1301:PRO:HA	1.46	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:620:MET:HG3	1:B:677:THR:HG21	1.64	0.77
1:B:1139:GLU:OE2	1:B:1216:LEU:HD11	1.84	0.77
1:B:23:TRP:CE2	1:B:350:HIS:CD2	2.73	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: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:1254:LEU:HD13	1:A:1316:VAL:HG12	1.67	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:87:TYR:O	1:A:91:VAL:HG22	1.85	0.76
1:A:1457:VAL:HG21	1:A:1473:LEU:HD22	1.67	0.76
1:A:309:VAL:HG11	1:A:373:ARG:HD2	1.67	0.76
1:A:2075:THR:HB	1:A:2077:ASP:H	1.51	0.76
1:B:47:LEU:HA	1:B:201:MET:HE1	1.65	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:132:MET:HE1	1:B:200:PHE:CE2	2.21	0.76
1:A:1207:GLU:O	1:A:1211:LEU:HB2	1.86	0.76
1:B:883:ARG:HH11	1:B:924:ILE:HD11	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1133:ASN:HD22	1:B:1136:LEU:HD12	1.51	0.76
1:A:504:GLN:HA	1:A:541:THR:HG21	1.67	0.76
1:A:1073:ASP:O	1:A:1074:THR:HG22	1.84	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
1:B:112:SER:CB	1:B:334:PRO:HG3	2.14	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:B:1456:MET:HG3	1:B:2036:PHE:HB2	1.68	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:944:PHE:HD2	1:A:959:VAL:HG22	1.51	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: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:963:GLU:O	1:A:965:PRO:HD3	1.86	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:416:GLN:O	1:A:420:LEU:HB2	1.87	0.74
1:B:944:PHE:HD2	1:B:959:VAL:HG22	1.52	0.74
1:B:1139:GLU:CD	1:B:1218:SER:HB2	2.12	0.74
1:B:1926:ALA:O	1:B:1930:ARG:HB2	1.87	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:384:ARG:HH11	1:A:384:ARG:CG	1.99	0.74
1:A:1003:TYR:CZ	1:A:1037:HIS:CE1	2.73	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:14:PRO:HG2	1:B:329:MET:HG3	1.67	0.74
1:B:1234:LEU:HD22	1:B:1262:LEU:HD22	1.69	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:326:LYS:HE3	1:B:336:SER:HB2	1.69	0.74
1:B:1476:ASN:O	1:B:1477:LEU:HD23	1.88	0.74
1:A:1460:LEU:HD11	1:A:1980:LEU:HD13	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:856:CYS:CB	1:B:856:CYS:SG	2.77	0.73
1:B:1616:MET:CE	1:B:1650:ILE:HD13	2.17	0.73
1:B:19:LEU:HD11	1:B:342:ILE:HD13	1.69	0.73
1:A:1223:ALA:HB1	1:A:1224:PRO:HD2	1.70	0.73
1:B:136:GLN:HE22	1:B:138:ALA:H	1.35	0.73
1:B:1223:ALA:HB1	1:B:1224:PRO:HD2	1.68	0.73
1:A:1725:ASP:OD1	1:A:1726:THR:N	2.22	0.73
1:B:322:ILE:HD12	1:B:374:LEU:HD13	1.69	0.73
1:B:1641:THR:HG23	1:B:1644:GLU:OE1	1.87	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:A:1616:MET:HE2	1:A:1800:PHE:CZ	2.23	0.72
1:B:1616:MET:HB3	1:B:1800:PHE:CE1	2.23	0.72
1:A:143:ARG:HG2	1:A:143:ARG:HH11	1.54	0.72
1:A:1208:ARG:HH11	1:A:1211:LEU:HD22	1.54	0.72
1:A:200:PHE:CE2	1:B:132:MET:HE1	2.24	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:HH11	1:A:1545:ARG:CG	2.02	0.72
1:B:1299:TRP:CZ3	1:B:1301:PRO:HA	2.24	0.72
1:A:504:GLN:HG2	1:A:541:THR:HG22	1.71	0.72
1:A:1857:ARG:HG2	1:A:1871:ILE:HD11	1.72	0.72
1:B:309:VAL:HG11	1:B:373:ARG:HD2	1.69	0.72
1:B:1725:ASP:OD2	1:B:1727:SER:HB3	1.89	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:963:GLU:O	1:B:965:PRO:HD3	1.91	0.71
1:B:1299:TRP:NE1	1:B:1306:PRO:HD2	2.04	0.71
1:A:1299:TRP:HE1	1:A:1306:PRO:HD2	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1903:TRP:HB2	1:A:2092:LEU:HD13	1.72	0.71
1:A:504:GLN:HG2	1:A:541:THR:CG2	2.20	0.71
1:A:1302:ALA:O	1:A:1304:PRO:HD3	1.91	0.71
1:B:1577:MET:HE3	1:B:1582:LYS:HD3	1.72	0.71
1:B:112:SER:HB2	1:B:334:PRO:CG	2.19	0.71
1:A:443:ARG:HG3	1:A:443:ARG:NH1	2.05	0.71
1:B:982:THR:HG23	1:B:983:ALA:H	1.55	0.71
1:B:1903:TRP:HB2	1:B:2092:LEU:HD13	1.71	0.71
1:B:506:MET:HE1	1:B:555:SER:HB3	1.73	0.71
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: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:A:1614:MET:HE3	1:A:1634:TRP:HB2	1.71	0.69
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:A:506:MET:HE1	1:A:555:SER:HB3	1.73	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:B:1603:PHE:HE2	1:B:1615:GLY:C	2.00	0.69
1:A:39:ARG:NH1	1:A:57:LEU:HD22	2.07	0.69
1:A:54:LEU:HG	1:A:226:GLU:HG3	1.74	0.69
1:A:1694:ARG:HG3	1:A:1694:ARG:HH11	1.57	0.69
1:B:913:VAL:HG23	1:B:962:TRP:HB2	1.74	0.69
1:B:2053:LEU:HD22	1:B:2054:PRO:HD2	1.74	0.69
1:A:853:GLY:O	1:A:854:SER:HB3	1.92	0.69
1:A:782:ILE:HD12	1:A:803:LEU:CD2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2064:GLY:O	1:A:2066:VAL:N	2.22	0.69
1:A:159:THR:CG2	1:A:398:SER:HB3	2.23	0.69
1:A:1777:ASN:HD22	1:B:1783:ALA:H	1.39	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:B:1034:ALA:O	1:B:1037:HIS:HB2	1.93	0.69
1:A:913:VAL:HG23	1:A:962:TRP:HB2	1.75	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:B:1299:TRP:HE1	1:B:1306:PRO:HD2	1.57	0.69
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:A:1486:MET:HE3	1:A:1506:TYR:HB3	1.76	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:B:1036:LEU:HD21	1:B:1096:PHE:HE1	1.58	0.68
1:A:502:GLN:HG2	1:A:556:LEU:CD1	2.22	0.68
1:A:1034:ALA:O	1:A:1037:HIS:HB2	1.93	0.68
1:A:1616:MET:HE3	1:A:1650:ILE:HA	1.75	0.68
1:B:615:VAL:HG22	1:B:686:PHE:HD2	1.57	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: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:B:420:LEU:HD11	1:B:512:ARG:HD2	1.76	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:B:1060:ASP:OD1	1:B:1062:VAL:HG23	1.93	0.68
1:A:50:ARG:HD3	1:A:210:GLY:O	1.94	0.68
1:A:1705:ARG:HG2	1:A:1720:PHE:HD2	1.59	0.68
1:B:1214:ASP:HB3	1:B:1215:PRO:HD3	1.74	0.68
1:A:953:LEU:HD12	1:A:954:ILE:N	2.09	0.68
1:A:1252:GLY:HA2	1:A:1318:ASN:HD22	1.59	0.68
1:A:976:VAL:O	1:A:978:PRO:HD3	1.93	0.68
1:B:1454:VAL:CG1	1:B:1503:MET:HE1	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1302:ALA:O	1:A:1303:ASN:HB2	1.92	0.67
1:B:550:VAL:HG23	1:B:611:LYS:HD3	1.75	0.67
1:B:917:VAL:CG1	1:B:1054:PHE:HB2	2.24	0.67
1:B:1003:TYR:CE2	1:B:1037:HIS:CE1	2.78	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: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
1:B:1554:ALA:O	1:B:1556:PRO:HD3	1.93	0.67
1:B:953:LEU:HD12	1:B:954:ILE:N	2.09	0.67
1:B:1363:THR:O	1:B:1363:THR:HG22	1.93	0.67
1:A:254:ASP:HB2	1:A:257:LYS:HE2	1.76	0.67
1:A:808:VAL:HG12	1:A:809:SER:N	2.08	0.67
1:A:1234:LEU:HD22	1:A:1262:LEU:HD22	1.76	0.67
1:B:98:ALA:HA	1:B:101:ARG:HG3	1.77	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: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:159:THR:O	1:B:159:THR:HG22	1.94	0.66
1:B:1456:MET:HE2	1:B:1460:LEU:HD21	1.77	0.66
1:B:1887:TYR:CD2	1:B:1967:GLY:HA3	2.30	0.66
1:A:1577:MET:HE3	1:A:1582:LYS:HD3	1.76	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:139:MET:HE1	1:B:396:GLY:CA	2.26	0.66
1:A:460:VAL:HG21	1:A:465:MET:HG3	1.78	0.66
1:A:1703:GLU:O	1:A:1706:ALA:HB3	1.94	0.66
1:B:359:TYR:OH	1:B:362:PRO:HG3	1.95	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: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:289:TYR:HB3	1:A:388:VAL:HG22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1350:LEU:HD22	1:A:1373:LEU:O	1.96	0.66
1:B:9:MET:HE1	1:B:345:LEU:HB2	1.77	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:56:ASP:OD2	1:A:59:ARG:HD3	1.96	0.66
1:A:78:GLN:HB3	1:A:188:LEU:HD13	1.77	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: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:A:77:PRO:O	1:A:81:MET:HG2	1.95	0.66
1:A:1890:THR:HA	1:A:1915:THR:HB	1.76	0.66
1:B:506:MET:HE3	1:B:559:ILE:CD1	2.24	0.66
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:64:PHE:HB2	1:A:429:ARG:HH21	1.61	0.65
1:A:545:VAL:HG22	1:A:551:SER:CB	2.26	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:A:1783:ALA:H	1:B:1777:ASN:HD22	1.44	0.65
1:B:82:LEU:HG	1:B:144:LEU:HD13	1.78	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:98:ALA:HA	1:A:101:ARG:HG3	1.79	0.65
1:A:1060:ASP:OD1	1:A:1062:VAL:HG23	1.95	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:139:MET:HE1	1:B:396:GLY:HA3	1.79	0.65
1:A:254:ASP:CB	1:A:257:LYS:HE2	2.27	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: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:B:1207:GLU:O	1:B:1211:LEU:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1566:VAL:HG12	1:B:1856:VAL:HG21	1.77	0.65
1:A:1140:LEU:HD21	1:A:1354:PRO:HG2	1.77	0.65
1:A:1475:SER:O	1:A:1486:MET:HE1	1.97	0.65
1:A:1484:PRO:O	1:A:1485:GLU:HB2	1.97	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:200:PHE:CD2	1:B:132:MET:HE1	2.31	0.64
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:662:LEU:HD13	1:B:672:VAL:HG12	1.79	0.64
1:A:366:ILE:HD11	1:A:369:LEU:HD11	1.78	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:132:MET:HE1	1:B:200:PHE:CD2	2.33	0.64
1:A:1268:MET:HA	1:A:1268:MET:HE2	1.79	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
1:B:1407:GLN:CG	1:B:1409:PRO:HD2	2.27	0.64
1:B:1554:ALA:C	1:B:1556:PRO:HD3	2.23	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:333:GLU:CB	1:A:334:PRO:HD3	2.18	0.64
1:A:1653:THR:HG22	1:A:1810:VAL:CG1	2.28	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:A:1302:ALA:C	1:A:1304:PRO:HD3	2.21	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:B:64:PHE:CE2	1:B:464:ALA:HB1	2.33	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:B:1463:GLU:OE1	1:B:1980:LEU:HB2	1.98	0.64
1:B:1614:MET:HG2	1:B:1614:MET:O	1.98	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2101:GLN:HG3	1:A:2102:PRO:HD2	1.80	0.63
1:B:157:ILE:HD12	1:B:166:LEU:HD23	1.80	0.63
1:B:1338:LEU:HD13	1:B:1406:GLN:CG	2.29	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: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:2075:THR:HG22	1:B:2076:ASN:N	2.14	0.63
1:A:64:PHE:HE2	1:A:464:ALA:HB1	1.64	0.63
1:A:82:LEU:HG	1:A:144:LEU:HD13	1.78	0.63
1:A:1180:LEU:HB2	1:A:1181:PRO:HD3	1.78	0.63
1:B:56:ASP:OD2	1:B:59:ARG:HD3	1.98	0.63
1:B:1470:ARG:HG3	1:B:1470:ARG:O	1.97	0.63
1:A:499:MET:SD	1:A:502:GLN:NE2	2.71	0.63
1:A:506:MET:HE3	1:A:559:ILE:CD1	2.27	0.63
1:A:616:LEU:HD23	1:A:617:PRO:CD	2.18	0.63
1:A:1216:LEU:CD1	1:A:1218:SER:H	2.08	0.63
1:A:1476:ASN:HA	1:A:1486:MET:HE1	1.80	0.63
1:A:1658:SER:O	1:A:1767:LEU:HD13	1.98	0.63
1:B:1408:THR:N	1:B:1409:PRO:CD	2.61	0.63
1:B:1454:VAL:HG13	1:B:1503:MET:CE	2.25	0.63
1:B:1520:GLU:O	1:B:1522:ASP:N	2.32	0.63
1:A:47:LEU:HA	1:A:201:MET:CE	2.27	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:945:GLU:OE2	1:B:941:SER:HB2	1.99	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:1211:LEU:HG	1:B:1211:LEU:O	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:1126:GLU:HB3	1:A:1129:CYS:SG	2.38	0.63
1:A:252:ASN:ND2	1:A:272:LEU:HB2	2.13	0.62
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:B:259:GLN:HB2	1:B:263:PHE:CD1	2.34	0.62
1:B:1433:LEU:HD21	1:B:1465:GLY:HA3	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1422:SER:O	1:A:1423:PHE:HB2	1.98	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:39:ARG:NH1	1:B:57:LEU:HD22	2.14	0.62
1:B:1890:THR:HA	1:B:1915:THR:HB	1.81	0.62
1:A:423:LEU:HB2	1:A:797:LEU:HD22	1.82	0.62
1:B:304:GLU:HG3	1:B:393:PHE:HE2	1.63	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: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:A:1036:LEU:HD21	1:A:1096:PHE:CE1	2.35	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:O	1:A:1461:ARG:HG3	1.99	0.62
1:B:859:VAL:HG13	1:B:936:ARG:HG2	1.81	0.62
1:A:142:ASN:HD22	1:B:396:GLY:HA3	1.64	0.62
1:A:263:PHE:HE2	1:A:303:GLN:HE21	1.48	0.62
1:A:2018:ILE:HG12	1:A:2041:MET:HE2	1.82	0.62
1:B:1409:PRO:CB	1:B:1439:ARG:HH12	2.12	0.62
1:A:765:ALA:HB1	1:A:768:GLN:CG	2.29	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:B:319:PRO:HB2	1:B:320:LEU:HD23	1.82	0.62
1:B:1016:GLU:HA	1:B:1043:PRO:HG3	1.81	0.62
1:A:64:PHE:CE2	1:A:464:ALA:HB1	2.34	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:B:1422:SER:O	1:B:1423:PHE:HB2	2.00	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: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:1318:ASN:O	1:A:1321:LEU:HD22	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:302:PRO:HA	1:A:366:ILE:HG21	1.82	0.61
1:A:2098:PHE:O	1:A:2101:GLN:HB2	2.00	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:207:SER:OG	1:B:209:ASP:HB3	2.01	0.61
1:B:1273:THR:HA	1:B:1295:THR:O	2.00	0.61
1:B:1616:MET:HE2	1:B:1800:PHE:HE1	1.66	0.61
1:A:111:VAL:CG2	1:A:188:LEU:HB2	2.30	0.61
1:B:82:LEU:HG	1:B:144:LEU:CD1	2.31	0.61
1:B:1720:PHE:N	1:B:1720:PHE:HD1	1.99	0.61
1:A:1036:LEU:CD2	1:A:1096:PHE:HE1	2.12	0.61
1:B:344:VAL:HG11	1:B:388:VAL:HG11	1.83	0.61
1:B:1991:VAL:HG21	1:B:2033:ASN:ND2	2.16	0.61
1:A:878:HIS:HB2	1:A:1007:PHE:CE1	2.34	0.61
1:A:1422:SER:CB	1:A:1424:ARG:HG3	2.30	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
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:9:MET:HE1	1:A:345:LEU:HB2	1.83	0.61
1:A:159:THR:O	1:A:159:THR:HG22	2.00	0.61
1:A:1802:GLU:HG2	1:A:1802:GLU:O	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:118:GLU:CD	1:B:118:GLU:HG3	2.26	0.60
1:A:259:GLN:HB2	1:A:263:PHE:CD1	2.35	0.60
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:B:252:ASN:ND2	1:B:272:LEU:HB2	2.15	0.60
1:B:1200:LEU:O	1:B:1203:VAL:HG23	2.00	0.60
1:A:1316:VAL:HG13	1:A:1345:LEU:HB3	1.82	0.60
1:A:1782:MET:HE3	1:B:1773:ASP:HB3	1.82	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:1694:ARG:HH11	1:B:1694:ARG:HG3	1.67	0.60
1:B:117:SER:HB3	1:B:135:CYS:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1011:LEU:HD21	1:B:1023:GLN:HB2	1.83	0.60
1:A:671:PHE:HE2	1:A:773:ARG:NH2	1.95	0.60
1:B:861:VAL:CG2	1:B:934:GLU:HB3	2.31	0.60
1:B:1429:LEU:HD11	1:B:1443:LEU:HD11	1.84	0.60
1:B:1616:MET:HE2	1:B:1800:PHE:CE1	2.36	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:A:861:VAL:CG2	1:A:934:GLU:HB3	2.32	0.60
1:B:64:PHE:HB2	1:B:429:ARG:HH21	1.65	0.60
1:B:442:LEU:HD23	1:B:473:LEU:HD22	1.84	0.60
1:B:982:THR:C	1:B:984:GLU:N	2.58	0.60
1:A:1259:PRO:HB2	1:A:1292:LEU:HD22	1.83	0.60
1:A:1773:ASP:HB3	1:B:1782:MET:HE3	1.83	0.60
1:B:353:TRP:HH2	1:B:388:VAL:HG21	1.67	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:A:118:GLU:HG3	1:B:118:GLU:CG	2.32	0.60
1:A:207:SER:OG	1:A:209:ASP:HB3	2.02	0.60
1:A:1182:ARG:NH2	1:A:1217:LEU:HB3	2.17	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
1:A:118:GLU:CG	1:B:118:GLU:HG3	2.32	0.60
1:A:856:CYS:O	1:A:856:CYS:SG	2.60	0.60
1:A:925:LEU:HD22	1:A:931:VAL:HG21	1.84	0.60
1:A:1349:LEU:CD1	1:A:1359:VAL:HG11	2.32	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:B:1126:GLU:HB3	1:B:1129:CYS:SG	2.42	0.60
1:A:81:MET:HG3	1:A:228:VAL:HG11	1.83	0.59
1:B:384:ARG:HG3	1:B:384:ARG:NH1	2.02	0.59
1:A:1419:GLU:CD	1:A:1447:GLY:HA3	2.28	0.59
1:B:273:ILE:O	1:B:277:TYR:HD1	1.85	0.59
1:B:1694:ARG:HG3	1:B:1694:ARG:NH1	2.16	0.59
1:A:663:GLN:O	1:A:667:ARG:HD2	2.03	0.59
1:A:1437:SER:O	1:A:1439:ARG:N	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1240:PRO:O	1:B:1268:MET:HE2	2.03	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:A:1133:ASN:HD22	1:A:1136:LEU:CD1	2.12	0.59
1:A:1662:ARG:HG2	1:A:1662:ARG:NH1	2.17	0.59
1:B:2098:PHE:O	1:B:2101:GLN:HB2	2.02	0.59
1:A:1043:PRO:HA	1:A:1927:ARG:NH1	2.18	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: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: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:A:200:PHE:CB	1:A:206:LEU:HD12	2.33	0.59
1:A:1801:GLU:C	1:A:1803:GLY:H	2.10	0.59
1:B:93:GLY:HA2	1:B:241:ARG:HD2	1.84	0.59
1:B:236:LYS:HG3	1:B:237:SER:N	2.17	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:644:ASN:HB3	1:A:770:VAL:HG11	1.85	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: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: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: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:1734:ARG:C	1:A:1736:THR:H	2.10	0.58
1:A:1955:LEU:O	1:A:1958:GLU:HB2	2.02	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:82:LEU:HG	1:A:144:LEU:CD1	2.33	0.58
1:A:442:LEU:HD23	1:A:473:LEU:HD22	1.84	0.58
1:A:859:VAL:HG13	1:A:936:ARG:HG2	1.84	0.58
1:A:1711:ARG:HG2	1:A:1712:PHE:CE1	2.37	0.58
1:B:1603:PHE:N	1:B:1603:PHE:CD2	2.69	0.58
1:B:1711:ARG:HG2	1:B:1712:PHE:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:118:GLU:HG3	1:B:118:GLU:CD	2.29	0.58
1:A:322:ILE:O	1:A:377:VAL:HG23	2.03	0.58
1:A:1528:THR:HG22	1:A:1530:HIS:N	2.14	0.58
1:B:594:LEU:HD13	1:B:599:ALA:HA	1.84	0.58
1:B:1338:LEU:HD13	1:B:1406:GLN:HG3	1.85	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: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: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:B:371:ASP:CG	1:B:371:ASP:O	2.46	0.58
1:A:371:ASP:CG	1:A:371:ASP:O	2.46	0.58
1:A:423:LEU:HD23	1:A:812:PRO:HG3	1.85	0.58
1:A:1457:VAL:HG21	1:A:1473:LEU:HB3	1.86	0.58
1:B:234:THR:HG22	1:B:235:LYS:O	2.03	0.58
1:B:1995:LYS:HB3	1:B:2041:MET:SD	2.44	0.58
1:A:188:LEU:HD22	1:A:228:VAL:HG12	1.85	0.58
1:A:997:ARG:HA	1:A:1001:TYR:O	2.04	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:B:655:GLN:O	1:B:655:GLN:HG2	2.03	0.58
1:B:1824:GLN:HG3	1:B:1825:PRO:HD2	1.86	0.58
1:A:586:ALA:O	1:A:589:TYR:HB3	2.03	0.58
1:A:1275:THR:HG22	1:A:1299:TRP:HB2	1.85	0.58
1:B:640:PRO:HA	1:B:651:ILE:HG22	1.85	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:1532:PHE:CD1	1:B:1532:PHE:C	2.81	0.58
1:A:426:ALA:HA	1:A:458:ALA:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:765:ALA:HB1	1:A:768:GLN:HG3	1.85	0.57
1:A:1735:HIS:CD2	1:A:1735:HIS:H	2.21	0.57
1:B:48:PRO:HD3	1:B:201:MET:CE	2.34	0.57
1:B:111:VAL:CG2	1:B:188:LEU:HB2	2.33	0.57
1:B:993:TYR:CZ	1:B:1008:GLN:HA	2.39	0.57
1:B:997:ARG:HA	1:B:1001:TYR:O	2.04	0.57
1:B:1222:ASP:HA	1:B:1226:LEU:CD1	2.34	0.57
1:B:1719:CYS:C	1:B:1720:PHE:HD1	2.12	0.57
1:B:1836:VAL:HG13	1:B:1854:ILE:CD1	2.33	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: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:B:662:LEU:HD22	1:B:672:VAL:HG11	1.86	0.57
1:B:1220:LEU:CB	1:B:1257:ARG:HH22	2.10	0.57
1:A:215:PHE:O	1:A:363:ASN:HB2	2.04	0.57
1:A:1137:GLN:NE2	1:A:1396:PHE:CE1	2.72	0.57
1:A:1182:ARG:NE	1:A:1217:LEU:H	2.01	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:B:1665:MET:HE1	1:B:1688:ALA:HA	1.86	0.57
1:B:1734:ARG:C	1:B:1736:THR:H	2.12	0.57
1:A:273:ILE:O	1:A:277:TYR:HD1	1.87	0.57
1:A:1345:LEU:HD12	1:A:1402:PHE:O	2.04	0.57
1:A:1528:THR:HG21	1:A:1552:HIS:HB2	1.87	0.57
1:A:1560:GLN:C	1:A:1562:ARG:H	2.13	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:38:ARG:HB2	1:B:53:LYS:HD2	1.87	0.57
1:B:1762:GLN:NE2	1:B:1787:LYS:HA	2.19	0.57
1:A:633:ARG:HG2	1:A:633:ARG:O	2.04	0.57
1:A:1673:ILE:HD13	1:A:1684:ALA:CB	2.35	0.57
1:B:1209:PRO:O	1:B:1210:LEU:HG	2.05	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:A:1001:TYR:HB3	1:A:1003:TYR:CE1	2.39	0.57
1:A:1418:VAL:O	1:A:1418:VAL:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1719:CYS:C	1:A:1720:PHE:HD1	2.12	0.57
1:B:275:SER:C	1:B:276:LEU:HD23	2.29	0.57
1:B:1299:TRP:CZ2	1:B:1305:ALA:HA	2.40	0.57
1:A:275:SER:C	1:A:276:LEU:HD23	2.30	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:351:GLY:C	1:B:383:ILE:HG22	2.29	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:290:ILE:HD13	1:A:308:ILE:HD13	1.87	0.56
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:B:77:PRO:O	1:B:81:MET:HG2	2.04	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: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:455:ASN:HB2	1:B:813:ASN:HD21	1.69	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:A:321:LEU:HD23	1:A:381:LEU:HD12	1.86	0.56
1:A:343:LYS:CE	1:A:354:ALA:HB3	2.26	0.56
1:A:1477:LEU:CD1	1:A:2043:ARG:HD2	2.23	0.56
1:A:1528:THR:HG22	1:A:1529:GLU:N	2.19	0.56
1:A:1672:LEU:N	1:A:1741:VAL:HG11	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:2101:GLN:HG3	1:A:2102:PRO:CD	2.35	0.56
1:B:302:PRO:HA	1:B:366:ILE:HG21	1.85	0.56
1:B:627:TRP:HB2	1:B:643:HIS:CE1	2.40	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:A:564:ILE:HD13	1:A:590:ALA:HB2	1.87	0.56
1:A:1204:LEU:HD21	1:A:1365:PRO:CG	2.34	0.56
1:B:440:GLN:HG3	1:B:833:HIS:CG	2.39	0.56
1:B:1451:SER:O	1:B:1452:GLY:C	2.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2018:ILE:HG12	1:B:2041:MET:HE2	1.87	0.56
1:B:2065:ASP:C	1:B:2070:LEU:HD12	2.30	0.56
1:A:1252:GLY:N	1:A:1321:LEU:HD11	2.20	0.56
1:A:1265:GLN:HE21	1:A:2026:ARG:NH1	2.01	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:B:81:MET:HG3	1:B:228:VAL:HG11	1.87	0.56
1:B:209:ASP:OD2	1:B:213:ARG:NE	2.38	0.56
1:B:1183:LEU:HD22	1:B:1213:ASP:O	2.05	0.56
1:A:251:THR:HB	1:A:399:ASN:O	2.06	0.56
1:A:734:TYR:C	1:A:734:TYR:CD2	2.83	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: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:51:MET:CE	1:A:191:LEU:HD13	2.27	0.56
1:A:278:ALA:CB	1:A:279:PRO:CD	2.84	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: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: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:A:159:THR:O	1:A:160:ALA:HB3	2.05	0.56
1:A:1720:PHE:HD1	1:A:1720:PHE:N	2.04	0.56
1:B:468:ARG:HD3	1:B:485:VAL:HG21	1.88	0.56
1:B:1180:LEU:HB2	1:B:1181:PRO:HD3	1.88	0.56
1:A:594:LEU:HD13	1:A:599:ALA:HA	1.88	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:B:1237:MET:SD	1:B:1242:MET:HG3	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:VAL:HG12	1:B:624:GLY:N	2.19	0.56
1:B:665:LEU:HB2	1:B:672:VAL:HG21	1.87	0.56
1:A:396:GLY:HA3	1:B:139:MET:HE1	1.88	0.55
1:A:1556:PRO:O	1:A:1557:ALA:C	2.49	0.55
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:A:379:ARG:O	1:A:381:LEU:HG	2.06	0.55
1:A:633:ARG:NH2	1:A:668:GLU:OE1	2.39	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:B:1138:GLU:HG3	1:B:1142:LEU:HD12	1.88	0.55
1:A:122:ARG:O	1:A:124:PRO:HD3	2.05	0.55
1:A:776:GLU:HB3	1:A:778:SER:OG	2.06	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:B:353:TRP:CH2	1:B:388:VAL:HG21	2.41	0.55
1:B:1611:ARG:HG2	1:B:1612:ARG:H	1.71	0.55
1:A:128:VAL:HG11	1:A:130:TYR:CZ	2.40	0.55
1:A:287:LEU:HA	1:A:387:ASN:O	2.07	0.55
1:A:1390:VAL:HG22	1:A:1501:LEU:HD21	1.89	0.55
1:B:734:TYR:C	1:B:734:TYR:CD2	2.82	0.55
1:A:38:ARG:HB2	1:A:53:LYS:HD2	1.87	0.55
1:A:1606:ARG:HH21	1:A:1860:GLU:HG3	1.71	0.55
1:A:1662:ARG:HH11	1:A:1662:ARG:HG3	1.68	0.55
1:A:1674:HIS:O	1:A:1675:SER:HB2	2.07	0.55
1:B:438:LEU:O	1:B:442:LEU:HG	2.06	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:A:396:GLY:CA	1:B:139:MET:HE1	2.37	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:1085:ASN:C	1:B:1086:LEU:HD23	2.31	0.55
1:B:1523:ARG:NH1	1:B:1545:ARG:HE	2.03	0.55
1:A:241:ARG:NH2	1:A:827:THR:O	2.40	0.55
1:A:1231:ASP:HB3	1:A:1515:ARG:HD2	1.89	0.55
1:B:1115:ILE:HD11	1:B:2111:LEU:HD12	1.88	0.55
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:1311:LYS:O	1:B:1312:ALA:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1422:SER:HB3	1:B:1424:ARG:HG3	1.87	0.55
1:B:1431:ASP:C	1:B:1433:LEU:H	2.14	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: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:A:1720:PHE:N	1:A:1720:PHE:CD1	2.75	0.55
1:A:1851:LYS:HG3	1:A:1852:VAL:N	2.21	0.55
1:A:2065:ASP:C	1:A:2070:LEU:HD12	2.32	0.55
1:B:128:VAL:HG11	1:B:130:TYR:CZ	2.41	0.55
1:B:1183:LEU:HB3	1:B:1216:LEU:HD23	1.89	0.55
1:B:1614:MET:HE3	1:B:1634:TRP:HB2	1.88	0.55
1:B:1662:ARG:HD3	1:B:1794:ILE:HG12	1.88	0.55
1:A:887:PRO:HB2	1:A:890:GLY:H	1.72	0.55
1:A:1041:LEU:HG	1:A:1041:LEU:O	2.07	0.55
1:A:1842:TYR:HE2	1:A:1848:HIS:HB3	1.71	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:A:662:LEU:C	1:A:664:GLN:N	2.63	0.54
1:B:162:SER:OG	1:B:163:SER:N	2.39	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:B:1735:HIS:H	1:B:1735:HIS:CD2	2.25	0.54
1:A:100:LEU:O	1:A:103:THR:OG1	2.24	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:100:LEU:O	1:B:101:ARG:C	2.50	0.54
1:B:136:GLN:NE2	1:B:138:ALA:H	2.04	0.54
1:A:475:GLY:C	1:A:477:ALA:H	2.15	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:1442:TRP:HB3	1:A:1444:MET:HE1	1.90	0.54
1:B:1611:ARG:HG2	1:B:1612:ARG:N	2.22	0.54
1:A:87:TYR:CE2	1:A:97:PRO:HG2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ARG:HG3	1:A:384:ARG:NH1	2.03	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
1:B:379:ARG:O	1:B:381:LEU:HG	2.07	0.54
1:B:745:PHE:CE2	1:B:767:LEU:HD13	2.43	0.54
1:B:1316:VAL:HG13	1:B:1345:LEU:HB3	1.90	0.54
1:A:333:GLU:CB	1:A:334:PRO:CD	2.84	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:348:LEU:HD13	1:A:406:PRO:HB3	1.89	0.54
1:A:1455:GLY:HA3	1:A:2039:SER:HB2	1.90	0.54
1:B:36:ASP:HB3	1:B:38:ARG:HG3	1.90	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: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:734:TYR:C	1:B:734:TYR:HD2	2.16	0.54
1:B:883:ARG:HE	1:B:1107:ARG:HD3	1.72	0.54
1:B:1533:VAL:HG21	1:B:1836:VAL:HG11	1.89	0.54
1:A:734:TYR:C	1:A:734:TYR:HD2	2.15	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:953:LEU:HD12	1:B:954:ILE:H	1.70	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: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:A:1315:LEU:O	1:A:1344:LEU:HD13	2.07	0.54
1:B:127:LEU:O	1:B:127:LEU:HG	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:491:PRO:HD2	1:A:756:ALA:HA	1.90	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:B:1243:LYS:HA	1:B:1271:ASP:HB2	1.90	0.54
1:A:275:SER:HB2	1:A:276:LEU:HD23	1.88	0.53
1:A:1011:LEU:HD21	1:A:1023:GLN:HB2	1.91	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: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:580:HIS:O	1:A:581:SER:HB3	2.07	0.53
1:A:1652:TYR:CE1	1:A:1823:VAL:HB	2.43	0.53
1:A:606:ARG:HH12	1:A:739:LEU:HG	1.72	0.53
1:A:988:SER:O	1:A:989:GLN:C	2.51	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:HA	1:A:1486:MET:CE	2.38	0.53
1:A:1476:ASN:HB3	1:A:1486:MET:SD	2.49	0.53
1:A:1594:THR:OG1	1:A:1596:ASP:HB2	2.08	0.53
1:B:642:CYS:HB2	1:B:650:THR:HB	1.89	0.53
1:B:1420:ASP:HB3	1:B:1425:TRP:HZ3	1.72	0.53
1:B:1540:ASP:HB3	1:B:1542:SER:OG	2.09	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:B:475:GLY:C	1:B:477:ALA:H	2.17	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:122:ARG:NH1	1:B:849:ASP:O	2.42	0.53
1:B:278:ALA:CB	1:B:279:PRO:CD	2.81	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: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:A:1451:SER:O	1:A:1452:GLY:C	2.51	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:B:23:TRP:CZ2	1:B:350:HIS:HD2	2.26	0.53
1:B:988:SER:O	1:B:989:GLN:C	2.47	0.53
1:B:1476:ASN:C	1:B:1477:LEU:HD23	2.33	0.53
1:B:2006:THR:O	1:B:2010:CYS:HB2	2.08	0.53
1:A:234:THR:HG22	1:A:235:LYS:O	2.09	0.53
1:A:737:ASN:C	1:A:737:ASN:HD22	2.17	0.53
1:A:1477:LEU:HB3	1:A:1507:ARG:HE	1.73	0.53
1:A:1585:PRO:CB	1:A:1598:MET:HE1	2.25	0.53
1:B:586:ALA:O	1:B:589:TYR:HB3	2.08	0.53
1:B:1246:GLU:CD	1:B:1254:LEU:HB2	2.34	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:A:1973:MET:SD	2:A:3002:NAP:H3D	2.49	0.53
1:A:1986:GLU:HB3	1:A:1989:GLN:NE2	2.24	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:1995:LYS:HD3	1:B:2038:ASN:OD1	2.09	0.53
1:A:23:TRP:CZ2	1:A:350:HIS:HD2	2.26	0.53
1:A:236:LYS:C	1:A:238:LEU:H	2.17	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: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: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: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:A:662:LEU:O	1:A:663:GLN:C	2.52	0.53
1:B:572:LEU:HD23	1:B:572:LEU:C	2.34	0.53
1:B:972:THR:HG23	1:B:1081:VAL:HG21	1.90	0.53
1:B:997:ARG:HH21	1:B:2070:LEU:HD12	1.73	0.53
1:B:1371:HIS:O	1:B:1371:HIS:CG	2.62	0.53
1:B:1567:TYR:C	1:B:1856:VAL:HG23	2.34	0.53
1:B:1616:MET:HE3	1:B:1650:ILE:HA	1.91	0.53
1:B:1656:TYR:CE1	1:B:1687:ILE:HD11	2.44	0.53
1:A:6:ILE:HG21	1:A:345:LEU:CD1	2.38	0.52
1:A:1456:MET:HE2	1:A:1460:LEU:HD21	1.89	0.52
1:B:424:LEU:CD2	1:B:441:GLY:HA3	2.39	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:A:100:LEU:O	1:A:101:ARG:C	2.52	0.52
1:A:945:GLU:OE2	1:B:941:SER:N	2.42	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:1786:LEU:C	1:A:1788:ASN:H	2.17	0.52
1:B:321:LEU:HD12	1:B:321:LEU:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:MET:HE2	1:B:677:THR:HG22	1.90	0.52
1:B:624:GLY:O	1:B:625:LEU:HD23	2.09	0.52
1:B:1842:TYR:CE2	1:B:1848:HIS:HB3	2.45	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:A:1085:ASN:C	1:A:1086:LEU:HD23	2.34	0.52
1:B:808:VAL:HG12	1:B:809:SER:N	2.25	0.52
1:B:1343:PHE:O	1:B:1344:LEU:HD22	2.10	0.52
1:B:1456:MET:HG3	1:B:2036:PHE:CD1	2.45	0.52
1:A:581:SER:OG	1:A:582:LEU:N	2.37	0.52
1:A:645:SER:C	1:A:746:GLN:HG3	2.35	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: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:A:91:VAL:HG21	1:A:834:ILE:CD1	2.40	0.52
1:A:605:TRP:O	1:A:606:ARG:C	2.53	0.52
1:A:1424:ARG:O	1:A:1426:VAL:N	2.42	0.52
1:A:1486:MET:HE3	1:A:1506:TYR:CB	2.38	0.52
1:A:1602:GLU:OE2	1:A:1650:ILE:N	2.42	0.52
1:B:1363:THR:O	1:B:1363:THR:CG2	2.58	0.52
1:A:1489:SER:HA	1:A:1493:LEU:HD22	1.91	0.52
1:B:297:THR:HB	1:B:300:GLY:H	1.74	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: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:A:137:ARG:NH1	1:B:137:ARG:HD2	2.24	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:1299:TRP:CH2	1:A:1333:ASN:CG	2.88	0.52
1:A:1456:MET:HG3	1:A:2036:PHE:HD1	1.75	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: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:A:98:ALA:O	1:A:101:ARG:HG3	2.10	0.52
1:A:504:GLN:HG3	1:A:546:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1011:LEU:CD2	1:B:1023:GLN:HB2	2.40	0.52
1:B:1771:LYS:O	1:B:1775:SER:HB2	2.09	0.52
1:A:808:VAL:HG12	1:A:809:SER:H	1.74	0.52
1:A:1300:ASP:O	1:A:1302:ALA:N	2.43	0.52
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:1578:LEU:C	1:A:1580:THR:H	2.17	0.52
1:B:776:GLU:HB3	1:B:778:SER:OG	2.10	0.52
1:B:276:LEU:HD23	1:B:276:LEU:N	2.25	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: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:1578:LEU:C	1:B:1580:THR:H	2.16	0.52
1:A:525:GLN:NE2	1:A:525:GLN:HA	2.24	0.51
1:A:1528:THR:CG2	1:A:1552:HIS:HB2	2.40	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:B:1470:ARG:O	1:B:1470:ARG:CG	2.57	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:A:1123:PRO:HB3	1:A:1510:ALA:HB1	1.92	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:O	1:A:866:VAL:HG13	2.10	0.51
1:A:994:LYS:HA	1:A:997:ARG:NH1	2.25	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:B:331:HIS:C	1:B:333:GLU:H	2.18	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:A:709:SER:OG	1:A:711:ARG:HB2	2.10	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:B:217:ALA:CB	1:B:364:PRO:HD3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:SER:O	1:B:409:ARG:HB2	2.11	0.51
1:B:980:ASP:CG	1:B:982:THR:HG22	2.35	0.51
1:A:331:HIS:C	1:A:333:GLU:H	2.18	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
1:B:889:THR:CG2	1:B:1032:LEU:HB2	2.41	0.51
1:B:895:THR:HA	1:B:935:VAL:HG11	1.91	0.51
1:B:1477:LEU:CD1	1:B:2043:ARG:HD2	2.40	0.51
1:A:1673:ILE:HD13	1:A:1684:ALA:HB1	1.92	0.51
1:B:1239:SER:C	1:B:1241:LYS:H	2.19	0.51
1:B:2102:PRO:HD2	1:B:2103:HIS:CD2	2.46	0.51
1:A:322:ILE:HG22	1:A:376:VAL:HA	1.92	0.51
1:A:1766:PHE:CD2	1:A:1791:PHE:CE1	2.98	0.51
1:B:1353:HIS:HB2	1:B:1354:PRO:CD	2.39	0.51
1:A:143:ARG:HG2	1:A:143:ARG:NH1	2.25	0.51
1:A:162:SER:OG	1:A:163:SER:N	2.40	0.51
1:A:469:GLY:HA2	1:A:805:LEU:HD21	1.93	0.51
1:A:1122:THR:HG21	1:A:1517:PHE:HZ	1.76	0.51
1:A:1420:ASP:HB3	1:A:1425:TRP:CZ3	2.46	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:B:209:ASP:CG	1:B:213:ARG:HH21	2.18	0.51
1:B:433:ALA:HB2	1:B:835:LYS:O	2.10	0.51
1:B:876:VAL:O	1:B:876:VAL:HG12	2.11	0.51
1:A:169:GLN:HE21	1:A:169:GLN:C	2.19	0.51
1:A:1064:HIS:O	1:A:1065:ARG:C	2.54	0.51
1:A:1246:GLU:CD	1:A:1254:LEU:HB2	2.36	0.51
1:A:1390:VAL:HG22	1:A:1501:LEU:CD2	2.41	0.51
1:A:1999:THR:HG1	1:A:2041:MET:HE3	1.76	0.51
1:B:127:LEU:C	1:B:127:LEU:HD12	2.36	0.51
1:B:515:ARG:HH22	1:B:817:PRO:HA	1.76	0.51
1:B:887:PRO:O	1:B:888:GLY:C	2.54	0.51
1:B:973:ARG:O	1:B:974:ALA:HB3	2.10	0.51
1:B:1303:ASN:H	1:B:1304:PRO:HD3	1.74	0.51
1:A:64:PHE:HB2	1:A:429:ARG:NH2	2.25	0.51
1:A:1247:VAL:HG21	1:A:1334:MET:HE1	1.93	0.51
1:A:1894:GLY:O	1:A:1895:GLY:C	2.53	0.51
1:A:768:GLN:CD	1:A:783:PRO:HG3	2.36	0.50
1:A:965:PRO:O	1:A:967:PRO:HD3	2.11	0.50
1:A:2002:LEU:O	1:A:2006:THR:HB	2.11	0.50
1:B:612:GLU:O	1:B:612:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:983:ALA:O	1:B:985:PHE:N	2.41	0.50
1:B:1234:LEU:HD11	1:B:1268:MET:HE1	1.93	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:1430:LYS:CE	1:B:1981:GLU:O	2.56	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:1999:THR:HG1	1:B:2041:MET:HE3	1.75	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: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:B:1674:HIS:HE1	1:B:1756:SER:OG	1.94	0.50
1:A:325:THR:OG1	1:A:343:LYS:HG2	2.11	0.50
1:A:1886:SER:HA	1:A:1911:LYS:HB2	1.92	0.50
1:B:6:ILE:HG21	1:B:345:LEU:CD1	2.39	0.50
1:B:209:ASP:CG	1:B:213:ARG:NH2	2.70	0.50
1:B:1279:PRO:HG3	1:B:1298:GLN:HE22	1.75	0.50
1:A:297:THR:HB	1:A:300:GLY:H	1.76	0.50
1:B:23:TRP:O	1:B:24:ALA:C	2.54	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: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:A:1411:ASP:OD2	1:A:1439:ARG:HB2	2.12	0.50
1:A:1424:ARG:C	1:A:1426:VAL:N	2.70	0.50
1:A:1841:ARG:O	1:A:1844:ALA:HB3	2.12	0.50
1:B:143:ARG:HH11	1:B:143:ARG:CG	2.19	0.50
1:B:159:THR:O	1:B:160:ALA:HB3	2.12	0.50
1:B:1442:TRP:HB3	1:B:1444:MET:HE1	1.92	0.50
1:B:1833:ARG:NH2	1:B:1872:ALA:O	2.45	0.50
1:A:277:TYR:O	1:A:278:ALA:C	2.54	0.50
1:A:289:TYR:HE2	1:A:291:GLU:CA	2.25	0.50
1:A:470:TYR:CD1	1:A:470:TYR:C	2.90	0.50
1:A:1651:VAL:HG12	1:A:1683:ALA:HB2	1.94	0.50
1:A:1999:THR:OG1	1:A:2041:MET:HE3	2.12	0.50
1:B:275:SER:HB2	1:B:276:LEU:HD23	1.93	0.50
1:B:367:PRO:C	1:B:369:LEU:H	2.20	0.50
1:B:866:VAL:HG13	1:B:866:VAL:O	2.12	0.50
1:B:1894:GLY:O	1:B:1896:PHE:N	2.45	0.50
1:A:128:VAL:HG11	1:A:130:TYR:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:HIS:HB2	1:A:1007:PHE:HE1	1.75	0.50
1:A:1896:PHE:HB2	2:A:3002:NAP:O2N	2.12	0.50
1:B:403:ILE:C	1:B:404:LEU:HD23	2.37	0.50
1:B:903:LEU:O	1:B:905:GLN:HG3	2.12	0.50
1:B:1422:SER:CB	1:B:1424:ARG:HG3	2.42	0.50
1:B:1616:MET:C	1:B:1800:PHE:HZ	2.20	0.50
1:A:112:SER:CB	1:A:334:PRO:CG	2.85	0.50
1:A:1369:GLY:C	1:A:1371:HIS:H	2.20	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: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:B:605:TRP:O	1:B:606:ARG:C	2.55	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:1894:GLY:O	1:B:1895:GLY:C	2.54	0.50
1:A:23:TRP:CZ2	1:A:350:HIS:CD2	3.00	0.50
1:A:72:ALA:HB3	1:A:842:TRP:CZ3	2.47	0.50
1:A:286:SER:HB2	1:A:387:ASN:HD22	1.77	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:CD2	1:A:1735:HIS:N	2.79	0.50
1:B:1041:LEU:O	1:B:1041:LEU:HG	2.12	0.50
1:B:1786:LEU:C	1:B:1788:ASN:H	2.20	0.50
1:A:5:VAL:HG12	1:A:245:THR:HA	1.94	0.49
1:A:23:TRP:O	1:A:24:ALA:C	2.54	0.49
1:A:895:THR:HA	1:A:935:VAL:HG11	1.92	0.49
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
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: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:1800:PHE:C	1:B:1800:PHE:CD2	2.90	0.49
1:B:1801:GLU:C	1:B:1803:GLY:H	2.20	0.49
1:A:59:ARG:N	1:A:59:ARG:HD2	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:495:ILE:CD1	1:B:578:ILE:HB	2.41	0.49
1:B:1285:ALA:HB1	1:B:1289:LEU:HG	1.94	0.49
1:B:1419:GLU:CD	1:B:1447:GLY:HA3	2.37	0.49
1:B:1458:ASN:O	1:B:2027:GLY:HA3	2.13	0.49
1:A:276:LEU:HD23	1:A:276:LEU:N	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:A:1672:LEU:HD12	1:A:1696:PHE:O	2.11	0.49
1:B:112:SER:CB	1:B:334:PRO:CG	2.85	0.49
1:B:272:LEU:O	1:B:276:LEU:HG	2.12	0.49
1:B:1568:TYR:CE2	1:B:1855:GLN:HB2	2.47	0.49
1:B:1603:PHE:CE2	1:B:1615:GLY:C	2.85	0.49
1:A:166:LEU:CD1	1:A:251:THR:HG21	2.32	0.49
1:A:737:ASN:C	1:A:737:ASN:ND2	2.69	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:CD2	1:A:2103:HIS:H	2.30	0.49
1:B:59:ARG:HD2	1:B:59:ARG:N	2.28	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: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:1999:THR:OG1	1:B:2041:MET:HE3	2.12	0.49
1:B:2086:GLN:HG2	1:B:2110:VAL:HG23	1.93	0.49
1:B:2103:HIS:CD2	1:B:2103:HIS:H	2.29	0.49
1:A:572:LEU:C	1:A:572:LEU:HD23	2.37	0.49
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:143:ARG:HG2	1:B:143:ARG:NH1	2.21	0.49
1:B:389:GLY:O	1:B:390:ILE:HG13	2.12	0.49
1:B:972:THR:HG23	1:B:1081:VAL:CG2	2.42	0.49
1:B:1123:PRO:HB3	1:B:1510:ALA:HB1	1.94	0.49
1:B:1364:SER:OG	1:B:1370:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1418:VAL:HG13	1:B:1425:TRP:CD2	2.46	0.49
1:B:1476:ASN:N	1:B:1476:ASN:OD1	2.44	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:A:384:ARG:CG	1:A:384:ARG:NH1	2.66	0.49
1:A:497:SER:OG	1:A:767:LEU:HG	2.13	0.49
1:A:1001:TYR:CD2	1:A:1003:TYR:HE1	2.29	0.49
1:B:305:LEU:O	1:B:309:VAL:HG23	2.13	0.49
1:B:1150:LEU:HB2	1:B:1192:LEU:HD21	1.94	0.49
1:B:1603:PHE:HD2	1:B:1603:PHE:H	1.59	0.49
1:A:1038:MET:HE3	1:A:1041:LEU:HD23	1.94	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:169:GLN:HE21	1:B:169:GLN:C	2.21	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:B:1424:ARG:C	1:B:1426:VAL:N	2.71	0.49
1:B:1694:ARG:HH11	1:B:1694:ARG:CG	2.26	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: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:B:491:PRO:HA	1:B:575:ASP:OD2	2.13	0.49
1:B:1117:GLU:HB2	1:B:2107:SER:HB2	1.94	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
1:B:1969:PHE:CD2	1:B:2017:VAL:HB	2.48	0.49
1:A:408:SER:O	1:A:409:ARG:HB2	2.12	0.49
1:A:1140:LEU:O	1:A:1140:LEU:HD22	2.12	0.49
1:A:2086:GLN:HG2	1:A:2110:VAL:HG23	1.94	0.49
1:B:1086:LEU:HD23	1:B:1086:LEU:N	2.28	0.49
1:B:1647:SER:HB2	1:B:1851:LYS:HG3	1.95	0.49
1:A:997:ARG:HH21	1:A:2070:LEU:HD12	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1989:GLN:HG2	1:A:1990:ASP:N	2.28	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: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:A:137:ARG:O	1:A:140:MET:HG2	2.13	0.48
1:A:846:SER:O	1:A:849:ASP:HB2	2.13	0.48
1:A:856:CYS:HB2	1:B:856:CYS:HG	1.77	0.48
1:A:1214:ASP:O	1:A:1216:LEU:N	2.41	0.48
1:A:2006:THR:O	1:A:2010:CYS:HB2	2.13	0.48
1:B:610:ILE:CG2	1:B:680:ILE:HD12	2.43	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: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:1996:TYR:C	1:B:1996:TYR:CD2	2.91	0.48
1:A:276:LEU:O	1:A:281:GLY:HA3	2.12	0.48
1:A:506:MET:HB3	1:A:559:ILE:HD11	1.93	0.48
1:A:1429:LEU:HD21	1:A:1443:LEU:HD21	1.95	0.48
1:A:2068:VAL:N	2:A:3002:NAP:O1N	2.46	0.48
1:B:112:SER:O	1:B:137:ARG:NH2	2.46	0.48
1:B:143:ARG:CG	1:B:143:ARG:NH1	2.76	0.48
1:B:525:GLN:NE2	1:B:525:GLN:HA	2.23	0.48
1:B:1504:ASN:HB3	1:B:1511:TRP:HZ3	1.77	0.48
1:A:903:LEU:O	1:A:904:SER:HB3	2.13	0.48
1:A:1231:ASP:O	1:A:1232:THR:C	2.56	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:B:98:ALA:O	1:B:101:ARG:HG3	2.13	0.48
1:B:662:LEU:HD13	1:B:672:VAL:CG1	2.43	0.48
1:B:1841:ARG:O	1:B:1844:ALA:HB3	2.14	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:A:1416:LEU:HD21	1:A:1425:TRP:HB2	1.94	0.48
1:B:87:TYR:CE2	1:B:97:PRO:HG2	2.48	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:1123:PRO:HA	1:B:1512:GLY:HA3	1.96	0.48
1:B:1729:GLU:OE1	1:B:1758:ARG:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLN:NE2	1:A:138:ALA:H	2.06	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:A:1237:MET:HB3	1:A:1237:MET:HE2	1.65	0.48
1:A:1240:PRO:HD2	1:A:1462:LYS:HE3	1.95	0.48
1:A:1651:VAL:HG13	1:A:1679:GLY:C	2.38	0.48
1:A:1694:ARG:HH11	1:A:1694:ARG:CG	2.26	0.48
1:B:12:LYS:HD2	1:B:81:MET:CE	2.44	0.48
1:B:277:TYR:O	1:B:278:ALA:C	2.56	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:2046:GLU:HG2	1:B:2104:PRO:HG2	1.95	0.48
1:A:39:ARG:NH1	1:A:226:GLU:OE2	2.47	0.48
1:A:450:PHE:CE2	1:A:828:PRO:HB2	2.49	0.48
1:A:645:SER:OG	1:A:648:THR:N	2.47	0.48
1:A:917:VAL:HG12	1:A:1054:PHE:HB2	1.93	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:B:1220:LEU:HB3	1:B:1257:ARG:NH2	2.14	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:B:128:VAL:HG11	1:B:130:TYR:OH	2.14	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:737:ASN:C	1:B:737:ASN:HD22	2.18	0.48
1:B:1390:VAL:HG13	1:B:1501:LEU:HD22	1.95	0.48
1:B:1904:LEU:HA	1:B:1904:LEU:HD23	1.56	0.48
1:A:226:GLU:O	1:A:227:ALA:HB2	2.14	0.48
1:A:1252:GLY:CA	1:A:1318:ASN:HD22	2.25	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:768:GLN:CD	1:B:783:PRO:HG3	2.39	0.48
1:B:981:SER:HA	1:B:986:ARG:NH2	2.29	0.48
1:B:1424:ARG:C	1:B:1426:VAL:H	2.21	0.48
1:A:103:THR:HG22	1:A:104:SER:H	1.77	0.48
1:A:225:ALA:O	1:A:332:PRO:HA	2.14	0.48
1:A:937:LEU:HD12	1:A:937:LEU:HA	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1476:ASN:ND2	1:A:1486:MET:HE2	2.29	0.48
1:A:1580:THR:HG22	1:A:1581:GLY:N	2.29	0.48
1:B:1069:TYR:CD1	1:B:1077:ALA:O	2.67	0.48
1:B:1636:VAL:O	1:B:1636:VAL:HG22	2.13	0.48
1:B:2023:SER:O	1:B:2027:GLY:HA2	2.14	0.48
1:A:146:PHE:O	1:B:256:SER:HB3	2.13	0.47
1:A:642:CYS:SG	1:A:743:VAL:CG2	3.02	0.47
1:A:661:PHE:CG	1:A:661:PHE:O	2.67	0.47
1:A:886:PHE:HA	1:A:887:PRO:HD3	1.63	0.47
1:A:1121:PHE:CE2	1:A:1507:ARG:HB2	2.49	0.47
1:A:1265:GLN:HG2	1:A:1266:PRO:HD2	1.94	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:B:297:THR:HG22	1:B:299:VAL:H	1.79	0.47
1:B:620:MET:HE2	1:B:677:THR:CG2	2.43	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:B:2003:ASP:O	1:B:2007:ARG:HG3	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:2076:ASN:HA	1:A:2085:PRO:HG2	1.96	0.47
1:B:606:ARG:O	1:B:610:ILE:HG13	2.13	0.47
1:B:1071:LEU:HD12	1:B:1075:THR:OG1	2.14	0.47
1:B:1363:THR:HG22	1:B:1367:GLN:NE2	2.29	0.47
1:B:1915:THR:CG2	2:B:3002:NAP:H2A	2.43	0.47
1:A:330:GLY:O	1:A:332:PRO:HD3	2.13	0.47
1:A:856:CYS:HB2	1:B:856:CYS:SG	2.53	0.47
1:B:211:THR:HG22	1:B:212:CYS:N	2.28	0.47
1:B:1183:LEU:HB3	1:B:1216:LEU:CD2	2.44	0.47
1:B:1228:ALA:HB2	1:B:1517:PHE:CZ	2.49	0.47
1:B:1231:ASP:O	1:B:1232:THR:C	2.58	0.47
1:B:1327:PRO:O	1:B:1331:VAL:HG23	2.14	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: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:1996:TYR:C	1:A:1996:TYR:CD2	2.92	0.47
1:A:2046:GLU:HG2	1:A:2104:PRO:HG2	1.95	0.47
1:A:132:MET:CE	1:B:200:PHE:CE2	2.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:GLY:O	1:A:511:MET:HE2	2.14	0.47
1:A:1067:LYS:HB3	1:A:1092:GLY:HA2	1.95	0.47
1:B:299:VAL:O	1:B:302:PRO:HD2	2.13	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:CD2	1:B:1735:HIS:N	2.83	0.47
1:B:1769:ILE:HG23	2:B:3001:NAP:C2N	2.45	0.47
1:B:1814:LEU:O	1:B:1818:ILE:HG13	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:A:1424:ARG:C	1:A:1426:VAL:H	2.22	0.47
1:A:1435:ASP:CG	1:A:1438:SER:HB3	2.40	0.47
1:A:1619:ALA:O	1:A:1620:GLU:HB2	2.15	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: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:A:76:ASP:CG	1:A:116:ALA:HB3	2.40	0.47
1:A:351:GLY:C	1:A:383:ILE:HG22	2.40	0.47
1:A:504:GLN:HG3	1:A:546:LEU:CD1	2.45	0.47
1:A:782:ILE:HG22	1:A:783:PRO:O	2.14	0.47
1:A:844:VAL:O	1:A:845:PRO:C	2.56	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:A:1182:ARG:CB	1:A:1216:LEU:HB2	2.33	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:1774:LEU:CD2	1:B:1785:PHE:HB2	2.45	0.47
1:A:1791:PHE:CD2	1:A:1791:PHE:C	2.92	0.47
1:B:67:VAL:O	1:B:68:HIS:C	2.57	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:O	1:B:633:ARG:HG2	2.14	0.47
1:B:709:SER:OG	1:B:711:ARG:HB2	2.14	0.47
1:B:1276:ASP:OD2	1:B:1281:ALA:HB3	2.14	0.47
1:B:1469:ILE:O	1:B:1469:ILE:CG2	2.61	0.47
1:B:1781:GLY:O	1:B:1784:VAL:HG23	2.15	0.47
1:A:64:PHE:HB2	1:A:429:ARG:HE	1.80	0.47
1:A:420:LEU:HD11	1:A:512:ARG:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:PRO:HA	1:A:575:ASP:OD2	2.15	0.47
1:A:1670:SER:OG	1:A:1741:VAL:HA	2.15	0.47
1:B:285:GLU:HG3	1:B:315:THR:OG1	2.15	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: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: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: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:1685:ILE:O	1:B:1686:ALA:C	2.58	0.47
1:B:1766:PHE:O	1:B:1792:HIS:HB2	2.14	0.47
1:A:88:GLU:HB3	1:A:831:SER:HB2	1.97	0.47
1:A:542:ASP:C	1:A:542:ASP:OD1	2.58	0.47
1:A:561:ILE:HG23	1:A:589:TYR:CE2	2.50	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:1584:SER:C	1:A:1586:ASP:H	2.23	0.47
1:A:1653:THR:HG22	1:A:1810:VAL:HG12	1.96	0.47
1:B:831:SER:N	1:B:832:PRO:CD	2.77	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:A:91:VAL:CG2	1:A:834:ILE:CD1	2.94	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: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
1:A:2099:LEU:HD23	1:A:2099:LEU:HA	1.70	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:470:TYR:C	1:B:470:TYR:CD1	2.92	0.46
1:B:556:LEU:O	1:B:560:GLN:HG3	2.15	0.46
1:B:1515:ARG:HD3	1:B:1515:ARG:HA	1.56	0.46
1:A:59:ARG:HG3	1:A:838:HIS:HB3	1.96	0.46
1:A:168:LEU:O	1:A:168:LEU:HG	2.14	0.46
1:A:509:SER:O	1:A:512:ARG:HG3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:ASP:OD1	1:A:839:SER:HB3	2.16	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:B:168:LEU:O	1:B:168:LEU:HG	2.14	0.46
1:B:297:THR:HB	1:B:300:GLY:N	2.31	0.46
1:B:1014:ASP:OD1	1:B:1015:LEU:N	2.49	0.46
1:B:1147:ALA:C	1:B:1149:ALA:H	2.23	0.46
1:B:1556:PRO:C	1:B:1558:SER:H	2.23	0.46
1:B:1578:LEU:C	1:B:1580:THR:N	2.73	0.46
1:B:1662:ARG:NH1	1:B:1662:ARG:CG	2.50	0.46
1:B:1857:ARG:CZ	1:B:1871:ILE:CD1	2.93	0.46
1:A:188:LEU:CD2	1:A:228:VAL:HG12	2.44	0.46
1:A:1136:LEU:HD21	1:A:1217:LEU:HG	1.97	0.46
1:A:1240:PRO:O	1:A:1268:MET:HE2	2.16	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:B:1216:LEU:CD1	1:B:1217:LEU:N	2.78	0.46
1:B:1540:ASP:C	1:B:1542:SER:H	2.21	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:A:67:VAL:O	1:A:68:HIS:C	2.58	0.46
1:A:248:ASN:HD22	1:A:249:ALA:H	1.61	0.46
1:A:925:LEU:CD2	1:A:931:VAL:HG21	2.46	0.46
1:A:1086:LEU:HD23	1:A:1086:LEU:N	2.31	0.46
1:A:1568:TYR:HE2	1:A:1855:GLN:HB2	1.80	0.46
1:A:1573:PHE:HD2	2:A:3001:NAP:HO3N	1.61	0.46
1:A:1798:SER:O	1:A:1802:GLU:OE1	2.33	0.46
1:B:117:SER:CB	1:B:135:CYS:HB3	2.44	0.46
1:B:283:ASP:C	1:B:285:GLU:H	2.22	0.46
1:B:309:VAL:CG2	1:B:374:LEU:HD11	2.45	0.46
1:B:1420:ASP:CB	1:B:1425:TRP:HZ3	2.28	0.46
1:B:1669:GLU:HG2	1:B:1742:ASP:OD2	2.15	0.46
1:A:1439:ARG:O	1:A:1470:ARG:HB3	2.15	0.46
1:B:147:PHE:CD2	1:B:147:PHE:C	2.94	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:B:1460:LEU:O	1:B:1462:LYS:N	2.49	0.46
1:A:494:PHE:CD1	1:A:574:PRO:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1466:GLY:HA2	1:A:1469:ILE:CG1	2.46	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:B:161:CYS:HB2	1:B:394:GLY:HA2	1.97	0.46
1:B:532:LEU:HD22	1:B:604:TYR:CE1	2.51	0.46
1:B:533:ARG:HH11	1:B:533:ARG:HB2	1.81	0.46
1:B:643:HIS:CD2	1:B:746:GLN:HB3	2.50	0.46
1:B:912:VAL:HG22	1:B:913:VAL:N	2.31	0.46
1:B:1452:GLY:O	1:B:2036:PHE:CD1	2.68	0.46
1:B:1697:THR:HG23	1:B:1698:THR:N	2.30	0.46
1:B:1762:GLN:O	1:B:1763:HIS:HB2	2.14	0.46
1:A:62:ALA:O	1:A:67:VAL:HG22	2.16	0.46
1:A:142:ASN:ND2	1:B:396:GLY:HA3	2.30	0.46
1:A:440:GLN:HG3	1:A:833:HIS:CG	2.50	0.46
1:B:119:ALA:HB2	1:B:850:PHE:CE2	2.51	0.46
1:B:438:LEU:HD23	1:B:438:LEU:N	2.30	0.46
1:B:1036:LEU:CD2	1:B:1096:PHE:CE1	2.94	0.46
1:B:1245:VAL:HB	1:B:1315:LEU:HD13	1.97	0.46
1:B:1311:LYS:O	1:B:1312:ALA:CB	2.63	0.46
1:B:1448:CYS:C	1:B:1450:THR:H	2.24	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
1:A:33:VAL:HG13	1:A:51:MET:C	2.39	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:384:ARG:CG	1:B:384:ARG:NH1	2.65	0.46
1:B:886:PHE:HA	1:B:887:PRO:HD3	1.64	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:A:36:ASP:C	1:A:38:ARG:H	2.24	0.46
1:A:556:LEU:O	1:A:560:GLN:HG3	2.15	0.46
1:A:1234:LEU:HD11	1:A:1268:MET:HE1	1.97	0.46
1:A:1975:LEU:HD22	1:A:1977:ASP:OD1	2.16	0.46
1:B:1361:PHE:CZ	1:B:1370:ARG:HD3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1208:ARG:H	1:A:1209:PRO:CD	2.29	0.46
1:A:1214:ASP:C	1:A:1216:LEU:N	2.74	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:HA	1:A:2043:ARG:HD3	1.61	0.46
1:B:1984:THR:C	1:B:1986:GLU:H	2.22	0.46
1:B:2017:VAL:HG21	1:B:2099:LEU:HD21	1.97	0.46
1:B:2099:LEU:HA	1:B:2099:LEU:HD23	1.71	0.46
1:A:240:ARG:HG2	1:A:821:PHE:CD2	2.51	0.45
1:A:356:ASN:HD22	1:A:356:ASN:HA	1.50	0.45
1:A:426:ALA:HA	1:A:458:ALA:CB	2.46	0.45
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:B:103:THR:HG22	1:B:104:SER:H	1.81	0.45
1:B:201:MET:HA	1:B:206:LEU:HB2	1.97	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:B:1214:ASP:CG	1:B:1321:LEU:HD21	2.40	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:A:984:GLU:HG2	1:A:986:ARG:NE	2.27	0.45
1:A:1115:ILE:HD11	1:A:2111:LEU:HG	1.99	0.45
1:A:1307:GLY:C	1:A:1309:LEU:H	2.24	0.45
1:A:1330:ALA:O	1:A:1334:MET:HG2	2.16	0.45
1:A:1371:HIS:CD2	1:A:1371:HIS:O	2.69	0.45
1:A:1785:PHE:HB2	1:B:1774:LEU:HD22	1.98	0.45
1:A:2018:ILE:HG23	1:A:2041:MET:HE2	1.97	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:1540:ASP:C	1:B:1542:SER:N	2.73	0.45
1:B:1647:SER:CA	1:B:1851:LYS:HG3	2.46	0.45
1:B:1674:HIS:CE1	1:B:1756:SER:OG	2.68	0.45
1:A:336:SER:OG	1:A:337:GLY:N	2.49	0.45
1:A:593:CYS:SG	1:A:708:ARG:HA	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:76:ASP:CG	1:B:116:ALA:HB3	2.41	0.45
1:B:122:ARG:HG3	1:B:123:ASP:H	1.80	0.45
1:B:1413:PRO:CA	1:B:1440:PRO:HB2	2.47	0.45
1:B:1418:VAL:O	1:B:1418:VAL:HG12	2.15	0.45
1:B:1442:TRP:CD2	1:B:1472:VAL:HB	2.51	0.45
1:B:1473:LEU:N	1:B:1473:LEU:HD23	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: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: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:1734:ARG:C	1:A:1736:THR:N	2.75	0.45
1:B:236:LYS:C	1:B:238:LEU:H	2.24	0.45
1:B:288:GLU:CD	1:B:385:GLY:H	2.24	0.45
1:B:399:ASN:N	1:B:399:ASN:ND2	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
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:A:762:ALA:HB1	1:A:763:PRO:HD2	1.99	0.45
1:A:1237:MET:SD	1:A:1242:MET:HG3	2.56	0.45
1:B:19:LEU:HD23	1:B:19:LEU:HA	1.76	0.45
1:B:40:TRP:CZ3	1:B:194:PRO:HA	2.51	0.45
1:B:62:ALA:O	1:B:67:VAL:HG22	2.17	0.45
1:B:136:GLN:NE2	1:B:138:ALA:N	2.64	0.45
1:B:416:GLN:C	1:B:418:ALA:H	2.25	0.45
1:B:1572:ASN:OD1	1:B:1851:LYS:NZ	2.49	0.45
1:A:416:GLN:C	1:A:418:ALA:H	2.24	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:A:1251:ASP:HB2	1:A:1321:LEU:HG	1.97	0.45
1:A:1408:THR:CG2	1:A:1409:PRO:HD2	2.46	0.45
1:A:1662:ARG:HH12	1:B:1790:THR:CG2	2.29	0.45
1:A:1766:PHE:O	1:A:1792:HIS:HB2	2.17	0.45
1:B:234:THR:HG22	1:B:235:LYS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ARG:C	1:B:276:LEU:N	2.75	0.45
1:B:782:ILE:CD1	1:B:803:LEU:HD23	2.40	0.45
1:B:944:PHE:CD1	1:B:944:PHE:C	2.94	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:297:THR:HB	1:A:300:GLY:N	2.32	0.45
1:A:1118:LYS:HB3	1:A:1519:LEU:HD13	1.99	0.45
1:A:1236:ASN:HA	1:A:1502:VAL:HG21	1.98	0.45
1:B:258:GLU:H	1:B:259:GLN:NE2	2.15	0.45
1:B:561:ILE:HG23	1:B:589:TYR:CE2	2.51	0.45
1:B:1338:LEU:CB	1:B:1406:GLN:HE21	2.29	0.45
1:B:1339:LYS:O	1:B:1340:GLU:HB2	2.17	0.45
1:B:1453:VAL:O	1:B:1454:VAL:C	2.59	0.45
1:B:1627:LEU:HD22	1:B:1627:LEU:HA	1.67	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:375:GLN:O	1:A:376:VAL:C	2.59	0.45
1:A:642:CYS:HB2	1:A:650:THR:HB	1.99	0.45
1:A:1350:LEU:HD13	1:A:1374:SER:HA	1.99	0.45
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:1674:HIS:HD2	1:B:1698:THR:OG1	1.97	0.45
1:B:2104:PRO:HD2	1:B:2105:VAL:H	1.82	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:759:VAL:O	1:A:759:VAL:HG23	2.17	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: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:B:426:ALA:HA	1:B:458:ALA:CB	2.46	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:1456:MET:HE3	1:B:1988:PHE:CZ	2.52	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:A:58:SER:HB3	1:A:844:VAL:CG2	2.47	0.45
1:A:363:ASN:HA	1:A:364:PRO:HD3	1.81	0.45
1:A:1385:ALA:O	1:A:1386:SER:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1925:GLN:O	1:A:1926:ALA:C	2.58	0.45
1:B:903:LEU:O	1:B:904:SER:HB3	2.17	0.45
1:B:1412:SER:HA	1:B:1413:PRO:HD3	1.61	0.45
1:B:1436:ALA:C	1:B:1438:SER:H	2.24	0.45
1:B:1728:PHE:CD1	1:B:1728:PHE:C	2.94	0.45
1:B:1817:GLY:C	1:B:1823:VAL:HG12	2.42	0.45
1:A:94:GLY:HA3	1:A:453:MET:HG2	1.97	0.44
1:A:283:ASP:C	1:A:285:GLU:H	2.25	0.44
1:A:606:ARG:O	1:A:610:ILE:HG13	2.18	0.44
1:A:970:PHE:O	1:A:1067:LYS:NZ	2.48	0.44
1:A:1111:HIS:O	1:A:1112:LEU:HD23	2.17	0.44
1:A:1515:ARG:HA	1:A:1515:ARG:HD3	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:B:542:ASP:O	1:B:545:VAL:HG12	2.17	0.44
1:B:1000:GLY:HA2	1:B:1106:ARG:NH2	2.32	0.44
1:B:1028:TRP:O	1:B:1032:LEU:HB2	2.17	0.44
1:B:1221:LEU:O	1:B:1221:LEU:HG	2.17	0.44
1:A:211:THR:HG22	1:A:212:CYS:N	2.32	0.44
1:A:366:ILE:O	1:A:366:ILE:CG1	2.65	0.44
1:A:396:GLY:HA3	1:B:142:ASN:ND2	2.31	0.44
1:A:856:CYS:C	1:A:858:SER:H	2.25	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
1:A:1411:ASP:HB2	1:A:1440:PRO:HD3	2.00	0.44
1:A:1473:LEU:N	1:A:1473:LEU:HD23	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:B:206:LEU:HD23	1:B:206:LEU:HA	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:B:1472:VAL:HG12	1:B:1473:LEU:N	2.32	0.44
1:B:1898:LEU:HD23	1:B:1898:LEU:HA	1.78	0.44
1:B:1901:ALA:O	1:B:1902:GLN:C	2.60	0.44
1:B:2053:LEU:CD2	1:B:2054:PRO:HD2	2.47	0.44
1:A:903:LEU:O	1:A:905:GLN:HG3	2.18	0.44
1:A:944:PHE:CD1	1:A:944:PHE:C	2.95	0.44
1:B:51:MET:CE	1:B:191:LEU:HD13	2.35	0.44
1:B:123:ASP:HA	1:B:124:PRO:HD3	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:737:ASN:C	1:B:737:ASN:ND2	2.70	0.44
1:B:1662:ARG:NH1	1:B:1792:HIS:ND1	2.66	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:A:887:PRO:O	1:A:888:GLY:C	2.58	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:B:254:ASP:O	1:B:255:GLY:O	2.36	0.44
1:B:274:ARG:C	1:B:276:LEU:H	2.24	0.44
1:B:642:CYS:O	1:B:649:VAL:HG13	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: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: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:732:ALA:O	1:B:733:GLU:C	2.61	0.44
1:B:994:LYS:HE2	1:B:1924:TYR:CE2	2.52	0.44
1:B:1036:LEU:HD13	1:B:1051:PRO:HG3	1.99	0.44
1:B:1251:ASP:CB	1:B:1321:LEU:HD22	2.47	0.44
1:B:1265:GLN:HE21	1:B:2026:ARG:NH1	2.16	0.44
1:B:1345:LEU:HD12	1:B:1402:PHE:O	2.17	0.44
1:A:22:PHE:CE2	1:A:26:LEU:HD11	2.53	0.44
1:A:103:THR:HG22	1:A:104:SER:N	2.32	0.44
1:A:136:GLN:HE22	1:A:138:ALA:N	2.09	0.44
1:A:169:GLN:HE21	1:A:170:SER:N	2.15	0.44
1:A:274:ARG:C	1:A:276:LEU:H	2.26	0.44
1:A:1011:LEU:CD2	1:A:1023:GLN:HB2	2.47	0.44
1:A:1234:LEU:HD22	1:A:1262:LEU:CD2	2.46	0.44
1:A:1234:LEU:HD13	1:A:1242:MET:SD	2.58	0.44
1:A:1584:SER:C	1:A:1586:ASP:N	2.75	0.44
1:A:1673:ILE:CD1	1:A:1684:ALA:HB1	2.48	0.44
1:A:1685:ILE:O	1:A:1686:ALA:C	2.60	0.44
1:A:1812:GLU:HA	1:A:1815:LYS:HB2	1.99	0.44
1:B:55:LYS:HB3	1:B:55:LYS:HE2	1.77	0.44
1:B:165:LEU:HD22	1:B:392:SER:HB2	1.98	0.44
1:B:699:ARG:O	1:B:703:LEU:HD23	2.18	0.44
1:B:784:LEU:HD23	1:B:784:LEU:HA	1.73	0.44
1:B:1389:LEU:HA	1:B:1389:LEU:HD23	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1472:VAL:HG12	1:B:1473:LEU:H	1.82	0.44
1:B:1535:VAL:O	1:B:1535:VAL:HG12	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:2031:GLN:HB3	1:B:2034:TYR:HB3	1.99	0.44
1:A:40:TRP:CZ3	1:A:194:PRO:HA	2.52	0.44
1:A:191:LEU:O	1:A:192:LEU:HD23	2.18	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:A:1147:ALA:HB1	1:A:1358:MET:CE	2.39	0.44
1:A:1390:VAL:HG13	1:A:1501:LEU:HD22	1.99	0.44
1:A:1488:PRO:O	1:A:1489:SER:HB2	2.17	0.44
1:A:1726:THR:O	1:A:1726:THR:CG2	2.66	0.44
1:A:1941:VAL:O	1:A:1941:VAL:HG12	2.16	0.44
1:B:64:PHE:HB2	1:B:429:ARG:HE	1.82	0.44
1:B:78:GLN:HE21	1:B:190:VAL:H	1.65	0.44
1:B:497:SER:HB2	1:B:762:ALA:CB	2.47	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:1897:GLY:HA2	1:B:1971:LEU:HD12	2.00	0.44
1:A:84:GLU:CD	1:A:838:HIS:HE2	2.26	0.44
1:A:440:GLN:HG3	1:A:833:HIS:CD2	2.53	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:1725:ASP:CG	1:A:1727:SER:H	2.25	0.44
1:A:1837:GLU:O	1:A:1840:PHE:HB2	2.18	0.44
1:B:159:THR:HG22	1:B:398:SER:HB3	1.98	0.44
1:B:368:ALA:HB1	1:B:374:LEU:HG	2.00	0.44
1:B:690:ILE:C	1:B:692:PRO:HD2	2.42	0.44
1:B:1038:MET:HE3	1:B:1041:LEU:HD23	1.99	0.44
1:B:1444:MET:HB2	1:B:1474:VAL:HB	2.00	0.44
1:B:1656:TYR:CD2	1:B:1687:ILE:HD13	2.53	0.44
1:B:1663:GLY:O	1:B:1664:ARG:C	2.61	0.44
1:A:83:LEU:HD23	1:A:144:LEU:HD12	1.99	0.44
1:A:896:TRP:CD2	1:A:907:LEU:HD11	2.53	0.44
1:A:1456:MET:HG3	1:A:2036:PHE:CD1	2.53	0.44
1:A:1616:MET:HE2	1:A:1800:PHE:HZ	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1532:PHE:HA	1:B:1546:TRP:HZ3	1.83	0.44
1:B:1941:VAL:O	1:B:1941:VAL:HG12	2.16	0.44
1:A:327:SER:HG	1:A:357:LEU:H	1.66	0.43
1:A:399:ASN:ND2	1:A:399:ASN:H	2.16	0.43
1:A:584:GLU:O	1:A:587:CYS:HB2	2.18	0.43
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:B:135:CYS:O	1:B:136:GLN:C	2.61	0.43
1:B:276:LEU:HD12	1:B:401:HIS:HB3	2.00	0.43
1:B:336:SER:OG	1:B:337:GLY:N	2.51	0.43
1:B:642:CYS:HA	1:B:743:VAL:HG23	2.00	0.43
1:B:643:HIS:CD2	1:B:746:GLN:CB	3.02	0.43
1:B:1477:LEU:HD12	1:B:1507:ARG:HH21	1.82	0.43
1:B:1697:THR:CG2	1:B:1698:THR:N	2.76	0.43
1:A:159:THR:HG22	1:A:398:SER:HB3	2.00	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:690:ILE:C	1:A:692:PRO:HD2	2.43	0.43
1:A:784:LEU:HD23	1:A:784:LEU:HA	1.73	0.43
1:A:1418:VAL:HG21	1:A:1443:LEU:HD13	2.00	0.43
1:A:1616:MET:HB3	1:A:1800:PHE:HE2	1.83	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:128:VAL:HG12	1:A:129:GLY:H	1.83	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:A:1234:LEU:HD21	1:A:1268:MET:HE3	2.00	0.43
1:A:1389:LEU:HD23	1:A:1389:LEU:HA	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
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:B:5:VAL:HG12	1:B:245:THR:HA	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:ILE:O	1:B:761:ILE:HG22	2.18	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: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:A:403:ILE:C	1:A:404:LEU:HD23	2.43	0.43
1:A:1069:TYR:CD1	1:A:1077:ALA:O	2.71	0.43
1:A:1578:LEU:C	1:A:1580:THR:N	2.74	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:B:264:PRO:HG2	1:B:300:GLY:HA2	1.99	0.43
1:B:289:TYR:HE2	1:B:291:GLU:HA	1.83	0.43
1:B:762:ALA:HB1	1:B:763:PRO:HD2	1.99	0.43
1:B:998:LEU:HA	1:B:998:LEU:HD23	1.87	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:1791:PHE:C	1:B:1791:PHE:CD2	2.97	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:A:274:ARG:C	1:A:276:LEU:N	2.76	0.43
1:A:899:LEU:HD12	1:A:899:LEU:O	2.18	0.43
1:A:1216:LEU:HD11	1:A:1218:SER:HB3	2.00	0.43
1:A:1236:ASN:ND2	1:A:1502:VAL:H	2.16	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: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:B:65:PHE:CE2	1:B:83:LEU:HB3	2.54	0.43
1:B:594:LEU:HD23	1:B:594:LEU:HA	1.70	0.43
1:B:615:VAL:CG2	1:B:686:PHE:HD2	2.27	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
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:A:583:GLY:O	1:A:584:GLU:C	2.61	0.43
1:A:830:ILE:C	1:A:832:PRO:HD2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1963:GLY:O	1:A:1964:PRO:C	2.61	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:765:ALA:HB2	1:B:783:PRO:HB3	2.00	0.43
1:B:782:ILE:HG22	1:B:783:PRO:O	2.19	0.43
1:B:1896:PHE:HB2	2:B:3002:NAP:O2N	2.19	0.43
1:A:67:VAL:O	1:A:67:VAL:HG23	2.19	0.43
1:A:504:GLN:N	1:A:546:LEU:HD11	2.34	0.43
1:A:594:LEU:HD23	1:A:594:LEU:HA	1.69	0.43
1:A:703:LEU:O	1:A:703:LEU:HG	2.19	0.43
1:A:981:SER:HA	1:A:986:ARG:NH2	2.34	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:O	1:A:1552:HIS:CG	2.71	0.43
1:A:1796:LEU:HD12	1:A:1796:LEU:HA	1.88	0.43
1:A:2058:VAL:HG22	1:A:2098:PHE:HD2	1.83	0.43
1:B:103:THR:HG22	1:B:104:SER:N	2.33	0.43
1:B:159:THR:CG2	1:B:398:SER:CB	2.94	0.43
1:B:321:LEU:HD23	1:B:381:LEU:CD1	2.49	0.43
1:B:494:PHE:CD1	1:B:574:PRO:HB3	2.53	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: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:B:1554:ALA:HB2	1:B:1882:PRO:CG	2.46	0.43
1:B:1562:ARG:HB3	1:B:1627:LEU:HD13	1.99	0.43
1:B:1617:VAL:HG13	1:B:1618:PRO:HD2	2.01	0.43
1:A:212:CYS:O	1:A:213:ARG:C	2.61	0.43
1:A:494:PHE:CZ	1:A:574:PRO:HG3	2.54	0.43
1:A:1014:ASP:OD1	1:A:1015:LEU:N	2.51	0.43
1:A:1015:LEU:HD23	1:A:1015:LEU:HA	1.76	0.43
1:A:1068:LEU:CD1	1:A:1078:ALA:HB2	2.49	0.43
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:HD12	1:A:1956:ILE:HA	1.84	0.43
1:B:608:TYR:O	1:B:611:LYS:N	2.51	0.43
1:B:844:VAL:O	1:B:845:PRO:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:915:GLU:O	1:B:916:ASP:HB2	2.18	0.43
1:B:1231:ASP:O	1:B:1234:LEU:N	2.50	0.43
1:B:1347:HIS:CD2	1:B:1347:HIS:C	2.96	0.43
1:B:1480:THR:HG22	1:B:1481:SER:H	1.83	0.43
1:B:1584:SER:C	1:B:1586:ASP:H	2.26	0.43
1:B:1629:LEU:O	1:B:1630:GLN:C	2.60	0.43
1:B:1893:LEU:HB3	1:B:1925:GLN:HE21	1.79	0.43
1:B:1925:GLN:O	1:B:1926:ALA:C	2.60	0.43
1:B:2075:THR:CG2	1:B:2076:ASN:N	2.82	0.43
1:B:2075:THR:C	1:B:2077:ASP:H	2.26	0.43
1:A:90:ILE:HG12	1:A:232:LEU:HD22	2.00	0.43
1:A:202:LYS:HB2	1:B:129:GLY:HA3	2.01	0.43
1:A:658:MET:O	1:A:659:SER:C	2.62	0.43
1:A:876:VAL:O	1:A:876:VAL:HG12	2.19	0.43
1:A:1476:ASN:C	1:A:1477:LEU:HD23	2.44	0.43
1:A:1653:THR:HG21	1:A:1807:TRP:CH2	2.53	0.43
1:A:2088:ILE:O	1:A:2089:ALA:C	2.60	0.43
1:B:193:LYS:O	1:B:193:LYS:HG3	2.19	0.43
1:B:193:LYS:HA	1:B:194:PRO:HD3	1.87	0.43
1:B:521:LEU:O	1:B:524:ASP:HB2	2.19	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:2043:ARG:NH1	1:B:2046:GLU:OE1	2.51	0.43
1:A:254:ASP:HB3	1:A:257:LYS:HE2	2.00	0.43
1:A:1212:CYS:C	1:A:1214:ASP:H	2.27	0.43
1:A:2086:GLN:NE2	1:A:2108:SER:OG	2.49	0.43
1:B:1288:LYS:O	1:B:1291:GLN:HG2	2.19	0.43
1:B:1658:SER:C	1:B:1767:LEU:HD13	2.44	0.43
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:A:830:ILE:C	1:A:832:PRO:CD	2.92	0.42
1:A:1405:ARG:HH22	1:A:1470:ARG:NH2	2.16	0.42
1:A:1817:GLY:C	1:A:1823:VAL:HG12	2.44	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:B:33:VAL:HG13	1:B:51:MET:C	2.44	0.42
1:B:36:ASP:CB	1:B:38:ARG:HG3	2.49	0.42
1:B:1064:HIS:O	1:B:1065:ARG:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1068:LEU:CD1	1:B:1078:ALA:HB2	2.49	0.42
1:B:1119:PHE:CZ	1:B:1514:PHE:HB3	2.53	0.42
1:B:1459:CYS:CB	1:B:2032:ALA:HA	2.49	0.42
1:B:2105:VAL:O	1:B:2106:LEU:HD23	2.19	0.42
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:A:1444:MET:HB3	1:A:1444:MET:HE2	1.48	0.42
1:A:1733:LEU:HA	1:A:1733:LEU:HD23	1.77	0.42
1:A:1735:HIS:H	1:A:1735:HIS:HD2	1.64	0.42
1:A:1932:TRP:O	1:A:1937:VAL:HB	2.18	0.42
1:B:22:PHE:CE2	1:B:26:LEU:HD11	2.54	0.42
1:B:136:GLN:HE22	1:B:138:ALA:N	2.09	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:B:1220:LEU:HD21	1:B:1318:ASN:HD21	1.83	0.42
1:B:1237:MET:HB3	1:B:1237:MET:HE2	1.54	0.42
1:B:1384:GLY:C	1:B:1386:SER:H	2.27	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:A:265:SER:O	1:A:269:GLN:HG3	2.20	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:1345:LEU:C	1:A:1346:LEU:HD23	2.43	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: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:B:2088:ILE:O	1:B:2089:ALA:C	2.62	0.42
1:A:195:ASN:O	1:A:196:SER:C	2.62	0.42
1:A:234:THR:HG22	1:A:235:LYS:N	2.35	0.42
1:A:532:LEU:HD22	1:A:604:TYR:CE1	2.55	0.42
1:A:1565:SER:O	1:A:1605:GLY:HA3	2.19	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:B:213:ARG:HD3	1:B:218:GLU:O	2.19	0.42
1:B:1584:SER:C	1:B:1586:ASP:N	2.78	0.42
1:B:1733:LEU:O	1:B:1736:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2066:VAL:HG22	1:B:2088:ILE:CD1	2.50	0.42
1:A:65:PHE:CE2	1:A:83:LEU:HB3	2.54	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:685:TYR:CD1	1:A:685:TYR:C	2.97	0.42
1:A:851:PRO:HB2	1:B:122:ARG:HA	2.01	0.42
1:A:1617:VAL:O	1:A:1617:VAL:HG12	2.19	0.42
1:B:276:LEU:CD1	1:B:401:HIS:HB3	2.50	0.42
1:B:507:GLY:O	1:B:511:MET:HE2	2.19	0.42
1:B:572:LEU:C	1:B:572:LEU:CD2	2.92	0.42
1:B:976:VAL:O	1:B:977:ASP:C	2.61	0.42
1:B:1253:GLN:HB3	1:B:1255:TYR:CE2	2.53	0.42
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:A:47:LEU:HD21	1:A:198:LEU:HA	2.01	0.42
1:A:739:LEU:HD23	1:A:739:LEU:HA	1.76	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: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: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:A:55:LYS:HE2	1:A:55:LYS:HB3	1.74	0.42
1:A:147:PHE:CD2	1:A:147:PHE:C	2.96	0.42
1:A:236:LYS:C	1:A:238:LEU:N	2.78	0.42
1:A:275:SER:CB	1:A:276:LEU:HD23	2.49	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:A:963:GLU:C	1:A:965:PRO:HD3	2.43	0.42
1:A:2105:VAL:O	1:A:2106:LEU:HD23	2.18	0.42
1:B:128:VAL:O	1:B:131:SER:OG	2.34	0.42
1:B:283:ASP:C	1:B:285:GLU:N	2.77	0.42
1:B:454:LEU:HD23	1:B:454:LEU:HA	1.80	0.42
1:B:876:VAL:HA	1:B:884:VAL:HG11	2.01	0.42
1:B:979:ALA:O	1:B:980:ASP:C	2.62	0.42
1:B:1009:LEU:HD22	1:B:1023:GLN:O	2.20	0.42
1:A:276:LEU:HD12	1:A:401:HIS:HB3	2.02	0.42
1:A:290:ILE:HG23	1:A:290:ILE:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ARG:C	1:A:317:ARG:O	2.63	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:1448:CYS:C	1:A:1450:THR:H	2.27	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
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:1473:LEU:HD11	1:B:1503:MET:SD	2.60	0.42
1:B:1496:VAL:HG21	1:B:1511:TRP:CH2	2.55	0.42
1:B:1565:SER:HB2	1:B:1857:ARG:CZ	2.50	0.42
1:B:1577:MET:CE	1:B:1582:LYS:HD3	2.46	0.42
1:B:1671:VAL:HG23	1:B:1743:LEU:CD1	2.49	0.42
1:B:1704:LYS:NZ	2:B:3001:NAP:O3X	2.45	0.42
1:A:189:ASN:HB2	1:A:334:PRO:HD2	2.02	0.42
1:A:299:VAL:O	1:A:302:PRO:HD2	2.19	0.42
1:A:506:MET:HB3	1:A:559:ILE:CD1	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: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:B:23:TRP:NE1	1:B:350:HIS:CD2	2.87	0.42
1:B:47:LEU:HD21	1:B:198:LEU:HA	2.01	0.42
1:B:491:PRO:HG2	1:B:753:PRO:HG2	2.02	0.42
1:B:638:ILE:HD11	1:B:657:ALA:O	2.20	0.42
1:B:1238:ALA:HB2	1:B:1468:ARG:HD3	2.02	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:A:283:ASP:C	1:A:285:GLU:N	2.78	0.42
1:A:1121:PHE:HE1	1:A:1512:GLY:O	2.03	0.42
1:A:1124:HIS:NE2	1:A:1512:GLY:HA2	2.35	0.42
1:A:1316:VAL:HA	1:A:1345:LEU:O	2.20	0.42
1:A:1322:ALA:O	1:A:1323:THR:C	2.61	0.42
1:A:1586:ASP:C	1:A:1588:ILE:H	2.27	0.42
1:A:1897:GLY:HA2	1:A:1971:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLU:O	1:B:88:GLU:HG3	2.20	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:1015:LEU:HD23	1:B:1015:LEU:HA	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:1538:ARG:NH1	1:B:1585:PRO:HG2	2.35	0.42
1:B:1556:PRO:C	1:B:1558:SER:N	2.76	0.42
1:A:633:ARG:NH2	1:A:668:GLU:CD	2.77	0.41
1:A:1302:ALA:O	1:A:1303:ASN:CB	2.65	0.41
1:A:1469:ILE:O	1:A:1469:ILE:CG2	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
1:A:2031:GLN:HB3	1:A:2034:TYR:HB3	2.01	0.41
1:B:47:LEU:HA	1:B:48:PRO:HD3	1.85	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:1068:LEU:HD13	1:B:1078:ALA:HB2	2.01	0.41
1:B:1115:ILE:HD11	1:B:2111:LEU:CD1	2.49	0.41
1:B:1251:ASP:HB3	1:B:1321:LEU:HD22	2.01	0.41
1:B:1350:LEU:N	1:B:1350:LEU:HD23	2.34	0.41
1:B:1442:TRP:HB3	1:B:1444:MET:CE	2.50	0.41
1:B:1563:LEU:HD12	1:B:1563:LEU:HA	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:A:120:LEU:HA	1:A:127:LEU:HD13	2.02	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:1235:GLU:OE2	1:A:1515:ARG:CZ	2.68	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: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:B:1394:ARG:HA	1:B:1400:VAL:HG22	2.02	0.41
1:B:1529:GLU:C	1:B:1530:HIS:CD2	2.98	0.41
1:B:1704:LYS:O	1:B:1705:ARG:C	2.63	0.41
1:B:1746:ASN:HD21	1:B:1753:LEU:HD12	1.85	0.41
1:A:89:ALA:O	1:A:92:ASP:HB3	2.21	0.41
1:A:91:VAL:O	1:A:457:ILE:HD11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:915:GLU:O	1:A:916:ASP:HB2	2.20	0.41
1:A:1252:GLY:N	1:A:1321:LEU:HD21	2.35	0.41
1:A:1466:GLY:O	1:A:1467:HIS:C	2.62	0.41
1:A:1644:GLU:HB3	1:A:1825:PRO:CG	2.50	0.41
1:A:1663:GLY:O	1:A:1664:ARG:C	2.62	0.41
1:A:1983:GLN:NE2	1:A:2033:ASN:CG	2.78	0.41
1:A:2073:MET:HE2	1:A:2073:MET:HB3	1.88	0.41
1:B:98:ALA:CA	1:B:101:ARG:HG3	2.47	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:B:1236:ASN:CG	1:B:1502:VAL:HG23	2.46	0.41
1:B:1456:MET:HE3	1:B:1988:PHE:HZ	1.85	0.41
1:B:1460:LEU:C	1:B:1462:LYS:N	2.79	0.41
1:B:1477:LEU:CD1	1:B:1507:ARG:HH21	2.33	0.41
1:B:1500:ASP:O	1:B:1501:LEU:C	2.62	0.41
1:B:1653:THR:O	1:B:1654:THR:C	2.62	0.41
1:B:2058:VAL:HG11	1:B:2060:TRP:CE2	2.54	0.41
1:B:2097:LEU:C	1:B:2097:LEU:HD12	2.44	0.41
1:A:14:PRO:HB2	1:A:32:MET:HB2	2.03	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: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:A:1068:LEU:HD13	1:A:1078:ALA:HB2	2.01	0.41
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: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:B:83:LEU:HD23	1:B:83:LEU:HA	1.89	0.41
1:B:595:THR:OG1	1:B:598:GLU:HG3	2.20	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:1433:LEU:HD11	1:B:1465:GLY:O	2.20	0.41
1:B:1963:GLY:O	1:B:1964:PRO:C	2.62	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:1456:MET:O	1:B:1457:VAL:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:200:PHE:CE2	1:B:132:MET:CE	2.98	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:667:ARG:C	1:A:668:GLU:HG3	2.43	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:A:999:ARG:HD3	1:A:1046:LEU:C	2.45	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: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:581:SER:HA	1:B:738:ASN:HD21	1.85	0.41
1:B:719:GLU:HA	1:B:722:TRP:NE1	2.35	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:A:40:TRP:CE3	1:A:194:PRO:HG3	2.56	0.41
1:A:128:VAL:O	1:A:131:SER:OG	2.39	0.41
1:A:132:MET:HB3	1:A:132:MET:HE2	1.59	0.41
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.76	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:A:1422:SER:O	1:A:1423:PHE:CB	2.68	0.41
1:A:1463:GLU:O	1:A:1464:PRO:C	2.64	0.41
1:A:1898:LEU:HD23	1:A:1898:LEU:HA	1.72	0.41
1:B:14:PRO:HB2	1:B:32:MET:HB2	2.02	0.41
1:B:291:GLU:OE2	1:B:325:THR:N	2.53	0.41
1:B:375:GLN:O	1:B:376:VAL:C	2.63	0.41
1:B:687:MET:HE2	1:B:687:MET:HA	2.03	0.41
1:B:827:THR:HA	1:B:828:PRO:HD3	1.96	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:A:63:SER:O	1:A:66:GLY:N	2.49	0.41
1:A:96:ASN:ND2	1:A:98:ALA:HB3	2.36	0.41
1:A:139:MET:HE1	1:B:396:GLY:HA2	2.00	0.41
1:A:165:LEU:HD23	1:A:400:VAL:CG2	2.30	0.41
1:A:305:LEU:CD2	1:A:308:ILE:HD12	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:GLY:N	1:A:679:GLY:O	2.50	0.41
1:A:854:SER:OG	1:A:855:SER:N	2.52	0.41
1:A:976:VAL:CG2	1:A:977:ASP:H	2.23	0.41
1:A:997:ARG:HE	1:A:2070:LEU:CD1	2.34	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:O	1:A:1614:MET:HG2	2.19	0.41
1:A:1762:GLN:HB3	1:A:1763:HIS:CD2	2.55	0.41
1:A:1816:ALA:C	1:A:1818:ILE:N	2.78	0.41
1:B:169:GLN:HG3	1:B:249:ALA:HB1	2.02	0.41
1:B:197:SER:OG	1:B:224:ARG:HD3	2.21	0.41
1:B:533:ARG:HB2	1:B:533:ARG:NH1	2.35	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:1541:LEU:CD1	1:B:1840:PHE:HB3	2.44	0.41
1:B:2018:ILE:HG23	1:B:2041:MET:HE2	2.01	0.41
1:A:81:MET:HG2	1:A:81:MET:H	1.72	0.41
1:A:135:CYS:O	1:A:136:GLN:C	2.63	0.41
1:A:193:LYS:O	1:A:193:LYS:HG3	2.21	0.41
1:A:193:LYS:HA	1:A:194:PRO:HD3	1.88	0.41
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:A:460:VAL:O	1:A:461:SER:C	2.64	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:1185:ALA:O	1:A:1189:GLN:CD	2.64	0.41
1:A:1321:LEU:HD12	1:A:1321:LEU:HA	1.90	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:1654:THR:HG21	2:A:3001:NAP:C4N	2.51	0.41
1:A:1765:ARG:CD	1:A:1765:ARG:N	2.84	0.41
1:A:1766:PHE:C	1:A:1767:LEU:HD23	2.46	0.41
1:A:1893:LEU:CB	1:A:1925:GLN:NE2	2.75	0.41
1:A:1921:ARG:HE	1:A:1921:ARG:HB2	1.47	0.41
1:B:25:ASN:CB	1:B:32:MET:SD	3.09	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:132:MET:HG2	1:B:136:GLN:HB2	2.02	0.41
1:B:214:SER:HB3	1:B:327:SER:HB3	2.03	0.41
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.79	0.41
1:B:399:ASN:H	1:B:399:ASN:HD22	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:ILE:HA	1:B:690:ILE:HD13	2.02	0.41
1:B:898:THR:HG22	1:B:937:LEU:HD22	2.02	0.41
1:B:1224:PRO:O	1:B:1225:ALA:C	2.63	0.41
1:B:1569:THR:HG23	1:B:1602:GLU:O	2.20	0.41
1:B:1586:ASP:C	1:B:1588:ILE:H	2.28	0.41
1:B:1695:VAL:HG12	1:B:1696:PHE:N	2.36	0.41
1:B:1999:THR:HG23	1:B:2018:ILE:HD11	2.02	0.41
1:A:92:ASP:O	1:A:241:ARG:NH1	2.52	0.41
1:A:119:ALA:HB2	1:A:850:PHE:CE2	2.56	0.41
1:A:545:VAL:HG22	1:A:551:SER:HB3	2.02	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:2018:ILE:CG2	1:A:2041:MET:HE2	2.50	0.41
1:B:59:ARG:HH21	1:B:841:ALA:HB2	1.86	0.41
1:B:128:VAL:HG12	1:B:130:TYR:CE2	2.56	0.41
1:B:137:ARG:O	1:B:138:ALA:C	2.64	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:ND2	1:B:737:ASN:O	2.52	0.41
1:B:903:LEU:C	1:B:905:GLN:H	2.29	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:HD3	1:B:2043:ARG:HA	1.61	0.41
1:B:2086:GLN:NE2	1:B:2108:SER:OG	2.50	0.41
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: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:1653:THR:CG2	1:A:1810:VAL:HG12	2.52	0.40
1:A:1728:PHE:CD1	1:A:1728:PHE:C	2.99	0.40
1:A:1733:LEU:O	1:A:1736:THR:HG22	2.20	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:B:36:ASP:C	1:B:38:ARG:H	2.29	0.40
1:B:82:LEU:HD22	1:B:188:LEU:HD11	2.03	0.40
1:B:96:ASN:HD21	1:B:98:ALA:HB3	1.85	0.40
1:B:411:ALA:HA	1:B:412:PRO:HD3	1.85	0.40
1:B:460:VAL:O	1:B:461:SER:C	2.63	0.40
1:B:570:LEU:HD11	1:B:800:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1433:LEU:C	1:B:1435:ASP:H	2.28	0.40
1:B:1698:THR:HA	1:B:1721:ALA:O	2.20	0.40
1:B:2072:THR:HB	1:B:2073:MET:H	1.69	0.40
1:A:254:ASP:O	1:A:255:GLY:O	2.39	0.40
1:A:473:LEU:N	1:A:473:LEU:HD23	2.36	0.40
1:A:1345:LEU:HD12	1:A:1345:LEU:HA	1.93	0.40
1:A:1431:ASP:C	1:A:1433:LEU:H	2.29	0.40
1:A:1713:PRO:C	1:A:1715:LEU:H	2.29	0.40
1:B:163:SER:O	1:B:164:SER:C	2.62	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:B:908:GLU:CD	1:B:1065:ARG:HH21	2.27	0.40
1:B:1001:TYR:HD2	1:B:1003:TYR:CE1	2.39	0.40
1:B:1153:LYS:CD	1:B:1195:ASN:HD22	2.35	0.40
1:B:1236:ASN:HD21	1:B:1502:VAL:H	1.69	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:1816:ALA:C	1:B:1818:ILE:N	2.79	0.40
1:B:1858:GLU:HG3	1:B:1859:GLU:N	2.37	0.40
1:A:289:TYR:CD2	1:A:289:TYR:C	3.00	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:N	2.80	0.40
1:A:762:ALA:C	1:A:764:HIS:H	2.30	0.40
1:B:232:LEU:HD12	1:B:233:LEU:N	2.36	0.40
1:B:290:ILE:O	1:B:290:ILE:HG23	2.21	0.40
1:B:719:GLU:HA	1:B:722:TRP:CE2	2.56	0.40
1:B:979:ALA:O	1:B:980:ASP:O	2.40	0.40
1:A:98:ALA:HA	1:A:101:ARG:CG	2.50	0.40
1:A:368:ALA:CA	1:A:371:ASP:HB3	2.51	0.40
1:A:1223:ALA:CB	1:A:1224:PRO:HD2	2.39	0.40
1:A:1325:GLY:C	1:A:1326:ASP:OD1	2.65	0.40
1:A:1472:VAL:CG1	1:A:1473:LEU:H	2.33	0.40
1:B:30:VAL:O	1:B:32:MET:HG2	2.21	0.40
1:B:195:ASN:O	1:B:196:SER:C	2.63	0.40
1:B:316:ARG:O	1:B:317:ARG:O	2.40	0.40
1:B:461:SER:HA	1:B:462:PRO:HD3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1343:PHE:CE2	1:B:1405:ARG:HD2	2.57	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:1984:THR:C	1:B:1986:GLU:N	2.79	0.40
1:A:51:MET:HE2	1:A:191:LEU:CD1	2.32	0.40
1:A:165:LEU:HD22	1:A:392:SER:HB2	2.03	0.40
1:A:1657:TYR:CZ	1:A:1799:LEU:HD11	2.57	0.40
1:A:1976:ARG:HB2	1:A:2033:ASN:ND2	2.36	0.40
2:A:3001:NAP:H52N	2:A:3001:NAP:H52A	2.03	0.40
1:B:47:LEU:HD22	1:B:197:SER:HB3	2.04	0.40
1:B:159:THR:CG2	1:B:159:THR:O	2.65	0.40
1:B:166:LEU:HB2	1:B:400:VAL:HG11	2.04	0.40
1:B:537:LEU:HD23	1:B:537:LEU:HA	1.74	0.40
1:B:980:ASP:HB2	1:B:981:SER:H	1.44	0.40
1:B:1493:LEU:HD23	1:B:1494:GLN:HE21	1.87	0.40
1:B:1612:ARG:CG	1:B:1642:LEU:HD21	2.51	0.40
1:B:1796:LEU:HD12	1:B:1796:LEU:HA	1.89	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	13
1	B	2080/2512 (83%)	1713 (82%)	276 (13%)	91 (4%)	2	13
All	All	4155/5024 (83%)	3396 (82%)	572 (14%)	187 (4%)	2	13

All (187) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	ALA

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	1471 (86%)	246 (14%)	3	14
1	B	1722/2072 (83%)	1492 (87%)	230 (13%)	4	16
All	All	3439/4144 (83%)	2963 (86%)	476 (14%)	3	15

All (476) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	MET
1	A	39	ARG
1	A	59	ARG
1	A	81	MET
1	A	86	THR

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Mol	Chain	Res	Type
1	A	95	ILE
1	A	100	LEU
1	A	103	THR
1	A	111	VAL
1	A	113	SER
1	A	120	LEU
1	A	121	SER
1	A	126	THR
1	A	128	VAL
1	A	131	SER
1	A	132	MET
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	224	ARG
1	A	237	SER
1	A	241	ARG
1	A	251	THR
1	A	273	ILE
1	A	276	LEU
1	A	295	THR
1	A	317	ARG
1	A	318	GLU
1	A	320	LEU
1	A	325	THR
1	A	329	MET
1	A	343	LYS
1	A	347	SER
1	A	356	ASN
1	A	366	ILE
1	A	371	ASP
1	A	375	GLN
1	A	381	LEU
1	A	383	ILE
1	A	384	ARG
1	A	399	ASN

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Mol	Chain	Res	Type
1	A	400	VAL
1	A	402	VAL
1	A	407	ASN
1	A	439	GLU
1	A	443	ARG
1	A	460	VAL
1	A	468	ARG
1	A	473	LEU
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	534	VAL
1	A	545	VAL
1	A	549	ILE
1	A	557	THR
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	649	VAL
1	A	658	MET
1	A	659	SER
1	A	660	GLU
1	A	665	LEU
1	A	668	GLU
1	A	670	VAL
1	A	675	VAL
1	A	676	ARG
1	A	677	THR
1	A	680	ILE
1	A	689	SER
1	A	697	GLN
1	A	701	VAL
1	A	703	LEU
1	A	704	ASP
1	A	723	GLN

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Mol	Chain	Res	Type
1	A	734	TYR
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	830	ILE
1	A	845	PRO
1	A	846	SER
1	A	858	SER
1	A	861	VAL
1	A	866	VAL
1	A	892	LEU
1	A	894	LEU
1	A	910	THR
1	A	919	LEU
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	1011	LEU
1	A	1019	ARG
1	A	1038	MET
1	A	1039	SER
1	A	1055	THR
1	A	1062	VAL
1	A	1063	THR
1	A	1068	LEU
1	A	1069	TYR
1	A	1070	THR
1	A	1072	GLN
1	A	1086	LEU
1	A	1087	ASN
1	A	1088	THR
1	A	1090	VAL
1	A	1101	SER
1	A	1102	SER
1	A	1103	VAL

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Mol	Chain	Res	Type
1	A	1107	ARG
1	A	1112	LEU
1	A	1122	THR
1	A	1140	LEU
1	A	1182	ARG
1	A	1216	LEU
1	A	1237	MET
1	A	1264	THR
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	1316	VAL
1	A	1319	CYS
1	A	1321	LEU
1	A	1324	LEU
1	A	1329	VAL
1	A	1333	ASN
1	A	1346	LEU
1	A	1350	LEU
1	A	1374	SER
1	A	1421	THR
1	A	1433	LEU
1	A	1443	LEU
1	A	1444	MET
1	A	1446	VAL
1	A	1449	SER
1	A	1469	ILE
1	A	1473	LEU
1	A	1476	ASN
1	A	1477	LEU
1	A	1480	THR
1	A	1481	SER
1	A	1501	LEU
1	A	1505	VAL
1	A	1537	SER
1	A	1544	ILE
1	A	1545	ARG
1	A	1551	LEU
1	A	1561	ASP

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Mol	Chain	Res	Type
1	A	1571	LEU
1	A	1573	PHE
1	A	1580	THR
1	A	1583	LEU
1	A	1587	SER
1	A	1601	MET
1	A	1614	MET
1	A	1617	VAL
1	A	1626	VAL
1	A	1628	LEU
1	A	1629	LEU
1	A	1636	VAL
1	A	1638	SER
1	A	1639	THR
1	A	1653	THR
1	A	1661	VAL
1	A	1662	ARG
1	A	1664	ARG
1	A	1671	VAL
1	A	1697	THR
1	A	1699	VAL
1	A	1714	GLN
1	A	1720	PHE
1	A	1726	THR
1	A	1735	HIS
1	A	1736	THR
1	A	1756	SER
1	A	1760	LEU
1	A	1765	ARG
1	A	1768	GLU
1	A	1769	ILE
1	A	1782	MET
1	A	1789	VAL
1	A	1790	THR
1	A	1797	ASP
1	A	1800	PHE
1	A	1813	LEU
1	A	1815	LYS
1	A	1818	ILE
1	A	1823	VAL
1	A	1841	ARG
1	A	1856	VAL

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Mol	Chain	Res	Type
1	A	1860	GLU
1	A	1868	LEU
1	A	1873	LEU
1	A	1877	SER
1	A	1899	GLN
1	A	1906	LEU
1	A	1915	THR
1	A	1916	SER
1	A	1922	THR
1	A	1927	ARG
1	A	1930	ARG
1	A	1939	VAL
1	A	1940	LEU
1	A	1941	VAL
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	2018	ILE
1	A	2026	ARG
1	A	2063	ILE
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	39	ARG
1	B	59	ARG
1	B	81	MET
1	B	86	THR
1	B	95	ILE
1	B	100	LEU
1	B	103	THR
1	B	111	VAL
1	B	113	SER
1	B	120	LEU

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Mol	Chain	Res	Type
1	B	126	THR
1	B	127	LEU
1	B	128	VAL
1	B	131	SER
1	B	132	MET
1	B	144	LEU
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	251	THR
1	B	273	ILE
1	B	276	LEU
1	B	295	THR
1	B	309	VAL
1	B	317	ARG
1	B	318	GLU
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	366	ILE
1	B	371	ASP
1	B	375	GLN
1	B	381	LEU
1	B	383	ILE
1	B	384	ARG
1	B	399	ASN
1	B	400	VAL
1	B	402	VAL
1	B	407	ASN
1	B	439	GLU
1	B	443	ARG
1	B	460	VAL
1	B	468	ARG

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Mol	Chain	Res	Type
1	B	473	LEU
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	534	VAL
1	B	549	ILE
1	B	557	THR
1	B	568	THR
1	B	569	SER
1	B	593	CYS
1	B	597	GLU
1	B	615	VAL
1	B	649	VAL
1	B	664	GLN
1	B	675	VAL
1	B	680	ILE
1	B	689	SER
1	B	697	GLN
1	B	701	VAL
1	B	734	TYR
1	B	743	VAL
1	B	746	GLN
1	B	776	GLU
1	B	778	SER
1	B	798	SER
1	B	819	VAL
1	B	821	PHE
1	B	825	ARG
1	B	830	ILE
1	B	856	CYS
1	B	861	VAL
1	B	866	VAL
1	B	892	LEU
1	B	894	LEU
1	B	910	THR
1	B	931	VAL
1	B	937	LEU
1	B	947	SER
1	B	959	VAL

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Mol	Chain	Res	Type
1	B	972	THR
1	B	976	VAL
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	1055	THR
1	B	1062	VAL
1	B	1063	THR
1	B	1068	LEU
1	B	1069	TYR
1	B	1070	THR
1	B	1072	GLN
1	B	1086	LEU
1	B	1087	ASN
1	B	1088	THR
1	B	1090	VAL
1	B	1101	SER
1	B	1102	SER
1	B	1103	VAL
1	B	1107	ARG
1	B	1122	THR
1	B	1140	LEU
1	B	1184	LEU
1	B	1216	LEU
1	B	1224	PRO
1	B	1264	THR
1	B	1275	THR
1	B	1299	TRP
1	B	1316	VAL
1	B	1321	LEU
1	B	1329	VAL
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

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Mol	Chain	Res	Type
1	B	1444	MET
1	B	1449	SER
1	B	1456	MET
1	B	1469	ILE
1	B	1471	CYS
1	B	1473	LEU
1	B	1476	ASN
1	B	1477	LEU
1	B	1480	THR
1	B	1481	SER
1	B	1501	LEU
1	B	1505	VAL
1	B	1528	THR
1	B	1532	PHE
1	B	1535	VAL
1	B	1543	SER
1	B	1549	SER
1	B	1551	LEU
1	B	1573	PHE
1	B	1580	THR
1	B	1583	LEU
1	B	1587	SER
1	B	1597	CYS
1	B	1601	MET
1	B	1603	PHE
1	B	1612	ARG
1	B	1614	MET
1	B	1616	MET
1	B	1627	LEU
1	B	1629	LEU
1	B	1636	VAL
1	B	1639	THR
1	B	1643	GLU
1	B	1653	THR
1	B	1661	VAL
1	B	1662	ARG
1	B	1666	GLN
1	B	1669	GLU
1	B	1671	VAL
1	B	1694	ARG
1	B	1697	THR
1	B	1699	VAL

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Mol	Chain	Res	Type
1	B	1714	GLN
1	B	1720	PHE
1	B	1726	THR
1	B	1735	HIS
1	B	1736	THR
1	B	1756	SER
1	B	1760	LEU
1	B	1765	ARG
1	B	1768	GLU
1	B	1769	ILE
1	B	1782	MET
1	B	1789	VAL
1	B	1790	THR
1	B	1797	ASP
1	B	1815	LYS
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	1889	ILE
1	B	1899	GLN
1	B	1906	LEU
1	B	1915	THR
1	B	1916	SER
1	B	1922	THR
1	B	1927	ARG
1	B	1930	ARG
1	B	1939	VAL
1	B	1941	VAL
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

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Mol	Chain	Res	Type
1	B	2006	THR
1	B	2018	ILE
1	B	2026	ARG
1	B	2063	ILE
1	B	2079	VAL
1	B	2084	LEU
1	B	2088	ILE
1	B	2105	VAL
1	B	2107	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) 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	328	ASN
1	A	331	HIS
1	A	350	HIS
1	A	356	ASN
1	A	387	ASN
1	A	399	ASN
1	A	416	GLN
1	A	440	GLN
1	A	525	GLN
1	A	643	HIS
1	A	644	ASN
1	A	697	GLN
1	A	746	GLN
1	A	792	ASN
1	A	833	HIS
1	A	1018	ASN
1	A	1037	HIS
1	A	1109	GLN
1	A	1111	HIS
1	A	1124	HIS
1	A	1133	ASN

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Mol	Chain	Res	Type
1	A	1189	GLN
1	A	1191	GLN
1	A	1206	GLN
1	A	1265	GLN
1	A	1303	ASN
1	A	1318	ASN
1	A	1353	HIS
1	A	1406	GLN
1	A	1458	ASN
1	A	1467	HIS
1	A	1476	ASN
1	A	1504	ASN
1	A	1516	HIS
1	A	1735	HIS
1	A	1762	GLN
1	A	1777	ASN
1	A	1855	GLN
1	A	1899	GLN
1	A	1982	ASN
1	A	2028	ASN
1	A	2076	ASN
1	A	2086	GLN
1	A	2103	HIS
1	B	25	ASN
1	B	78	GLN
1	B	136	GLN
1	B	142	ASN
1	B	169	GLN
1	B	199	GLN
1	B	248	ASN
1	B	259	GLN
1	B	306	ASN
1	B	328	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

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Mol	Chain	Res	Type
1	B	614	ASN
1	B	643	HIS
1	B	697	GLN
1	B	723	GLN
1	B	738	ASN
1	B	746	GLN
1	B	833	HIS
1	B	1037	HIS
1	B	1066	GLN
1	B	1109	GLN
1	B	1111	HIS
1	B	1124	HIS
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	1406	GLN
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	1899	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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	50,52,52	1.36	6 (12%)	71,80,80	1.82	14 (19%)
2	NAP	B	3001	-	50,52,52	1.31	3 (6%)	71,80,80	1.72	13 (18%)
2	NAP	A	3001	-	50,52,52	1.38	5 (10%)	71,80,80	1.71	13 (18%)
2	NAP	A	3002	-	50,52,52	1.22	5 (10%)	71,80,80	1.64	10 (14%)

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	-	-	9/35/67/67	0/5/5/5
2	NAP	B	3001	-	-	2/35/67/67	0/5/5/5
2	NAP	A	3001	-	-	12/35/67/67	0/5/5/5
2	NAP	A	3002	-	-	10/35/67/67	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3002	NAP	C2N-N1N	5.62	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3001	NAP	C2N-N1N	5.49	1.41	1.35
2	A	3002	NAP	C2N-N1N	5.17	1.40	1.35
2	A	3001	NAP	C2N-N1N	4.86	1.40	1.35
2	A	3001	NAP	C2A-N3A	3.53	1.40	1.33
2	A	3001	NAP	C2A-N1A	3.33	1.39	1.33
2	B	3001	NAP	C2A-N1A	3.30	1.39	1.33
2	B	3002	NAP	C2A-N3A	3.01	1.39	1.33
2	B	3001	NAP	C2A-N3A	2.75	1.38	1.33
2	B	3002	NAP	C6N-N1N	2.56	1.41	1.35
2	A	3002	NAP	C2A-N3A	2.44	1.38	1.33
2	A	3001	NAP	PN-O3	2.42	1.62	1.59
2	A	3002	NAP	C2A-N1A	2.27	1.38	1.33
2	B	3002	NAP	C2A-N1A	2.21	1.37	1.33
2	A	3001	NAP	C8A-N7A	2.11	1.35	1.31
2	B	3002	NAP	PN-O3	2.07	1.61	1.59
2	A	3002	NAP	C8A-N7A	2.05	1.35	1.31
2	B	3002	NAP	C8A-N7A	2.02	1.35	1.31
2	A	3002	NAP	C6N-N1N	2.01	1.39	1.35

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	NAP	N3A-C2A-N1A	-6.08	119.37	128.58
2	A	3002	NAP	N3A-C2A-N1A	-5.54	120.20	128.58
2	B	3001	NAP	N3A-C2A-N1A	-5.41	120.39	128.58
2	A	3001	NAP	C2B-C1B-N9A	-5.37	104.91	113.75
2	A	3002	NAP	C2B-C1B-N9A	-5.19	105.21	113.75
2	B	3002	NAP	N3A-C2A-N1A	-5.12	120.84	128.58
2	B	3002	NAP	C5A-C4A-N3A	-4.95	119.90	126.72
2	B	3001	NAP	C2B-C1B-N9A	-4.81	105.84	113.75
2	A	3002	NAP	C5A-C4A-N3A	-4.73	120.21	126.72
2	B	3002	NAP	C2B-C1B-N9A	-4.69	106.04	113.75
2	B	3002	NAP	N9A-C8A-N7A	-4.63	107.37	113.94
2	B	3001	NAP	C3N-C7N-N7N	-4.23	112.52	117.74
2	A	3002	NAP	N9A-C8A-N7A	-4.05	108.20	113.94
2	B	3001	NAP	N9A-C8A-N7A	-4.02	108.23	113.94
2	A	3001	NAP	N9A-C8A-N7A	-3.94	108.34	113.94
2	A	3001	NAP	C5A-C4A-N3A	-3.92	121.32	126.72
2	B	3002	NAP	O4B-C1B-N9A	3.87	115.52	108.09
2	B	3002	NAP	C5A-N7A-C8A	3.73	109.31	103.45
2	A	3002	NAP	C2A-N3A-C4A	3.56	120.52	111.83
2	B	3002	NAP	N3A-C4A-N9A	3.54	133.19	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3002	NAP	C2A-N3A-C4A	3.53	120.44	111.83
2	A	3002	NAP	N3A-C4A-N9A	3.53	133.16	127.17
2	B	3001	NAP	C5A-C4A-N3A	-3.50	121.90	126.72
2	B	3002	NAP	C6N-N1N-C2N	-3.42	118.97	121.88
2	A	3001	NAP	C5A-N7A-C8A	3.27	108.59	103.45
2	B	3001	NAP	C5A-N7A-C8A	3.27	108.59	103.45
2	A	3001	NAP	C2A-N3A-C4A	3.18	119.59	111.83
2	A	3002	NAP	C5A-N7A-C8A	3.09	108.30	103.45
2	A	3001	NAP	N3A-C4A-N9A	3.04	132.33	127.17
2	B	3002	NAP	C4A-N9A-C8A	2.94	108.82	105.74
2	B	3001	NAP	N3A-C4A-N9A	2.76	131.86	127.17
2	B	3001	NAP	C2A-N3A-C4A	2.76	118.56	111.83
2	B	3001	NAP	O7N-C7N-C3N	2.73	122.93	119.60
2	B	3001	NAP	C4A-N9A-C8A	2.64	108.51	105.74
2	B	3002	NAP	C4A-C5A-N7A	-2.62	107.58	110.58
2	B	3002	NAP	C4B-O4B-C1B	-2.54	103.85	109.47
2	B	3001	NAP	O4B-C1B-N9A	2.53	112.96	108.09
2	A	3001	NAP	C4A-N9A-C8A	2.48	108.34	105.74
2	A	3002	NAP	C4A-N9A-C8A	2.45	108.31	105.74
2	A	3001	NAP	C3B-C2B-C1B	2.38	107.36	102.81
2	A	3001	NAP	C4D-O4D-C1D	2.28	112.02	109.92
2	A	3002	NAP	O4B-C1B-N9A	2.27	112.46	108.09
2	B	3001	NAP	C5D-C4D-C3D	-2.27	107.03	115.21
2	B	3002	NAP	C3N-C7N-N7N	-2.26	114.95	117.74
2	A	3001	NAP	O4B-C1B-N9A	2.12	112.16	108.09
2	A	3001	NAP	O2A-PA-O3	2.11	112.98	107.27
2	B	3002	NAP	C6A-C5A-C4A	2.09	120.03	117.18
2	B	3001	NAP	C6A-C5A-C4A	2.08	120.02	117.18
2	A	3001	NAP	O2B-C2B-C1B	-2.06	102.80	110.05
2	A	3002	NAP	C3N-C7N-N7N	-2.05	115.21	117.74

There are no chirality outliers.

All (33) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	A	3002	NAP	C3B-C4B-C5B-O5B
2	B	3002	NAP	O4D-C4D-C5D-O5D
2	A	3001	NAP	O4B-C4B-C5B-O5B
2	A	3002	NAP	O4B-C4B-C5B-O5B
2	B	3002	NAP	O4B-C4B-C5B-O5B
2	A	3001	NAP	C3B-C4B-C5B-O5B
2	A	3002	NAP	C3D-C4D-C5D-O5D
2	B	3002	NAP	C3D-C4D-C5D-O5D
2	B	3002	NAP	PA-O3-PN-O5D
2	B	3001	NAP	O4B-C4B-C5B-O5B
2	A	3001	NAP	C5B-O5B-PA-O1A
2	A	3001	NAP	C5B-O5B-PA-O2A
2	A	3001	NAP	C5B-O5B-PA-O3
2	A	3001	NAP	C5D-O5D-PN-O1N
2	B	3001	NAP	C4B-C5B-O5B-PA
2	B	3002	NAP	C1B-C2B-O2B-P2B
2	A	3001	NAP	PA-O3-PN-O2N
2	A	3001	NAP	C2B-O2B-P2B-O2X
2	A	3001	NAP	O4D-C1D-N1N-C2N
2	A	3002	NAP	O4D-C1D-N1N-C6N
2	A	3001	NAP	C2B-O2B-P2B-O1X
2	A	3002	NAP	PN-O3-PA-O1A
2	A	3001	NAP	PA-O3-PN-O1N
2	A	3002	NAP	C4B-C5B-O5B-PA
2	A	3002	NAP	PN-O3-PA-O2A
2	B	3002	NAP	PN-O3-PA-O2A

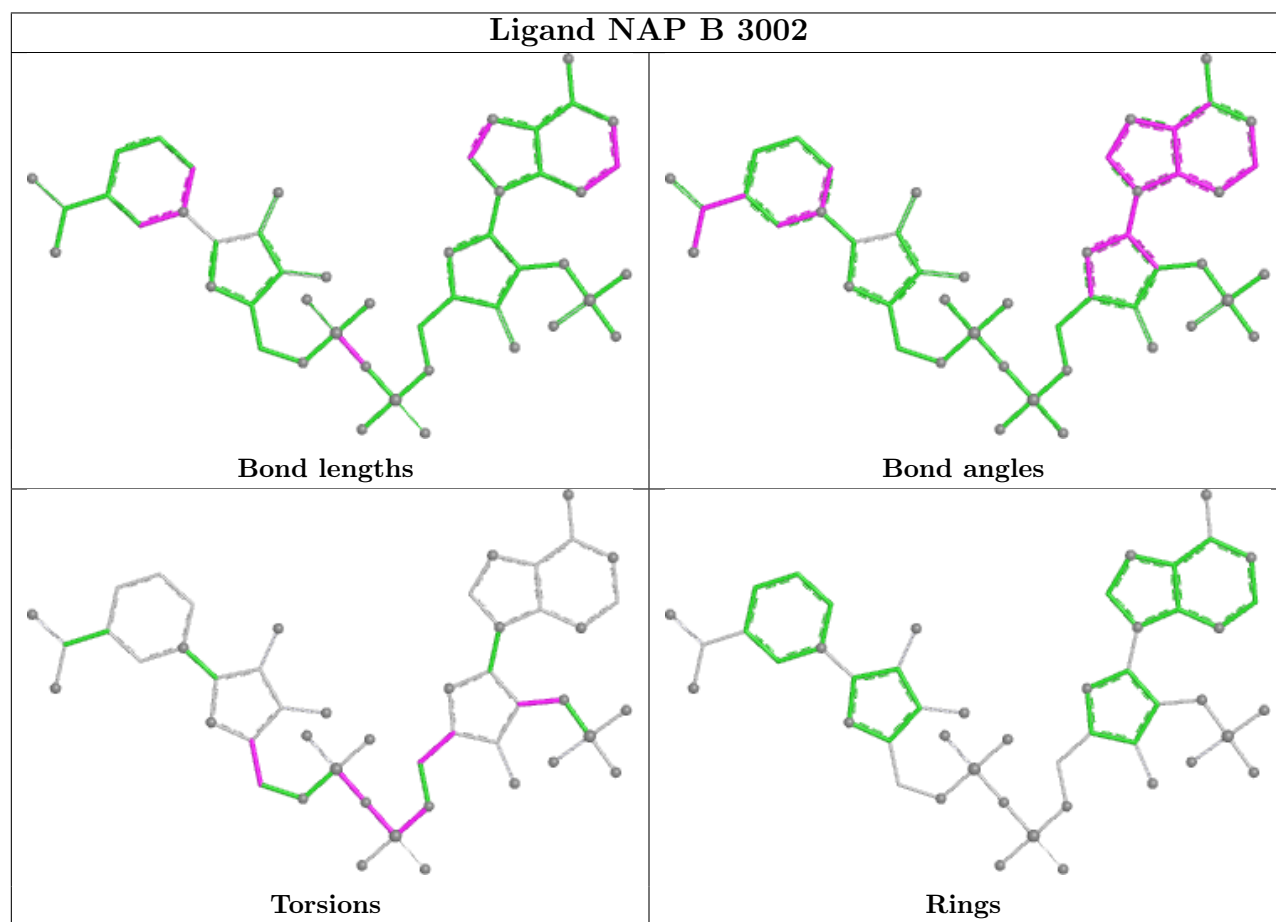
There are no ring outliers.

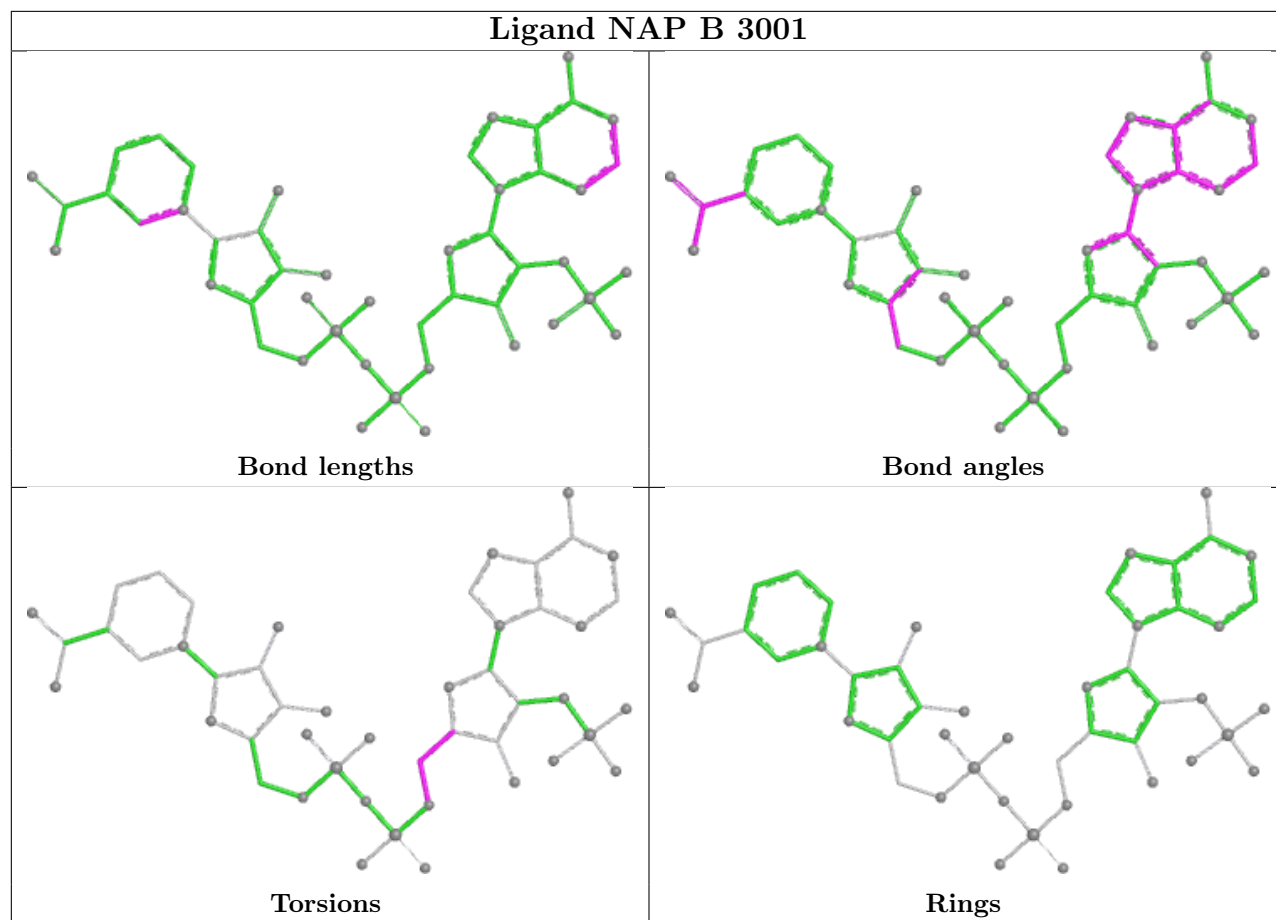
4 monomers are involved in 16 short contacts:

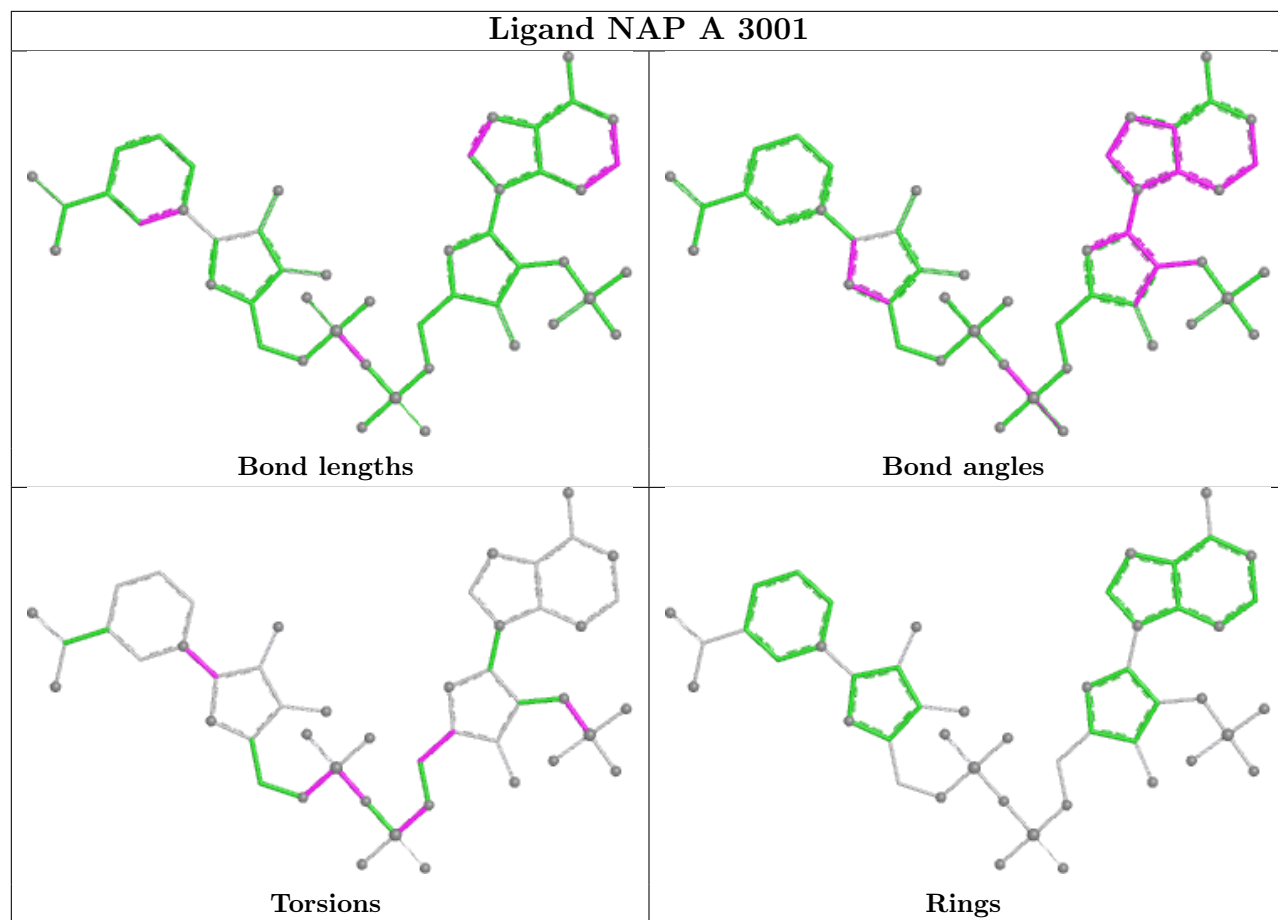
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3002	NAP	2	0
2	B	3001	NAP	2	0
2	A	3001	NAP	8	0
2	A	3002	NAP	4	0

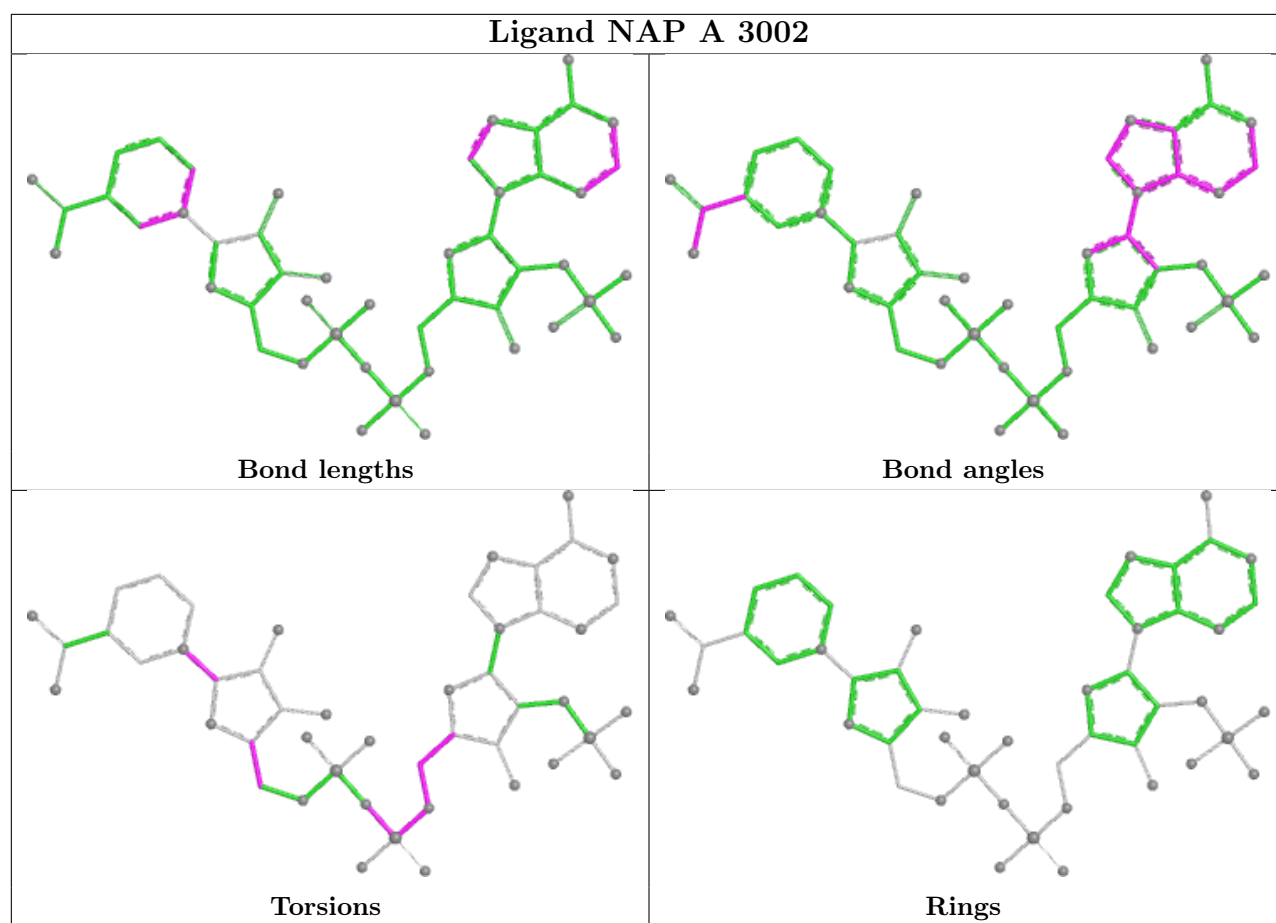
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	2081/2512 (82%)	-0.68	4 (0%)	91 86	73, 131, 230, 299	0
1	B	2086/2512 (83%)	-0.62	2 (0%)	92 90	72, 166, 228, 299	0
All	All	4167/5024 (82%)	-0.65	6 (0%)	92 90	72, 145, 229, 299	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1191	GLN	3.2
1	A	457	ILE	2.6
1	A	977	ASP	2.3
1	B	1475	SER	2.2
1	A	1312	ALA	2.2
1	A	427	SER	2.1

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

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

6.3 Carbohydrates [i](#)

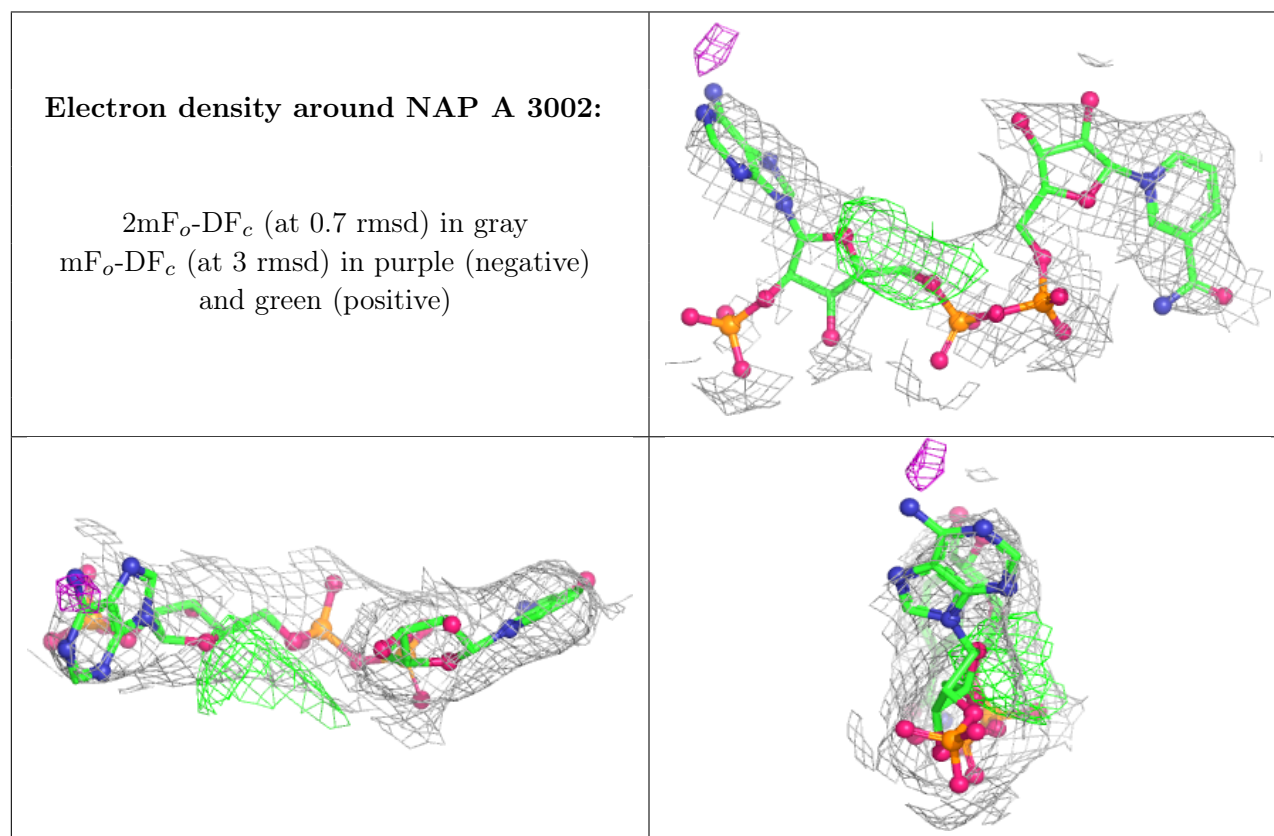
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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.

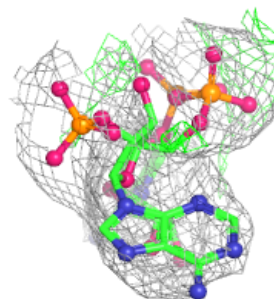
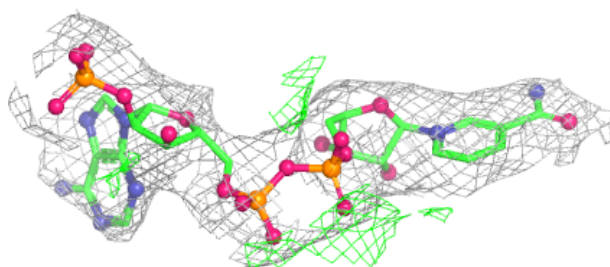
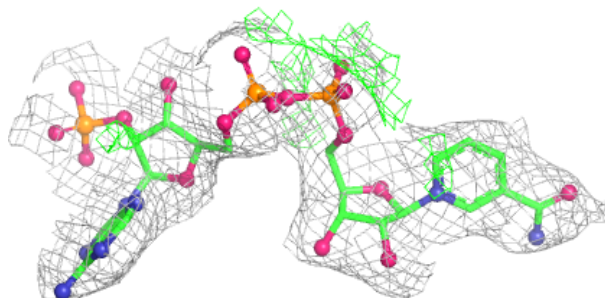
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	A	3002	48/48	0.95	0.07	96,135,161,194	0
2	NAP	A	3001	48/48	0.96	0.07	100,122,179,189	0
2	NAP	B	3001	48/48	0.96	0.06	99,123,160,163	0
2	NAP	B	3002	48/48	0.96	0.07	99,122,153,198	0

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.

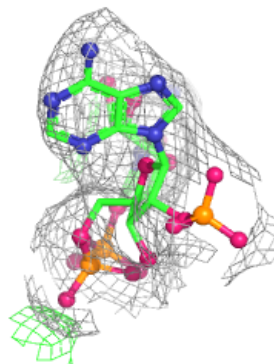
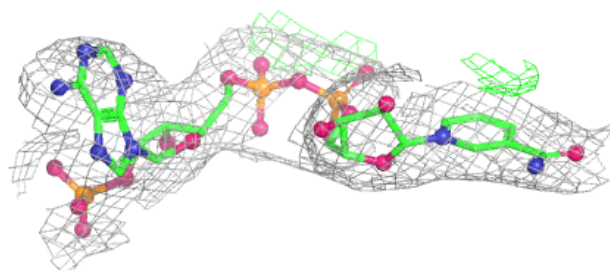
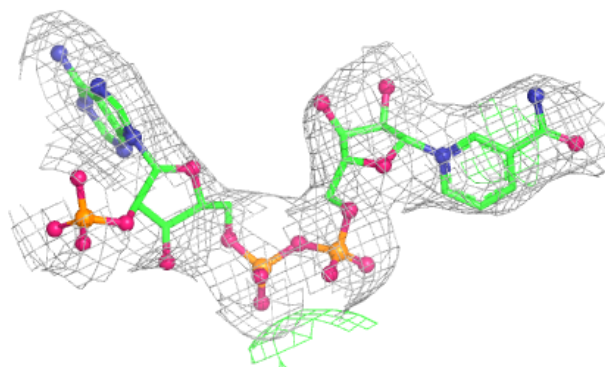


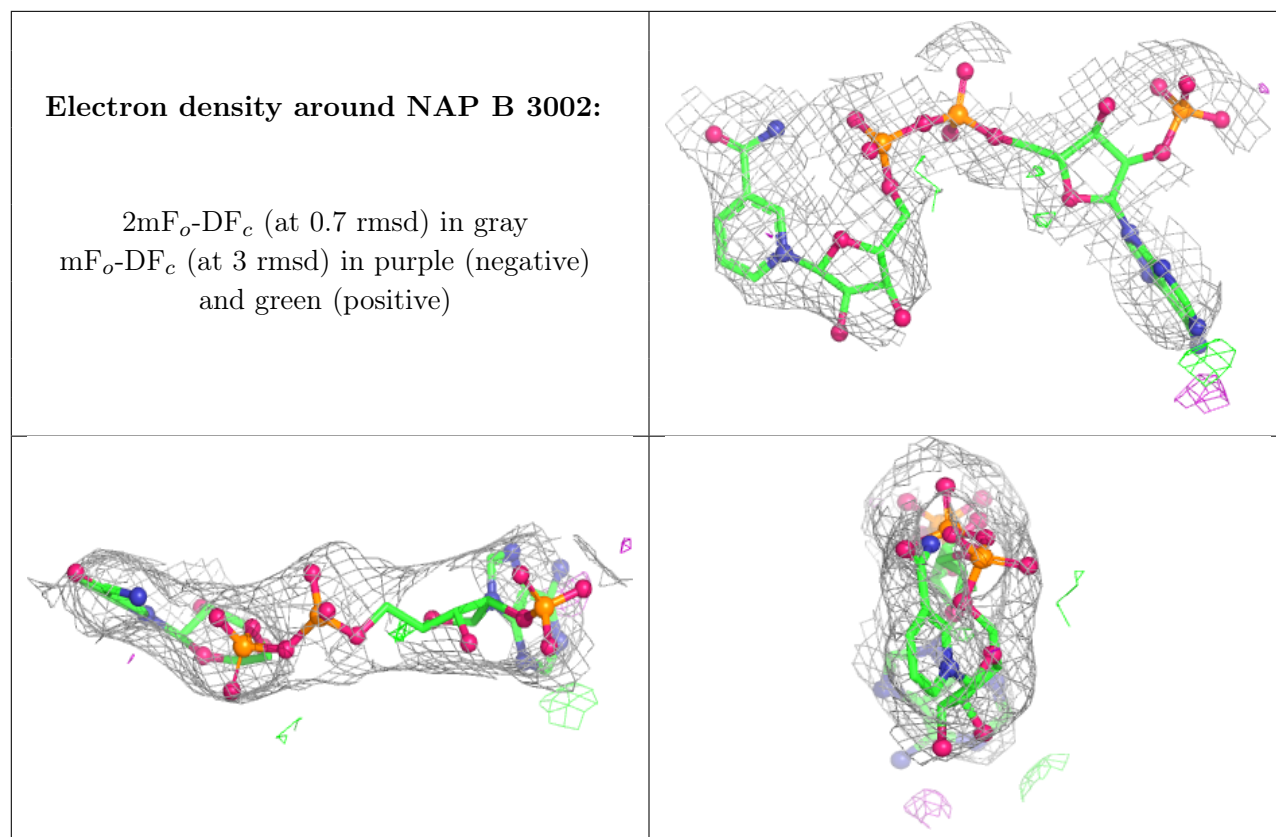
Electron density around NAP A 3001:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.