



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:09 PM UTC

PDB ID : 8G4U / pdb_00008g4u
Title : Final ketosynthase+acyltransferase of the erythromycin modular polyketide synthase
Authors : Keatinge-Clay, A.T.
Deposited on : 2023-02-10
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

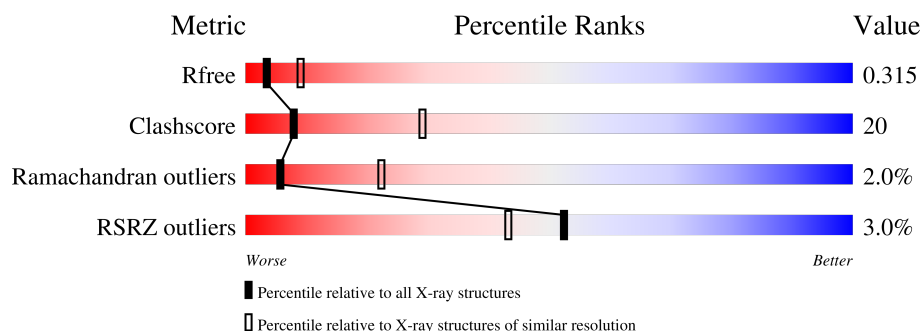
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	881	0% 57% 34% 7%
1	B	881	2% 52% 35% 11%
1	C	881	5% 54% 30% 15%
1	D	881	2% 59% 33% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22987 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 EryAIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	818	Total	C	N	O	S	0	0	0
			5950	3723	1077	1131	19			
1	B	786	Total	C	N	O	S	0	0	0
			5696	3567	1032	1079	18			
1	C	750	Total	C	N	O	S	0	0	0
			5423	3396	990	1021	16			
1	D	815	Total	C	N	O	S	0	0	0
			5910	3696	1072	1123	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1480	GLY	-	expression tag	UNP Q5UNP4
A	1481	SER	-	expression tag	UNP Q5UNP4
A	1482	HIS	-	expression tag	UNP Q5UNP4
A	1483	MET	-	expression tag	UNP Q5UNP4
A	2357	GLN	ALA	engineered mutation	UNP Q5UNP4
B	1480	GLY	-	expression tag	UNP Q5UNP4
B	1481	SER	-	expression tag	UNP Q5UNP4
B	1482	HIS	-	expression tag	UNP Q5UNP4
B	1483	MET	-	expression tag	UNP Q5UNP4
B	2357	GLN	ALA	engineered mutation	UNP Q5UNP4
C	1480	GLY	-	expression tag	UNP Q5UNP4
C	1481	SER	-	expression tag	UNP Q5UNP4
C	1482	HIS	-	expression tag	UNP Q5UNP4
C	1483	MET	-	expression tag	UNP Q5UNP4
C	2357	GLN	ALA	engineered mutation	UNP Q5UNP4
D	1480	GLY	-	expression tag	UNP Q5UNP4
D	1481	SER	-	expression tag	UNP Q5UNP4
D	1482	HIS	-	expression tag	UNP Q5UNP4
D	1483	MET	-	expression tag	UNP Q5UNP4
D	2357	GLN	ALA	engineered mutation	UNP Q5UNP4

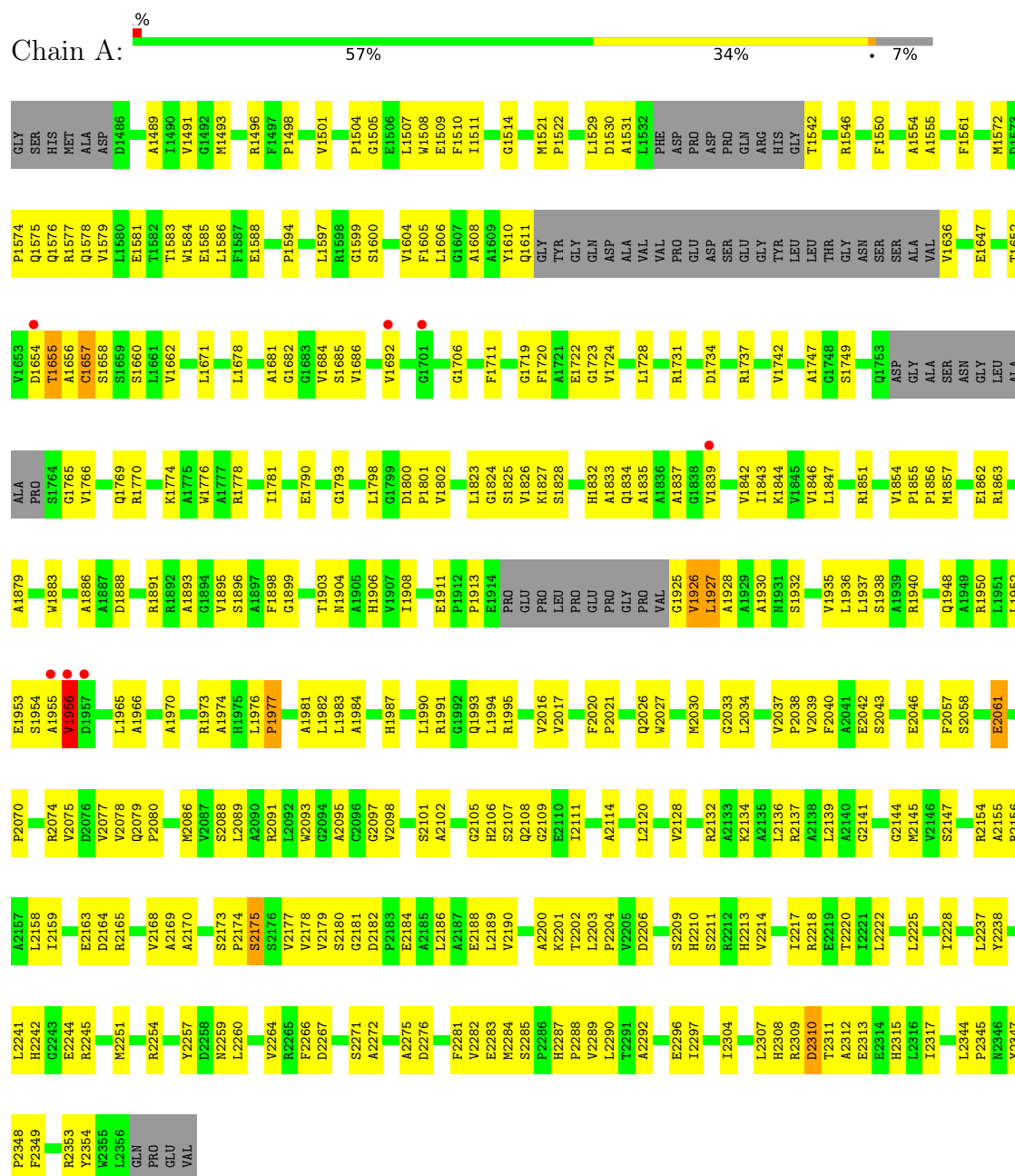
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	O 1	0	0
2	B	3	Total 3	O 3	0	0
2	C	3	Total 3	O 3	0	0
2	D	1	Total 1	O 1	0	0

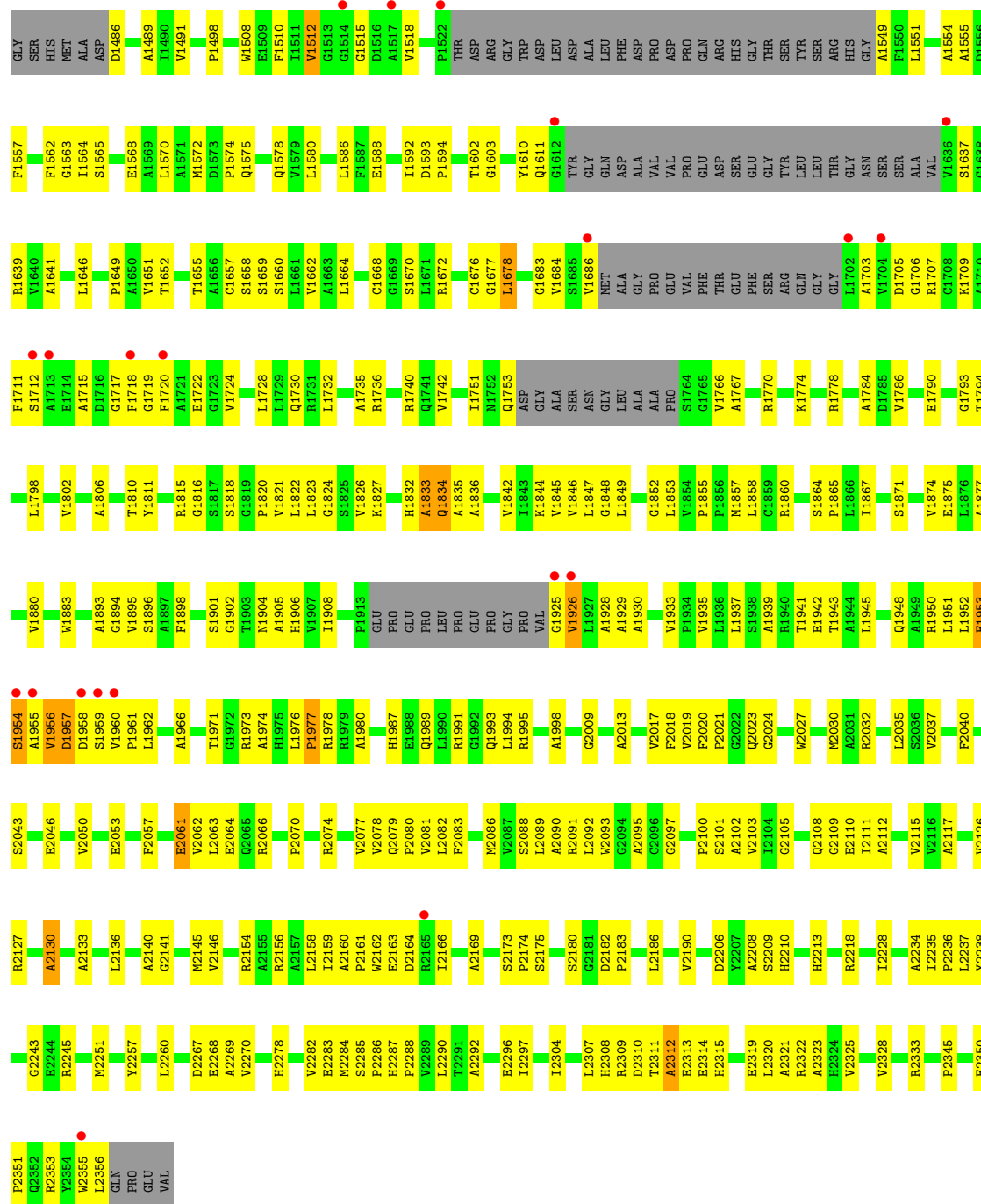
3 Residue-property plots

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

• Molecule 1: EryAIII

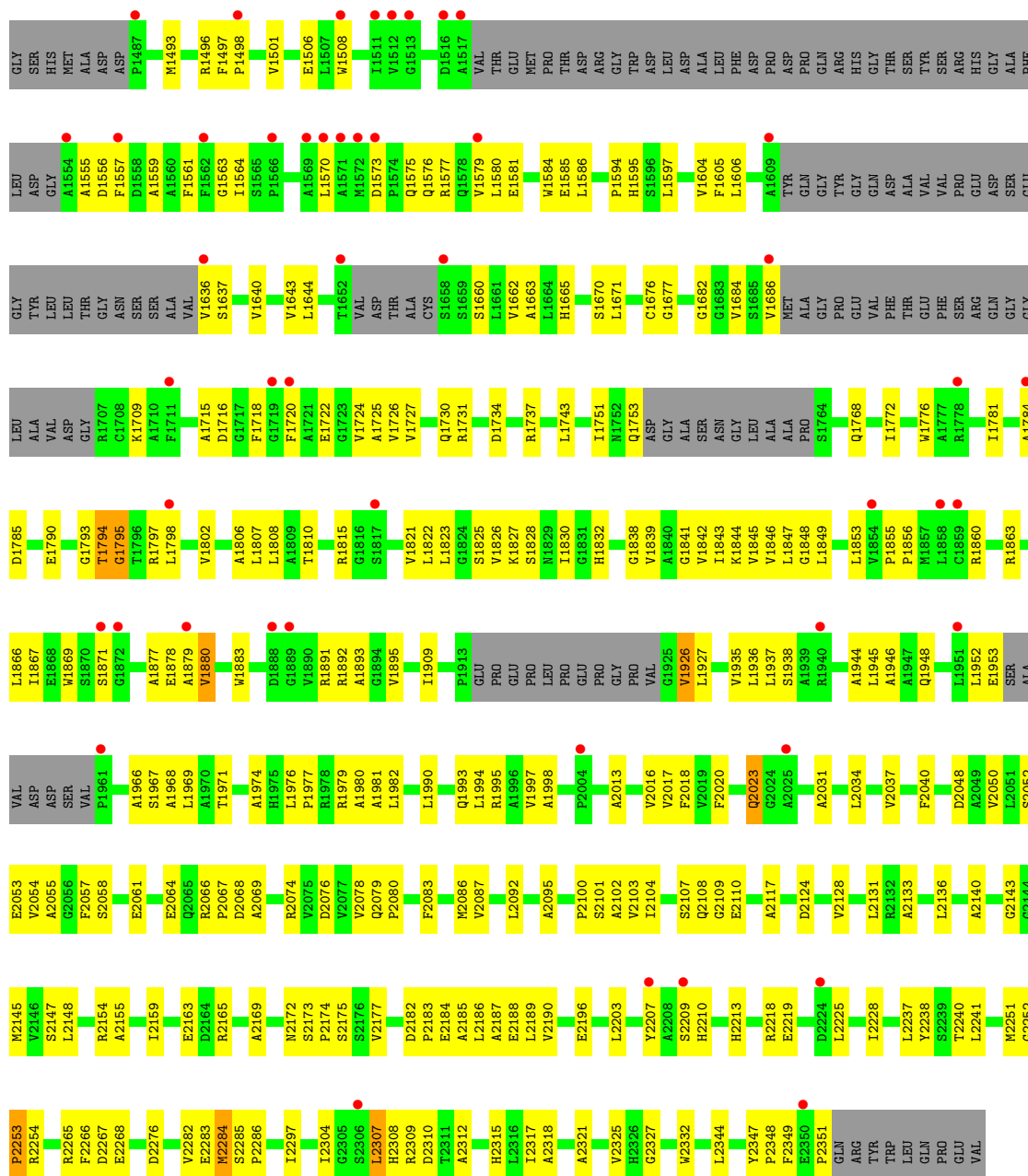


• Molecule 1: EryAIII

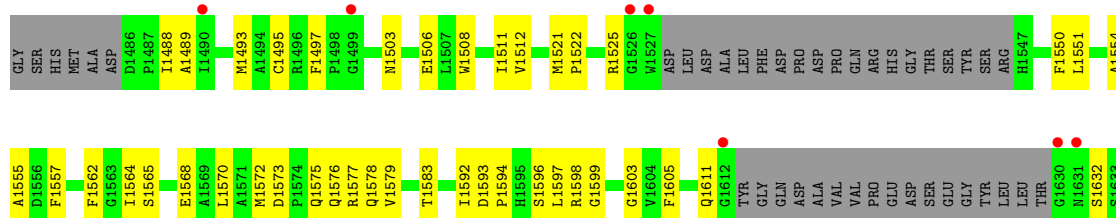


• Molecule 1: EryAIII





• Molecule 1: EryAIII



L2344	L2225	V2119	V2016	PRO	P1820	L1732	A1634
E2350	R2231	D2124	V2017	VAL	V1821	A1735	V1635
R2353	R2232	G2125	F2018	V1925	L1822	R1736	R1639
W2355	L2237	V2126	V2019	V1926	L1823	G1824	V1643
L2356	Y2238	R2127	F2020	L1927	S1825	G1739	E1647
G1N	Y2354	V2128	Q2026	V1933	V1826	R1740	G1648
PRO	W2239	V2129	W2027	P1934	A1835	L1743	P1649
GLU	T2240	A2130	E2028	V1935	G1838	G1748	T1652
VAL	L2131	L2131	G2029	L1937	V1839	S1749	T1655
	L2136	R2137	M2030	S1938	V1842	N1752	A1656
	A2249	R2137	A2031	G1939	I1843	Q1753	C1657
	D2250	G2141	R2032	R1940	D1754	GLY	S1658
	M2251	G2145	L2035	T1941	V1845	ALA	S1659
	R2254	M2145	S2036	A1944	V1846	SER	S1660
	Y2255	V2146	V2037	A1947	L1847	ASN	L1661
	Y2257	A2160	E2042	Q1948	G1852	GLY	V1662
	L2260	P2161	S2043	A1949	L1853	ALA	C1668
	L2262	W2162	I2044	R1950	V1854	ALA	G1677
	V2264	E2163	A2045	L1951	P1855	PRO	V1680
	R2265	D2164	E2046	L1952	P1856	S1764	A1681
	F2266	R2165	V2050	E1953	M1857	R1770	G1682
	A2269	I2166	L2051	V1956	L1858	V1771	G1683
	V2274	S2173	A2055	D1957	C1859	I1772	V1684
	D2276	P2174	E2064	D1958	R1860	R1773	M1687
	G2277	S2175	Q2065	S1959	S1864	W1776	A1688
	A2278	S2180	D2068	V1960	I1867	A1779	G1689
	H2280	E2184	A2069	A1968	S1871	G1783	P1690
	M2284	L2186	L2072	A1974	W1883	A1784	E1691
	S2285	A2185	D2076	P1977	A1893	D1785	V1692
	P2286	L2187	V2077	R1978	F1898	V1786	F1693
	H2287	E2188	Q2078	R1979	S1901	V1789	E1695
	L2290	L2189	V2079	L1982	M1904	E1790	F1696
	V2294	C2193	V2087	L1983	V1907	A1791	S1697
	Q2295	E2194	S2088	G1985	E1911	H1792	R1698
	E2296	R2199	L2089	D1986	P1912	G1793	D1705
	T2297	T2202	A2090	Q1989	V1907	T1794	G1706
	A2298	D2206	R2091	L1990	E1911	L1798	K1709
	L2307	Y2207	A2102	R1991	P1912	G1801	F1718
	H2308	H2210	V2103	G1992	F1913	L1807	G1719
	R2309	S2211	I2104	Q1993	GLU	F1720	F1726
	D2310	R2212	G2105	L1994	PRO	Y1811	V1727
	T2311	R2212	H2106	E1999	GLU	R1815	L1728
	A2312	E2215	S2107	G2000	PRO	Q1729	L1729
	H2315	R2218	Q2108	V2001	LEU	Q1730	R1731
	L2316	E2219	G2109	G2009	PRO	G1816	
	T2317		I2111	A2013	GLY	G1819	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.21Å 167.94Å 184.23Å 90.00° 99.43° 90.00°	Depositor
Resolution (Å)	76.23 – 2.90 76.23 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (76.23-2.90) 85.5 (76.23-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.53 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.239 , 0.314 0.239 , 0.315	Depositor DCC
R_{free} test set	2006 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	22987	wwPDB-VP
Average B, all atoms (Å ²)	60.0	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 39.64 % 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 3.0818e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.49	0/6065	0.73	2/8264 (0.0%)
1	B	0.50	0/5803	0.74	0/7908
1	C	0.40	0/5522	0.63	0/7517
1	D	0.40	0/6024	0.65	0/8208
All	All	0.45	0/23414	0.69	2/31897 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1956	VAL	CA-C-N	-6.54	112.42	122.62
1	A	1956	VAL	C-N-CA	-6.54	112.42	122.62

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1657	CYS	Peptide
1	A	1954	SER	Peptide
1	B	1953	GLU	Peptide
1	B	1956	VAL	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	1957	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5950	0	5885	226	0
1	B	5696	0	5658	238	0
1	C	5423	0	5410	221	1
1	D	5910	0	5845	227	1
2	A	1	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
All	All	22987	0	22798	903	1

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 20.

All (903) 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:D:1934:PRO:HD3	1:D:2317:ILE:HD11	1.42	1.00
1:B:1926:VAL:HG11	1:B:2037:VAL:HG22	1.48	0.96
1:B:1824:GLY:HA2	1:B:1857:MET:HE2	1.48	0.94
1:D:1687:MET:HE1	1:D:1720:PHE:HB3	1.49	0.94
1:D:1824:GLY:HA2	1:D:1857:MET:HE2	1.52	0.91
1:C:2308:HIS:ND1	1:C:2309:ARG:O	2.05	0.89
1:B:1826:VAL:HB	1:B:1844:LYS:HD2	1.53	0.88
1:C:2064:GLU:OE1	1:C:2066:ARG:NH1	2.06	0.88
1:A:2308:HIS:ND1	1:A:2309:ARG:O	2.07	0.87
1:A:1660:SER:OG	1:A:1835:ALA:O	1.92	0.86
1:A:1655:THR:O	1:A:1657:CYS:N	2.09	0.85
1:A:2145:MET:HG2	1:A:2180:SER:HB2	1.57	0.84
1:D:1682:GLY:HA2	1:D:1839:VAL:HG21	1.60	0.84
1:C:1815:ARG:HH12	1:C:1821:VAL:HB	1.43	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2282:VAL:HG13	1:C:2304:ILE:HG22	1.59	0.83
1:C:1686:VAL:HA	1:C:1722:GLU:HG2	1.59	0.83
1:B:1574:PRO:HB2	1:B:1686:VAL:HG11	1.60	0.83
1:C:1926:VAL:HG13	1:C:1927:LEU:H	1.43	0.83
1:C:1682:GLY:HA2	1:C:1839:VAL:HG21	1.62	0.82
1:D:2308:HIS:ND1	1:D:2309:ARG:O	2.13	0.82
1:A:1935:VAL:HG12	1:A:1966:ALA:HB2	1.62	0.81
1:B:1945:LEU:HD21	1:B:1980:ALA:HB2	1.61	0.81
1:A:2058:SER:HB2	1:A:2061:GLU:HG3	1.63	0.81
1:A:2218:ARG:HB2	1:A:2257:TYR:CE1	2.15	0.81
1:D:1999:GLU:OE1	1:D:1999:GLU:N	2.13	0.81
1:D:1572:MET:HE2	1:D:1577:ARG:HG2	1.60	0.80
1:C:1883:TRP:CD1	1:C:1891:ARG:HB3	2.17	0.80
1:D:1927:LEU:HD21	1:D:1933:VAL:HG12	1.62	0.79
1:B:2017:VAL:HG22	1:B:2102:ALA:HB3	1.63	0.79
1:C:2023:GLN:HG3	1:C:2108:GLN:HE21	1.43	0.79
1:B:1660:SER:OG	1:B:1835:ALA:O	2.02	0.78
1:A:2145:MET:HE2	1:A:2209:SER:H	1.49	0.78
1:D:2286:PRO:HA	1:D:2307:LEU:HB2	1.65	0.78
1:A:2132:ARG:HH12	1:A:2259:ASN:HD22	1.32	0.77
1:B:1925:GLY:O	1:B:1926:VAL:HG13	1.83	0.77
1:A:1496:ARG:NH2	1:A:1581:GLU:HB3	2.00	0.77
1:A:1658:SER:HB3	1:A:1903:THR:HB	1.67	0.76
1:A:1660:SER:HB3	1:A:1839:VAL:HG23	1.67	0.76
1:A:1976:LEU:HB3	1:A:1977:PRO:HD2	1.68	0.76
1:A:2021:PRO:HB3	1:A:2290:LEU:HD12	1.69	0.75
1:A:2027:TRP:CD1	1:A:2309:ARG:HB3	2.22	0.75
1:D:2105:GLY:HA3	1:D:2110:GLU:HG2	1.69	0.74
1:A:1926:VAL:O	1:A:1928:ALA:N	2.21	0.74
1:C:1806:ALA:O	1:C:1810:THR:OG1	2.06	0.74
1:B:2267:ASP:HB2	1:B:2297:ILE:HG12	1.70	0.74
1:C:2076:ASP:HA	1:C:2133:ALA:HB1	1.69	0.74
1:C:2103:VAL:HG21	1:C:2117:ALA:HB2	1.68	0.73
1:C:1594:PRO:HD2	1:C:1974:ALA:HB2	1.70	0.73
1:B:2043:SER:HA	1:B:2046:GLU:HG3	1.70	0.73
1:B:1572:MET:HE2	1:B:1639:ARG:HD3	1.70	0.72
1:B:1637:SER:H	1:B:1652:THR:HG22	1.55	0.72
1:C:2145:MET:HE2	1:C:2209:SER:H	1.54	0.72
1:C:2154:ARG:HH22	1:C:2196:GLU:HG2	1.54	0.72
1:D:1655:THR:HG21	1:D:1835:ALA:HB2	1.72	0.72
1:C:1827:LYS:HG2	1:C:1832:HIS:HA	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2114:ALA:HB1	1:A:2120:LEU:HD12	1.71	0.71
1:A:1493:MET:HE3	1:A:1843:ILE:HG23	1.71	0.71
1:A:2154:ARG:NH1	1:A:2158:LEU:HD11	2.05	0.71
1:B:1954:SER:OG	1:B:1955:ALA:N	2.22	0.71
1:C:1935:VAL:HG21	1:C:1990:LEU:HD11	1.71	0.71
1:A:2038:PRO:O	1:A:2042:GLU:HG3	1.91	0.71
1:A:2086:MET:HG2	1:A:2284:MET:O	1.90	0.71
1:C:1496:ARG:NH2	1:C:1585:GLU:OE2	2.23	0.71
1:A:1844:LYS:HE3	1:A:1855:PRO:HB2	1.73	0.71
1:B:1937:LEU:HD23	1:B:1948:GLN:HB3	1.72	0.70
1:D:1657:CYS:O	1:D:1901:SER:OG	2.10	0.70
1:D:1937:LEU:HD23	1:D:1948:GLN:HB3	1.73	0.70
1:D:1593:ASP:O	1:D:1596:SER:OG	2.06	0.69
1:B:2145:MET:HE2	1:B:2209:SER:H	1.58	0.69
1:A:2046:GLU:OE2	1:A:2091:ARG:NH2	2.25	0.69
1:C:2218:ARG:NH1	1:D:2250:ASP:OD1	2.26	0.69
1:B:1711:PHE:CE1	1:B:1823:LEU:HD21	2.28	0.69
1:C:2154:ARG:NH2	1:C:2196:GLU:HG2	2.08	0.69
1:A:1734:ASP:HA	1:A:1737:ARG:HG2	1.75	0.68
1:A:2217:ILE:O	1:A:2220:THR:HG22	1.92	0.68
1:C:2267:ASP:HB2	1:C:2297:ILE:HG12	1.74	0.68
1:A:2106:HIS:CE1	1:A:2264:VAL:HG11	2.28	0.68
1:C:1842:VAL:HG22	1:C:1895:VAL:HG11	1.73	0.68
1:D:2199:ARG:H	1:D:2199:ARG:HD2	1.58	0.68
1:A:1842:VAL:O	1:A:1846:VAL:HG23	1.93	0.68
1:B:1842:VAL:O	1:B:1846:VAL:HG23	1.94	0.68
1:A:2107:SER:OG	1:A:2108:GLN:N	2.21	0.68
1:B:2286:PRO:HA	1:B:2307:LEU:HB2	1.76	0.68
1:A:2267:ASP:O	1:A:2271:SER:OG	2.12	0.68
1:B:2282:VAL:HG22	1:B:2304:ILE:HB	1.74	0.68
1:D:1511:ILE:HG13	1:D:1512:VAL:N	2.09	0.68
1:B:1774:LYS:HG3	1:B:1778:ARG:HH21	1.59	0.67
1:C:1797:ARG:HH11	1:C:1866:LEU:HD11	1.59	0.67
1:C:2017:VAL:HG22	1:C:2102:ALA:HB3	1.76	0.67
1:C:1982:LEU:HD13	1:C:1993:GLN:HB3	1.77	0.67
1:B:1751:ILE:HG22	1:B:1905:ALA:HB2	1.76	0.67
1:C:1967:SER:O	1:C:1971:THR:HG22	1.94	0.67
1:C:1844:LYS:HE3	1:C:1855:PRO:HB2	1.77	0.67
1:A:1692:VAL:HG22	1:A:1720:PHE:CE2	2.29	0.66
1:B:1586:LEU:HD21	1:B:1728:LEU:HB2	1.76	0.66
1:C:1856:PRO:HB3	1:C:1879:ALA:HA	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2145:MET:HG2	1:D:2180:SER:HB2	1.78	0.66
1:B:1845:VAL:O	1:B:1849:LEU:HD12	1.96	0.66
1:D:1947:ALA:O	1:D:1950:ARG:HG3	1.95	0.66
1:A:1938:SER:HB3	1:A:1976:LEU:H	1.60	0.65
1:B:2237:LEU:HD22	1:B:2251:MET:HE1	1.79	0.65
1:C:1845:VAL:HB	1:C:1909:ILE:HD11	1.78	0.65
1:C:1935:VAL:HG12	1:C:1966:ALA:HB2	1.77	0.65
1:B:2105:GLY:HA3	1:B:2110:GLU:HG2	1.79	0.65
1:B:2043:SER:OG	1:B:2088:SER:OG	2.12	0.65
1:A:2292:ALA:O	1:A:2296:GLU:HG3	1.97	0.65
1:C:1841:GLY:O	1:C:1845:VAL:HG23	1.97	0.64
1:D:1883:TRP:HZ2	1:D:1893:ALA:HB2	1.62	0.64
1:B:2019:VAL:HG12	1:B:2021:PRO:HD3	1.77	0.64
1:B:1941:THR:OG1	1:B:1943:THR:OG1	2.14	0.64
1:D:1754:ASP:HB2	1:D:1764:SER:HB3	1.79	0.64
1:A:2027:TRP:CH2	1:A:2030:MET:HA	2.33	0.64
1:C:2018:PHE:CG	1:C:2100:PRO:HB3	2.33	0.64
1:B:1941:THR:HG1	1:B:1943:THR:HG1	1.46	0.64
1:D:2050:VAL:HB	1:D:2126:VAL:HG21	1.79	0.64
1:C:1776:TRP:HB3	1:C:1781:ILE:O	1.97	0.64
1:C:1604:VAL:HG12	1:C:1637:SER:HB2	1.79	0.64
1:B:1821:VAL:HG12	1:B:1874:VAL:HG22	1.79	0.63
1:C:1580:LEU:HG	1:C:1640:VAL:HG12	1.80	0.63
1:D:2027:TRP:O	1:D:2030:MET:HG2	1.98	0.63
1:B:1798:LEU:O	1:B:1802:VAL:HG23	1.98	0.63
1:C:1842:VAL:O	1:C:1846:VAL:HG23	1.98	0.63
1:C:1570:LEU:HD13	1:C:1577:ARG:HH22	1.63	0.63
1:C:2058:SER:HB2	1:C:2061:GLU:H	1.64	0.63
1:C:1952:LEU:HD13	1:C:1952:LEU:O	1.98	0.63
1:A:1883:TRP:CD1	1:A:1891:ARG:HB3	2.34	0.63
1:B:2086:MET:HG2	1:B:2284:MET:O	1.99	0.63
1:B:2169:ALA:HB2	1:B:2180:SER:HB3	1.80	0.63
1:D:1692:VAL:HG12	1:D:1720:PHE:CE1	2.34	0.63
1:D:1503:ASN:ND2	1:D:1506:GLU:H	1.96	0.62
1:B:1952:LEU:HB3	1:B:1994:LEU:HD13	1.81	0.62
1:C:1982:LEU:HD12	1:C:1994:LEU:HD23	1.80	0.62
1:A:2147:SER:OG	1:A:2203:LEU:HD21	1.99	0.62
1:C:1643:VAL:HG13	1:C:1644:LEU:HD12	1.80	0.62
1:D:1508:TRP:HB2	1:D:1847:LEU:HD13	1.81	0.62
1:D:1493:MET:HE3	1:D:1843:ILE:HG23	1.82	0.62
1:C:1883:TRP:HZ2	1:C:1893:ALA:HB2	1.64	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2103:VAL:HG23	1:D:2237:LEU:HD13	1.81	0.61
1:D:1807:LEU:HD13	1:D:1823:LEU:HD11	1.82	0.61
1:C:1573:ASP:HB3	1:C:1575:GLN:HE22	1.64	0.61
1:A:1828:SER:OG	1:A:1857:MET:HE3	2.00	0.61
1:B:1784:ALA:HB2	1:B:1815:ARG:HA	1.82	0.61
1:A:2132:ARG:HH22	1:A:2259:ASN:ND2	1.98	0.61
1:D:1521:MET:HE3	1:D:1550:PHE:CZ	2.36	0.61
1:D:1864:SER:HB3	1:D:1867:ILE:HD12	1.83	0.61
1:B:1718:PHE:HB3	1:B:1794:THR:HG22	1.81	0.61
1:C:1605:PHE:O	1:C:1606:LEU:HD23	2.01	0.61
1:D:1570:LEU:HG	1:D:2356:LEU:HD21	1.81	0.60
1:B:2159:ILE:HD12	1:B:2166:ILE:HG22	1.83	0.60
1:B:1491:VAL:HB	1:B:1740:ARG:HG2	1.83	0.60
1:B:1637:SER:H	1:B:1652:THR:CG2	2.13	0.60
1:A:2114:ALA:CB	1:A:2120:LEU:HD12	2.31	0.60
1:A:1671:LEU:O	1:A:1731:ARG:NH1	2.35	0.60
1:D:1736:ARG:O	1:D:1739:GLY:N	2.31	0.60
1:B:2186:LEU:O	1:B:2190:VAL:HG13	2.02	0.60
1:C:2016:VAL:N	1:C:2101:SER:OG	2.34	0.60
1:B:1712:SER:OG	1:B:1860:ARG:O	2.12	0.60
1:A:2046:GLU:CD	1:A:2091:ARG:HH22	2.10	0.59
1:D:2107:SER:HB3	1:D:2210:HIS:NE2	2.16	0.59
1:B:1610:TYR:O	1:B:1611:GLN:HG3	2.02	0.59
1:C:1952:LEU:HD21	1:C:1969:LEU:HD11	1.84	0.59
1:C:1926:VAL:H	1:C:2037:VAL:HG11	1.67	0.59
1:B:1720:PHE:HE1	1:B:1834:GLN:HB2	1.68	0.59
1:B:1953:GLU:O	1:B:1956:VAL:HG23	2.03	0.59
1:C:2163:GLU:HG3	1:D:2276:ASP:OD2	2.02	0.59
1:B:2287:HIS:ND1	1:B:2309:ARG:HG2	2.18	0.59
1:B:1826:VAL:HB	1:B:1844:LYS:CD	2.31	0.59
1:A:2186:LEU:O	1:A:2190:VAL:HG23	2.02	0.59
1:B:1570:LEU:HB2	1:B:2356:LEU:HD11	1.85	0.59
1:B:1943:THR:OG1	1:B:2350:GLU:OE1	2.21	0.59
1:C:1581:GLU:O	1:C:1585:GLU:HG3	2.02	0.59
1:A:2033:GLY:HA3	1:A:2313:GLU:CD	2.28	0.59
1:D:1512:VAL:HG23	1:D:1856:PRO:HG3	1.84	0.59
1:A:1790:GLU:HB3	1:A:1895:VAL:HG22	1.84	0.58
1:B:2050:VAL:HG23	1:B:2126:VAL:HG11	1.84	0.58
1:A:1983:LEU:O	1:A:1993:GLN:NE2	2.27	0.58
1:C:2104:ILE:HG12	1:C:2238:TYR:HB2	1.84	0.58
1:B:1883:TRP:CZ2	1:B:1893:ALA:HB2	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2076:ASP:CG	1:D:2137:ARG:HD3	2.29	0.58
1:A:1898:PHE:CD1	1:A:1904:ASN:HB3	2.38	0.58
1:B:2208:ALA:HB3	1:B:2213:HIS:CD2	2.37	0.58
1:C:2155:ALA:O	1:C:2159:ILE:HG12	2.04	0.58
1:A:1491:VAL:HG23	1:A:1728:LEU:HD23	1.85	0.58
1:A:2267:ASP:HB2	1:A:2297:ILE:HG12	1.85	0.58
1:B:1811:TYR:OH	1:B:1906:HIS:NE2	2.29	0.58
1:C:2023:GLN:HG3	1:C:2108:GLN:NE2	2.17	0.58
1:A:1511:ILE:O	1:A:1514:GLY:N	2.36	0.58
1:A:1599:GLY:HA2	1:A:1647:GLU:HG3	1.86	0.58
1:A:2201:LYS:HD3	1:A:2202:THR:N	2.18	0.58
1:A:1932:SER:OG	1:A:1984:ALA:N	2.37	0.58
1:B:2046:GLU:CD	1:B:2091:ARG:HH12	2.12	0.58
1:D:1937:LEU:HD11	1:D:1952:LEU:HD22	1.86	0.58
1:D:2173:SER:O	1:D:2175:SER:N	2.36	0.58
1:C:1497:PHE:HB2	1:C:1501:VAL:HG13	1.86	0.57
1:B:2308:HIS:ND1	1:B:2309:ARG:O	2.37	0.57
1:C:1576:GLN:HG3	1:C:1636:VAL:HG13	1.85	0.57
1:C:2321:ALA:O	1:C:2325:VAL:HG23	2.05	0.57
1:D:1709:LYS:HG2	1:D:1860:ARG:HG3	1.86	0.57
1:D:2119:VAL:HG11	1:D:2251:MET:HE2	1.86	0.57
1:B:1956:VAL:O	1:B:1957:ASP:HB2	2.03	0.57
1:A:2287:HIS:ND1	1:A:2288:PRO:HD2	2.20	0.57
1:B:2018:PHE:CG	1:B:2100:PRO:HB3	2.40	0.57
1:C:2067:PRO:HD2	1:C:2068:ASP:H	1.69	0.57
1:D:2173:SER:OG	1:D:2296:GLU:OE1	2.22	0.57
1:A:2034:LEU:HD11	1:A:2307:LEU:HD21	1.87	0.57
1:D:1489:ALA:HB2	1:D:1732:LEU:HD13	1.86	0.57
1:D:1936:LEU:O	1:D:1937:LEU:HD12	2.04	0.57
1:D:2027:TRP:CH2	1:D:2030:MET:HA	2.40	0.57
1:D:2218:ARG:NH1	1:D:2219:GLU:OE2	2.37	0.57
1:C:2124:ASP:O	1:C:2128:VAL:HG23	2.05	0.57
1:D:2274:VAL:HG21	1:D:2298:ALA:HB2	1.86	0.57
1:C:1945:LEU:HD11	1:C:1980:ALA:HB2	1.87	0.57
1:A:1586:LEU:HD21	1:A:1728:LEU:HB2	1.85	0.56
1:C:1575:GLN:O	1:C:1579:VAL:HG12	2.05	0.56
1:D:1864:SER:HB3	1:D:1867:ILE:CD1	2.34	0.56
1:A:2017:VAL:HG22	1:A:2102:ALA:HB3	1.87	0.56
1:D:2218:ARG:HD3	1:D:2257:TYR:CE2	2.41	0.56
1:A:2132:ARG:NH1	1:A:2259:ASN:HD22	2.01	0.56
1:A:2165:ARG:HB3	1:A:2182:ASP:HB2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1883:TRP:CZ2	1:C:1893:ALA:HB2	2.40	0.56
1:A:1493:MET:CE	1:A:1843:ILE:HG23	2.36	0.56
1:B:1720:PHE:CE1	1:B:1834:GLN:HB2	2.40	0.56
1:D:1956:VAL:HG21	1:D:1991:ARG:HG2	1.88	0.56
1:D:2232:ARG:NH1	1:D:2247:ASP:OD2	2.39	0.56
1:C:1684:VAL:HG23	1:C:1724:VAL:HB	1.88	0.56
1:C:1981:ALA:C	1:C:1982:LEU:HD23	2.31	0.56
1:C:2140:ALA:HA	1:C:2207:TYR:HB3	1.88	0.56
1:D:1692:VAL:HG12	1:D:1720:PHE:HE1	1.71	0.55
1:B:1942:GLU:HG3	1:B:1978:ARG:HD2	1.87	0.55
1:D:1926:VAL:H	1:D:2037:VAL:HG22	1.71	0.55
1:C:2282:VAL:HG13	1:C:2304:ILE:CG2	2.34	0.55
1:D:2128:VAL:HG13	1:D:2225:LEU:HD13	1.88	0.55
1:A:1747:ALA:HB3	1:A:1908:ILE:HG22	1.88	0.55
1:A:2276:ASP:OD2	1:B:2163:GLU:HG3	2.07	0.55
1:B:1489:ALA:HB1	1:B:1742:VAL:HG13	1.88	0.55
1:C:1826:VAL:HG22	1:C:1830:ILE:HD12	1.89	0.55
1:D:2119:VAL:HG21	1:D:2251:MET:HE2	1.89	0.55
1:B:2057:PHE:HB2	1:B:2061:GLU:OE1	2.07	0.55
1:B:2173:SER:C	1:B:2175:SER:H	2.15	0.55
1:D:2124:ASP:O	1:D:2128:VAL:HG23	2.07	0.55
1:C:1557:PHE:CD2	1:C:1577:ARG:HD3	2.42	0.55
1:C:1684:VAL:HB	1:C:1724:VAL:HG23	1.89	0.55
1:D:1695:GLU:O	1:D:1698:ARG:HG2	2.06	0.55
1:D:2016:VAL:HG23	1:D:2280:THR:HB	1.89	0.55
1:D:2035:LEU:HD12	1:D:2035:LEU:H	1.72	0.55
1:B:1657:CYS:HA	1:B:1901:SER:HB3	1.89	0.54
1:B:2282:VAL:HG12	1:B:2284:MET:HE3	1.89	0.54
1:C:2040:PHE:HD2	1:C:2092:LEU:HD12	1.71	0.54
1:A:1682:GLY:HA2	1:A:1839:VAL:HG21	1.90	0.54
1:B:1565:SER:HB3	1:B:1568:GLU:OE2	2.07	0.54
1:B:2173:SER:O	1:B:2175:SER:N	2.39	0.54
1:C:1845:VAL:O	1:C:1849:LEU:HD12	2.06	0.54
1:D:1603:GLY:HA2	1:D:1649:PRO:O	2.07	0.54
1:D:1635:VAL:HG13	1:D:1639:ARG:HD3	1.88	0.54
1:C:2218:ARG:HH12	1:D:2250:ASP:HA	1.72	0.54
1:B:2112:ALA:O	1:B:2115:VAL:HG22	2.08	0.54
1:B:2154:ARG:NH1	1:B:2158:LEU:HD11	2.21	0.54
1:D:1952:LEU:O	1:D:1956:VAL:HG23	2.06	0.54
1:A:1581:GLU:O	1:A:1585:GLU:HG3	2.08	0.54
1:B:1896:SER:OG	1:B:1906:HIS:ND1	2.32	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2021:PRO:HB3	1:B:2290:LEU:HD12	1.90	0.54
1:B:2210:HIS:ND1	1:B:2260:LEU:O	2.41	0.54
1:D:1594:PRO:HD2	1:D:1974:ALA:HB2	1.88	0.54
1:A:2237:LEU:HD22	1:A:2251:MET:HE1	1.90	0.54
1:C:2283:GLU:O	1:C:2285:SER:N	2.39	0.54
1:D:1687:MET:CE	1:D:1720:PHE:HB3	2.31	0.54
1:D:1605:PHE:O	1:D:1681:ALA:HA	2.07	0.54
1:D:1984:ALA:HB2	1:D:1993:GLN:OE1	2.08	0.54
1:D:2287:HIS:HE1	1:D:2308:HIS:CE1	2.26	0.54
1:A:1706:GLY:O	1:A:1719:GLY:HA3	2.08	0.54
1:B:2077:VAL:O	1:B:2080:PRO:HD2	2.08	0.54
1:C:1575:GLN:HB2	1:C:1684:VAL:HG13	1.90	0.54
1:A:2136:LEU:HD12	1:A:2139:LEU:HG	1.90	0.54
1:B:1486:ASP:N	1:B:1672:ARG:NH2	2.55	0.54
1:C:1580:LEU:HD21	1:C:1643:VAL:HG11	1.89	0.54
1:D:1959:SER:O	1:D:1960:VAL:HG12	2.07	0.54
1:D:2311:THR:OG1	1:D:2315:HIS:HB2	2.07	0.54
1:B:1678:LEU:HD12	1:B:1730:GLN:HB2	1.90	0.53
1:B:2321:ALA:O	1:B:2325:VAL:HG23	2.07	0.53
1:C:1497:PHE:HB2	1:C:1501:VAL:CG1	2.39	0.53
1:C:1671:LEU:HB3	1:C:1731:ARG:HG2	1.90	0.53
1:C:1715:ALA:HB1	1:C:1795:GLY:O	2.09	0.53
1:D:1706:GLY:O	1:D:1719:GLY:HA3	2.08	0.53
1:D:2128:VAL:HG13	1:D:2225:LEU:CD1	2.38	0.53
1:C:2218:ARG:NE	1:C:2219:GLU:OE1	2.36	0.53
1:D:1522:PRO:HB2	1:D:1525:ARG:HD2	1.89	0.53
1:D:1944:ALA:HB2	1:D:2350:GLU:OE1	2.07	0.53
1:D:2266:PHE:O	1:D:2269:ALA:N	2.40	0.53
1:A:1883:TRP:NE1	1:A:1891:ARG:HB3	2.23	0.53
1:B:1510:PHE:CZ	1:B:1515:GLY:HA2	2.44	0.53
1:C:1563:GLY:O	1:C:1564:ILE:HD13	2.09	0.53
1:D:1599:GLY:HA2	1:D:1647:GLU:HG3	1.91	0.53
1:B:2108:GLN:O	1:B:2111:ILE:HD12	2.08	0.53
1:B:2117:ALA:HA	1:B:2235:ILE:HD13	1.90	0.53
1:B:2130:ALA:O	1:B:2133:ALA:N	2.41	0.53
1:D:1935:VAL:HG21	1:D:1990:LEU:HD11	1.90	0.53
1:D:2164:ASP:O	1:D:2166:ILE:N	2.39	0.53
1:A:1572:MET:HE3	1:A:1576:GLN:HG2	1.90	0.53
1:A:1973:ARG:HH22	1:A:2344:LEU:HB2	1.74	0.53
1:C:1946:ALA:HB1	1:C:1998:ALA:O	2.09	0.53
1:D:1554:ALA:HA	1:D:1578:GLN:NE2	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1856:PRO:HB3	1:A:1879:ALA:HA	1.91	0.53
1:D:1740:ARG:HB2	1:D:1740:ARG:NH1	2.23	0.53
1:D:1784:ALA:HA	1:D:1815:ARG:HH21	1.73	0.53
1:D:2184:GLU:HG2	1:D:2188:GLU:OE2	2.09	0.53
1:B:1641:ALA:HA	1:B:1646:LEU:HD12	1.90	0.53
1:B:1790:GLU:OE2	1:B:1826:VAL:HG12	2.09	0.53
1:C:1498:PRO:HD3	1:C:1722:GLU:O	2.09	0.53
1:A:2164:ASP:OD1	1:A:2165:ARG:N	2.41	0.52
1:B:1786:VAL:HG13	1:B:1893:ALA:HA	1.91	0.52
1:D:1941:THR:CG2	1:D:1944:ALA:H	2.22	0.52
1:B:1592:ILE:HD11	1:B:1740:ARG:NH1	2.24	0.52
1:B:1989:GLN:HG2	1:B:1993:GLN:HE21	1.74	0.52
1:A:1489:ALA:HB1	1:A:1742:VAL:HG13	1.92	0.52
1:A:1883:TRP:HZ2	1:A:1893:ALA:HB2	1.75	0.52
1:B:1822:LEU:HB3	1:B:1877:ALA:HB2	1.91	0.52
1:D:2290:LEU:O	1:D:2294:VAL:HG23	2.09	0.52
1:A:1824:GLY:HA2	1:A:1857:MET:HG2	1.91	0.52
1:A:2214:VAL:HG11	1:A:2260:LEU:HG	1.91	0.52
1:B:2292:ALA:O	1:B:2296:GLU:HG3	2.10	0.52
1:C:1938:SER:HB3	1:C:1976:LEU:H	1.74	0.52
1:D:1941:THR:HG23	1:D:1944:ALA:H	1.74	0.52
1:A:2017:VAL:HB	1:A:2281:PHE:CD1	2.45	0.52
1:B:1593:ASP:OD2	1:B:1974:ALA:HA	2.09	0.52
1:B:1953:GLU:N	1:B:1953:GLU:OE1	2.43	0.52
1:C:2048:ASP:O	1:C:2052:SER:N	2.31	0.52
1:D:1786:VAL:HG13	1:D:1893:ALA:HA	1.90	0.52
1:B:2062:VAL:HG11	1:B:2081:VAL:HG21	1.91	0.52
1:D:1511:ILE:HG13	1:D:1512:VAL:H	1.73	0.52
1:B:2309:ARG:O	1:B:2309:ARG:HG3	2.09	0.52
1:C:1576:GLN:HE21	1:C:1636:VAL:HA	1.75	0.52
1:C:1794:THR:OG1	1:C:1795:GLY:N	2.40	0.52
1:D:1842:VAL:O	1:D:1846:VAL:HG22	2.10	0.52
1:D:2145:MET:HE2	1:D:2207:TYR:O	2.10	0.52
1:A:1684:VAL:HG23	1:A:1724:VAL:HG22	1.92	0.52
1:B:1705:ASP:O	1:B:1707:ARG:NH1	2.42	0.52
1:B:2103:VAL:HG21	1:B:2117:ALA:HB2	1.92	0.52
1:B:1557:PHE:HZ	1:B:1580:LEU:HD23	1.75	0.52
1:C:1798:LEU:O	1:C:1802:VAL:HG23	2.10	0.52
1:A:1930:ALA:HB2	1:A:2317:ILE:HD13	1.92	0.52
1:B:2140:ALA:HA	1:B:2206:ASP:O	2.08	0.52
1:D:1749:SER:HB3	1:D:1907:VAL:HG23	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2018:PHE:HB3	1:D:2020:PHE:CE1	2.45	0.52
1:A:1597:LEU:O	1:A:1600:SER:HB2	2.10	0.51
1:A:2173:SER:C	1:A:2175:SER:H	2.18	0.51
1:C:1555:ALA:O	1:C:1577:ARG:NH1	2.43	0.51
1:C:1576:GLN:NE2	1:C:1636:VAL:HA	2.25	0.51
1:C:1807:LEU:HD13	1:C:1823:LEU:HD11	1.92	0.51
1:C:1993:GLN:O	1:C:1997:VAL:HG23	2.10	0.51
1:D:1925:GLY:O	1:D:1926:VAL:HG12	2.10	0.51
1:C:1878:GLU:H	1:C:1878:GLU:CD	2.18	0.51
1:A:1983:LEU:HD21	1:A:2317:ILE:HG22	1.92	0.51
1:A:1987:HIS:O	1:A:1991:ARG:HG3	2.10	0.51
1:B:1816:GLY:C	1:B:1818:SER:H	2.19	0.51
1:A:1575:GLN:O	1:A:1579:VAL:HG12	2.11	0.51
1:A:1827:LYS:HE3	1:A:1832:HIS:ND1	2.26	0.51
1:A:1886:ALA:HB3	1:A:1888:ASP:OD1	2.11	0.51
1:A:1936:LEU:HD12	1:A:1970:ALA:HA	1.91	0.51
1:A:2079:GLN:HB2	1:A:2080:PRO:HD3	1.93	0.51
1:A:2168:VAL:HA	1:A:2179:VAL:HG12	1.92	0.51
1:C:1579:VAL:HG21	1:C:1606:LEU:HD11	1.92	0.51
1:C:2254:ARG:HD3	1:D:2254:ARG:HG2	1.92	0.51
1:D:1634:ALA:HA	1:D:1652:THR:HB	1.92	0.51
1:D:1659:SER:C	1:D:1661:LEU:N	2.68	0.51
1:D:2032:ARG:HA	1:D:2035:LEU:CD1	2.41	0.51
1:A:1594:PRO:HD2	1:A:1974:ALA:HB2	1.91	0.51
1:A:1765:GLY:O	1:A:1769:GLN:HG3	2.11	0.51
1:B:1594:PRO:HD2	1:B:1974:ALA:HB2	1.93	0.51
1:B:2218:ARG:HB2	1:B:2257:TYR:CE1	2.46	0.51
1:D:1659:SER:C	1:D:1661:LEU:H	2.19	0.51
1:A:1498:PRO:HB3	1:A:1550:PHE:O	2.10	0.51
1:A:1678:LEU:HD21	1:A:1728:LEU:HD11	1.91	0.51
1:A:2184:GLU:O	1:A:2188:GLU:HG3	2.11	0.51
1:C:1501:VAL:HG23	1:C:1506:GLU:CB	2.41	0.51
1:A:2225:LEU:O	1:A:2228:ILE:HG12	2.11	0.50
1:B:1898:PHE:CD1	1:B:1904:ASN:HB3	2.46	0.50
1:B:1973:ARG:HH11	1:B:1973:ARG:HG2	1.76	0.50
1:C:1671:LEU:O	1:C:1731:ARG:HD3	2.11	0.50
1:A:1948:GLN:HG3	1:A:2348:PRO:HD2	1.93	0.50
1:B:1956:VAL:HG12	1:B:1987:HIS:HB3	1.94	0.50
1:B:2023:GLN:HG3	1:B:2024:GLY:N	2.26	0.50
1:C:2186:LEU:O	1:C:2190:VAL:HG13	2.12	0.50
1:A:1950:ARG:HG2	1:A:1995:ARG:HH12	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2134:LYS:O	1:A:2137:ARG:HB2	2.11	0.50
1:B:1518:VAL:HG22	1:B:1549:ALA:HB2	1.93	0.50
1:B:1926:VAL:HG11	1:B:2037:VAL:CG2	2.33	0.50
1:B:1935:VAL:HG12	1:B:1966:ALA:HB2	1.92	0.50
1:C:1968:ALA:HB1	1:C:2344:LEU:HD11	1.94	0.50
1:C:1709:LYS:HG2	1:C:1860:ARG:HD2	1.94	0.50
1:D:1789:VAL:HG23	1:D:1823:LEU:HD12	1.93	0.50
1:A:1774:LYS:HZ2	1:A:1778:ARG:CD	2.24	0.50
1:A:1862:GLU:HG2	1:A:1863:ARG:H	1.76	0.50
1:B:2162:TRP:O	1:B:2164:ASP:O	2.29	0.50
1:B:2355:TRP:C	1:B:2356:LEU:HD12	2.36	0.50
1:C:2067:PRO:CD	1:C:2068:ASP:H	2.24	0.50
1:A:2244:GLU:OE1	1:B:2156:ARG:NH1	2.43	0.50
1:B:2304:ILE:HD13	1:B:2322:ARG:NH2	2.27	0.50
1:D:1740:ARG:HB2	1:D:1740:ARG:CZ	2.42	0.50
1:B:1572:MET:CE	1:B:1639:ARG:HD3	2.39	0.50
1:B:2027:TRP:CD1	1:B:2309:ARG:HB3	2.47	0.50
1:B:2243:GLY:HA3	1:B:2268:GLU:HB3	1.92	0.50
1:C:1926:VAL:CG1	1:C:1927:LEU:H	2.19	0.50
1:C:1944:ALA:O	1:C:1948:GLN:HG3	2.12	0.50
1:C:2148:LEU:HB2	1:C:2177:VAL:HG23	1.93	0.50
1:D:1857:MET:HG2	1:D:1858:LEU:N	2.26	0.50
1:D:2046:GLU:CD	1:D:2091:ARG:HH22	2.20	0.50
1:A:1925:GLY:HA3	1:A:2037:VAL:HG13	1.92	0.50
1:B:1883:TRP:HZ2	1:B:1893:ALA:HB2	1.75	0.50
1:C:1797:ARG:NH1	1:C:1866:LEU:HD11	2.24	0.50
1:C:2023:GLN:H	1:C:2108:GLN:HE21	1.58	0.50
1:D:2017:VAL:HG13	1:D:2102:ALA:HB3	1.94	0.50
1:B:1989:GLN:O	1:B:1993:GLN:HG3	2.12	0.50
1:C:1570:LEU:HD13	1:C:1577:ARG:NH2	2.26	0.50
1:C:1662:VAL:HG13	1:C:1663:ALA:H	1.77	0.50
1:C:2347:TYR:HE1	1:C:2349:PHE:HA	1.76	0.50
1:B:1637:SER:OG	1:B:1651:VAL:O	2.19	0.49
1:C:1604:VAL:CG1	1:C:1637:SER:HB2	2.41	0.49
1:C:1990:LEU:HG	1:C:1994:LEU:HD11	1.92	0.49
1:D:1657:CYS:HA	1:D:1901:SER:HB3	1.93	0.49
1:B:1720:PHE:CZ	1:B:1832:HIS:CD2	2.99	0.49
1:D:1718:PHE:CD1	1:D:1720:PHE:HE2	2.30	0.49
1:D:2111:ILE:HG21	1:D:2129:VAL:HB	1.93	0.49
1:A:1555:ALA:HB1	1:A:2353:ARG:HG3	1.92	0.49
1:C:1863:ARG:HD3	1:C:1869:TRP:CD1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1573:ASP:HB3	1:C:1575:GLN:NE2	2.27	0.49
1:D:1488:ILE:HG21	1:D:1668:CYS:SG	2.53	0.49
1:D:1677:GLY:O	1:D:1730:GLN:HG3	2.12	0.49
1:D:2136:LEU:HD13	1:D:2260:LEU:HD21	1.94	0.49
1:A:1824:GLY:HA2	1:A:1857:MET:CG	2.43	0.49
1:A:2201:LYS:HD3	1:A:2202:THR:H	1.75	0.49
1:C:2020:PHE:O	1:C:2109:GLY:HA3	2.13	0.49
1:D:1525:ARG:HG2	1:D:2355:TRP:CZ2	2.48	0.49
1:C:2159:ILE:HG22	1:C:2189:LEU:HD22	1.95	0.49
1:D:1911:GLU:HG2	1:D:1912:PRO:HD2	1.93	0.49
1:D:2119:VAL:O	1:D:2231:ARG:HG2	2.12	0.49
1:D:2237:LEU:HD12	1:D:2238:TYR:N	2.27	0.49
1:A:2027:TRP:CZ2	1:A:2030:MET:HA	2.47	0.49
1:A:1636:VAL:HG12	1:A:1652:THR:HG23	1.95	0.49
1:A:1774:LYS:HZ2	1:A:1778:ARG:HD3	1.76	0.49
1:A:1883:TRP:CZ2	1:A:1893:ALA:HB2	2.48	0.49
1:A:2170:ALA:HB3	1:A:2178:VAL:HB	1.95	0.49
1:C:1665:HIS:CD2	1:C:1751:ILE:HG12	2.48	0.49
1:C:1768:GLN:O	1:C:1772:ILE:HG13	2.12	0.49
1:C:2079:GLN:HB2	1:C:2080:PRO:HD3	1.94	0.49
1:A:1956:VAL:HG21	1:A:1965:LEU:CD1	2.43	0.49
1:C:2013:ALA:H	1:C:2327:GLY:HA3	1.77	0.49
1:D:1883:TRP:CZ2	1:D:1893:ALA:HB2	2.45	0.49
1:A:1898:PHE:HD1	1:A:1904:ASN:HB3	1.78	0.49
1:B:1939:ALA:HB2	1:B:1948:GLN:OE1	2.13	0.49
1:B:2311:THR:HB	1:B:2315:HIS:HB2	1.93	0.49
1:C:1822:LEU:HB3	1:C:1877:ALA:HB2	1.94	0.49
1:D:1659:SER:O	1:D:1661:LEU:N	2.46	0.49
1:B:2018:PHE:HA	1:B:2282:VAL:O	2.13	0.48
1:C:1936:LEU:HD21	1:C:2332:TRP:CZ2	2.48	0.48
1:C:2124:ASP:HB3	1:C:2228:ILE:HD12	1.94	0.48
1:D:1521:MET:HB3	1:D:1521:MET:HE2	1.62	0.48
1:D:1852:GLY:O	1:D:1853:LEU:HD23	2.12	0.48
1:D:1986:ASP:OD1	1:D:1989:GLN:N	2.30	0.48
1:A:2020:PHE:HB2	1:A:2105:GLY:HA2	1.93	0.48
1:B:2245:ARG:HE	1:B:2245:ARG:HB3	1.41	0.48
1:B:2304:ILE:HG23	1:B:2319:GLU:OE1	2.13	0.48
1:A:1896:SER:OG	1:A:1906:HIS:ND1	2.36	0.48
1:B:2092:LEU:O	1:B:2095:ALA:HB3	2.12	0.48
1:C:2018:PHE:HB3	1:C:2020:PHE:CE1	2.49	0.48
1:A:2155:ALA:O	1:A:2159:ILE:HG12	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2285:SER:OG	1:B:2287:HIS:O	2.28	0.48
1:C:2165:ARG:HD3	1:C:2185:ALA:HB2	1.95	0.48
1:D:1568:GLU:O	1:D:1572:MET:HG3	2.13	0.48
1:A:2308:HIS:CE1	1:A:2309:ARG:O	2.65	0.48
1:A:2311:THR:OG1	1:A:2315:HIS:HB2	2.14	0.48
1:B:2070:PRO:HB2	1:B:2077:VAL:HG21	1.95	0.48
1:D:1844:LYS:HE3	1:D:1855:PRO:HB2	1.95	0.48
1:A:2141:GLY:N	1:A:2206:ASP:O	2.46	0.48
1:B:1857:MET:HG2	1:B:1858:LEU:N	2.28	0.48
1:B:2090:ALA:HA	1:B:2284:MET:SD	2.53	0.48
1:C:1790:GLU:OE1	1:C:1826:VAL:N	2.46	0.48
1:D:2017:VAL:HG22	1:D:2278:HIS:ND1	2.28	0.48
1:D:2190:VAL:HA	1:D:2193:CYS:SG	2.53	0.48
1:A:1584:TRP:CZ2	1:A:1594:PRO:HG2	2.49	0.48
1:B:1958:ASP:O	1:B:1960:VAL:N	2.47	0.48
1:C:1725:ALA:HB1	1:C:1843:ILE:HD12	1.95	0.48
1:D:1935:VAL:HG23	1:D:1982:LEU:HB2	1.95	0.48
1:A:1505:GLY:O	1:A:1509:GLU:HG3	2.14	0.48
1:A:2241:LEU:HD22	1:A:2242:HIS:CE1	2.49	0.48
1:C:2317:ILE:HD12	1:C:2318:ALA:N	2.28	0.48
1:C:1866:LEU:HD12	1:C:1866:LEU:H	1.79	0.48
1:D:2026:GLN:OE1	1:D:2026:GLN:N	2.46	0.48
1:A:2241:LEU:HD23	1:A:2241:LEU:C	2.39	0.48
1:B:1956:VAL:HB	1:B:1991:ARG:HE	1.78	0.48
1:B:1971:THR:HG21	1:B:2333:ARG:HH11	1.79	0.48
1:A:1981:ALA:O	1:A:1982:LEU:HD23	2.14	0.47
1:C:1496:ARG:HB2	1:C:1724:VAL:CG1	2.44	0.47
1:C:1662:VAL:HG13	1:C:1663:ALA:N	2.29	0.47
1:D:2079:GLN:HG2	1:D:2108:GLN:OE1	2.13	0.47
1:D:2173:SER:C	1:D:2175:SER:H	2.22	0.47
1:A:1798:LEU:O	1:A:1801:PRO:HD2	2.14	0.47
1:B:2083:PHE:O	1:B:2086:MET:N	2.47	0.47
1:C:1493:MET:HG2	1:C:1727:VAL:HG12	1.96	0.47
1:D:1730:GLN:OE1	1:D:1740:ARG:NH1	2.47	0.47
1:D:2218:ARG:HB2	1:D:2257:TYR:CE1	2.49	0.47
1:A:1685:SER:N	1:A:1723:GLY:O	2.45	0.47
1:A:1798:LEU:O	1:A:1802:VAL:HG23	2.14	0.47
1:B:1858:LEU:HG	1:B:1860:ARG:HD2	1.95	0.47
1:B:1929:ALA:HB1	1:B:2313:GLU:HG2	1.96	0.47
1:C:1496:ARG:NH2	1:C:1581:GLU:HB3	2.29	0.47
1:C:1781:ILE:HD12	1:C:1785:ASP:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2165:ARG:O	1:A:2181:GLY:HA3	2.13	0.47
1:C:1843:ILE:O	1:C:1847:LEU:HG	2.14	0.47
1:C:2031:ALA:HB2	1:C:2307:LEU:HD11	1.97	0.47
1:A:1508:TRP:HB2	1:A:1847:LEU:HD13	1.97	0.47
1:A:2210:HIS:ND1	1:A:2260:LEU:O	2.45	0.47
1:C:2055:ALA:HB1	1:C:2057:PHE:CE1	2.49	0.47
1:D:1680:VAL:HG22	1:D:1728:LEU:HD12	1.96	0.47
1:A:1554:ALA:HA	1:A:1578:GLN:NE2	2.29	0.47
1:A:1936:LEU:O	1:A:1937:LEU:HG	2.13	0.47
1:A:2089:LEU:HD23	1:A:2089:LEU:HA	1.79	0.47
1:A:2169:ALA:HB1	1:A:2210:HIS:HB2	1.97	0.47
1:B:1491:VAL:HG23	1:B:1728:LEU:HD23	1.96	0.47
1:B:1518:VAL:HG13	1:B:1549:ALA:N	2.30	0.47
1:B:1871:SER:O	1:B:1871:SER:OG	2.27	0.47
1:B:2020:PHE:O	1:B:2109:GLY:HA3	2.14	0.47
1:B:2308:HIS:CE1	1:B:2309:ARG:O	2.67	0.47
1:C:1508:TRP:CZ3	1:C:1848:GLY:HA2	2.50	0.47
1:C:2172:ASN:O	1:C:2267:ASP:HB3	2.14	0.47
1:D:1562:PHE:HB2	1:D:1564:ILE:HD12	1.97	0.47
1:D:1743:LEU:HA	1:D:1743:LEU:HD23	1.58	0.47
1:D:1793:GLY:HA3	1:D:1825:SER:HB2	1.95	0.47
1:A:2218:ARG:HB2	1:A:2257:TYR:CZ	2.49	0.47
1:B:1790:GLU:HB3	1:B:1895:VAL:HG22	1.97	0.47
1:B:1962:LEU:HD23	1:B:1962:LEU:HA	1.55	0.47
1:B:1806:ALA:O	1:B:1810:THR:OG1	2.25	0.47
1:C:2187:ALA:O	1:C:2190:VAL:HG22	2.13	0.47
1:A:1686:VAL:HA	1:A:1722:GLU:HG2	1.97	0.47
1:A:2266:PHE:CE2	1:A:2290:LEU:HD22	2.50	0.47
1:B:1709:LYS:HB2	1:B:1715:ALA:HA	1.97	0.47
1:C:1936:LEU:O	1:C:1937:LEU:HD12	2.15	0.47
1:A:1952:LEU:HD23	1:A:1994:LEU:HD11	1.97	0.46
1:B:1958:ASP:C	1:B:1960:VAL:H	2.22	0.46
1:B:2032:ARG:HG3	1:B:2063:LEU:O	2.15	0.46
1:C:2086:MET:HG2	1:C:2284:MET:O	2.16	0.46
1:D:1579:VAL:O	1:D:1583:THR:OG1	2.31	0.46
1:D:1784:ALA:HA	1:D:1815:ARG:NH2	2.30	0.46
1:D:2237:LEU:CD2	1:D:2251:MET:HE1	2.45	0.46
1:D:2294:VAL:HA	1:D:2297:ILE:HD12	1.97	0.46
1:B:1815:ARG:NH1	1:B:1821:VAL:HB	2.31	0.46
1:B:1832:HIS:C	1:B:1834:GLN:H	2.23	0.46
1:B:2027:TRP:O	1:B:2030:MET:HG2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2093:TRP:CD1	1:B:2284:MET:HE1	2.50	0.46
1:C:1677:GLY:O	1:C:1730:GLN:HG3	2.16	0.46
1:C:1883:TRP:NE1	1:C:1891:ARG:HB3	2.31	0.46
1:C:1953:GLU:HG3	1:C:1995:ARG:NH1	2.29	0.46
1:C:2286:PRO:HA	1:C:2307:LEU:HB2	1.97	0.46
1:A:2241:LEU:HD23	1:A:2241:LEU:O	2.15	0.46
1:C:1580:LEU:HD21	1:C:1643:VAL:CG1	2.45	0.46
1:D:1695:GLU:HG3	1:D:1698:ARG:NH1	2.31	0.46
1:D:2141:GLY:N	1:D:2206:ASP:O	2.49	0.46
1:B:2019:VAL:HG12	1:B:2283:GLU:HG3	1.96	0.46
1:D:2028:GLU:OE1	1:D:2065:GLN:HG2	2.15	0.46
1:D:2240:THR:HG22	1:D:2266:PHE:HA	1.96	0.46
1:C:2237:LEU:HD22	1:C:2251:MET:HE1	1.98	0.46
1:A:1496:ARG:HH22	1:A:1581:GLU:HB3	1.75	0.46
1:A:2070:PRO:HB2	1:A:2077:VAL:HG21	1.97	0.46
1:A:2147:SER:O	1:A:2200:ALA:HA	2.16	0.46
1:B:1551:LEU:HD23	1:B:1551:LEU:HA	1.79	0.46
1:A:1883:TRP:HB3	1:A:1891:ARG:HE	1.81	0.46
1:A:2021:PRO:HD3	1:A:2283:GLU:HG3	1.97	0.46
1:B:1670:SER:HB3	1:B:1676:CYS:SG	2.56	0.46
1:D:1554:ALA:HA	1:D:1578:GLN:HE21	1.81	0.46
1:A:1572:MET:HE2	1:A:1577:ARG:HG2	1.97	0.46
1:B:1588:GLU:HB3	1:B:1973:ARG:NH2	2.31	0.46
1:C:1716:ASP:N	1:C:1716:ASP:OD1	2.46	0.46
1:C:2184:GLU:O	1:C:2188:GLU:HG3	2.16	0.46
1:A:2057:PHE:CZ	1:A:2077:VAL:HG22	2.51	0.46
1:A:2211:SER:OG	1:A:2213:HIS:HB2	2.15	0.46
1:C:1586:LEU:HD22	1:C:1726:VAL:HG23	1.98	0.46
1:D:2131:LEU:HD13	1:D:2131:LEU:HA	1.77	0.46
1:A:1508:TRP:CE2	1:A:1851:ARG:HD3	2.51	0.45
1:A:1926:VAL:HG22	1:A:2317:ILE:HD11	1.98	0.45
1:A:2282:VAL:HG12	1:A:2304:ILE:HB	1.97	0.45
1:B:1820:PRO:HB2	1:B:1875:GLU:OE1	2.16	0.45
1:C:2169:ALA:HB1	1:C:2210:HIS:HB2	1.99	0.45
1:B:1575:GLN:HG2	1:B:1686:VAL:HG13	1.98	0.45
1:B:1844:LYS:HE2	1:B:1855:PRO:HB2	1.99	0.45
1:C:1559:ALA:HB1	1:C:1564:ILE:HB	1.98	0.45
1:C:1660:SER:HB3	1:C:1838:GLY:HA3	1.98	0.45
1:A:2272:ALA:O	1:A:2275:ALA:HB3	2.16	0.45
1:B:1508:TRP:CD1	1:B:1508:TRP:C	2.94	0.45
1:B:1973:ARG:HG2	1:B:1973:ARG:NH1	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1753:GLN:OE1	1:C:1753:GLN:N	2.49	0.45
1:C:1969:LEU:HD23	1:C:1969:LEU:HA	1.80	0.45
1:A:1658:SER:HB3	1:A:1903:THR:CB	2.42	0.45
1:A:1800:ASP:HB2	1:A:1801:PRO:HD3	1.98	0.45
1:A:1953:GLU:OE2	1:A:1995:ARG:HB2	2.17	0.45
1:B:1833:ALA:HB1	1:B:1836:ALA:HB3	1.98	0.45
1:B:2009:GLY:HA3	1:B:2325:VAL:HG12	1.98	0.45
1:B:2234:ALA:HB3	1:B:2235:ILE:HD12	1.96	0.45
1:B:2311:THR:O	1:B:2312:ALA:C	2.59	0.45
1:C:1575:GLN:CD	1:C:1575:GLN:H	2.24	0.45
1:C:1926:VAL:HG13	1:C:1927:LEU:N	2.21	0.45
1:A:1956:VAL:HG21	1:A:1965:LEU:HD11	1.99	0.45
1:B:2023:GLN:HG3	1:B:2024:GLY:H	1.82	0.45
1:D:1718:PHE:CD1	1:D:1720:PHE:CE2	3.05	0.45
1:D:1785:ASP:OD1	1:D:1785:ASP:N	2.49	0.45
1:D:2072:LEU:HD22	1:D:2078:VAL:HG23	1.98	0.45
1:A:1658:SER:HB2	1:A:1662:VAL:HG21	1.98	0.45
1:A:2136:LEU:HD12	1:A:2136:LEU:HA	1.79	0.45
1:B:1575:GLN:CD	1:B:1686:VAL:HG22	2.42	0.45
1:D:1838:GLY:O	1:D:1842:VAL:HG23	2.16	0.45
1:D:1927:LEU:HD21	1:D:1933:VAL:CG1	2.42	0.45
1:D:1968:ALA:CB	1:D:2344:LEU:HD11	2.47	0.45
1:D:2210:HIS:HA	1:D:2260:LEU:O	2.16	0.45
1:D:2248:GLY:O	1:D:2251:MET:HG3	2.16	0.45
1:A:1521:MET:HG3	1:A:1546:ARG:C	2.41	0.45
1:A:2089:LEU:O	1:A:2093:TRP:HD1	2.00	0.45
1:B:1736:ARG:O	1:B:1736:ARG:HD3	2.16	0.45
1:C:1825:SER:O	1:C:1828:SER:HB3	2.17	0.45
1:A:1774:LYS:NZ	1:A:1778:ARG:HH11	2.15	0.45
1:A:2309:ARG:O	1:A:2310:ASP:HB2	2.17	0.45
1:B:2173:SER:C	1:B:2175:SER:N	2.75	0.45
1:B:2210:HIS:HA	1:B:2260:LEU:O	2.17	0.45
1:B:2237:LEU:C	1:B:2237:LEU:HD23	2.41	0.45
1:D:1748:GLY:O	1:D:1907:VAL:HG23	2.17	0.45
1:C:1867:ILE:HB	1:C:1869:TRP:CE2	2.51	0.45
1:D:1941:THR:HG21	1:D:2350:GLU:OE2	2.17	0.45
1:D:2160:ALA:HB3	1:D:2161:PRO:HD3	1.99	0.45
1:A:1833:ALA:HB3	1:A:1837:ALA:HA	1.98	0.45
1:A:2033:GLY:HA3	1:A:2313:GLU:OE2	2.17	0.45
1:B:1557:PHE:CZ	1:B:1580:LEU:HD23	2.52	0.45
1:B:1960:VAL:O	1:B:1987:HIS:HE1	2.00	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2276:ASP:OD2	1:D:2163:GLU:HG3	2.16	0.45
1:A:1501:VAL:HG11	1:A:1507:LEU:HB2	1.98	0.44
1:B:1753:GLN:N	1:B:1753:GLN:CD	2.75	0.44
1:B:1767:ALA:HA	1:B:1770:ARG:HG3	1.98	0.44
1:C:1501:VAL:HG23	1:C:1506:GLU:HB3	1.99	0.44
1:D:1565:SER:OG	1:D:1568:GLU:HG3	2.17	0.44
1:D:2190:VAL:O	1:D:2194:GLU:HG3	2.17	0.44
1:B:1602:THR:HG23	1:B:1678:LEU:O	2.17	0.44
1:B:2320:LEU:HA	1:B:2320:LEU:HD23	1.50	0.44
1:C:1938:SER:CB	1:C:1976:LEU:H	2.29	0.44
1:D:1573:ASP:O	1:D:1576:GLN:HB2	2.18	0.44
1:A:1927:LEU:HD23	1:A:1927:LEU:HA	1.65	0.44
1:A:2139:LEU:HD13	1:A:2213:HIS:HB3	1.99	0.44
1:B:1951:LEU:O	1:B:2345:PRO:HG3	2.17	0.44
1:B:2074:ARG:O	1:B:2078:VAL:HG12	2.18	0.44
1:C:1976:LEU:O	1:C:1979:ARG:HG3	2.18	0.44
1:D:1592:ILE:HG21	1:D:1597:LEU:HD11	1.99	0.44
1:A:1711:PHE:CZ	1:A:1823:LEU:HD21	2.53	0.44
1:A:2039:VAL:HG13	1:A:2040:PHE:N	2.32	0.44
1:A:2154:ARG:HH11	1:A:2158:LEU:HD11	1.83	0.44
1:D:1898:PHE:CD1	1:D:1904:ASN:HB3	2.52	0.44
1:B:1592:ILE:O	1:B:1594:PRO:HD3	2.16	0.44
1:C:2128:VAL:HA	1:C:2225:LEU:HD22	1.99	0.44
1:C:2147:SER:OG	1:C:2203:LEU:HD21	2.17	0.44
1:A:2039:VAL:HG13	1:A:2040:PHE:H	1.82	0.44
1:B:1575:GLN:CG	1:B:1686:VAL:HG22	2.48	0.44
1:C:1496:ARG:HB2	1:C:1724:VAL:HG12	1.99	0.44
1:C:1597:LEU:N	1:C:1597:LEU:HD22	2.33	0.44
1:C:1990:LEU:O	1:C:1994:LEU:HG	2.16	0.44
1:D:1953:GLU:HA	1:D:1994:LEU:HD13	1.99	0.44
1:A:2177:VAL:HG12	1:A:2178:VAL:N	2.33	0.44
1:B:1960:VAL:O	1:B:1960:VAL:HG13	2.17	0.44
1:B:2145:MET:HE1	1:B:2209:SER:HB2	1.98	0.44
1:C:1508:TRP:HZ3	1:C:1848:GLY:HA2	1.83	0.44
1:C:2050:VAL:O	1:C:2053:GLU:N	2.48	0.44
1:D:1871:SER:O	1:D:1871:SER:OG	2.35	0.44
1:D:1936:LEU:C	1:D:1937:LEU:HD12	2.43	0.44
1:D:2162:TRP:CH2	1:D:2189:LEU:HA	2.52	0.44
1:A:1749:SER:O	1:A:1778:ARG:NH2	2.51	0.44
1:A:2163:GLU:CD	1:B:2245:ARG:HD3	2.42	0.44
1:B:1976:LEU:HB3	1:B:1977:PRO:HD2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1575:GLN:HB3	1:C:1686:VAL:HG22	1.99	0.44
1:C:1586:LEU:HD22	1:C:1726:VAL:CG2	2.47	0.44
1:C:2347:TYR:CE1	1:C:2349:PHE:HA	2.52	0.44
1:D:2042:GLU:O	1:D:2045:ALA:HB3	2.17	0.44
1:D:2145:MET:HG2	1:D:2180:SER:CB	2.48	0.44
1:D:2173:SER:C	1:D:2175:SER:N	2.75	0.44
1:A:1577:ARG:NH1	1:A:2354:TYR:HB2	2.33	0.44
1:A:2159:ILE:HG22	1:A:2189:LEU:HD22	1.99	0.44
1:C:2218:ARG:NH1	1:D:2250:ASP:HA	2.32	0.44
1:D:1770:ARG:HD2	1:D:1770:ARG:HA	1.26	0.44
1:D:2251:MET:HA	1:D:2255:TYR:HB2	1.99	0.44
1:B:2017:VAL:HG23	1:B:2278:HIS:ND1	2.33	0.43
1:C:1493:MET:HE2	1:C:1743:LEU:HD13	1.99	0.43
1:C:1776:TRP:HH2	1:C:1810:THR:O	2.00	0.43
1:D:1732:LEU:O	1:D:1735:ALA:N	2.51	0.43
1:B:1684:VAL:HG23	1:B:1724:VAL:HG22	2.01	0.43
1:B:2323:ALA:HB1	1:B:2328:VAL:HG21	1.99	0.43
1:D:1555:ALA:O	1:D:1577:ARG:NH1	2.51	0.43
1:D:1659:SER:O	1:D:1662:VAL:HG12	2.18	0.43
1:A:1561:PHE:HA	1:A:1940:ARG:HD2	2.00	0.43
1:A:1938:SER:CB	1:A:1976:LEU:H	2.28	0.43
1:B:2182:ASP:HA	1:B:2183:PRO:HD3	1.91	0.43
1:C:2172:ASN:HA	1:C:2266:PHE:HB3	1.99	0.43
1:D:1564:ILE:HG23	1:D:1568:GLU:HB2	2.00	0.43
1:D:1570:LEU:HD11	1:D:2355:TRP:N	2.33	0.43
1:A:2043:SER:OG	1:A:2088:SER:OG	2.36	0.43
1:A:2074:ARG:O	1:A:2078:VAL:HG12	2.19	0.43
1:A:2222:LEU:HD21	1:A:2254:ARG:HA	1.99	0.43
1:C:1797:ARG:HH11	1:C:1866:LEU:CD1	2.27	0.43
1:C:2265:ARG:HD3	1:C:2268:GLU:OE2	2.17	0.43
1:B:1864:SER:HB3	1:B:1867:ILE:HD12	2.00	0.43
1:C:1784:ALA:HB2	1:C:1815:ARG:HD2	2.01	0.43
1:C:1827:LYS:HG2	1:C:1832:HIS:CA	2.46	0.43
1:D:1632:SER:HB3	1:D:1635:VAL:HG23	1.99	0.43
1:A:1608:ALA:HA	1:A:1835:ALA:CB	2.48	0.43
1:A:1636:VAL:HG12	1:A:1652:THR:CG2	2.49	0.43
1:B:2082:LEU:HD23	1:B:2082:LEU:HA	1.69	0.43
1:C:1853:LEU:HD23	1:C:1880:VAL:HG13	2.00	0.43
1:C:2136:LEU:HA	1:C:2136:LEU:HD23	1.84	0.43
1:D:1521:MET:HE3	1:D:1550:PHE:HZ	1.81	0.43
1:D:1792:HIS:CD2	1:D:1794:THR:HG23	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2027:TRP:CZ2	1:D:2030:MET:HA	2.53	0.43
1:A:1511:ILE:C	1:A:1514:GLY:H	2.22	0.43
1:A:1973:ARG:HH12	1:A:2344:LEU:HD12	1.82	0.43
1:A:2111:ILE:HD13	1:A:2128:VAL:HG12	2.00	0.43
1:A:2283:GLU:OE2	1:A:2285:SER:OG	2.32	0.43
1:D:1551:LEU:HD23	1:D:1551:LEU:HA	1.82	0.43
1:A:1654:ASP:O	1:A:1655:THR:C	2.62	0.43
1:B:1753:GLN:HA	1:B:1902:GLY:O	2.19	0.43
1:C:2110:GLU:OE2	1:C:2240:THR:N	2.40	0.43
1:D:2018:PHE:CE1	1:D:2284:MET:HE3	2.54	0.43
1:D:1690:PRO:O	1:D:1694:THR:HG23	2.19	0.43
1:D:1752:ASN:ND2	1:D:1771:VAL:HB	2.33	0.43
1:D:1798:LEU:C	1:D:1801:PRO:HD2	2.43	0.43
1:D:2087:VAL:O	1:D:2090:ALA:HB3	2.18	0.43
1:D:2251:MET:HA	1:D:2255:TYR:CB	2.49	0.43
1:A:1521:MET:HG3	1:A:1546:ARG:O	2.18	0.43
1:C:1867:ILE:HB	1:C:1869:TRP:NE1	2.33	0.43
1:C:2173:SER:C	1:C:2175:SER:H	2.27	0.43
1:A:1610:TYR:C	1:A:1611:GLN:HG2	2.43	0.42
1:A:2287:HIS:O	1:A:2289:VAL:HG13	2.19	0.42
1:A:2347:TYR:HE1	1:A:2349:PHE:HA	1.84	0.42
1:B:1664:LEU:HD23	1:B:1668:CYS:SG	2.59	0.42
1:B:1894:GLY:HA2	1:B:1908:ILE:HD13	2.00	0.42
1:B:2027:TRP:CH2	1:B:2030:MET:HA	2.53	0.42
1:B:2032:ARG:HA	1:B:2035:LEU:CD1	2.49	0.42
1:B:2238:TYR:HB3	1:B:2269:ALA:HB1	2.01	0.42
1:C:1595:HIS:CD2	1:C:1974:ALA:HB1	2.54	0.42
1:C:1785:ASP:O	1:C:1892:ARG:HB2	2.18	0.42
1:D:1660:SER:HB3	1:D:1835:ALA:O	2.19	0.42
1:D:1939:ALA:HB2	1:D:1948:GLN:OE1	2.19	0.42
1:A:2144:GLY:O	1:A:2186:LEU:HD11	2.18	0.42
1:A:2209:SER:HB2	1:A:2260:LEU:HD11	2.02	0.42
1:A:2238:TYR:HA	1:A:2245:ARG:HA	2.00	0.42
1:B:2136:LEU:HA	1:B:2136:LEU:HD23	1.76	0.42
1:C:2058:SER:CB	1:C:2061:GLU:HG3	2.48	0.42
1:C:2107:SER:OG	1:C:2108:GLN:N	2.52	0.42
1:D:1977:PRO:O	1:D:1979:ARG:HG3	2.18	0.42
1:D:2043:SER:HG	1:D:2088:SER:HG	1.66	0.42
1:A:1507:LEU:O	1:A:1510:PHE:N	2.50	0.42
1:A:1531:ALA:O	1:A:1542:THR:HG22	2.19	0.42
1:A:1579:VAL:O	1:A:1583:THR:OG1	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1781:ILE:HD11	1:A:1908:ILE:HG12	2.00	0.42
1:B:1926:VAL:C	1:B:1928:ALA:N	2.76	0.42
1:B:2101:SER:O	1:B:2236:PRO:HD2	2.19	0.42
1:D:1705:ASP:OD1	1:D:1709:LYS:NZ	2.53	0.42
1:D:1815:ARG:HD3	1:D:1819:GLY:O	2.19	0.42
1:A:1657:CYS:O	1:A:1899:GLY:HA3	2.19	0.42
1:A:1955:ALA:HB1	1:A:2345:PRO:HD3	2.01	0.42
1:A:2156:ARG:HD2	1:A:2156:ARG:HA	1.75	0.42
1:B:1706:GLY:O	1:B:1719:GLY:HA3	2.19	0.42
1:B:1950:ARG:C	1:B:1952:LEU:H	2.26	0.42
1:C:2083:PHE:O	1:C:2087:VAL:HG12	2.20	0.42
1:D:2212:ARG:O	1:D:2215:GLU:HG3	2.18	0.42
1:A:2020:PHE:O	1:A:2109:GLY:HA3	2.19	0.42
1:A:2282:VAL:HA	1:A:2304:ILE:O	2.19	0.42
1:B:1655:THR:OG1	1:B:1834:GLN:NE2	2.53	0.42
1:B:1827:LYS:HD3	1:B:1832:HIS:HA	2.00	0.42
1:B:1852:GLY:O	1:B:1853:LEU:HD23	2.18	0.42
1:B:1995:ARG:O	1:B:1998:ALA:HB3	2.20	0.42
1:C:1784:ALA:HA	1:C:1815:ARG:NE	2.34	0.42
1:C:2061:GLU:HA	1:C:2066:ARG:HG3	2.02	0.42
1:D:1752:ASN:C	1:D:1753:GLN:HG2	2.43	0.42
1:D:2199:ARG:H	1:D:2199:ARG:CD	2.26	0.42
1:A:2043:SER:HG	1:A:2088:SER:HG	1.64	0.42
1:B:1508:TRP:CZ3	1:B:1848:GLY:HA2	2.54	0.42
1:C:2048:ASP:O	1:C:2052:SER:HB3	2.19	0.42
1:D:1958:ASP:OD1	1:D:1991:ARG:NH2	2.34	0.42
1:A:1983:LEU:CD2	1:A:2317:ILE:HG22	2.50	0.42
1:B:1512:VAL:HG13	1:B:1880:VAL:HG21	2.01	0.42
1:B:1865:PRO:C	1:B:1867:ILE:H	2.27	0.42
1:B:1953:GLU:O	1:B:1954:SER:C	2.63	0.42
1:B:2079:GLN:HB2	1:B:2080:PRO:HD3	2.01	0.42
1:C:1561:PHE:HZ	1:C:1584:TRP:CZ2	2.38	0.42
1:C:1670:SER:HB3	1:C:1676:CYS:SG	2.58	0.42
1:D:1681:ALA:O	1:D:1726:VAL:HA	2.20	0.42
1:D:2027:TRP:CZ3	1:D:2030:MET:HA	2.54	0.42
1:A:1891:ARG:HD2	1:A:1911:GLU:OE2	2.20	0.42
1:A:2075:VAL:HA	1:A:2078:VAL:HG12	2.01	0.42
1:B:1659:SER:OG	1:B:1660:SER:N	2.52	0.42
1:B:1933:VAL:HG11	1:B:1962:LEU:HB3	2.01	0.42
1:C:1563:GLY:C	1:C:1564:ILE:HD13	2.45	0.42
1:C:2252:GLY:O	1:C:2253:PRO:C	2.63	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2051:LEU:HD12	1:D:2055:ALA:HB3	2.01	0.42
1:B:2160:ALA:HB3	1:B:2161:PRO:HD3	2.02	0.42
1:C:1606:LEU:HD22	1:C:1682:GLY:C	2.45	0.42
1:C:2034:LEU:O	1:C:2037:VAL:HG22	2.20	0.42
1:D:1783:GLY:O	1:D:1815:ARG:NH2	2.49	0.42
1:D:2106:HIS:CE1	1:D:2264:VAL:HG11	2.55	0.42
1:A:1678:LEU:CD2	1:A:1728:LEU:HD11	2.49	0.42
1:B:1498:PRO:HD3	1:B:1722:GLU:O	2.20	0.42
1:D:2079:GLN:HG2	1:D:2108:GLN:CD	2.45	0.42
1:A:1926:VAL:HG22	1:A:1927:LEU:H	1.85	0.41
1:B:1930:ALA:HB1	1:B:2314:GLU:HG3	2.02	0.41
1:C:1734:ASP:HA	1:C:1737:ARG:HB3	2.01	0.41
1:C:1866:LEU:HD12	1:C:1866:LEU:N	2.35	0.41
1:D:1575:GLN:NE2	1:D:1611:GLN:OE1	2.53	0.41
1:D:1598:ARG:CZ	1:D:1598:ARG:HB3	2.50	0.41
1:D:2353:ARG:CZ	1:D:2355:TRP:HB3	2.50	0.41
1:A:1604:VAL:HG12	1:A:1606:LEU:HG	2.01	0.41
1:A:1692:VAL:O	1:A:1720:PHE:HE2	2.03	0.41
1:A:2095:ALA:C	1:A:2097:GLY:H	2.27	0.41
1:B:1554:ALA:HA	1:B:1578:GLN:NE2	2.35	0.41
1:B:1898:PHE:HD1	1:B:1904:ASN:HB3	1.83	0.41
1:B:2141:GLY:N	1:B:2206:ASP:O	2.48	0.41
1:C:2347:TYR:HA	1:C:2348:PRO:HD2	1.94	0.41
1:D:1557:PHE:CD1	1:D:1577:ARG:HB3	2.55	0.41
1:D:2032:ARG:NH2	1:D:2064:GLU:O	2.53	0.41
1:D:2126:VAL:HA	1:D:2129:VAL:HG12	2.01	0.41
1:D:2248:GLY:HA2	1:D:2251:MET:HG3	2.02	0.41
1:A:1793:GLY:HA3	1:A:1825:SER:HB2	2.01	0.41
1:B:1603:GLY:HA2	1:B:1649:PRO:O	2.20	0.41
1:B:1732:LEU:O	1:B:1735:ALA:N	2.51	0.41
1:B:2018:PHE:CD2	1:B:2100:PRO:HB3	2.55	0.41
1:B:2050:VAL:HA	1:B:2053:GLU:HB2	2.03	0.41
1:C:2131:LEU:HD23	1:C:2131:LEU:HA	1.79	0.41
1:D:1572:MET:HE3	1:D:1576:GLN:HB3	2.02	0.41
1:D:2076:ASP:OD2	1:D:2137:ARG:HD3	2.19	0.41
1:A:1678:LEU:HD21	1:A:1728:LEU:HD21	2.01	0.41
1:B:2105:GLY:CA	1:B:2110:GLU:HG2	2.48	0.41
1:C:2182:ASP:OD1	1:C:2213:HIS:NE2	2.52	0.41
1:D:1953:GLU:HB2	1:D:1994:LEU:HB3	2.01	0.41
1:A:1529:LEU:HD12	1:A:1530:ASP:N	2.34	0.41
1:A:1605:PHE:O	1:A:1681:ALA:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1862:GLU:HG2	1:A:1863:ARG:N	2.35	0.41
1:B:1508:TRP:CE3	1:B:1847:LEU:HB3	2.56	0.41
1:B:2057:PHE:CZ	1:B:2077:VAL:HG22	2.56	0.41
1:C:1808:LEU:HB3	1:C:1871:SER:HB2	2.01	0.41
1:C:1839:VAL:O	1:C:1843:ILE:HG13	2.20	0.41
1:C:2017:VAL:HG11	1:C:2104:ILE:HD12	2.02	0.41
1:D:2127:ARG:HG3	1:D:2131:LEU:HD23	2.03	0.41
1:B:1659:SER:O	1:B:1662:VAL:HG23	2.20	0.41
1:B:2270:VAL:HB	1:B:2297:ILE:HD13	2.02	0.41
1:C:1718:PHE:CE1	1:C:1720:PHE:CZ	3.09	0.41
1:C:2237:LEU:HD23	1:C:2238:TYR:C	2.44	0.41
1:B:1562:PHE:CE2	1:B:1580:LEU:HG	2.55	0.41
1:B:1658:SER:HB3	1:B:1662:VAL:HG21	2.02	0.41
1:C:2241:LEU:HD23	1:C:2241:LEU:O	2.21	0.41
1:D:1968:ALA:HB1	1:D:2344:LEU:HD11	2.01	0.41
1:A:1574:PRO:HA	1:A:1577:ARG:HG3	2.02	0.41
1:A:1766:VAL:O	1:A:1770:ARG:HG3	2.21	0.41
1:A:1990:LEU:O	1:A:1994:LEU:HB2	2.21	0.41
1:B:1518:VAL:O	1:B:1707:ARG:NH2	2.53	0.41
1:C:2031:ALA:HB2	1:C:2307:LEU:CD1	2.50	0.41
1:D:1575:GLN:HB3	1:D:1684:VAL:HG13	2.02	0.41
1:D:1811:TYR:HB3	1:D:1821:VAL:HG11	2.03	0.41
1:D:2105:GLY:CA	1:D:2110:GLU:HG2	2.45	0.41
1:A:1834:GLN:HE21	1:A:1834:GLN:HB3	1.69	0.41
1:A:2016:VAL:O	1:A:2101:SER:N	2.51	0.41
1:C:1945:LEU:HD23	1:C:1945:LEU:O	2.20	0.41
1:C:2018:PHE:CD2	1:C:2100:PRO:HB3	2.54	0.41
1:C:2092:LEU:O	1:C:2095:ALA:N	2.54	0.41
1:D:1639:ARG:O	1:D:1643:VAL:HG23	2.21	0.41
1:D:2146:VAL:HG12	1:D:2202:THR:HA	2.03	0.41
1:D:2175:SER:O	1:D:2175:SER:OG	2.33	0.41
1:A:1588:GLU:HG2	1:A:1973:ARG:NE	2.36	0.41
1:B:2146:VAL:HG23	1:B:2186:LEU:HD22	2.01	0.41
1:C:2148:LEU:HB2	1:C:2177:VAL:CG2	2.51	0.41
1:A:1522:PRO:HD3	1:A:1550:PHE:CE1	2.56	0.40
1:A:1826:VAL:HB	1:A:1844:LYS:HD3	2.02	0.40
1:C:2040:PHE:CD2	1:C:2092:LEU:HD12	2.54	0.40
1:D:1635:VAL:CG1	1:D:1639:ARG:HD3	2.50	0.40
1:D:1776:TRP:HZ2	1:D:1811:TYR:CE1	2.39	0.40
1:D:1786:VAL:O	1:D:1815:ARG:NH2	2.47	0.40
1:D:1999:GLU:HG2	1:D:2001:VAL:HG13	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2186:LEU:O	1:D:2190:VAL:HG13	2.21	0.40
1:B:1555:ALA:HB3	1:B:2353:ARG:HG3	2.03	0.40
1:B:1683:GLY:HA3	1:B:1835:ALA:O	2.21	0.40
1:B:1703:ALA:HB2	1:B:1717:GLY:O	2.21	0.40
1:B:2040:PHE:CE1	1:B:2089:LEU:HD23	2.56	0.40
1:B:2095:ALA:C	1:B:2097:GLY:H	2.29	0.40
1:B:2133:ALA:HA	1:B:2136:LEU:HB2	2.03	0.40
1:B:2287:HIS:CG	1:B:2288:PRO:HD2	2.56	0.40
1:D:2027:TRP:CD1	1:D:2309:ARG:HB3	2.56	0.40
1:D:2105:GLY:HA3	1:D:2110:GLU:HA	2.03	0.40
1:B:1766:VAL:O	1:B:1770:ARG:HG3	2.22	0.40
1:B:2064:GLU:OE1	1:B:2066:ARG:NE	2.51	0.40
1:C:1580:LEU:HA	1:C:1580:LEU:HD23	1.78	0.40
1:A:1776:TRP:HB3	1:A:1781:ILE:O	2.20	0.40
1:A:1854:VAL:HA	1:A:1855:PRO:HD2	1.93	0.40
1:B:1508:TRP:HB2	1:B:1847:LEU:HD13	2.03	0.40
1:B:1677:GLY:O	1:B:1678:LEU:HB2	2.21	0.40
1:C:1575:GLN:HB2	1:C:1684:VAL:CG1	2.51	0.40
1:C:1982:LEU:CD1	1:C:1994:LEU:HD23	2.49	0.40
1:C:2308:HIS:HB2	1:C:2315:HIS:ND1	2.37	0.40
1:D:1790:GLU:OE2	1:D:1826:VAL:HB	2.22	0.40
1:A:2093:TRP:O	1:A:2098:VAL:N	2.52	0.40
1:A:2309:ARG:O	1:A:2310:ASP:CB	2.69	0.40
1:B:1563:GLY:C	1:B:1564:ILE:HD13	2.46	0.40
1:C:1556:ASP:HB3	1:C:2351:PRO:HB3	2.04	0.40
1:C:2074:ARG:O	1:C:2078:VAL:HG12	2.22	0.40
1:C:2143:GLY:HA2	1:C:2183:PRO:HD3	2.04	0.40
1:D:1495:CYS:HB2	1:D:1497:PHE:CE2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2054:VAL:O	1:D:1773:ARG:NH1[2_656]	1.85	0.35

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	808/881 (92%)	725 (90%)	68 (8%)	15 (2%)	6	23
1	B	774/881 (88%)	687 (89%)	67 (9%)	20 (3%)	4	17
1	C	734/881 (83%)	666 (91%)	54 (7%)	14 (2%)	6	23
1	D	805/881 (91%)	733 (91%)	59 (7%)	13 (2%)	7	27
All	All	3121/3524 (89%)	2811 (90%)	248 (8%)	62 (2%)	6	22

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1656	ALA
1	A	1913	PRO
1	A	1926	VAL
1	A	2026	GLN
1	A	2310	ASP
1	A	2312	ALA
1	B	1793	GLY
1	B	1926	VAL
1	B	1954	SER
1	B	1957	ASP
1	B	2310	ASP
1	B	2312	ALA
1	C	1793	GLY
1	C	1794	THR
1	C	1880	VAL
1	C	2069	ALA
1	C	2312	ALA
1	D	1957	ASP
1	D	2069	ALA
1	D	2310	ASP
1	D	2312	ALA
1	A	1927	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1956	VAL
1	B	1977	PRO
1	B	2174	PRO
1	C	1926	VAL
1	C	2023	GLN
1	C	2284	MET
1	C	2310	ASP
1	D	1956	VAL
1	A	2061	GLU
1	A	2175	SER
1	B	1833	ALA
1	B	2013	ALA
1	B	2061	GLU
1	B	2127	ARG
1	C	1977	PRO
1	D	1816	GLY
1	D	2174	PRO
1	A	1977	PRO
1	B	1678	LEU
1	B	1959	SER
1	B	2130	ALA
1	C	1795	GLY
1	D	1660	SER
1	D	1960	VAL
1	D	2013	ALA
1	A	1504	PRO
1	A	1655	THR
1	B	1834	GLN
1	D	1977	PRO
1	D	2068	ASP
1	A	2174	PRO
1	C	2174	PRO
1	C	2253	PRO
1	C	2307	LEU
1	D	1658	SER
1	B	2351	PRO
1	B	2228	ILE
1	A	2204	PRO
1	B	1512	VAL
1	B	1961	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	818/881 (92%)	0.28	7 (0%) 81 75	25, 48, 77, 99	0
1	B	786/881 (89%)	0.31	21 (2%) 56 47	24, 49, 81, 98	0
1	C	750/881 (85%)	0.86	48 (6%) 25 20	41, 74, 103, 119	0
1	D	815/881 (92%)	0.53	18 (2%) 62 53	40, 63, 85, 109	0
All	All	3169/3524 (89%)	0.49	94 (2%) 52 43	24, 59, 91, 119	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1511	ILE	6.3
1	A	1956	VAL	5.4
1	C	1720	PHE	5.4
1	C	1570	LEU	4.5
1	C	1569	ALA	4.3
1	B	1636	VAL	4.0
1	B	1959	SER	4.0
1	D	1925	GLY	3.9
1	B	1718	PHE	3.9
1	C	2025	ALA	3.8
1	B	1702	LEU	3.7
1	C	1636	VAL	3.7
1	C	1872	GLY	3.5
1	D	2355	TRP	3.5
1	B	1612	GLY	3.3
1	C	1562	PHE	3.3
1	C	1871	SER	3.3
1	C	1798	LEU	3.3
1	C	1940	ARG	3.3
1	C	1566	PRO	3.3
1	C	1889	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	1631	ASN	3.2
1	B	1720	PHE	3.1
1	C	1784	ALA	3.1
1	C	1572	MET	3.1
1	B	1925	GLY	3.0
1	D	1527	TRP	2.9
1	C	1512	VAL	2.9
1	C	2207	TYR	2.9
1	A	1955	ALA	2.9
1	C	1817	SER	2.9
1	C	1719	GLY	2.9
1	C	2209	SER	2.9
1	C	1516	ASP	2.8
1	B	1955	ALA	2.8
1	C	1652	THR	2.8
1	C	1517	ALA	2.7
1	C	1554	ALA	2.7
1	C	1557	PHE	2.7
1	B	1514	GLY	2.7
1	D	1499	GLY	2.6
1	C	1609	ALA	2.6
1	D	1779	ALA	2.6
1	B	1954	SER	2.6
1	A	1654	ASP	2.6
1	C	1686	VAL	2.6
1	D	1720	PHE	2.5
1	A	1701	GLY	2.5
1	C	1961	PRO	2.5
1	C	2004	PRO	2.5
1	D	2356	LEU	2.5
1	C	1879	ALA	2.5
1	C	2224	ASP	2.5
1	B	1522	PRO	2.5
1	D	2009	GLY	2.5
1	B	2355	TRP	2.5
1	C	1498	PRO	2.4
1	B	1713	ALA	2.4
1	B	1712	SER	2.4
1	B	1960	VAL	2.3
1	B	1958	ASP	2.3
1	C	1513	GLY	2.3
1	C	1508	TRP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	2306	SER	2.3
1	B	2165	ARG	2.3
1	B	1704	VAL	2.3
1	D	1696	PHE	2.3
1	C	1858	LEU	2.3
1	D	1635	VAL	2.3
1	D	1688	ALA	2.2
1	C	1579	VAL	2.2
1	D	1526	GLY	2.2
1	D	2162	TRP	2.2
1	C	1571	ALA	2.2
1	D	1490	ILE	2.2
1	C	1573	ASP	2.2
1	B	1517	ALA	2.2
1	C	1888	ASP	2.2
1	D	1612	GLY	2.2
1	C	1658	SER	2.2
1	C	1778	ARG	2.1
1	D	1689	GLY	2.1
1	C	1711	PHE	2.1
1	B	1686	VAL	2.1
1	C	1951	LEU	2.1
1	C	1859	CYS	2.1
1	A	1692	VAL	2.1
1	D	1630	GLY	2.1
1	A	1957	ASP	2.1
1	B	1926	VAL	2.0
1	C	2350	GLU	2.0
1	C	1487	PRO	2.0
1	A	1839	VAL	2.0
1	C	1854	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.