



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:27 am BST

PDB ID : 4R7Y
Title : Crystal structure of an active MCM hexamer
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Deposited on : 2014-08-28
Resolution : 2.70 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

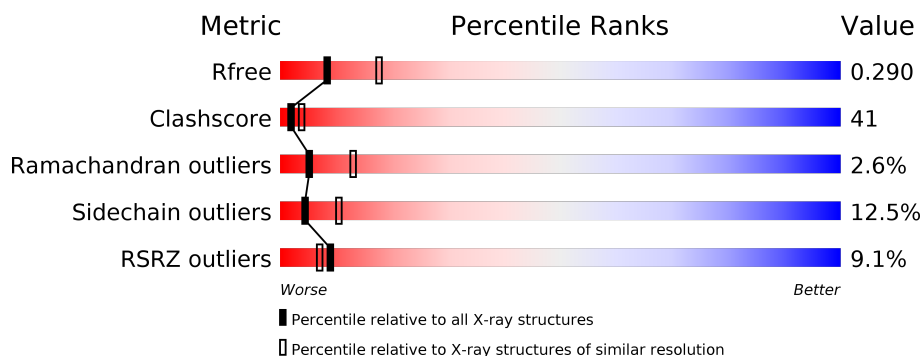
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	613	
1	B	613	

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
5	CL	A	2006	-	-	X	-
5	CL	B	2006	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9494 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.

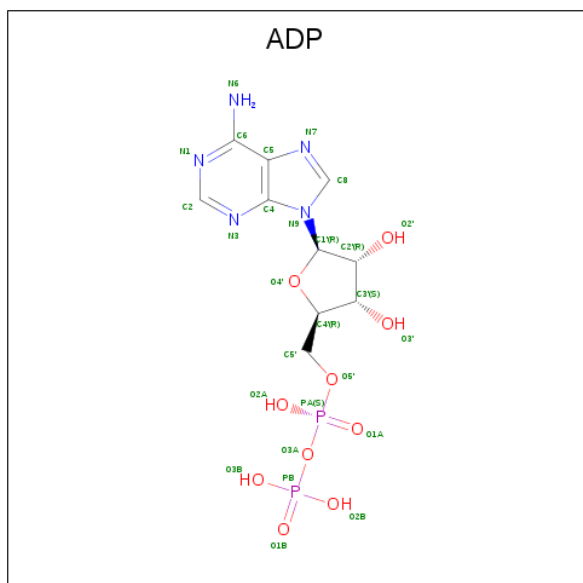
- Molecule 1 is a protein called Minichromosome maintenance protein MCM, Cell division control protein 21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	0	0
			4715	3001	822	878	14			
1	B	591	Total	C	N	O	S	0	0	0
			4715	3001	822	878	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q9UXG1
A	1	LEU	-	EXPRESSION TAG	UNP Q9UXG1
B	0	SER	-	EXPRESSION TAG	UNP Q9UXG1
B	1	LEU	-	EXPRESSION TAG	UNP Q9UXG1

- 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		
2	B	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	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Cl	0	0
			3	3		
5	A	3	Total	Cl	0	0
			3	3		

GLU	ILE	PRO	PRO	ILE	P1919	L1852	H1773	R1319	S260	K173	I103	SER
GLY	PRO	PRO	PRO	ILE	I1920	R1853	E1774	G1320	S261	C174	I104	LEU
ILE	PRO	PRO	PRO	ILE	T1921	V1854	A1775	I1322	I262	G175	P105	GLU
ILE	PRO	PRO	PRO	ILE	I1922	R1855	A1775	I1322	E263	K176	R105	PRO
ILE	PRO	PRO	PRO	ILE	I1923	R1856	Q1779	L1325	K267	P177	E108	SER
ILE	PRO	PRO	PRO	ILE	I1924	R1857	T1780	L1326	I1261	G178	L109	SER
ILE	PRO	PRO	PRO	ILE	I1925	R1858	I1781	V1327	I1264	F180	R110	LYS
ILE	PRO	PRO	PRO	ILE	I1926	E1859	S1782	G1328	E1265	R181	R111	LYS
ILE	PRO	PRO	PRO	ILE	I1927	E1860	I1783	D1329	E1266	L182	R112	LYS
ILE	PRO	PRO	PRO	ILE	I1928	V1861	T1789	I1332	Q1267	I183	R113	LYS
ILE	PRO	PRO	PRO	ILE	I1929	A1863	T1796	A1333	Q1268	K186	R114	LYS
ILE	PRO	PRO	PRO	ILE	I1930	K1864	T1796	K1334	I1268	T187	R115	LYS
ILE	PRO	PRO	PRO	ILE	I1931	K1865	A1800	S1335	I1269	K188	R116	LYS
ILE	PRO	PRO	PRO	ILE	I1932	I1866	A1800	Q1336	I1270	Q193	R117	LYS
ILE	PRO	PRO	PRO	ILE	I1933	P1867	M1803	I1337	E1271	I123	R118	LYS
ILE	PRO	PRO	PRO	ILE	I1934	E1868	P1804	I1340	L1272	R200	R119	LYS
ILE	PRO	PRO	PRO	ILE	I1935	E1869	K1805	V1341	A1273	P201	R120	LYS
ILE	PRO	PRO	PRO	ILE	I1936	I1870	K1805	A1342	K1274	E202	R121	LYS
ILE	PRO	PRO	PRO	ILE	I1937	L1871	R1808	N1343	A1275	E203	R122	LYS
ILE	PRO	PRO	PRO	ILE	I1938	R1872	F1809	M1344	K1276	P205	R123	LYS
ILE	PRO	PRO	PRO	ILE	I1939	K1873	M1810	A1345	D1277	Q208	R124	LYS
ILE	PRO	PRO	PRO	ILE	I1940	Y1874	M1811	A1346	I1278	L209	R125	LYS
ILE	PRO	PRO	PRO	ILE	I1941	I1875	M1812	R1347	V1279	R211	R126	LYS
ILE	PRO	PRO	PRO	ILE	I1942	A1878	K1813	A1348	D1280	E214	R127	LYS
ILE	PRO	PRO	PRO	ILE	I1943	R1879	M1814	I1349	I1281	K143	R128	LYS
ILE	PRO	PRO	PRO	ILE	I1944	K1880	M1815	S1352	D1284	R144	R129	LYS
ILE	PRO	PRO	PRO	ILE	I1945	I1881	M1816	G1353	I1285	I146	R130	LYS
ILE	PRO	PRO	PRO	ILE	I1946	I1882	F1817	V1733	I1286	P147	R131	LYS
ILE	PRO	PRO	PRO	ILE	I1947	I1883	Q1818	D1735	G1292	P148	R132	LYS
ILE	PRO	PRO	PRO	ILE	I1948	P1884	I1819	G1746	I1293	C149	R133	LYS
ILE	PRO	PRO	PRO	ILE	I1949	V1885	P1823	A1747	V1296	R150	R134	LYS
ILE	PRO	PRO	PRO	ILE	I1950	I1886	L1824	L1748	K1297	Q151	R135	LYS
ILE	PRO	PRO	PRO	ILE	I1951	I1887	L1825	L1748	K1298	E152	R136	LYS
ILE	PRO	PRO	PRO	ILE	I1952	E1888	L1826	A1751	G1299	F153	R137	LYS
ILE	PRO	PRO	PRO	ILE	I1953	E1889	S1827	D1752	I1300	E154	R138	LYS
ILE	PRO	PRO	PRO	ILE	I1954	A1890	R1828	L1757	A1301	V155	R139	LYS
ILE	PRO	PRO	PRO	ILE	I1955	E1891	F1829	I1758	A1302	P156	R140	LYS
ILE	PRO	PRO	PRO	ILE	I1956	E1892	D1830	D1759	L1303	E157	R141	LYS
ILE	PRO	PRO	PRO	ILE	I1957	E1893	F1833	E1760	L1304	D158	R142	LYS
ILE	PRO	PRO	PRO	ILE	I1958	I1894	A1751	L1761	I1308	E159	R143	LYS
ILE	PRO	PRO	PRO	ILE	I1959	K1895	D1752	D1762	V1309	R161	R144	LYS
ILE	PRO	PRO	PRO	ILE	I1960	K1896	I1836	K1763	R1310	P162	R145	LYS
ILE	PRO	PRO	PRO	ILE	I1961	Y1897	D1837	M1764	K1311	E163	R146	LYS
ILE	PRO	PRO	PRO	ILE	I1962	Y1898	E1838	S1765	L1312	E166	R147	LYS
ILE	PRO	PRO	PRO	ILE	I1963	V1899	P1839	D1766	P1313	M167	R148	LYS
ILE	PRO	PRO	PRO	ILE	I1964	R1900	D1840	R1767	D1314	P168	R149	LYS
ILE	PRO	PRO	PRO	ILE	I1965	M1901	D1841	A1761	G1315	T169	R150	LYS
ILE	PRO	PRO	PRO	ILE	I1966	R1902	K1842	L1762	R1316	I170	R151	LYS
ILE	PRO	PRO	PRO	ILE	I1967	K1903	I1843	D1762	T1317	P172	R152	LYS
ILE	PRO	PRO	PRO	ILE	I1968	S1904	D1844	K1763	K258		R153	LYS
ILE	PRO	PRO	PRO	ILE	I1969	VAL	S1845	M1764	R1317		R154	LYS
ILE	PRO	PRO	PRO	ILE	I1970	LYS	E1846	D1766	R1318		R155	LYS
ILE	PRO	PRO	PRO	ILE	I1971	LYS	V1847	R1767			R156	LYS
ILE	PRO	PRO	PRO	ILE	I1972	THR	A1848	A1767			R157	LYS
ILE	PRO	PRO	PRO	ILE	I1973	LYS	R1849				R158	LYS
ILE	PRO	PRO	PRO	ILE	I1974	GLY	H1850				R159	LYS
ILE	PRO	PRO	PRO	ILE	I1975	GLU	I1851				R160	LYS
ILE	PRO	PRO	PRO	ILE	I1976	GLU					R161	LYS
ILE	PRO	PRO	PRO	ILE	I1977	GLU					R162	LYS
ILE	PRO	PRO	PRO	ILE	I1978	GLU					R163	LYS
ILE	PRO	PRO	PRO	ILE	I1979	GLU					R164	LYS
ILE	PRO	PRO	PRO	ILE	I1980	GLU					R165	LYS
ILE	PRO	PRO	PRO	ILE	I1981	GLU					R166	LYS
ILE	PRO	PRO	PRO	ILE	I1982	GLU					R167	LYS
ILE	PRO	PRO	PRO	ILE	I1983	GLU					R168	LYS
ILE	PRO	PRO	PRO	ILE	I1984	GLU					R169	LYS
ILE	PRO	PRO	PRO	ILE	I1985	GLU					R170	LYS
ILE	PRO	PRO	PRO	ILE	I1986	GLU					R171	LYS
ILE	PRO	PRO	PRO	ILE	I1987	GLU					R172	LYS
ILE	PRO	PRO	PRO	ILE	I1988	GLU					R173	LYS
ILE	PRO	PRO	PRO	ILE	I1989	GLU					R174	LYS
ILE	PRO	PRO	PRO	ILE	I1990	GLU					R175	LYS
ILE	PRO	PRO	PRO	ILE	I1991	GLU					R176	LYS
ILE	PRO	PRO	PRO	ILE	I1992	GLU					R177	LYS
ILE	PRO	PRO	PRO	ILE	I1993	GLU					R178	LYS
ILE	PRO	PRO	PRO	ILE	I1994	GLU					R179	LYS
ILE	PRO	PRO	PRO	ILE	I1995	GLU					R180	LYS
ILE	PRO	PRO	PRO	ILE	I1996	GLU					R181	LYS
ILE	PRO	PRO	PRO	ILE	I1997	GLU					R182	LYS
ILE	PRO	PRO	PRO	ILE	I1998	GLU					R183	LYS
ILE	PRO	PRO	PRO	ILE	I1999	GLU					R184	LYS
ILE	PRO	PRO	PRO	ILE	I2000	GLU					R185	LYS
ILE	PRO	PRO	PRO	ILE	I2001	GLU					R186	LYS
ILE	PRO	PRO	PRO	ILE	I2002	GLU					R187	LYS
ILE	PRO	PRO	PRO	ILE	I2003	GLU					R188	LYS
ILE	PRO	PRO	PRO	ILE	I2004	GLU					R189	LYS
ILE	PRO	PRO	PRO	ILE	I2005	GLU					R190	LYS
ILE	PRO	PRO	PRO	ILE	I2006	GLU					R191	LYS
ILE	PRO	PRO	PRO	ILE	I2007	GLU					R192	LYS
ILE	PRO	PRO	PRO	ILE	I2008	GLU					R193	LYS
ILE	PRO	PRO	PRO	ILE	I2009	GLU					R194	LYS
ILE	PRO	PRO	PRO	ILE	I2010	GLU					R195	LYS
ILE	PRO	PRO	PRO	ILE	I2011	GLU					R196	LYS
ILE	PRO	PRO	PRO	ILE	I2012	GLU					R197	LYS
ILE	PRO	PRO	PRO	ILE	I2013	GLU					R198	LYS
ILE	PRO	PRO	PRO	ILE	I2014	GLU					R199	LYS
ILE	PRO	PRO	PRO	ILE	I2015	GLU					R200	LYS
ILE	PRO	PRO	PRO	ILE	I2016	GLU					R201	LYS
ILE	PRO	PRO	PRO	ILE	I2017	GLU					R202	LYS
ILE	PRO	PRO	PRO	ILE	I2018	GLU					R203	LYS
ILE	PRO	PRO	PRO	ILE	I2019	GLU					R204	LYS
ILE	PRO	PRO	PRO	ILE	I2020	GLU					R205	LYS
ILE	PRO	PRO	PRO	ILE	I2021	GLU					R206	LYS
ILE	PRO	PRO	PRO	ILE	I2022	GLU					R207	LYS
ILE	PRO	PRO	PRO	ILE	I2023	GLU					R208	LYS
ILE	PRO	PRO	PRO	ILE	I2024	GLU					R209	LYS
ILE	PRO	PRO	PRO	ILE	I2025	GLU					R210	LYS
ILE	PRO	PRO	PRO	ILE	I2026	GLU					R211	LYS
ILE	PRO	PRO	PRO	ILE	I2027	GLU					R212	LYS
ILE	PRO	PRO	PRO	ILE	I2028	GLU					R213	LYS
ILE	PRO	PRO	PRO	ILE	I2029	GLU					R214	LYS
ILE	PRO	PRO	PRO	ILE	I2030	GLU					R215	LYS
ILE	PRO	PRO	PRO	ILE	I2031	GLU					R216	LYS
ILE	PRO	PRO	PRO	ILE	I2032	GLU					R217	LYS
ILE	PRO	PRO	PRO	ILE	I2033	GLU					R218	LYS
ILE	PRO	PRO	PRO	ILE	I2034	GLU					R219	LYS
ILE	PRO	PRO	PRO	ILE	I2035	GLU					R220	LYS
ILE	PRO	PRO	PRO	ILE	I2036	GLU					R221	LYS
ILE	PRO	PRO	PRO	ILE	I2037	GLU					R222	LYS
ILE	PRO	PRO	PRO	ILE	I2038	GLU					R223	LYS
ILE	PRO	PRO	PRO	ILE	I2039	GLU					R224	LYS
ILE	PRO	PRO	PRO	ILE	I2040	GLU					R225	LYS
ILE	PRO	PRO	PRO	ILE	I2041	GLU					R226	LYS
ILE	PRO	PRO	PRO	ILE	I2042	GLU					R227	LYS
ILE	PRO	PRO	PRO	ILE	I2043	GLU					R228	LYS
ILE	PRO	PRO	PRO	ILE	I2044	GLU					R229	LYS
ILE	PRO	PRO	PRO	ILE	I2045	GLU					R230	LYS
ILE	PRO	PRO	PRO	ILE	I2046	GLU					R231	LYS
ILE	PRO	PRO	PRO	ILE	I2047	GLU					R232	LYS
ILE	PRO	PRO	PRO	ILE	I2048	GLU					R233	LYS
ILE	PRO	PRO	PRO	ILE	I2049	GLU					R234	LYS
ILE	PRO	PRO	PRO	ILE	I2050	GLU					R235	LYS
ILE	PRO	PRO	PRO	ILE	I2051	GLU					R236	LYS
ILE	PRO	PRO	PRO	ILE	I2052	GLU					R237	LYS
ILE	PRO											

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	118.90Å 118.90Å 199.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.83 – 2.70 49.83 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.7 (49.83-2.70) 89.7 (49.83-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.69Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.263 , 0.295 0.254 , 0.290	Depositor DCC
R_{free} test set	1976 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9494	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4816e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: ZN, MG, ADP, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/4793	0.69	0/6476
1	B	0.45	0/4793	0.70	0/6476
All	All	0.45	0/9586	0.70	0/12952

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4715	0	4876	420	0
1	B	4715	0	4876	393	0
2	A	27	0	12	3	0
2	B	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	3	0	0	2	0
5	B	3	0	0	2	0
All	All	9494	0	9776	798	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 41.

All (798) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1346:PRO:HB3	1:B:1872:ARG:HD3	1.29	1.10
1:A:156:PRO:HB2	1:A:159:GLU:O	1.53	1.07
1:B:1261:ILE:HA	1:B:1873:LYS:HZ1	1.17	1.05
1:A:1878:ALA:HA	1:A:1882:ILE:HD11	1.37	1.05
1:B:1261:ILE:HA	1:B:1873:LYS:NZ	1.73	1.04
1:A:1902:ARG:HB3	1:A:1903:LYS:HZ3	1.22	1.02
1:A:105:ARG:NH1	5:A:2006:CL:CL	2.32	1.00
1:A:1260:GLU:O	1:A:1873:LYS:HE2	1.62	0.99
1:A:1345:ALA:HB1	1:A:1348:ALA:HB3	1.44	0.97
1:A:1809:PHE:HD1	1:A:1809:PHE:H	1.10	0.96
1:B:105:ARG:NH1	5:B:2006:CL:CL	2.35	0.96
1:B:1949:ALA:O	1:B:1953:ILE:HG22	1.65	0.96
1:B:1311:LYS:HE2	1:B:1317:ARG:HH11	1.31	0.95
1:B:1809:PHE:HD1	1:B:1809:PHE:H	1.10	0.95
1:B:1894:ILE:HG13	1:B:1928:LEU:HD23	1.49	0.95
1:A:1920:ILE:HG23	1:A:1924:GLN:HG3	1.47	0.94
1:A:1882:ILE:HD13	1:A:1882:ILE:N	1.82	0.92
1:B:156:PRO:HB2	1:B:159:GLU:O	1.67	0.92
1:A:170:ILE:HG23	1:A:175:GLY:O	1.70	0.92
1:B:103:ILE:HD13	1:B:103:ILE:H	1.36	0.90
1:A:162:PRO:HG2	1:A:164:VAL:O	1.70	0.90
1:B:1290:ILE:HD11	1:B:1297:LYS:HE2	1.51	0.90
1:B:1261:ILE:H	1:B:1261:ILE:HD13	1.35	0.90
1:A:1889:GLU:HB3	1:A:1946:ARG:CG	2.02	0.89
1:B:214:GLU:OE2	1:B:240:LYS:HE2	1.74	0.88
1:A:143:LYS:HB2	1:A:183:ILE:HD11	1.52	0.88
1:B:1886:ILE:H	1:B:1886:ILE:HD12	1.39	0.88
1:B:1317:ARG:NH2	1:B:1779:GLN:HG3	1.88	0.87
1:A:1889:GLU:HB3	1:A:1946:ARG:HG2	1.56	0.86
1:A:161:MET:HE1	1:A:165:LEU:HD13	1.58	0.86
1:B:1863:ALA:HB1	1:B:1864:PRO:HD2	1.58	0.85
1:B:25:ASN:H	1:B:27:GLN:NE2	1.76	0.84
1:B:1317:ARG:HH21	1:B:1779:GLN:HG3	1.42	0.84
1:B:143:LYS:HG3	1:B:152:GLU:HG2	1.60	0.84
1:A:144:HIS:HB3	1:A:149:CYS:SG	2.17	0.83
1:B:1329:ASP:O	1:B:1332:VAL:HG22	1.78	0.83
1:A:1312:LEU:HB3	1:A:1313:PRO:HD2	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1329:ASP:OD1	1:B:1808:ARG:HA	1.78	0.82
1:B:1269:ILE:HD11	1:B:1874:TYR:HA	1.62	0.82
1:A:1893:GLU:OE1	1:A:1950:ARG:HD2	1.79	0.82
1:B:1752:ASP:HA	1:B:1796:THR:HG22	1.61	0.82
1:B:1276:LYS:HE2	1:B:1276:LYS:HA	1.62	0.82
1:B:156:PRO:HG3	1:B:161:MET:HG2	1.62	0.82
1:A:1960:LEU:O	1:A:1963:ILE:HG13	1.81	0.81
1:A:41:ARG:NH2	1:A:88:THR:HG22	1.96	0.81
1:B:1281:ALA:HB1	1:B:1866:ILE:HD11	1.62	0.80
1:A:1882:ILE:HD13	1:A:1882:ILE:H	1.40	0.80
1:A:1901:MET:SD	1:A:1920:ILE:HG21	2.21	0.80
1:B:1310:ARG:O	1:B:1318:LEU:HB2	1.81	0.79
1:A:25:ASN:H	1:A:27:GLN:HE21	1.28	0.79
1:B:1317:ARG:HH22	1:B:1779:GLN:HE21	1.30	0.79
1:B:1823:PRO:HA	1:B:1826:LEU:HD12	1.65	0.79
1:A:1760:GLU:HG3	1:A:1763:LYS:CG	2.13	0.79
1:A:1760:GLU:HG3	1:A:1763:LYS:HG3	1.65	0.79
1:B:1946:ARG:HD3	1:B:1950:ARG:HH12	1.46	0.79
1:B:25:ASN:H	1:B:27:GLN:HE21	1.30	0.79
1:A:1265:GLU:O	1:A:1269:ILE:HG22	1.82	0.78
1:A:249:SER:O	1:A:250:ARG:HG3	1.83	0.78
1:B:86:ASP:OD1	1:B:88:THR:HB	1.82	0.78
1:B:1311:LYS:NZ	1:B:1317:ARG:HB2	1.99	0.78
1:A:1276:LYS:HA	1:A:1276:LYS:HE2	1.65	0.78
1:A:1901:MET:SD	1:A:1920:ILE:HG13	2.24	0.77
1:B:41:ARG:NH2	1:B:88:THR:HG22	1.99	0.77
1:B:1345:ALA:HB1	1:B:1348:ALA:HB3	1.64	0.77
1:B:1810:ASN:HD21	1:B:1836:ILE:CG2	1.97	0.77
1:B:1946:ARG:HD3	1:B:1950:ARG:NH1	1.99	0.77
1:A:1878:ALA:O	1:A:1882:ILE:HG12	1.83	0.77
1:B:1311:LYS:HZ3	1:B:1317:ARG:HB2	1.48	0.77
1:A:1779:GLN:CG	1:A:1795:ARG:HA	2.15	0.77
1:A:1902:ARG:HB3	1:A:1903:LYS:NZ	1.99	0.77
1:A:1752:ASP:HA	1:A:1796:THR:HG22	1.66	0.76
1:B:1850:HIS:O	1:B:1854:VAL:HG23	1.85	0.76
1:B:1336:GLN:HG3	1:B:1340:TYR:HE1	1.51	0.76
1:A:1729:THR:HB	1:A:1781:ILE:HD13	1.66	0.76
1:A:1264:GLU:O	1:A:1268:ILE:HG13	1.86	0.75
1:B:1332:VAL:HG23	1:B:1334:LYS:HD2	1.69	0.75
1:A:1828:ARG:HE	1:A:1923:ARG:NH2	1.83	0.75
1:A:1899:VAL:O	1:A:1903:LYS:HE2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1289:ALA:HB3	1:A:1340:TYR:CE2	2.21	0.75
1:B:1327:VAL:HG13	1:B:1819:ILE:HG21	1.67	0.75
1:A:1345:ALA:CB	1:A:1348:ALA:HB3	2.17	0.75
1:B:1332:VAL:CG2	1:B:1334:LYS:HD2	2.17	0.74
1:A:1280:ASP:O	1:A:1283:VAL:HG13	1.88	0.74
1:B:1336:GLN:HG3	1:B:1340:TYR:CE1	2.23	0.73
1:B:1874:TYR:OH	1:B:1940:LEU:HD11	1.88	0.73
1:A:1278:ILE:HG23	1:A:1279:VAL:H	1.53	0.73
1:B:143:LYS:HB2	1:B:183:ILE:HD11	1.69	0.73
1:A:1839:PRO:HB3	1:B:1902:ARG:HH11	1.53	0.73
1:A:161:MET:HE1	1:A:165:LEU:HA	1.71	0.72
1:A:1278:ILE:HG23	1:A:1279:VAL:N	2.04	0.72
1:A:1332:VAL:O	1:A:1332:VAL:HG12	1.88	0.72
1:A:1878:ALA:HA	1:A:1882:ILE:CD1	2.18	0.72
1:A:1878:ALA:CA	1:A:1882:ILE:HD11	2.19	0.72
1:A:1828:ARG:NE	1:A:1923:ARG:HH22	1.87	0.72
1:A:1289:ALA:HB3	1:A:1340:TYR:HE2	1.56	0.71
1:A:1815:PRO:HG2	1:A:1963:ILE:HG22	1.72	0.71
1:A:1809:PHE:HB2	1:A:1818:GLN:OE1	1.90	0.71
1:B:1901:MET:SD	1:B:1920:ILE:HG13	2.30	0.71
1:A:1261:ILE:HA	1:A:1873:LYS:NZ	2.05	0.71
1:A:211:ARG:NH1	1:B:132:PRO:HA	2.07	0.70
1:B:1919:PRO:HG2	1:B:1920:ILE:H	1.57	0.70
1:B:1809:PHE:HD1	1:B:1809:PHE:N	1.88	0.70
1:B:1843:ILE:HA	1:B:1846:GLU:HG3	1.74	0.70
1:A:1348:ALA:C	1:A:1349:ILE:HD12	2.11	0.70
1:A:156:PRO:HG3	1:A:161:MET:HG2	1.73	0.70
1:A:1869:GLU:HA	1:A:1872:ARG:HH11	1.57	0.70
1:B:1312:LEU:O	1:B:1316:THR:HA	1.92	0.69
1:B:1809:PHE:CD1	1:B:1809:PHE:N	2.60	0.69
1:B:1810:ASN:HD21	1:B:1836:ILE:HG23	1.57	0.69
1:A:1960:LEU:HA	1:A:1963:ILE:HD11	1.74	0.69
1:B:140:ALA:HA	1:B:187:THR:HG23	1.73	0.69
1:A:171:CYS:HB3	1:A:174:CYS:SG	2.33	0.69
1:A:1779:GLN:HG3	1:A:1795:ARG:HA	1.74	0.69
1:B:144:HIS:HB3	1:B:149:CYS:SG	2.33	0.69
1:B:1944:VAL:HG12	1:B:1948:ASP:CB	2.22	0.69
1:A:1871:LEU:O	1:A:1874:TYR:HB3	1.92	0.69
1:B:1333:ALA:O	1:B:1337:ILE:HG13	1.93	0.69
1:A:1867:PRO:HG2	1:A:1870:ILE:HD12	1.75	0.69
1:A:1886:ILE:HA	1:A:1944:VAL:CG2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1884:PRO:HA	1:B:1942:PRO:HB2	1.75	0.69
1:A:1267:GLN:O	1:A:1271:GLU:HG2	1.92	0.68
1:A:1760:GLU:HA	1:A:1760:GLU:OE2	1.92	0.68
1:A:1773:HIS:HB3	1:A:1828:ARG:HH12	1.58	0.68
1:A:202:GLU:HG2	1:A:267:LYS:NZ	2.07	0.68
1:B:1316:THR:OG1	1:B:1317:ARG:N	2.25	0.68
1:A:161:MET:CE	1:A:165:LEU:HA	2.23	0.68
1:B:170:ILE:HG23	1:B:175:GLY:O	1.93	0.68
1:A:1290:ILE:HD11	1:A:1297:LYS:HE2	1.75	0.68
1:B:1871:LEU:O	1:B:1874:TYR:HB3	1.94	0.68
1:B:155:TRP:O	1:B:157:GLU:N	2.27	0.68
1:A:1828:ARG:HE	1:A:1923:ARG:HH22	1.41	0.68
1:B:1893:GLU:HG3	1:B:1946:ARG:HG2	1.76	0.67
1:A:1929:ILE:O	1:A:1933:GLU:HG3	1.94	0.67
1:A:130:VAL:HG23	1:A:227:PRO:HG3	1.76	0.67
1:A:1287:ALA:O	1:A:1290:ILE:HG12	1.95	0.67
1:B:1936:ALA:HB2	1:B:1948:ASP:OD1	1.94	0.67
1:B:25:ASN:N	1:B:27:GLN:HE21	1.93	0.67
1:B:1899:VAL:O	1:B:1903:LYS:HE3	1.95	0.67
1:A:1342:ALA:HA	1:A:1345:ALA:HB2	1.74	0.67
1:A:1308:VAL:HB	1:A:1933:GLU:OE2	1.94	0.67
1:A:1920:ILE:CG2	1:A:1924:GLN:HG3	2.23	0.67
1:B:1312:LEU:O	1:B:1316:THR:CA	2.43	0.67
1:B:141:THR:HG22	1:B:183:ILE:HB	1.76	0.67
1:B:1311:LYS:HE2	1:B:1317:ARG:NH1	2.07	0.67
1:A:1280:ASP:HA	1:A:1283:VAL:CG1	2.25	0.66
1:A:161:MET:CE	1:A:165:LEU:HD13	2.24	0.66
1:A:1839:PRO:HB3	1:B:1902:ARG:NH1	2.10	0.66
1:B:242:ASP:O	1:B:244:PRO:HD3	1.95	0.66
1:A:155:TRP:O	1:A:157:GLU:N	2.29	0.66
1:B:1276:LYS:CE	1:B:1276:LYS:HA	2.25	0.66
1:B:1327:VAL:CG1	1:B:1819:ILE:HG21	2.26	0.66
1:B:1867:PRO:HB2	1:B:1870:ILE:HB	1.76	0.66
1:B:1280:ASP:O	1:B:1283:VAL:HG22	1.95	0.66
1:B:211:ARG:HH11	1:B:211:ARG:HG3	1.61	0.66
1:A:1809:PHE:N	1:A:1809:PHE:CD1	2.61	0.66
1:B:1812:MET:SD	1:B:1812:MET:N	2.69	0.65
1:B:1943:ILE:HG22	1:B:1944:VAL:O	1.95	0.65
1:B:1890:ALA:O	1:B:1894:ILE:HG22	1.97	0.65
1:A:165:LEU:HD12	1:A:166:GLU:N	2.12	0.65
1:B:1288:PRO:C	1:B:1290:ILE:H	2.00	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1941:SER:CB	1:B:1943:ILE:H	2.10	0.65
1:A:143:LYS:HE3	1:A:150:MET:HG3	1.80	0.64
1:B:1748:LEU:O	1:B:1796:THR:HG21	1.97	0.64
1:A:1848:ALA:HB2	1:B:1898:TYR:HD2	1.61	0.64
1:B:161:MET:HE1	1:B:166:GLU:H	1.61	0.64
1:A:1958:TYR:O	1:A:1962:GLN:HG3	1.98	0.64
1:A:1939:ARG:HH12	1:A:1948:ASP:CG	2.00	0.64
1:B:1311:LYS:HZ3	1:B:1317:ARG:CB	2.09	0.64
1:A:168:PRO:O	1:A:180:PHE:CE2	2.51	0.64
1:B:1758:ILE:O	1:B:1800:ALA:HA	1.97	0.64
1:B:1317:ARG:NH2	1:B:1779:GLN:HE21	1.95	0.64
1:A:1949:ALA:O	1:A:1953:ILE:HG22	1.98	0.64
1:B:1939:ARG:C	1:B:1940:LEU:HD12	2.18	0.64
1:A:30:TYR:CE1	1:A:47:ILE:HD13	2.32	0.64
1:A:1850:HIS:O	1:A:1854:VAL:HG23	1.98	0.63
1:B:1729:THR:HB	1:B:1781:ILE:HD13	1.79	0.63
1:B:1767:ARG:CZ	1:B:1767:ARG:HB3	2.26	0.63
1:B:1856:ARG:HB2	1:B:1860:GLU:OE2	1.97	0.63
1:B:1292:GLY:O	1:B:1297:LYS:HE3	1.98	0.63
1:A:1285:SER:OG	1:A:1866:ILE:HG13	1.97	0.63
1:B:1348:ALA:C	1:B:1349:ILE:HD12	2.19	0.63
1:B:1886:ILE:HA	1:B:1944:VAL:HG21	1.81	0.63
1:A:1290:ILE:HD11	1:A:1297:LYS:CE	2.29	0.63
1:A:1848:ALA:O	1:A:1852:LEU:HD23	1.98	0.63
1:B:1342:ALA:O	1:B:1345:ALA:HB3	1.98	0.63
1:A:105:ARG:HH12	1:A:119:LYS:HZ3	1.46	0.63
1:A:155:TRP:HB3	1:A:156:PRO:CD	2.29	0.63
1:B:156:PRO:CG	1:B:161:MET:HG2	2.29	0.63
1:A:1290:ILE:HA	2:A:2001:ADP:N1	2.15	0.62
1:A:1887:SER:HB3	1:A:1944:VAL:O	1.99	0.62
1:B:1729:THR:HG21	1:B:1771:VAL:HG23	1.80	0.62
1:A:1837:ASP:OD2	1:B:1902:ARG:NH2	2.32	0.62
1:A:1261:ILE:HA	1:A:1873:LYS:HZ3	1.65	0.62
1:A:1758:ILE:O	1:A:1800:ALA:HA	1.99	0.62
1:A:1882:ILE:N	1:A:1882:ILE:CD1	2.56	0.62
1:B:1878:ALA:HA	1:B:1882:ILE:HG12	1.81	0.62
1:A:1329:ASP:OD1	1:A:1808:ARG:HA	1.99	0.62
1:A:1879:ARG:HG2	1:A:1879:ARG:HH11	1.64	0.62
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.64	0.62
1:A:1959:THR:O	1:A:1962:GLN:HB2	2.00	0.61
1:B:1273:ALA:HA	1:B:1278:ILE:CD1	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:MET:HB3	1:A:168:PRO:HD2	1.82	0.61
1:A:1734:ARG:HG3	1:A:1734:ARG:HH11	1.66	0.61
1:A:1281:ALA:HB3	1:A:1866:ILE:HD11	1.83	0.61
1:A:119:LYS:HD2	5:A:2006:CL:CL	2.38	0.61
1:B:1273:ALA:HA	1:B:1278:ILE:HD12	1.82	0.61
1:B:1963:ILE:O	1:B:1965:MET:HG3	2.00	0.61
1:A:1840:ASP:HB3	1:A:1843:ILE:HG23	1.83	0.61
1:A:1945:THR:O	1:A:1948:ASP:HB2	2.00	0.61
1:A:169:THR:HB	1:A:170:ILE:HD12	1.83	0.60
1:B:1903:LYS:HE2	1:B:1903:LYS:HA	1.84	0.60
1:A:1939:ARG:C	1:A:1940:LEU:HD12	2.22	0.60
1:B:1287:ALA:O	1:B:1290:ILE:HG12	2.00	0.60
1:A:1333:ALA:O	1:A:1337:ILE:HG13	2.00	0.60
1:B:1867:PRO:CB	1:B:1870:ILE:HD13	2.31	0.60
1:B:49:PHE:CZ	1:B:64:ILE:HD11	2.36	0.60
1:A:1875:ILE:O	1:A:1878:ALA:HB3	2.01	0.60
1:A:1890:ALA:O	1:A:1894:ILE:HG22	2.02	0.60
1:A:1920:ILE:HG22	1:A:1921:THR:N	2.15	0.60
1:B:1336:GLN:O	1:B:1340:TYR:HD1	1.85	0.60
1:A:1856:ARG:NH1	1:A:1860:GLU:OE1	2.34	0.60
1:A:181:ARG:O	1:A:183:ILE:HD12	2.02	0.60
1:B:1864:PRO:HB3	1:B:1868:HIS:CD2	2.37	0.60
1:B:1920:ILE:HG23	1:B:1924:GLN:HG3	1.82	0.60
1:B:1812:MET:H	1:B:1812:MET:HE2	1.67	0.59
1:B:1866:ILE:N	1:B:1866:ILE:HD12	2.16	0.59
1:B:88:THR:O	1:B:91:ARG:HG2	2.01	0.59
1:A:1329:ASP:O	1:A:1332:VAL:HG23	2.02	0.59
1:B:1311:LYS:O	1:B:1312:LEU:HD23	2.02	0.59
1:B:168:PRO:O	1:B:180:PHE:CE2	2.55	0.59
1:B:1899:VAL:O	1:B:1903:LYS:HG2	2.01	0.59
1:B:1853:ARG:O	1:B:1856:ARG:HG3	2.02	0.59
1:B:144:HIS:CE1	1:B:176:LYS:O	2.56	0.59
1:B:1760:GLU:OE2	1:B:1803:ASN:ND2	2.36	0.59
1:B:1332:VAL:HG23	1:B:1334:LYS:CD	2.32	0.59
1:B:155:TRP:O	1:B:156:PRO:C	2.41	0.59
1:A:142:TYR:OH	1:A:165:LEU:HD11	2.03	0.58
1:B:1810:ASN:HD21	1:B:1836:ILE:HG21	1.67	0.58
1:B:1290:ILE:CD1	1:B:1297:LYS:HE2	2.29	0.58
1:B:1811:ARG:CD	1:B:1813:LYS:HB2	2.32	0.58
1:B:141:THR:HG21	1:B:186:LYS:HB2	1.84	0.58
1:A:1317:ARG:NH2	1:A:1779:GLN:HE21	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1308:VAL:CG1	1:A:1309:SER:N	2.65	0.58
1:A:1342:ALA:O	1:A:1345:ALA:HB3	2.03	0.58
1:A:1840:ASP:O	1:A:1843:ILE:N	2.35	0.58
1:A:1860:GLU:OE1	1:A:1860:GLU:HA	2.04	0.58
1:A:246:LYS:HG2	1:A:247:ARG:N	2.18	0.58
1:B:1311:LYS:HG2	1:B:1317:ARG:HA	1.85	0.58
1:B:1941:SER:HB2	1:B:1943:ILE:H	1.69	0.58
1:B:1813:LYS:N	1:B:1813:LYS:HD2	2.18	0.58
1:B:1896:LYS:O	1:B:1899:VAL:HG12	2.03	0.58
1:A:168:PRO:HG2	1:A:180:PHE:CE2	2.39	0.57
1:A:143:LYS:CB	1:A:183:ILE:HD11	2.30	0.57
1:B:108:GLU:OE2	1:B:111:LYS:HE3	2.04	0.57
1:B:1812:MET:H	1:B:1812:MET:CE	2.16	0.57
1:B:1886:ILE:HA	1:B:1944:VAL:CG2	2.34	0.57
1:A:1332:VAL:O	1:A:1333:ALA:HB3	2.04	0.57
1:A:1769:ARG:O	1:A:1772:ILE:HG22	2.03	0.57
1:A:1886:ILE:HA	1:A:1944:VAL:HG21	1.85	0.57
1:A:114:SER:HB3	1:B:135:GLU:OE1	2.05	0.57
1:B:1900:ARG:HH11	1:B:1900:ARG:HG3	1.68	0.57
1:A:1894:ILE:HG23	1:A:1895:GLU:N	2.20	0.57
1:A:1896:LYS:O	1:A:1899:VAL:HG12	2.05	0.57
1:A:1886:ILE:HA	1:A:1944:VAL:HG23	1.86	0.57
1:B:1856:ARG:HB2	1:B:1860:GLU:CD	2.25	0.57
1:A:245:VAL:HG23	1:A:245:VAL:O	2.04	0.57
1:A:1748:LEU:O	1:A:1796:THR:HG21	2.05	0.57
1:B:41:ARG:HH22	1:B:88:THR:HG22	1.69	0.57
1:A:1902:ARG:O	1:A:1919:PRO:HD2	2.05	0.57
1:A:23:GLY:HA3	1:A:27:GLN:HE22	1.69	0.57
1:B:143:LYS:HB2	1:B:183:ILE:CD1	2.35	0.56
1:B:1284:ASP:O	1:B:1288:PRO:HG3	2.04	0.56
1:B:1902:ARG:HG2	1:B:1902:ARG:HH11	1.70	0.56
1:B:1264:GLU:O	1:B:1268:ILE:HG13	2.05	0.56
1:B:1309:SER:HB2	1:B:1320:GLY:HA3	1.86	0.56
1:B:1941:SER:HB2	1:B:1943:ILE:N	2.19	0.56
1:A:1811:ARG:HD3	1:A:1813:LYS:HG3	1.87	0.56
1:B:1304:LEU:O	1:B:1879:ARG:HD2	2.05	0.56
1:A:125:GLY:HA3	1:A:197:ILE:HD11	1.86	0.56
1:A:1342:ALA:HB2	1:A:1757:LEU:HD12	1.88	0.56
1:B:1773:HIS:HB3	1:B:1828:ARG:NH1	2.21	0.56
1:B:1308:VAL:HG13	1:B:1309:SER:N	2.19	0.56
1:B:143:LYS:HD2	1:B:152:GLU:OE2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1302:LEU:HD22	1:A:1934:ALA:HB3	1.87	0.56
1:A:202:GLU:HG2	1:A:267:LYS:HZ2	1.70	0.56
1:B:1284:ASP:CB	1:B:1865:LYS:HG3	2.36	0.56
1:B:1311:LYS:HZ3	1:B:1317:ARG:HD2	1.71	0.56
1:B:1848:ALA:O	1:B:1852:LEU:HD23	2.05	0.56
1:B:1929:ILE:O	1:B:1933:GLU:HG3	2.05	0.56
1:A:1302:LEU:HD22	1:A:1934:ALA:CB	2.35	0.56
1:A:41:ARG:HH21	1:A:88:THR:HG22	1.66	0.56
1:B:1847:VAL:O	1:B:1851:ILE:HG13	2.06	0.56
1:A:116:ASP:HA	1:A:119:LYS:NZ	2.21	0.56
1:A:1279:VAL:O	1:A:1283:VAL:HG12	2.05	0.56
1:A:1329:ASP:OD2	1:A:1836:ILE:HG23	2.05	0.56
1:B:1261:ILE:CD1	1:B:1261:ILE:H	2.14	0.56
1:B:1278:ILE:CG2	1:B:1279:VAL:N	2.68	0.56
1:A:1812:MET:SD	1:A:1812:MET:N	2.73	0.55
1:B:1815:PRO:HD3	1:B:1965:MET:HE2	1.88	0.55
1:A:63:ILE:HD13	1:A:100:ILE:HD13	1.89	0.55
1:A:1939:ARG:NH1	1:A:1948:ASP:OD2	2.39	0.55
1:A:1308:VAL:HG13	1:A:1309:SER:N	2.19	0.55
1:A:1753:GLY:N	1:A:1795:ARG:O	2.38	0.55
1:A:1950:ARG:HG2	1:A:1950:ARG:NH1	2.21	0.55
1:B:1849:ARG:O	1:B:1853:ARG:HG3	2.07	0.55
1:A:1278:ILE:CG2	1:A:1279:VAL:H	2.18	0.55
1:A:1760:GLU:HG3	1:A:1763:LYS:HG2	1.88	0.55
1:B:1882:ILE:HG22	1:B:1884:PRO:HD3	1.89	0.55
1:A:156:PRO:CG	1:A:161:MET:HG2	2.37	0.55
1:B:1289:ALA:HB3	1:B:1340:TYR:CE2	2.41	0.55
1:B:7:GLN:HG2	1:B:8:ILE:N	2.21	0.55
1:A:1767:ARG:CZ	1:A:1767:ARG:HB3	2.37	0.55
1:A:1273:ALA:HB1	1:A:1940:LEU:HD13	1.89	0.55
1:B:1328:GLY:O	1:B:1804:PRO:HD3	2.07	0.55
1:A:1296:VAL:HG22	1:A:1833:PHE:CD2	2.42	0.54
1:B:1901:MET:HG3	1:B:1920:ILE:HG13	1.88	0.54
1:A:1760:GLU:OE2	1:A:1803:ASN:ND2	2.40	0.54
1:A:1946:ARG:C	1:A:1950:ARG:HE	2.11	0.54
1:B:202:GLU:HG2	1:B:267:LYS:NZ	2.21	0.54
1:A:1856:ARG:O	1:A:1857:GLY:O	2.26	0.54
1:A:217:LEU:CD2	1:A:259:VAL:HG21	2.37	0.54
1:B:63:ILE:HG21	1:B:100:ILE:HD13	1.89	0.54
1:A:1278:ILE:CG2	1:A:1279:VAL:N	2.71	0.54
1:A:1941:SER:CB	1:A:1943:ILE:H	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1325:LEU:O	1:B:1326:LEU:HD23	2.07	0.54
1:B:155:TRP:CH2	1:B:168:PRO:HB3	2.43	0.54
1:B:1261:ILE:HA	1:B:1873:LYS:HZ3	1.69	0.54
1:B:1853:ARG:HD3	1:B:1856:ARG:HH21	1.73	0.54
1:A:1311:LYS:C	1:A:1312:LEU:HG	2.28	0.54
1:A:1860:GLU:OE1	1:A:1860:GLU:CA	2.56	0.54
1:A:1894:ILE:HD11	1:A:1925:LEU:HD12	1.90	0.54
1:B:1267:GLN:O	1:B:1271:GLU:HG2	2.07	0.54
1:A:1855:ARG:HD3	1:B:1318:LEU:HD11	1.88	0.54
1:B:1332:VAL:O	1:B:1333:ALA:HB3	2.08	0.54
1:A:88:THR:O	1:A:91:ARG:HG3	2.08	0.54
1:A:250:ARG:NE	1:B:163:GLU:HG3	2.22	0.54
1:B:181:ARG:O	1:B:183:ILE:HD12	2.08	0.54
1:A:116:ASP:HA	1:A:119:LYS:HZ1	1.72	0.54
1:A:183:ILE:HG22	1:A:186:LYS:H	1.72	0.54
1:A:71:LEU:O	1:A:75:GLU:HG3	2.08	0.54
1:B:144:HIS:HE1	1:B:176:LYS:O	1.91	0.54
1:B:1288:PRO:O	1:B:1290:ILE:N	2.41	0.53
1:B:1901:MET:CG	1:B:1920:ILE:HG13	2.38	0.53
1:A:1853:ARG:HD3	1:A:1856:ARG:NH2	2.24	0.53
1:B:1269:ILE:HG12	1:B:1874:TYR:HD1	1.73	0.53
1:B:1261:ILE:HG22	1:B:1873:LYS:HZ3	1.73	0.53
1:A:1809:PHE:N	1:A:1809:PHE:HD1	1.89	0.53
1:A:1896:LYS:HE3	1:A:1900:ARG:HG3	1.90	0.53
1:A:30:TYR:O	1:A:34:ILE:HG13	2.07	0.53
1:A:1929:ILE:N	1:A:1929:ILE:HD12	2.24	0.53
1:B:1284:ASP:HB3	1:B:1865:LYS:HG3	1.88	0.53
1:B:1819:ILE:HD12	1:B:1819:ILE:O	2.07	0.53
1:A:1853:ARG:CD	1:A:1856:ARG:NH2	2.72	0.53
1:B:1939:ARG:HH21	1:B:1947:GLU:HB2	1.74	0.53
1:A:155:TRP:HB3	1:A:156:PRO:HD2	1.90	0.53
1:B:1887:SER:HG	1:B:1943:ILE:HG22	1.74	0.53
1:B:262:ILE:O	1:B:262:ILE:HG23	2.09	0.53
1:A:108:GLU:OE2	1:A:111:LYS:HE3	2.08	0.52
1:B:155:TRP:CZ3	1:B:168:PRO:HB3	2.44	0.52
1:B:1298:LYS:HG2	1:B:1955:LEU:HD22	1.91	0.52
1:A:1901:MET:O	1:A:1904:SER:HB3	2.08	0.52
1:B:1325:LEU:C	1:B:1326:LEU:HD23	2.29	0.52
1:B:143:LYS:CG	1:B:152:GLU:HG2	2.37	0.52
1:B:1884:PRO:CA	1:B:1942:PRO:HB2	2.37	0.52
1:A:1322:ILE:HD13	1:A:1931:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1290:ILE:O	1:B:1290:ILE:HG13	2.07	0.52
1:B:1302:LEU:HD22	1:B:1934:ALA:HB3	1.91	0.52
1:B:1842:LYS:O	1:B:1846:GLU:HG2	2.09	0.52
1:A:1311:LYS:CD	1:A:1317:ARG:HB2	2.39	0.52
1:A:1779:GLN:HG2	1:A:1795:ARG:HG2	1.91	0.52
1:A:250:ARG:CZ	1:B:163:GLU:HG3	2.39	0.52
1:B:1281:ALA:CB	1:B:1866:ILE:HD11	2.37	0.52
1:A:183:ILE:N	1:A:183:ILE:HD12	2.25	0.52
1:A:1261:ILE:HA	1:A:1873:LYS:CE	2.39	0.52
1:A:1950:ARG:HH11	1:A:1950:ARG:HG2	1.74	0.52
1:B:140:ALA:O	1:B:154:GLU:HA	2.10	0.52
1:A:133:VAL:HG22	1:A:222:VAL:HG13	1.92	0.52
1:A:1771:VAL:O	1:A:1771:VAL:HG12	2.10	0.52
1:A:1897:TYR:CG	1:A:1953:ILE:HD12	2.45	0.52
1:A:1941:SER:HB2	1:A:1943:ILE:N	2.25	0.52
1:B:155:TRP:HB3	1:B:156:PRO:CD	2.39	0.52
1:A:23:GLY:HA3	1:A:27:GLN:NE2	2.24	0.52
1:A:262:ILE:HG23	1:A:262:ILE:O	2.09	0.52
1:B:153:PHE:HZ	1:B:168:PRO:HG3	1.75	0.52
1:B:1903:LYS:HE2	1:B:1903:LYS:CA	2.40	0.52
1:A:1855:ARG:HG2	1:B:1929:ILE:HG21	1.91	0.51
1:B:1261:ILE:HG12	1:B:1261:ILE:O	2.10	0.51
1:B:1288:PRO:C	1:B:1290:ILE:N	2.63	0.51
1:A:1339:ARG:HG2	1:A:1350:TYR:CE2	2.45	0.51
1:A:1899:VAL:HG13	1:A:1900:ARG:N	2.25	0.51
1:B:100:ILE:HG22	1:B:103:ILE:HG23	1.92	0.51
1:B:1278:ILE:HG23	1:B:1279:VAL:N	2.25	0.51
1:B:9:ASP:OD2	1:B:11:ARG:HB2	2.09	0.51
1:A:233:VAL:HG12	1:A:257:MET:HE3	1.93	0.51
1:B:1283:VAL:HG23	1:B:1284:ASP:N	2.26	0.51
1:B:257:MET:HE3	1:B:259:VAL:HG22	1.91	0.51
1:A:1288:PRO:C	1:A:1290:ILE:H	2.14	0.51
1:B:1289:ALA:CB	1:B:1340:TYR:CE2	2.94	0.51
1:B:1317:ARG:HH11	1:B:1317:ARG:HG3	1.76	0.51
1:B:1322:ILE:HD13	1:B:1931:LEU:HD23	1.93	0.51
1:B:14:PHE:CE2	1:B:74:LEU:HB3	2.45	0.51
1:A:1960:LEU:HA	1:A:1963:ILE:CD1	2.40	0.51
1:A:1325:LEU:O	1:A:1326:LEU:HD23	2.10	0.51
1:A:1898:TYR:CE1	1:A:1902:ARG:HD2	2.46	0.51
1:A:202:GLU:CD	1:A:202:GLU:H	2.14	0.51
1:A:240:LYS:HB3	1:A:256:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1296:VAL:HA	1:A:1833:PHE:CE2	2.45	0.51
1:A:155:TRP:CB	1:A:156:PRO:CD	2.89	0.51
1:A:1920:ILE:CG2	1:A:1921:THR:N	2.74	0.51
1:B:193:GLN:HB2	1:B:222:VAL:HG22	1.93	0.51
1:A:69:ILE:O	1:A:72:PRO:HD2	2.11	0.50
1:B:1317:ARG:HG3	1:B:1317:ARG:NH1	2.26	0.50
1:B:1939:ARG:HG3	1:B:1939:ARG:HH11	1.76	0.50
1:A:1852:LEU:HD11	1:B:1894:ILE:HD13	1.91	0.50
1:B:1864:PRO:HB2	1:B:1866:ILE:O	2.11	0.50
1:B:244:PRO:O	1:B:246:LYS:N	2.39	0.50
1:A:41:ARG:HH22	1:A:88:THR:HG22	1.75	0.50
1:B:1342:ALA:HB2	1:B:1757:LEU:HD12	1.92	0.50
1:B:241:GLN:NE2	1:B:253:PHE:CE2	2.80	0.50
1:A:1317:ARG:O	1:A:1317:ARG:HG3	2.11	0.50
1:A:1282:ILE:HD12	1:A:1938:MET:CE	2.41	0.50
1:A:1816:PHE:O	1:A:1819:ILE:HG12	2.11	0.50
1:A:1844:ASP:OD2	1:B:1902:ARG:HD3	2.12	0.50
1:A:1840:ASP:O	1:A:1842:LYS:N	2.45	0.50
1:B:1773:HIS:CD2	1:B:1828:ARG:NH1	2.80	0.50
1:A:1840:ASP:HB3	1:A:1843:ILE:CG2	2.42	0.50
1:A:240:LYS:HG3	1:A:241:GLN:N	2.26	0.50
1:A:1943:ILE:HG22	1:A:1944:VAL:O	2.11	0.50
1:A:1773:HIS:HB3	1:A:1828:ARG:NH1	2.24	0.50
1:A:1840:ASP:O	1:A:1841:ASP:C	2.50	0.50
1:A:1920:ILE:HG23	1:A:1924:GLN:CG	2.33	0.50
1:A:211:ARG:HG3	1:A:211:ARG:NH1	2.27	0.50
1:B:1853:ARG:HD3	1:B:1856:ARG:NH2	2.27	0.50
1:B:41:ARG:HH21	1:B:88:THR:HG22	1.77	0.50
1:A:161:MET:HE3	1:A:166:GLU:H	1.77	0.49
1:A:1928:LEU:HD22	1:A:1956:MET:CE	2.42	0.49
1:B:1293:TYR:HB3	1:B:1296:VAL:HB	1.93	0.49
1:B:181:ARG:O	1:B:183:ILE:CD1	2.59	0.49
1:B:1332:VAL:HG12	1:B:1837:ASP:HB3	1.94	0.49
1:B:1815:PRO:HD3	1:B:1965:MET:CE	2.41	0.49
1:A:1304:LEU:O	1:A:1879:ARG:HD2	2.12	0.49
1:A:1759:ASP:OD1	1:A:1760:GLU:N	2.46	0.49
1:B:156:PRO:CD	1:B:161:MET:HG2	2.43	0.49
1:A:1767:ARG:HH11	1:A:1767:ARG:HG3	1.77	0.49
1:A:1752:ASP:CA	1:A:1796:THR:HG22	2.38	0.49
1:A:1848:ALA:HB2	1:B:1898:TYR:CD2	2.46	0.49
1:A:1869:GLU:HA	1:A:1872:ARG:NH1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1312:LEU:O	1:B:1316:THR:N	2.45	0.49
1:B:156:PRO:CB	1:B:159:GLU:O	2.52	0.49
1:B:233:VAL:HG12	1:B:257:MET:HE1	1.93	0.49
1:B:30:TYR:CE1	1:B:47:ILE:HD13	2.48	0.49
1:A:1290:ILE:O	1:A:1290:ILE:HG13	2.10	0.49
1:B:1329:ASP:OD1	1:B:1808:ARG:CA	2.54	0.49
1:B:1869:GLU:HA	1:B:1872:ARG:HH11	1.78	0.49
1:B:1939:ARG:HG3	1:B:1939:ARG:NH1	2.27	0.49
1:A:246:LYS:HG2	1:A:247:ARG:H	1.75	0.49
1:B:1293:TYR:O	1:B:1297:LYS:HG3	2.13	0.49
1:B:167:MET:HB2	1:B:168:PRO:HD2	1.95	0.49
1:A:153:PHE:CD2	1:A:172:PRO:HG3	2.48	0.49
1:A:1868:HIS:O	1:A:1871:LEU:N	2.43	0.49
1:A:1928:LEU:HD22	1:A:1956:MET:HE2	1.95	0.49
1:B:1266:GLU:O	1:B:1269:ILE:HG22	2.12	0.49
1:B:139:LYS:NZ	1:B:156:PRO:O	2.45	0.49
1:B:1816:PHE:O	1:B:1819:ILE:HG13	2.13	0.49
1:A:1879:ARG:NH1	1:A:1879:ARG:HG2	2.27	0.48
1:A:1886:ILE:H	1:A:1886:ILE:HD12	1.78	0.48
1:B:155:TRP:O	1:B:157:GLU:HG3	2.13	0.48
1:A:1322:ILE:O	1:A:1797:THR:HG23	2.13	0.48
1:B:1867:PRO:HB3	1:B:1870:ILE:HD13	1.95	0.48
1:B:1830:ASP:CG	1:B:1930:ARG:HH21	2.17	0.48
1:A:1312:LEU:O	1:A:1316:THR:HA	2.12	0.48
1:A:168:PRO:HG2	1:A:180:PHE:CZ	2.49	0.48
1:A:200:ARG:O	1:A:203:GLU:HG2	2.14	0.48
1:A:44:SER:HA	1:A:97:HIS:O	2.13	0.48
1:B:1938:MET:O	1:B:1940:LEU:HD12	2.14	0.48
1:A:1311:LYS:HA	1:A:1317:ARG:HA	1.95	0.48
1:A:1319:ARG:O	1:A:1930:ARG:HD3	2.14	0.48
1:A:1730:ALA:CB	1:A:1783:ILE:HD11	2.43	0.48
1:A:1856:ARG:HG3	1:A:1860:GLU:OE2	2.14	0.48
1:B:1939:ARG:CG	1:B:1939:ARG:HH11	2.26	0.48
1:A:1804:PRO:CG	1:A:1807:GLY:O	2.62	0.48
1:A:1889:GLU:HB3	1:A:1946:ARG:HG3	1.90	0.48
1:A:1902:ARG:CB	1:A:1903:LYS:HZ3	2.10	0.48
1:B:1345:ALA:CB	1:B:1348:ALA:HB3	2.38	0.48
1:B:1809:PHE:HB2	1:B:1818:GLN:CD	2.33	0.48
1:B:1867:PRO:HB2	1:B:1870:ILE:HD13	1.95	0.48
1:B:119:LYS:HD3	5:B:2006:CL:CL	2.51	0.48
1:A:1261:ILE:HD11	1:A:1880:LYS:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1281:ALA:O	1:A:1285:SER:OG	2.23	0.48
1:A:155:TRP:HA	1:A:155:TRP:CE3	2.49	0.48
1:B:1312:LEU:HB3	1:B:1313:PRO:HD2	1.95	0.48
1:B:211:ARG:NH1	1:B:211:ARG:HG3	2.26	0.48
1:B:1879:ARG:HH11	1:B:1879:ARG:HG2	1.77	0.48
1:B:1936:ALA:O	1:B:1939:ARG:HB2	2.14	0.48
1:A:1939:ARG:NH2	1:A:1945:THR:OG1	2.46	0.48
1:B:103:ILE:CD1	1:B:103:ILE:H	2.16	0.48
1:B:1944:VAL:HG12	1:B:1948:ASP:CG	2.33	0.48
1:B:1945:THR:O	1:B:1948:ASP:HB2	2.13	0.48
1:B:161:MET:HE3	1:B:162:PRO:HD2	1.96	0.47
1:A:171:CYS:CB	1:A:174:CYS:SG	2.99	0.47
1:A:1853:ARG:O	1:A:1856:ARG:HG2	2.13	0.47
1:B:1948:ASP:O	1:B:1949:ALA:C	2.52	0.47
1:A:1346:PRO:HG2	1:A:1347:ARG:HG3	1.95	0.47
1:A:1898:TYR:CE2	1:A:1925:LEU:HD22	2.49	0.47
1:B:1948:ASP:O	1:B:1951:GLU:N	2.46	0.47
1:B:202:GLU:CD	1:B:202:GLU:H	2.18	0.47
1:A:1839:PRO:HA	1:A:1844:ASP:OD1	2.13	0.47
1:B:1828:ARG:HE	1:B:1923:ARG:NH2	2.13	0.47
1:A:1311:LYS:HD3	1:A:1317:ARG:HB2	1.96	0.47
1:A:155:TRP:O	1:A:156:PRO:C	2.51	0.47
1:A:1847:VAL:O	1:A:1851:ILE:HG13	2.14	0.47
1:A:8:ILE:CG1	1:A:9:ASP:N	2.76	0.47
1:B:1298:LYS:HZ1	1:B:1935:HIS:CD2	2.32	0.47
1:A:1262:SER:HB3	1:A:1265:GLU:OE2	2.14	0.47
1:A:1278:ILE:HD11	1:A:1874:TYR:OH	2.14	0.47
1:A:1346:PRO:C	1:A:1347:ARG:HG3	2.34	0.47
1:A:171:CYS:O	1:A:175:GLY:N	2.42	0.47
1:A:1922:ALA:O	1:A:1925:LEU:HB3	2.15	0.47
1:B:1853:ARG:O	1:B:1855:ARG:N	2.48	0.47
1:A:1257:GLN:HG3	1:A:1257:GLN:O	2.14	0.47
1:A:1263:PRO:HA	1:A:1266:GLU:HB3	1.95	0.47
1:A:1332:VAL:O	1:A:1332:VAL:CG1	2.59	0.47
1:A:170:ILE:HG23	1:A:175:GLY:C	2.35	0.47
1:B:65:ASN:ND2	1:B:263:GLU:HG3	2.30	0.47
1:A:1276:LYS:HA	1:A:1276:LYS:CE	2.30	0.47
1:A:1311:LYS:HD2	1:A:1317:ARG:NH1	2.30	0.47
1:B:1311:LYS:HG2	1:B:1317:ARG:CA	2.44	0.47
1:B:1346:PRO:HG2	1:B:1347:ARG:N	2.30	0.47
1:B:1815:PRO:HG3	1:B:1963:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1840:ASP:HB3	1:B:1843:ILE:CG2	2.45	0.47
1:B:1882:ILE:CG2	1:B:1942:PRO:HB3	2.45	0.47
1:A:1853:ARG:HD3	1:A:1856:ARG:HH21	1.80	0.47
1:A:239:ILE:HG13	1:A:239:ILE:O	2.15	0.47
1:B:153:PHE:CZ	1:B:168:PRO:HG3	2.50	0.47
1:A:1856:ARG:O	1:A:1860:GLU:OE2	2.33	0.47
1:A:1925:LEU:O	1:A:1929:ILE:HD13	2.15	0.47
1:B:145:ILE:HG22	1:B:145:ILE:O	2.15	0.47
1:A:1276:LYS:HE2	1:A:1276:LYS:CA	2.40	0.46
1:A:1325:LEU:C	1:A:1326:LEU:HD23	2.35	0.46
1:B:1319:ARG:O	1:B:1930:ARG:HD3	2.15	0.46
1:B:137:ILE:HG23	1:B:187:THR:CG2	2.45	0.46
1:A:1310:ARG:HB3	1:A:1312:LEU:HD11	1.96	0.46
1:B:103:ILE:HD13	1:B:103:ILE:N	2.15	0.46
1:A:164:VAL:CG2	1:A:244:PRO:HB2	2.46	0.46
1:A:1804:PRO:HG2	1:A:1807:GLY:O	2.15	0.46
1:A:1843:ILE:HG13	1:A:1844:ASP:N	2.30	0.46
1:B:155:TRP:CG	1:B:156:PRO:N	2.82	0.46
1:B:1920:ILE:CG2	1:B:1921:THR:N	2.78	0.46
1:B:1939:ARG:O	1:B:1940:LEU:HB2	2.15	0.46
1:A:1779:GLN:HG2	1:A:1795:ARG:HA	1.97	0.46
1:B:9:ASP:OD1	1:B:9:ASP:O	2.34	0.46
1:A:1311:LYS:HD2	1:A:1317:ARG:HB2	1.98	0.46
1:A:1867:PRO:CG	1:A:1870:ILE:HD12	2.45	0.46
1:B:155:TRP:CB	1:B:156:PRO:CD	2.94	0.46
1:A:182:LEU:O	1:A:184:PRO:HD3	2.16	0.46
1:B:1317:ARG:NH2	1:B:1779:GLN:CG	2.72	0.46
1:A:1853:ARG:HA	1:A:1856:ARG:HG2	1.98	0.46
1:B:71:LEU:HB3	1:B:72:PRO:HD3	1.98	0.46
1:A:1288:PRO:O	1:A:1290:ILE:N	2.44	0.46
1:A:233:VAL:CG1	1:A:257:MET:HE3	2.45	0.46
1:B:65:ASN:OD1	1:B:232:LYS:HD2	2.16	0.46
1:B:61:TYR:HD1	1:B:64:ILE:HD12	1.81	0.46
1:A:1798:VAL:O	1:A:1799:ILE:HD13	2.17	0.45
1:A:25:ASN:H	1:A:27:GLN:NE2	2.05	0.45
1:B:1269:ILE:HG22	1:B:1270:LYS:N	2.31	0.45
1:A:1272:LEU:HD12	1:A:1272:LEU:H	1.81	0.45
1:A:1317:ARG:HH21	1:A:1779:GLN:HE21	1.62	0.45
1:B:1352:SER:OG	1:B:1353:GLY:N	2.50	0.45
1:A:1893:GLU:HG2	1:A:1946:ARG:NH2	2.31	0.45
1:A:1945:THR:O	1:A:1948:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:GLN:HG3	1:A:199:GLU:O	2.16	0.45
1:B:88:THR:O	1:B:91:ARG:CG	2.64	0.45
1:A:123:ILE:HG22	1:A:124:ASP:N	2.32	0.45
1:A:1946:ARG:HB3	1:A:1950:ARG:NE	2.32	0.45
1:A:1951:GLU:OE1	1:A:1951:GLU:HA	2.17	0.45
1:A:258:LYS:HA	1:A:258:LYS:HD2	1.78	0.45
1:B:1296:VAL:HG22	1:B:1833:PHE:CD2	2.51	0.45
1:B:1322:ILE:HG23	1:B:1830:ASP:CG	2.36	0.45
1:A:1353:GLY:N	1:A:1759:ASP:O	2.50	0.45
1:A:217:LEU:HD23	1:A:259:VAL:HG21	1.99	0.45
1:B:123:ILE:HG22	1:B:124:ASP:N	2.31	0.45
1:B:1272:LEU:O	1:B:1275:ARG:HB3	2.16	0.45
1:B:1760:GLU:CG	1:B:1763:LYS:HD2	2.46	0.45
1:A:1729:THR:OG1	1:A:1730:ALA:N	2.48	0.45
1:A:1752:ASP:HA	1:A:1796:THR:CG2	2.44	0.45
1:A:1779:GLN:HG2	1:A:1795:ARG:CG	2.47	0.45
1:A:1871:LEU:HD12	1:A:1874:TYR:HB3	1.99	0.45
1:B:1853:ARG:C	1:B:1855:ARG:N	2.70	0.45
1:B:1900:ARG:CG	1:B:1900:ARG:HH11	2.30	0.45
1:B:1946:ARG:O	1:B:1950:ARG:HB2	2.17	0.45
1:B:202:GLU:HG2	1:B:267:LYS:HZ2	1.80	0.45
1:A:1858:GLU:O	1:A:1859:SER:HB3	2.16	0.45
1:A:1866:ILE:HG22	1:A:1867:PRO:CD	2.46	0.45
1:A:1956:MET:O	1:A:1959:THR:OG1	2.28	0.45
1:B:1276:LYS:HE2	1:B:1276:LYS:CA	2.41	0.45
1:B:200:ARG:HB2	1:B:203:GLU:HG2	1.99	0.45
1:A:1260:GLU:HA	1:A:1260:GLU:OE2	2.17	0.45
1:A:1831:LEU:HD11	1:A:1955:LEU:HD23	1.99	0.45
1:B:1760:GLU:HA	1:B:1760:GLU:OE2	2.17	0.45
1:A:1844:ASP:OD2	1:B:1902:ARG:NH1	2.50	0.45
1:A:1897:TYR:CE1	1:A:1901:MET:HB3	2.52	0.45
1:B:1308:VAL:CG1	1:B:1309:SER:N	2.80	0.45
1:A:1946:ARG:CB	1:A:1950:ARG:HE	2.30	0.44
1:A:86:ASP:OD1	1:A:88:THR:HB	2.17	0.44
1:B:174:CYS:SG	1:B:176:LYS:N	2.81	0.44
1:B:25:ASN:CA	1:B:27:GLN:HE21	2.29	0.44
1:A:1760:GLU:OE1	1:A:1763:LYS:HE3	2.17	0.44
1:A:1950:ARG:O	1:A:1953:ILE:HG23	2.17	0.44
1:A:242:ASP:O	1:A:244:PRO:HD3	2.18	0.44
1:B:1843:ILE:HG13	1:B:1844:ASP:N	2.30	0.44
1:B:1897:TYR:CE1	1:B:1901:MET:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1921:THR:H	1:B:1924:GLN:HG3	1.82	0.44
1:A:1346:PRO:HG2	1:A:1347:ARG:N	2.32	0.44
1:B:1775:ALA:O	1:B:1779:GLN:HA	2.17	0.44
1:B:1869:GLU:N	1:B:1869:GLU:OE1	2.45	0.44
1:A:161:MET:HB3	1:A:161:MET:HE2	1.49	0.44
1:A:1897:TYR:CE2	1:A:1901:MET:HE3	2.53	0.44
1:B:108:GLU:HB2	1:B:111:LYS:HG3	1.99	0.44
1:B:153:PHE:CD2	1:B:172:PRO:HG3	2.53	0.44
1:A:1262:SER:HB3	1:A:1265:GLU:HB2	2.00	0.44
1:A:1730:ALA:HB3	1:A:1783:ILE:HD11	1.99	0.44
1:A:1282:ILE:HG12	1:A:1866:ILE:HD12	2.00	0.44
1:A:1334:LYS:HB2	2:A:2001:ADP:O2B	2.18	0.44
1:B:1805:LYS:N	1:B:1818:GLN:O	2.40	0.44
1:A:1807:GLY:O	1:A:1808:ARG:C	2.56	0.44
1:B:1810:ASN:ND2	1:B:1836:ILE:HG21	2.33	0.44
1:B:1840:ASP:O	1:B:1843:ILE:HG23	2.18	0.44
1:B:200:ARG:O	1:B:203:GLU:HG2	2.18	0.44
1:A:1322:ILE:HG23	1:A:1830:ASP:HB2	1.99	0.44
1:A:1956:MET:O	1:A:1960:LEU:HG	2.18	0.44
1:B:1311:LYS:HZ3	1:B:1317:ARG:CD	2.31	0.44
1:B:1804:PRO:O	1:B:1805:LYS:C	2.56	0.44
1:B:1853:ARG:C	1:B:1855:ARG:H	2.22	0.44
1:A:1894:ILE:HD11	1:A:1925:LEU:CD1	2.47	0.43
1:A:1960:LEU:HA	1:A:1963:ILE:CG1	2.48	0.43
1:A:237:LEU:HD23	1:A:257:MET:HB2	2.00	0.43
1:B:182:LEU:C	1:B:183:ILE:HD12	2.39	0.43
1:A:1346:PRO:HB3	1:A:1872:ARG:HD3	2.00	0.43
1:B:1269:ILE:CG2	1:B:1270:LYS:N	2.80	0.43
1:B:169:THR:HB	1:B:170:ILE:HD12	2.00	0.43
1:B:1902:ARG:NH1	1:B:1902:ARG:HG2	2.32	0.43
1:B:215:ILE:HD12	1:B:217:LEU:HD21	1.99	0.43
1:A:1266:GLU:O	1:A:1269:ILE:HG23	2.19	0.43
1:A:164:VAL:HG21	1:A:244:PRO:HB2	2.00	0.43
1:B:1899:VAL:HG13	1:B:1900:ARG:N	2.33	0.43
1:A:168:PRO:O	1:A:168:PRO:HG2	2.17	0.43
1:B:1759:ASP:OD1	1:B:1760:GLU:N	2.51	0.43
1:B:1809:PHE:HB2	1:B:1818:GLN:NE2	2.33	0.43
1:B:1851:ILE:HG12	2:B:2001:ADP:O2'	2.18	0.43
1:B:233:VAL:HG12	1:B:257:MET:CE	2.48	0.43
1:A:1265:GLU:OE2	1:A:1873:LYS:HE3	2.18	0.43
1:A:153:PHE:CD1	1:A:153:PHE:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1311:LYS:HG2	1:B:1317:ARG:CB	2.48	0.43
1:B:1919:PRO:CG	1:B:1920:ILE:H	2.29	0.43
1:B:204:VAL:HG21	1:B:210:PRO:HB3	2.00	0.43
1:B:130:VAL:HG23	1:B:227:PRO:HG3	2.01	0.43
1:A:1286:ILE:HA	1:A:1286:ILE:HD13	1.91	0.43
1:A:1308:VAL:O	1:A:1309:SER:HB3	2.19	0.43
1:A:1311:LYS:NZ	1:A:1319:ARG:HA	2.34	0.43
1:A:1353:GLY:O	1:A:1764:MET:HA	2.19	0.43
1:A:191:ASP:HB3	1:A:222:VAL:HG21	2.00	0.43
1:A:1350:TYR:C	1:A:1350:TYR:CD1	2.92	0.43
1:A:140:ALA:O	1:A:154:GLU:HA	2.19	0.43
1:A:138:TYR:OH	1:A:188:LYS:HD2	2.18	0.43
1:A:1290:ILE:HA	2:A:2001:ADP:C2	2.53	0.43
1:B:1300:ILE:O	1:B:1304:LEU:HG	2.18	0.43
1:B:1939:ARG:NH1	1:B:1948:ASP:OD2	2.52	0.43
1:B:121:ILE:HD12	1:B:123:ILE:HD11	1.99	0.43
1:B:1885:VAL:O	1:B:1944:VAL:HG23	2.19	0.43
1:A:1328:GLY:HA3	1:A:1334:LYS:HD2	2.01	0.43
1:A:161:MET:HE3	1:A:165:LEU:HA	2.00	0.43
1:B:1811:ARG:HG3	1:B:1813:LYS:HB2	2.01	0.43
1:A:1261:ILE:HG23	1:A:1873:LYS:HZ1	1.84	0.43
1:B:1308:VAL:O	1:B:1309:SER:HB3	2.18	0.43
1:B:162:PRO:HG2	1:B:166:GLU:OE2	2.18	0.43
1:B:1842:LYS:O	1:B:1845:SER:HB3	2.19	0.43
1:B:1926:GLU:O	1:B:1930:ARG:HG3	2.19	0.43
1:B:205:PRO:O	1:B:208:GLN:HB2	2.19	0.43
1:A:105:ARG:NH2	1:A:116:ASP:OD1	2.50	0.42
1:A:1311:LYS:HE3	1:A:1317:ARG:NH2	2.34	0.42
1:A:165:LEU:C	1:A:165:LEU:HD12	2.39	0.42
1:B:1318:LEU:HA	1:B:1318:LEU:HD22	1.89	0.42
1:B:241:GLN:HE21	1:B:241:GLN:HB2	1.50	0.42
1:A:1840:ASP:HB3	1:A:1843:ILE:HG12	2.02	0.42
1:A:1860:GLU:HB2	1:A:1862:VAL:HG22	2.00	0.42
1:A:1862:VAL:HG23	1:A:1862:VAL:O	2.18	0.42
1:A:1935:HIS:CE1	1:A:1951:GLU:HG3	2.54	0.42
1:A:1762:ASP:OD1	1:A:1820:ASP:HB3	2.20	0.42
1:A:1894:ILE:HG23	1:A:1895:GLU:H	1.83	0.42
1:A:1929:ILE:H	1:A:1929:ILE:HD12	1.84	0.42
1:A:1947:GLU:O	1:A:1951:GLU:HG2	2.19	0.42
1:A:204:VAL:HA	1:A:205:PRO:HD3	1.77	0.42
1:B:110:ARG:O	1:B:113:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ASP:O	1:B:16:GLU:HB2	2.18	0.42
1:B:245:VAL:HG22	1:B:245:VAL:O	2.19	0.42
1:A:1733:VAL:HG12	1:A:1734:ARG:N	2.34	0.42
1:A:1919:PRO:HG2	1:A:1920:ILE:H	1.84	0.42
1:A:1828:ARG:NE	1:A:1923:ARG:NH2	2.51	0.42
1:A:78:LEU:O	1:A:82:ILE:HG13	2.20	0.42
1:B:11:ARG:HG2	1:B:77:ALA:HB2	2.02	0.42
1:B:143:LYS:HA	1:B:151:GLN:O	2.18	0.42
1:B:1733:VAL:CG1	1:B:1734:ARG:N	2.82	0.42
1:B:1839:PRO:O	1:B:1843:ILE:HG23	2.18	0.42
1:B:1878:ALA:HA	1:B:1882:ILE:CG1	2.47	0.42
1:B:241:GLN:HG2	1:B:243:SER:O	2.19	0.42
1:A:1751:ALA:O	1:A:1752:ASP:C	2.57	0.42
1:B:1296:VAL:HA	1:B:1833:PHE:CE2	2.55	0.42
1:B:1289:ALA:CB	1:B:1340:TYR:HE2	2.32	0.42
1:B:1344:LEU:O	1:B:1346:PRO:HD3	2.20	0.42
1:B:1335:SER:HA	1:B:1759:ASP:OD2	2.20	0.42
1:B:1882:ILE:HG23	1:B:1942:PRO:HB3	2.01	0.42
1:A:1811:ARG:HH11	1:A:1813:LYS:HD2	1.84	0.42
1:A:1316:THR:HB	1:A:1317:ARG:H	1.62	0.42
1:A:1342:ALA:HB2	1:A:1757:LEU:CD1	2.50	0.42
1:A:1811:ARG:HD3	1:A:1813:LYS:CG	2.47	0.42
1:A:1327:VAL:HG11	1:A:1819:ILE:HG21	2.02	0.42
1:B:1283:VAL:CG2	1:B:1284:ASP:N	2.83	0.42
1:B:1342:ALA:O	1:B:1345:ALA:CB	2.65	0.42
1:B:1761:LEU:HD11	1:B:1764:MET:HE1	2.01	0.42
1:B:1879:ARG:NH1	1:B:1879:ARG:HG2	2.32	0.42
1:A:1312:LEU:HB3	1:A:1313:PRO:CD	2.43	0.42
1:A:155:TRP:HA	1:A:155:TRP:HE3	1.83	0.42
1:A:1899:VAL:CG1	1:A:1900:ARG:N	2.83	0.42
1:B:1814:ASN:ND2	1:B:1817:GLU:OE2	2.53	0.42
1:A:1734:ARG:HH11	1:A:1734:ARG:CG	2.33	0.41
1:A:53:LEU:HA	1:A:60:ALA:HB2	2.01	0.41
1:B:1940:LEU:O	1:B:1941:SER:C	2.58	0.41
1:A:1942:PRO:HG2	1:A:1942:PRO:O	2.20	0.41
1:A:25:ASN:N	1:A:27:GLN:HE21	2.07	0.41
1:A:155:TRP:CG	1:A:156:PRO:N	2.88	0.41
1:A:156:PRO:CD	1:A:161:MET:HG2	2.49	0.41
1:A:1941:SER:CB	1:A:1943:ILE:N	2.84	0.41
1:A:1884:PRO:HA	1:A:1942:PRO:HB2	2.01	0.41
1:B:1810:ASN:O	1:B:1811:ARG:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ILE:HG22	1:B:186:LYS:H	1.85	0.41
1:A:1308:VAL:CG1	1:A:1309:SER:H	2.33	0.41
1:A:143:LYS:HB2	1:A:183:ILE:CD1	2.37	0.41
1:A:156:PRO:HD3	1:A:161:MET:HG2	2.02	0.41
1:A:240:LYS:HB3	1:A:256:TYR:CD1	2.56	0.41
1:A:1278:ILE:O	1:A:1282:ILE:HG13	2.20	0.41
1:A:1851:ILE:HD12	1:B:1925:LEU:HD23	2.03	0.41
1:A:1928:LEU:HA	1:A:1928:LEU:HD13	1.70	0.41
1:A:1945:THR:O	1:A:1946:ARG:C	2.58	0.41
1:A:37:LEU:C	1:A:37:LEU:HD23	2.41	0.41
1:B:1729:THR:O	1:B:1746:GLY:N	2.46	0.41
1:B:1773:HIS:HD2	1:B:1828:ARG:NH1	2.19	0.41
1:B:1869:GLU:HA	1:B:1872:ARG:NH1	2.35	0.41
1:B:1898:TYR:CD1	1:B:1925:LEU:HD13	2.56	0.41
1:B:82:ILE:CD1	1:B:96:VAL:HG11	2.51	0.41
1:A:155:TRP:O	1:A:157:GLU:HG3	2.20	0.41
1:A:1772:ILE:HG23	1:A:1773:HIS:N	2.35	0.41
1:A:1882:ILE:H	1:A:1882:ILE:CD1	2.15	0.41
1:B:138:TYR:CZ	1:B:188:LYS:HB3	2.55	0.41
1:B:30:TYR:O	1:B:34:ILE:HG13	2.21	0.41
1:A:1335:SER:HA	1:A:1759:ASP:OD2	2.21	0.41
1:A:1342:ALA:C	1:A:1345:ALA:H	2.24	0.41
1:A:1767:ARG:CG	1:A:1767:ARG:HH11	2.33	0.41
1:B:1760:GLU:HG2	1:B:1763:LYS:HD2	2.02	0.41
1:B:1880:LYS:O	1:B:1883:HIS:HE1	2.03	0.41
1:A:161:MET:SD	1:A:165:LEU:HD13	2.61	0.41
1:A:1946:ARG:HB3	1:A:1950:ARG:HE	1.86	0.41
1:B:1287:ALA:O	1:B:1290:ILE:CG1	2.68	0.41
1:B:1735:ASP:C	1:B:1735:ASP:OD1	2.59	0.41
1:B:1944:VAL:HG12	1:B:1948:ASP:HB3	2.01	0.41
1:B:61:TYR:OH	1:B:260:SER:HB3	2.21	0.41
1:A:121:ILE:HD12	1:A:123:ILE:HD11	2.03	0.41
1:B:1783:ILE:O	1:B:1789:THR:HA	2.21	0.41
1:B:1868:HIS:O	1:B:1871:LEU:N	2.53	0.41
1:A:1281:ALA:O	1:A:1285:SER:N	2.54	0.41
1:A:1811:ARG:O	1:A:1813:LYS:N	2.54	0.41
1:B:1733:VAL:HG12	1:B:1734:ARG:N	2.35	0.41
1:B:1814:ASN:OD1	1:B:1814:ASN:N	2.54	0.41
1:B:1863:ALA:HB1	1:B:1864:PRO:CD	2.42	0.41
1:B:1920:ILE:HA	1:B:1920:ILE:HD13	1.87	0.41
1:A:144:HIS:CE1	1:A:174:CYS:SG	3.13	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:TYR:HD2	1:B:155:TRP:HB2	1.86	0.41
1:A:1336:GLN:HE21	1:A:1340:TYR:HE1	1.69	0.40
1:A:1344:LEU:O	1:A:1346:PRO:HD3	2.21	0.40
1:A:1761:LEU:HD11	1:A:1764:MET:CE	2.51	0.40
1:A:142:TYR:CE1	1:A:182:LEU:HB2	2.56	0.40
1:A:185:GLU:H	1:A:185:GLU:CD	2.24	0.40
1:A:221:LEU:O	1:A:222:VAL:C	2.60	0.40
1:A:233:VAL:HB	1:A:257:MET:HE3	2.03	0.40
1:B:1311:LYS:HZ3	1:B:1317:ARG:CG	2.34	0.40
1:B:1875:ILE:HG22	1:B:1879:ARG:HD3	2.03	0.40
1:A:182:LEU:HG	1:A:183:ILE:N	2.34	0.40
1:B:1751:ALA:O	1:B:1752:ASP:C	2.58	0.40
1:B:1939:ARG:O	1:B:1940:LEU:HD12	2.20	0.40
1:B:1939:ARG:NH2	1:B:1945:THR:OG1	2.55	0.40
1:A:1361:LEU:HB2	1:A:1768:ASP:OD2	2.20	0.40
1:A:144:HIS:ND1	1:A:171:CYS:HB2	2.35	0.40
1:A:1843:ILE:HG13	1:A:1844:ASP:H	1.86	0.40
1:B:152:GLU:OE1	1:B:186:LYS:NZ	2.32	0.40
1:B:155:TRP:HB3	1:B:156:PRO:HD2	2.04	0.40
1:B:70:ILE:HG23	1:B:71:LEU:N	2.37	0.40
1:A:1950:ARG:HH11	1:A:1950:ARG:CG	2.35	0.40
1:B:1899:VAL:CG1	1:B:1900:ARG:N	2.84	0.40
1:B:69:ILE:O	1:B:72:PRO:HD2	2.22	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	587/613 (96%)	519 (88%)	53 (9%)	15 (3%)	5	13
1	B	587/613 (96%)	524 (89%)	47 (8%)	16 (3%)	5	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1174/1226 (96%)	1043 (89%)	100 (8%)	31 (3%)	5	13

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	TRP
1	A	247	ARG
1	A	1841	ASP
1	A	1857	GLY
1	B	155	TRP
1	B	245	VAL
1	B	1841	ASP
1	B	1861	VAL
1	B	1948	ASP
1	A	245	VAL
1	A	1812	MET
1	A	1858	GLU
1	B	1289	ALA
1	B	1811	ARG
1	B	1839	PRO
1	A	139	LYS
1	A	156	PRO
1	A	1289	ALA
1	A	1868	HIS
1	B	156	PRO
1	B	1346	PRO
1	B	1859	SER
1	A	250	ARG
1	A	1346	PRO
1	B	1309	SER
1	B	1854	VAL
1	B	89	TYR
1	A	168	PRO
1	B	1941	SER
1	A	1942	PRO
1	B	1942	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	517/537 (96%)	444 (86%)	73 (14%)	3	8
1	B	517/537 (96%)	461 (89%)	56 (11%)	6	15
All	All	1034/1074 (96%)	905 (88%)	129 (12%)	4	10

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	8	ILE
1	A	27	GLN
1	A	48	GLU
1	A	71	LEU
1	A	91	ARG
1	A	158	ASP
1	A	161	MET
1	A	163	GLU
1	A	165	LEU
1	A	168	PRO
1	A	169	THR
1	A	181	ARG
1	A	182	LEU
1	A	188	LYS
1	A	241	GLN
1	A	245	VAL
1	A	247	ARG
1	A	254	ASP
1	A	264	VAL
1	A	265	SER
1	A	269	LEU
1	A	1267	GLN
1	A	1269	ILE
1	A	1276	LYS
1	A	1283	VAL
1	A	1285	SER
1	A	1308	VAL
1	A	1311	LYS
1	A	1316	THR
1	A	1318	LEU
1	A	1347	ARG
1	A	1352	SER

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Mol	Chain	Res	Type
1	A	1355	SER
1	A	1734	ARG
1	A	1760	GLU
1	A	1762	ASP
1	A	1763	LYS
1	A	1764	MET
1	A	1766	ASP
1	A	1770	SER
1	A	1779	GLN
1	A	1805	LYS
1	A	1806	GLN
1	A	1808	ARG
1	A	1809	PHE
1	A	1818	GLN
1	A	1825	LEU
1	A	1830	ASP
1	A	1841	ASP
1	A	1844	ASP
1	A	1855	ARG
1	A	1858	GLU
1	A	1861	VAL
1	A	1869	GLU
1	A	1882	ILE
1	A	1886	ILE
1	A	1888	GLU
1	A	1892	GLU
1	A	1894	ILE
1	A	1896	LYS
1	A	1903	LYS
1	A	1921	THR
1	A	1928	LEU
1	A	1939	ARG
1	A	1940	LEU
1	A	1941	SER
1	A	1942	PRO
1	A	1943	ILE
1	A	1944	VAL
1	A	1950	ARG
1	A	1953	ILE
1	A	1963	ILE
1	B	9	ASP
1	B	27	GLN

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Mol	Chain	Res	Type
1	B	48	GLU
1	B	68	LYS
1	B	91	ARG
1	B	96	VAL
1	B	103	ILE
1	B	139	LYS
1	B	143	LYS
1	B	158	ASP
1	B	161	MET
1	B	163	GLU
1	B	166	GLU
1	B	171	CYS
1	B	233	VAL
1	B	241	GLN
1	B	242	ASP
1	B	247	ARG
1	B	254	ASP
1	B	1261	ILE
1	B	1269	ILE
1	B	1272	LEU
1	B	1276	LYS
1	B	1314	ASP
1	B	1316	THR
1	B	1318	LEU
1	B	1329	ASP
1	B	1347	ARG
1	B	1762	ASP
1	B	1766	ASP
1	B	1770	SER
1	B	1808	ARG
1	B	1809	PHE
1	B	1812	MET
1	B	1813	LYS
1	B	1814	ASN
1	B	1824	THR
1	B	1825	LEU
1	B	1830	ASP
1	B	1842	LYS
1	B	1843	ILE
1	B	1850	HIS
1	B	1860	GLU
1	B	1862	VAL

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Mol	Chain	Res	Type
1	B	1869	GLU
1	B	1873	LYS
1	B	1879	ARG
1	B	1892	GLU
1	B	1896	LYS
1	B	1900	ARG
1	B	1902	ARG
1	B	1939	ARG
1	B	1941	SER
1	B	1944	VAL
1	B	1948	ASP
1	B	1953	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	27	GLN
1	A	212	GLN
1	A	241	GLN
1	A	1267	GLN
1	A	1779	GLN
1	A	1814	ASN
1	A	1962	GLN
1	B	27	GLN
1	B	241	GLN
1	B	1336	GLN
1	B	1779	GLN
1	B	1810	ASN
1	B	1850	HIS
1	B	1962	GLN

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 12 ligands modelled in this entry, 10 are 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
2	ADP	B	2001	3	24,29,29	1.44	3 (12%)	29,45,45	1.80	4 (13%)
2	ADP	A	2001	3	24,29,29	1.32	3 (12%)	29,45,45	1.86	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
2	ADP	B	2001	3	-	0/12/32/32	0/3/3/3
2	ADP	A	2001	3	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	ADP	O4'-C1'	3.67	1.46	1.41
2	B	2001	ADP	PB-O1B	3.31	1.61	1.50
2	A	2001	ADP	O4'-C1'	3.18	1.45	1.41
2	A	2001	ADP	PB-O1B	3.13	1.60	1.50
2	B	2001	ADP	C8-N7	-2.80	1.29	1.34
2	A	2001	ADP	C8-N7	-2.13	1.30	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	ADP	PA-O3A-PB	-6.59	110.20	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	ADP	PA-O3A-PB	-6.43	110.77	132.83
2	A	2001	ADP	N3-C2-N1	-4.61	121.48	128.68
2	B	2001	ADP	N3-C2-N1	-4.13	122.22	128.68
2	B	2001	ADP	C3'-C2'-C1'	2.99	105.48	100.98
2	A	2001	ADP	C3'-C2'-C1'	2.85	105.28	100.98
2	A	2001	ADP	PA-O5'-C5'	-2.29	108.23	121.68
2	B	2001	ADP	PA-O5'-C5'	-2.23	108.62	121.68

There are no chirality outliers.

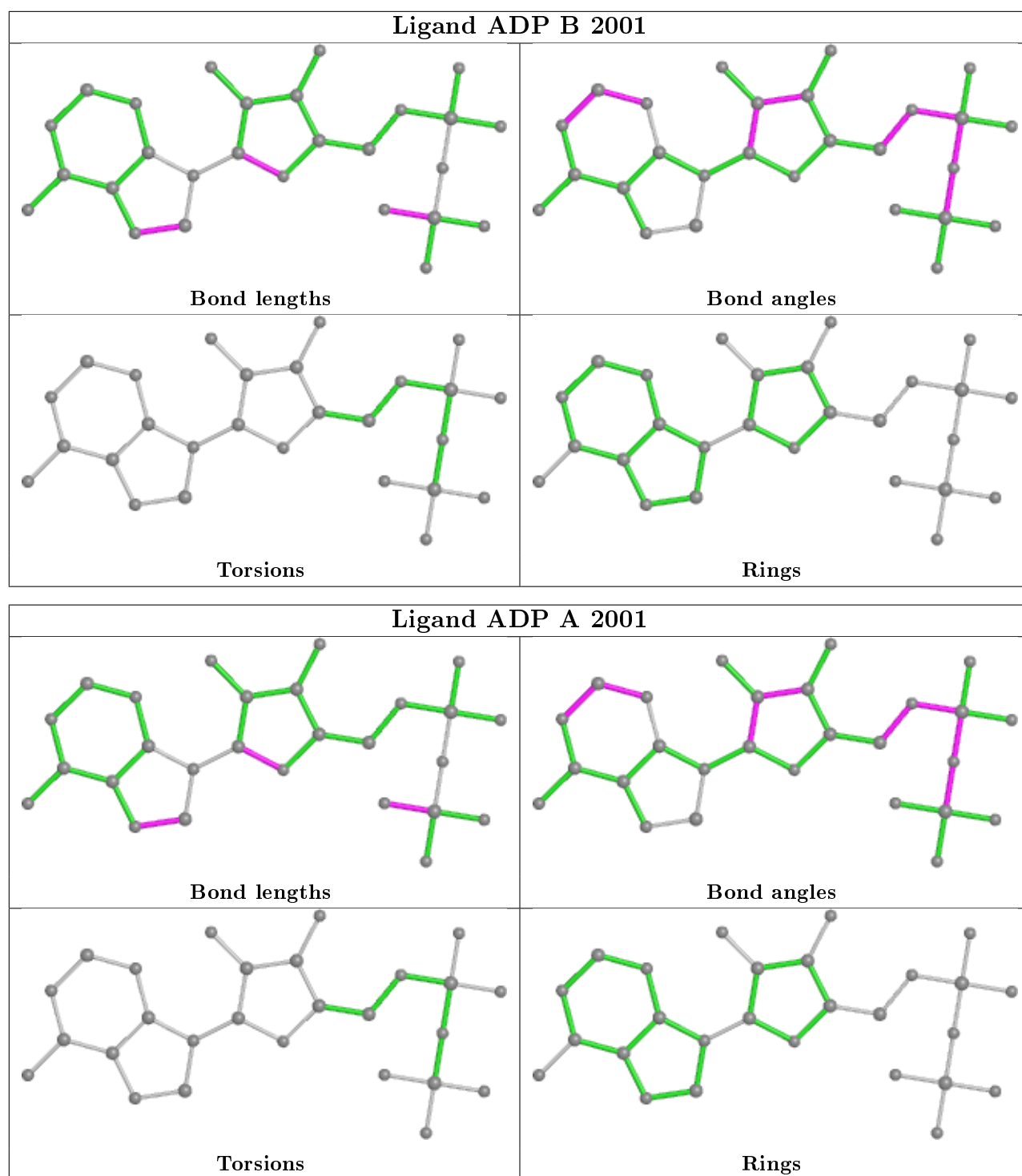
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	ADP	1	0
2	A	2001	ADP	3	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	591/613 (96%)	0.54	56 (9%) 8 6	10, 63, 109, 125	0
1	B	591/613 (96%)	0.47	51 (8%) 10 8	9, 61, 110, 128	0
All	All	1182/1226 (96%)	0.51	107 (9%) 9 7	9, 62, 110, 128	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	GLY	8.0
1	B	249	SER	7.7
1	A	249	SER	7.6
1	B	1315	GLY	6.6
1	B	146	HIS	6.4
1	A	1886	ILE	5.9
1	A	1315	GLY	5.4
1	A	177	PRO	5.3
1	B	179	GLN	5.2
1	B	147	PRO	5.0
1	A	1859	SER	4.8
1	B	1861	VAL	4.4
1	A	248	GLY	4.3
1	A	1810	ASN	4.3
1	A	147	PRO	4.2
1	A	1855	ARG	4.2
1	B	145	ILE	4.1
1	A	176	LYS	4.1
1	A	155	TRP	4.1
1	B	1291	TYR	4.1
1	B	181	ARG	4.0
1	A	1901	MET	4.0
1	B	177	PRO	3.9
1	B	150	MET	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	151	GLN	3.8
1	B	151	GLN	3.7
1	B	1849	ARG	3.6
1	B	1317	ARG	3.6
1	A	1311	LYS	3.6
1	B	1901	MET	3.6
1	B	178	GLY	3.6
1	B	1311	LYS	3.6
1	B	1857	GLY	3.6
1	B	1886	ILE	3.5
1	B	1858	GLU	3.5
1	B	1852	LEU	3.5
1	B	1949	ALA	3.4
1	A	149	CYS	3.4
1	A	159	GLU	3.4
1	A	1862	VAL	3.4
1	B	148	ASP	3.3
1	B	1850	HIS	3.2
1	A	143	LYS	3.2
1	B	149	CYS	3.1
1	B	1919	PRO	3.1
1	B	1316	THR	3.1
1	A	152	GLU	3.1
1	A	1852	LEU	3.0
1	A	1843	ILE	3.0
1	A	1310	ARG	3.0
1	B	176	LYS	3.0
1	A	1885	VAL	2.9
1	A	148	ASP	2.9
1	A	1943	ILE	2.9
1	B	7	GLN	2.8
1	B	1853	ARG	2.8
1	A	173	LYS	2.8
1	B	1859	SER	2.8
1	B	250	ARG	2.7
1	B	1346	PRO	2.7
1	A	1346	PRO	2.7
1	B	1943	ILE	2.7
1	A	178	GLY	2.6
1	A	1944	VAL	2.6
1	A	1899	VAL	2.6
1	A	1289	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1291	TYR	2.5
1	B	1310	ARG	2.5
1	A	7	GLN	2.5
1	B	1810	ASN	2.4
1	B	172	PRO	2.4
1	A	1273	ALA	2.4
1	B	1904	SER	2.4
1	B	1856	ARG	2.4
1	A	1858	GLU	2.4
1	A	146	HIS	2.4
1	B	157	GLU	2.4
1	A	172	PRO	2.3
1	A	150	MET	2.3
1	A	1850	HIS	2.3
1	A	1942	PRO	2.3
1	A	1904	SER	2.3
1	A	1963	ILE	2.3
1	B	1841	ASP	2.3
1	A	181	ARG	2.3
1	B	1950	ARG	2.3
1	A	1340	TYR	2.3
1	A	138	TYR	2.2
1	A	142	TYR	2.2
1	B	8	ILE	2.2
1	B	1870	ILE	2.1
1	A	250	ARG	2.1
1	A	1274	LYS	2.1
1	A	1939	ARG	2.1
1	A	1314	ASP	2.1
1	A	1292	GLY	2.1
1	A	1861	VAL	2.1
1	B	1340	TYR	2.1
1	B	1854	VAL	2.1
1	B	1888	GLU	2.1
1	B	173	LYS	2.0
1	B	1267	GLN	2.0
1	A	1313	PRO	2.0
1	A	1947	GLU	2.0
1	B	159	GLU	2.0
1	A	144	HIS	2.0
1	A	1259	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

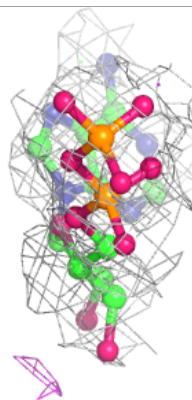
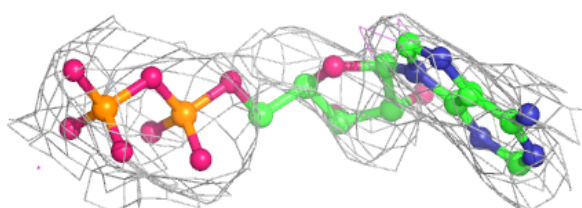
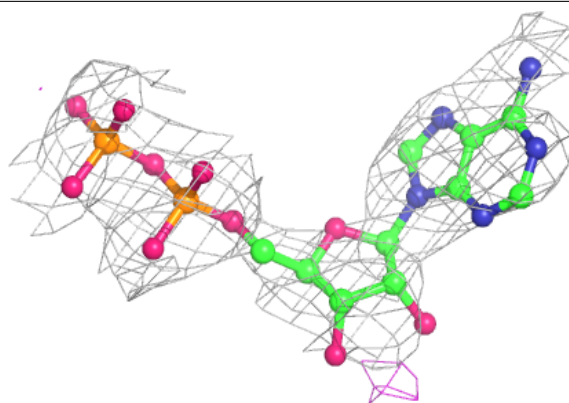
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ADP	A	2001	27/27	0.80	0.27	113,114,115,115	0
2	ADP	B	2001	27/27	0.82	0.27	118,121,127,128	0
4	ZN	B	2003	1/1	0.88	0.05	169,169,169,169	0
5	CL	B	2006	1/1	0.92	0.09	39,39,39,39	0
4	ZN	A	2003	1/1	0.93	0.09	163,163,163,163	0
3	MG	B	2002	1/1	0.94	0.19	64,64,64,64	0
3	MG	A	2002	1/1	0.95	0.13	64,64,64,64	0
5	CL	B	2004	1/1	0.96	0.23	48,48,48,48	0
5	CL	A	2005	1/1	0.96	0.21	59,59,59,59	0
5	CL	B	2005	1/1	0.96	0.17	53,53,53,53	0
5	CL	A	2004	1/1	0.97	0.25	48,48,48,48	0
5	CL	A	2006	1/1	0.99	0.22	41,41,41,41	0

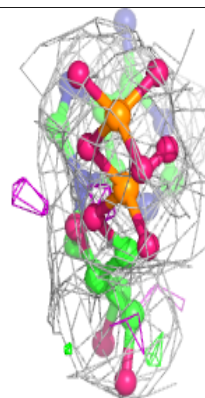
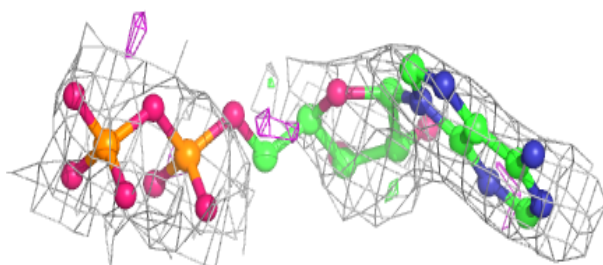
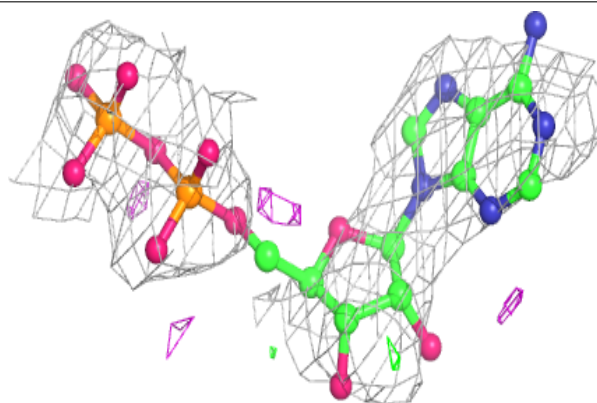
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 2001:

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

**Electron density around ADP B 2001:**

$2mF_o-DF_c$ (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.