



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 08:00 am BST

PDB ID : 3LC6
Title : The alternative conformation structure of isocitrate dehydrogenase kinase/phosphatase from E. Coli
Authors : Zheng, J.; Jia, Z.
Deposited on : 2010-01-09
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

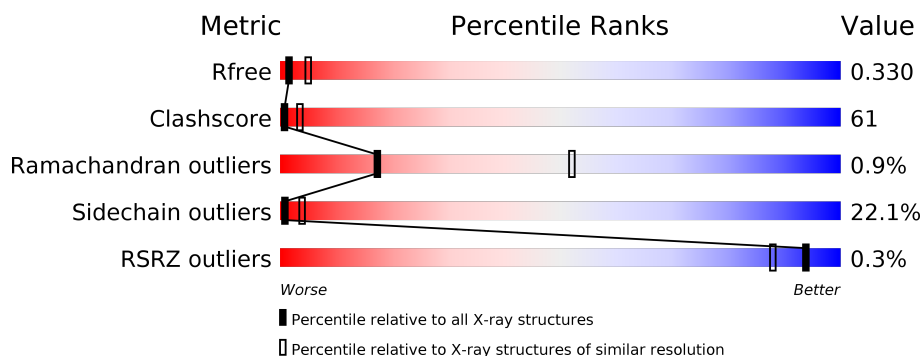
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	578	<div> <div></div> <div>24%</div> <div>56%</div> <div>14%</div> <div>• 5%</div> </div>
1	B	578	<div> <div>27%</div> <div>52%</div> <div>14%</div> <div>7%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9107 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 Isocitrate dehydrogenase kinase/phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4526	2906	800	799	21			
1	B	539	Total	C	N	O	S	0	0	0
			4454	2861	785	788	20			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

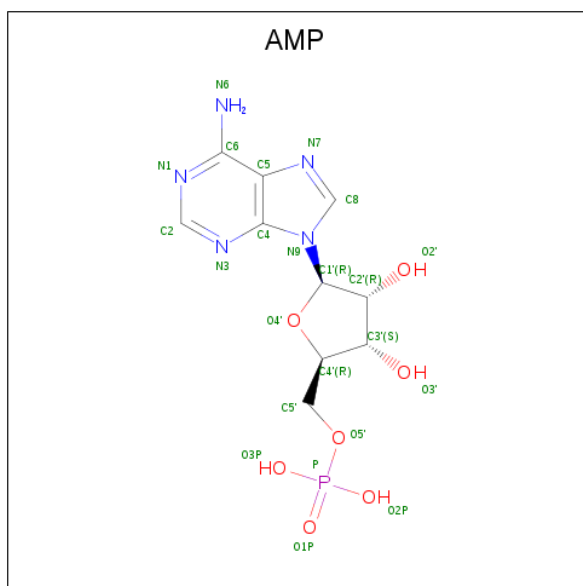


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O P 23 10 5 7 1	0	0

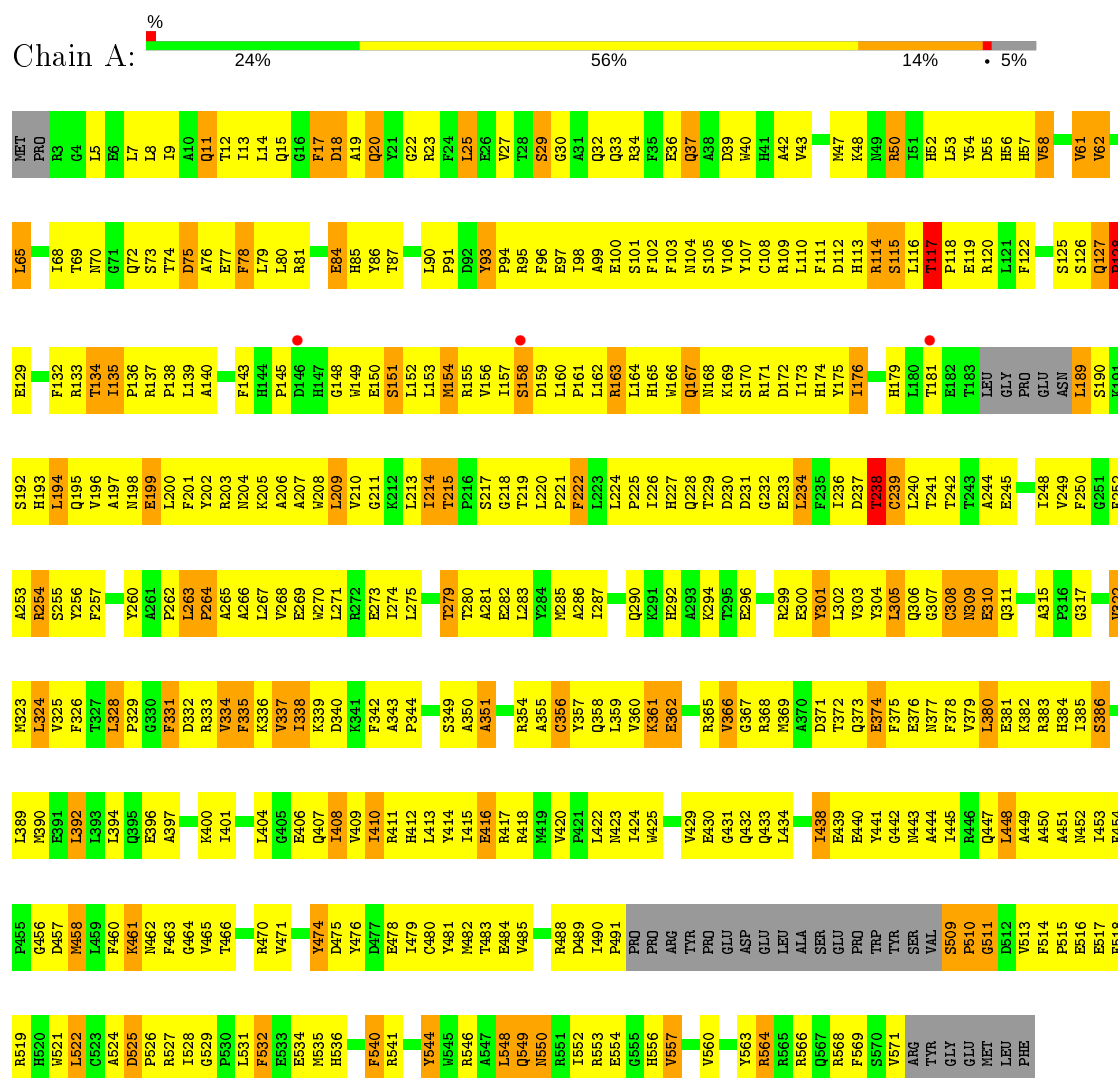
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	31	Total O 31 31	0	0
5	B	45	Total O 45 45	0	0

3 Residue-property plots

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

- Molecule 1: Isocitrate dehydrogenase kinase/phosphatase



- Molecule 1: Isocitrate dehydrogenase kinase/phosphatase



F518	F519	F520	F521	F522	F523	F524	F525	F526	F527	F528	F529	F530	F531	F532	F533	F534	F535	F536	F537	F538	F539	F540	F541	F542	F543	F544	F545	F546	F547	F548	F549	F550	F551	F552	F553	F554	F555	F556	F557	F558	F559	F560	F561	F562	F563	F564	F565	F566	F567	F568	F569	F570	F571	F572	F573	F574	F575	F576	F577	F578	F579	F580	F581	F582	F583	F584	F585	F586	F587	F588	F589	F590	F591	F592	F593	F594	F595	F596	F597	F598	F599	F600	F601	F602	F603	F604	F605	F606	F607	F608	F609	F610	F611	F612	F613	F614	F615	F616	F617	F618	F619	F620	F621	F622	F623	F624	F625	F626	F627	F628	F629	F630	F631	F632	F633	F634	F635	F636	F637	F638	F639	F640	F641	F642	F643	F644	F645	F646	F647	F648	F649	F650	F651	F652	F653	F654	F655	F656	F657	F658	F659	F660	F661	F662	F663	F664	F665	F666	F667	F668	F669	F670	F671	F672	F673	F674	F675	F676	F677	F678	F679	F680	F681	F682	F683	F684	F685	F686	F687	F688	F689	F690	F691	F692	F693	F694	F695	F696	F697	F698	F699	F700	F701	F702	F703	F704	F705	F706	F707	F708	F709	F710	F711	F712	F713	F714	F715	F716	F717	F718	F719	F720	F721	F722	F723	F724	F725	F726	F727	F728	F729	F730	F731	F732	F733	F734	F735	F736	F737	F738	F739	F740	F741	F742	F743	F744	F745	F746	F747	F748	F749	F750	F751	F752	F753	F754	F755	F756	F757	F758	F759	F760	F761	F762	F763	F764	F765	F766	F767	F768	F769	F770	F771	F772	F773	F774	F775	F776	F777	F778	F779	F780	F781	F782	F783	F784	F785	F786	F787	F788	F789	F790	F791	F792	F793	F794	F795	F796	F797	F798	F799	F800	F801	F802	F803	F804	F805	F806	F807	F808	F809	F810	F811	F812	F813	F814	F815	F816	F817	F818	F819	F820	F821	F822	F823	F824	F825	F826	F827	F828	F829	F830	F831	F832	F833	F834	F835	F836	F837	F838	F839	F840	F841	F842	F843	F844	F845	F846	F847	F848	F849	F850	F851	F852	F853	F854	F855	F856	F857	F858	F859	F860	F861	F862	F863	F864	F865	F866	F867	F868	F869	F870	F871	F872	F873	F874	F875	F876	F877	F878	F879	F880	F881	F882	F883	F884	F885	F886	F887	F888	F889	F890	F891	F892	F893	F894	F895	F896	F897	F898	F899	F900	F901	F902	F903	F904	F905	F906	F907	F908	F909	F910	F911	F912	F913	F914	F915	F916	F917	F918	F919	F920	F921	F922	F923	F924	F925	F926	F927	F928	F929	F930	F931	F932	F933	F934	F935	F936	F937	F938	F939	F940	F941	F942	F943	F944	F945	F946	F947	F948	F949	F950	F951	F952	F953	F954	F955	F956	F957	F958	F959	F960	F961	F962	F963	F964	F965	F966	F967	F968	F969	F970	F971	F972	F973	F974	F975	F976	F977	F978	F979	F980	F981	F982	F983	F984	F985	F986	F987	F988	F989	F990	F991	F992	F993	F994	F995	F996	F997	F998	F999	1000																																																																	
1453	1454	1455	1456	1457	1458	1459	1460	1461	1462	1463	1464	1465	1466	1467	1468	1469	1470	1471	1472	1473	1474	1475	1476	1477	1478	1479	1480	1481	1482	1483	1484	1485	1486	1487	1488	1489	1490	1491	1492	1493	1494	1495	1496	1497	1498	1499	1500	1501	1502	1503	1504	1505	1506	1507	1508	1509	1510	1511	1512	1513	1514	1515	1516	1517	1518	1519	1520	1521	1522	1523	1524	1525	1526	1527	1528	1529	1530	1531	1532	1533	1534	1535	1536	1537	1538	1539	1540	1541	1542	1543	1544	1545	1546	1547	1548	1549	1550	1551	1552	1553	1554	1555	1556	1557	1558	1559	1560	1561	1562	1563	1564	1565	1566	1567	1568	1569	1570	1571	1572	1573	1574	1575	1576	1577	1578	1579	1580	1581	1582	1583	1584	1585	1586	1587	1588	1589	1590	1591	1592	1593	1594	1595	1596	1597	1598	1599	1600	1601	1602	1603	1604	1605	1606	1607	1608	1609	1610	1611	1612	1613	1614	1615	1616	1617	1618	1619	1620	1621	1622	1623	1624	1625	1626	1627	1628	1629	1630	1631	1632	1633	1634	1635	1636	1637	1638	1639	1640	1641	1642	1643	1644	1645	1646	1647	1648	1649	1650	1651	1652	1653	1654	1655	1656	1657	1658	1659	1660	1661	1662	1663	1664	1665	1666	1667	1668	1669	1670	1671	1672	1673	1674	1675	1676	1677	1678	1679	1680	1681	1682	1683	1684	1685	1686	1687	1688	1689	1690	1691	1692	1693	1694	1695	1696	1697	1698	1699	1700	1701	1702	1703	1704	1705	1706	1707	1708	1709	1710	1711	1712	1713	1714	1715	1716	1717	1718	1719	1720	1721	1722	1723	1724	1725	1726	1727	1728	1729	1730	1731	1732	1733	1734	1735	1736	1737	1738	1739	1740	1741	1742	1743	1744	1745	1746	1747	1748	1749	1750	1751	1752	1753	1754	1755	1756	1757	1758	1759	1760	1761	1762	1763	1764	1765	1766	1767	1768	1769	1770	1771	1772	1773	1774	1775	1776	1777	1778	1779	1780	1781	1782	1783	1784	1785	1786	1787	1788	1789	1790	1791	1792	1793	1794	1795	1796	1797	1798	1799	1800	1801	1802	1803	1804	1805	1806	1807	1808	1809	1810	1811	1812	1813	1814	1815	1816	1817	1818	1819	1820	1821	1822	1823	1824	1825	1826	1827	1828	1829	1830	1831	1832	1833	1834	1835	1836	1837	1838	1839	1840	1841	1842	1843	1844	1845	1846	1847	1848	1849	1850	1851	1852	1853	1854	1855	1856	1857	1858	1859	1860	1861	1862	1863	1864	1865	1866	1867	1868	1869	1870	1871	1872	1873	1874	1875	1876	1877	1878	1879	1880	1881	1882	1883	1884	1885	1886	1887	1888	1889	1890	1891	1892	1893	1894	1895	1896	1897	1898	1899	1900	1901	1902	1903	1904	1905	1906	1907	1908	1909	1910	1911	1912	1913	1914	1915	1916	1917	1918	1919	1920	1921	1922	1923	1924	1925	1926	1927	1928	1929	1930	1931	1932	1933	1934	1935	1936	1937	1938	1939	1940	1941	1942	1943	1944	1945	1946	1947	1948	1949	1950	1951	1952	1953	1954	1955	1956	1957	1958	1959	1960	1961	1962	1963	1964	1965	1966	1967	1968	1969	1970	1971	1972	1973	1974	1975	1976	1977	1978	1979	1980	1981	1982	1983	1984	1985	1986	1987	1988	1989	1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000
Q72	D75	F78	L79	L80	R81	V82	H85	Y86	T87	L88	L89	L90	P91	D92	Y93	P94	R95	F96	T97	I98	A99	E100	S101	F102	F103	N104	K105	S106	V107	C108	R109	L110	PHE	D112	H113	R114	S115	L116	T117	P118	E119	R120	L121	F122	I123	F124	S125	V126	Q127	E128	Q129	G130	L131	L132	L133	L134	L135	L136	L137	L138	L139	L140	L141	L142	L143	L144	L145	L146	L147	L148	L149	L150	L151	L152	L153	L154	L155	L156	L157	L158	L159	L160	L161	L162	L163	L164	L165	L166	L167	L168	L169	L170	L171	L172	L173	L174	L175	L176	L177	L178	L179	L180	L181	L182	L183	L184	L185	L186	L187	L188	L189	L190	L191	L192	L193	L194	L195	L196	L197	L198	L199	L200	L201	L202	L203	L204	L205	L206	L207	L208	L209	L210	L211	L212	L213	L214	L215	L216	L217	L218	L219	L220	L221	L222	L223	L224	L225	L226	L227	L228	L229	L230	L231	L232	L233	L234	L235	L236	L237	L238	L239	L240	L241	L242	L243	L244	L245	L246	L247	L248	L249	L250	L251	L252	L253	L254	L255	L256	L257	L258	L259	L260	L261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L5																																																																																																																			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.14Å 133.76Å 187.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10 10.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	83.1 (10.00-3.10) 83.7 (10.00-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	16.46 (at 3.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.287 , 0.332 0.292 , 0.330	Depositor DCC
R_{free} test set	1191 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 82.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	9107	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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: AMP, MG, ADP

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	0.62	2/4643 (0.0%)	0.80	7/6283 (0.1%)
1	B	0.57	1/4567 (0.0%)	0.77	1/6179 (0.0%)
All	All	0.60	3/9210 (0.0%)	0.79	8/12462 (0.1%)

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	1	5
1	B	0	2
All	All	1	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	239	CYS	CB-SG	-6.93	1.70	1.82
1	A	511	GLY	N-CA	6.30	1.55	1.46
1	A	356	CYS	CB-SG	-5.39	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	PRO	N-CA-C	-8.62	89.69	112.10
1	A	239	CYS	N-CA-C	7.35	130.85	111.00
1	A	509	SER	N-CA-CB	-6.98	100.02	110.50
1	A	238	THR	N-CA-C	6.78	129.31	111.00
1	B	240	LEU	CA-CB-CG	6.74	130.80	115.30
1	A	75	ASP	N-CA-C	-6.36	93.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	PRO	N-CA-C	5.33	125.96	112.10
1	A	117	THR	C-N-CD	-5.26	109.03	120.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	239	CYS	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	THR	Peptide
1	A	128	PRO	Peptide
1	A	230	ASP	Peptide
1	A	350	ALA	Peptide
1	A	510	PRO	Peptide
1	B	117	THR	Peptide
1	B	278	LYS	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	4526	0	4449	592	7
1	B	4454	0	4376	518	7
2	A	27	0	12	5	0
3	A	1	0	0	0	0
4	B	23	0	12	2	0
5	A	31	0	0	12	0
5	B	45	0	0	11	0
All	All	9107	0	8849	1095	7

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 61.

All (1095) 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:279:THR:OG1	1:A:282:GLU:HG3	1.16	1.29
1:A:128:PRO:HB2	1:A:129:GLU:CA	1.56	1.29
1:A:200:LEU:HD23	1:A:201:PHE:N	1.48	1.29
1:B:550:ASN:O	1:B:554:GLU:HG3	1.31	1.29
1:A:23:ARG:O	1:A:27:VAL:HG23	1.37	1.25
1:A:128:PRO:CB	1:A:129:GLU:HA	1.57	1.24
1:B:434:LEU:O	1:B:438:ILE:HG23	1.38	1.24
1:B:376:GLU:O	1:B:411:ARG:HA	1.38	1.23
1:A:200:LEU:HD23	1:A:200:LEU:C	1.56	1.23
1:A:8:LEU:HD12	5:A:596:HOH:O	1.33	1.21
1:A:416:GLU:OE2	2:A:1762:ADP:N6	1.71	1.21
1:B:228:GLN:HB2	1:B:233:GLU:O	1.37	1.20
1:B:5:LEU:O	1:B:9:ILE:CG2	1.89	1.20
1:A:279:THR:OG1	1:A:282:GLU:CG	1.90	1.17
1:A:311:GLN:NE2	5:A:590:HOH:O	1.74	1.17
1:B:237:ASP:O	1:B:238:THR:HG22	1.41	1.16
1:B:124:PHE:HB2	1:B:299:ARG:CG	1.75	1.16
1:B:382:LYS:NZ	1:B:403:ASP:OD1	1.79	1.16
1:A:240:LEU:CD2	1:A:245:GLU:HG3	1.75	1.15
1:B:124:PHE:HB2	1:B:299:ARG:HG2	1.28	1.14
1:B:117:THR:OG1	1:B:118:PRO:HA	1.45	1.12
1:B:5:LEU:O	1:B:9:ILE:HG22	0.95	1.11
1:A:107:TYR:HE2	1:A:115:SER:HB3	1.16	1.10
1:B:304:TYR:CD2	1:B:305:LEU:HD12	1.88	1.08
1:B:413:LEU:HD23	1:B:413:LEU:O	1.54	1.07
1:B:203:ARG:NH2	1:B:254:ARG:HD2	1.70	1.07
1:A:308:CYS:C	1:A:309:ASN:HD22	1.56	1.07
1:A:168:ASN:HD22	1:A:171:ARG:HB2	1.18	1.07
1:B:124:PHE:CB	1:B:299:ARG:HG2	1.84	1.06
1:A:30:GLY:O	1:A:34:ARG:HG3	1.55	1.06
1:B:253:ALA:CB	1:B:367:GLY:HA2	1.87	1.05
1:B:178:ARG:HA	1:B:181:THR:HG22	1.07	1.04
1:B:304:TYR:HD2	1:B:305:LEU:CD1	1.69	1.04
1:A:155:ARG:O	1:A:159:ASP:OD2	1.74	1.04
1:A:189:LEU:C	1:A:189:LEU:HD23	1.79	1.03
1:B:127:GLN:HB3	1:B:128:PRO:HD3	1.38	1.03
1:B:253:ALA:HB3	1:B:367:GLY:HA2	1.35	1.03
1:B:304:TYR:CD2	1:B:305:LEU:CD1	2.42	1.03
1:A:126:SER:O	1:A:128:PRO:HD3	1.57	1.02
1:A:167:GLN:HG2	1:A:233:GLU:HB2	1.39	1.01
1:B:257:PHE:HB2	1:B:286:ALA:O	1.58	1.01
1:A:168:ASN:ND2	1:A:171:ARG:HB2	1.77	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:O	1:A:189:LEU:HD23	1.60	0.99
1:A:200:LEU:CD2	1:A:200:LEU:C	2.29	0.99
1:A:240:LEU:HD22	1:A:245:GLU:HG3	1.39	0.99
1:B:404:LEU:HB2	1:B:407:GLN:HE21	1.28	0.99
1:A:238:THR:HG23	1:A:238:THR:O	1.63	0.99
1:A:328:LEU:HD12	1:A:329:PRO:HD2	1.44	0.99
1:B:538:ASP:OD1	5:B:580:HOH:O	1.82	0.97
1:A:101:SER:HA	1:A:104:ASN:ND2	1.79	0.97
1:B:178:ARG:HA	1:B:181:THR:CG2	1.95	0.97
1:A:8:LEU:CD1	5:A:596:HOH:O	1.99	0.97
1:A:429:VAL:HG12	1:A:433:GLN:OE1	1.64	0.97
1:A:430:GLU:OE2	1:A:527:ARG:NH1	1.97	0.96
1:A:107:TYR:CE2	1:A:115:SER:HB3	2.00	0.96
1:B:61:VAL:O	1:B:65:LEU:N	1.96	0.96
1:A:546:ARG:O	1:A:550:ASN:HB2	1.66	0.95
1:B:516:GLU:O	1:B:519:ARG:HG2	1.64	0.95
1:B:296:GLU:O	1:B:300:GLU:HG3	1.66	0.95
1:B:338:ILE:HG12	1:B:353:VAL:HG21	1.49	0.95
1:A:96:PHE:CE1	1:A:128:PRO:CG	2.51	0.94
1:B:24:PHE:O	1:B:28:THR:OG1	1.86	0.94
1:B:366:VAL:HG11	1:B:447:GLN:HG2	1.47	0.94
1:B:108:CYS:HB3	1:B:113:HIS:CE1	2.03	0.93
1:B:404:LEU:O	1:B:407:GLN:NE2	2.01	0.93
1:B:327:THR:CG2	1:B:328:LEU:H	1.82	0.92
1:B:541:ARG:NH2	1:B:544:TYR:HB2	1.84	0.92
1:A:305:LEU:H	1:A:305:LEU:HD13	1.30	0.92
1:B:201:PHE:HB3	1:B:257:PHE:CE1	2.04	0.92
1:B:117:THR:OG1	1:B:118:PRO:CA	2.18	0.92
1:B:442:GLY:HA3	1:B:536:HIS:CD2	2.04	0.92
1:B:361:LYS:HE2	1:B:372:THR:O	1.69	0.91
1:A:105:SER:O	1:A:109:ARG:HG2	1.69	0.91
1:A:86:TYR:OH	1:A:99:ALA:O	1.88	0.91
1:B:455:PRO:HB2	1:B:458:MET:HB3	1.53	0.91
1:B:267:LEU:O	1:B:271:LEU:HD12	1.70	0.91
1:B:253:ALA:HB1	1:B:367:GLY:C	1.91	0.91
1:A:135:ILE:HG12	1:A:266:ALA:HB1	1.52	0.90
1:A:192:SER:HB2	1:A:214:ILE:O	1.71	0.90
1:B:327:THR:HG22	1:B:328:LEU:H	1.35	0.90
1:A:356:CYS:HB2	1:A:476:TYR:O	1.71	0.90
1:A:125:SER:CB	1:A:129:GLU:HG3	2.02	0.90
1:A:189:LEU:HD23	1:A:190:SER:OG	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ILE:HG23	5:B:601:HOH:O	1.69	0.89
1:A:454:PHE:HB2	1:A:482:MET:SD	2.13	0.89
1:B:178:ARG:CA	1:B:181:THR:HG22	1.98	0.89
1:A:96:PHE:CE1	1:A:128:PRO:HG2	2.08	0.89
1:B:81:ARG:HH21	1:B:81:ARG:HG2	1.37	0.89
1:B:310:GLU:HG3	1:B:328:LEU:HD23	1.54	0.88
1:B:450:ALA:HB1	1:B:558:GLU:CG	2.03	0.88
1:A:193:HIS:NE2	1:A:214:ILE:HG21	1.88	0.88
1:B:228:GLN:CB	1:B:233:GLU:O	2.21	0.88
1:B:304:TYR:HD2	1:B:305:LEU:HD12	1.28	0.88
1:B:551:ARG:O	1:B:556:HIS:HB3	1.72	0.88
1:A:309:ASN:HD22	1:A:309:ASN:N	1.68	0.88
1:B:535:MET:O	5:B:580:HOH:O	1.92	0.88
1:A:65:LEU:O	1:A:69:THR:OG1	1.90	0.88
1:A:356:CYS:CB	1:A:476:TYR:O	2.22	0.88
1:B:137:ARG:HB3	1:B:138:PRO:HD2	1.54	0.87
1:A:132:PHE:O	1:A:134:THR:HG23	1.74	0.87
1:A:193:HIS:CD2	1:A:214:ILE:HG21	2.09	0.87
1:B:382:LYS:HZ3	1:B:403:ASP:CG	1.76	0.87
1:B:336:LYS:HD2	1:B:416:GLU:OE2	1.74	0.87
1:B:327:THR:HG22	1:B:328:LEU:N	1.87	0.87
1:A:23:ARG:O	1:A:27:VAL:CG2	2.23	0.86
1:A:75:ASP:HB2	1:A:77:GLU:HG2	1.53	0.86
1:A:443:ASN:O	1:A:447:GLN:HG3	1.76	0.86
1:A:126:SER:C	1:A:128:PRO:CD	2.43	0.86
1:A:381:GLU:O	1:A:385:ILE:HG12	1.74	0.86
1:B:284:TYR:CE1	1:B:292:HIS:HD2	1.93	0.86
1:A:489:ASP:HA	1:A:514:PHE:CD1	2.11	0.86
1:A:252:PHE:CE2	1:A:417:ARG:HD2	2.11	0.85
1:A:221:PRO:O	1:A:241:THR:HG23	1.77	0.85
1:A:96:PHE:CE1	1:A:128:PRO:HG3	2.11	0.85
1:A:294:LYS:HG3	1:A:373:GLN:HG2	1.59	0.85
1:B:5:LEU:C	1:B:9:ILE:HG22	1.97	0.84
1:B:127:GLN:HB3	1:B:128:PRO:CD	2.07	0.84
1:A:167:GLN:OE1	1:A:167:GLN:HA	1.77	0.84
1:A:240:LEU:HD22	1:A:245:GLU:CG	2.07	0.83
1:B:90:LEU:HD22	1:B:96:PHE:HB2	1.58	0.83
1:A:444:ALA:O	1:A:448:LEU:HD22	1.78	0.83
1:B:253:ALA:CB	1:B:367:GLY:CA	2.56	0.83
1:A:113:HIS:HB2	1:A:376:GLU:HB3	1.61	0.82
1:A:465:VAL:HA	1:A:470:ARG:O	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:SER:CB	1:A:214:ILE:O	2.27	0.82
1:A:525:ASP:HB3	1:A:528:ILE:HG12	1.61	0.82
1:B:7:LEU:O	1:B:11:GLN:HG2	1.79	0.82
1:A:335:PHE:HB3	1:A:413:LEU:HD11	1.60	0.82
5:A:596:HOH:O	1:B:60:LEU:HD11	1.78	0.82
1:A:125:SER:HB3	1:A:129:GLU:HG3	1.62	0.82
1:A:489:ASP:OD1	1:A:516:GLU:HB3	1.80	0.82
1:B:124:PHE:CB	1:B:299:ARG:CG	2.52	0.82
1:A:257:PHE:N	1:A:286:ALA:O	2.10	0.81
1:B:108:CYS:HB3	1:B:113:HIS:ND1	1.95	0.81
1:B:482:MET:O	1:B:549:GLN:NE2	2.13	0.81
1:B:95:ARG:HH22	1:B:262:PRO:HB3	1.43	0.81
1:A:332:ASP:OD1	1:A:333:ARG:HG3	1.80	0.81
1:A:338:ILE:HD12	1:A:338:ILE:N	1.96	0.81
1:A:338:ILE:O	1:A:400:LYS:HD2	1.80	0.81
1:A:107:TYR:HE2	1:A:115:SER:CB	1.94	0.81
1:A:20:GLN:HA	1:A:57:HIS:CD2	2.16	0.81
1:A:325:VAL:HG11	2:A:1762:ADP:O4'	1.80	0.80
1:A:294:LYS:HG3	1:A:373:GLN:CG	2.10	0.80
1:B:538:ASP:HB3	1:B:541:ARG:NH2	1.95	0.80
1:A:203:ARG:O	5:A:594:HOH:O	1.99	0.80
1:A:382:LYS:HB3	1:A:406:GLU:O	1.82	0.80
1:B:450:ALA:HB1	1:B:558:GLU:HG2	1.64	0.80
1:A:96:PHE:HE1	1:A:128:PRO:HG2	1.43	0.80
1:A:366:VAL:HG13	1:A:560:VAL:HB	1.64	0.80
1:A:126:SER:C	1:A:128:PRO:HD2	2.02	0.80
1:A:252:PHE:CD2	1:A:417:ARG:HD2	2.17	0.80
1:B:153:LEU:O	1:B:157:ILE:HD12	1.82	0.80
1:A:238:THR:CG2	1:A:238:THR:O	2.29	0.80
1:A:47:MET:SD	1:A:362:GLU:O	2.40	0.80
1:B:245:GLU:O	1:B:248:ILE:HG22	1.82	0.79
1:A:167:GLN:CG	1:A:233:GLU:HB2	2.13	0.79
1:B:438:ILE:HG13	1:B:439:GLU:N	1.97	0.79
1:A:189:LEU:O	1:A:189:LEU:CD2	2.30	0.79
1:B:201:PHE:HB3	1:B:257:PHE:CD1	2.17	0.79
1:B:366:VAL:CG1	1:B:447:GLN:HG2	2.11	0.79
1:A:126:SER:O	1:A:128:PRO:CD	2.30	0.79
1:A:400:LYS:NZ	1:A:412:HIS:NE2	2.31	0.79
1:A:268:VAL:HG13	1:A:283:LEU:HB3	1.63	0.79
1:B:100:GLU:O	1:B:104:ASN:ND2	2.16	0.79
1:B:208:TRP:CE3	1:B:223:LEU:HD22	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLN:OE1	5:B:615:HOH:O	2.01	0.78
1:B:97:GLU:O	1:B:100:GLU:HG2	1.82	0.78
1:B:317:GLY:HA2	1:B:424:ILE:HD11	1.64	0.78
1:A:108:CYS:O	1:A:113:HIS:N	2.15	0.78
1:A:189:LEU:CD2	1:A:190:SER:OG	2.30	0.78
1:A:509:SER:N	1:A:510:PRO:CD	2.47	0.78
1:A:279:THR:OG1	1:A:282:GLU:CD	2.21	0.78
1:A:47:MET:HG3	1:A:48:LYS:H	1.48	0.78
1:A:167:GLN:OE1	1:A:167:GLN:CA	2.30	0.78
1:A:305:LEU:CD1	1:A:305:LEU:H	1.96	0.77
1:B:322:VAL:HG11	1:B:475:ASP:OD2	1.85	0.77
1:A:340:ASP:OD1	1:A:400:LYS:HG3	1.84	0.77
1:B:208:TRP:CE3	1:B:223:LEU:CD2	2.68	0.77
1:B:237:ASP:O	1:B:238:THR:CG2	2.29	0.77
1:B:304:TYR:HD2	1:B:305:LEU:HD13	1.48	0.77
1:B:387:PRO:HA	1:B:390:MET:CB	2.14	0.77
1:B:366:VAL:HG11	1:B:447:GLN:CG	2.14	0.77
1:A:128:PRO:HB2	1:A:129:GLU:HA	0.80	0.77
1:B:29:SER:HB3	1:B:260:TYR:CD1	2.20	0.77
1:B:304:TYR:CD2	1:B:305:LEU:HD13	2.20	0.77
1:B:61:VAL:HG23	1:B:62:VAL:N	2.00	0.77
1:A:47:MET:HG3	1:A:48:LYS:N	2.00	0.77
1:A:488:ARG:O	1:A:514:PHE:CE1	2.37	0.77
1:B:117:THR:HG1	1:B:118:PRO:HA	1.49	0.77
1:B:550:ASN:O	1:B:554:GLU:CG	2.24	0.77
1:A:139:LEU:C	1:A:198:ASN:OD1	2.24	0.76
1:B:427:GLU:C	1:B:429:VAL:H	1.83	0.76
1:A:125:SER:HB2	1:A:129:GLU:HG3	1.67	0.76
1:B:368:ARG:NH1	5:B:590:HOH:O	2.17	0.76
1:A:381:GLU:HB2	1:A:384:HIS:HB2	1.67	0.76
1:B:89:LEU:C	1:B:91:PRO:HD3	2.05	0.76
1:B:203:ARG:HH21	1:B:254:ARG:HD2	1.49	0.76
1:B:418:ARG:HG3	1:B:418:ARG:O	1.84	0.76
1:A:137:ARG:NH2	1:B:199:GLU:OE1	2.19	0.75
1:B:68:ILE:HG13	1:B:69:THR:H	1.51	0.75
1:A:423:ASN:OD1	1:A:461:LYS:CB	2.35	0.75
1:B:296:GLU:O	1:B:300:GLU:CG	2.35	0.75
1:B:90:LEU:N	1:B:91:PRO:HD3	2.02	0.75
1:A:268:VAL:HG13	1:A:283:LEU:CB	2.17	0.74
1:A:304:TYR:CE2	1:A:328:LEU:HD21	2.21	0.74
1:B:564:ARG:HG3	1:B:564:ARG:HH21	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ARG:NH2	1:B:262:PRO:HB3	2.02	0.74
1:B:253:ALA:HB3	1:B:367:GLY:CA	2.13	0.74
1:B:326:PHE:HE2	1:B:337:VAL:HG12	1.52	0.74
1:A:292:HIS:CD2	1:A:296:GLU:HG2	2.23	0.74
1:B:450:ALA:CB	1:B:558:GLU:HG2	2.17	0.74
1:B:81:ARG:HH21	1:B:81:ARG:CG	2.00	0.74
1:A:76:ALA:HA	1:A:79:LEU:HB2	1.68	0.74
1:B:275:LEU:O	1:B:277:GLY:N	2.21	0.74
1:B:376:GLU:HA	1:B:412:HIS:H	1.52	0.73
1:A:108:CYS:HB3	1:A:113:HIS:CD2	2.23	0.73
1:B:25:LEU:HB3	1:B:260:TYR:CE1	2.23	0.73
1:A:128:PRO:CG	1:A:129:GLU:HA	2.18	0.73
1:A:304:TYR:HE2	1:A:328:LEU:HD21	1.53	0.73
1:A:420:VAL:O	1:A:420:VAL:HG23	1.86	0.73
1:B:482:MET:HE2	1:B:545:TRP:HZ3	1.52	0.73
1:A:361:LYS:NZ	1:A:372:THR:OG1	2.22	0.73
1:A:101:SER:HA	1:A:104:ASN:HD22	1.52	0.73
1:A:90:LEU:N	1:A:91:PRO:HD3	2.03	0.73
1:B:387:PRO:HA	1:B:390:MET:HB2	1.69	0.73
1:B:525:ASP:HB3	1:B:528:ILE:HD12	1.70	0.73
1:B:541:ARG:HH22	1:B:544:TYR:HB2	1.51	0.73
1:A:338:ILE:HD12	1:A:338:ILE:H	1.54	0.73
1:A:107:TYR:CE2	1:A:115:SER:CB	2.71	0.72
1:A:192:SER:HB3	1:A:215:THR:HA	1.71	0.72
1:A:452:ASN:OD1	1:A:552:ILE:HG21	1.89	0.72
1:A:452:ASN:O	1:A:453:ILE:HD13	1.89	0.72
1:A:429:VAL:CG1	1:A:433:GLN:OE1	2.37	0.72
1:A:440:GLU:HB3	1:A:471:VAL:HG23	1.71	0.72
1:B:397:ALA:O	1:B:401:ILE:HD12	1.89	0.72
1:B:399:GLU:OE2	5:B:617:HOH:O	2.06	0.72
1:B:242:THR:O	1:B:245:GLU:HG3	1.88	0.72
1:A:254:ARG:C	1:A:365:ARG:NH2	2.43	0.72
1:B:118:PRO:HD2	1:B:119:GLU:H	1.55	0.72
1:B:413:LEU:HD23	1:B:413:LEU:C	2.10	0.72
1:A:549:GLN:O	1:A:553:ARG:HG3	1.90	0.72
1:B:323:MET:SD	1:B:338:ILE:HG13	2.29	0.72
1:B:372:THR:HA	1:B:415:ILE:O	1.90	0.72
1:A:454:PHE:CZ	1:A:513:VAL:HG11	2.25	0.71
1:B:275:LEU:O	1:B:275:LEU:HG	1.88	0.71
1:B:253:ALA:HB1	1:B:367:GLY:CA	2.20	0.71
1:B:438:ILE:CG1	1:B:439:GLU:N	2.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ARG:HH21	1:A:490:ILE:HB	1.54	0.71
1:A:488:ARG:O	1:A:514:PHE:CD1	2.43	0.71
1:B:215:THR:O	1:B:218:GLY:O	2.09	0.71
1:A:524:ALA:O	1:A:526:PRO:HD3	1.90	0.71
1:A:227:HIS:O	1:A:234:LEU:HB2	1.91	0.71
1:A:328:LEU:HD12	1:A:329:PRO:CD	2.18	0.71
1:B:229:THR:N	1:B:233:GLU:OE2	2.23	0.71
1:B:122:PHE:CD2	1:B:122:PHE:N	2.58	0.70
1:B:352:HIS:O	1:B:356:CYS:HB2	1.91	0.70
1:A:430:GLU:HA	1:A:434:LEU:HB2	1.72	0.70
1:A:461:LYS:HD3	1:A:461:LYS:H	1.56	0.70
1:A:30:GLY:O	1:A:34:ARG:CG	2.38	0.70
1:B:229:THR:HG22	1:B:233:GLU:OE2	1.90	0.70
1:A:97:GLU:OE2	1:A:265:ALA:HB2	1.92	0.70
1:A:48:LYS:HG2	1:A:362:GLU:HB2	1.72	0.70
1:B:354:ARG:NE	1:B:374:GLU:OE2	2.25	0.70
1:A:322:VAL:O	1:A:339:LYS:HG3	1.91	0.70
1:A:463:PHE:HB3	1:A:471:VAL:HG12	1.72	0.70
1:A:77:GLU:HG3	1:A:78:PHE:N	2.06	0.70
1:B:208:TRP:HE3	1:B:223:LEU:CD2	2.03	0.70
1:B:48:LYS:HE2	1:B:362:GLU:CD	2.12	0.70
1:B:122:PHE:H	1:B:122:PHE:HD2	1.38	0.69
1:A:166:TRP:C	1:A:167:GLN:OE1	2.30	0.69
1:A:228:GLN:HA	1:A:234:LEU:HA	1.74	0.69
1:A:281:ALA:O	1:A:285:MET:HG3	1.92	0.69
1:B:438:ILE:HD13	1:B:531:LEU:HB3	1.72	0.69
1:A:376:GLU:O	1:A:411:ARG:HA	1.90	0.69
1:A:357:TYR:CE1	1:A:476:TYR:HD2	2.09	0.69
1:A:95:ARG:NH2	1:B:26:GLU:HG2	2.06	0.69
1:B:220:LEU:HD12	1:B:221:PRO:HD2	1.74	0.69
1:B:412:HIS:CG	1:B:412:HIS:O	2.46	0.69
1:B:48:LYS:O	1:B:52:HIS:ND1	2.25	0.69
1:B:270:TRP:CE3	1:B:271:LEU:HG	2.28	0.69
1:B:274:ILE:HG13	1:B:275:LEU:H	1.56	0.69
1:B:87:THR:CG2	1:B:122:PHE:HE1	2.05	0.69
1:A:93:TYR:O	1:A:96:PHE:HB3	1.91	0.69
1:B:68:ILE:HG13	1:B:69:THR:N	2.05	0.69
1:A:153:LEU:CD2	1:A:176:ILE:HG21	2.23	0.69
1:A:136:PRO:O	1:B:163:ARG:NH1	2.25	0.69
1:B:253:ALA:CB	1:B:367:GLY:C	2.62	0.69
1:A:139:LEU:O	1:A:198:ASN:OD1	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HD23	1:A:201:PHE:CA	2.22	0.68
1:A:255:SER:HA	1:A:365:ARG:HH21	1.58	0.68
1:A:292:HIS:O	1:A:292:HIS:HD2	1.76	0.68
1:B:544:TYR:O	1:B:548:LEU:HB3	1.94	0.68
1:A:94:PRO:HB2	1:A:263:LEU:HD21	1.76	0.68
1:A:454:PHE:HZ	1:A:513:VAL:HG11	1.59	0.68
1:B:334:VAL:O	1:B:415:ILE:HG23	1.94	0.68
1:B:324:LEU:O	1:B:337:VAL:HG13	1.94	0.68
1:B:152:LEU:HD22	1:B:152:LEU:N	2.08	0.68
1:B:21:TYR:O	1:B:24:PHE:HB3	1.94	0.68
1:A:58:VAL:O	1:A:62:VAL:HB	1.93	0.67
1:B:124:PHE:CB	1:B:299:ARG:HD3	2.25	0.67
1:B:137:ARG:HB3	1:B:138:PRO:CD	2.23	0.67
1:A:371:ASP:CG	1:A:372:THR:H	1.98	0.67
1:B:54:TYR:OH	1:B:102:PHE:HA	1.93	0.67
1:B:93:TYR:HB3	1:B:96:PHE:HB3	1.75	0.67
1:B:118:PRO:CD	1:B:119:GLU:H	2.08	0.67
1:B:107:TYR:OH	1:B:115:SER:O	2.10	0.67
1:B:203:ARG:NH2	1:B:254:ARG:CD	2.53	0.67
1:A:95:ARG:NH2	1:B:26:GLU:OE1	2.27	0.67
1:A:343:ALA:HB3	1:A:344:PRO:HD3	1.76	0.67
1:A:52:HIS:NE2	1:A:362:GLU:OE1	2.26	0.67
1:B:97:GLU:OE1	1:B:265:ALA:HB2	1.95	0.67
1:B:376:GLU:O	1:B:411:ARG:CA	2.31	0.67
1:A:255:SER:HA	1:A:365:ARG:NH2	2.11	0.66
1:A:411:ARG:O	1:A:412:HIS:CD2	2.48	0.66
1:B:274:ILE:HG13	1:B:275:LEU:N	2.09	0.66
1:B:323:MET:HG3	1:B:338:ILE:HA	1.77	0.66
1:A:434:LEU:HD11	1:A:528:ILE:HG22	1.78	0.66
1:A:55:ASP:HA	1:A:58:VAL:CG1	2.25	0.66
1:B:65:LEU:O	1:B:68:ILE:HG12	1.96	0.66
1:A:222:PHE:O	1:A:222:PHE:HD2	1.79	0.66
1:B:448:LEU:HD13	1:B:453:ILE:CG2	2.26	0.66
1:A:462:ASN:CG	1:A:475:ASP:OD2	2.34	0.66
1:A:97:GLU:HB2	1:A:292:HIS:HE1	1.60	0.66
1:A:279:THR:CB	1:A:282:GLU:HG3	2.26	0.66
1:A:254:ARG:O	1:A:365:ARG:NH2	2.29	0.66
1:A:451:ALA:O	1:A:453:ILE:N	2.29	0.66
1:A:139:LEU:HD21	1:A:267:LEU:HD13	1.78	0.65
1:A:404:LEU:N	1:A:407:GLN:O	2.28	0.65
1:A:167:GLN:OE1	1:A:167:GLN:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:HG	1:A:221:PRO:HD3	1.78	0.65
1:B:123:ILE:O	1:B:123:ILE:HG12	1.95	0.65
1:B:366:VAL:HG12	1:B:366:VAL:O	1.96	0.65
1:A:337:VAL:HG22	1:A:413:LEU:HD13	1.77	0.65
1:A:199:GLU:N	1:A:199:GLU:OE1	2.30	0.65
1:A:95:ARG:CZ	1:B:26:GLU:HG2	2.26	0.65
1:A:157:ILE:CG2	1:A:169:LYS:HD2	2.26	0.65
1:A:202:TYR:O	1:A:257:PHE:HD1	1.80	0.65
1:A:95:ARG:NE	1:A:262:PRO:O	2.29	0.65
1:A:220:LEU:HG	1:A:221:PRO:CD	2.27	0.65
1:A:332:ASP:O	1:A:418:ARG:N	2.26	0.65
1:A:420:VAL:CG2	1:A:465:VAL:HB	2.27	0.65
1:B:427:GLU:C	1:B:429:VAL:N	2.51	0.65
1:A:101:SER:CA	1:A:104:ASN:ND2	2.59	0.65
1:A:150:GLU:OE1	1:A:173:ILE:HD12	1.97	0.65
1:A:377:ASN:ND2	1:A:411:ARG:HG2	2.12	0.65
1:A:132:PHE:C	1:A:134:THR:HG23	2.18	0.64
1:A:200:LEU:HD11	1:A:207:ALA:HB1	1.78	0.64
1:A:516:GLU:OE1	1:A:540:PHE:HD1	1.80	0.64
1:A:371:ASP:O	1:A:416:GLU:HB2	1.97	0.64
1:B:310:GLU:HG2	1:B:311:GLN:N	2.12	0.64
1:A:77:GLU:HG3	1:A:78:PHE:H	1.63	0.64
1:A:279:THR:HG1	1:A:282:GLU:CD	2.00	0.64
1:A:292:HIS:O	1:A:292:HIS:CD2	2.50	0.64
1:A:282:GLU:OE2	1:A:417:ARG:NH2	2.30	0.64
1:B:529:GLY:O	1:B:532:PHE:HB2	1.96	0.64
1:A:151:SER:O	1:A:154:MET:HB2	1.97	0.64
1:A:264:PRO:HB3	1:A:287:ILE:HD12	1.80	0.64
1:A:128:PRO:HB2	1:A:129:GLU:C	2.16	0.63
1:A:33:GLN:O	1:A:37:GLN:HB2	1.98	0.63
1:B:253:ALA:CB	1:B:367:GLY:O	2.46	0.63
1:B:284:TYR:CE1	1:B:292:HIS:CD2	2.83	0.63
1:A:152:LEU:O	1:A:155:ARG:HB2	1.98	0.63
1:A:229:THR:HB	1:A:233:GLU:HG2	1.78	0.63
1:A:308:CYS:C	1:A:309:ASN:ND2	2.41	0.63
1:B:305:LEU:N	1:B:305:LEU:HD13	2.12	0.63
1:B:420:VAL:HG13	1:B:465:VAL:HB	1.79	0.63
1:A:104:ASN:OD1	1:A:122:PHE:O	2.17	0.63
1:A:519:ARG:HD3	1:A:540:PHE:HB2	1.79	0.63
1:A:529:GLY:O	1:A:532:PHE:HB2	1.99	0.63
1:B:108:CYS:CB	1:B:113:HIS:ND1	2.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:TYR:HH	1:B:102:PHE:HA	1.63	0.63
1:A:420:VAL:O	1:A:420:VAL:CG2	2.45	0.62
1:A:489:ASP:CA	1:A:514:PHE:CD1	2.82	0.62
1:B:370:ALA:N	1:B:476:TYR:OH	2.28	0.62
1:A:143:PHE:O	1:A:194:LEU:N	2.31	0.62
1:A:145:PRO:HD2	1:A:193:HIS:HA	1.80	0.62
1:A:438:ILE:O	1:A:536:HIS:HE1	1.83	0.62
1:A:154:MET:O	1:A:158:SER:OG	2.16	0.62
1:A:206:ALA:HB3	5:A:594:HOH:O	1.99	0.62
1:A:309:ASN:N	1:A:309:ASN:ND2	2.43	0.62
1:B:245:GLU:O	1:B:248:ILE:CG2	2.47	0.62
1:B:61:VAL:CG2	1:B:62:VAL:N	2.62	0.62
1:B:338:ILE:HD11	1:B:414:TYR:HD2	1.64	0.62
1:A:292:HIS:HD2	1:A:296:GLU:HG2	1.63	0.62
1:A:304:TYR:CE2	1:A:328:LEU:CD2	2.82	0.62
1:A:54:TYR:O	1:A:58:VAL:HG12	1.99	0.62
1:B:58:VAL:O	1:B:61:VAL:HG22	2.00	0.62
1:A:200:LEU:CD2	1:A:201:PHE:N	2.43	0.61
1:B:102:PHE:O	1:B:106:VAL:HG23	2.00	0.61
1:B:124:PHE:HB2	1:B:299:ARG:CD	2.29	0.61
1:A:365:ARG:HB3	1:A:369:MET:HB2	1.83	0.61
1:A:422:LEU:HB3	1:A:460:PHE:O	2.01	0.61
1:A:516:GLU:OE1	1:A:540:PHE:CD1	2.53	0.61
1:A:75:ASP:CB	1:A:77:GLU:HG2	2.27	0.61
1:B:220:LEU:HD12	1:B:221:PRO:CD	2.30	0.61
1:A:170:SER:O	1:A:173:ILE:HG12	2.00	0.61
1:A:414:TYR:C	1:A:415:ILE:HD12	2.19	0.61
1:A:509:SER:N	1:A:510:PRO:HD2	2.13	0.61
1:A:240:LEU:HD23	1:A:245:GLU:HG3	1.75	0.61
1:B:124:PHE:HB2	1:B:299:ARG:HG3	1.80	0.61
1:B:215:THR:C	1:B:217:SER:H	2.04	0.61
1:B:253:ALA:HB1	1:B:367:GLY:O	2.00	0.61
1:A:423:ASN:OD1	1:A:461:LYS:HB2	2.00	0.61
1:B:228:GLN:HE21	1:B:232:GLY:HA2	1.64	0.61
1:B:413:LEU:O	1:B:413:LEU:CD2	2.41	0.61
1:A:127:GLN:N	1:A:128:PRO:CD	2.61	0.61
1:A:69:THR:HG22	1:A:73:SER:OG	2.01	0.61
1:B:448:LEU:HD13	1:B:453:ILE:HG22	1.82	0.61
1:A:119:GLU:OE1	1:A:119:GLU:N	2.34	0.61
1:A:133:ARG:O	1:A:133:ARG:HG3	2.01	0.61
1:A:108:CYS:SG	1:A:113:HIS:HA	2.40	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:PHE:C	1:A:134:THR:H	2.02	0.60
1:A:208:TRP:CZ3	1:A:225:PRO:HG3	2.36	0.60
1:B:389:LEU:O	1:B:389:LEU:HG	2.00	0.60
1:B:391:GLU:HA	1:B:394:LEU:HB3	1.83	0.60
1:B:95:ARG:NH2	1:B:262:PRO:O	2.25	0.60
1:B:265:ALA:O	1:B:269:GLU:HB2	2.01	0.60
1:A:101:SER:HA	1:A:104:ASN:HD21	1.63	0.60
1:A:132:PHE:O	1:A:134:THR:N	2.28	0.60
1:A:264:PRO:O	1:A:268:VAL:HG23	2.01	0.60
1:A:324:LEU:N	1:A:337:VAL:O	2.29	0.60
1:A:86:TYR:O	1:A:90:LEU:CD1	2.50	0.60
1:A:420:VAL:HG22	1:A:465:VAL:HB	1.84	0.60
1:A:127:GLN:N	1:A:128:PRO:HD2	2.17	0.60
1:A:266:ALA:O	1:A:269:GLU:HB3	2.02	0.60
1:A:557:VAL:O	1:A:557:VAL:CG1	2.49	0.60
1:A:126:SER:O	1:A:127:GLN:HB3	2.01	0.60
1:A:229:THR:N	1:A:233:GLU:O	2.33	0.60
1:B:315:ALA:HB3	1:B:325:VAL:HG11	1.84	0.60
1:B:514:PHE:HD2	1:B:517:GLU:HB2	1.66	0.60
1:B:270:TRP:HE3	1:B:271:LEU:HG	1.66	0.60
1:A:116:LEU:HD12	1:A:117:THR:H	1.66	0.59
1:A:331:PHE:HD1	1:A:332:ASP:H	1.49	0.59
1:A:463:PHE:HB3	1:A:471:VAL:CG1	2.31	0.59
1:B:525:ASP:CB	1:B:528:ILE:HD12	2.32	0.59
1:A:458:MET:HE2	5:A:601:HOH:O	2.02	0.59
1:A:488:ARG:O	1:A:514:PHE:HE1	1.83	0.59
1:B:108:CYS:CB	1:B:113:HIS:HD1	2.15	0.59
1:A:305:LEU:N	1:A:305:LEU:HD13	2.07	0.59
1:A:351:ALA:HB3	1:A:354:ARG:HG3	1.83	0.59
1:A:357:TYR:CE1	1:A:476:TYR:CD2	2.89	0.59
1:A:213:LEU:O	1:A:213:LEU:HG	2.01	0.59
1:A:86:TYR:O	1:A:90:LEU:HD12	2.03	0.59
1:B:124:PHE:CB	1:B:299:ARG:CD	2.80	0.59
1:B:420:VAL:HG21	1:B:425:TRP:HD1	1.67	0.59
1:B:482:MET:CE	1:B:545:TRP:HZ3	2.16	0.59
1:A:458:MET:CE	5:A:601:HOH:O	2.50	0.59
1:B:104:ASN:HB2	4:B:1604:AMP:O3'	2.03	0.59
1:A:19:ALA:O	1:A:22:GLY:N	2.36	0.59
1:B:261:ALA:HB2	1:B:267:LEU:HD22	1.84	0.59
1:B:359:LEU:O	1:B:363:HIS:HB2	2.01	0.59
1:A:58:VAL:HG23	1:A:106:VAL:HG22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:ASP:HB3	1:A:514:PHE:HB3	1.85	0.58
1:A:14:LEU:HD13	1:A:86:TYR:OH	2.01	0.58
1:A:61:VAL:O	1:A:65:LEU:HB2	2.03	0.58
1:B:116:LEU:C	1:B:117:THR:HG22	2.23	0.58
1:A:109:ARG:NH1	1:A:374:GLU:OE1	2.36	0.58
1:A:161:PRO:HB3	1:B:138:PRO:HB3	1.84	0.58
1:A:252:PHE:O	1:A:365:ARG:NH1	2.37	0.58
1:A:301:TYR:HA	1:A:331:PHE:HZ	1.67	0.58
1:B:208:TRP:CZ3	1:B:223:LEU:HD22	2.38	0.58
1:B:370:ALA:H	1:B:476:TYR:HH	1.51	0.58
1:B:433:GLN:HA	1:B:433:GLN:OE1	2.04	0.58
1:A:335:PHE:N	1:A:335:PHE:CD2	2.71	0.58
1:B:220:LEU:CD1	1:B:221:PRO:HD2	2.34	0.58
1:B:310:GLU:CG	1:B:328:LEU:HD23	2.31	0.58
1:A:101:SER:CA	1:A:104:ASN:HD22	2.16	0.58
1:A:245:GLU:O	1:A:249:VAL:HG12	2.03	0.58
1:A:304:TYR:HE2	1:A:328:LEU:CD2	2.15	0.58
1:B:442:GLY:O	1:B:446:ARG:HG3	2.04	0.58
1:B:95:ARG:NH2	1:B:262:PRO:CB	2.67	0.58
1:B:221:PRO:HG3	1:B:274:ILE:O	2.03	0.58
1:B:295:THR:HG22	1:B:296:GLU:N	2.16	0.58
1:B:541:ARG:O	1:B:541:ARG:HG2	2.04	0.58
1:A:39:ASP:O	1:A:42:ALA:HB3	2.04	0.57
1:B:32:GLN:HE22	1:B:161:PRO:HB3	1.69	0.57
1:B:327:THR:OG1	1:B:334:VAL:HA	2.04	0.57
1:B:253:ALA:HA	1:B:369:MET:O	2.05	0.57
1:B:450:ALA:HB1	1:B:558:GLU:CB	2.34	0.57
1:A:358:GLN:C	1:A:360:VAL:H	2.06	0.57
1:A:340:ASP:OD1	1:A:400:LYS:CG	2.53	0.57
1:A:325:VAL:HG11	2:A:1762:ADP:C1'	2.34	0.57
1:A:48:LYS:O	1:A:52:HIS:ND1	2.37	0.57
1:B:78:PHE:O	1:B:82:VAL:HG23	2.04	0.57
1:B:124:PHE:HB3	1:B:299:ARG:HG2	1.82	0.57
1:B:354:ARG:HE	1:B:412:HIS:CD2	2.23	0.57
1:A:215:THR:O	1:A:218:GLY:O	2.23	0.57
1:A:292:HIS:CD2	1:A:296:GLU:CG	2.88	0.57
1:A:145:PRO:CD	1:A:193:HIS:HA	2.35	0.57
1:A:449:ALA:CB	1:A:548:LEU:HD13	2.35	0.57
1:A:222:PHE:O	1:A:222:PHE:CD2	2.58	0.56
1:A:222:PHE:HE2	1:A:224:LEU:HD12	1.69	0.56
1:B:356:CYS:SG	1:B:479:ILE:HG22	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LYS:HG3	1:A:373:GLN:HG3	1.87	0.56
1:A:380:LEU:HD13	1:A:410:ILE:HG21	1.86	0.56
1:A:23:ARG:HB3	1:A:53:LEU:HD22	1.87	0.56
1:A:315:ALA:HB3	1:A:325:VAL:HG13	1.87	0.56
1:B:179:HIS:CD2	1:B:241:THR:OG1	2.57	0.56
1:B:334:VAL:HB	1:B:418:ARG:HB3	1.87	0.56
1:A:425:TRP:O	1:A:429:VAL:HG22	2.05	0.56
1:A:568:ARG:CG	1:A:571:VAL:HG12	2.35	0.56
1:A:489:ASP:HA	1:A:514:PHE:CE1	2.39	0.56
1:A:68:ILE:HG13	1:B:67:CYS:SG	2.45	0.56
1:B:93:TYR:HB3	1:B:96:PHE:CB	2.35	0.56
1:B:9:ILE:HG21	1:B:82:VAL:HG22	1.87	0.56
1:A:113:HIS:CB	1:A:376:GLU:HB3	2.35	0.56
1:B:325:VAL:HG22	1:B:334:VAL:HG22	1.87	0.56
1:A:325:VAL:O	1:A:325:VAL:HG13	2.06	0.56
1:A:442:GLY:HA3	1:A:536:HIS:NE2	2.21	0.56
1:B:326:PHE:CE2	1:B:337:VAL:HG12	2.36	0.56
1:A:308:CYS:SG	1:A:309:ASN:N	2.78	0.55
1:A:449:ALA:HB1	1:A:548:LEU:HD13	1.88	0.55
1:B:327:THR:CG2	1:B:328:LEU:N	2.46	0.55
1:A:237:ASP:C	1:A:237:ASP:OD1	2.43	0.55
1:A:299:ARG:O	1:A:303:VAL:HG23	2.06	0.55
1:A:408:ILE:O	1:A:408:ILE:HG12	2.05	0.55
1:B:411:ARG:O	1:B:412:HIS:HB3	2.06	0.55
1:B:54:TYR:HH	1:B:105:SER:HG	1.54	0.55
1:A:423:ASN:OD1	1:A:461:LYS:HB3	2.06	0.55
1:A:488:ARG:NH2	1:A:490:ILE:HB	2.21	0.55
1:B:149:TRP:HB3	1:B:177:ILE:HD11	1.87	0.55
1:B:318:ILE:HB	1:B:461:LYS:CE	2.37	0.55
1:B:95:ARG:NH1	5:B:603:HOH:O	2.02	0.55
1:A:108:CYS:CB	1:A:113:HIS:HA	2.36	0.55
1:B:394:LEU:HA	1:B:401:ILE:HD13	1.88	0.55
1:A:244:ALA:O	1:A:248:ILE:HG12	2.06	0.55
1:B:107:TYR:HE2	1:B:116:LEU:HA	1.72	0.55
1:B:171:ARG:O	1:B:175:TYR:HD2	1.90	0.55
1:B:51:ILE:HD11	1:B:256:TYR:HD2	1.72	0.55
1:B:529:GLY:O	1:B:532:PHE:N	2.27	0.55
1:A:23:ARG:HB3	1:A:53:LEU:CD2	2.37	0.55
1:B:441:TYR:O	1:B:444:ALA:HB3	2.06	0.55
1:A:127:GLN:O	1:A:128:PRO:C	2.42	0.55
1:A:209:LEU:HB3	1:A:224:LEU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:PHE:HB2	1:A:275:LEU:HD21	1.87	0.55
1:B:372:THR:HG22	1:B:415:ILE:O	2.07	0.55
1:A:153:LEU:HD21	1:A:176:ILE:HG21	1.87	0.55
1:A:20:GLN:C	1:A:20:GLN:NE2	2.61	0.55
1:A:201:PHE:O	1:A:208:TRP:HB2	2.07	0.54
1:A:189:LEU:O	1:A:190:SER:CB	2.55	0.54
1:A:255:SER:CA	1:A:365:ARG:HH21	2.18	0.54
1:A:371:ASP:CG	1:A:372:THR:N	2.60	0.54
1:B:134:THR:O	1:B:134:THR:HG22	2.06	0.54
1:B:312:PHE:CD2	1:B:384:HIS:HB3	2.42	0.54
1:B:338:ILE:HG22	1:B:339:LYS:O	2.08	0.54
1:B:237:ASP:OD2	1:B:563:TYR:OH	2.22	0.54
1:B:324:LEU:HD13	1:B:393:LEU:HD12	1.89	0.54
1:B:61:VAL:CG2	1:B:62:VAL:H	2.20	0.54
1:A:25:LEU:O	1:A:29:SER:HB3	2.06	0.54
1:B:231:ASP:OD1	1:B:231:ASP:N	2.29	0.54
1:A:221:PRO:HB3	1:A:274:ILE:HG23	1.90	0.54
1:A:442:GLY:HA3	1:A:536:HIS:CE1	2.43	0.54
1:A:128:PRO:CB	1:A:129:GLU:CA	2.38	0.54
1:B:195:GLN:O	1:B:212:LYS:N	2.33	0.54
1:B:255:SER:OG	1:B:364:ASP:OD1	2.26	0.54
1:A:170:SER:O	1:A:173:ILE:CG1	2.56	0.54
1:A:97:GLU:HB2	1:A:292:HIS:CE1	2.42	0.54
1:A:456:GLY:HA3	1:A:478:GLU:O	2.08	0.54
1:A:359:LEU:O	1:A:359:LEU:HD23	2.08	0.54
1:A:372:THR:HA	1:A:415:ILE:O	2.08	0.54
1:B:290:GLN:HA	1:B:293:ALA:HB3	1.90	0.54
1:B:403:ASP:C	1:B:404:LEU:HD23	2.28	0.54
1:B:462:ASN:HB3	1:B:475:ASP:HB2	1.90	0.54
1:B:118:PRO:CD	1:B:119:GLU:N	2.71	0.53
1:B:538:ASP:N	1:B:538:ASP:OD1	2.41	0.53
1:B:327:THR:C	1:B:328:LEU:HD12	2.29	0.53
1:B:353:VAL:O	1:B:357:TYR:HB2	2.09	0.53
1:B:375:PHE:HE2	1:B:415:ILE:HD12	1.73	0.53
1:A:366:VAL:O	1:A:366:VAL:HG12	2.09	0.53
1:B:280:THR:O	1:B:284:TYR:HD2	1.90	0.53
1:B:287:ILE:O	1:B:287:ILE:HG22	2.08	0.53
1:B:465:VAL:HA	1:B:470:ARG:O	2.08	0.53
1:A:490:ILE:O	1:A:491:PRO:O	2.25	0.53
1:A:96:PHE:CZ	1:A:128:PRO:CG	2.92	0.53
1:A:194:LEU:CD2	1:A:195:GLN:N	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:THR:OG1	1:A:282:GLU:OE1	2.26	0.53
1:A:292:HIS:HD2	1:A:296:GLU:CG	2.21	0.53
1:A:449:ALA:O	1:A:451:ALA:O	2.25	0.53
1:A:483:THR:HG23	1:A:553:ARG:HD3	1.91	0.53
1:B:561:TYR:HB3	1:B:563:TYR:CE1	2.43	0.53
1:A:358:GLN:O	1:A:361:LYS:N	2.38	0.53
1:A:489:ASP:HB3	1:A:514:PHE:CB	2.39	0.53
1:A:490:ILE:O	1:A:491:PRO:C	2.46	0.53
1:A:488:ARG:HB2	1:A:546:ARG:HH22	1.73	0.53
1:B:427:GLU:O	1:B:429:VAL:N	2.39	0.53
1:B:48:LYS:NZ	5:B:610:HOH:O	2.30	0.53
1:B:556:HIS:CE1	5:B:579:HOH:O	2.60	0.53
1:A:200:LEU:HD23	1:A:200:LEU:O	2.05	0.53
1:B:313:ILE:O	1:B:327:THR:N	2.40	0.53
1:B:79:LEU:HD12	1:B:120:ARG:HB3	1.90	0.53
1:A:194:LEU:HD23	1:A:195:GLN:H	1.73	0.53
1:A:200:LEU:CD2	1:A:200:LEU:O	2.55	0.53
1:A:78:PHE:C	1:A:80:LEU:H	2.11	0.53
1:B:294:LYS:HG3	1:B:373:GLN:OE1	2.09	0.53
1:A:334:VAL:O	1:A:415:ILE:HA	2.08	0.52
1:B:127:GLN:CB	1:B:128:PRO:HD3	2.26	0.52
1:B:251:GLY:O	1:B:254:ARG:HB2	2.09	0.52
1:B:85:HIS:O	1:B:88:ARG:HG2	2.08	0.52
1:A:317:GLY:HA2	1:A:424:ILE:HD11	1.91	0.52
1:A:359:LEU:HD21	1:A:481:TYR:CE1	2.44	0.52
1:B:338:ILE:HG21	1:B:353:VAL:HG11	1.90	0.52
1:A:40:TRP:HD1	1:A:43:VAL:HB	1.74	0.52
1:B:294:LYS:NZ	4:B:1604:AMP:O3P	2.30	0.52
1:B:177:ILE:O	1:B:181:THR:N	2.43	0.52
1:B:448:LEU:HD12	1:B:455:PRO:HG3	1.91	0.52
1:A:264:PRO:CB	1:A:287:ILE:HD12	2.40	0.52
1:B:278:LYS:HB2	1:B:282:GLU:OE2	2.10	0.52
1:B:286:ALA:O	1:B:287:ILE:HD12	2.09	0.52
1:B:63:GLU:O	1:B:67:CYS:HB2	2.10	0.52
1:A:200:LEU:CD2	1:A:201:PHE:C	2.78	0.52
1:A:445:ILE:HG22	1:A:445:ILE:O	2.10	0.52
1:B:186:PRO:HA	1:B:189:LEU:HD22	1.90	0.52
1:A:95:ARG:NH2	1:B:26:GLU:CG	2.72	0.52
1:B:101:SER:HA	1:B:104:ASN:ND2	2.25	0.52
1:B:80:LEU:HD11	1:B:119:GLU:O	2.08	0.52
1:B:338:ILE:HG12	1:B:353:VAL:CG2	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:ILE:C	1:B:554:GLU:H	2.10	0.52
1:A:323:MET:HE2	1:A:336:LYS:HB3	1.92	0.52
1:A:33:GLN:O	1:A:37:GLN:N	2.40	0.52
1:B:176:ILE:HD11	1:B:236:ILE:HD12	1.92	0.52
1:B:124:PHE:HB3	1:B:299:ARG:HD3	1.90	0.52
1:B:482:MET:CE	1:B:545:TRP:CZ3	2.92	0.52
1:A:200:LEU:HD23	1:A:201:PHE:C	2.29	0.52
1:B:569:PHE:O	1:B:573:TYR:O	2.28	0.52
1:A:336:LYS:HD2	1:A:416:GLU:OE1	2.09	0.52
1:A:358:GLN:HA	1:A:361:LYS:HB2	1.92	0.51
1:B:54:TYR:OH	1:B:105:SER:OG	2.25	0.51
1:B:438:ILE:HB	1:B:532:PHE:CE2	2.45	0.51
1:A:127:GLN:O	1:A:128:PRO:O	2.29	0.51
1:A:380:LEU:HD13	1:A:410:ILE:CG2	2.40	0.51
1:B:222:PHE:O	1:B:222:PHE:CD2	2.63	0.51
1:B:514:PHE:CD2	1:B:517:GLU:HB2	2.45	0.51
1:A:194:LEU:CD2	1:A:195:GLN:H	2.23	0.51
1:A:237:ASP:OD1	1:A:238:THR:N	2.43	0.51
1:B:204:ASN:ND2	1:B:560:VAL:HG11	2.24	0.51
1:B:564:ARG:HG3	1:B:564:ARG:NH2	2.24	0.51
1:A:194:LEU:HD22	1:A:195:GLN:N	2.25	0.51
1:B:430:GLU:N	1:B:430:GLU:OE2	2.44	0.51
1:B:40:TRP:HD1	1:B:43:VAL:HG21	1.76	0.51
1:A:189:LEU:O	1:A:190:SER:HB2	2.10	0.51
1:A:57:HIS:O	1:A:61:VAL:CG1	2.58	0.51
1:A:74:THR:HA	1:A:78:PHE:HE1	1.76	0.51
1:B:374:GLU:HB2	1:B:414:TYR:CE1	2.46	0.51
1:A:462:ASN:HB3	1:A:475:ASP:HB2	1.93	0.51
1:B:62:VAL:HG21	1:B:109:ARG:HB3	1.93	0.51
1:B:154:MET:HG3	1:B:173:ILE:HG21	1.92	0.51
1:B:515:PRO:HB3	1:B:545:TRP:NE1	2.25	0.51
1:B:569:PHE:O	1:B:573:TYR:HB2	2.11	0.51
1:A:138:PRO:HB2	1:A:140:ALA:O	2.11	0.51
1:A:81:ARG:O	1:A:85:HIS:CD2	2.63	0.51
1:A:33:GLN:HE22	1:B:134:THR:HG23	1.75	0.51
1:A:32:GLN:OE1	1:B:138:PRO:HD3	2.11	0.51
1:A:449:ALA:HB1	1:A:482:MET:CE	2.40	0.51
1:B:116:LEU:O	1:B:117:THR:HG22	2.11	0.51
1:B:312:PHE:HD2	1:B:384:HIS:HB3	1.74	0.51
1:B:422:LEU:O	1:B:425:TRP:N	2.44	0.51
1:B:81:ARG:CG	1:B:81:ARG:NH2	2.66	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:CYS:O	1:A:360:VAL:HG23	2.11	0.51
1:B:280:THR:HG22	1:B:284:TYR:CE2	2.46	0.51
1:B:327:THR:HG23	1:B:328:LEU:H	1.73	0.51
1:A:268:VAL:HG13	1:A:283:LEU:HB2	1.93	0.51
1:A:336:LYS:HB2	1:A:414:TYR:HB2	1.93	0.51
1:B:382:LYS:HG3	1:B:408:ILE:HG12	1.92	0.51
1:B:559:ASP:HB3	1:B:561:TYR:CE2	2.46	0.51
1:B:95:ARG:HD3	1:B:262:PRO:O	2.11	0.51
1:A:260:TYR:O	1:A:260:TYR:CD2	2.64	0.50
1:A:53:LEU:HA	1:A:56:HIS:HB3	1.93	0.50
1:B:96:PHE:CD1	1:B:96:PHE:C	2.84	0.50
1:B:54:TYR:CG	1:B:291:LYS:HD3	2.46	0.50
1:A:439:GLU:HG3	1:A:535:MET:HG3	1.94	0.50
1:B:334:VAL:CG1	1:B:416:GLU:HG3	2.41	0.50
1:B:518:PHE:O	1:B:522:LEU:HB2	2.11	0.50
1:B:525:ASP:HB3	1:B:528:ILE:CD1	2.40	0.50
1:B:315:ALA:HB3	1:B:325:VAL:CG1	2.41	0.50
1:A:149:TRP:CD1	1:A:189:LEU:HG	2.47	0.50
1:A:55:ASP:HA	1:A:58:VAL:HG13	1.93	0.50
1:B:29:SER:HB3	1:B:260:TYR:HD1	1.75	0.50
1:B:241:THR:N	1:B:245:GLU:OE1	2.37	0.50
1:B:353:VAL:O	1:B:354:ARG:C	2.50	0.50
1:B:239:CYS:HB2	1:B:569:PHE:HZ	1.77	0.50
1:B:318:ILE:HB	1:B:461:LYS:HE2	1.94	0.50
1:B:368:ARG:O	1:B:473:PHE:HB3	2.11	0.50
1:A:414:TYR:O	1:A:415:ILE:HD12	2.11	0.50
1:B:194:LEU:HD12	1:B:213:LEU:HA	1.94	0.50
1:A:95:ARG:NH2	1:B:26:GLU:CD	2.65	0.50
1:B:61:VAL:HG23	1:B:62:VAL:H	1.73	0.50
1:B:21:TYR:O	1:B:24:PHE:CB	2.59	0.50
1:A:198:ASN:OD1	1:A:198:ASN:O	2.30	0.49
1:A:20:GLN:NE2	1:A:20:GLN:O	2.45	0.49
1:A:375:PHE:O	1:A:412:HIS:HA	2.12	0.49
1:A:519:ARG:HD3	1:A:540:PHE:CB	2.42	0.49
1:B:448:LEU:HD13	1:B:453:ILE:HG21	1.94	0.49
1:B:176:ILE:HD11	1:B:236:ILE:CD1	2.41	0.49
1:B:275:LEU:C	1:B:277:GLY:N	2.65	0.49
1:B:287:ILE:O	1:B:287:ILE:CG2	2.60	0.49
1:B:366:VAL:CG1	1:B:366:VAL:O	2.59	0.49
1:A:382:LYS:CB	1:A:406:GLU:O	2.58	0.49
1:A:76:ALA:O	1:A:77:GLU:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:VAL:HG13	1:B:209:LEU:HD21	1.93	0.49
1:B:339:LYS:HD3	1:B:342:PHE:HA	1.93	0.49
1:B:376:GLU:HA	1:B:412:HIS:N	2.25	0.49
1:A:107:TYR:CZ	1:A:120:ARG:HG3	2.48	0.49
1:A:328:LEU:CD1	1:A:329:PRO:HD2	2.31	0.49
1:B:310:GLU:OE2	1:B:384:HIS:CE1	2.66	0.49
1:B:476:TYR:HB3	1:B:479:ILE:HD12	1.94	0.49
1:A:157:ILE:HG22	1:A:169:LYS:HD2	1.92	0.49
1:A:197:ALA:HB3	1:A:210:VAL:CG1	2.43	0.49
1:A:411:ARG:O	1:A:412:HIS:HD2	1.93	0.49
1:A:449:ALA:HB1	1:A:482:MET:HE2	1.93	0.49
1:B:223:LEU:HD13	1:B:249:VAL:HG11	1.94	0.49
1:A:470:ARG:HB3	1:A:470:ARG:CZ	2.43	0.49
1:A:525:ASP:CB	1:A:528:ILE:HG12	2.39	0.49
1:A:48:LYS:O	1:A:52:HIS:CE1	2.65	0.49
1:A:305:LEU:HD23	1:A:381:GLU:OE2	2.12	0.49
1:A:40:TRP:CD1	1:A:43:VAL:HB	2.48	0.49
1:B:322:VAL:HG23	1:B:323:MET:N	2.26	0.49
1:B:387:PRO:HA	1:B:390:MET:HB3	1.92	0.49
1:A:7:LEU:O	1:A:11:GLN:HB2	2.13	0.49
1:A:125:SER:HB2	1:A:129:GLU:CG	2.40	0.49
1:A:249:VAL:HG13	1:A:250:PHE:HD2	1.78	0.49
1:A:339:LYS:HD2	1:A:396:GLU:OE1	2.12	0.49
1:A:355:ALA:O	1:A:359:LEU:HB2	2.13	0.49
1:B:124:PHE:CD2	1:B:299:ARG:HD3	2.47	0.49
1:B:539:LEU:O	1:B:545:TRP:NE1	2.43	0.49
1:A:461:LYS:CD	1:A:461:LYS:H	2.24	0.49
1:A:453:ILE:HG23	1:A:479:ILE:HD12	1.95	0.49
1:A:165:HIS:H	1:A:165:HIS:CD2	2.30	0.48
1:B:304:TYR:HB3	1:B:305:LEU:HD13	1.95	0.48
1:A:338:ILE:CD1	1:A:338:ILE:H	2.24	0.48
1:A:333:ARG:HA	1:A:418:ARG:H	1.79	0.48
1:A:441:TYR:O	1:A:444:ALA:HB3	2.13	0.48
1:B:328:LEU:HB3	1:B:329:PRO:HD2	1.96	0.48
1:B:95:ARG:HH22	1:B:262:PRO:CB	2.20	0.48
1:A:132:PHE:C	1:A:134:THR:N	2.66	0.48
1:A:240:LEU:HD22	1:A:245:GLU:CB	2.43	0.48
1:A:338:ILE:CD1	1:A:338:ILE:N	2.67	0.48
1:B:168:ASN:C	1:B:170:SER:H	2.16	0.48
1:B:338:ILE:HD11	1:B:414:TYR:CD2	2.46	0.48
1:A:222:PHE:HE2	1:A:224:LEU:CD1	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:CYS:O	1:A:309:ASN:ND2	2.45	0.48
1:A:336:LYS:N	1:A:414:TYR:O	2.31	0.48
1:A:368:ARG:HH22	1:A:440:GLU:HG3	1.78	0.48
1:A:457:ASP:OD1	1:A:457:ASP:C	2.52	0.48
1:B:340:ASP:N	1:B:340:ASP:OD1	2.40	0.48
1:B:47:MET:O	1:B:47:MET:HG3	2.14	0.48
1:A:356:CYS:HB3	1:A:476:TYR:O	2.10	0.48
1:A:68:ILE:O	1:A:68:ILE:HG22	2.14	0.48
1:B:85:HIS:HA	1:B:88:ARG:HD3	1.96	0.48
1:A:116:LEU:CD1	1:A:117:THR:H	2.27	0.48
1:A:302:LEU:O	1:A:306:GLN:HB2	2.14	0.48
1:B:438:ILE:CD1	1:B:531:LEU:HB3	2.41	0.48
1:B:116:LEU:O	1:B:117:THR:CB	2.56	0.48
1:B:251:GLY:O	1:B:254:ARG:CG	2.62	0.48
1:A:241:THR:O	1:A:241:THR:HG22	2.13	0.48
1:B:304:TYR:CE2	1:B:305:LEU:HD12	2.45	0.48
1:A:189:LEU:HD21	1:A:190:SER:OG	2.13	0.48
1:A:335:PHE:CB	1:A:413:LEU:HD11	2.37	0.48
1:B:203:ARG:NH1	1:B:255:SER:O	2.47	0.48
1:B:222:PHE:C	1:B:222:PHE:CD2	2.87	0.48
1:B:538:ASP:HA	1:B:541:ARG:HD3	1.95	0.48
1:A:281:ALA:HB2	1:A:296:GLU:HB3	1.95	0.47
1:A:452:ASN:OD1	1:A:552:ILE:CG2	2.60	0.47
1:A:450:ALA:O	1:A:557:VAL:CG2	2.63	0.47
1:B:108:CYS:HB3	1:B:113:HIS:HD1	1.74	0.47
1:B:16:GLY:O	1:B:20:GLN:HB2	2.14	0.47
1:B:7:LEU:HD22	1:B:8:LEU:N	2.28	0.47
1:A:25:LEU:HB2	1:A:260:TYR:CE1	2.49	0.47
1:A:447:GLN:NE2	5:A:580:HOH:O	2.47	0.47
1:B:327:THR:HG21	1:B:418:ARG:HD3	1.96	0.47
1:A:97:GLU:HG2	1:A:98:ILE:N	2.30	0.47
1:B:375:PHE:CE2	1:B:415:ILE:HD12	2.49	0.47
1:A:25:LEU:HD13	5:B:603:HOH:O	2.14	0.47
1:A:305:LEU:HD22	1:A:306:GLN:N	2.29	0.47
1:B:122:PHE:HB3	1:B:127:GLN:HB2	1.96	0.47
1:B:145:PRO:HB3	1:B:149:TRP:CD1	2.49	0.47
1:B:259:VAL:HG11	1:B:267:LEU:HD21	1.95	0.47
1:B:420:VAL:CG2	1:B:425:TRP:HD1	2.28	0.47
1:A:100:GLU:O	1:A:103:PHE:HB3	2.15	0.47
1:A:156:VAL:O	1:A:160:LEU:HG	2.13	0.47
1:A:255:SER:CA	1:A:365:ARG:NH2	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:PHE:HZ	1:A:522:LEU:O	1.98	0.47
1:B:215:THR:C	1:B:217:SER:N	2.66	0.47
1:A:65:LEU:HD22	1:A:110:LEU:HD11	1.97	0.47
1:A:462:ASN:ND2	1:A:475:ASP:OD2	2.48	0.47
1:A:488:ARG:HD2	1:A:546:ARG:HH22	1.79	0.47
1:A:544:TYR:CE2	1:A:548:LEU:HD11	2.49	0.47
1:B:90:LEU:N	1:B:91:PRO:CD	2.74	0.47
1:A:189:LEU:HD23	1:A:190:SER:CB	2.44	0.47
1:B:259:VAL:CG1	1:B:267:LEU:HD21	2.45	0.47
1:B:290:GLN:O	1:B:294:LYS:N	2.41	0.47
1:B:378:PHE:HE2	1:B:380:LEU:HD21	1.80	0.47
1:B:539:LEU:HD23	1:B:539:LEU:O	2.15	0.47
1:B:90:LEU:HD21	1:B:99:ALA:CB	2.45	0.47
1:A:304:TYR:CD2	1:A:328:LEU:HD23	2.49	0.47
1:B:58:VAL:HG23	1:B:59:GLY:N	2.30	0.47
1:A:557:VAL:O	1:A:557:VAL:HG12	2.15	0.47
1:A:32:GLN:NE2	1:B:138:PRO:HD3	2.30	0.47
1:A:326:PHE:HE2	1:A:337:VAL:HG21	1.80	0.46
1:A:422:LEU:HD13	1:A:471:VAL:HG13	1.97	0.46
1:B:137:ARG:CB	1:B:138:PRO:CD	2.89	0.46
1:B:203:ARG:HH22	1:B:254:ARG:HG3	1.80	0.46
1:B:246:ALA:HA	1:B:249:VAL:CG1	2.45	0.46
1:B:380:LEU:CD1	1:B:410:ILE:HD11	2.45	0.46
1:B:376:GLU:CA	1:B:412:HIS:H	2.24	0.46
1:A:145:PRO:HB3	1:A:148:GLY:HA2	1.96	0.46
1:A:430:GLU:HG3	1:A:431:GLY:N	2.30	0.46
1:A:84:GLU:HG3	1:A:85:HIS:N	2.27	0.46
1:B:189:LEU:C	1:B:189:LEU:HD23	2.36	0.46
1:B:257:PHE:CB	1:B:286:ALA:O	2.46	0.46
1:A:480:CYS:HB2	1:A:484:GLU:OE1	2.16	0.46
1:A:5:LEU:O	1:A:9:ILE:HG13	2.16	0.46
1:A:86:TYR:CD2	1:A:90:LEU:HD11	2.50	0.46
1:B:173:ILE:N	5:B:601:HOH:O	2.48	0.46
1:B:271:LEU:O	1:B:274:ILE:HG23	2.14	0.46
1:B:295:THR:O	1:B:298:TYR:N	2.46	0.46
1:A:228:GLN:HG2	1:A:229:THR:N	2.29	0.46
1:A:448:LEU:O	1:A:451:ALA:O	2.32	0.46
1:A:441:TYR:OH	1:A:458:MET:O	2.30	0.46
1:B:368:ARG:C	1:B:369:MET:HG2	2.35	0.46
1:A:163:ARG:HD2	1:A:163:ARG:HA	1.66	0.46
1:A:304:TYR:CD2	1:A:328:LEU:CD2	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:VAL:HB	1:B:418:ARG:CB	2.45	0.46
1:A:160:LEU:C	1:A:162:LEU:H	2.19	0.46
1:A:412:HIS:CG	1:A:412:HIS:O	2.69	0.46
1:A:458:MET:HB2	5:A:601:HOH:O	2.14	0.46
1:A:516:GLU:C	1:A:518:PHE:N	2.69	0.46
1:B:149:TRP:HH2	1:B:194:LEU:HD13	1.80	0.46
1:B:304:TYR:C	1:B:304:TYR:CD2	2.89	0.46
1:A:101:SER:C	1:A:104:ASN:HD22	2.18	0.46
1:A:151:SER:O	1:A:154:MET:CB	2.62	0.46
1:A:438:ILE:CD1	1:A:531:LEU:HD23	2.45	0.46
1:B:204:ASN:HD22	1:B:560:VAL:CG1	2.28	0.46
1:B:290:GLN:O	1:B:293:ALA:HB3	2.15	0.46
1:A:365:ARG:O	1:A:366:VAL:HB	2.15	0.46
1:A:401:ILE:HA	1:A:409:VAL:O	2.15	0.46
1:A:552:ILE:HA	1:A:556:HIS:O	2.16	0.46
1:B:402:THR:O	1:B:408:ILE:HG22	2.16	0.46
1:B:450:ALA:HB1	1:B:558:GLU:CD	2.36	0.46
1:B:78:PHE:HD1	1:B:81:ARG:NH2	2.13	0.46
1:A:208:TRP:CE3	1:A:225:PRO:HG3	2.51	0.46
1:B:173:ILE:HG13	1:B:174:HIS:N	2.31	0.46
1:B:334:VAL:HG12	1:B:416:GLU:HG3	1.96	0.46
1:B:72:GLN:H	1:B:72:GLN:HG3	1.34	0.46
1:A:114:ARG:C	1:A:114:ARG:HD3	2.36	0.46
1:A:86:TYR:O	1:A:90:LEU:HD11	2.16	0.46
1:B:299:ARG:HD2	1:B:299:ARG:HA	1.32	0.46
1:B:434:LEU:O	1:B:438:ILE:CG2	2.33	0.46
1:B:450:ALA:HB1	1:B:558:GLU:HB2	1.98	0.46
1:A:228:GLN:OE1	1:A:231:ASP:HA	2.16	0.45
1:A:481:TYR:HB2	1:A:484:GLU:HG3	1.97	0.45
1:B:458:MET:O	1:B:458:MET:HG3	2.16	0.45
1:B:301:TYR:O	1:B:305:LEU:HD22	2.15	0.45
1:B:323:MET:CG	1:B:338:ILE:HA	2.44	0.45
1:B:33:GLN:O	1:B:33:GLN:HG3	2.16	0.45
1:A:488:ARG:HB2	1:A:546:ARG:NH2	2.30	0.45
1:B:376:GLU:OE2	1:B:411:ARG:NH2	2.48	0.45
1:B:454:PHE:HD1	1:B:482:MET:HE2	1.81	0.45
1:A:134:THR:OG1	1:A:134:THR:O	2.29	0.45
1:A:153:LEU:O	1:A:156:VAL:HG22	2.16	0.45
1:A:227:HIS:O	1:A:234:LEU:CB	2.62	0.45
1:A:337:VAL:HG22	1:A:413:LEU:CD1	2.45	0.45
1:A:78:PHE:C	1:A:80:LEU:N	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ARG:O	1:B:69:THR:O	2.33	0.45
1:A:245:GLU:OE1	1:A:245:GLU:HA	2.17	0.45
1:A:464:GLY:O	1:A:471:VAL:HA	2.16	0.45
1:A:568:ARG:HG3	1:A:571:VAL:HG12	1.98	0.45
1:A:90:LEU:N	1:A:91:PRO:CD	2.78	0.45
1:A:222:PHE:CD2	1:A:222:PHE:C	2.90	0.45
1:B:312:PHE:N	1:B:384:HIS:O	2.38	0.45
1:B:75:ASP:O	1:B:79:LEU:HB2	2.16	0.45
1:A:366:VAL:O	1:A:366:VAL:CG1	2.64	0.45
1:A:57:HIS:O	1:A:61:VAL:HG13	2.17	0.45
1:B:125:SER:HA	1:B:296:GLU:CG	2.47	0.45
1:B:274:ILE:CG1	1:B:275:LEU:H	2.25	0.45
1:B:37:GLN:O	1:B:38:ALA:HB3	2.17	0.45
1:A:173:ILE:HG13	1:A:174:HIS:N	2.32	0.45
1:B:310:GLU:OE2	1:B:384:HIS:ND1	2.49	0.45
1:A:203:ARG:HB2	1:A:257:PHE:CE1	2.52	0.45
1:A:430:GLU:HG3	1:A:431:GLY:H	1.82	0.45
1:A:357:TYR:CD1	1:A:476:TYR:HD2	2.35	0.45
1:A:47:MET:O	1:A:50:ARG:N	2.48	0.45
1:A:13:ILE:HA	1:A:61:VAL:HG21	1.98	0.45
1:A:126:SER:O	1:A:127:GLN:CB	2.63	0.45
1:B:466:THR:CG2	1:B:467:ARG:N	2.79	0.45
1:B:420:VAL:O	1:B:465:VAL:N	2.40	0.44
1:B:481:TYR:C	1:B:483:THR:H	2.21	0.44
1:A:36:GLU:HA	1:A:164:LEU:HD11	1.98	0.44
1:A:296:GLU:O	1:A:300:GLU:HG3	2.17	0.44
1:B:382:LYS:NZ	1:B:403:ASP:CG	2.54	0.44
1:A:234:LEU:O	1:A:234:LEU:HD22	2.16	0.44
1:A:371:ASP:OD2	1:A:372:THR:N	2.51	0.44
1:A:47:MET:CG	1:A:48:LYS:N	2.77	0.44
1:B:162:LEU:H	1:B:162:LEU:HD22	1.81	0.44
1:B:226:ILE:CG2	1:B:234:LEU:HD22	2.47	0.44
1:B:544:TYR:O	1:B:548:LEU:CB	2.64	0.44
1:A:103:PHE:C	1:A:103:PHE:CD2	2.91	0.44
1:A:153:LEU:HD11	1:A:224:LEU:HD11	2.00	0.44
1:A:301:TYR:HA	1:A:331:PHE:CZ	2.51	0.44
1:A:368:ARG:HB2	1:A:448:LEU:HD13	2.00	0.44
1:B:196:VAL:CG1	1:B:209:LEU:HD21	2.48	0.44
1:B:338:ILE:CG1	1:B:353:VAL:HG21	2.35	0.44
1:A:139:LEU:O	1:A:139:LEU:HD23	2.18	0.44
1:A:100:GLU:O	1:A:104:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HD12	1:A:117:THR:N	2.32	0.44
1:A:135:ILE:HG22	1:A:137:ARG:O	2.16	0.44
1:A:255:SER:N	1:A:365:ARG:NH2	2.66	0.44
1:B:87:THR:HG22	1:B:122:PHE:HE1	1.80	0.44
1:B:298:TYR:HA	1:B:301:TYR:HB3	1.99	0.44
1:B:565:ARG:O	1:B:567:GLN:N	2.51	0.44
1:A:127:GLN:O	1:A:127:GLN:HG3	2.17	0.44
1:B:152:LEU:N	1:B:152:LEU:CD2	2.79	0.44
1:B:375:PHE:O	1:B:413:LEU:N	2.50	0.44
1:B:387:PRO:HA	1:B:390:MET:H	1.83	0.44
1:A:153:LEU:HD22	1:A:176:ILE:HG21	1.99	0.44
1:A:17:PHE:CG	1:A:18:ASP:N	2.85	0.44
1:A:474:TYR:OH	2:A:1762:ADP:H2'	2.18	0.44
1:B:80:LEU:CD1	1:B:119:GLU:O	2.66	0.44
1:B:164:LEU:CD1	1:B:228:GLN:HE22	2.31	0.44
1:B:290:GLN:HB3	1:B:290:GLN:HE21	1.46	0.44
1:B:323:MET:HE3	1:B:323:MET:HB2	1.95	0.44
1:A:155:ARG:C	1:A:159:ASP:OD2	2.52	0.44
1:A:394:LEU:HD23	1:A:401:ILE:HD11	2.00	0.44
1:B:121:LEU:C	1:B:121:LEU:HD12	2.38	0.44
1:B:152:LEU:HD22	1:B:152:LEU:H	1.82	0.44
1:B:32:GLN:O	1:B:36:GLU:HB2	2.18	0.44
1:B:564:ARG:CG	1:B:564:ARG:HH21	2.25	0.44
1:B:565:ARG:C	1:B:567:GLN:N	2.71	0.44
1:B:454:PHE:HA	1:B:455:PRO:HD3	1.87	0.43
1:B:5:LEU:HB2	1:B:78:PHE:CZ	2.53	0.43
1:A:309:ASN:HA	1:A:310:GLU:HA	1.86	0.43
1:A:361:LYS:HZ3	1:A:372:THR:HG1	1.58	0.43
1:A:255:SER:N	1:A:365:ARG:HH21	2.17	0.43
1:A:23:ARG:HE	1:A:53:LEU:HD11	1.83	0.43
1:B:297:SER:HA	1:B:300:GLU:HG3	2.01	0.43
1:A:458:MET:HE3	5:A:601:HOH:O	2.17	0.43
1:A:23:ARG:CD	1:A:53:LEU:HD21	2.48	0.43
1:B:246:ALA:HA	1:B:249:VAL:HG13	2.00	0.43
1:B:274:ILE:CG1	1:B:275:LEU:N	2.80	0.43
1:B:5:LEU:HA	1:B:8:LEU:HB3	2.00	0.43
1:B:305:LEU:N	1:B:305:LEU:CD1	2.80	0.43
1:B:370:ALA:N	1:B:476:TYR:HH	2.14	0.43
1:B:430:GLU:N	1:B:430:GLU:CD	2.72	0.43
1:B:288:GLY:O	1:B:290:GLN:N	2.42	0.43
1:A:172:ASP:HA	1:A:175:TYR:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:TYR:HB3	1:A:286:ALA:O	2.19	0.43
1:A:432:GLN:HB3	5:A:607:HOH:O	2.18	0.43
1:A:513:VAL:O	1:A:515:PRO:HD3	2.19	0.43
1:B:438:ILE:HB	1:B:532:PHE:CZ	2.53	0.43
1:A:18:ASP:HB3	1:B:19:ALA:HA	1.99	0.43
1:A:371:ASP:OD2	1:A:372:THR:O	2.36	0.43
1:A:81:ARG:O	1:A:85:HIS:HB2	2.19	0.43
1:B:204:ASN:ND2	1:B:560:VAL:CG1	2.82	0.43
1:A:32:GLN:HE22	1:B:138:PRO:HD3	1.83	0.43
1:A:113:HIS:CG	1:A:376:GLU:HB3	2.53	0.43
1:A:490:ILE:HG23	1:A:491:PRO:HD3	2.00	0.43
1:B:448:LEU:HD11	1:B:473:PHE:CD2	2.53	0.43
1:B:434:LEU:HD11	1:B:528:ILE:HG23	2.00	0.43
1:A:116:LEU:O	1:A:120:ARG:HB3	2.19	0.43
1:A:193:HIS:CE1	1:A:214:ILE:HG21	2.50	0.43
1:A:253:ALA:O	1:A:367:GLY:N	2.50	0.43
1:A:385:ILE:HG22	1:A:386:SER:O	2.19	0.43
1:B:123:ILE:O	1:B:123:ILE:HG23	2.19	0.43
1:B:441:TYR:C	1:B:441:TYR:CD2	2.91	0.43
1:B:49:ASN:O	1:B:52:HIS:HB2	2.19	0.43
1:A:170:SER:HA	1:A:173:ILE:HG12	1.99	0.43
1:A:202:TYR:O	1:A:257:PHE:CD1	2.67	0.43
1:A:301:TYR:HD1	1:A:331:PHE:HE2	1.67	0.43
1:B:382:LYS:CE	1:B:403:ASP:OD1	2.64	0.43
1:B:564:ARG:CG	1:B:564:ARG:NH2	2.82	0.43
1:A:139:LEU:O	1:A:139:LEU:CD2	2.68	0.42
1:A:211:GLY:HA2	1:A:270:TRP:HH2	1.84	0.42
1:A:23:ARG:HD3	1:A:53:LEU:HD21	2.01	0.42
1:A:397:ALA:HB1	1:A:400:LYS:HB2	2.00	0.42
1:A:408:ILE:O	1:A:408:ILE:CG1	2.67	0.42
1:A:368:ARG:NH2	1:A:440:GLU:HG3	2.33	0.42
1:A:535:MET:HE3	1:A:535:MET:O	2.18	0.42
1:B:139:LEU:O	1:B:198:ASN:OD1	2.36	0.42
1:B:149:TRP:HZ2	1:B:192:SER:O	2.01	0.42
1:A:193:HIS:CD2	1:A:214:ILE:CG2	2.93	0.42
1:B:101:SER:C	1:B:104:ASN:HD22	2.22	0.42
1:A:112:ASP:O	1:A:113:HIS:C	2.57	0.42
1:A:175:TYR:HB3	1:A:569:PHE:CZ	2.53	0.42
1:A:197:ALA:HB3	1:A:210:VAL:HG13	2.01	0.42
1:B:301:TYR:O	1:B:305:LEU:CD2	2.67	0.42
1:B:331:PHE:CE2	1:B:333:ARG:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:HIS:CE1	1:B:451:ALA:O	2.71	0.42
1:B:9:ILE:HG13	1:B:65:LEU:HD21	2.02	0.42
1:A:549:GLN:HG3	1:A:553:ARG:HE	1.83	0.42
1:B:422:LEU:O	1:B:423:ASN:C	2.57	0.42
1:A:79:LEU:HD11	1:A:111:PHE:CZ	2.55	0.42
1:A:311:GLN:HB3	1:A:384:HIS:O	2.19	0.42
1:A:440:GLU:O	1:A:444:ALA:HB2	2.20	0.42
1:B:543:ASP:O	1:B:547:ALA:HB3	2.19	0.42
1:A:116:LEU:HB3	1:A:120:ARG:NH1	2.34	0.42
1:A:143:PHE:N	1:A:194:LEU:O	2.53	0.42
1:A:221:PRO:O	1:A:241:THR:CG2	2.60	0.42
1:A:221:PRO:HD2	1:A:241:THR:O	2.19	0.42
1:A:334:VAL:HG22	1:A:418:ARG:HA	2.01	0.42
1:A:465:VAL:HG12	1:A:466:THR:N	2.34	0.42
1:B:143:PHE:N	1:B:143:PHE:CD2	2.88	0.42
1:B:448:LEU:O	1:B:453:ILE:N	2.51	0.42
1:B:442:GLY:CA	1:B:536:HIS:CD2	2.88	0.42
1:B:450:ALA:HB3	1:B:558:GLU:HG2	1.98	0.42
1:A:157:ILE:HG21	1:A:169:LYS:HG3	2.02	0.42
1:A:488:ARG:O	1:A:514:PHE:HD1	1.95	0.42
1:B:89:LEU:C	1:B:91:PRO:CD	2.84	0.42
1:A:489:ASP:CB	1:A:514:PHE:CD1	3.02	0.42
1:B:121:LEU:O	1:B:121:LEU:HD12	2.20	0.42
1:B:226:ILE:HG22	1:B:234:LEU:HD22	2.02	0.42
1:B:459:LEU:O	1:B:463:PHE:HD2	2.03	0.42
1:A:200:LEU:HD21	1:A:208:TRP:H	1.85	0.41
1:A:32:GLN:HG3	1:A:202:TYR:OH	2.20	0.41
1:B:403:ASP:O	1:B:404:LEU:HD23	2.19	0.41
1:B:48:LYS:HE2	1:B:362:GLU:CG	2.49	0.41
1:A:80:LEU:CD2	1:A:119:GLU:O	2.68	0.41
1:A:196:VAL:HG13	1:A:209:LEU:HD23	2.02	0.41
1:A:315:ALA:HB3	1:A:325:VAL:CG1	2.50	0.41
1:A:379:VAL:O	1:A:379:VAL:HG13	2.21	0.41
1:A:325:VAL:CG1	2:A:1762:ADP:O4'	2.61	0.41
1:A:358:GLN:C	1:A:360:VAL:N	2.72	0.41
1:A:390:MET:O	1:A:394:LEU:N	2.35	0.41
1:B:168:ASN:C	1:B:170:SER:N	2.73	0.41
1:B:285:MET:HB2	1:B:285:MET:HE3	1.95	0.41
1:B:32:GLN:O	1:B:36:GLU:CB	2.68	0.41
1:B:466:THR:HG23	1:B:467:ARG:N	2.34	0.41
1:A:79:LEU:HD11	1:A:111:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ARG:C	1:A:566:ARG:H	2.23	0.41
1:B:318:ILE:O	1:B:319:ARG:C	2.59	0.41
1:B:354:ARG:HA	1:B:354:ARG:HD3	1.79	0.41
1:B:368:ARG:O	1:B:369:MET:HG2	2.19	0.41
1:B:514:PHE:CD2	1:B:517:GLU:OE2	2.73	0.41
1:A:157:ILE:CG2	1:A:169:LYS:CD	2.96	0.41
1:A:113:HIS:O	1:A:377:ASN:HB2	2.20	0.41
1:A:54:TYR:OH	1:A:102:PHE:HA	2.20	0.41
1:A:69:THR:O	1:A:73:SER:HB2	2.21	0.41
1:B:280:THR:HG22	1:B:284:TYR:HE2	1.85	0.41
1:B:432:GLN:O	1:B:436:ASP:N	2.34	0.41
1:B:93:TYR:CB	1:B:96:PHE:HB3	2.48	0.41
1:A:355:ALA:O	1:A:359:LEU:CB	2.68	0.41
1:A:362:GLU:HG2	1:A:362:GLU:H	1.73	0.41
1:A:334:VAL:HG23	1:A:416:GLU:O	2.20	0.41
1:B:340:ASP:OD1	1:B:396:GLU:O	2.37	0.41
1:B:525:ASP:CB	1:B:528:ILE:CD1	2.99	0.41
1:B:68:ILE:CG1	1:B:69:THR:H	2.26	0.41
1:B:78:PHE:CD1	1:B:81:ARG:NH2	2.88	0.41
1:A:222:PHE:CE2	1:A:224:LEU:CD1	3.03	0.41
1:A:438:ILE:O	1:A:441:TYR:HB3	2.21	0.41
1:B:525:ASP:CG	1:B:528:ILE:HD12	2.40	0.41
1:B:549:GLN:C	1:B:551:ARG:N	2.74	0.41
1:A:157:ILE:HG21	1:A:169:LYS:CD	2.51	0.41
1:A:509:SER:N	1:A:510:PRO:HD3	2.33	0.41
1:B:116:LEU:H	1:B:116:LEU:HG	1.64	0.41
1:B:253:ALA:O	1:B:365:ARG:HB3	2.21	0.41
1:B:541:ARG:HH22	1:B:544:TYR:CB	2.26	0.41
1:B:565:ARG:C	1:B:567:GLN:H	2.24	0.41
1:A:166:TRP:O	1:A:167:GLN:OE1	2.38	0.41
1:A:198:ASN:HA	1:A:199:GLU:HA	1.71	0.41
1:A:204:ASN:C	1:A:206:ALA:H	2.24	0.41
1:A:204:ASN:HB3	1:A:205:LYS:H	1.53	0.41
1:B:58:VAL:HG11	1:B:105:SER:HB2	2.03	0.41
1:A:305:LEU:C	1:A:307:GLY:H	2.24	0.41
1:A:389:LEU:O	1:A:392:LEU:HD23	2.21	0.41
1:B:57:HIS:O	1:B:61:VAL:HG13	2.21	0.41
1:B:68:ILE:CG1	1:B:69:THR:N	2.79	0.41
1:A:107:TYR:OH	1:A:120:ARG:CG	2.69	0.40
1:A:9:ILE:O	1:A:12:THR:HB	2.22	0.40
1:A:134:THR:H	1:A:134:THR:HG23	1.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:PHE:O	1:A:194:LEU:O	2.39	0.40
1:A:234:LEU:H	1:A:234:LEU:HD13	1.87	0.40
1:A:240:LEU:HD22	1:A:245:GLU:HB3	2.03	0.40
1:A:161:PRO:CB	1:B:138:PRO:HB3	2.49	0.40
1:B:529:GLY:O	1:B:532:PHE:CB	2.66	0.40
1:B:559:ASP:HB3	1:B:561:TYR:HE2	1.86	0.40
1:A:250:PHE:CB	1:A:275:LEU:HD21	2.51	0.40
1:A:474:TYR:CD1	1:A:474:TYR:C	2.95	0.40
1:B:200:LEU:HB3	1:B:208:TRP:O	2.21	0.40
1:B:24:PHE:CE1	1:B:50:ARG:HG2	2.56	0.40
1:B:271:LEU:HB2	1:B:283:LEU:HD11	2.02	0.40
1:B:34:ARG:HA	1:B:34:ARG:HD2	1.93	0.40
1:B:334:VAL:HG12	1:B:416:GLU:O	2.21	0.40
1:A:172:ASP:OD1	1:A:236:ILE:HB	2.21	0.40
1:B:155:ARG:HA	1:B:155:ARG:HD3	1.91	0.40
1:B:203:ARG:NH2	1:B:254:ARG:CG	2.83	0.40
1:B:425:TRP:CZ3	1:B:429:VAL:HG21	2.56	0.40
1:B:433:GLN:CA	1:B:433:GLN:OE1	2.68	0.40
1:A:229:THR:HB	1:A:233:GLU:CG	2.50	0.40
1:A:305:LEU:CD1	1:A:305:LEU:N	2.72	0.40
1:A:48:LYS:CG	1:A:362:GLU:HB2	2.45	0.40
1:A:516:GLU:O	1:A:517:GLU:C	2.60	0.40
1:B:101:SER:HA	1:B:104:ASN:HD22	1.85	0.40
1:B:126:SER:O	1:B:127:GLN:C	2.58	0.40
1:B:195:GLN:HB2	1:B:214:ILE:HD11	2.04	0.40
1:A:107:TYR:OH	1:A:120:ARG:HG3	2.21	0.40
1:A:220:LEU:HG	1:A:221:PRO:HD2	1.99	0.40
1:A:226:ILE:HG23	1:A:236:ILE:HG12	2.02	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ASN:ND2	1:B:427:GLU:CD[2_455]	1.48	0.72
1:A:423:ASN:CG	1:B:427:GLU:OE2[2_455]	1.55	0.65
1:A:423:ASN:ND2	1:B:427:GLU:OE1[2_455]	1.74	0.46
1:A:423:ASN:ND2	1:B:427:GLU:OE2[2_455]	1.98	0.22
1:A:423:ASN:CG	1:B:427:GLU:CD[2_455]	2.01	0.19
1:A:423:ASN:OD1	1:B:427:GLU:OE2[2_455]	2.09	0.11
1:A:423:ASN:CB	1:B:427:GLU:OE2[2_455]	2.13	0.07

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	541/578 (94%)	470 (87%)	65 (12%)	6 (1%)	14	46
1	B	529/578 (92%)	457 (86%)	68 (13%)	4 (1%)	19	54
All	All	1070/1156 (93%)	927 (87%)	133 (12%)	10 (1%)	17	52

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	232	GLY
1	A	366	VAL
1	A	511	GLY
1	B	118	PRO
1	B	566	ARG
1	A	264	PRO
1	A	351	ALA
1	B	90	LEU
1	B	216	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	480/508 (94%)	382 (80%)	98 (20%)	1	5
1	B	472/508 (93%)	360 (76%)	112 (24%)	1	2
All	All	952/1016 (94%)	742 (78%)	210 (22%)	1	4

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	15	GLN
1	A	17	PHE
1	A	18	ASP
1	A	20	GLN
1	A	25	LEU
1	A	29	SER
1	A	37	GLN
1	A	50	ARG
1	A	58	VAL
1	A	61	VAL
1	A	62	VAL
1	A	65	LEU
1	A	70	ASN
1	A	72	GLN
1	A	78	PHE
1	A	84	GLU
1	A	87	THR
1	A	93	TYR
1	A	114	ARG
1	A	115	SER
1	A	134	THR
1	A	135	ILE
1	A	151	SER
1	A	154	MET
1	A	158	SER
1	A	163	ARG
1	A	167	GLN
1	A	176	ILE
1	A	179	HIS
1	A	181	THR
1	A	189	LEU
1	A	194	LEU
1	A	199	GLU
1	A	209	LEU
1	A	214	ILE
1	A	215	THR
1	A	217	SER
1	A	219	THR
1	A	222	PHE
1	A	234	LEU
1	A	238	THR

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Mol	Chain	Res	Type
1	A	239	CYS
1	A	242	THR
1	A	254	ARG
1	A	263	LEU
1	A	271	LEU
1	A	273	GLU
1	A	279	THR
1	A	280	THR
1	A	290	GLN
1	A	301	TYR
1	A	305	LEU
1	A	308	CYS
1	A	309	ASN
1	A	310	GLU
1	A	322	VAL
1	A	324	LEU
1	A	328	LEU
1	A	331	PHE
1	A	334	VAL
1	A	335	PHE
1	A	337	VAL
1	A	338	ILE
1	A	342	PHE
1	A	349	SER
1	A	361	LYS
1	A	362	GLU
1	A	374	GLU
1	A	378	PHE
1	A	380	LEU
1	A	383	ARG
1	A	386	SER
1	A	392	LEU
1	A	408	ILE
1	A	410	ILE
1	A	416	GLU
1	A	438	ILE
1	A	448	LEU
1	A	458	MET
1	A	461	LYS
1	A	474	TYR
1	A	485	VAL
1	A	521	TRP

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Mol	Chain	Res	Type
1	A	522	LEU
1	A	525	ASP
1	A	532	PHE
1	A	534	GLU
1	A	540	PHE
1	A	541	ARG
1	A	544	TYR
1	A	548	LEU
1	A	549	GLN
1	A	550	ASN
1	A	554	GLU
1	A	557	VAL
1	A	563	TYR
1	A	564	ARG
1	B	3	ARG
1	B	5	LEU
1	B	6	GLU
1	B	7	LEU
1	B	33	GLN
1	B	35	PHE
1	B	44	GLN
1	B	47	MET
1	B	53	LEU
1	B	67	CYS
1	B	72	GLN
1	B	79	LEU
1	B	80	LEU
1	B	81	ARG
1	B	89	LEU
1	B	93	TYR
1	B	95	ARG
1	B	96	PHE
1	B	109	ARG
1	B	112	ASP
1	B	113	HIS
1	B	116	LEU
1	B	117	THR
1	B	121	LEU
1	B	122	PHE
1	B	124	PHE
1	B	134	THR
1	B	136	PRO

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Mol	Chain	Res	Type
1	B	141	LYS
1	B	152	LEU
1	B	158	SER
1	B	159	ASP
1	B	171	ARG
1	B	174	HIS
1	B	189	LEU
1	B	212	LYS
1	B	215	THR
1	B	219	THR
1	B	222	PHE
1	B	223	LEU
1	B	231	ASP
1	B	233	GLU
1	B	241	THR
1	B	243	THR
1	B	245	GLU
1	B	247	SER
1	B	249	VAL
1	B	257	PHE
1	B	258	MET
1	B	263	LEU
1	B	275	LEU
1	B	280	THR
1	B	287	ILE
1	B	290	GLN
1	B	291	LYS
1	B	294	LYS
1	B	295	THR
1	B	299	ARG
1	B	305	LEU
1	B	306	GLN
1	B	309	ASN
1	B	321	MET
1	B	324	LEU
1	B	325	VAL
1	B	329	PRO
1	B	337	VAL
1	B	341	LYS
1	B	352	HIS
1	B	353	VAL
1	B	354	ARG

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Mol	Chain	Res	Type
1	B	356	CYS
1	B	357	TYR
1	B	359	LEU
1	B	360	VAL
1	B	364	ASP
1	B	368	ARG
1	B	372	THR
1	B	376	GLU
1	B	379	VAL
1	B	383	ARG
1	B	392	LEU
1	B	400	LYS
1	B	401	ILE
1	B	402	THR
1	B	404	LEU
1	B	408	ILE
1	B	411	ARG
1	B	413	LEU
1	B	417	ARG
1	B	418	ARG
1	B	420	VAL
1	B	425	TRP
1	B	426	LEU
1	B	427	GLU
1	B	428	GLN
1	B	430	GLU
1	B	433	GLN
1	B	459	LEU
1	B	466	THR
1	B	472	VAL
1	B	474	TYR
1	B	478	GLU
1	B	479	ILE
1	B	485	VAL
1	B	489	ASP
1	B	514	PHE
1	B	516	GLU
1	B	521	TRP
1	B	531	LEU
1	B	538	ASP
1	B	559	ASP
1	B	571	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	33	GLN
1	A	45	GLN
1	A	64	GLN
1	A	72	GLN
1	A	85	HIS
1	A	104	ASN
1	A	165	HIS
1	A	168	ASN
1	A	227	HIS
1	A	292	HIS
1	A	309	ASN
1	A	407	GLN
1	A	447	GLN
1	A	536	HIS
1	A	550	ASN
1	B	32	GLN
1	B	64	GLN
1	B	72	GLN
1	B	168	ASN
1	B	179	HIS
1	B	204	ASN
1	B	228	GLN
1	B	290	GLN
1	B	292	HIS
1	B	309	ASN
1	B	363	HIS
1	B	407	GLN
1	B	412	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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
4	AMP	B	1604	-	22,25,25	1.04	1 (4%)	25,38,38	1.48	2 (8%)
2	ADP	A	1762	3	24,29,29	0.86	1 (4%)	29,45,45	1.61	4 (13%)

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
4	AMP	B	1604	-	-	5/6/26/26	0/3/3/3
2	ADP	A	1762	3	-	5/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1604	AMP	C5-C4	2.45	1.47	1.40
2	A	1762	ADP	C5-C4	2.02	1.46	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1762	ADP	PA-O3A-PB	-4.21	118.39	132.83
2	A	1762	ADP	N3-C2-N1	-4.13	122.23	128.68
4	B	1604	AMP	N3-C2-N1	-3.83	122.69	128.68
4	B	1604	AMP	C4-C5-N7	-3.38	105.88	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1762	ADP	C3'-C2'-C1'	2.82	105.22	100.98
2	A	1762	ADP	C4-C5-N7	-2.71	106.58	109.40

There are no chirality outliers.

All (10) torsion outliers are listed below:

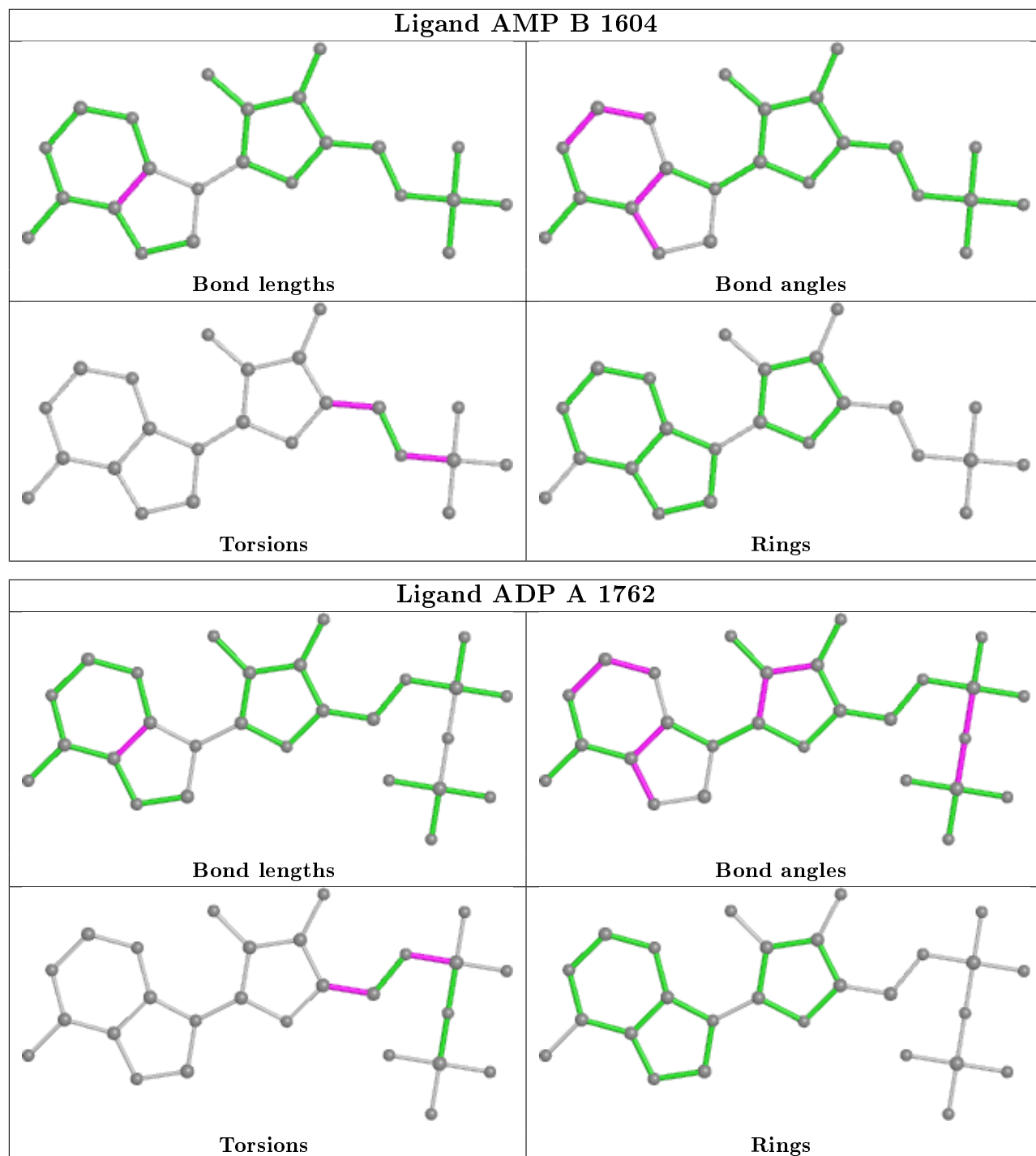
Mol	Chain	Res	Type	Atoms
4	B	1604	AMP	C5'-O5'-P-O2P
4	B	1604	AMP	C5'-O5'-P-O3P
2	A	1762	ADP	C5'-O5'-PA-O3A
2	A	1762	ADP	O4'-C4'-C5'-O5'
2	A	1762	ADP	C3'-C4'-C5'-O5'
4	B	1604	AMP	O4'-C4'-C5'-O5'
4	B	1604	AMP	C5'-O5'-P-O1P
4	B	1604	AMP	C3'-C4'-C5'-O5'
2	A	1762	ADP	C5'-O5'-PA-O1A
2	A	1762	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1604	AMP	2	0
2	A	1762	ADP	5	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	547/578 (94%)	-0.25	3 (0%) 91 81	2, 15, 29, 37	0
1	B	539/578 (93%)	-0.18	0 100 100	4, 18, 28, 34	0
All	All	1086/1156 (93%)	-0.22	3 (0%) 94 88	2, 17, 29, 37	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	THR	3.2
1	A	158	SER	2.3
1	A	146	ASP	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	AMP	B	1604	23/23	0.93	0.18	23,25,31,34	0
2	ADP	A	1762	27/27	0.95	0.15	6,10,11,12	0

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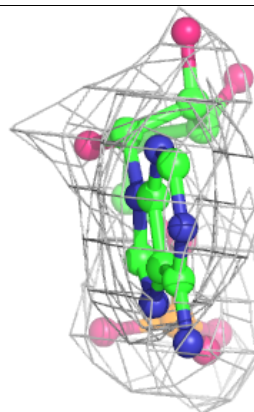
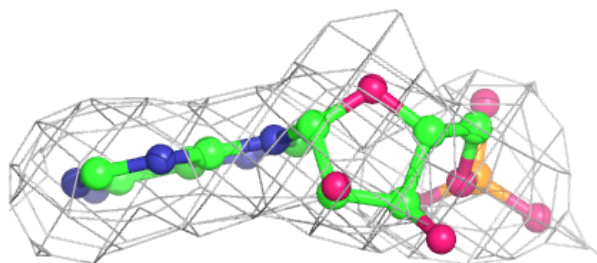
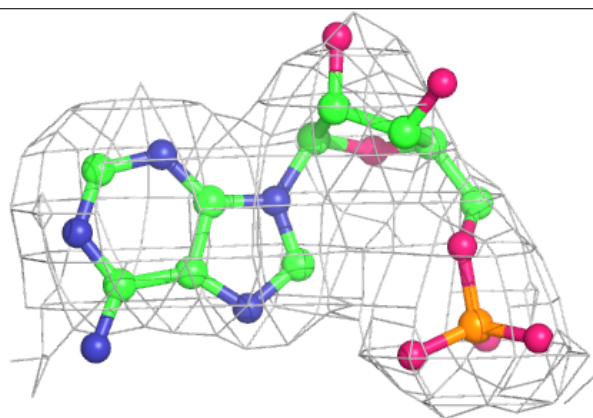
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	579	1/1	0.98	0.20	15,15,15,15	0

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.

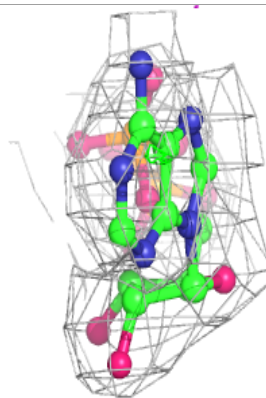
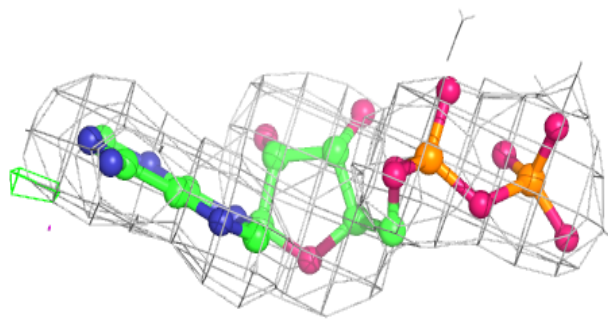
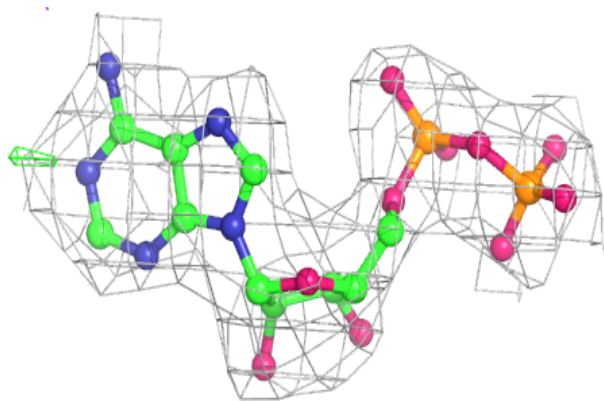
Electron density around AMP B 1604:

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 ADP A 1762:

$2mF_o - DF_c$ (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.