



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:05 am BST

PDB ID : 1OD2
Title : Acetyl-CoA Carboxylase Carboxyltransferase Domain
Authors : Zhang, H.; Yang, Z.; Shen, Y.; Tong, L.
Deposited on : 2003-02-12
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

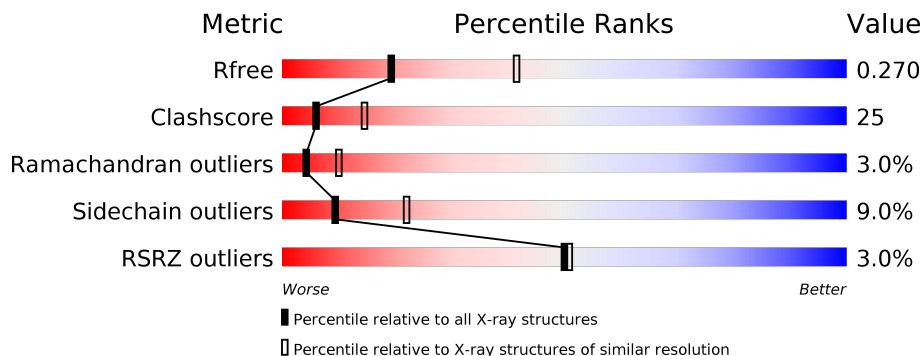
1 Overall quality at a glance i

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	805	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 52%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">3% 52% 32% 5% 11%</p>
1	B	805	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 44%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 37%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 44% 37% 5% 14%</p>

2 Entry composition i

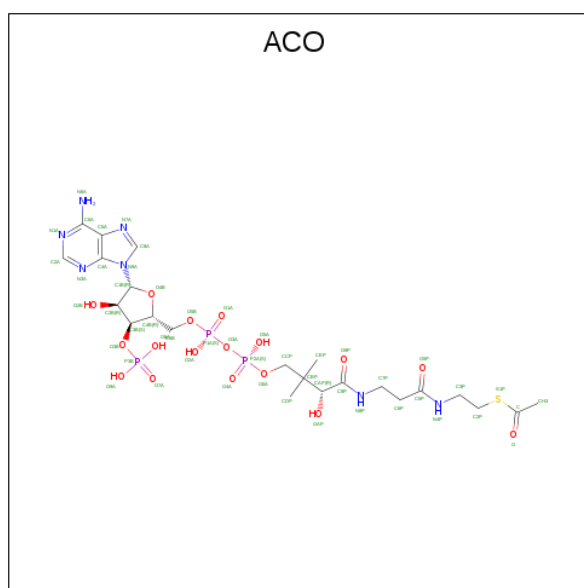
There are 4 unique types of molecules in this entry. The entry contains 11433 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYL-COENZYME A CARBOXYLASE.

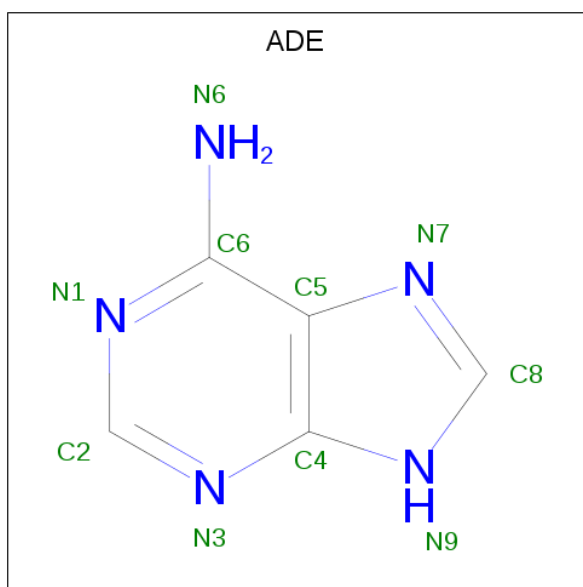
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	S				Se
1	A	720	Total	C	N	O	S	Se	0	0	1
			5742	3650	994	1079	2	17			
1	B	696	Total	C	N	O	S	Se	0	0	1
			5544	3518	963	1044	2	17			

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is ADENINE (three-letter code: ADE) (formula: $C_5H_5N_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			10	5	5		

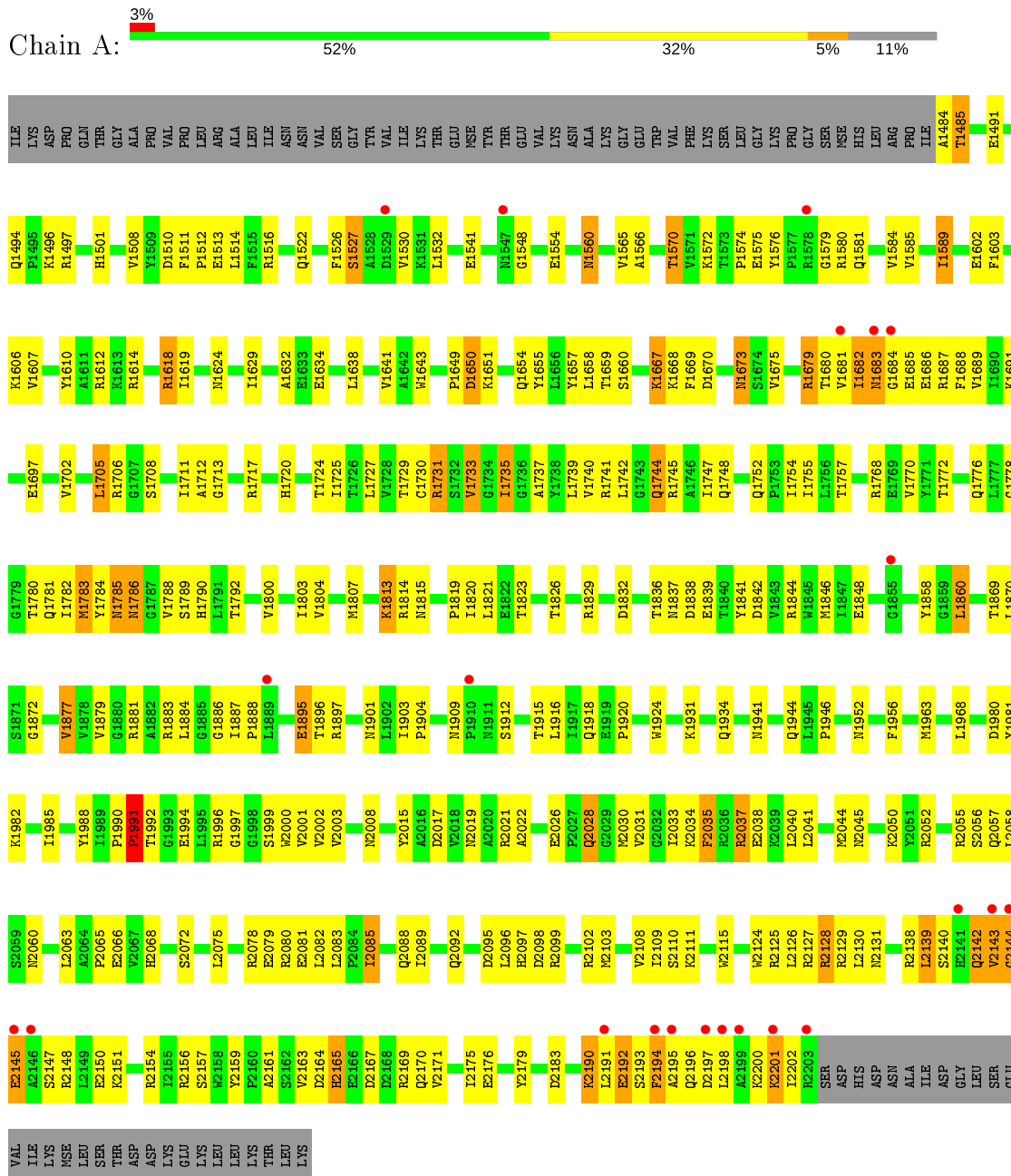
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		
4	B	42	Total	O	0	0
			42	42		

3 Residue-property plots [i](#)

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

● Molecule 1: ACETYL-COENZYME A CARBOXYLASE



● Molecule 1: ACETYL-COENZYME A CARBOXYLASE



ILE	VAL	M1560	M1643	A1742	D1796	R1883	V1975	R2061	Q2142	ILE
LYS	LYS	F1567	M1644	G1713	L1797	I1887	V1979	R2062	V2143	ASP
ASP	GLU	I1569	D1645	M1717	E1801	V1891	D1980	S2063	E2144	GLY
GLN	TRP	I1572	A1646	M1725	E1807	V1895	K1981	A2064	E2145	LEU
THR	LEU	K1572	A1647	I1726	M1807	E1895	K1982	V2067	S2147	SER
GLY	GLN	K1496	N1648	T1726	M1807	T1894	Q1983	Y2067	R2148	VAL
ALA	ALA	K1496	P1649	L1727	V1810	T1894	P1984	Q2070	E2148	L2149
PRO	PRO	R1497	D1650	H1727	V1810	R1897	I1985	Q2071	E2150	LYS
VAL	VAL	R1498	G1652	T1728	P1811	R1897	I1986	L2071	E2151	LYS
PRO	PRO	K1499	F1653	T1729	A1812	M1901	I1986	L2072	L2152	LEU
LEU	LEU	K1499	Q1654	C1730	K1813	L1902	I1987	L2073	A2153	THR
ARG	ARG	L1502	Q1655	R1731	K1814	I1903	I1987	L2074	R2154	SER
ALA	ALA	L1502	L1656	V1732	H1815	P1904	P1990	A2076	I2155	ASP
LEU	LEU	T1505	Y1657	G1734	M1816	A1905	T1992	D2077	W2158	ASP
LEU	LEU	T1506	L1658	I1735	P1817	D1906	G1993	R2078	W2159	LYS
ILE	ILE	T1507	L1658	I1735	V1818	D1906	G1993	E2079	P2160	LYS
ASN	ASN	Y1508	T1659	L1739	V1818	D1906	E1994	R2080	P2160	LYS
ASN	ASN	Y1508	E1661	V1740	V1819	P1910	L1995	R2081	P2160	LYS
VAL	VAL	T1590	E1662	M1741	I1820	M1911	R1996	E2081	P2160	LEU
SER	SER	T1590	G1663	R1741	W1827	S1912	G1997	L2082	V2163	LEU
GLY	GLY	F1591	E1664	Q1744	D1828	A1913	G1998	L2083	D2164	LYS
TYR	TYR	K1592	E1664	Q1744	R1829	E1914	G1998	L2083	D2165	LYS
TYR	TYR	I1593	E1664	Q1744	R1829	E1914	S1999	P2084	E2166	THR
ILE	ILE	G1594	K1668	I1747	R1830	I1917	W2000	L2085	D2167	LEU
LYS	LYS	W1523	F1669	I1748	V1831	I1917	V2001	Y2086	D2167	LEU
THR	THR	W1523	D1670	V1749	V1831	I1917	D2010	G2087	D2168	LYS
GLU	GLU	F1526	K1671	M1749	T1834	G1921	D2010	Q2088	V2171	LYS
MSE	MSE	S1527	E1672	Q1752	P1835	Q1922	Q2011	I2089	V2171	LYS
THR	THR	D1601	N1673	Q1752	T1836	V1923	M2012	S2090	N2178	ASP
THR	THR	A1528	S1674	M1755	M1837	H1924	E2013	L2091	Y2179	GLY
GLU	GLU	D1529	L1675	L1756	N1837	H1925	M2014	L2092	Y2179	GLY
VAL	VAL	V1530	L1676	L1757	D1838	P1926	M2014	Q2092	K2180	LYS
LYS	LYS	A1531	L1676	T1757	E1839	S1927	R2021	R2097	T2181	LYS
ASN	ASN	L1532	R1679	G1758	D1842	S1928	V2024	E2097	L2182	LYS
ALA	ALA	L1532	T1680	A1759	V1843	Q1934	L2025	S2100	D2184	LYS
LYS	LYS	T1533	V1681	P1760	R1844	Q1934	L2026	E2103	D2185	LYS
GLY	GLY	D1534	I1682	M1765	T1852	I1936	E2026	R2106	K2186	LEU
GLY	GLY	D1534	N1683	L1766	E1853	M1940	Q2027	G2107	L2187	LEU
TRP	TRP	F1537	G1684	G1767	S1854	M1940	P2027	V2108	L2188	LEU
VAL	VAL	T1538	E1686	M1768	G1855	M1947	Q2029	L2109	L2189	LEU
PHE	PHE	I1539	E1686	M1768	G1855	M1947	F2035	R2119	K2190	LEU
LYS	LYS	N1540	E1687	T1772	F1856	M1949	R2036	R2125	GLU	GLU
SER	SER	E1541	F1688	S1773	L1860	I1949	R2037	L2126	SER	SER
LEU	LEU	L1542	L1621	Q1776	L1860	L1950	E2038	L2127	PHE	PHE
GLY	GLY	L1543	A1622	Q1776	K1863	L1950	K2039	L2040	ALA	ALA
LYS	LYS	E1544	A1623	G1779	G1864	M1953	L2040	L2041	ALA	ALA
PRO	PRO	D1545	N1624	T1692	S1871	M1953	L2041	L2041	GLN	GLN
PRO	PRO	D1545	S1625	T1692	G1872	M1954	K2039	L2042	ASP	ASP
GLY	GLY	E1546	G1626	I1694	A1874	G1954	M2044	M2044	LEU	LEU
SER	SER	M1547	G1626	I1694	L1870	R1955	N2045	N2045	LEU	LEU
MSE	MSE	G1548	M1631	M1782	S1871	Q1960	R2046	R2046	ALA	ALA
HIS	HIS	E1549	A1632	M1782	G1871	R1961	R2046	R2046	LYS	LYS
LEU	LEU	E1552	E1633	M1783	G1872	R1961	L2047	L2047	LYS	LYS
ARG	ARG	V1553	E1634	Y1784	A1874	D1962	L2047	L2047	ILE	ILE
PRO	PRO	E1554	E1634	M1785	A1874	M1963	K2050	K2050	ARG	ARG
ILE	ILE	E1554	P1637	M1786	A1874	M1963	Y2051	Y2051	SER	SER
ALA	ALA	E1555	L1638	G1787	A1874	E1966	R2052	R2052	ASP	ASP
THR	THR	E1556	F1639	G1788	V1877	V1967	R2052	R2052	ASP	ASP
PRO	PRO	G1557	Q1640	S1789	V1878	L1968	R2055	R2055	HIS	HIS
TYR	TYR	P1558	V1641	L1790	V1878	L1968	R2055	R2055	ASP	ASP
PRO	PRO	A1559	A1642	T1792	R1881	K1969	L2058	L2058	ASN	ASN
PRO	PRO	A1559	A1642	T1792	A1882	K1969	L2058	L2058	ALA	ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.87Å 138.13Å 101.40Å 90.00° 114.42° 90.00°	Depositor
Resolution (Å)	28.85 – 2.70 28.85 – 2.69	Depositor EDS
% Data completeness (in resolution range)	93.2 (28.85-2.70) 92.7 (28.85-2.69)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.54 (at 2.68Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.279 0.217 , 0.270	Depositor DCC
R_{free} test set	6032 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtrriage
Anisotropy	0.414	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11433	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: ADE, ACO

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	0/5850	0.66	0/7893
1	B	0.45	0/5646	0.67	0/7615
All	All	0.45	0/11496	0.66	0/15508

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	5742	0	5688	271	0
1	B	5544	0	5483	318	0
2	A	48	0	31	4	0
3	B	10	0	4	0	0
4	A	47	0	0	1	0
4	B	42	0	0	2	0
All	All	11433	0	11206	558	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 25.

All (558) 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:2085:ILE:HD12	1:A:2085:ILE:H	1.17	1.06
1:A:2085:ILE:HG12	1:B:1650:ASP:HA	1.38	1.01
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.18	0.99
1:A:2034:LYS:HB2	1:B:1631:MSE:HE3	1.48	0.96
1:B:1940:ASN:HD22	1:B:1983:GLN:HE22	1.07	0.94
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	1.82	0.93
1:A:1560:ASN:HD22	1:A:1560:ASN:H	1.11	0.89
1:A:1570:THR:HB	1:A:1581:GLN:HG2	1.52	0.87
1:B:1772:THR:H	1:B:1776:GLN:NE2	1.73	0.87
1:B:1940:ASN:HD22	1:B:1983:GLN:NE2	1.75	0.85
1:B:1860:LEU:CD2	1:B:1948:MSE:HE1	2.06	0.85
1:A:2065:PRO:HG2	1:A:2066:GLU:OE2	1.75	0.84
1:B:1991:PRO:O	1:B:1993:GLY:N	2.09	0.84
1:A:2037:ARG:HB3	1:A:2037:ARG:HH11	1.39	0.84
1:A:1629:ILE:HG22	1:B:2024:VAL:HG11	1.60	0.84
1:A:1679:ARG:HG2	1:A:1680:THR:N	1.93	0.83
1:B:1772:THR:H	1:B:1776:GLN:HE22	1.25	0.83
1:A:1782:ILE:O	1:A:1786:ASN:HB2	1.81	0.81
1:A:2034:LYS:CB	1:B:1631:MSE:HE3	2.10	0.81
1:B:1505:THR:HB	1:B:1730:CYS:HB2	1.62	0.81
1:B:1829:ARG:CZ	1:B:2119:ARG:HE	1.93	0.81
1:A:2092:GLN:O	1:A:2096:LEU:HD23	1.81	0.81
1:B:2070:GLN:HE21	1:B:2074:GLN:HE21	1.29	0.81
1:A:2085:ILE:CD1	1:A:2085:ILE:H	1.94	0.81
1:B:1499:LYS:HE2	1:B:1590:THR:HB	1.60	0.81
1:B:1644:ASN:HD21	1:B:1654:GLN:HE21	1.25	0.80
1:A:1783:MSE:HE1	1:B:1963:MSE:HE3	1.62	0.79
1:A:1560:ASN:ND2	1:A:1560:ASN:H	1.80	0.79
1:B:1940:ASN:ND2	1:B:1983:GLN:HE22	1.81	0.79
1:B:2106:LYS:HA	1:B:2106:LYS:HE2	1.66	0.78
1:A:2031:VAL:HG13	1:A:2035:PHE:HB3	1.66	0.77
2:A:3203:ACO:H10	2:A:3203:ACO:O4A	1.84	0.77
1:B:2146:ALA:HB1	1:B:2150:GLU:OE2	1.84	0.77
1:B:2142:GLN:HE22	1:B:2144:GLY:N	1.84	0.75
1:A:1786:ASN:ND2	1:B:1966:GLU:HG3	2.00	0.75
1:B:1725:ILE:HD11	1:B:1747:ILE:HD11	1.69	0.75
1:B:2077:ASP:O	1:B:2081:GLU:HG3	1.85	0.74
1:B:1860:LEU:HD21	1:B:1948:MSE:HE1	1.68	0.74
1:A:1785:ASN:HD22	1:A:1785:ASN:N	1.85	0.74
1:B:1657:TYR:CD2	1:B:1687:ARG:HB2	2.23	0.73
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2070:GLN:HE21	1:B:2074:GLN:NE2	1.86	0.73
1:A:2142:GLN:HB3	1:A:2190:LYS:CE	2.19	0.73
1:A:1667:LYS:C	1:A:1669:PHE:H	1.91	0.72
1:A:1679:ARG:HG2	1:A:1680:THR:H	1.54	0.72
1:A:2079:GLU:O	1:A:2083:LEU:HB2	1.89	0.72
1:B:1790:HIS:HA	1:B:1870:LEU:HD23	1.70	0.72
1:B:1508:VAL:HG21	1:B:1588:ASP:HA	1.70	0.72
1:B:1499:LYS:HG2	1:B:1590:THR:HG22	1.71	0.71
1:B:1658:LEU:HG	1:B:1690:ILE:HD11	1.70	0.71
1:B:1921:GLY:O	1:B:1923:VAL:HG12	1.91	0.71
1:A:1815:ASN:ND2	1:A:1944:GLN:HE22	1.89	0.71
1:B:1766:LEU:O	1:B:1768:ARG:HG2	1.91	0.71
1:B:2046:ARG:CZ	1:B:2047:LEU:HD11	2.21	0.71
1:B:1954:ARG:HG3	1:B:1954:ARG:HH11	1.55	0.70
1:A:2080:ARG:O	1:A:2080:ARG:HG2	1.92	0.70
1:A:2142:GLN:HB3	1:A:2190:LYS:HE3	1.74	0.69
1:B:1539:SER:C	1:B:1540:ASN:HD22	1.95	0.69
1:B:2070:GLN:NE2	1:B:2074:GLN:HE21	1.91	0.69
1:A:1838:ASP:HB2	1:A:1839:GLU:OE1	1.91	0.69
1:A:1731:ARG:HH12	2:A:3203:ACO:H121	1.58	0.69
1:A:1815:ASN:HD22	1:A:1944:GLN:HE22	1.40	0.68
1:B:2167:ASP:O	1:B:2171:VAL:HG23	1.93	0.68
1:B:1773:SER:H	1:B:1776:GLN:HE21	1.42	0.68
1:B:2142:GLN:HE22	1:B:2144:GLY:CA	2.06	0.68
1:B:2125:ARG:NH1	1:B:2168:ASP:OD1	2.27	0.68
1:A:2033:ILE:HG22	1:A:2034:LYS:HG3	1.75	0.67
1:B:1634:GLU:O	1:B:1638:LEU:HD22	1.94	0.67
1:A:1643:TRP:CZ3	1:A:1649:PRO:HB3	2.29	0.67
1:B:1768:ARG:HB2	1:B:1768:ARG:HH11	1.58	0.67
1:A:1733:VAL:HG13	1:A:1755:ILE:HG13	1.76	0.67
1:A:1735:ILE:H	1:A:1735:ILE:HD12	1.60	0.67
1:B:1701:GLY:O	1:B:1704:CYS:HB2	1.95	0.67
1:A:1731:ARG:NH1	2:A:3203:ACO:H121	2.09	0.66
1:A:1513:GLU:OE2	1:A:1516:ARG:NH1	2.28	0.66
1:B:2039:LYS:HB2	1:B:2039:LYS:NZ	2.10	0.66
1:A:2147:SER:OG	1:A:2150:GLU:HG3	1.95	0.66
1:B:1540:ASN:N	1:B:1540:ASN:HD22	1.94	0.65
1:B:1733:VAL:HG22	1:B:1755:ILE:HD11	1.79	0.65
1:A:1650:ASP:OD2	1:A:1650:ASP:N	2.30	0.65
1:A:1733:VAL:HA	1:A:1755:ILE:O	1.97	0.65
1:B:1685:GLU:HG2	1:B:1686:GLU:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1637:PRO:HG2	1:B:1638:LEU:HD13	1.80	0.64
1:B:1836:THR:HB	1:B:1839:GLU:OE2	1.97	0.64
1:A:2096:LEU:HD12	1:B:1692:THR:HA	1.80	0.64
1:A:2191:LEU:C	1:A:2191:LEU:HD23	2.18	0.64
1:B:2010:ASP:CG	1:B:2148:ARG:HG3	2.18	0.64
1:B:2055:ARG:HG3	1:B:2055:ARG:HH11	1.63	0.64
1:B:1541:GLU:HG3	1:B:1567:PHE:HE2	1.63	0.64
1:B:2142:GLN:NE2	1:B:2144:GLY:N	2.46	0.64
1:A:1679:ARG:HG3	1:A:1679:ARG:HH11	1.62	0.64
1:A:2089:ILE:HD13	1:B:1641:VAL:HG21	1.80	0.63
1:A:1603:PHE:O	1:A:1607:VAL:HG23	1.99	0.63
1:A:1680:THR:HG22	1:A:1687:ARG:HB2	1.80	0.63
1:A:1682:ILE:C	1:A:1684:GLY:H	2.01	0.63
1:A:2041:LEU:HD12	1:A:2044:MSE:HE3	1.81	0.62
1:B:1780:THR:O	1:B:1784:TYR:HB3	1.97	0.62
1:B:2188:GLY:O	1:B:2189:LEU:HD23	1.99	0.62
1:A:1790:HIS:HB3	1:A:1869:THR:HG23	1.80	0.62
1:A:2138:ARG:HB3	1:A:2138:ARG:HH11	1.64	0.62
1:B:1749:VAL:O	1:B:1752:GLN:HB2	1.99	0.62
1:A:1641:VAL:HG21	1:B:2089:ILE:HD13	1.82	0.62
1:A:2200:LYS:HZ1	1:A:2202:ILE:HB	1.64	0.62
1:B:1755:ILE:HD13	1:B:1755:ILE:H	1.64	0.62
1:B:1813:LYS:HG3	1:B:1816:MSE:HG3	1.80	0.62
1:B:1552:GLU:O	1:B:1553:VAL:HG13	2.00	0.62
1:B:2064:ALA:HB3	1:B:2067:VAL:HG23	1.80	0.62
1:A:1712:ALA:O	1:A:1742:LEU:HD13	2.00	0.61
1:A:2200:LYS:HE2	1:A:2202:ILE:HD12	1.82	0.61
1:A:1629:ILE:HG22	1:B:2024:VAL:CG1	2.28	0.61
1:B:1779:GLY:HA3	1:B:1781:GLN:OE1	2.00	0.61
1:B:1543:ILE:HD12	1:B:1544:GLU:O	2.00	0.61
1:B:1813:LYS:HG3	1:B:1816:MSE:CG	2.31	0.61
1:A:2057:GLN:O	1:A:2063:LEU:HD11	2.01	0.61
1:A:2142:GLN:HB3	1:A:2190:LYS:NZ	2.15	0.61
1:B:1860:LEU:HD23	1:B:1948:MSE:HE1	1.82	0.61
1:A:1820:ILE:HD12	1:A:1886:GLY:C	2.21	0.60
1:A:2139:LEU:O	1:A:2151:LYS:HD3	2.00	0.60
1:A:1589:ILE:HD13	1:A:1589:ILE:O	2.02	0.60
1:B:1966:GLU:HG2	1:B:1969:LYS:HE3	1.82	0.60
1:B:1572:LYS:HA	1:B:1579:GLY:HA2	1.83	0.60
1:B:2139:LEU:HD11	1:B:2154:ARG:NH1	2.17	0.59
1:A:2097:HIS:HE1	1:B:1632:ALA:H	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2099:ARG:HH11	1:A:2099:ARG:HG3	1.67	0.59
1:B:1810:VAL:HG23	1:B:1811:PRO:HD2	1.84	0.59
1:A:2045:ASN:HD22	1:A:2055:ARG:HG3	1.68	0.59
1:B:1990:PRO:O	1:B:1991:PRO:O	2.20	0.59
1:A:1585:VAL:HG22	1:A:1607:VAL:HG11	1.84	0.59
1:A:1491:GLU:OE2	1:A:1501:HIS:HD2	1.86	0.59
1:B:1991:PRO:C	1:B:1993:GLY:H	2.03	0.59
1:B:1516:ARG:HH22	1:B:1534:ASP:HA	1.68	0.59
1:B:1772:THR:N	1:B:1776:GLN:NE2	2.49	0.59
1:B:1589:ILE:O	1:B:1589:ILE:HG13	2.03	0.59
1:A:2035:PHE:HB2	1:B:1631:MSE:HE1	1.84	0.58
1:A:2200:LYS:HA	1:A:2200:LYS:HZ3	1.67	0.58
1:A:1572:LYS:HA	1:A:1579:GLY:HA2	1.85	0.58
1:B:1679:ARG:CZ	1:B:1686:GLU:OE1	2.51	0.58
1:B:2025:LEU:HD12	1:B:2029:GLY:HA3	1.84	0.58
1:A:1527:SER:O	1:A:1530:VAL:HG22	2.04	0.58
1:A:1682:ILE:O	1:A:1684:GLY:N	2.34	0.58
1:B:1755:ILE:HD13	1:B:1755:ILE:N	2.18	0.58
1:B:2125:ARG:NH1	1:B:2128:ARG:HD2	2.19	0.58
1:A:2085:ILE:N	1:A:2085:ILE:HD12	2.02	0.58
1:B:2050:LYS:HD2	1:B:2078:ARG:CZ	2.33	0.58
1:B:2180:LYS:HB3	1:B:2180:LYS:NZ	2.19	0.58
1:B:2135:LEU:HB3	1:B:2155:ILE:HD13	1.86	0.58
1:A:2193:SER:C	1:A:2195:ALA:H	2.07	0.58
1:B:1925:HIS:HD2	4:B:5025:HOH:O	1.86	0.57
1:A:1786:ASN:HD21	1:B:1966:GLU:HG3	1.65	0.57
1:A:1848:GLU:HB2	4:A:5031:HOH:O	2.03	0.57
1:B:1541:GLU:HG3	1:B:1567:PHE:CE2	2.39	0.57
1:B:2010:ASP:OD1	1:B:2148:ARG:HG3	2.04	0.57
1:B:1917:ILE:HD12	1:B:1961:ARG:NH2	2.19	0.57
1:B:1711:ILE:HD12	1:B:1739:LEU:HD21	1.86	0.57
1:B:2119:ARG:HH11	1:B:2119:ARG:HG2	1.68	0.57
1:A:2037:ARG:O	1:A:2040:LEU:N	2.37	0.57
1:B:1948:MSE:HE3	1:B:1950:LEU:HD21	1.87	0.57
1:A:1560:ASN:HD22	1:A:1560:ASN:N	1.93	0.57
1:A:2052:ARG:HG3	1:A:2052:ARG:NH1	2.20	0.57
1:A:2142:GLN:HB3	1:A:2190:LYS:HG3	1.87	0.57
1:A:1741:ARG:CZ	1:A:1744:GLN:HE22	2.18	0.56
1:A:1813:LYS:HB2	1:A:1813:LYS:NZ	2.19	0.56
1:B:1786:ASN:OD1	1:B:1788:VAL:HG23	2.06	0.56
1:B:1527:SER:O	1:B:1530:VAL:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1730:CYS:CA	1:A:1752:GLN:HE21	2.06	0.56
1:A:2142:GLN:CD	1:A:2143:VAL:H	2.09	0.56
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.53	0.56
1:B:1654:GLN:O	1:B:1655:TYR:HB3	2.06	0.56
1:A:2148:ARG:HG2	1:A:2148:ARG:HH11	1.71	0.56
1:A:2200:LYS:HA	1:A:2200:LYS:NZ	2.21	0.56
1:B:1948:MSE:HE3	1:B:1950:LEU:HG	1.87	0.56
1:A:1903:ILE:HB	1:A:1915:THR:HG23	1.87	0.56
1:B:1560:ASN:HD22	1:B:1560:ASN:H	1.54	0.56
1:B:1657:TYR:HA	1:B:1690:ILE:HG12	1.87	0.56
1:A:2142:GLN:CD	1:A:2143:VAL:N	2.59	0.56
1:A:2164:ASP:OD1	1:A:2167:ASP:HB2	2.06	0.56
1:B:1948:MSE:HE3	1:B:1950:LEU:CD2	2.36	0.56
1:B:2061:LYS:O	1:B:2061:LYS:HD3	2.06	0.56
1:B:2164:ASP:O	1:B:2166:GLU:N	2.39	0.56
1:B:1730:CYS:CA	1:B:1752:GLN:HG3	2.36	0.56
1:B:1877:VAL:HG23	1:B:1928:SER:HB2	1.88	0.56
1:A:1632:ALA:H	1:B:2097:HIS:HE1	1.53	0.56
1:A:1980:ASP:O	1:A:1982:LYS:HD2	2.06	0.55
1:A:1776:GLN:O	1:B:1960:GLN:HG3	2.05	0.55
1:B:2082:LEU:N	1:B:2082:LEU:HD12	2.21	0.55
1:B:1940:ASN:HD21	1:B:1982:LYS:H	1.54	0.55
1:B:1955:GLY:HA2	1:B:1999:SER:HB3	1.88	0.55
1:A:2140:SER:HB3	1:A:2151:LYS:HE2	1.88	0.55
1:B:1516:ARG:NH2	1:B:1534:ASP:HA	2.22	0.55
1:B:2132:GLU:O	1:B:2136:ILE:HG12	2.07	0.55
1:A:1860:LEU:HD23	1:A:2115:TRP:CZ3	2.41	0.55
1:B:1556:GLU:O	1:B:1558:GLY:N	2.38	0.55
1:B:1643:TRP:CE3	1:B:1649:PRO:HB3	2.41	0.55
1:A:2142:GLN:HG2	1:A:2190:LYS:HZ1	1.71	0.55
1:B:2148:ARG:NH2	1:B:2152:ILE:HD11	2.22	0.55
1:A:1667:LYS:C	1:A:1669:PHE:N	2.59	0.55
1:B:2148:ARG:CZ	1:B:2152:ILE:HD11	2.37	0.55
1:A:2142:GLN:HG2	1:A:2190:LYS:NZ	2.22	0.55
1:B:1560:ASN:ND2	1:B:1560:ASN:H	2.05	0.55
1:B:2100:SER:HA	1:B:2103:MSE:HE3	1.88	0.54
1:B:2139:LEU:O	1:B:2141:HIS:N	2.40	0.54
1:A:2034:LYS:HB2	1:B:1631:MSE:CE	2.32	0.54
1:B:1948:MSE:HE3	1:B:1950:LEU:CG	2.37	0.54
1:B:1593:ILE:HB	1:B:1625:SER:OG	2.08	0.54
1:B:1620:TYR:HB3	1:B:1726:THR:HB	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1987:ILE:HB	1:B:2014:MSE:HG3	1.90	0.54
1:A:1968:LEU:HD21	1:B:1756:LEU:HD11	1.90	0.54
1:B:1829:ARG:NH2	1:B:2119:ARG:HE	2.06	0.54
1:B:2039:LYS:HZ2	1:B:2039:LYS:HB2	1.71	0.54
1:B:1505:THR:CB	1:B:1730:CYS:HB2	2.35	0.54
1:B:1922:GLN:HB2	1:B:1954:ARG:NH1	2.22	0.54
1:B:2037:ARG:NE	1:B:2083:LEU:HD11	2.21	0.54
1:A:2097:HIS:O	1:A:2102:ARG:HD3	2.08	0.54
1:A:1624:ASN:ND2	1:A:1733:VAL:H	2.05	0.54
1:A:2050:LYS:NZ	1:A:2078:ARG:HD3	2.23	0.54
1:B:2037:ARG:HE	1:B:2083:LEU:HD11	1.72	0.54
1:B:2158:TRP:NE1	1:B:2185:LYS:HE3	2.23	0.54
1:A:1918:GLN:O	1:A:1920:PRO:HD3	2.08	0.53
1:A:2196:GLN:NE2	1:A:2196:GLN:HA	2.22	0.53
1:B:1594:GLY:O	1:B:1624:ASN:HB2	2.08	0.53
1:B:1680:THR:HG22	1:B:1681:VAL:N	2.23	0.53
1:B:1730:CYS:C	1:B:1752:GLN:HG3	2.29	0.53
1:A:1735:ILE:N	1:A:1735:ILE:HD12	2.22	0.53
1:A:1946:PRO:HG3	1:A:2130:LEU:HD21	1.90	0.53
1:B:1741:ARG:HH22	1:B:1934:GLN:NE2	2.05	0.53
1:B:2075:LEU:O	1:B:2079:GLU:HG3	2.09	0.53
1:B:2164:ASP:C	1:B:2166:GLU:H	2.11	0.53
1:B:1966:GLU:HG2	1:B:1969:LYS:CE	2.38	0.53
1:B:2131:ASN:ND2	1:B:2179:TYR:OH	2.42	0.53
1:A:2167:ASP:OD1	1:A:2170:GLN:HB2	2.09	0.52
1:B:1592:LYS:O	1:B:1593:ILE:HG13	2.08	0.52
1:B:2046:ARG:C	1:B:2047:LEU:HD12	2.29	0.52
1:A:1883:ARG:HA	1:A:1887:ILE:O	2.08	0.52
1:A:1655:TYR:CE1	1:A:1689:VAL:HG12	2.44	0.52
1:A:1860:LEU:HD23	1:A:2115:TRP:CH2	2.45	0.52
1:B:1783:MSE:SE	1:B:1786:ASN:HD21	2.42	0.52
1:A:2052:ARG:HH11	1:A:2052:ARG:HG3	1.73	0.52
1:B:1922:GLN:CD	1:B:1954:ARG:HH12	2.12	0.52
1:B:1545:ASP:OD1	1:B:1549:GLU:N	2.42	0.52
1:B:2139:LEU:O	1:B:2140:SER:C	2.47	0.52
1:A:1548:GLY:O	1:A:1606:LYS:HE2	2.09	0.52
1:A:1820:ILE:HD12	1:A:1886:GLY:O	2.10	0.52
1:B:1537:PHE:CZ	1:B:1569:ILE:HD12	2.45	0.52
1:B:2147:SER:O	1:B:2148:ARG:C	2.48	0.52
1:A:2028:GLN:H	1:A:2028:GLN:CD	2.13	0.52
1:B:1952:ASN:OD1	1:B:1993:GLY:HA2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2082:LEU:CD1	1:B:2082:LEU:N	2.72	0.52
1:B:2148:ARG:O	1:B:2149:LEU:C	2.47	0.52
1:A:2124:TRP:CZ3	1:A:2169:ARG:HG3	2.45	0.52
1:B:2160:PRO:HD2	1:B:2163:VAL:HG21	1.90	0.52
1:A:1657:TYR:CE2	1:A:1687:ARG:HD2	2.44	0.52
1:A:1724:THR:H	1:A:1745:ARG:HH21	1.56	0.52
1:A:1727:LEU:HB2	1:A:1803:ILE:HD11	1.91	0.52
1:A:1877:VAL:HG23	1:A:1931:LYS:HD3	1.91	0.52
1:A:2142:GLN:HB3	1:A:2190:LYS:HZ2	1.74	0.52
1:A:1511:PHE:CZ	1:A:1729:THR:HG21	2.46	0.51
1:A:1508:VAL:HG21	1:A:1565:VAL:CG2	2.40	0.51
1:A:1655:TYR:CD1	1:A:1689:VAL:HG12	2.45	0.51
1:A:2127:ARG:NH2	1:A:2176:GLU:OE2	2.43	0.51
1:A:1673:ASN:N	1:A:1673:ASN:OD1	2.42	0.51
1:A:1881:ARG:HH11	1:A:1881:ARG:HG2	1.76	0.51
1:A:1846:MSE:HE2	1:A:2115:TRP:CH2	2.45	0.51
1:A:2099:ARG:NH1	1:A:2099:ARG:HG3	2.26	0.51
1:B:2035:PHE:CE2	1:B:2039:LYS:HG2	2.45	0.51
1:B:2139:LEU:HD21	1:B:2154:ARG:NH1	2.25	0.51
1:A:1679:ARG:HG3	1:A:1679:ARG:NH1	2.25	0.51
1:A:2143:VAL:HG12	1:A:2144:GLY:N	2.25	0.51
1:B:1954:ARG:NH1	1:B:1954:ARG:HG3	2.24	0.51
1:B:1940:ASN:ND2	1:B:1982:LYS:H	2.08	0.51
1:B:2010:ASP:OD2	1:B:2148:ARG:HG3	2.08	0.51
1:B:1528:ALA:O	1:B:1530:VAL:N	2.44	0.51
1:B:1917:ILE:HD12	1:B:1961:ARG:HH22	1.74	0.51
1:B:1713:GLY:O	1:B:1717:ARG:HG3	2.11	0.51
1:A:1963:MSE:HE3	1:B:1783:MSE:HE2	1.93	0.51
1:A:1667:LYS:O	1:A:1669:PHE:N	2.43	0.51
1:A:1754:ILE:HD12	1:A:1783:MSE:HG2	1.92	0.51
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	1.91	0.51
1:B:2055:ARG:HG3	1:B:2055:ARG:NH1	2.25	0.51
1:A:1991:PRO:HG3	1:A:2115:TRP:HB2	1.91	0.51
1:A:2022:ALA:HB3	1:A:2103:MSE:HE2	1.92	0.51
1:A:2191:LEU:HD23	1:A:2191:LEU:O	2.11	0.51
1:A:1705:LEU:HB3	1:B:2000:TRP:CD1	2.46	0.51
1:A:1790:HIS:HB3	1:A:1869:THR:CG2	2.41	0.50
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	2.09	0.50
1:A:1785:ASN:ND2	1:A:1785:ASN:N	2.56	0.50
1:B:1856:PHE:CD2	1:B:1863:LYS:HE2	2.45	0.50
1:A:2131:ASN:HD22	1:A:2175:ILE:CG2	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1785:ASN:HD22	1:B:1785:ASN:N	2.09	0.50
1:B:2119:ARG:HH11	1:B:2119:ARG:CG	2.24	0.50
1:B:1661:GLU:O	1:B:1664:GLU:N	2.44	0.50
1:A:1988:TYR:HA	1:A:2015:TYR:O	2.12	0.50
1:B:1584:VAL:HG22	1:B:1619:ILE:HB	1.91	0.50
1:A:1682:ILE:CG1	1:A:1683:ASN:N	2.74	0.50
1:B:1772:THR:HG23	1:B:1776:GLN:HE22	1.76	0.50
1:B:1663:MSE:HB2	1:B:1688:PHE:CE1	2.47	0.50
1:A:2085:ILE:O	1:A:2088:GLN:HB2	2.12	0.50
1:A:2167:ASP:HB3	1:A:2170:GLN:HB2	1.94	0.50
1:A:2102:ARG:HH11	1:B:1694:ILE:HG23	1.76	0.50
1:B:1936:ILE:HG12	1:B:1947:MSE:SE	2.61	0.50
1:A:1778:GLY:HA2	1:A:1783:MSE:HE2	1.93	0.50
1:A:2192:GLU:O	1:A:2196:GLN:HB2	2.11	0.49
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.59	0.49
1:A:1737:ALA:O	1:A:1740:VAL:CG1	2.60	0.49
1:B:1513:GLU:O	1:B:1517:GLN:HG3	2.11	0.49
1:B:1660:SER:HA	1:B:1688:PHE:HE1	1.77	0.49
1:B:1730:CYS:O	1:B:1731:ARG:HB3	2.13	0.49
1:A:1654:GLN:O	1:A:1655:TYR:HB3	2.12	0.49
1:A:1837:ASN:OD1	1:A:1992:THR:HG22	2.12	0.49
1:A:2017:ASP:OD2	1:A:2115:TRP:HB2	2.12	0.49
1:A:2193:SER:O	1:A:2195:ALA:N	2.46	0.49
1:A:2097:HIS:CE1	1:B:1632:ALA:H	2.30	0.49
1:A:1497:ARG:HD3	1:A:1510:ASP:OD2	2.12	0.49
1:B:1711:ILE:HD11	1:B:1735:ILE:HG12	1.95	0.49
1:B:1747:ILE:HD12	1:B:1747:ILE:N	2.27	0.49
1:B:1966:GLU:HG2	1:B:1969:LYS:HD2	1.94	0.49
1:A:1682:ILE:HG23	1:A:1687:ARG:HG3	1.94	0.49
1:A:1768:ARG:HD2	1:A:1770:VAL:HG22	1.94	0.49
1:A:2058:LEU:HD22	1:A:2068:HIS:CE1	2.46	0.49
1:B:1836:THR:HG22	1:B:1838:ASP:N	2.26	0.49
1:A:1494:GLN:OE1	1:A:1496:LYS:HG2	2.13	0.49
1:A:2041:LEU:HD12	1:A:2044:MSE:CE	2.42	0.49
1:B:1772:THR:HG23	1:B:1776:GLN:NE2	2.27	0.49
1:A:1744:GLN:HA	1:A:1744:GLN:NE2	2.28	0.49
1:B:2160:PRO:HD2	1:B:2163:VAL:CG2	2.43	0.49
1:A:1711:ILE:HD12	1:A:1739:LEU:HD11	1.94	0.49
1:A:1511:PHE:HZ	1:A:1729:THR:HG21	1.77	0.49
1:A:2125:ARG:HH12	1:A:2128:ARG:HH21	1.61	0.49
1:B:1748:GLN:O	1:B:1792:THR:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1495:PRO:HG2	1:B:1496:LYS:H	1.78	0.48
1:B:1994:GLU:HA	1:B:2021:ARG:O	2.13	0.48
1:A:1803:ILE:HG22	1:A:1807:MSE:CE	2.44	0.48
1:A:1963:MSE:HE1	1:B:1755:ILE:HA	1.94	0.48
1:A:1968:LEU:HD12	1:B:1783:MSE:HE1	1.96	0.48
1:A:1629:ILE:HG12	2:A:3203:ACO:C6A	2.43	0.48
1:B:1643:TRP:HA	1:B:1653:PHE:HA	1.95	0.48
1:B:1883:ARG:HA	1:B:1887:ILE:O	2.13	0.48
1:A:1841:TYR:CZ	1:A:1896:THR:HG21	2.48	0.48
1:B:1575:GLU:H	1:B:1575:GLU:CD	2.17	0.48
1:B:1682:ILE:HG13	1:B:1685:GLU:O	2.14	0.48
1:B:1676:LEU:HD12	1:B:1692:THR:HG21	1.95	0.48
1:B:1975:VAL:O	1:B:1979:VAL:HG23	2.12	0.48
1:A:1735:ILE:H	1:A:1735:ILE:CD1	2.22	0.48
1:A:2156:ARG:HG2	1:A:2159:TYR:CE1	2.49	0.48
1:B:1600:GLU:OE1	1:B:1600:GLU:N	2.45	0.48
1:A:2083:LEU:HD12	1:A:2083:LEU:HA	1.72	0.48
1:A:1748:GLN:O	1:A:1792:THR:HA	2.13	0.48
1:A:1508:VAL:HG21	1:A:1565:VAL:HG21	1.96	0.48
1:A:1651:LYS:HG3	1:A:1651:LYS:O	2.14	0.48
1:B:1625:SER:OG	1:B:1731:ARG:NH2	2.45	0.48
1:B:1645:ASP:O	1:B:1647:ALA:O	2.32	0.47
1:A:1484:ALA:O	1:A:1485:THR:O	2.32	0.47
1:A:1682:ILE:C	1:A:1684:GLY:N	2.68	0.47
1:A:1720:HIS:HD2	1:A:1941:ASN:ND2	2.13	0.47
1:A:1842:ASP:HA	1:A:1897:ARG:HH11	1.79	0.47
1:A:2082:LEU:HA	1:A:2085:ILE:HD13	1.96	0.47
1:B:1766:LEU:O	1:B:1767:GLY:C	2.52	0.47
1:B:2058:LEU:HD21	1:B:2071:ILE:HB	1.96	0.47
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.62	0.47
1:A:1909:ASN:HB3	1:A:1912:SER:HB2	1.96	0.47
1:B:1966:GLU:HG2	1:B:1969:LYS:CD	2.44	0.47
1:B:2138:ARG:HH11	1:B:2138:ARG:HG3	1.79	0.47
1:B:1985:ILE:HD12	1:B:2012:MSE:HG2	1.96	0.47
1:B:2164:ASP:C	1:B:2166:GLU:N	2.68	0.47
1:A:1689:VAL:HG23	1:A:1691:LYS:HE2	1.97	0.47
1:B:1598:PRO:HG2	1:B:1698:ASP:OD1	2.15	0.47
1:A:1522:GLN:NE2	1:A:1574:PRO:HD2	2.30	0.47
1:A:2197:ASP:O	1:A:2201:LYS:HB3	2.15	0.47
1:A:1508:VAL:CG2	1:A:1565:VAL:HG21	2.44	0.47
1:A:1842:ASP:OD1	1:A:1844:ARG:NH1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1583:VAL:HG22	1:B:1584:VAL:N	2.29	0.47
1:A:1667:LYS:NZ	1:A:1670:ASP:HA	2.29	0.47
1:A:2128:ARG:HD3	1:A:2171:VAL:HG11	1.97	0.47
1:A:2138:ARG:HB3	1:A:2138:ARG:NH1	2.29	0.47
1:B:1797:LEU:O	1:B:1801:GLU:HG3	2.15	0.47
1:B:2180:LYS:HZ2	1:B:2180:LYS:HB3	1.80	0.47
1:B:2041:LEU:HA	1:B:2044:MSE:HG3	1.97	0.47
1:B:1852:THR:C	1:B:1854:SER:H	2.18	0.46
1:A:2002:VAL:HG23	1:A:2003:VAL:HG13	1.97	0.46
1:B:1523:TRP:HB3	1:B:1530:VAL:HG21	1.98	0.46
1:B:1810:VAL:HG23	1:B:1811:PRO:CD	2.45	0.46
1:B:2078:ARG:CZ	1:B:2082:LEU:HD11	2.45	0.46
1:B:1682:ILE:C	1:B:1682:ILE:HD12	2.35	0.46
1:A:1881:ARG:NH1	1:A:1881:ARG:HG2	2.31	0.46
1:B:1940:ASN:ND2	1:B:1983:GLN:NE2	2.50	0.46
1:B:2064:ALA:HB3	1:B:2067:VAL:CG2	2.45	0.46
1:A:1681:VAL:HA	1:A:1685:GLU:O	2.15	0.46
1:A:2191:LEU:C	1:A:2191:LEU:CD2	2.83	0.46
1:A:2143:VAL:O	1:A:2145:GLU:N	2.49	0.46
1:B:1499:LYS:NZ	1:B:1499:LYS:HB2	2.31	0.46
1:B:2139:LEU:HD11	1:B:2154:ARG:HH11	1.81	0.46
1:B:1917:ILE:O	1:B:1917:ILE:HG12	2.14	0.46
1:A:2196:GLN:NE2	1:A:2196:GLN:CA	2.77	0.46
1:B:1514:LEU:HD22	1:B:1797:LEU:HD13	1.97	0.46
1:B:1729:THR:HG22	1:B:1796:ASP:OD1	2.16	0.46
1:B:1759:ALA:N	1:B:1760:PRO:CD	2.79	0.46
1:A:1657:TYR:HB2	1:A:1688:PHE:O	2.16	0.46
1:A:1963:MSE:CE	1:B:1755:ILE:HA	2.46	0.46
1:B:1906:ASP:H	1:B:1912:SER:HB2	1.80	0.46
1:A:1730:CYS:O	1:A:1731:ARG:HB3	2.16	0.45
1:A:2110:SER:O	1:A:2111:LYS:HG3	2.16	0.45
1:A:2102:ARG:NH2	1:B:1700:LEU:HB2	2.31	0.45
1:B:1733:VAL:HG22	1:B:1755:ILE:CD1	2.44	0.45
1:B:1906:ASP:H	1:B:1912:SER:CB	2.29	0.45
1:A:1575:GLU:HG2	1:A:1576:TYR:CD1	2.51	0.45
1:A:2037:ARG:CB	1:A:2037:ARG:HH11	2.20	0.45
1:A:2148:ARG:HG2	1:A:2148:ARG:NH1	2.32	0.45
1:B:1901:ASN:HB3	1:B:1917:ILE:HG23	1.99	0.45
1:A:1619:ILE:HD12	1:A:1725:ILE:CG2	2.45	0.45
1:B:1671:LYS:C	1:B:1673:ASN:H	2.20	0.45
1:B:1985:ILE:HD12	1:B:2012:MSE:CG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1903:ILE:HD12	1:A:1903:ILE:N	2.32	0.45
1:B:2108:VAL:HG23	1:B:2109:ILE:HG23	1.99	0.45
1:A:2021:ARG:HE	1:A:2095:ASP:CG	2.20	0.45
1:A:2129:ARG:HG3	1:A:2129:ARG:HH11	1.82	0.45
1:A:2030:MSE:HG3	1:B:1631:MSE:HE2	1.99	0.45
1:B:2044:MSE:HB3	1:B:2044:MSE:HE3	1.84	0.45
1:B:2126:LEU:HD22	1:B:2130:LEU:HD13	1.99	0.45
1:A:1720:HIS:HD2	1:A:1941:ASN:HD21	1.63	0.45
1:A:1901:ASN:O	1:A:1916:LEU:HD12	2.16	0.45
1:B:2188:GLY:C	1:B:2189:LEU:HD23	2.36	0.45
1:A:1612:ARG:O	1:A:1814:ARG:NH2	2.37	0.45
1:A:1610:TYR:CE1	1:A:1614:ARG:CZ	3.00	0.45
1:A:1667:LYS:HD3	1:A:1667:LYS:O	2.17	0.45
1:A:1784:TYR:CD1	1:A:1792:THR:HG23	2.51	0.45
1:A:1956:PHE:HB2	1:B:1756:LEU:HD23	1.99	0.44
1:B:1593:ILE:HB	1:B:1625:SER:HG	1.82	0.44
1:B:1903:ILE:HA	1:B:1904:PRO:HD3	1.77	0.44
1:B:1951:ALA:O	1:B:1990:PRO:HD2	2.18	0.44
1:B:2142:GLN:C	1:B:2142:GLN:CD	2.75	0.44
1:B:1744:GLN:O	1:B:1790:HIS:CE1	2.70	0.44
1:B:1874:ALA:HB2	1:B:1927:ASN:HB2	1.98	0.44
1:A:1708:SER:OG	1:A:1735:ILE:HG12	2.18	0.44
1:A:1803:ILE:HG22	1:A:1807:MSE:HE2	2.00	0.44
1:A:1991:PRO:O	1:A:2019:ASN:O	2.34	0.44
1:A:1996:ARG:NE	1:A:2026:GLU:HG2	2.32	0.44
1:B:1657:TYR:HB2	1:B:1688:PHE:O	2.18	0.44
1:B:2126:LEU:CD2	1:B:2130:LEU:HD13	2.48	0.44
1:B:1818:VAL:O	1:B:1820:ILE:HD12	2.17	0.44
1:A:1713:GLY:O	1:A:1717:ARG:HG3	2.18	0.44
1:B:1877:VAL:HG12	1:B:1878:VAL:N	2.33	0.44
1:B:1496:LYS:HB3	1:B:1507:TYR:CE2	2.53	0.44
1:B:1532:LEU:HD13	1:B:1536:PHE:CE1	2.52	0.44
1:A:2000:TRP:CD1	1:B:1705:LEU:HB3	2.53	0.44
1:B:2082:LEU:HB3	1:B:2086:TYR:CD1	2.53	0.44
1:A:2066:GLU:H	1:A:2066:GLU:CD	2.21	0.44
1:B:1657:TYR:CD2	1:B:1687:ARG:CB	2.99	0.44
1:B:1783:MSE:HA	1:B:1786:ASN:ND2	2.33	0.44
1:A:2144:GLY:O	1:A:2145:GLU:C	2.55	0.43
1:B:1640:GLN:O	1:B:1656:LEU:HA	2.17	0.43
1:B:1669:PHE:CD2	1:B:1669:PHE:N	2.86	0.43
1:B:2047:LEU:N	1:B:2047:LEU:HD12	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1735:ILE:O	1:A:1739:LEU:HG	2.18	0.43
1:A:2072:SER:O	1:A:2075:LEU:HB3	2.18	0.43
1:B:1594:GLY:O	1:B:1624:ASN:CB	2.66	0.43
1:B:1844:ARG:HH11	1:B:1844:ARG:HG3	1.82	0.43
1:B:2100:SER:CA	1:B:2103:MSE:HE3	2.48	0.43
1:B:1607:VAL:O	1:B:1610:TYR:HB3	2.17	0.43
1:B:2070:GLN:HG3	1:B:2074:GLN:NE2	2.33	0.43
1:B:1602:GLU:O	1:B:1606:LYS:HB2	2.18	0.43
1:B:1644:ASN:OD1	1:B:1651:LYS:O	2.37	0.43
1:A:1903:ILE:HA	1:A:1904:PRO:HD3	1.86	0.43
1:B:1676:LEU:HD12	1:B:1692:THR:CG2	2.48	0.43
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.48	0.43
1:B:1827:TRP:CD2	1:B:1828:ASP:N	2.87	0.43
1:B:1829:ARG:CZ	1:B:2119:ARG:NE	2.74	0.43
1:A:1895:GLU:HA	1:A:1895:GLU:OE2	2.18	0.43
1:A:1990:PRO:HB2	1:A:1991:PRO:HD2	2.01	0.43
1:A:2197:ASP:O	1:A:2200:LYS:O	2.36	0.43
1:B:1644:ASN:ND2	1:B:1654:GLN:HE21	2.03	0.43
1:B:1895:GLU:OE2	1:B:1897:ARG:NH2	2.35	0.43
1:A:1566:ALA:HA	1:A:1584:VAL:O	2.19	0.43
1:A:2138:ARG:C	1:A:2140:SER:H	2.22	0.43
1:A:2165:HIS:ND1	1:A:2165:HIS:N	2.65	0.43
1:B:1881:ARG:HH11	1:B:1881:ARG:HG3	1.83	0.43
1:A:1735:ILE:HG23	1:B:2001:VAL:HG21	2.00	0.43
1:A:1511:PHE:N	1:A:1512:PRO:CD	2.82	0.43
1:A:2198:LEU:C	1:A:2198:LEU:HD23	2.37	0.43
1:B:1617:PRO:HG2	1:B:1807:MSE:HE3	2.00	0.43
1:B:1865:SER:O	1:B:1882:ALA:HA	2.18	0.43
1:A:1702:VAL:HA	1:A:1705:LEU:HD22	2.01	0.43
1:B:1660:SER:HA	1:B:1688:PHE:CE1	2.53	0.43
1:A:1747:ILE:HD12	1:A:1803:ILE:HG13	2.02	0.42
1:B:1785:ASN:HA	1:B:1872:GLY:O	2.19	0.42
1:B:1541:GLU:HA	1:B:1567:PHE:HD2	1.84	0.42
1:B:1728:VAL:HG12	1:B:1752:GLN:HB3	2.01	0.42
1:A:1783:MSE:HB3	1:A:1789:SER:OG	2.20	0.42
1:A:2154:ARG:O	1:A:2157:SER:OG	2.38	0.42
1:B:1786:ASN:C	1:B:1786:ASN:OD1	2.57	0.42
1:B:2070:GLN:OE1	1:B:2070:GLN:HA	2.19	0.42
1:A:1702:VAL:HA	1:A:1705:LEU:HB2	2.00	0.42
1:B:1765:MSE:C	1:B:1766:LEU:HD12	2.39	0.42
1:B:2082:LEU:O	1:B:2083:LEU:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1681:VAL:O	1:B:1681:VAL:HG22	2.20	0.42
1:A:2052:ARG:HH11	1:A:2052:ARG:CG	2.32	0.42
1:B:2179:TYR:O	1:B:2183:ASP:HB2	2.20	0.42
1:B:1644:ASN:HD21	1:B:1654:GLN:NE2	2.05	0.42
1:B:1836:THR:O	1:B:1838:ASP:N	2.52	0.42
1:B:2083:LEU:HA	1:B:2083:LEU:HD23	1.90	0.42
1:A:2108:VAL:HG11	1:B:1702:VAL:HG23	2.01	0.42
1:A:1638:LEU:CD1	1:A:1658:LEU:HD22	2.50	0.41
1:A:1819:PRO:O	1:A:1888:PRO:HG3	2.20	0.41
1:A:1901:ASN:ND2	1:A:1903:ILE:HD11	2.35	0.41
1:A:1952:ASN:HA	1:A:1994:GLU:O	2.20	0.41
1:A:1981:TYR:CG	1:A:1985:ILE:HD11	2.55	0.41
1:B:1831:VAL:HG22	1:B:2119:ARG:HB2	2.02	0.41
1:A:1659:THR:O	1:A:1660:SER:C	2.57	0.41
1:B:1702:VAL:HA	1:B:1705:LEU:HD12	2.01	0.41
1:B:1766:LEU:CD1	1:B:1766:LEU:N	2.84	0.41
1:B:1813:LYS:HG3	1:B:1816:MSE:HG2	2.02	0.41
1:B:1881:ARG:HG3	1:B:1881:ARG:NH1	2.36	0.41
1:B:1998:GLY:O	1:B:2001:VAL:CG1	2.68	0.41
1:B:2148:ARG:NE	1:B:2152:ILE:HD11	2.36	0.41
1:A:1686:GLU:C	1:A:1687:ARG:HG2	2.40	0.41
1:A:1737:ALA:O	1:A:1740:VAL:HG13	2.20	0.41
1:A:1785:ASN:HA	1:A:1872:GLY:O	2.20	0.41
1:A:1800:VAL:O	1:A:1804:VAL:HG23	2.20	0.41
1:A:1680:THR:CG2	1:A:1681:VAL:N	2.82	0.41
1:A:1680:THR:HB	1:A:1687:ARG:O	2.21	0.41
1:B:1643:TRP:CZ3	1:B:1649:PRO:HB3	2.56	0.41
1:A:1643:TRP:CH2	1:A:1649:PRO:HB3	2.55	0.41
1:A:1686:GLU:O	1:A:1687:ARG:HG2	2.21	0.41
1:A:2078:ARG:HA	1:A:2081:GLU:HG2	2.02	0.41
1:B:1702:VAL:HG23	1:B:1703:GLU:N	2.36	0.41
1:A:1836:THR:O	1:A:1838:ASP:N	2.46	0.41
1:B:1671:LYS:C	1:B:1673:ASN:N	2.74	0.41
1:B:1834:THR:HA	1:B:1835:PRO:HD3	1.83	0.41
1:B:1842:ASP:OD1	1:B:1844:ARG:HG3	2.20	0.41
1:A:1526:PHE:C	1:A:1526:PHE:CD1	2.94	0.41
1:A:2108:VAL:HG23	1:A:2109:ILE:HG23	2.03	0.41
1:B:1615:GLY:HA2	1:B:1814:ARG:NH1	2.36	0.41
1:B:1755:ILE:CD1	1:B:1755:ILE:N	2.83	0.41
1:A:2022:ALA:O	1:A:2098:ASP:HA	2.21	0.41
1:B:1619:ILE:N	1:B:1619:ILE:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2102:ARG:NH1	1:B:1694:ILE:HG23	2.36	0.41
1:B:1968:LEU:HB2	4:B:5028:HOH:O	2.20	0.41
1:A:1783:MSE:HG3	1:A:1788:VAL:HB	2.02	0.41
1:A:1832:ASP:HB2	1:A:1858:TYR:N	2.35	0.40
1:B:1852:THR:O	1:B:1854:SER:N	2.49	0.40
1:B:2061:LYS:O	1:B:2062:SER:HB3	2.21	0.40
1:B:2091:LEU:HA	1:B:2091:LEU:HD12	1.90	0.40
1:B:2136:ILE:HD13	1:B:2155:ILE:HD12	2.03	0.40
1:B:2140:SER:O	1:B:2142:GLN:N	2.54	0.40
1:A:1618:ARG:C	1:A:1618:ARG:HE	2.24	0.40
1:A:1869:THR:HG22	1:A:1870:LEU:N	2.36	0.40
1:A:2056:SER:O	1:A:2060:ASN:N	2.54	0.40
1:A:2125:ARG:HH12	1:A:2128:ARG:NH2	2.20	0.40
1:A:2167:ASP:CG	1:A:2170:GLN:HB2	2.42	0.40
1:B:1668:LYS:HD3	1:B:1668:LYS:HA	1.91	0.40
1:B:1728:VAL:O	1:B:1749:VAL:HG23	2.21	0.40
1:A:1968:LEU:HD12	1:B:1783:MSE:CE	2.52	0.40
1:B:2144:GLY:O	1:B:2145:GLU:C	2.59	0.40
1:A:1803:ILE:CG2	1:A:1807:MSE:HE2	2.51	0.40
1:B:1902:LEU:HD21	1:B:1914:GLU:CD	2.42	0.40
1:B:2187:LYS:C	1:B:2189:LEU:H	2.24	0.40
1:A:1530:VAL:HG23	1:A:1530:VAL:O	2.20	0.40
1:B:1545:ASP:O	1:B:1548:GLY:N	2.45	0.40
1:B:2052:ARG:HG2	1:B:2052:ARG:HH11	1.87	0.40
1:B:2178:ASN:HD22	1:B:2181:THR:CB	2.34	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	718/805 (89%)	640 (89%)	61 (8%)	17 (2%)	6 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	694/805 (86%)	608 (88%)	61 (9%)	25 (4%)	3	7
All	All	1412/1610 (88%)	1248 (88%)	122 (9%)	42 (3%)	4	10

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1683	ASN
1	A	1991	PRO
1	A	2144	GLY
1	A	2194	PHE
1	B	1838	ASP
1	B	1991	PRO
1	B	1992	THR
1	A	1679	ARG
1	A	1997	GLY
1	A	2142	GLN
1	B	1529	ASP
1	B	1683	ASN
1	B	1684	GLY
1	B	2140	SER
1	B	2141	HIS
1	B	2143	VAL
1	B	2165	HIS
1	A	1485	THR
1	A	1668	LYS
1	A	1744	GLN
1	B	1526	PHE
1	B	2061	LYS
1	B	2084	PRO
1	B	2148	ARG
1	A	1527	SER
1	A	1826	THR
1	A	2161	ALA
1	B	1558	GLY
1	B	1837	ASN
1	A	1731	ARG
1	A	2139	LEU
1	B	1731	ARG
1	B	1853	GLU
1	A	1682	ILE
1	B	1508	VAL
1	B	1534	ASP

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Mol	Chain	Res	Type
1	B	2038	GLU
1	B	2145	GLU
1	A	2143	VAL
1	B	1843	VAL
1	B	2144	GLY
1	B	1557	PRO

5.3.2 Protein sidechains [i](#)

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	612/668 (92%)	556 (91%)	56 (9%)	9 21
1	B	591/668 (88%)	539 (91%)	52 (9%)	10 23
All	All	1203/1336 (90%)	1095 (91%)	108 (9%)	9 22

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1514	LEU
1	A	1532	LEU
1	A	1541	GLU
1	A	1554	GLU
1	A	1560	ASN
1	A	1570	THR
1	A	1580	ARG
1	A	1589	ILE
1	A	1602	GLU
1	A	1618	ARG
1	A	1634	GLU
1	A	1650	ASP
1	A	1667	LYS
1	A	1673	ASN
1	A	1675	VAL
1	A	1697	GLU
1	A	1705	LEU

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Mol	Chain	Res	Type
1	A	1706	ARG
1	A	1733	VAL
1	A	1735	ILE
1	A	1757	THR
1	A	1772	THR
1	A	1780	THR
1	A	1781	GLN
1	A	1783	MSE
1	A	1785	ASN
1	A	1786	ASN
1	A	1813	LYS
1	A	1821	LEU
1	A	1823	THR
1	A	1860	LEU
1	A	1877	VAL
1	A	1879	VAL
1	A	1884	LEU
1	A	1895	GLU
1	A	1924	TRP
1	A	1991	PRO
1	A	1999	SER
1	A	2001	VAL
1	A	2008	ASN
1	A	2028	GLN
1	A	2035	PHE
1	A	2037	ARG
1	A	2038	GLU
1	A	2085	ILE
1	A	2126	LEU
1	A	2128	ARG
1	A	2145	GLU
1	A	2163	VAL
1	A	2165	HIS
1	A	2179	TYR
1	A	2183	ASP
1	A	2190	LYS
1	A	2192	GLU
1	A	2194	PHE
1	A	2201	LYS
1	B	1499	LYS
1	B	1513	GLU
1	B	1527	SER

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Mol	Chain	Res	Type
1	B	1534	ASP
1	B	1540	ASN
1	B	1553	VAL
1	B	1555	ARG
1	B	1560	ASN
1	B	1568	LYS
1	B	1575	GLU
1	B	1602	GLU
1	B	1618	ARG
1	B	1621	LEU
1	B	1638	LEU
1	B	1675	VAL
1	B	1726	THR
1	B	1739	LEU
1	B	1755	ILE
1	B	1757	THR
1	B	1768	ARG
1	B	1772	THR
1	B	1781	GLN
1	B	1810	VAL
1	B	1839	GLU
1	B	1891	VAL
1	B	1902	LEU
1	B	1910	PRO
1	B	1917	ILE
1	B	1923	VAL
1	B	1924	TRP
1	B	1980	ASP
1	B	1981	TYR
1	B	1991	PRO
1	B	1996	ARG
1	B	2001	VAL
1	B	2026	GLU
1	B	2027	PRO
1	B	2035	PHE
1	B	2037	ARG
1	B	2044	MSE
1	B	2055	ARG
1	B	2063	LEU
1	B	2088	GLN
1	B	2091	LEU
1	B	2092	GLN

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Mol	Chain	Res	Type
1	B	2125	ARG
1	B	2126	LEU
1	B	2128	ARG
1	B	2130	LEU
1	B	2142	GLN
1	B	2166	GLU
1	B	2182	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1501	HIS
1	A	1560	ASN
1	A	1599	GLN
1	A	1624	ASN
1	A	1640	GLN
1	A	1654	GLN
1	A	1720	HIS
1	A	1744	GLN
1	A	1748	GLN
1	A	1785	ASN
1	A	1786	ASN
1	A	1790	HIS
1	A	1815	ASN
1	A	1901	ASN
1	A	1909	ASN
1	A	1934	GLN
1	A	1941	ASN
1	A	1983	GLN
1	A	2008	ASN
1	A	2011	GLN
1	A	2045	ASN
1	A	2060	ASN
1	A	2097	HIS
1	A	2131	ASN
1	A	2178	ASN
1	A	2196	GLN
1	B	1525	ASN
1	B	1540	ASN
1	B	1560	ASN
1	B	1581	GLN
1	B	1587	ASN

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Mol	Chain	Res	Type
1	B	1605	ASN
1	B	1624	ASN
1	B	1644	ASN
1	B	1744	GLN
1	B	1748	GLN
1	B	1776	GLN
1	B	1785	ASN
1	B	1925	HIS
1	B	1934	GLN
1	B	1940	ASN
1	B	2057	GLN
1	B	2074	GLN
1	B	2097	HIS
1	B	2131	ASN
1	B	2141	HIS
1	B	2178	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADE	B	3190	-	9,11,11	1.53	2 (22%)	7,15,15	0.92	0
2	ACO	A	3203	-	41,50,53	1.22	4 (9%)	52,75,79	1.65	6 (11%)

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
3	ADE	B	3190	-	-	-	0/2/2/2
2	ACO	A	3203	-	-	9/44/64/67	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3190	ADE	C2-N3	3.30	1.37	1.32
2	A	3203	ACO	C2A-N3A	3.06	1.37	1.32
2	A	3203	ACO	C4A-N3A	2.84	1.39	1.35
3	B	3190	ADE	C4-N9	2.48	1.39	1.34
2	A	3203	ACO	C8A-N7A	-2.34	1.30	1.34
2	A	3203	ACO	C9P-N8P	2.06	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3203	ACO	C3P-N4P-C5P	5.53	133.10	122.84
2	A	3203	ACO	O6A-CCP-CBP	5.46	119.33	110.55
2	A	3203	ACO	P2A-O3A-P1A	-3.42	121.08	132.83
2	A	3203	ACO	C2P-C3P-N4P	-3.36	104.64	112.31
2	A	3203	ACO	O2B-C2B-C3B	2.09	117.09	111.17
2	A	3203	ACO	CEP-CBP-CAP	2.07	112.41	108.82

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3203	ACO	C5B-O5B-P1A-O1A
2	A	3203	ACO	C5B-O5B-P1A-O2A
2	A	3203	ACO	CBP-CCP-O6A-P2A
2	A	3203	ACO	N8P-C9P-CAP-CBP

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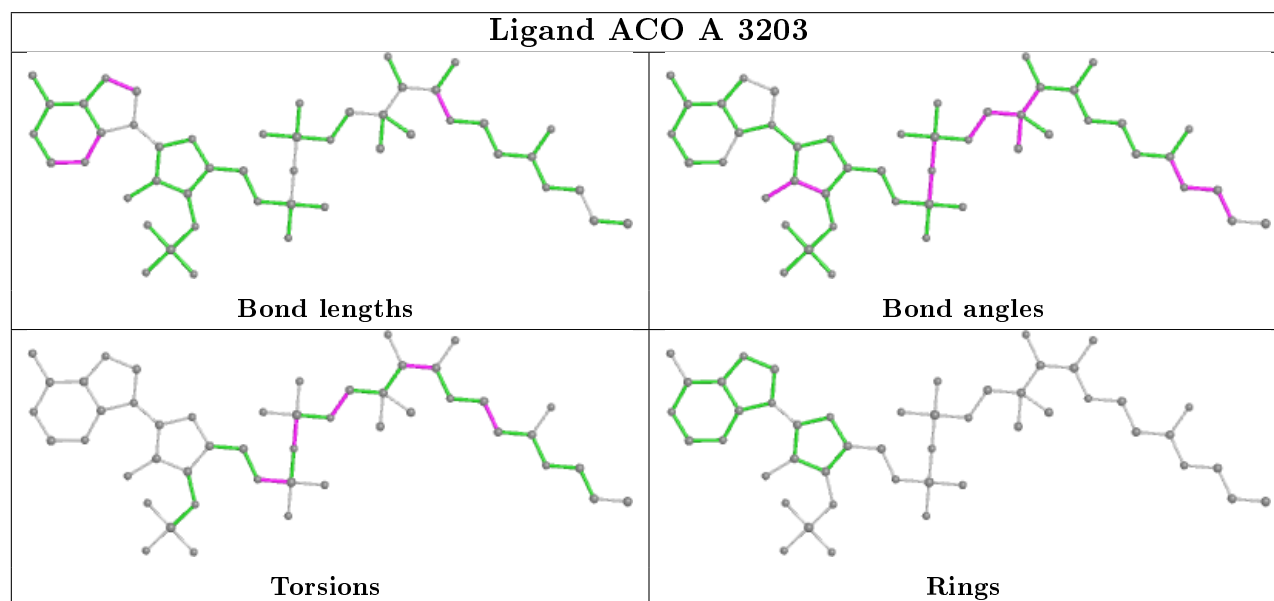
Mol	Chain	Res	Type	Atoms
2	A	3203	ACO	P1A-O3A-P2A-O5A
2	A	3203	ACO	C5P-C6P-C7P-N8P
2	A	3203	ACO	O9P-C9P-CAP-CBP
2	A	3203	ACO	C5B-O5B-P1A-O3A
2	A	3203	ACO	P1A-O3A-P2A-O4A

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3203	ACO	4	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	703/805 (87%)	-0.01	22 (3%) 49 49	22, 37, 58, 74	0
1	B	679/805 (84%)	-0.05	19 (2%) 53 54	20, 38, 59, 69	0
All	All	1382/1610 (85%)	-0.03	41 (2%) 50 51	20, 38, 59, 74	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2143	VAL	7.9
1	A	2194	PHE	5.1
1	A	2146	ALA	4.5
1	A	2203	ARG	4.3
1	A	2201	LYS	4.2
1	B	1529	ASP	4.0
1	A	2198	LEU	3.9
1	B	1681	VAL	3.7
1	B	1527	SER	3.6
1	B	2144	GLY	3.5
1	A	2145	GLU	3.5
1	A	2191	LEU	3.3
1	B	2190	LYS	3.2
1	B	1839	GLU	3.2
1	A	2143	VAL	3.0
1	A	2199	ALA	2.9
1	B	1682	ILE	2.8
1	A	1683	ASN	2.8
1	B	1498	TYR	2.8
1	A	2195	ALA	2.8
1	B	1726	THR	2.7
1	A	1855	GLY	2.7
1	A	1547	ASN	2.6
1	A	2144	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1578	ARG	2.5
1	B	1621	LEU	2.5
1	A	1681	VAL	2.4
1	A	2197	ASP	2.4
1	A	1684	GLY	2.4
1	B	1547	ASN	2.2
1	B	1585	VAL	2.2
1	B	1502	LEU	2.2
1	A	1889	LEU	2.2
1	B	1497	ARG	2.2
1	B	1556	GLU	2.1
1	A	2141	HIS	2.1
1	B	1620	TYR	2.1
1	B	1852	THR	2.1
1	B	1584	VAL	2.1
1	A	1529	ASP	2.0
1	A	1910	PRO	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](#)

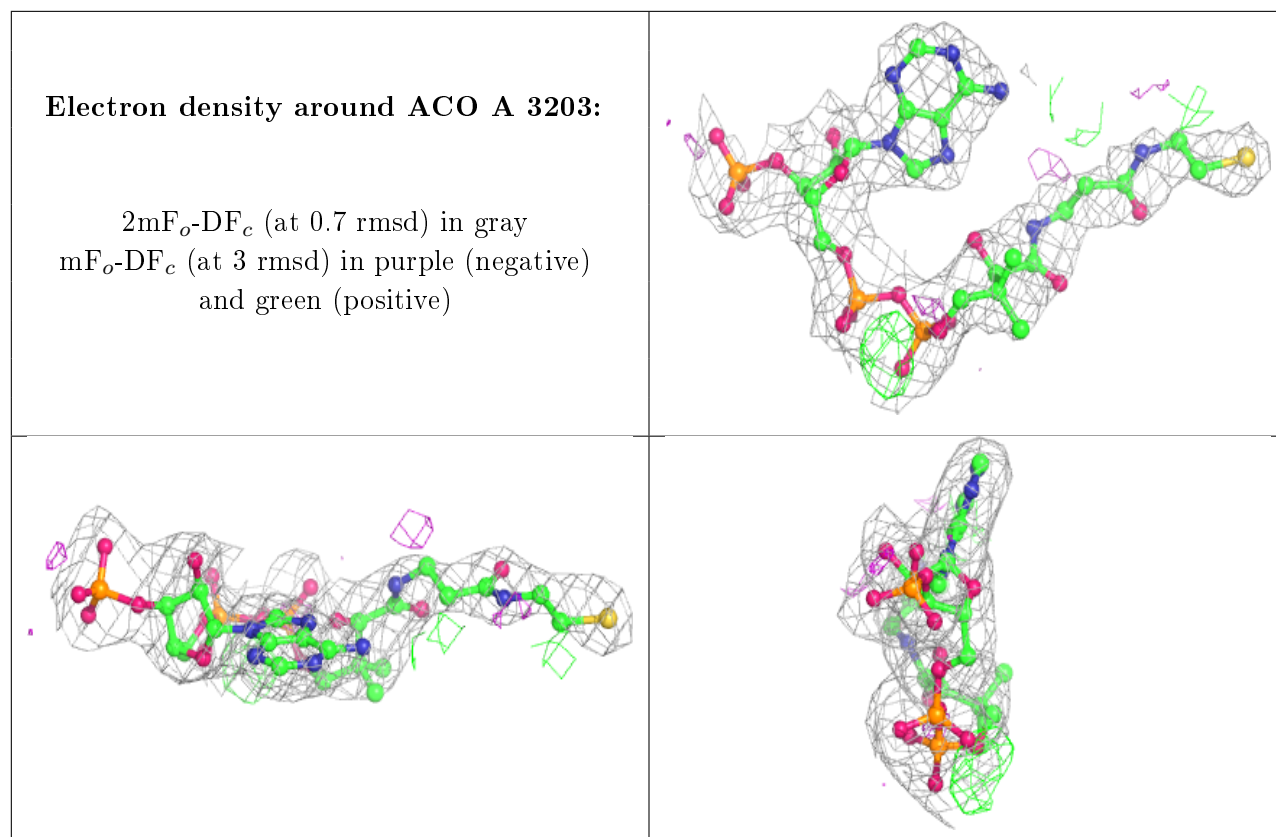
There are no carbohydrates in this entry.

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
3	ADE	B	3190	10/10	0.85	0.28	61,63,63,64	0
2	ACO	A	3203	48/51	0.91	0.17	56,68,77,79	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.