



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3T8L / pdb_00003t8l
Title : Crystal Structure of adenine deaminase with Mn/Fe
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Deposited on : 2011-08-01
Resolution : 2.80 Å(reported)

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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
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

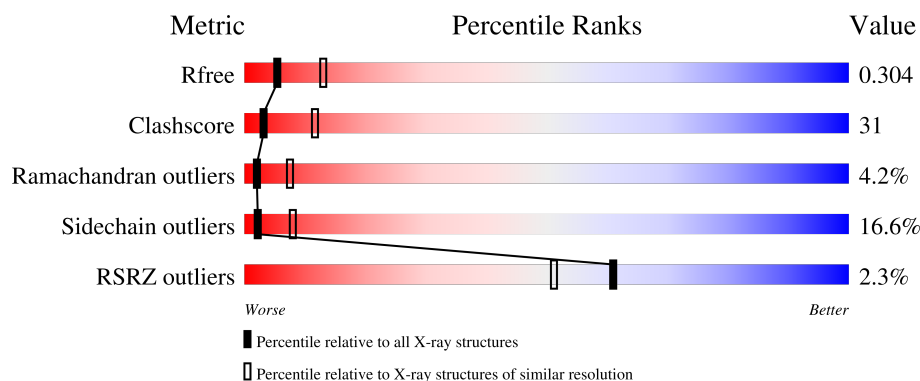
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

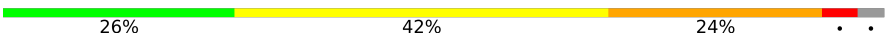
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	608	
1	B	608	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNX	A	606	-	-	-	X
2	UNX	A	607	-	-	-	X
2	UNX	A	608	-	-	-	X
2	UNX	B	607	-	-	-	X
2	UNX	B	608	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8761 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 Adenine deaminase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	Se	0	0	0
			4337	2723	775	817	6	16			
1	B	587	Total	C	N	O	S	Se	0	0	0
			4335	2721	775	817	6	16			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MSE	-	expression tag	UNP Q7CUX4
A	-1	SER	-	expression tag	UNP Q7CUX4
A	0	LEU	-	expression tag	UNP Q7CUX4
A	598	GLU	-	expression tag	UNP Q7CUX4
A	599	GLY	-	expression tag	UNP Q7CUX4
A	600	HIS	-	expression tag	UNP Q7CUX4
A	601	HIS	-	expression tag	UNP Q7CUX4
A	602	HIS	-	expression tag	UNP Q7CUX4
A	603	HIS	-	expression tag	UNP Q7CUX4
A	604	HIS	-	expression tag	UNP Q7CUX4
A	605	HIS	-	expression tag	UNP Q7CUX4
B	-2	MSE	-	expression tag	UNP Q7CUX4
B	-1	SER	-	expression tag	UNP Q7CUX4
B	0	LEU	-	expression tag	UNP Q7CUX4
B	598	GLU	-	expression tag	UNP Q7CUX4
B	599	GLY	-	expression tag	UNP Q7CUX4
B	600	HIS	-	expression tag	UNP Q7CUX4
B	601	HIS	-	expression tag	UNP Q7CUX4
B	602	HIS	-	expression tag	UNP Q7CUX4
B	603	HIS	-	expression tag	UNP Q7CUX4
B	604	HIS	-	expression tag	UNP Q7CUX4
B	605	HIS	-	expression tag	UNP Q7CUX4

- Molecule 2 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	X 3	0	0
2	B	3	Total 3	X 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total 33	O 33	0	0
3	B	50	Total 50	O 50	0	0

1570	G571	P572	H573	A509	T574	D576	M577	G505	H506	A507	V508	T510	H511	L512	P513	A514	H515	L516	T517	H518	L519	P520	A521	H522	L523	P524	A525	H526	L527	P528	A529	H530	L531	P532	A533	H534	L535	P536	A537	H538	L539	P540	A541	H542	L543	P544	A545	H546	L547	P548	A549	H550	L551	P552	A553	H554	L555	P556	A557	H558	L559	P560	A561	H562	L563	P564	A565	H566	L567	P568	A569	H570	L571	P572	A573	H574	L575	P576	A577	H578	L579	P580	A581	H582	L583	P584	A585	H586	L587	P588	A589	H590	L591	P592	A593	H594	L595	P596	A597	H598	L599	P600	A601	H602	L603	P604	A605	H606	L607	P608	A609	H610	L611	P612	A613	H614	L615	P616	A617	H618	L619	P620	A621	H622	L623	P624	A625	H626	L627	P628	A629	H630	L631	P632	A633	H634	L635	P636	A637	H638	L639	P640	A641	H642	L643	P644	A645	H646	L647	P648	A649	H650	L651	P652	A653	H654	L655	P656	A657	H658	L659	P660	A661	H662	L663	P664	A665	H666	L667	P668	A669	H670	L671	P672	A673	H674	L675	P676	A677	H678	L679	P680	A681	H682	L683	P684	A685	H686	L687	P688	A689	H690	L691	P692	A693	H694	L695	P696	A697	H698	L699	P700	A701	H702	L703	P704	A705	H706	L707	P708	A709	H710	L711	P712	A713	H714	L715	P716	A717	H718	L719	P720	A721	H722	L723	P724	A725	H726	L727	P728	A729	H730	L731	P732	A733	H734	L735	P736	A737	H738	L739	P740	A741	H742	L743	P744	A745	H746	L747	P748	A749	H750	L751	P752	A753	H754	L755	P756	A757	H758	L759	P760	A761	H762	L763	P764	A765	H766	L767	P768	A769	H770	L771	P772	A773	H774	L775	P776	A777	H778	L779	P780	A781	H782	L783	P784	A785	H786	L787	P788	A789	H790	L791	P792	A793	H794	L795	P796	A797	H798	L799	P800	A801	H802	L803	P804	A805	H806	L807	P808	A809	H810	L811	P812	A813	H814	L815	P816	A817	H818	L819	P820	A821	H822	L823	P824	A825	H826	L827	P828	A829	H830	L831	P832	A833	H834	L835	P836	A837	H838	L839	P840	A841	H842	L843	P844	A845	H846	L847	P848	A849	H850	L851	P852	A853	H854	L855	P856	A857	H858	L859	P860	A861	H862	L863	P864	A865	H866	L867	P868	A869	H870	L871	P872	A873	H874	L875	P876	A877	H878	L879	P880	A881	H882	L883	P884	A885	H886	L887	P888	A889	H890	L891	P892	A893	H894	L895	P896	A897	H898	L899	P900	A901	H902	L903	P904	A905	H906	L907	P908	A909	H910	L911	P912	A913	H914	L915	P916	A917	H918	L919	P920	A921	H922	L923	P924	A925	H926	L927	P928	A929	H930	L931	P932	A933	H934	L935	P936	A937	H938	L939	P940	A941	H942	L943	P944	A945	H946	L947	P948	A949	H950	L951	P952	A953	H954	L955	P956	A957	H958	L959	P960	A961	H962	L963	P964	A965	H966	L967	P968	A969	H970	L971	P972	A973	H974	L975	P976	A977	H978	L979	P980	A981	H982	L983	P984	A985	H986	L987	P988	A989	H990	L991	P992	A993	H994	L995	P996	A997	H998	L999	P1000	A1001	H1002	L1003	P1004	A1005	H1006	L1007	P1008	A1009	H1010	L1011	P1012	A1013	H1014	L1015	P1016	A1017	H1018	L1019	P1020	A1021	H1022	L1023	P1024	A1025	H1026	L1027	P1028	A1029	H1030	L1031	P1032	A1033	H1034	L1035	P1036	A1037	H1038	L1039	P1040	A1041	H1042	L1043	P1044	A1045	H1046	L1047	P1048	A1049	H1050	L1051	P1052	A1053	H1054	L1055	P1056	A1057	H1058	L1059	P1060	A1061	H1062	L1063	P1064	A1065	H1066	L1067	P1068	A1069	H1070	L1071	P1072	A1073	H1074	L1075	P1076	A1077	H1078	L1079	P1080	A1081	H1082	L1083	P1084	A1085	H1086	L1087	P1088	A1089	H1090	L1091	P1092	A1093	H1094	L1095	P1096	A1097	H1098	L1099	P1100	A1101	H1102	L1103	P1104	A1105	H1106	L1107	P1108	A1109	H1110	L1111	P1112	A1113	H1114	L1115	P1116	A1117	H1118	L1119	P1120	A1121	H1122	L1123	P1124	A1125	H1126	L1127	P1128	A1129	H1130	L1131	P1132	A1133	H1134	L1135	P1136	A1137	H1138	L1139	P1140	A1141	H1142	L1143	P1144	A1145	H1146	L1147	P1148	A1149	H1150	L1151	P1152	A1153	H1154	L1155	P1156	A1157	H1158	L1159	P1160	A1161	H1162	L1163	P1164	A1165	H1166	L1167	P1168	A1169	H1170	L1171	P1172	A1173	H1174	L1175	P1176	A1177	H1178	L1179	P1180	A1181	H1182	L1183	P1184	A1185	H1186	L1187	P1188	A1189	H1190	L1191	P1192	A1193	H1194	L1195	P1196	A1197	H1198	L1199	P1200	A1201	H1202	L1203	P1204	A1205	H1206	L1207	P1208	A1209	H1210	L1211	P1212	A1213	H1214	L1215	P1216	A1217	H1218	L1219	P1220	A1221	H1222	L1223	P1224	A1225	H1226	L1227	P1228	A1229	H1230	L1231	P1232	A1233	H1234	L1235	P1236	A1237	H1238	L1239	P1240	A1241	H1242	L1243	P1244	A1245	H1246	L1247	P1248	A1249	H1250	L1251	P1252	A1253	H1254	L1255	P1256	A1257	H1258	L1259	P1260	A1261	H1262	L1263	P1264	A1265	H1266	L1267	P1268	A1269	H1270	L1271	P1272	A1273	H1274	L1275	P1276	A1277	H1278	L1279	P1280	A1281	H1282	L1283	P1284	A1285	H1286	L1287	P1288	A1289	H1290	L1291	P1292	A1293	H1294	L1295	P1296	A1297	H1298	L1299	P1300	A1301	H1302	L1303	P1304	A1305	H1306	L1307	P1308	A1309	H1310	L1311	P1312	A1313	H1314	L1315	P1316	A1317	H1318	L1319	P1320	A1321	H1322	L1323	P1324	A1325	H1326	L1327	P1328	A1329	H1330	L1331	P1332	A1333	H1334	L1335	P1336	A1337	H1338	L1339	P1340	A1341	H1342	L1343	P1344	A1345	H1346	L1347	P1348	A1349	H1350	L1351	P1352	A1353	H1354	L1355	P1356	A1357	H1358	L1359	P1360	A1361	H1362	L1363	P1364	A1365	H1366	L1367	P1368	A1369	H1370	L1371	P1372	A1373	H1374	L1375	P1376	A1377	H1378	L1379	P1380	A1381	H1382	L1383	P1384	A1385	H1386	L1387	P1388	A1389	H1390	L1391	P1392	A1393	H1394	L1395	P1396	A1397	H1398	L1399	P1400	A1401	H1402	L1403	P1404	A1405	H1406	L1407	P1408	A1409	H1410	L1411	P1412	A1413	H1414	L1415	P1416	A1417	H1418	L1419	P1420	A1421	H1422	L1423	P1424	A1425	H1426	L1427	P1428	A1429	H1430	L1431	P1432	A1433	H1434	L1435	P1436	A1437	H1438	L1439	P1440	A1441	H1442	L1443	P1444	A1445	H1446	L1447	P1448	A1449	H1450	L1451	P1452	A1453	H1454	L1455	P1456	A1457	H1458	L1459	P1460	A1461	H1462	L1463	P1464	A1465	H1466	L1467	P1468	A1469	H1470	L1471	P1472	A1473	H1474	L1475	P1476	A1477	H1478	L1479	P1480	A1481	H1482	L1483	P1484	A1485	H1486	L1487	P1488	A1489	H1490	L1491	P1492	A1493	H1494	L1495	P1496	A1497	H1498	L1499	P1500	A1501	H1502	L1503	P1504	A1505	H1506	L1507	P1508	A1509	H1510	L1511	P1512	A1513	H1514	L1515	P1516	A1517	H1518	L1519	P1520	A1521	H1522	L1523	P1524	A1525	H1526	L1527	P1528	A1529	H1530	L1531	P1532	A1533	H1534	L1535	P1536	A1537	H1538	L1539	P1540	A1541	H1542	L1543	P1544	A1545	H1546	L1547	P1548	A1549	H1550	L1551	P1552	A1553	H1554	L1555	P1556	A1557	H1558	L1559	P1560	A1561	H1562	L1563	P1564	A1565	H1566	L1567	P1568	A1569	H1570	L1571	P1572	A1573	H1574	L1575	P1576	A1577	H1578	L1579	P1580	A1581	H1582	L1583	P1584	A1585	H1586	L1587	P1588	A1589	H1590	L1591	P1592	A1593	H1594	L1595	P1596	A1597	H1598	L1599	P1600	A1601	H1602	L1603	P1604	A1605	H1606	L1607	P1608	A1609	H1610	L1611	P1612	A1613	H1614	L1615	P1616	A1617	H1618	L1619	P1620	A1621	H1622	L1623	P1624	A1625	H1626	L1627	P1628	A1629	H1630	L1631	P1632	A1633	H1634	L1635	P1636	A1637	H1638	L1639	P1640	A1641	H1642	L1643	P1644	A1645	H1646	L1647	P1648	A1649	H1650	L1651	P1652	A1653	H1654	L1655	P1656	A1657	H1658	L1659	P1660	A1661	H1662	L1663	P1664	A1665	H1666	L1667	P1668	A1669	H1670	L1671	P1672	A1673	H1674	L1675	P1676	A1677	H1678	L1679	P1680	A1681	H1682	L1683	P1684	A1685	H1686	L1687	P1688	A1689	H1690	L1691	P1692	A1693	H1694	L1695	P1696	A1697	H1698	L1699	P1700	A1701	H1702	L1703	P1704	A1705	H1706	L1707	P1708	A1709	H1710	L1711	P1712	A1713	H1714	L1715	P1716	A1717	H1718	L1719	P1720	A1721	H1722	L1723	P1724	A1725	H1726	L1727	P1728	A1729	H1730	L1731	P1732	A1733	H1734	L1735	P1736	A1737	H1738	L1739	P1740	A1741	H1742	L1743	P1744	A1745	H1746	L1747	P1748	A1749	H1750	L1751	P1752	A1753	H1754	L1755	P1756	A1757	H1758	L1759	P1760	A1761	H1762	L1763	P1764	A1765	H1766	L1767	P1768	A1769	H1770	L1771	P1772	A1773	H1774	L1775	P1776	A1777	H1778	L1779	P1780	A1781	H1782	L1783	P1784	A1785	H1786	L1787	P1788	A1789	H1790	L1791	P1792	A1793	H1794	L1795	P1796	A1797	H1798	L1799	P1800	A1801	H1802	L1803	P1804	A1805	H1806	L1807	P1808	A1809	H1810	L1811	P1812	A1813	H1814	L1815	P1816	A1817	H1818	L1819	P1820	A1821	H1822	L1823	P1824	A1825	H1826	L1827	P1828	A1829	H1830	L1831	P1832	A1833	H1834	L1835	P1836	A1837	H1838	L1839	P1840	A1841	H1842	L1843	P1844	A1845	H1846	L1847	P1848	A1849	H1850	L1851	P1852	A1853	H1854	L1855	P1856	A1857	H1858	L1859	P1860	A1861	H1862	L1863	P1864	A1865	H1866	L1867	P1868	A1869	H1870	L1871	P1872	A1873	H1874	L1875	P1876	A1877	H1878	L1879	P1880	A1881	H1882	L1883	P1884	A1885	H1886	L1887	P1888	A1889	H1890	L1891	P1892	A1893	H1894	L1895	P1896	A1897	H1898	L1899	P1900	A1901	H1902	L1903	P1904	A1905	H1906	L1907	P1908	A1909	H1910	L1911	P1912	A1913	H191
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.54Å 131.17Å 69.28Å 90.00° 97.04° 90.00°	Depositor
Resolution (Å)	48.73 – 2.80 48.73 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.73-2.80) 99.7 (48.73-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.301 0.182 , 0.304	Depositor DCC
R_{free} test set	1362 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8761	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: UNX

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	2.66	265/4402 (6.0%)	2.19	191/5964 (3.2%)
1	B	2.53	231/4400 (5.2%)	2.17	191/5961 (3.2%)
All	All	2.59	496/8802 (5.6%)	2.18	382/11925 (3.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	6
All	All	0	8

All (496) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	451	MSE	SE-CE	24.10	2.67	1.95
1	A	396	MSE	SE-CE	23.09	2.64	1.95
1	B	189	MSE	SE-CE	22.53	2.63	1.95
1	A	189	MSE	SE-CE	22.34	2.62	1.95
1	B	191	MSE	SE-CE	19.62	2.54	1.95
1	B	396	MSE	SE-CE	19.30	2.53	1.95
1	A	577	MSE	SE-CE	17.32	2.47	1.95
1	A	99	MSE	SE-CE	17.07	2.46	1.95
1	B	451	MSE	SE-CE	16.07	2.43	1.95
1	B	201	MSE	SE-CE	13.44	2.35	1.95
1	A	588	MSE	SE-CE	13.09	2.34	1.95
1	A	248	MSE	SE-CE	12.65	2.33	1.95
1	B	588	MSE	SE-CE	12.38	2.32	1.95
1	B	127	VAL	C-O	-11.79	1.12	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	231	MSE	SE-CE	11.51	2.29	1.95
1	A	233	ALA	CA-CB	-11.40	1.34	1.53
1	A	582	VAL	CA-CB	-11.18	1.40	1.54
1	A	319	ALA	CA-CB	-10.97	1.36	1.53
1	A	163	ARG	CZ-NH1	10.96	1.48	1.32
1	A	52	ALA	CA-CB	-10.69	1.35	1.53
1	B	248	MSE	SE-CE	10.69	2.27	1.95
1	A	174	ALA	N-CA	10.63	1.59	1.46
1	A	201	MSE	SE-CE	10.60	2.27	1.95
1	A	548	VAL	CA-CB	10.57	1.67	1.54
1	B	442	MSE	SE-CE	10.55	2.27	1.95
1	B	254	GLY	C-O	-10.45	1.10	1.24
1	B	355	GLY	C-O	9.88	1.37	1.23
1	B	280	LEU	C-O	-9.82	1.11	1.24
1	B	188	ILE	N-CA	-9.49	1.33	1.46
1	A	593	ILE	CA-C	9.44	1.64	1.52
1	B	390	MSE	SE-CE	9.38	2.23	1.95
1	A	137	ALA	CA-CB	-9.25	1.38	1.53
1	B	584	THR	CA-CB	9.14	1.69	1.53
1	A	208	GLY	N-CA	-9.12	1.34	1.45
1	A	374	MSE	SE-CE	9.09	2.22	1.95
1	B	420	THR	N-CA	9.04	1.56	1.45
1	A	514	VAL	CA-CB	9.02	1.65	1.54
1	B	171	ALA	CA-CB	9.02	1.67	1.53
1	B	409	VAL	N-CA	8.97	1.56	1.46
1	A	560	ALA	CA-CB	-8.93	1.38	1.53
1	A	103	ALA	CA-CB	8.77	1.67	1.53
1	B	147	ALA	C-O	-8.66	1.14	1.24
1	A	592	VAL	CA-CB	8.64	1.64	1.53
1	A	56	ILE	CA-CB	8.57	1.66	1.54
1	A	129	GLY	C-O	8.48	1.35	1.23
1	B	135	TRP	C-O	8.45	1.33	1.24
1	B	211	ALA	CA-CB	-8.39	1.39	1.53
1	A	509	ALA	CA-C	8.38	1.63	1.52
1	A	64	VAL	C-O	8.33	1.33	1.24
1	B	434	VAL	CA-CB	8.28	1.65	1.54
1	B	24	ALA	CA-CB	-8.26	1.40	1.53
1	A	328	ALA	CA-CB	-8.24	1.40	1.53
1	A	320	LEU	C-O	8.11	1.33	1.24
1	A	41	LEU	N-CA	-8.11	1.35	1.46
1	A	54	ILE	CA-CB	8.06	1.65	1.54
1	B	344	ARG	C-O	-8.06	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	GLY	C-O	8.00	1.36	1.24
1	B	64	VAL	CA-CB	7.99	1.64	1.54
1	A	40	THR	C-O	7.95	1.33	1.24
1	A	208	GLY	C-O	7.90	1.33	1.23
1	B	235	VAL	C-O	7.89	1.32	1.24
1	A	131	ASP	C-O	7.84	1.33	1.24
1	B	174	ALA	CA-CB	-7.80	1.40	1.53
1	B	202	SER	C-O	-7.79	1.15	1.24
1	B	307	ARG	C-O	7.74	1.32	1.24
1	B	207	ALA	CA-CB	-7.72	1.40	1.53
1	B	24	ALA	C-O	7.72	1.32	1.24
1	A	20	ALA	N-CA	7.71	1.55	1.46
1	A	329	GLN	CD-NE2	7.69	1.49	1.33
1	A	36	ILE	CA-C	-7.66	1.43	1.52
1	A	225	ALA	CA-CB	-7.65	1.41	1.53
1	B	52	ALA	CA-CB	-7.65	1.41	1.53
1	B	31	ARG	CZ-NH2	7.64	1.43	1.33
1	A	588	MSE	CA-C	7.63	1.61	1.53
1	B	593	ILE	CA-CB	7.59	1.64	1.54
1	A	105	TYR	C-O	-7.59	1.15	1.24
1	A	166	ALA	CA-CB	7.58	1.68	1.54
1	B	290	ASP	N-CA	7.58	1.55	1.46
1	B	148	ILE	CA-CB	7.56	1.63	1.54
1	B	141	GLU	CD-OE2	7.56	1.39	1.25
1	A	148	ILE	C-O	-7.52	1.16	1.24
1	A	185	ILE	CA-CB	-7.51	1.45	1.54
1	B	17	THR	CA-CB	7.48	1.65	1.53
1	A	216	CYS	CA-C	-7.47	1.44	1.52
1	B	496	ALA	CA-CB	-7.43	1.41	1.53
1	B	113	GLY	C-O	7.42	1.34	1.24
1	B	236	SER	CA-CB	-7.38	1.42	1.53
1	A	385	VAL	CB-CG1	7.38	1.76	1.52
1	A	231	MSE	SE-CE	7.37	2.17	1.95
1	A	424	GLU	C-O	7.36	1.32	1.23
1	B	354	ASN	CA-C	7.35	1.59	1.52
1	A	390	MSE	CG-SE	7.34	2.17	1.95
1	B	110	VAL	CA-CB	-7.33	1.45	1.54
1	A	207	ALA	C-O	7.33	1.32	1.24
1	B	382	ASP	CA-C	7.32	1.62	1.52
1	A	304	ASP	C-O	7.32	1.32	1.24
1	A	171	ALA	C-O	7.29	1.32	1.24
1	B	11	ALA	CA-CB	-7.27	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249	ALA	CA-CB	-7.27	1.41	1.53
1	B	175	ASP	N-CA	7.26	1.55	1.46
1	A	172	ILE	CA-CB	7.26	1.63	1.54
1	B	151	ALA	CA-CB	-7.23	1.42	1.53
1	B	201	MSE	CG-SE	7.21	2.17	1.95
1	B	88	LEU	C-O	7.16	1.33	1.23
1	A	215	VAL	C-O	7.14	1.32	1.24
1	A	557	VAL	CA-C	7.14	1.61	1.52
1	B	9	GLU	CA-C	-7.14	1.42	1.52
1	A	267	LEU	CA-CB	-7.13	1.43	1.53
1	B	544	ALA	CA-C	7.11	1.62	1.52
1	B	257	ILE	CA-CB	-7.10	1.45	1.54
1	B	516	ALA	CA-C	-7.10	1.43	1.52
1	B	76	VAL	C-O	-7.07	1.16	1.24
1	B	384	THR	N-CA	7.04	1.54	1.46
1	B	518	LEU	N-CA	-7.04	1.38	1.46
1	A	269	GLU	N-CA	-7.03	1.38	1.46
1	A	100	ILE	C-O	-7.02	1.16	1.23
1	A	93	MSE	N-CA	-7.01	1.37	1.46
1	B	66	GLU	CA-C	7.01	1.61	1.53
1	A	76	VAL	CA-C	-7.00	1.44	1.52
1	A	220	ARG	C-O	7.00	1.32	1.23
1	A	34	VAL	C-O	7.00	1.31	1.23
1	B	37	THR	CA-C	-6.99	1.44	1.52
1	B	195	ILE	CA-CB	-6.97	1.46	1.54
1	B	353	LEU	C-O	-6.96	1.13	1.23
1	A	535	ALA	C-O	6.95	1.32	1.24
1	A	183	GLY	C-N	6.93	1.39	1.33
1	A	471	PHE	C-O	-6.93	1.15	1.23
1	A	192	ARG	CG-CD	6.92	1.73	1.52
1	A	253	ALA	CA-CB	-6.92	1.41	1.53
1	B	222	LEU	CA-C	6.92	1.61	1.52
1	B	346	ASP	CA-C	6.91	1.61	1.52
1	A	562	PHE	C-O	6.83	1.33	1.24
1	B	165	GLY	N-CA	6.83	1.55	1.45
1	B	306	VAL	CA-C	6.83	1.61	1.52
1	A	594	GLU	N-CA	6.80	1.56	1.46
1	A	80	GLY	N-CA	6.79	1.55	1.45
1	A	270	PHE	C-O	6.78	1.31	1.24
1	A	170	ALA	CA-CB	-6.76	1.42	1.53
1	A	287	CYS	N-CA	-6.76	1.37	1.45
1	A	579	ILE	C-O	6.75	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	LYS	CG-CD	6.72	1.72	1.52
1	A	212	GLU	CG-CD	6.72	1.68	1.52
1	A	213	LYS	C-O	6.69	1.32	1.23
1	A	147	ALA	N-CA	6.69	1.54	1.46
1	B	202	SER	N-CA	-6.69	1.38	1.46
1	B	535	ALA	N-CA	6.67	1.54	1.46
1	A	311	ARG	CD-NE	6.65	1.55	1.46
1	A	133	VAL	C-O	-6.64	1.16	1.24
1	B	25	ALA	CA-C	-6.64	1.44	1.52
1	A	488	ASN	N-CA	6.64	1.54	1.46
1	B	533	GLU	CA-C	-6.62	1.43	1.52
1	A	518	LEU	CA-C	6.61	1.60	1.52
1	B	409	VAL	CA-CB	6.61	1.64	1.55
1	A	108	ALA	CA-CB	-6.60	1.42	1.53
1	A	472	ALA	CA-CB	-6.60	1.44	1.53
1	A	545	VAL	N-CA	-6.59	1.38	1.46
1	B	294	ASP	CA-C	6.59	1.61	1.52
1	A	358	ALA	CA-CB	6.58	1.61	1.53
1	B	232	ALA	CA-CB	6.57	1.64	1.53
1	B	577	MSE	SE-CE	6.55	2.15	1.95
1	A	169	ASP	CA-C	6.54	1.62	1.53
1	A	155	VAL	CA-C	6.54	1.58	1.53
1	B	25	ALA	CA-CB	-6.54	1.43	1.53
1	B	119	TRP	CA-CB	-6.53	1.44	1.53
1	B	174	ALA	N-CA	-6.53	1.38	1.46
1	B	128	HIS	CA-C	6.52	1.60	1.52
1	A	220	ARG	CA-C	6.51	1.61	1.52
1	B	297	LEU	CA-C	-6.50	1.46	1.53
1	B	231	MSE	CG-SE	6.50	2.15	1.95
1	A	489	ALA	CA-C	6.49	1.61	1.52
1	A	499	VAL	C-O	-6.49	1.15	1.24
1	A	354	ASN	CG-OD1	6.49	1.35	1.23
1	A	428	ASP	CA-C	-6.46	1.43	1.53
1	A	532	GLU	CD-OE1	6.46	1.37	1.25
1	A	82	ALA	CA-CB	6.45	1.64	1.53
1	B	451	MSE	CA-C	-6.45	1.44	1.52
1	A	492	MSE	SE-CE	6.44	2.14	1.95
1	B	535	ALA	CA-CB	-6.44	1.43	1.53
1	B	570	ILE	CA-CB	6.44	1.62	1.54
1	A	195	ILE	CA-CB	-6.43	1.46	1.54
1	A	444	SER	C-O	6.42	1.31	1.24
1	B	188	ILE	CA-C	-6.42	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	390	MSE	CA-C	-6.42	1.44	1.53
1	A	116	THR	C-O	6.41	1.31	1.23
1	B	11	ALA	CA-C	6.41	1.61	1.52
1	B	28	GLY	CA-C	6.39	1.60	1.51
1	A	335	ASP	N-CA	-6.39	1.37	1.46
1	A	514	VAL	C-O	-6.39	1.16	1.24
1	A	442	MSE	CA-C	-6.37	1.44	1.52
1	A	295	ASP	C-O	6.37	1.31	1.24
1	A	53	ASP	N-CA	-6.37	1.37	1.45
1	A	207	ALA	CA-C	6.37	1.61	1.52
1	B	61	ILE	N-CA	-6.37	1.39	1.46
1	B	310	VAL	C-O	-6.37	1.17	1.24
1	A	177	LEU	N-CA	6.34	1.54	1.46
1	B	16	ASP	C-O	6.34	1.32	1.24
1	B	134	ARG	CZ-NH1	6.34	1.41	1.32
1	B	303	ASP	N-CA	6.34	1.54	1.46
1	B	265	HIS	N-CA	6.33	1.54	1.46
1	A	148	ILE	CA-CB	-6.33	1.46	1.54
1	A	484	VAL	CA-CB	6.32	1.64	1.55
1	B	62	ALA	CA-CB	-6.30	1.43	1.53
1	A	324	THR	N-CA	-6.30	1.38	1.46
1	A	442	MSE	CA-CB	-6.30	1.43	1.53
1	B	225	ALA	CA-CB	6.29	1.64	1.53
1	A	326	ASN	C-O	6.29	1.31	1.24
1	A	477	HIS	CA-CB	-6.29	1.42	1.53
1	A	500	ILE	N-CA	-6.28	1.39	1.46
1	A	231	MSE	N-CA	-6.28	1.38	1.46
1	A	194	VAL	CA-CB	6.27	1.61	1.54
1	A	421	GLN	N-CA	6.27	1.53	1.46
1	B	292	PHE	CA-C	-6.25	1.46	1.53
1	B	542	ARG	CZ-NH2	6.25	1.41	1.33
1	B	246	ASP	CA-C	6.24	1.60	1.52
1	A	9	GLU	N-CA	6.24	1.58	1.46
1	B	445	VAL	N-CA	-6.22	1.38	1.46
1	B	248	MSE	CG-SE	6.21	2.14	1.95
1	B	218	HIS	CA-CB	6.21	1.61	1.52
1	A	586	LYS	N-CA	-6.21	1.38	1.46
1	A	351	GLU	C-O	-6.20	1.17	1.24
1	B	21	ARG	CZ-NH2	6.20	1.41	1.33
1	A	31	ARG	N-CA	-6.19	1.38	1.45
1	A	114	VAL	CA-CB	-6.19	1.46	1.53
1	B	439	GLY	C-O	6.18	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	525	LEU	N-CA	-6.18	1.37	1.46
1	A	361	VAL	CA-CB	6.17	1.62	1.54
1	B	155	VAL	N-CA	6.17	1.52	1.46
1	B	197	ARG	CZ-NH2	6.16	1.41	1.33
1	B	73	ALA	N-CA	6.16	1.53	1.45
1	B	242	VAL	C-O	6.16	1.31	1.24
1	B	99	MSE	SE-CE	6.15	2.13	1.95
1	A	575	THR	N-CA	6.15	1.54	1.45
1	B	273	ALA	C-O	6.14	1.31	1.24
1	A	92	HIS	CA-C	-6.14	1.44	1.52
1	B	255	LEU	C-O	6.13	1.31	1.23
1	A	259	LEU	CG-CD1	-6.12	1.32	1.52
1	A	225	ALA	C-O	6.12	1.32	1.24
1	B	474	THR	N-CA	-6.12	1.37	1.46
1	A	186	ALA	C-O	-6.12	1.15	1.23
1	A	167	ASP	CA-C	6.11	1.59	1.52
1	B	306	VAL	C-O	6.11	1.31	1.24
1	A	80	GLY	C-O	6.09	1.32	1.23
1	B	169	ASP	N-CA	6.09	1.53	1.45
1	A	595	VAL	CA-CB	6.08	1.70	1.54
1	A	544	ALA	CA-C	6.08	1.60	1.52
1	B	580	ALA	C-O	6.07	1.31	1.23
1	A	386	LEU	N-CA	-6.07	1.38	1.46
1	B	582	VAL	C-O	6.07	1.29	1.24
1	B	342	GLY	C-O	-6.07	1.15	1.24
1	A	304	ASP	N-CA	-6.07	1.38	1.46
1	A	379	PRO	N-CA	-6.07	1.39	1.47
1	B	301	GLY	C-O	-6.06	1.17	1.24
1	A	334	SER	N-CA	6.05	1.54	1.46
1	B	274	LEU	C-O	-6.05	1.16	1.24
1	A	27	ARG	C-O	-6.05	1.16	1.24
1	A	280	LEU	C-N	6.04	1.41	1.33
1	A	32	PHE	C-O	-6.04	1.16	1.23
1	A	321	ARG	CA-C	-6.04	1.45	1.52
1	A	443	ILE	N-CA	-6.02	1.38	1.46
1	B	322	ALA	N-CA	-6.01	1.38	1.46
1	B	200	ARG	C-O	-6.01	1.17	1.24
1	B	54	ILE	N-CA	-6.00	1.39	1.46
1	A	218	HIS	CA-C	-6.00	1.45	1.52
1	A	393	PRO	CB-CG	6.00	1.79	1.49
1	B	406	GLY	C-O	6.00	1.29	1.23
1	B	494	LEU	CA-C	-5.99	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	462	THR	C-O	5.99	1.31	1.24
1	A	76	VAL	CA-CB	-5.98	1.46	1.54
1	B	83	TYR	CA-C	-5.97	1.45	1.52
1	A	495	ALA	C-O	-5.97	1.16	1.24
1	B	245	GLU	CG-CD	5.96	1.67	1.52
1	B	517	ILE	CA-CB	5.96	1.62	1.54
1	B	71	ARG	C-O	-5.96	1.16	1.24
1	B	294	ASP	N-CA	5.95	1.53	1.46
1	A	326	ASN	N-CA	-5.93	1.39	1.46
1	A	207	ALA	CA-CB	5.92	1.62	1.53
1	A	333	ARG	C-O	-5.92	1.17	1.23
1	A	534	VAL	C-O	5.91	1.31	1.24
1	B	318	TRP	N-CA	-5.91	1.39	1.46
1	B	536	ARG	C-O	5.91	1.31	1.24
1	B	374	MSE	SE-CE	5.91	2.13	1.95
1	B	189	MSE	CG-SE	5.90	2.13	1.95
1	B	246	ASP	C-O	5.90	1.30	1.24
1	A	593	ILE	C-N	5.89	1.39	1.33
1	B	570	ILE	CB-CG2	5.89	1.72	1.52
1	A	250	LYS	C-O	5.88	1.31	1.24
1	B	248	MSE	CA-C	-5.88	1.44	1.52
1	A	271	VAL	C-O	5.87	1.31	1.24
1	B	139	ALA	CA-CB	-5.86	1.44	1.53
1	A	279	HIS	C-O	-5.86	1.16	1.23
1	A	421	GLN	CA-C	-5.85	1.45	1.52
1	B	111	ALA	CA-CB	-5.85	1.42	1.53
1	B	517	ILE	C-O	5.85	1.31	1.24
1	A	59	ALA	CA-C	5.84	1.60	1.52
1	B	537	ALA	CA-CB	-5.84	1.44	1.53
1	A	15	ASP	CG-OD2	5.83	1.36	1.25
1	A	235	VAL	C-O	-5.83	1.16	1.24
1	A	68	ALA	CA-CB	5.82	1.63	1.53
1	B	435	VAL	CB-CG2	5.82	1.71	1.52
1	A	130	VAL	CB-CG1	5.82	1.71	1.52
1	A	155	VAL	CA-CB	5.80	1.59	1.53
1	B	41	LEU	C-O	5.80	1.31	1.23
1	B	559	LYS	CG-CD	5.80	1.69	1.52
1	B	455	THR	CA-CB	5.79	1.61	1.53
1	B	264	ASP	C-O	-5.77	1.17	1.24
1	A	63	SER	C-O	5.77	1.31	1.23
1	A	570	ILE	C-O	5.77	1.30	1.24
1	B	386	LEU	N-CA	5.77	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	ILE	C-O	5.76	1.29	1.23
1	A	559	LYS	CG-CD	5.76	1.69	1.52
1	B	548	VAL	CA-CB	5.75	1.61	1.54
1	B	351	GLU	C-O	-5.75	1.17	1.24
1	A	213	LYS	N-CA	-5.75	1.38	1.45
1	B	347	ILE	CA-CB	-5.75	1.46	1.55
1	B	593	ILE	CA-C	5.73	1.60	1.52
1	B	336	LEU	CG-CD2	5.73	1.71	1.52
1	B	243	SER	N-CA	-5.71	1.38	1.45
1	A	51	PRO	CA-C	-5.71	1.45	1.52
1	A	504	GLY	C-O	5.70	1.31	1.23
1	A	232	ALA	C-O	-5.69	1.17	1.24
1	B	122	HIS	C-O	-5.68	1.16	1.24
1	A	572	PRO	CA-C	5.67	1.59	1.52
1	A	341	ALA	N-CA	-5.67	1.38	1.46
1	A	387	LYS	N-CA	5.66	1.52	1.45
1	A	513	LYS	CA-C	5.66	1.59	1.52
1	B	327	ALA	CA-C	-5.66	1.45	1.52
1	B	328	ALA	CA-CB	-5.66	1.44	1.53
1	B	271	VAL	CA-CB	-5.66	1.46	1.54
1	B	329	GLN	CD-NE2	5.65	1.45	1.33
1	A	73	ALA	CA-C	5.65	1.58	1.52
1	B	394	LEU	CA-C	-5.64	1.45	1.52
1	A	506	MSE	CA-C	-5.64	1.45	1.52
1	A	149	LEU	CA-C	-5.63	1.45	1.52
1	A	366	ARG	N-CA	5.63	1.52	1.46
1	A	348	VAL	CB-CG1	-5.63	1.33	1.52
1	A	192	ARG	C-O	-5.63	1.17	1.24
1	B	161	LEU	CA-C	5.62	1.60	1.52
1	A	178	SER	CA-C	5.62	1.60	1.52
1	A	522	LEU	CG-CD1	-5.62	1.34	1.52
1	A	583	LEU	N-CA	5.61	1.53	1.46
1	A	22	ALA	C-O	5.61	1.31	1.24
1	A	344	ARG	CZ-NH2	-5.60	1.26	1.33
1	A	237	SER	N-CA	5.60	1.53	1.46
1	A	487	GLY	C-O	-5.60	1.16	1.24
1	A	71	ARG	NE-CZ	5.59	1.39	1.33
1	A	48	GLU	C-O	5.59	1.30	1.23
1	A	323	ALA	CA-CB	-5.59	1.43	1.53
1	B	240	GLU	C-O	-5.59	1.17	1.23
1	A	226	ASP	CA-C	-5.58	1.45	1.52
1	A	343	ARG	C-O	5.58	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	ASP	CA-C	-5.58	1.46	1.52
1	A	21	ARG	CZ-NH1	5.56	1.40	1.32
1	A	338	LEU	CA-C	-5.55	1.45	1.52
1	B	213	LYS	C-O	5.55	1.30	1.23
1	B	381	CYS	CA-C	-5.54	1.46	1.52
1	B	396	MSE	CA-C	-5.54	1.45	1.52
1	A	179	TRP	CA-C	5.53	1.59	1.52
1	B	150	LEU	N-CA	-5.53	1.39	1.45
1	B	227	LEU	CA-C	5.53	1.59	1.52
1	B	183	GLY	C-O	5.53	1.31	1.23
1	A	131	ASP	CA-CB	-5.53	1.44	1.53
1	B	108	ALA	CA-C	5.52	1.60	1.52
1	B	461	LEU	C-O	5.52	1.30	1.24
1	A	492	MSE	N-CA	-5.51	1.39	1.46
1	A	403	LYS	CG-CD	5.51	1.69	1.52
1	B	13	LEU	N-CA	5.50	1.53	1.46
1	A	350	PHE	CD1-CE1	5.50	1.55	1.38
1	B	507	ALA	CA-CB	5.50	1.62	1.53
1	B	493	ALA	C-O	5.50	1.31	1.24
1	A	185	ILE	C-O	5.49	1.30	1.24
1	B	376	VAL	N-CA	5.47	1.52	1.46
1	B	298	GLN	CA-C	5.47	1.59	1.52
1	A	173	LEU	CA-C	-5.47	1.45	1.52
1	B	220	ARG	CA-C	5.47	1.60	1.52
1	A	133	VAL	CA-C	-5.47	1.45	1.53
1	A	64	VAL	CA-C	-5.46	1.45	1.52
1	A	35	LEU	CA-C	-5.46	1.45	1.52
1	A	311	ARG	CA-C	5.46	1.60	1.52
1	A	31	ARG	CZ-NH2	5.45	1.40	1.33
1	A	116	THR	CA-CB	5.45	1.62	1.53
1	B	420	THR	CA-C	5.45	1.59	1.52
1	A	345	ALA	CA-CB	-5.42	1.44	1.53
1	A	190	ASN	N-CA	-5.41	1.39	1.46
1	A	139	ALA	N-CA	5.41	1.53	1.46
1	A	374	MSE	CG-SE	5.41	2.11	1.95
1	A	479	SER	CB-OG	5.41	1.52	1.42
1	A	484	VAL	N-CA	5.41	1.52	1.46
1	A	434	VAL	CA-CB	5.40	1.61	1.54
1	A	67	PRO	C-O	5.40	1.30	1.23
1	A	549	VAL	N-CA	5.39	1.53	1.46
1	B	368	VAL	C-O	5.39	1.30	1.24
1	A	189	MSE	CG-SE	5.39	2.11	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	343	ARG	CA-C	-5.39	1.45	1.52
1	B	522	LEU	C-O	5.39	1.30	1.24
1	B	582	VAL	N-CA	5.38	1.53	1.46
1	A	289	ASP	CA-C	5.38	1.59	1.52
1	B	314	LEU	C-O	-5.38	1.17	1.24
1	A	107	ALA	C-O	-5.38	1.17	1.24
1	B	134	ARG	CD-NE	5.36	1.53	1.46
1	A	390	MSE	SE-CE	5.35	2.11	1.95
1	B	115	THR	C-O	-5.35	1.17	1.24
1	A	319	ALA	N-CA	5.35	1.52	1.46
1	B	144	PRO	C-O	-5.35	1.17	1.24
1	B	495	ALA	CA-C	-5.34	1.45	1.52
1	A	33	ASP	C-O	5.34	1.30	1.24
1	B	507	ALA	C-O	-5.33	1.16	1.23
1	A	71	ARG	C-O	-5.32	1.16	1.24
1	B	435	VAL	CA-C	5.32	1.57	1.53
1	B	407	ALA	CA-C	5.32	1.59	1.52
1	B	171	ALA	N-CA	5.31	1.52	1.46
1	B	361	VAL	CA-C	-5.31	1.46	1.52
1	A	110	VAL	C-O	-5.31	1.18	1.24
1	A	442	MSE	SE-CE	5.31	2.11	1.95
1	A	53	ASP	CA-C	-5.30	1.46	1.52
1	A	242	VAL	CA-CB	5.30	1.61	1.54
1	B	310	VAL	N-CA	-5.30	1.40	1.46
1	B	192	ARG	CA-C	5.30	1.59	1.52
1	A	139	ALA	CA-CB	-5.29	1.44	1.53
1	A	343	ARG	N-CA	5.29	1.52	1.45
1	A	593	ILE	CA-CB	5.29	1.60	1.54
1	A	315	LYS	C-N	5.27	1.39	1.34
1	B	510	SER	N-CA	5.27	1.52	1.46
1	A	61	ILE	CA-CB	5.27	1.60	1.54
1	B	403	LYS	N-CA	5.26	1.52	1.45
1	B	17	THR	CA-C	5.26	1.59	1.52
1	B	320	LEU	C-O	5.25	1.30	1.24
1	A	468	ASN	CA-C	5.24	1.59	1.53
1	A	396	MSE	CA-C	-5.23	1.45	1.52
1	A	452	ALA	C-O	-5.22	1.17	1.23
1	A	119	TRP	N-CA	5.22	1.52	1.46
1	B	279	HIS	N-CA	-5.22	1.39	1.46
1	B	534	VAL	CA-C	-5.22	1.46	1.52
1	A	212	GLU	C-O	-5.21	1.17	1.23
1	A	206	GLN	N-CA	5.21	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	513	LYS	C-O	-5.21	1.17	1.23
1	B	383	THR	C-O	5.21	1.31	1.24
1	A	435	VAL	CA-CB	5.19	1.60	1.54
1	B	138	LYS	CA-C	5.19	1.59	1.52
1	A	485	PHE	N-CA	5.18	1.52	1.45
1	B	108	ALA	N-CA	-5.18	1.39	1.46
1	B	172	ILE	CG1-CD1	5.18	1.72	1.51
1	B	529	ALA	C-N	5.18	1.40	1.33
1	A	417	PRO	CA-C	-5.17	1.47	1.52
1	B	176	LEU	CA-C	5.17	1.59	1.52
1	B	145	LEU	C-O	5.17	1.30	1.23
1	B	424	GLU	N-CA	5.17	1.52	1.45
1	B	74	ALA	CA-CB	5.17	1.61	1.53
1	A	573	HIS	N-CA	-5.16	1.39	1.46
1	A	189	MSE	C-O	-5.16	1.17	1.24
1	A	333	ARG	CA-C	-5.15	1.46	1.53
1	A	516	ALA	N-CA	5.15	1.52	1.46
1	B	399	ASP	CB-CG	5.14	1.65	1.52
1	B	573	HIS	N-CA	5.13	1.52	1.46
1	A	567	ALA	CA-CB	-5.12	1.45	1.53
1	B	215	VAL	CB-CG1	-5.10	1.35	1.52
1	B	521	PRO	C-O	5.10	1.31	1.24
1	A	415	ASP	N-CA	-5.10	1.39	1.46
1	A	154	CYS	CA-C	-5.10	1.46	1.53
1	B	498	ALA	C-O	5.10	1.30	1.24
1	A	582	VAL	CA-C	5.09	1.59	1.52
1	A	332	GLY	N-CA	-5.09	1.38	1.45
1	A	374	MSE	C-O	-5.09	1.17	1.23
1	A	362	LEU	N-CA	-5.09	1.39	1.46
1	B	529	ALA	C-O	5.08	1.30	1.23
1	B	40	THR	CA-C	-5.07	1.46	1.52
1	B	329	GLN	CD-OE1	5.07	1.33	1.23
1	A	218	HIS	CA-CB	-5.06	1.44	1.53
1	B	72	ASP	N-CA	-5.06	1.39	1.46
1	B	114	VAL	CA-C	-5.06	1.46	1.52
1	B	565	THR	CB-OG1	5.06	1.51	1.43
1	B	20	ALA	C-O	5.06	1.29	1.24
1	B	115	THR	CA-C	-5.06	1.46	1.52
1	B	589	GLU	CA-C	5.06	1.59	1.52
1	A	230	PHE	C-O	5.06	1.30	1.24
1	A	18	LEU	N-CA	5.06	1.52	1.46
1	A	292	PHE	CA-CB	-5.05	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	ARG	NE-CZ	5.05	1.38	1.33
1	A	533	GLU	CD-OE2	5.05	1.34	1.25
1	A	191	MSE	SE-CE	5.05	2.10	1.95
1	A	146	ARG	C-O	-5.05	1.17	1.24
1	B	141	GLU	CD-OE1	5.04	1.34	1.25
1	B	148	ILE	C-O	5.04	1.29	1.24
1	A	99	MSE	N-CA	-5.04	1.39	1.46
1	A	250	LYS	CA-C	5.03	1.59	1.52
1	B	352	ASP	CA-CB	-5.03	1.47	1.53
1	A	134	ARG	CZ-NH1	5.02	1.39	1.32
1	B	234	GLY	C-O	5.02	1.30	1.23
1	A	546	GLY	CA-C	5.02	1.58	1.51
1	B	91	THR	N-CA	-5.02	1.39	1.46
1	A	170	ALA	C-O	-5.01	1.18	1.24
1	B	408	LYS	N-CA	5.01	1.51	1.45
1	B	233	ALA	CA-CB	-5.01	1.45	1.53
1	B	172	ILE	C-O	5.01	1.29	1.24
1	B	327	ALA	C-O	-5.01	1.18	1.24
1	A	28	GLY	C-O	5.00	1.30	1.24
1	A	536	ARG	CG-CD	5.00	1.67	1.52

All (382) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	548	VAL	N-CA-C	-13.68	99.65	113.47
1	B	420	THR	N-CA-C	13.13	130.73	109.72
1	A	210	ALA	N-CA-C	-13.10	97.08	111.36
1	A	502	THR	N-CA-C	-12.08	98.52	113.02
1	B	552	GLN	CA-C-N	11.04	131.75	120.38
1	B	552	GLN	C-N-CA	11.04	131.75	120.38
1	A	64	VAL	N-CA-C	-10.84	92.94	108.11
1	B	416	ARG	CA-C-N	10.75	133.28	119.84
1	B	416	ARG	C-N-CA	10.75	133.28	119.84
1	B	218	HIS	N-CA-C	-10.72	89.33	107.23
1	B	54	ILE	CA-C-N	-10.28	115.09	122.18
1	B	54	ILE	C-N-CA	-10.28	115.09	122.18
1	A	77	ILE	CA-C-N	-10.28	108.03	122.93
1	A	77	ILE	C-N-CA	-10.28	108.03	122.93
1	B	197	ARG	NE-CZ-NH1	-10.25	111.25	121.50
1	A	163	ARG	NE-CZ-NH2	-10.25	109.97	119.20
1	A	272	ALA	N-CA-C	-9.75	100.64	111.07
1	B	494	LEU	N-CA-C	-9.46	100.31	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	LEU	CA-C-N	9.27	129.31	119.76
1	A	280	LEU	C-N-CA	9.27	129.31	119.76
1	B	120	ASP	N-CA-CB	-9.19	98.50	110.17
1	B	72	ASP	N-CA-CB	-9.18	94.97	110.49
1	B	502	THR	N-CA-C	-9.18	101.78	113.16
1	A	251	LEU	N-CA-C	-8.93	101.49	111.14
1	B	542	ARG	N-CA-C	-8.91	101.52	111.14
1	A	492	MSE	CG-SE-CE	8.90	118.50	98.92
1	B	260	ARG	N-CA-C	8.86	123.90	109.72
1	A	93	MSE	N-CA-C	8.82	122.00	108.42
1	A	53	ASP	N-CA-C	-8.76	96.10	109.41
1	B	189	MSE	CG-SE-CE	8.72	118.11	98.92
1	A	344	ARG	CA-C-N	-8.65	110.03	122.06
1	A	344	ARG	C-N-CA	-8.65	110.03	122.06
1	B	304	ASP	N-CA-C	8.65	121.85	111.82
1	B	381	CYS	N-CA-C	-8.65	96.19	109.85
1	B	441	THR	N-CA-C	8.62	122.81	109.96
1	B	127	VAL	N-CA-C	-8.35	101.11	113.39
1	B	214	LEU	N-CA-C	8.35	121.70	110.35
1	B	25	ALA	N-CA-C	-8.33	101.12	111.11
1	B	434	VAL	CA-C-N	-8.21	114.48	123.02
1	B	434	VAL	C-N-CA	-8.21	114.48	123.02
1	B	61	ILE	N-CA-C	-8.17	98.05	108.84
1	B	137	ALA	N-CA-C	8.16	120.18	111.28
1	B	207	ALA	CA-C-N	8.16	129.00	119.94
1	B	207	ALA	C-N-CA	8.16	129.00	119.94
1	B	192	ARG	N-CA-C	-8.16	102.39	111.28
1	A	507	ALA	CA-C-N	-8.14	112.67	122.93
1	A	507	ALA	C-N-CA	-8.14	112.67	122.93
1	A	318	TRP	CA-C-O	-8.11	112.35	120.70
1	A	231	MSE	CG-SE-CE	8.10	116.73	98.92
1	B	355	GLY	N-CA-C	-8.05	94.11	113.18
1	B	396	MSE	CG-SE-CE	7.99	116.50	98.92
1	B	338	LEU	CA-C-N	-7.98	113.05	122.22
1	B	338	LEU	C-N-CA	-7.98	113.05	122.22
1	B	249	ALA	N-CA-C	-7.96	104.08	113.88
1	B	9	GLU	N-CA-C	-7.93	98.35	110.32
1	B	321	ARG	N-CA-C	-7.92	102.64	111.28
1	A	467	TRP	N-CA-C	7.86	122.37	107.75
1	A	64	VAL	CB-CA-C	-7.86	99.00	110.63
1	A	215	VAL	CA-C-N	-7.59	110.65	122.87
1	A	215	VAL	C-N-CA	-7.59	110.65	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	LEU	CA-CB-CG	-7.54	89.90	116.30
1	B	442	MSE	N-CA-C	7.49	121.25	110.24
1	B	269	GLU	N-CA-C	7.47	119.21	111.14
1	A	351	GLU	N-CA-C	-7.47	103.07	111.14
1	A	407	ALA	N-CA-C	-7.45	104.43	113.97
1	A	396	MSE	CB-CA-C	-7.44	96.79	109.51
1	A	204	ILE	N-CA-C	7.43	117.56	110.42
1	B	274	LEU	N-CA-C	-7.42	102.57	111.69
1	B	266	LEU	N-CA-C	7.37	120.37	111.82
1	B	71	ARG	N-CA-C	-7.34	102.71	114.09
1	A	343	ARG	NE-CZ-NH1	7.34	128.84	121.50
1	A	52	ALA	CA-C-N	-7.26	110.62	122.82
1	A	52	ALA	C-N-CA	-7.26	110.62	122.82
1	A	448	ARG	N-CA-C	7.26	121.85	112.41
1	A	127	VAL	CA-C-O	7.26	128.09	120.25
1	B	93	MSE	N-CA-C	7.26	117.45	107.73
1	A	109	VAL	N-CA-C	-7.23	106.45	113.53
1	B	82	ALA	CA-C-O	-7.21	113.25	121.40
1	A	207	ALA	CA-C-N	7.18	128.10	119.99
1	A	207	ALA	C-N-CA	7.18	128.10	119.99
1	A	178	SER	CA-C-N	-7.15	111.09	120.67
1	A	178	SER	C-N-CA	-7.15	111.09	120.67
1	A	118	VAL	N-CA-C	-7.12	94.52	109.34
1	A	454	PRO	CA-C-N	-7.11	113.19	123.00
1	A	454	PRO	C-N-CA	-7.11	113.19	123.00
1	A	588	MSE	N-CA-C	7.07	121.45	108.58
1	B	537	ALA	N-CA-C	-7.06	103.58	111.28
1	A	390	MSE	CA-C-N	-7.05	113.34	122.79
1	A	390	MSE	C-N-CA	-7.05	113.34	122.79
1	A	229	ALA	N-CA-C	7.04	119.03	111.36
1	B	120	ASP	CA-C-N	7.02	128.62	119.84
1	B	120	ASP	C-N-CA	7.02	128.62	119.84
1	B	382	ASP	CB-CA-C	7.01	120.78	110.26
1	A	518	LEU	CA-C-N	-6.93	112.50	119.99
1	A	518	LEU	C-N-CA	-6.93	112.50	119.99
1	A	506	MSE	N-CA-C	6.92	119.96	109.23
1	B	248	MSE	CA-C-N	-6.88	110.53	122.36
1	B	248	MSE	C-N-CA	-6.88	110.53	122.36
1	B	465	GLY	N-CA-C	-6.84	100.67	110.38
1	B	141	GLU	N-CA-C	6.83	119.60	111.33
1	A	405	GLN	N-CA-C	6.82	118.40	110.97
1	B	588	MSE	N-CA-C	6.81	120.59	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	HIS	O-C-N	-6.80	114.94	123.17
1	A	503	GLY	N-CA-C	6.80	125.77	114.48
1	A	252	ARG	N-CA-C	-6.78	104.87	113.01
1	A	354	ASN	N-CA-C	6.78	125.24	110.80
1	B	197	ARG	NE-CZ-NH2	6.78	125.30	119.20
1	B	382	ASP	N-CA-CB	-6.75	99.32	109.71
1	B	207	ALA	N-CA-C	-6.74	104.01	111.82
1	A	184	GLY	N-CA-C	6.71	119.61	110.69
1	B	451	MSE	CG-SE-CE	6.71	113.67	98.92
1	B	73	ALA	N-CA-C	6.70	119.61	109.23
1	B	236	SER	N-CA-C	6.67	121.49	112.88
1	A	195	ILE	N-CA-C	6.66	118.21	110.62
1	B	220	ARG	CA-C-N	-6.65	115.53	123.44
1	B	220	ARG	C-N-CA	-6.65	115.53	123.44
1	B	335	ASP	N-CA-C	-6.65	104.39	113.30
1	B	463	GLY	N-CA-C	-6.63	97.45	113.18
1	A	431	ASP	N-CA-C	6.61	120.93	112.86
1	B	246	ASP	N-CA-C	-6.61	103.76	110.97
1	A	470	ALA	N-CA-C	6.60	118.79	108.96
1	A	98	SER	CA-CB-OG	-6.60	97.90	111.10
1	A	501	GLY	CA-C-N	-6.58	111.25	122.56
1	A	501	GLY	C-N-CA	-6.58	111.25	122.56
1	A	37	THR	N-CA-C	6.52	119.33	109.41
1	A	329	GLN	N-CA-C	-6.51	104.10	111.07
1	B	104	ALA	N-CA-C	-6.50	104.61	112.54
1	B	390	MSE	CG-SE-CE	6.50	113.22	98.92
1	B	380	THR	CA-C-N	-6.50	111.89	122.81
1	B	380	THR	C-N-CA	-6.50	111.89	122.81
1	B	285	THR	CB-CA-C	-6.44	97.60	110.42
1	A	366	ARG	N-CA-C	-6.43	99.23	109.59
1	B	145	LEU	N-CA-C	-6.41	99.24	109.76
1	A	196	GLU	N-CA-C	-6.41	105.41	112.72
1	A	343	ARG	NE-CZ-NH2	-6.38	113.46	119.20
1	A	163	ARG	NE-CZ-NH1	6.37	127.87	121.50
1	B	455	THR	CB-CA-C	-6.35	99.87	110.29
1	B	435	VAL	CA-C-N	6.35	126.92	120.38
1	B	435	VAL	C-N-CA	6.35	126.92	120.38
1	A	265	HIS	N-CA-C	-6.34	105.37	113.23
1	A	535	ALA	N-CA-C	-6.34	104.29	111.07
1	B	66	GLU	CA-C-N	6.34	127.76	119.84
1	B	66	GLU	C-N-CA	6.34	127.76	119.84
1	A	559	LYS	N-CA-C	-6.32	105.43	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	ASP	CA-C-N	-6.29	115.68	122.85
1	A	377	ASP	C-N-CA	-6.29	115.68	122.85
1	A	184	GLY	O-C-N	-6.24	117.93	123.92
1	A	402	VAL	N-CA-CB	-6.24	104.16	111.83
1	B	64	VAL	CA-C-N	-6.23	111.66	121.87
1	B	64	VAL	C-N-CA	-6.23	111.66	121.87
1	A	509	ALA	O-C-N	-6.22	116.00	123.03
1	A	315	LYS	CA-C-N	-6.21	113.73	119.82
1	A	315	LYS	C-N-CA	-6.21	113.73	119.82
1	B	264	ASP	CA-C-O	-6.21	113.97	120.92
1	A	109	VAL	CB-CA-C	-6.20	104.57	110.65
1	B	525	LEU	N-CA-C	-6.20	105.61	113.43
1	A	373	ARG	N-CA-C	6.20	119.64	109.85
1	A	593	ILE	CA-C-O	-6.19	114.66	121.29
1	B	257	ILE	N-CA-C	6.19	117.70	108.23
1	B	462	THR	CB-CA-C	-6.17	98.14	110.42
1	B	11	ALA	N-CA-C	6.16	118.79	111.33
1	B	184	GLY	CA-C-N	-6.16	114.67	122.37
1	B	184	GLY	C-N-CA	-6.16	114.67	122.37
1	B	302	LEU	N-CA-C	6.16	118.50	111.11
1	B	226	ASP	N-CA-C	-6.15	104.13	111.69
1	B	189	MSE	CA-C-N	-6.13	112.97	122.16
1	B	189	MSE	C-N-CA	-6.13	112.97	122.16
1	A	130	VAL	N-CA-C	-6.11	103.46	111.09
1	B	332	GLY	CA-C-N	-6.08	113.88	123.12
1	B	332	GLY	C-N-CA	-6.08	113.88	123.12
1	A	127	VAL	O-C-N	-6.07	113.50	121.82
1	A	141	GLU	CA-C-N	-6.07	112.41	123.34
1	A	141	GLU	C-N-CA	-6.07	112.41	123.34
1	B	373	ARG	N-CA-C	6.06	119.08	109.50
1	B	448	ARG	CB-CA-C	-6.06	101.73	111.18
1	A	88	LEU	CA-C-O	-6.06	114.96	121.56
1	B	441	THR	CB-CA-C	-6.05	101.44	110.16
1	A	181	GLU	CA-C-N	-6.03	115.33	122.93
1	A	181	GLU	C-N-CA	-6.03	115.33	122.93
1	B	451	MSE	N-CA-C	-6.02	104.05	113.02
1	A	400	PHE	N-CA-C	6.02	120.62	113.16
1	B	260	ARG	CA-C-O	6.01	127.90	121.11
1	B	216	CYS	CA-C-O	-6.00	114.14	120.80
1	A	119	TRP	CA-C-O	-5.95	113.78	120.32
1	A	520	LEU	CA-C-N	5.93	127.26	119.84
1	A	520	LEU	C-N-CA	5.93	127.26	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	501	GLY	N-CA-C	-5.90	106.45	115.66
1	B	90	ASP	CA-C-N	-5.90	111.70	122.38
1	B	90	ASP	C-N-CA	-5.90	111.70	122.38
1	B	205	VAL	CB-CA-C	-5.89	101.63	111.29
1	A	351	GLU	O-C-N	-5.88	115.74	122.09
1	B	272	ALA	N-CA-C	-5.87	104.47	111.69
1	B	451	MSE	CB-CA-C	-5.87	100.58	110.44
1	A	338	LEU	CB-CA-C	-5.86	99.31	109.86
1	B	458	THR	N-CA-C	5.86	119.61	110.17
1	A	64	VAL	N-CA-CB	5.85	119.48	111.41
1	A	161	LEU	N-CA-C	5.84	118.59	111.82
1	A	76	VAL	CB-CA-C	-5.83	101.06	110.28
1	A	346	ASP	N-CA-C	-5.83	97.68	107.99
1	B	123	GLU	CA-C-O	-5.82	114.71	120.70
1	A	322	ALA	N-CA-C	-5.81	105.45	112.54
1	B	454	PRO	CA-C-N	5.81	130.15	121.72
1	B	454	PRO	C-N-CA	5.81	130.15	121.72
1	A	98	SER	N-CA-C	5.81	120.06	113.15
1	B	326	ASN	N-CA-C	5.80	117.28	111.07
1	B	138	LYS	CD-CE-NZ	-5.79	93.38	111.90
1	B	245	GLU	CA-C-N	-5.78	113.03	120.65
1	B	245	GLU	C-N-CA	-5.78	113.03	120.65
1	A	220	ARG	CB-CG-CD	5.77	124.57	111.30
1	B	318	TRP	N-CA-C	-5.77	104.63	111.03
1	B	365	GLY	N-CA-C	-5.77	107.04	113.79
1	A	91	THR	OG1-CB-CG2	-5.76	97.78	109.30
1	A	276	THR	N-CA-C	-5.75	106.39	113.41
1	A	528	ASP	N-CA-C	5.75	119.56	112.54
1	A	16	ASP	N-CA-C	5.74	117.34	111.14
1	B	284	VAL	N-CA-C	5.74	116.48	109.30
1	A	114	VAL	CB-CA-C	-5.73	105.04	111.23
1	B	366	ARG	CA-C-N	-5.73	114.11	122.19
1	B	366	ARG	C-N-CA	-5.73	114.11	122.19
1	A	133	VAL	N-CA-C	-5.73	104.27	112.35
1	B	103	ALA	N-CA-C	5.73	117.98	111.11
1	B	409	VAL	N-CA-C	5.73	116.61	108.42
1	B	517	ILE	CA-CB-CG2	5.73	120.23	110.50
1	A	387	LYS	N-CA-C	5.72	118.88	110.59
1	A	593	ILE	N-CA-C	5.71	115.84	110.30
1	A	385	VAL	CG1-CB-CG2	5.71	123.36	110.80
1	A	86	PRO	CA-C-O	-5.71	114.78	122.08
1	A	321	ARG	O-C-N	5.71	127.95	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	LEU	N-CA-C	-5.70	102.46	110.50
1	A	554	PRO	N-CA-C	-5.70	97.27	112.10
1	A	594	GLU	CA-C-O	-5.68	115.05	120.56
1	B	391	LYS	N-CA-CB	-5.68	103.30	110.45
1	A	173	LEU	N-CA-CB	5.67	118.39	109.94
1	A	471	PHE	N-CA-C	5.67	118.39	107.44
1	A	486	GLY	N-CA-C	5.66	119.01	110.75
1	B	442	MSE	CB-CG-SE	-5.62	95.82	112.70
1	B	543	GLU	CA-CB-CG	-5.61	102.88	114.10
1	B	518	LEU	CA-C-N	5.61	125.79	119.90
1	B	518	LEU	C-N-CA	5.61	125.79	119.90
1	A	198	ASP	N-CA-C	5.60	116.88	109.93
1	A	84	VAL	N-CA-C	5.58	116.34	108.36
1	A	182	ILE	N-CA-CB	-5.58	104.29	110.99
1	A	518	LEU	CB-CA-C	5.57	116.45	110.65
1	B	71	ARG	CA-C-O	5.57	125.09	118.79
1	A	498	ALA	CA-C-N	-5.57	110.71	120.29
1	A	498	ALA	C-N-CA	-5.57	110.71	120.29
1	B	257	ILE	CB-CA-C	-5.56	104.23	110.96
1	A	194	VAL	CB-CA-C	-5.56	104.86	111.81
1	A	433	PHE	N-CA-C	5.56	118.31	110.14
1	B	333	ARG	O-C-N	-5.56	116.75	122.64
1	B	119	TRP	N-CA-CB	-5.55	101.83	110.55
1	B	455	THR	CA-C-N	-5.53	113.51	121.42
1	B	455	THR	C-N-CA	-5.53	113.51	121.42
1	A	367	ALA	CA-C-N	-5.53	115.20	122.16
1	A	367	ALA	C-N-CA	-5.53	115.20	122.16
1	B	489	ALA	N-CA-C	5.51	116.97	111.07
1	A	214	LEU	N-CA-C	5.51	117.84	110.35
1	B	349	VAL	CB-CA-C	-5.51	103.53	111.19
1	A	394	LEU	CA-C-N	-5.51	112.72	122.74
1	A	394	LEU	C-N-CA	-5.51	112.72	122.74
1	A	541	LEU	N-CA-C	-5.50	105.69	112.90
1	A	179	TRP	N-CA-C	5.50	117.59	109.50
1	A	364	SER	N-CA-C	-5.50	105.20	112.24
1	A	371	GLY	CA-C-N	-5.50	113.94	122.69
1	A	371	GLY	C-N-CA	-5.50	113.94	122.69
1	A	495	ALA	N-CA-C	-5.50	105.44	111.82
1	A	218	HIS	CB-CA-C	-5.48	99.67	109.71
1	B	544	ALA	N-CA-C	5.48	118.77	111.75
1	A	31	ARG	N-CA-CB	-5.48	102.41	110.85
1	A	35	LEU	CA-C-N	-5.47	116.03	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	LEU	C-N-CA	-5.47	116.03	122.93
1	B	161	LEU	N-CA-C	5.46	120.01	113.23
1	A	249	ALA	N-CA-C	-5.46	105.41	111.36
1	A	155	VAL	CB-CA-C	5.45	117.44	111.18
1	B	72	ASP	CA-C-N	-5.45	113.30	122.29
1	B	72	ASP	C-N-CA	-5.45	113.30	122.29
1	B	147	ALA	O-C-N	-5.43	116.97	123.27
1	A	552	GLN	CA-C-N	5.40	125.94	120.38
1	A	552	GLN	C-N-CA	5.40	125.94	120.38
1	B	37	THR	CA-C-O	-5.40	115.01	121.11
1	A	495	ALA	O-C-N	-5.39	115.63	122.27
1	B	157	SER	N-CA-C	-5.39	106.20	112.89
1	B	17	THR	CB-CA-C	5.39	120.02	110.85
1	B	289	ASP	N-CA-C	-5.39	99.32	110.80
1	A	125	GLY	CA-C-N	-5.38	112.65	120.29
1	A	125	GLY	C-N-CA	-5.38	112.65	120.29
1	A	467	TRP	CA-C-O	5.38	126.65	120.84
1	A	238	ASP	N-CA-C	5.37	117.25	108.76
1	B	84	VAL	CB-CA-C	-5.37	103.63	110.98
1	A	333	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	B	267	LEU	O-C-N	5.35	125.64	120.55
1	A	505	GLY	CA-C-O	-5.35	116.19	120.79
1	A	232	ALA	CA-C-O	-5.34	114.86	120.63
1	A	299	GLY	CA-C-N	-5.34	115.00	122.85
1	A	299	GLY	C-N-CA	-5.34	115.00	122.85
1	B	148	ILE	N-CA-C	-5.34	100.06	107.80
1	A	474	THR	CA-C-O	5.34	125.16	119.34
1	B	192	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	A	57	VAL	N-CA-C	-5.32	100.45	108.12
1	A	321	ARG	CB-CA-C	-5.32	102.53	110.88
1	A	148	ILE	CB-CA-C	5.32	117.30	111.08
1	A	21	ARG	NE-CZ-NH2	-5.32	114.42	119.20
1	A	164	GLY	N-CA-C	-5.31	104.91	112.55
1	A	178	SER	CA-CB-OG	-5.29	100.52	111.10
1	B	339	ILE	N-CA-CB	-5.29	106.93	112.06
1	A	426	GLU	CA-C-O	-5.29	116.06	122.03
1	A	189	MSE	CB-CA-C	-5.29	100.45	109.65
1	B	56	ILE	CB-CA-C	-5.29	101.93	110.28
1	B	263	HIS	N-CA-C	-5.28	101.10	108.54
1	B	27	ARG	N-CA-C	-5.27	105.70	111.82
1	B	321	ARG	CA-CB-CG	-5.27	103.56	114.10
1	B	406	GLY	N-CA-C	5.27	118.71	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	PRO	CA-C-O	-5.27	115.53	121.43
1	B	584	THR	N-CA-CB	5.27	119.39	110.49
1	A	110	VAL	N-CA-C	-5.26	105.58	110.53
1	A	195	ILE	CB-CA-C	-5.26	105.15	112.04
1	B	34	VAL	CB-CA-C	-5.26	103.70	111.80
1	B	419	PHE	CB-CA-C	5.26	119.04	109.62
1	B	376	VAL	CB-CA-C	-5.26	102.56	110.55
1	A	275	ASN	CA-C-N	-5.25	112.69	122.09
1	A	275	ASN	C-N-CA	-5.25	112.69	122.09
1	B	403	LYS	N-CA-C	5.25	117.60	110.35
1	A	579	ILE	CB-CA-C	-5.25	103.01	110.83
1	A	458	THR	N-CA-C	5.24	118.60	110.17
1	B	466	ARG	CA-C-N	5.23	130.88	123.14
1	B	466	ARG	C-N-CA	5.23	130.88	123.14
1	A	494	LEU	N-CA-C	-5.22	105.50	111.14
1	B	40	THR	CA-CB-OG1	-5.22	101.77	109.60
1	B	182	ILE	CB-CA-C	-5.22	104.44	110.91
1	B	277	LEU	N-CA-C	-5.22	106.06	112.90
1	B	477	HIS	N-CA-C	-5.22	100.73	109.24
1	A	524	GLY	N-CA-C	-5.21	107.05	115.08
1	B	294	ASP	CB-CA-C	5.21	119.13	110.90
1	B	342	GLY	O-C-N	-5.21	116.35	122.50
1	B	40	THR	OG1-CB-CG2	-5.21	98.89	109.30
1	A	214	LEU	CB-CG-CD1	-5.20	95.11	110.70
1	B	152	PRO	CA-C-N	-5.19	112.94	121.92
1	B	152	PRO	C-N-CA	-5.19	112.94	121.92
1	B	12	ASP	CA-C-O	-5.18	113.50	119.61
1	A	64	VAL	O-C-N	5.17	128.84	123.26
1	A	417	PRO	CB-CA-C	-5.17	107.53	111.87
1	B	524	GLY	CA-C-N	-5.16	111.90	122.58
1	B	524	GLY	C-N-CA	-5.16	111.90	122.58
1	B	112	ARG	N-CA-C	5.15	119.66	113.17
1	A	384	THR	N-CA-C	5.14	117.28	111.11
1	A	78	ASP	N-CA-C	5.13	117.86	109.59
1	B	260	ARG	CG-CD-NE	-5.13	100.71	112.00
1	B	321	ARG	CB-CG-CD	5.13	123.10	111.30
1	B	435	VAL	CB-CA-C	5.13	116.68	110.78
1	A	592	VAL	CB-CA-C	5.13	116.94	111.35
1	A	99	MSE	CA-C-N	-5.12	114.59	122.68
1	A	99	MSE	C-N-CA	-5.12	114.59	122.68
1	A	309	LEU	N-CA-C	-5.12	105.70	111.28
1	A	592	VAL	N-CA-CB	5.12	116.94	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	ASN	O-C-N	5.11	127.33	122.07
1	B	245	GLU	N-CA-C	-5.10	105.90	111.82
1	A	38	GLY	CA-C-N	5.10	127.07	120.64
1	A	38	GLY	C-N-CA	5.10	127.07	120.64
1	A	201	MSE	CG-SE-CE	5.09	110.13	98.92
1	B	124	PHE	CB-CA-C	-5.09	102.34	110.79
1	B	41	LEU	CA-C-N	-5.07	116.29	122.93
1	B	41	LEU	C-N-CA	-5.07	116.29	122.93
1	B	96	GLU	N-CA-C	5.07	121.60	110.80
1	B	277	LEU	CD1-CG-CD2	-5.07	99.64	110.80
1	B	110	VAL	N-CA-C	-5.07	105.45	110.62
1	B	262	SER	CA-C-N	-5.07	116.21	123.20
1	B	262	SER	C-N-CA	-5.07	116.21	123.20
1	B	327	ALA	CA-C-O	-5.07	115.50	120.82
1	B	367	ALA	CA-C-N	-5.06	115.83	121.85
1	B	367	ALA	C-N-CA	-5.06	115.83	121.85
1	B	134	ARG	CA-C-N	5.05	127.32	120.65
1	B	134	ARG	C-N-CA	5.05	127.32	120.65
1	A	167	ASP	CB-CA-C	5.05	118.48	109.65
1	A	339	ILE	CB-CA-C	-5.04	105.38	111.88
1	A	492	MSE	CA-CB-CG	-5.04	104.02	114.10
1	B	127	VAL	O-C-N	-5.04	117.29	122.23
1	B	380	THR	N-CA-C	-5.02	104.05	110.53
1	B	422	TRP	N-CA-C	5.01	117.86	110.59
1	A	322	ALA	CA-C-N	-5.01	113.31	122.38
1	A	322	ALA	C-N-CA	-5.01	113.31	122.38
1	A	498	ALA	N-CA-C	-5.01	106.01	111.82
1	B	593	ILE	CB-CA-C	5.00	119.50	111.29

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	396	MSE	Peptide
1	A	430	LYS	Peptide
1	B	152	PRO	Peptide
1	B	412	ALA	Peptide
1	B	417	PRO	Peptide
1	B	419	PHE	Peptide
1	B	460	PHE	Peptide
1	B	553	PRO	Peptide

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	4337	0	4344	237	0
1	B	4335	0	4339	315	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	33	0	0	5	0
3	B	50	0	0	16	0
All	All	8761	0	8683	539	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 31.

All (539) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:VAL:CB	1:A:385:VAL:CG1	1.76	1.58
1:B:231:MSE:SE	1:B:231:MSE:CG	2.14	1.44
1:A:492:MSE:SE	1:A:492:MSE:CE	2.14	1.44
1:A:393:PRO:CB	1:A:393:PRO:CG	1.79	1.43
1:A:231:MSE:SE	1:A:231:MSE:CE	2.17	1.42
1:A:390:MSE:CG	1:A:390:MSE:SE	2.17	1.42
1:B:577:MSE:CE	1:B:577:MSE:SE	2.15	1.42
1:B:201:MSE:CG	1:B:201:MSE:SE	2.17	1.42
1:A:374:MSE:SE	1:A:374:MSE:CE	2.22	1.36
1:B:189:MSE:HG3	1:B:568:CYS:SG	1.64	1.36
1:B:390:MSE:CE	1:B:390:MSE:SE	2.23	1.35
1:A:201:MSE:SE	1:A:201:MSE:CE	2.27	1.33
1:B:442:MSE:SE	1:B:442:MSE:CE	2.27	1.32
1:B:248:MSE:SE	1:B:248:MSE:CE	2.27	1.32
1:B:231:MSE:SE	1:B:231:MSE:CE	2.30	1.30
1:B:588:MSE:SE	1:B:588:MSE:CE	2.32	1.27
1:A:248:MSE:SE	1:A:248:MSE:CE	2.33	1.26
1:A:588:MSE:SE	1:A:588:MSE:CE	2.34	1.26
1:B:201:MSE:SE	1:B:201:MSE:CE	2.35	1.23
1:B:451:MSE:CE	1:B:451:MSE:SE	2.43	1.17
1:B:420:THR:HB	1:B:572:PRO:HD2	1.29	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:GLN:H	1:B:556:LEU:HD23	1.09	1.14
1:A:99:MSE:SE	1:A:99:MSE:CE	2.46	1.12
1:A:577:MSE:SE	1:A:577:MSE:CE	2.47	1.11
1:A:120:ASP:OD1	1:A:122:HIS:HB3	1.50	1.11
1:B:191:MSE:SE	1:B:191:MSE:CE	2.54	1.05
1:B:396:MSE:SE	1:B:396:MSE:CE	2.53	1.05
1:B:441:THR:HG1	1:B:467:TRP:CD1	1.75	1.03
1:B:552:GLN:H	1:B:556:LEU:CD2	1.70	1.02
1:B:552:GLN:N	1:B:556:LEU:HD23	1.73	1.02
1:A:588:MSE:HE2	1:A:590:SER:O	1.60	1.00
1:B:583:LEU:O	1:B:585:GLY:N	1.94	1.00
1:A:189:MSE:SE	1:A:189:MSE:CE	2.62	0.97
1:A:308:ARG:HG2	1:A:311:ARG:NH2	1.80	0.97
1:B:189:MSE:SE	1:B:189:MSE:CE	2.63	0.96
1:A:396:MSE:SE	1:A:396:MSE:CE	2.64	0.95
1:A:396:MSE:HB3	1:A:398:ASN:H	1.31	0.94
1:B:488:ASN:O	1:B:492:MSE:HG3	1.67	0.93
1:A:451:MSE:SE	1:A:451:MSE:CE	2.67	0.93
1:B:476:SER:H	1:B:480:HIS:HD2	1.05	0.93
1:A:518:LEU:C	1:A:518:LEU:HD12	1.92	0.92
1:B:31:ARG:HA	1:B:72:ASP:OD2	1.71	0.91
1:B:402:VAL:HB	1:B:434:VAL:HG23	1.54	0.90
1:A:448:ARG:H	1:A:481:ASN:HD22	1.19	0.90
1:A:420:THR:HG21	1:A:572:PRO:O	1.71	0.90
1:A:286:LEU:HD12	1:A:323:ALA:HB2	1.55	0.89
1:A:200:ARG:HB3	3:A:635:HOH:O	1.74	0.88
1:B:189:MSE:CG	1:B:568:CYS:SG	2.57	0.88
1:B:476:SER:H	1:B:480:HIS:CD2	1.93	0.86
1:B:505:GLY:HA2	1:B:520:LEU:HB2	1.58	0.86
1:A:373:ARG:HG3	1:A:373:ARG:HH11	1.39	0.85
1:A:416:ARG:HB3	1:A:419:PHE:O	1.77	0.84
1:A:99:MSE:HG2	1:A:520:LEU:HD21	1.60	0.84
1:B:477:HIS:HB3	1:B:478:ASP:OD1	1.78	0.84
1:A:259:LEU:HD12	1:A:259:LEU:C	1.98	0.83
1:B:64:VAL:HG21	3:B:643:HOH:O	1.78	0.83
1:B:351:GLU:OE1	1:B:359:ARG:HB2	1.78	0.82
1:B:196:GLU:HG3	3:B:646:HOH:O	1.78	0.82
1:B:551:TRP:C	1:B:553:PRO:HD3	2.04	0.82
1:B:190:ASN:HB3	1:B:201:MSE:SE	2.30	0.81
1:B:486:GLY:HA3	1:B:492:MSE:SE	2.31	0.81
1:B:462:THR:HG22	1:B:463:GLY:N	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ARG:H	1:A:481:ASN:ND2	1.78	0.81
1:B:420:THR:HB	1:B:572:PRO:CD	2.09	0.81
1:B:295:ASP:O	1:B:300:GLY:HA2	1.80	0.81
1:B:374:MSE:HE2	1:B:378:ILE:HD11	1.62	0.80
1:A:554:PRO:O	1:A:555:TYR:HB2	1.82	0.79
1:A:308:ARG:CG	1:A:311:ARG:NH2	2.45	0.79
1:B:79:ALA:O	1:B:82:ALA:HB3	1.83	0.78
1:B:239:HIS:CD2	1:B:240:GLU:HG2	2.19	0.77
1:B:239:HIS:HD2	1:B:240:GLU:HG2	1.50	0.77
1:B:407:ALA:O	1:B:429:VAL:HB	1.85	0.77
1:B:476:SER:N	1:B:480:HIS:HD2	1.83	0.77
1:A:373:ARG:HH11	1:A:373:ARG:CG	1.97	0.77
1:B:440:ALA:HB1	1:B:461:LEU:O	1.83	0.76
1:A:496:ALA:O	1:A:500:ILE:HG13	1.83	0.76
1:B:267:LEU:HD23	1:B:267:LEU:N	1.99	0.76
1:B:161:LEU:N	1:B:161:LEU:HD12	2.00	0.76
1:B:90:ASP:OD1	1:B:287:CYS:HA	1.86	0.75
1:B:462:THR:CG2	1:B:463:GLY:N	2.49	0.75
1:A:110:VAL:HG23	1:A:145:LEU:HD13	1.68	0.75
1:A:92:HIS:HE1	1:A:187:GLU:HG2	1.52	0.74
1:A:259:LEU:HD12	1:A:260:ARG:N	2.02	0.74
1:B:505:GLY:CA	1:B:520:LEU:HB2	2.17	0.74
1:B:231:MSE:SE	1:B:231:MSE:CB	2.85	0.74
1:B:267:LEU:HD23	1:B:267:LEU:H	1.52	0.74
1:A:380:THR:OG1	1:A:381:CYS:N	2.21	0.73
1:A:93:MSE:HE1	1:A:95:ILE:HG12	1.70	0.73
1:A:99:MSE:HE2	1:A:506:MSE:HE1	1.68	0.73
1:B:175:ASP:HB3	3:B:658:HOH:O	1.87	0.73
1:A:385:VAL:CG1	1:A:385:VAL:HB	2.12	0.73
1:A:488:ASN:ND2	1:A:491:ASP:H	1.85	0.73
1:B:583:LEU:C	1:B:585:GLY:H	1.95	0.73
1:A:88:LEU:HB3	1:A:302:LEU:HD23	1.68	0.72
1:A:468:ASN:O	1:A:548:VAL:HG22	1.88	0.72
1:A:420:THR:HG22	1:A:571:GLY:HA3	1.70	0.72
1:B:248:MSE:O	1:B:252:ARG:HG3	1.89	0.72
1:A:63:SER:OG	1:A:65:HIS:HD2	1.73	0.72
1:B:294:ASP:HA	1:B:535:ALA:HB1	1.72	0.71
1:B:464:TRP:O	1:B:556:LEU:CD1	2.38	0.71
1:B:63:SER:OG	1:B:65:HIS:HD2	1.73	0.71
1:A:99:MSE:HG2	1:A:520:LEU:CD2	2.20	0.71
1:B:425:THR:HG22	3:B:615:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:THR:O	1:A:386:LEU:HB2	1.90	0.70
1:B:427:ALA:HB1	1:B:434:VAL:HG13	1.72	0.70
1:B:122:HIS:HB3	1:B:152:PRO:HB3	1.73	0.70
1:B:551:TRP:O	1:B:553:PRO:HD3	1.91	0.69
1:B:485:PHE:HZ	1:B:561:CYS:O	1.75	0.69
1:B:419:PHE:HA	3:B:647:HOH:O	1.92	0.69
1:A:110:VAL:CG2	1:A:145:LEU:HD13	2.22	0.69
1:B:427:ALA:CB	1:B:434:VAL:HG13	2.24	0.68
1:A:385:VAL:CG1	1:A:385:VAL:CA	2.70	0.68
1:B:476:SER:O	1:B:480:HIS:CD2	2.46	0.68
1:B:402:VAL:HB	1:B:434:VAL:CG2	2.24	0.68
1:A:414:ILE:HG23	1:A:572:PRO:HB2	1.75	0.68
1:B:128:HIS:HE1	3:B:656:HOH:O	1.75	0.67
1:B:122:HIS:CB	1:B:152:PRO:HB3	2.23	0.67
1:A:228:ASN:ND2	1:B:64:VAL:H	1.93	0.67
1:B:474:THR:HG21	1:B:505:GLY:H	1.59	0.67
1:A:99:MSE:HE2	1:A:506:MSE:CE	2.25	0.67
1:A:402:VAL:HB	1:A:434:VAL:HG13	1.77	0.66
1:B:425:THR:CG2	3:B:615:HOH:O	2.43	0.66
1:A:82:ALA:HB1	1:A:350:PHE:O	1.97	0.65
1:B:318:TRP:O	1:B:319:ALA:C	2.36	0.65
1:B:182:ILE:HG22	1:B:184:GLY:H	1.62	0.65
1:A:458:THR:CG2	1:A:459:GLY:N	2.59	0.65
1:B:305:VAL:O	1:B:306:VAL:C	2.38	0.65
1:B:430:LYS:HD2	1:B:431:ASP:N	2.12	0.64
1:B:161:LEU:N	1:B:161:LEU:CD1	2.60	0.64
1:B:464:TRP:O	1:B:556:LEU:HD13	1.98	0.64
1:A:341:ALA:HB2	1:B:228:ASN:HD22	1.63	0.64
1:A:396:MSE:HB3	1:A:398:ASN:N	2.08	0.64
1:B:428:ASP:O	1:B:435:VAL:HG12	1.98	0.64
1:A:405:GLN:O	1:A:406:GLY:O	2.16	0.64
1:B:163:ARG:O	1:B:447:HIS:HD2	1.79	0.64
1:B:556:LEU:O	1:B:556:LEU:HG	1.99	0.63
1:A:38:GLY:O	1:A:80:GLY:HA2	1.98	0.63
1:A:428:ASP:O	1:A:435:VAL:HG23	1.99	0.63
1:B:393:PRO:O	1:B:395:ARG:NH1	2.30	0.63
1:A:467:TRP:O	1:A:487:GLY:HA3	1.99	0.63
1:A:146:ARG:NH2	1:A:344:ARG:HD3	2.14	0.63
1:A:202:SER:O	1:A:206:GLN:HG2	1.99	0.63
1:A:22:ALA:HA	1:A:57:VAL:HG21	1.81	0.62
1:B:296:LEU:O	1:B:300:GLY:HA3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:GLY:O	1:B:429:VAL:HG11	1.98	0.62
1:B:446:THR:OG1	1:B:456:THR:HB	1.98	0.62
1:A:250:LYS:HB3	1:A:255:LEU:HD12	1.82	0.62
1:B:485:PHE:CZ	1:B:561:CYS:O	2.52	0.62
1:A:453:GLU:OE2	1:A:453:GLU:HA	2.00	0.62
1:B:570:ILE:HG13	1:B:583:LEU:HD11	1.81	0.62
1:A:448:ARG:HG3	1:A:481:ASN:HD22	1.65	0.62
1:B:583:LEU:C	1:B:585:GLY:N	2.55	0.61
1:A:403:LYS:HE3	1:A:432:GLY:CA	2.31	0.61
1:B:143:LEU:HD23	1:B:143:LEU:N	2.15	0.61
1:B:395:ARG:HD2	1:B:395:ARG:N	2.14	0.61
1:B:542:ARG:O	1:B:545:VAL:HG12	2.00	0.61
1:A:239:HIS:HB3	1:A:258:GLU:HB2	1.82	0.61
1:A:518:LEU:C	1:A:518:LEU:CD1	2.70	0.61
1:B:572:PRO:O	1:B:573:HIS:CG	2.54	0.61
1:B:247:LEU:O	1:B:251:LEU:HB2	2.01	0.61
1:B:405:GLN:HG3	3:B:619:HOH:O	2.00	0.61
1:A:351:GLU:OE1	1:A:359:ARG:HB2	2.00	0.60
1:B:464:TRP:O	1:B:556:LEU:HD11	2.00	0.60
1:A:505:GLY:HA2	1:A:520:LEU:HB2	1.81	0.60
1:B:177:LEU:HD21	1:B:185:ILE:HG13	1.83	0.60
1:B:586:LYS:C	1:B:587:VAL:HG23	2.26	0.59
1:A:554:PRO:O	1:A:555:TYR:CB	2.48	0.59
1:A:90:ASP:HB3	1:A:117:ILE:HG22	1.84	0.59
1:B:386:LEU:HD12	1:B:522:LEU:HB3	1.85	0.59
1:A:304:ASP:OD1	1:A:307:ARG:HD2	2.01	0.59
1:B:267:LEU:N	1:B:267:LEU:CD2	2.65	0.59
1:B:415:ASP:HA	1:B:462:THR:HB	1.84	0.59
1:A:215:VAL:HG12	1:A:235:VAL:HA	1.83	0.59
1:A:373:ARG:CG	1:A:373:ARG:NH1	2.65	0.59
1:B:409:VAL:O	1:B:426:GLU:HA	2.03	0.58
1:B:474:THR:CG2	1:B:505:GLY:H	2.16	0.58
1:B:128:HIS:O	1:B:131:ASP:HB2	2.02	0.58
1:B:112:ARG:HD3	1:B:303:ASP:OD2	2.03	0.58
1:B:150:LEU:O	1:B:152:PRO:HD3	2.04	0.58
1:A:441:THR:C	1:A:442:MSE:HE3	2.28	0.58
1:B:466:ARG:O	1:B:549:VAL:HG23	2.04	0.58
1:A:67:PRO:C	1:A:69:SER:H	2.12	0.58
1:B:86:PRO:HD3	1:B:339:ILE:HD12	1.87	0.57
1:B:154:CYS:O	1:B:189:MSE:HE2	2.03	0.57
1:B:477:HIS:CB	1:B:478:ASP:OD1	2.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:PRO:HG3	1:A:339:ILE:HG12	1.85	0.57
1:A:394:LEU:C	1:A:395:ARG:HD2	2.30	0.57
1:B:172:ILE:HA	1:B:175:ASP:OD2	2.05	0.57
1:B:570:ILE:HG12	1:B:571:GLY:N	2.18	0.57
1:A:53:ASP:OD2	1:A:67:PRO:HA	2.04	0.57
1:A:243:SER:OG	1:A:246:ASP:HB2	2.05	0.57
1:B:532:GLU:CD	1:B:532:GLU:H	2.12	0.57
1:A:53:ASP:C	1:A:54:ILE:HD13	2.30	0.56
1:A:581:ASP:OD1	1:A:583:LEU:HD22	2.05	0.56
1:B:94:HIS:O	1:B:95:ILE:C	2.45	0.56
1:B:461:LEU:HD22	1:B:464:TRP:NE1	2.19	0.56
1:B:21:ARG:O	1:B:24:ALA:HB3	2.06	0.56
1:B:136:ALA:HB1	1:B:149:LEU:HD21	1.87	0.56
1:B:155:VAL:HG22	1:B:168:PHE:CG	2.40	0.56
1:B:441:THR:O	1:B:461:LEU:HB2	2.05	0.56
1:B:245:GLU:O	1:B:246:ASP:C	2.48	0.56
1:A:67:PRO:O	1:A:69:SER:N	2.38	0.56
1:B:163:ARG:O	1:B:447:HIS:CD2	2.58	0.56
1:A:588:MSE:CE	1:A:590:SER:O	2.47	0.56
1:A:485:PHE:N	1:A:485:PHE:CD2	2.73	0.56
1:A:105:TYR:CE2	1:A:109:VAL:HG11	2.41	0.56
1:A:308:ARG:CG	1:A:311:ARG:HH21	2.19	0.55
1:B:244:GLY:O	1:B:247:LEU:HB3	2.06	0.55
1:A:197:ARG:HH22	1:A:206:GLN:NE2	2.04	0.55
1:A:488:ASN:HD21	1:A:491:ASP:H	1.52	0.55
1:A:18:LEU:HD12	1:A:57:VAL:HG12	1.89	0.55
1:B:63:SER:OG	1:B:65:HIS:CD2	2.58	0.55
1:A:556:LEU:HG	1:A:556:LEU:O	2.05	0.55
1:A:420:THR:CG2	1:A:572:PRO:O	2.52	0.55
1:A:329:GLN:HB3	1:B:329:GLN:HE21	1.71	0.55
1:B:37:THR:HA	1:B:53:ASP:CG	2.32	0.55
1:B:93:MSE:HE3	1:B:105:TYR:CZ	2.42	0.55
1:A:413:THR:OG1	1:A:423:GLY:HA3	2.07	0.55
1:B:430:LYS:HB2	1:B:435:VAL:CG1	2.37	0.55
1:A:529:ALA:HB1	1:A:530:PRO:CD	2.38	0.54
1:B:31:ARG:CA	1:B:72:ASP:OD2	2.49	0.54
1:B:462:THR:CG2	1:B:463:GLY:H	2.21	0.54
1:A:416:ARG:CB	1:A:419:PHE:O	2.53	0.54
1:B:58:GLY:O	1:B:365:GLY:HA3	2.08	0.54
1:B:494:LEU:O	1:B:494:LEU:HD12	2.08	0.54
1:A:370:GLU:HB3	1:A:375:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:MSE:HE3	1:A:442:MSE:N	2.23	0.54
1:B:187:GLU:OE2	1:B:218:HIS:HB2	2.07	0.54
1:A:474:THR:HG23	1:A:524:GLY:O	2.07	0.54
1:B:440:ALA:HB1	1:B:462:THR:HA	1.90	0.53
1:A:197:ARG:HH22	1:A:206:GLN:HE21	1.57	0.53
1:A:522:LEU:HB2	1:A:526:VAL:CG2	2.38	0.53
1:A:386:LEU:HD22	1:A:523:SER:OG	2.08	0.53
1:B:551:TRP:CH2	1:B:558:PHE:HA	2.43	0.53
1:B:223:LYS:O	1:B:224:ASN:C	2.51	0.53
1:B:413:THR:HB	1:B:460:PHE:O	2.09	0.53
1:B:467:TRP:O	1:B:487:GLY:HA3	2.09	0.53
1:B:447:HIS:CE1	1:B:451:MSE:H	2.26	0.53
1:B:280:LEU:HB2	1:B:318:TRP:CE3	2.43	0.53
1:B:554:PRO:O	1:B:555:TYR:HB2	2.08	0.53
1:B:49:LEU:HD11	1:B:317:GLU:OE2	2.08	0.53
1:A:106:ALA:O	1:A:110:VAL:HB	2.09	0.52
1:B:239:HIS:HD2	1:B:240:GLU:CG	2.20	0.52
1:B:586:LYS:C	1:B:587:VAL:CG2	2.81	0.52
1:B:196:GLU:O	1:B:197:ARG:CB	2.55	0.52
1:A:68:ALA:O	1:A:70:ARG:N	2.43	0.52
1:A:415:ASP:O	1:A:416:ARG:HB2	2.08	0.52
1:A:66:GLU:CG	1:A:69:SER:HB3	2.39	0.52
1:A:263:HIS:HB3	1:A:265:HIS:CE1	2.44	0.52
1:B:449:HIS:CD2	1:B:481:ASN:ND2	2.78	0.52
1:B:409:VAL:HB	1:B:429:VAL:CG2	2.40	0.51
1:A:20:ALA:HB2	1:B:197:ARG:HE	1.75	0.51
1:A:162:GLU:HA	1:A:577:MSE:HG3	1.93	0.51
1:A:359:ARG:HG2	1:A:360:HIS:CD2	2.45	0.51
1:A:458:THR:HG22	1:A:459:GLY:N	2.23	0.51
1:B:395:ARG:C	1:B:396:MSE:HG3	2.34	0.51
1:A:395:ARG:HD2	1:A:395:ARG:N	2.26	0.51
1:A:23:VAL:CG2	1:B:233:ALA:HB2	2.41	0.51
1:B:126:ASN:N	1:B:126:ASN:HD22	2.08	0.51
1:B:505:GLY:HA2	1:B:520:LEU:HD12	1.92	0.51
1:B:574:GLN:HG3	1:B:575:THR:N	2.26	0.51
1:B:35:LEU:HD12	1:B:73:ALA:HB2	1.93	0.51
1:A:46:THR:HB	1:B:277:LEU:HD11	1.93	0.50
1:A:137:ALA:O	1:A:140:ILE:HG13	2.11	0.50
1:A:403:LYS:HA	1:A:432:GLY:O	2.11	0.50
1:B:558:PHE:O	1:B:561:CYS:HB2	2.11	0.50
1:B:83:TYR:N	1:B:83:TYR:CD2	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ALA:HB2	1:B:228:ASN:ND2	2.26	0.50
1:B:311:ARG:HB3	1:B:312:TYR:HD2	1.76	0.50
1:B:35:LEU:HD23	1:B:54:ILE:O	2.12	0.50
1:B:427:ALA:HB1	1:B:434:VAL:CG1	2.40	0.50
1:A:324:THR:HB	1:A:337:GLY:HA2	1.94	0.50
1:A:520:LEU:N	1:A:521:PRO:HD3	2.25	0.50
1:B:427:ALA:HB2	1:B:437:PRO:HG3	1.92	0.50
1:B:513:LYS:HG2	1:B:514:VAL:N	2.27	0.50
1:B:168:PHE:O	1:B:200:ARG:NH2	2.45	0.49
1:A:475:VAL:HB	1:A:506:MSE:HE2	1.94	0.49
1:B:268:PRO:HD3	1:B:312:TYR:CD1	2.47	0.49
1:A:187:GLU:HA	1:A:216:CYS:O	2.12	0.49
1:B:432:GLY:HA2	3:B:640:HOH:O	2.12	0.49
1:B:440:ALA:CB	1:B:462:THR:HA	2.43	0.49
1:B:551:TRP:CH2	1:B:558:PHE:HD1	2.31	0.49
1:A:131:ASP:HB2	3:A:612:HOH:O	2.12	0.49
1:B:572:PRO:O	1:B:573:HIS:CD2	2.65	0.49
1:A:179:TRP:N	1:A:179:TRP:CD1	2.80	0.49
1:A:191:MSE:HE1	1:A:220:ARG:O	2.13	0.49
1:B:414:ILE:HB	1:B:461:LEU:HD23	1.94	0.49
1:A:15:ASP:OD2	1:A:17:THR:HB	2.13	0.49
1:A:542:ARG:HG3	1:A:558:PHE:HD2	1.78	0.49
1:B:191:MSE:HE1	1:B:220:ARG:O	2.12	0.49
1:B:92:HIS:O	1:B:287:CYS:HB2	2.13	0.49
1:B:505:GLY:N	1:B:520:LEU:HB2	2.28	0.49
1:A:447:HIS:HE1	1:A:451:MSE:H	1.60	0.48
1:A:467:TRP:CD1	1:A:467:TRP:N	2.79	0.48
1:A:542:ARG:HG3	1:A:558:PHE:CD2	2.48	0.48
1:B:88:LEU:HG	1:B:113:GLY:O	2.13	0.48
1:B:469:GLY:HA3	1:B:509:ALA:O	2.13	0.48
1:A:63:SER:OG	1:A:65:HIS:CD2	2.59	0.48
1:B:370:GLU:O	1:B:371:GLY:C	2.56	0.48
1:A:442:MSE:HG2	1:A:458:THR:HG21	1.95	0.48
1:A:413:THR:HG23	1:A:425:THR:HG22	1.95	0.48
1:B:8:ALA:O	1:B:12:ASP:HB3	2.14	0.48
1:B:416:ARG:HB3	3:B:626:HOH:O	2.13	0.48
1:B:430:LYS:HD2	1:B:431:ASP:H	1.77	0.48
1:B:488:ASN:O	1:B:492:MSE:CG	2.52	0.48
1:B:56:ILE:HG23	1:B:60:LEU:O	2.13	0.48
1:A:471:PHE:HD1	1:A:508:VAL:HG23	1.78	0.48
1:B:55:GLY:O	1:B:62:ALA:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:VAL:O	1:B:426:GLU:HG3	2.13	0.48
1:B:448:ARG:O	1:B:448:ARG:CD	2.62	0.48
1:A:40:THR:O	1:A:83:TYR:HA	2.14	0.47
1:A:144:PRO:HG2	1:A:374:MSE:HE1	1.95	0.47
1:B:485:PHE:CZ	1:B:561:CYS:HA	2.48	0.47
1:B:520:LEU:HD22	1:B:526:VAL:C	2.38	0.47
1:A:392:LEU:O	1:A:392:LEU:HG	2.12	0.47
1:B:545:VAL:C	1:B:547:LYS:H	2.22	0.47
1:A:34:VAL:HG12	1:A:35:LEU:N	2.29	0.47
1:B:242:VAL:HG22	1:B:246:ASP:OD2	2.15	0.47
1:B:394:LEU:C	1:B:395:ARG:HD2	2.40	0.47
1:A:161:LEU:N	1:A:161:LEU:HD13	2.30	0.47
1:A:228:ASN:HD21	1:B:64:VAL:H	1.60	0.47
1:B:346:ASP:HA	1:B:362:LEU:O	2.13	0.47
1:B:469:GLY:N	1:B:548:VAL:HG13	2.29	0.47
1:A:92:HIS:O	1:A:287:CYS:HB2	2.14	0.47
1:A:395:ARG:N	1:A:497:ASN:OD1	2.41	0.47
1:B:185:ILE:HG22	1:B:186:ALA:O	2.15	0.47
1:B:251:LEU:HD12	1:B:251:LEU:HA	1.64	0.47
1:A:67:PRO:C	1:A:69:SER:N	2.72	0.47
1:A:99:MSE:HA	1:A:526:VAL:HA	1.97	0.47
1:A:216:CYS:HB3	1:A:237:SER:OG	2.14	0.47
1:B:485:PHE:CD2	1:B:485:PHE:N	2.80	0.47
1:B:409:VAL:HB	1:B:429:VAL:HG23	1.96	0.47
1:A:301:GLY:O	1:A:302:LEU:C	2.56	0.47
1:B:204:ILE:HD13	1:B:204:ILE:HG21	1.61	0.47
1:A:248:MSE:O	1:A:252:ARG:HG3	2.15	0.46
1:B:517:ILE:O	1:B:519:PRO:HD3	2.15	0.46
1:A:136:ALA:HB1	1:A:149:LEU:HD21	1.97	0.46
1:A:522:LEU:HB2	1:A:526:VAL:HG23	1.98	0.46
1:B:311:ARG:HG2	1:B:311:ARG:HH11	1.79	0.46
1:A:231:MSE:HE1	1:A:253:ALA:O	2.15	0.46
1:B:182:ILE:CG2	1:B:184:GLY:H	2.28	0.46
1:B:266:LEU:CD2	1:B:269:GLU:OE1	2.63	0.46
1:B:533:GLU:CB	3:B:645:HOH:O	2.63	0.46
1:A:403:LYS:HE3	1:A:432:GLY:HA2	1.96	0.46
1:B:318:TRP:N	1:B:318:TRP:CD1	2.81	0.46
1:A:25:ALA:HB1	1:A:32:PHE:CD1	2.51	0.46
1:B:129:GLY:O	1:B:130:VAL:C	2.59	0.46
1:B:265:HIS:CD2	1:B:266:LEU:HG	2.50	0.46
1:B:468:ASN:N	1:B:548:VAL:HG13	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:HA	1:A:116:THR:O	2.16	0.46
1:B:24:ALA:O	1:B:25:ALA:C	2.56	0.46
1:B:122:HIS:CA	1:B:152:PRO:HB3	2.45	0.46
1:B:89:ILE:HG12	1:B:116:THR:HB	1.98	0.45
1:B:449:HIS:HD2	1:B:481:ASN:HD21	1.64	0.45
1:A:112:ARG:NH1	1:A:303:ASP:OD2	2.49	0.45
1:A:424:GLU:C	1:A:425:THR:HG22	2.40	0.45
1:B:566:LEU:HG	1:B:566:LEU:O	2.16	0.45
1:B:95:ILE:HG13	1:B:119:TRP:CD2	2.51	0.45
1:B:113:GLY:HA3	1:B:348:VAL:HG21	1.97	0.45
1:B:250:LYS:HE2	3:B:649:HOH:O	2.16	0.45
1:B:448:ARG:C	1:B:448:ARG:HD2	2.41	0.45
1:A:66:GLU:HG3	1:A:69:SER:HB3	1.98	0.45
1:A:109:VAL:HG23	1:A:114:VAL:HB	1.98	0.45
1:A:144:PRO:HG2	1:A:374:MSE:CE	2.46	0.45
1:A:508:VAL:HG12	1:A:515:THR:OG1	2.16	0.45
1:B:449:HIS:CD2	1:B:481:ASN:HD21	2.34	0.45
1:B:556:LEU:O	1:B:556:LEU:CG	2.63	0.45
1:B:348:VAL:O	1:B:348:VAL:HG13	2.15	0.45
1:A:568:CYS:HB3	3:A:628:HOH:O	2.16	0.45
1:B:185:ILE:CD1	1:B:208:GLY:HA3	2.47	0.45
1:B:398:ASN:O	1:B:400:PHE:N	2.50	0.45
1:A:140:ILE:HD13	1:A:147:ALA:HB3	1.99	0.45
1:A:490:GLY:C	1:A:492:MSE:H	2.25	0.45
1:B:9:GLU:HA	1:B:10:PRO:HA	1.50	0.45
1:B:317:GLU:HB3	3:B:638:HOH:O	2.17	0.45
1:B:448:ARG:CD	1:B:448:ARG:C	2.90	0.45
1:B:457:LYS:HA	1:B:457:LYS:NZ	2.32	0.45
1:A:494:LEU:HD22	1:A:514:VAL:HG23	1.99	0.45
1:A:485:PHE:C	1:A:492:MSE:HE3	2.41	0.45
1:B:282:GLN:HA	1:B:326:ASN:ND2	2.32	0.45
1:B:383:THR:HB	1:B:522:LEU:HD22	1.98	0.45
1:A:146:ARG:HH22	1:A:344:ARG:HD3	1.82	0.45
1:A:305:VAL:O	1:A:306:VAL:C	2.60	0.45
1:B:279:HIS:O	1:B:281:PRO:HD3	2.17	0.45
1:B:422:TRP:NE1	1:B:572:PRO:HG3	2.32	0.45
1:A:146:ARG:HB2	1:A:146:ARG:CZ	2.48	0.44
1:A:529:ALA:HB1	1:A:530:PRO:HD2	2.00	0.44
1:B:259:LEU:HD11	1:B:270:PHE:CD2	2.52	0.44
1:B:474:THR:HG23	1:B:524:GLY:O	2.16	0.44
1:A:295:ASP:O	1:A:299:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:THR:CG2	1:A:571:GLY:HA3	2.45	0.44
1:B:93:MSE:HE1	1:B:95:ILE:HG12	1.99	0.44
1:B:385:VAL:O	1:B:385:VAL:HG13	2.17	0.44
1:A:120:ASP:C	1:A:122:HIS:H	2.26	0.44
1:A:327:ALA:HB2	3:A:634:HOH:O	2.18	0.44
1:A:477:HIS:HA	1:A:478:ASP:HA	1.60	0.44
1:A:23:VAL:HG21	1:B:233:ALA:HB2	1.99	0.44
1:A:161:LEU:N	1:A:161:LEU:CD1	2.80	0.44
1:B:151:ALA:N	1:B:184:GLY:O	2.49	0.44
1:B:257:ILE:O	1:B:285:THR:OG1	2.31	0.44
1:B:447:HIS:HE1	1:B:451:MSE:H	1.66	0.44
1:A:280:LEU:HD23	3:A:632:HOH:O	2.18	0.44
1:B:19:ARG:HA	1:B:19:ARG:HD3	1.81	0.44
1:A:558:PHE:C	1:A:560:ALA:N	2.75	0.44
1:B:477:HIS:HA	1:B:478:ASP:HA	1.40	0.44
1:A:436:PRO:HA	1:A:437:PRO:HD3	1.84	0.44
1:B:36:ILE:O	1:B:53:ASP:HA	2.18	0.44
1:A:45:VAL:HG23	1:A:338:LEU:HD13	1.99	0.44
1:B:350:PHE:CE1	1:B:356:PHE:HB3	2.53	0.44
1:B:584:THR:O	1:B:586:LYS:N	2.51	0.44
1:B:90:ASP:HA	1:B:302:LEU:HD13	1.99	0.43
1:B:270:PHE:CD1	1:B:270:PHE:N	2.84	0.43
1:B:435:VAL:HG23	1:B:436:PRO:HD2	1.99	0.43
1:B:446:THR:O	1:B:481:ASN:HB3	2.17	0.43
1:B:494:LEU:HD13	1:B:494:LEU:HA	1.66	0.43
1:B:533:GLU:HB2	3:B:645:HOH:O	2.18	0.43
1:A:158:ALA:HB1	1:A:161:LEU:HD22	2.00	0.43
1:B:582:VAL:HG13	1:B:583:LEU:H	1.82	0.43
1:B:98:SER:O	1:B:100:ILE:HG23	2.18	0.43
1:B:435:VAL:CG2	1:B:436:PRO:HD2	2.49	0.43
1:A:192:ARG:HA	1:A:192:ARG:HD3	1.59	0.43
1:A:522:LEU:HB2	1:A:526:VAL:HG22	2.01	0.43
1:B:390:MSE:HE3	1:B:392:LEU:HD21	2.01	0.43
1:B:569:ASN:HA	3:B:635:HOH:O	2.18	0.43
1:A:437:PRO:O	1:A:438:GLU:C	2.60	0.43
1:A:461:LEU:HD13	1:A:464:TRP:CE2	2.53	0.43
1:A:519:PRO:C	1:A:521:PRO:HD3	2.43	0.43
1:B:182:ILE:HG22	1:B:184:GLY:N	2.30	0.43
1:A:548:VAL:HG13	1:A:548:VAL:O	2.18	0.43
1:A:554:PRO:O	1:A:554:PRO:CD	2.62	0.43
1:B:122:HIS:HA	1:B:152:PRO:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:ARG:HG2	1:B:311:ARG:NH1	2.34	0.43
1:A:145:LEU:HA	1:A:145:LEU:HD12	1.84	0.43
1:A:261:GLY:O	1:A:308:ARG:NH2	2.52	0.43
1:A:373:ARG:HG3	1:A:373:ARG:NH1	2.17	0.43
1:A:510:SER:N	1:A:513:LYS:O	2.39	0.43
1:B:89:ILE:HG21	1:B:327:ALA:HB1	2.00	0.43
1:B:123:GLU:OE1	1:B:480:HIS:CE1	2.72	0.43
1:A:20:ALA:HB2	1:B:197:ARG:NE	2.34	0.42
1:A:128:HIS:HB2	1:A:132:GLY:CA	2.49	0.42
1:B:86:PRO:N	1:B:339:ILE:HD11	2.35	0.42
1:B:168:PHE:CD1	1:B:172:ILE:HG21	2.54	0.42
1:B:183:GLY:O	1:B:214:LEU:HD12	2.18	0.42
1:B:457:LYS:HB3	1:B:574:GLN:HE21	1.84	0.42
1:B:484:VAL:HG12	1:B:492:MSE:HE3	2.00	0.42
1:B:520:LEU:HD23	1:B:520:LEU:HA	1.93	0.42
1:A:195:ILE:O	1:A:195:ILE:HG22	2.15	0.42
1:B:513:LYS:HE2	1:B:513:LYS:HB3	1.41	0.42
1:A:228:ASN:HD22	1:B:341:ALA:HB2	1.85	0.42
1:B:23:VAL:O	1:B:26:ALA:HB3	2.19	0.42
1:A:35:LEU:HA	1:A:54:ILE:O	2.20	0.42
1:B:22:ALA:HB1	1:B:62:ALA:HB2	2.00	0.42
1:B:85:SER:C	1:B:339:ILE:HD11	2.44	0.42
1:B:104:ALA:O	1:B:107:ALA:HB3	2.20	0.42
1:B:231:MSE:SE	1:B:231:MSE:HB3	2.70	0.42
1:A:18:LEU:HG	1:A:60:LEU:HD12	2.01	0.42
1:A:130:VAL:O	1:A:134:ARG:N	2.48	0.42
1:A:417:PRO:O	1:A:418:ARG:HB3	2.20	0.42
1:A:475:VAL:HG22	1:A:525:LEU:HD23	2.00	0.42
1:B:11:ALA:HA	1:B:14:ASN:ND2	2.34	0.42
1:B:518:LEU:HD13	1:B:537:ALA:HB3	2.01	0.42
1:A:34:VAL:CG1	1:A:35:LEU:N	2.82	0.42
1:A:416:ARG:HA	1:A:417:PRO:HD3	1.91	0.42
1:A:545:VAL:C	1:A:547:LYS:H	2.27	0.42
1:B:99:MSE:HA	1:B:526:VAL:HA	2.01	0.42
1:B:268:PRO:HD3	1:B:312:TYR:CE1	2.55	0.42
1:B:340:ALA:O	1:B:341:ALA:C	2.58	0.42
1:B:474:THR:CG2	1:B:524:GLY:O	2.68	0.42
1:A:514:VAL:HG11	1:A:517:ILE:HD11	2.00	0.42
1:B:475:VAL:HG22	1:B:525:LEU:HA	2.01	0.42
1:B:571:GLY:O	1:B:573:HIS:CD2	2.73	0.42
1:A:448:ARG:N	1:A:481:ASN:ND2	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:VAL:C	1:A:547:LYS:N	2.78	0.42
1:B:395:ARG:O	1:B:396:MSE:HG3	2.20	0.42
1:A:457:LYS:HB3	1:A:574:GLN:NE2	2.34	0.42
1:A:490:GLY:C	1:A:492:MSE:N	2.77	0.42
1:B:548:VAL:O	1:B:548:VAL:CG1	2.68	0.42
1:A:582:VAL:H	1:A:582:VAL:HG12	1.42	0.42
1:B:198:ASP:O	1:B:202:SER:HB2	2.19	0.42
1:B:505:GLY:HA2	1:B:520:LEU:CB	2.37	0.42
1:B:506:MSE:HE3	1:B:520:LEU:HD11	2.02	0.42
1:A:167:ASP:O	1:A:168:PHE:HD1	2.03	0.41
1:A:198:ASP:HA	1:A:199:PRO:HD3	1.83	0.41
1:A:277:LEU:HD12	1:A:277:LEU:HA	1.64	0.41
1:A:418:ARG:HD3	1:A:419:PHE:CE2	2.55	0.41
1:B:192:ARG:O	1:B:193:GLY:C	2.61	0.41
1:B:282:GLN:HA	1:B:326:ASN:HD21	1.85	0.41
1:A:66:GLU:HG2	1:A:69:SER:HB3	2.02	0.41
1:A:252:ARG:HG2	1:B:46:THR:HG21	2.00	0.41
1:B:151:ALA:O	1:B:152:PRO:C	2.60	0.41
1:B:520:LEU:HD22	1:B:526:VAL:CA	2.50	0.41
1:A:46:THR:OG1	1:A:48:GLU:HG3	2.20	0.41
1:A:119:TRP:CD1	1:A:119:TRP:C	2.94	0.41
1:B:294:ASP:CA	1:B:535:ALA:HB1	2.47	0.41
1:B:218:HIS:CE1	1:B:240:GLU:CD	2.98	0.41
1:A:90:ASP:O	1:A:118:VAL:HB	2.20	0.41
1:A:155:VAL:HG22	1:A:168:PHE:CG	2.56	0.41
1:A:443:ILE:HB	1:A:461:LEU:HD21	2.02	0.41
1:B:119:TRP:CD1	1:B:119:TRP:C	2.95	0.41
1:B:155:VAL:O	1:B:155:VAL:HG23	2.20	0.41
1:A:92:HIS:CE1	1:A:187:GLU:HG2	2.42	0.41
1:A:428:ASP:C	1:A:435:VAL:HG23	2.46	0.41
1:A:520:LEU:HD13	1:A:525:LEU:O	2.21	0.41
1:B:175:ASP:O	1:B:178:SER:OG	2.38	0.41
1:A:95:ILE:O	1:A:96:GLU:C	2.61	0.41
1:A:491:ASP:CG	1:A:511:GLU:H	2.29	0.41
1:B:429:VAL:HA	1:B:435:VAL:H	1.86	0.41
1:A:54:ILE:CG2	1:A:61:ILE:HG23	2.51	0.41
1:A:136:ALA:O	1:A:140:ILE:HG12	2.21	0.41
1:A:558:PHE:C	1:A:560:ALA:H	2.29	0.41
1:B:31:ARG:CB	1:B:72:ASP:OD2	2.69	0.41
1:B:155:VAL:HA	1:B:156:PRO:HA	1.65	0.41
1:B:447:HIS:HB2	1:B:576:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LYS:O	1:A:224:ASN:C	2.64	0.41
1:B:398:ASN:C	1:B:400:PHE:N	2.79	0.41
1:B:399:ASP:OD1	1:B:456:THR:HG23	2.21	0.41
1:B:584:THR:C	1:B:586:LYS:N	2.79	0.41
1:A:36:ILE:N	1:A:54:ILE:O	2.45	0.40
1:A:447:HIS:HD2	1:A:576:ASP:OD1	2.04	0.40
1:B:13:LEU:HD23	1:B:13:LEU:HA	1.93	0.40
1:B:196:GLU:O	1:B:197:ARG:HB3	2.21	0.40
1:B:375:LEU:HD23	1:B:375:LEU:HA	1.92	0.40
1:B:433:PHE:CD2	1:B:433:PHE:N	2.89	0.40
1:B:451:MSE:O	1:B:452:ALA:HB2	2.20	0.40
1:B:554:PRO:O	1:B:555:TYR:CB	2.70	0.40
1:A:252:ARG:HB3	1:B:50:ARG:NH2	2.36	0.40
1:A:485:PHE:N	1:A:485:PHE:HD2	2.18	0.40
1:A:13:LEU:O	1:A:19:ARG:NE	2.53	0.40
1:B:135:TRP:O	1:B:136:ALA:C	2.64	0.40
1:A:471:PHE:CD1	1:A:508:VAL:HG23	2.55	0.40
1:B:155:VAL:O	1:B:155:VAL:CG2	2.69	0.40
1:B:161:LEU:CD1	1:B:161:LEU:H	2.31	0.40
1:B:185:ILE:HD11	1:B:208:GLY:CA	2.51	0.40
1:A:413:THR:OG1	1:A:423:GLY:CA	2.70	0.40
1:B:69:SER:O	1:B:70:ARG:HG2	2.22	0.40
1:B:388:GLY:HA2	3:B:634:HOH:O	2.21	0.40
1:B:395:ARG:N	1:B:497:ASN:OD1	2.49	0.40
1:B:506:MSE:HE3	1:B:520:LEU:CD1	2.52	0.40
1:B:563:GLY:O	1:B:565:THR:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	585/608 (96%)	520 (89%)	49 (8%)	16 (3%)	4	15
1	B	585/608 (96%)	483 (83%)	69 (12%)	33 (6%)	1	4
All	All	1170/1216 (96%)	1003 (86%)	118 (10%)	49 (4%)	2	7

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
1	A	406	GLY
1	B	72	ASP
1	B	224	ASN
1	B	418	ARG
1	B	428	ASP
1	B	429	VAL
1	B	461	LEU
1	B	583	LEU
1	B	584	THR
1	B	585	GLY
1	B	593	ILE
1	A	69	SER
1	A	418	ARG
1	A	555	TYR
1	A	589	GLU
1	B	299	GLY
1	B	303	ASP
1	B	364	SER
1	B	371	GLY
1	B	399	ASP
1	B	555	TYR
1	A	74	ALA
1	A	380	THR
1	A	397	ALA
1	A	416	ARG
1	A	543	GLU
1	A	544	ALA
1	B	247	LEU
1	B	311	ARG
1	B	388	GLY
1	B	397	ALA
1	A	583	LEU
1	B	186	ALA
1	B	197	ARG

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Mol	Chain	Res	Type
1	B	404	SER
1	B	411	LEU
1	B	416	ARG
1	B	523	SER
1	B	564	ALA
1	B	573	HIS
1	B	576	ASP
1	A	136	ALA
1	A	302	LEU
1	A	425	THR
1	B	68	ALA
1	B	414	ILE
1	B	587	VAL
1	B	417	PRO

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	445/444 (100%)	371 (83%)	74 (17%)	2	8
1	B	444/444 (100%)	370 (83%)	74 (17%)	2	8
All	All	889/888 (100%)	741 (83%)	148 (17%)	2	8

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	23	VAL
1	A	31	ARG
1	A	35	LEU
1	A	66	GLU
1	A	72	ASP
1	A	77	ILE
1	A	78	ASP
1	A	84	VAL

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Mol	Chain	Res	Type
1	A	94	HIS
1	A	98	SER
1	A	99	MSE
1	A	109	VAL
1	A	120	ASP
1	A	122	HIS
1	A	131	ASP
1	A	134	ARG
1	A	140	ILE
1	A	152	PRO
1	A	155	VAL
1	A	161	LEU
1	A	172	ILE
1	A	175	ASP
1	A	182	ILE
1	A	189	MSE
1	A	191	MSE
1	A	192	ARG
1	A	201	MSE
1	A	209	LEU
1	A	227	LEU
1	A	235	VAL
1	A	245	GLU
1	A	259	LEU
1	A	280	LEU
1	A	290	ASP
1	A	334	SER
1	A	347	ILE
1	A	354	ASN
1	A	359	ARG
1	A	373	ARG
1	A	380	THR
1	A	396	MSE
1	A	408	LYS
1	A	420	THR
1	A	425	THR
1	A	426	GLU
1	A	430	LYS
1	A	434	VAL
1	A	435	VAL
1	A	438	GLU
1	A	442	MSE

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Mol	Chain	Res	Type
1	A	444	SER
1	A	453	GLU
1	A	461	LEU
1	A	462	THR
1	A	466	ARG
1	A	476	SER
1	A	483	THR
1	A	494	LEU
1	A	508	VAL
1	A	515	THR
1	A	518	LEU
1	A	528	ASP
1	A	536	ARG
1	A	543	GLU
1	A	548	VAL
1	A	552	GLN
1	A	577	MSE
1	A	583	LEU
1	A	584	THR
1	A	587	VAL
1	A	588	MSE
1	A	592	VAL
1	A	594	GLU
1	B	10	PRO
1	B	12	ASP
1	B	17	THR
1	B	30	GLN
1	B	35	LEU
1	B	42	VAL
1	B	71	ARG
1	B	75	GLN
1	B	95	ILE
1	B	96	GLU
1	B	97	SER
1	B	101	THR
1	B	126	ASN
1	B	155	VAL
1	B	161	LEU
1	B	173	LEU
1	B	178	SER
1	B	189	MSE
1	B	192	ARG

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Mol	Chain	Res	Type
1	B	196	GLU
1	B	218	HIS
1	B	226	ASP
1	B	228	ASN
1	B	241	LEU
1	B	242	VAL
1	B	243	SER
1	B	245	GLU
1	B	251	LEU
1	B	255	LEU
1	B	267	LEU
1	B	280	LEU
1	B	290	ASP
1	B	295	ASP
1	B	302	LEU
1	B	311	ARG
1	B	357	SER
1	B	362	LEU
1	B	382	ASP
1	B	385	VAL
1	B	402	VAL
1	B	408	LYS
1	B	409	VAL
1	B	411	LEU
1	B	414	ILE
1	B	416	ARG
1	B	420	THR
1	B	425	THR
1	B	428	ASP
1	B	430	LYS
1	B	441	THR
1	B	442	MSE
1	B	444	SER
1	B	445	VAL
1	B	455	THR
1	B	456	THR
1	B	457	LYS
1	B	474	THR
1	B	483	THR
1	B	485	PHE
1	B	492	MSE
1	B	494	LEU

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Mol	Chain	Res	Type
1	B	499	VAL
1	B	510	SER
1	B	517	ILE
1	B	523	SER
1	B	526	VAL
1	B	531	LEU
1	B	556	LEU
1	B	559	LYS
1	B	570	ILE
1	B	575	THR
1	B	590	SER
1	B	592	VAL
1	B	593	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	65	HIS
1	A	126	ASN
1	A	206	GLN
1	A	228	ASN
1	A	279	HIS
1	A	282	GLN
1	A	326	ASN
1	A	398	ASN
1	A	447	HIS
1	A	481	ASN
1	A	488	ASN
1	A	573	HIS
1	B	14	ASN
1	B	65	HIS
1	B	126	ASN
1	B	128	HIS
1	B	228	ASN
1	B	265	HIS
1	B	279	HIS
1	B	329	GLN
1	B	447	HIS
1	B	480	HIS
1	B	481	ASN
1	B	552	GLN

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Mol	Chain	Res	Type
1	B	573	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	571/608 (93%)	-0.64	0	100 100	28, 44, 66, 80	0
1	B	571/608 (93%)	-0.27	26 (4%)	37 29	23, 47, 83, 98	27 (4%)
All	All	1142/1216 (93%)	-0.46	26 (2%)	61 51	23, 46, 75, 98	27 (2%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	419	PHE	7.9
1	B	418	ARG	6.1
1	B	427	ALA	5.7
1	B	417	PRO	5.4
1	B	593	ILE	5.3
1	B	422	TRP	4.9
1	B	423	GLY	4.8
1	B	589	GLU	4.8
1	B	590	SER	4.4
1	B	415	ASP	4.4
1	B	414	ILE	4.4
1	B	428	ASP	4.3
1	B	430	LYS	4.3
1	B	411	LEU	4.2
1	B	429	VAL	4.1
1	B	420	THR	4.1
1	B	421	GLN	3.9
1	B	425	THR	3.8
1	B	591	PRO	3.7
1	B	592	VAL	3.5
1	B	413	THR	3.3
1	B	412	ALA	3.3
1	B	594	GLU	2.9
1	B	416	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	426	GLU	2.5
1	B	410	ARG	2.3

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	UNX	A	606	1/1	0.39	0.55	53,53,53,53	0
2	UNX	B	607	1/1	0.47	0.41	60,60,60,60	0
2	UNX	A	608	1/1	0.52	0.52	43,43,43,43	0
2	UNX	A	607	1/1	0.54	0.49	43,43,43,43	0
2	UNX	B	608	1/1	0.80	0.42	50,50,50,50	0
2	UNX	B	606	1/1	0.84	0.42	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.