Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 09:56 pm BST

PDB ID	:	1UYV
Title	:	Acetyl-CoA carboxylase carboxyltransferase domain L1705I/V1967I mutant
Authors	:	Zhang, H.; Tweel, B.; Tong, L.
Deposited on	:	2004-03-02
Resolution	:	2.60 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:

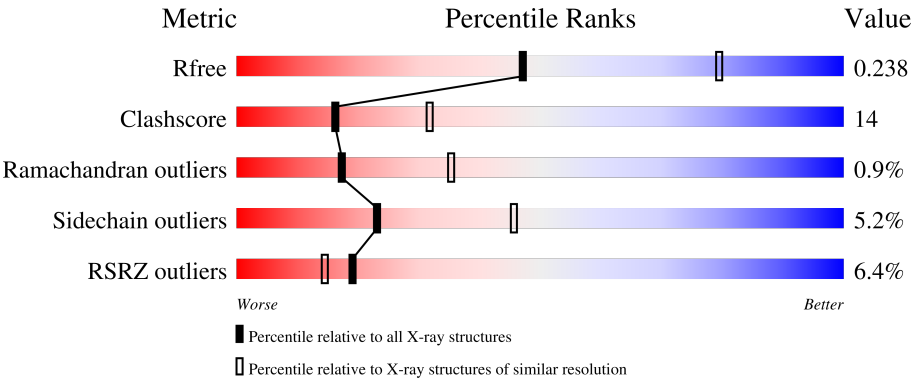
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	737	5% 54% 22% · 22%
1	B	737	4% 51% 23% · 25%
1	C	737	6% 53% 22% · 23%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13666 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-COA CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	1
			4542	2895	786	845	16			
1	B	553	Total	C	N	O	S	0	0	1
			4399	2805	759	821	14			
1	C	571	Total	C	N	O	S	0	0	1
			4533	2884	786	847	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1705	ILE	LEU	engineered mutation	UNP Q00955
A	1967	ILE	VAL	engineered mutation	UNP Q00955
B	1705	ILE	LEU	engineered mutation	UNP Q00955
B	1967	ILE	VAL	engineered mutation	UNP Q00955
C	1705	ILE	LEU	engineered mutation	UNP Q00955
C	1967	ILE	VAL	engineered mutation	UNP Q00955

- Molecule 2 is water.

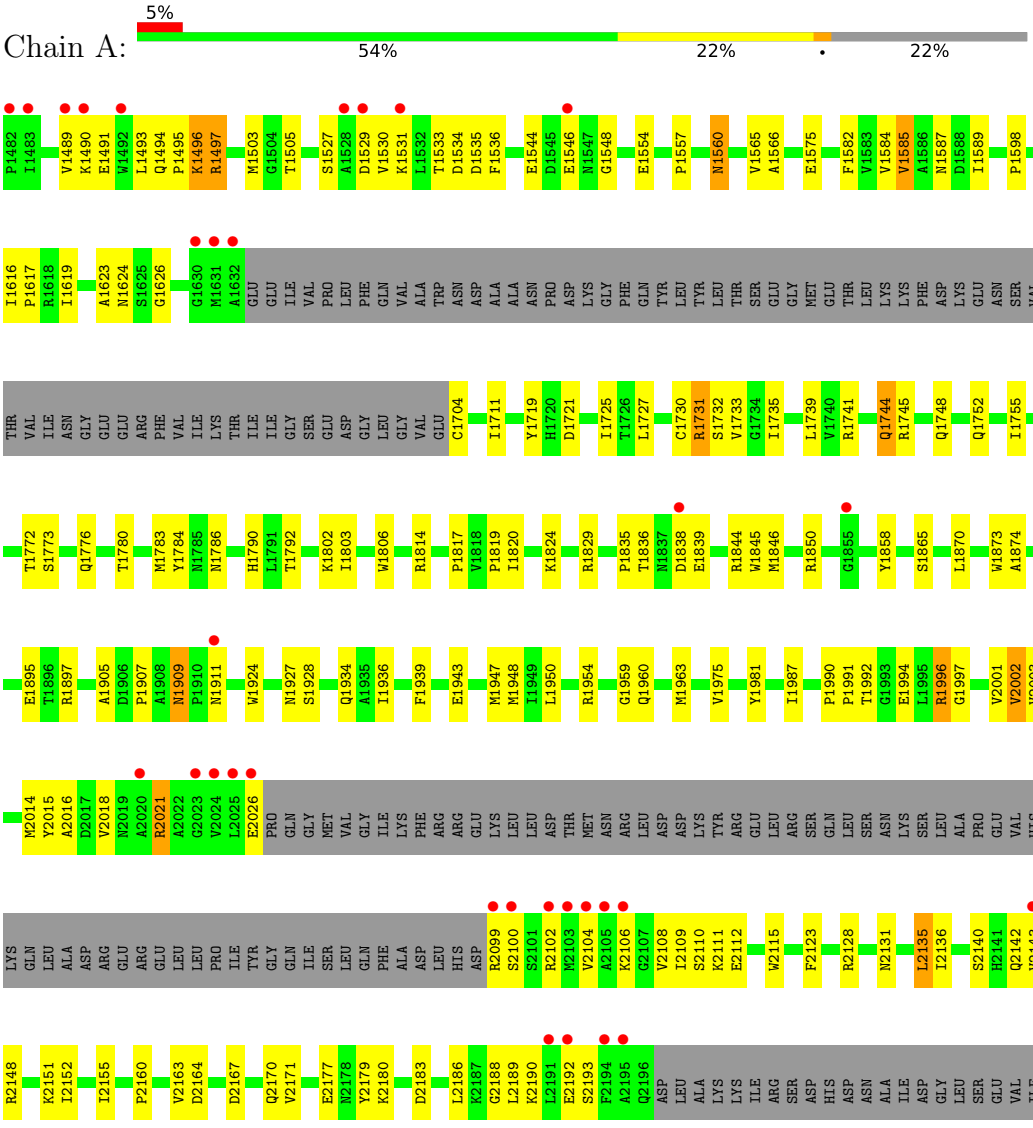
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	75	Total	O	0	0
			75	75		
2	B	68	Total	O	0	0
			68	68		
2	C	49	Total	O	0	0
			49	49		

3 Residue-property plots (i)

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.

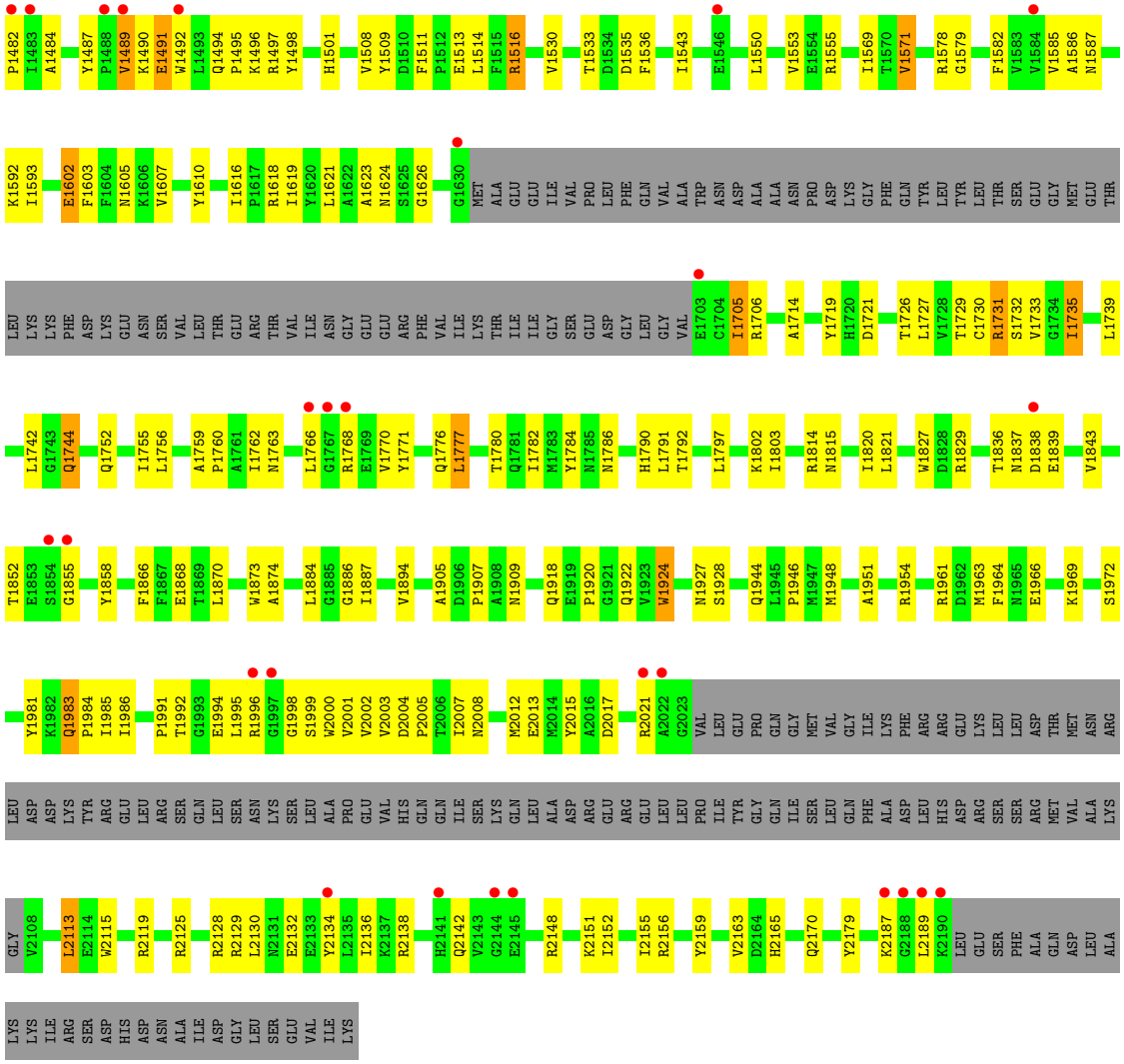
• Molecule 1: ACETYL-COA CARBOXYLASE

Chain A:



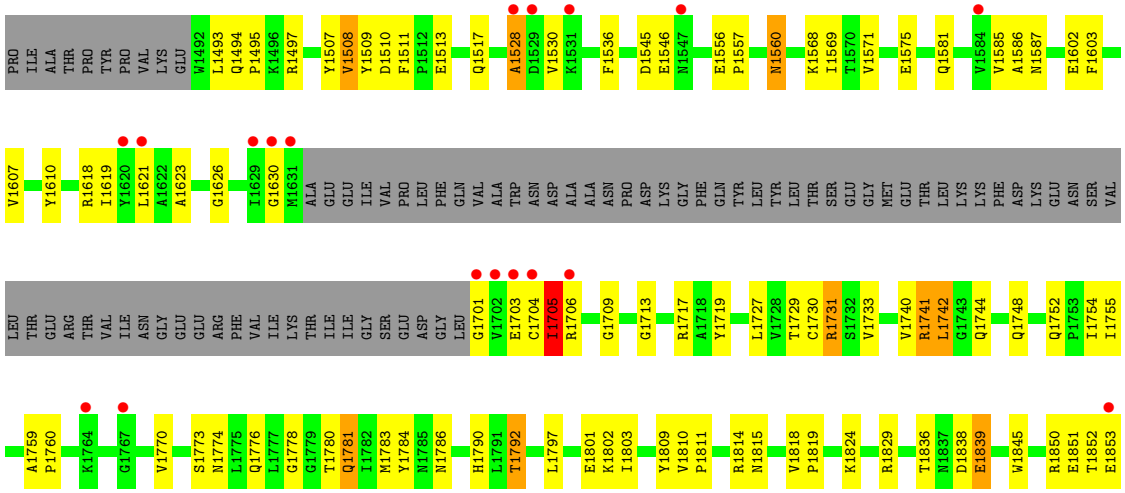
• Molecule 1: ACETYL-COA CARBOXYLASE

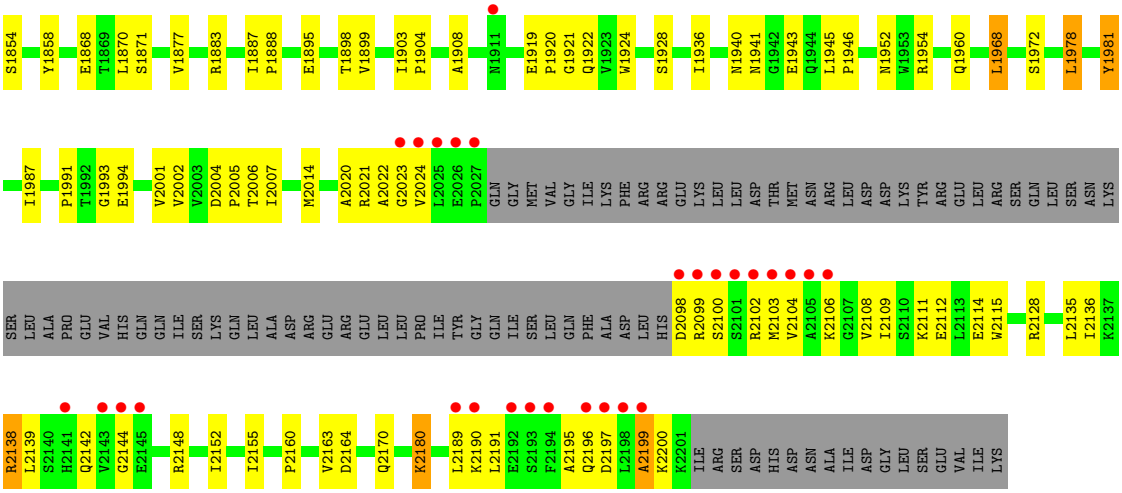
Chain B:



• Molecule 1: ACETYL-COA CARBOXYLASE

Chain C:




S1854 Y1858 E1868 T1869 L1870 S1871 V1877 R1883 I1887 P1888 E1895 T1898 V1899 I1903 P1904 A1908 N1911 E1919 P1920 G1921 Q1922 V1923 W1924 S1928 I1936 N1940 N1941 G1942 E1943 Q1944 L1945 P1946 N1952 W1953 R1954 Q1960 L1968 S1972 L1978 Y1981
I1987 P1991 T1992 G1993 E1994 V2001 V2002 V2003 D2004 P2005 T2006 I2007 M2014 A2020 R2021 A2022 G2023 V2024 L2025 E2026 P2027 GLN GLY MET VAL GLY ILE LYS PHE ARG ARG GLU LYS LEU LEU ASP THR MET ASN ARG LEU ASP ASP LYS TYR ARG GLU LEU ARG SER GLN LEU SER ASN LYS
SER LEU ALA PRO GLU VAL HIS GLN GLN ILE SER LYS GLN LEU ALA ASP ARG GLU ARG GLU LEU LEU PRO ILE TYR GLY GLN ILE SER LEU GLN PHE ALA ASP LEU HIS D2098 R2099 S2100 S2101 R2102 M2103 V2104 A2105 K2106 G2107 V2108 I2109 S2110 K2111 E2112 L2113 E2114 W2115 R2128 L2135 I2136 K2137
R2138 L2139 S2140 H2141 Q2142 V2143 G2144 E2145 R2148 I2152 I2155 P2160 V2163 D2164 Q2170 K2180 L2189 K2190 L2191 E2192 S2193 F2194 A2195 Q2196 D2197 L2198 A2199 K2200 K2201 ILE ARG SER ASP HIS ASP ASN ALA ILE ASP GLY LEU SER GLU VAL ILE LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	247.17Å 123.73Å 145.64Å 90.00° 94.20° 90.00°	Depositor
Resolution (Å)	27.56 – 2.60 27.56 – 2.52	Depositor EDS
% Data completeness (in resolution range)	87.2 (27.56-2.60) 88.8 (27.56-2.52)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.237 0.213 , 0.238	Depositor DCC
R_{free} test set	12751 reflections (9.38%)	wwPDB-VP
Wilson B-factor (Å^2)	42.2	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13666	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.40	0/4647	0.58	0/6299
1	B	0.40	0/4503	0.58	0/6109
1	C	0.39	0/4635	0.56	0/6280
All	All	0.40	0/13785	0.57	0/18688

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	4542	0	4484	128	0
1	B	4399	0	4326	137	0
1	C	4533	0	4467	137	0
2	A	75	0	0	0	0
2	B	68	0	0	1	0
2	C	49	0	0	2	0
All	All	13666	0	13277	386	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 14.

All (386) 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:C:2144:GLY:HA3	1:C:2197:ASP:HB3	1.46	0.94
1:C:1759:ALA:H	1:C:1774:ASN:HD21	1.07	0.92
1:B:1815:ASN:H	1:B:1944:GLN:HE22	0.97	0.92
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.36	0.90
1:A:1772:THR:H	1:A:1776:GLN:HE22	1.16	0.90
1:A:2135:LEU:HB3	1:A:2155:ILE:HD13	1.54	0.87
1:B:1766:LEU:HD13	1:B:1770:VAL:HG21	1.57	0.87
1:A:2164:ASP:H	1:A:2170:GLN:NE2	1.74	0.86
1:B:1705:ILE:HD13	1:B:1705:ILE:H	1.39	0.86
1:A:1496:LYS:H	1:A:1496:LYS:HD2	1.41	0.86
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.74	0.85
1:A:1909:ASN:HD21	1:A:1911:ASN:HB3	1.42	0.84
1:B:1582:PHE:HA	1:B:1616:ILE:HG23	1.58	0.83
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.26	0.81
1:B:1843:VAL:HG11	1:B:1894:VAL:O	1.80	0.81
1:A:1773:SER:H	1:A:1776:GLN:HE21	1.27	0.80
1:A:1494:GLN:HE22	1:A:1557:PRO:HB2	1.46	0.80
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.30	0.80
1:A:1497:ARG:HH11	1:A:1497:ARG:HB2	1.47	0.79
1:A:2164:ASP:H	1:A:2170:GLN:HE22	1.29	0.79
1:B:1852:THR:HG23	1:B:1855:GLY:H	1.48	0.78
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.28	0.77
1:C:1781:GLN:H	1:C:1781:GLN:HE21	1.34	0.75
1:C:1493:LEU:HD21	1:C:1557:PRO:HB2	1.68	0.75
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.54	0.72
1:B:2163:VAL:HG13	1:B:2170:GLN:HG2	1.71	0.72
1:B:1836:THR:HB	1:B:1839:GLU:HB2	1.70	0.72
1:A:1582:PHE:HA	1:A:1616:ILE:HG23	1.73	0.71
1:A:1991:PRO:HG3	1:A:2115:TRP:HB2	1.73	0.71
1:B:2008:ASN:HB3	1:B:2012:MET:HE2	1.71	0.71
1:A:1936:ILE:HG23	1:A:1947:MET:HE1	1.72	0.70
1:C:1936:ILE:HD13	1:C:1978:LEU:HD13	1.73	0.69
1:C:2142:GLN:HB3	1:C:2190:LYS:HG2	1.73	0.69
1:C:2104:VAL:HG22	1:C:2109:ILE:HD11	1.74	0.69
1:B:1815:ASN:H	1:B:1944:GLN:NE2	1.82	0.69
1:B:1827:TRP:HA	1:B:2119:ARG:HH11	1.57	0.69
1:B:1776:GLN:O	1:C:1960:GLN:HG3	1.94	0.68
1:B:1533:THR:HB	1:B:1535:ASP:OD1	1.94	0.68
1:A:1560:ASN:H	1:A:1560:ASN:HD22	1.40	0.68
1:B:1511:PHE:HZ	1:B:1729:THR:HG21	1.60	0.67
1:C:1585:VAL:HG22	1:C:1607:VAL:HG11	1.77	0.67
1:B:1585:VAL:HG22	1:B:1607:VAL:HG11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2108:VAL:HG23	1:A:2109:ILE:HG23	1.76	0.67
1:C:1852:THR:HG22	1:C:1854:SER:H	1.60	0.67
1:B:1815:ASN:N	1:B:1944:GLN:HE22	1.82	0.66
1:B:2008:ASN:N	1:B:2012:MET:HE3	2.10	0.66
1:C:1630:GLY:HA2	1:C:1701:GLY:HA2	1.78	0.66
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.42	0.65
1:A:1772:THR:N	1:A:1776:GLN:HE22	1.93	0.65
1:B:1730:CYS:HA	1:B:1752:GLN:NE2	2.10	0.65
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.61	0.64
1:C:1921:GLY:HA2	2:C:3029:HOH:O	1.97	0.64
1:A:1773:SER:H	1:A:1776:GLN:NE2	1.96	0.63
1:B:1730:CYS:CA	1:B:1752:GLN:HE21	2.11	0.63
1:C:2164:ASP:H	1:C:2170:GLN:NE2	1.97	0.63
1:C:2020:ALA:O	1:C:2021:ARG:HG2	1.99	0.62
1:C:2138:ARG:HH11	1:C:2138:ARG:HB3	1.65	0.62
1:A:1491:GLU:O	1:A:1495:PRO:HA	2.00	0.62
1:B:1735:ILE:HD13	1:B:1735:ILE:O	2.00	0.62
1:C:1824:LYS:H	1:C:1824:LYS:HE2	1.65	0.61
1:B:1511:PHE:CZ	1:B:1729:THR:HG21	2.35	0.61
1:C:2196:GLN:NE2	1:C:2200:LYS:HD3	2.15	0.61
1:A:1909:ASN:ND2	1:A:1911:ASN:HB3	2.14	0.61
1:A:1624:ASN:HD22	1:A:1626:GLY:H	1.49	0.60
1:B:1705:ILE:H	1:B:1705:ILE:CD1	2.12	0.60
1:A:2003:VAL:HG12	1:A:2003:VAL:O	2.00	0.60
1:C:1877:VAL:HG23	1:C:1928:SER:HB2	1.84	0.59
1:C:2100:SER:HA	1:C:2103:MET:CE	2.32	0.59
1:A:1959:GLY:O	1:A:1963:MET:HB2	2.02	0.59
1:A:1772:THR:H	1:A:1776:GLN:NE2	1.95	0.59
1:B:1543:ILE:HD11	1:B:1553:VAL:HG11	1.84	0.59
1:B:1966:GLU:HB3	1:B:1969:LYS:HD2	1.83	0.59
1:C:1586:ALA:HB2	1:C:1621:LEU:HB2	1.84	0.59
1:A:1783:MET:HA	1:A:1786:ASN:HB2	1.83	0.59
1:C:2139:LEU:O	1:C:2142:GLN:HG2	2.03	0.59
1:A:2189:LEU:O	1:A:2192:GLU:HG2	2.03	0.58
1:B:1721:ASP:OD2	1:B:1814:ARG:NH1	2.36	0.58
1:B:1991:PRO:CG	1:B:2115:TRP:HB2	2.33	0.58
1:C:1773:SER:HB3	1:C:1776:GLN:HE21	1.69	0.58
1:B:2007:ILE:HB	1:B:2012:MET:HE1	1.85	0.58
1:A:1497:ARG:HH11	1:A:1497:ARG:CB	2.17	0.58
1:B:1705:ILE:HD13	1:B:1705:ILE:N	2.16	0.58
1:A:1835:PRO:HB2	1:A:1992:THR:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1759:ALA:N	1:C:1774:ASN:HD21	1.88	0.58
1:B:2008:ASN:H	1:B:2012:MET:HE3	1.68	0.57
1:C:1773:SER:N	1:C:1776:GLN:NE2	2.52	0.57
1:A:1836:THR:HG22	1:A:1838:ASP:H	1.70	0.57
1:B:2008:ASN:HB3	1:B:2012:MET:CE	2.34	0.57
1:A:1546:GLU:CD	1:A:1546:GLU:H	2.07	0.57
1:A:1846:MET:HE1	1:A:1990:PRO:HB3	1.85	0.57
1:C:1730:CYS:HA	1:C:1752:GLN:OE1	2.05	0.57
1:A:2021:ARG:NH1	1:A:2021:ARG:HB3	2.20	0.57
1:B:1569:ILE:HG22	1:B:1571:VAL:HG22	1.86	0.57
1:C:1513:GLU:O	1:C:1517:GLN:HG3	2.05	0.57
1:C:2138:ARG:O	1:C:2190:LYS:HD3	2.04	0.57
1:B:1494:GLN:NE2	1:B:1496:LYS:HG3	2.21	0.56
1:A:2183:ASP:OD1	1:B:1482:PRO:HD3	2.06	0.56
1:C:2100:SER:HA	1:C:2103:MET:HE2	1.86	0.56
1:C:2195:ALA:O	1:C:2199:ALA:HB3	2.06	0.56
1:C:2100:SER:HB2	1:C:2112:GLU:OE2	2.06	0.56
1:A:1996:ARG:HD2	1:A:1996:ARG:N	2.21	0.56
1:C:1922:GLN:CD	1:C:1954:ARG:HH12	2.08	0.56
1:C:1790:HIS:HD2	2:C:3027:HOH:O	1.89	0.56
1:A:1598:PRO:HG3	1:A:1704:CYS:HA	1.88	0.56
1:B:1991:PRO:HG2	1:B:2115:TRP:HB2	1.88	0.56
1:A:1527:SER:O	1:A:1530:VAL:HG22	2.06	0.55
1:A:1503:MET:HG2	1:A:1589:ILE:HG12	1.87	0.55
1:A:2110:SER:O	1:A:2111:LYS:HG3	2.06	0.55
1:B:1494:GLN:HG3	1:B:1496:LYS:HB2	1.89	0.55
1:A:1975:VAL:HG23	1:A:2002:VAL:HG23	1.89	0.55
1:B:1582:PHE:HA	1:B:1616:ILE:CG2	2.32	0.55
1:C:1560:ASN:ND2	1:C:1560:ASN:H	2.05	0.55
1:A:1954:ARG:O	1:A:1996:ARG:HB2	2.07	0.55
1:A:1745:ARG:HG2	1:A:1806:TRP:CZ2	2.42	0.55
1:A:1954:ARG:HG2	1:A:1994:GLU:OE2	2.07	0.55
1:C:1868:GLU:HG2	1:C:1871:SER:HB3	1.88	0.55
1:A:2021:ARG:HH12	1:A:2099:ARG:HH12	1.54	0.55
1:B:1946:PRO:HG3	1:B:2130:LEU:HD21	1.87	0.54
1:B:1491:GLU:HG3	1:B:1497:ARG:HB3	1.88	0.54
1:B:1905:ALA:O	1:B:1907:PRO:HD3	2.07	0.54
1:C:1586:ALA:CB	1:C:1621:LEU:HB2	2.38	0.53
1:C:1790:HIS:HA	1:C:1870:LEU:HD23	1.89	0.53
1:A:2190:LYS:C	1:A:2192:GLU:H	2.10	0.53
1:A:2136:ILE:HD11	1:A:2152:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2013:GLU:OE1	1:B:2125:ARG:NH2	2.42	0.53
1:B:2156:ARG:HG2	1:B:2159:TYR:CE1	2.43	0.53
1:C:1936:ILE:HD13	1:C:1978:LEU:CD1	2.39	0.53
1:A:1844:ARG:HG3	1:A:1844:ARG:HH11	1.73	0.53
1:C:1568:LYS:HE2	1:C:1581:GLN:NE2	2.24	0.53
1:B:1706:ARG:HB2	1:C:2108:VAL:HG12	1.90	0.52
1:B:2000:TRP:NE1	1:C:1705:ILE:HG23	2.24	0.52
1:C:1883:ARG:HA	1:C:1887:ILE:O	2.10	0.52
1:A:1792:THR:O	1:A:1802:LYS:HE3	2.08	0.52
1:A:1927:ASN:OD1	1:A:1928:SER:N	2.43	0.52
1:C:1845:TRP:CE2	1:C:1850:ARG:HD3	2.44	0.52
1:B:1587:ASN:ND2	1:B:1623:ALA:H	2.03	0.52
1:C:1623:ALA:HB2	1:C:1729:THR:HG23	1.91	0.52
1:A:1585:VAL:HG13	1:A:1607:VAL:HG11	1.92	0.52
1:B:1998:GLY:O	1:B:2001:VAL:HG12	2.09	0.51
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.57	0.51
1:A:1987:ILE:HB	1:A:2014:MET:HG3	1.92	0.51
1:A:1711:ILE:HD11	1:A:1735:ILE:HG12	1.92	0.51
1:C:1494:GLN:N	1:C:1495:PRO:HD2	2.24	0.51
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	2.25	0.51
1:B:1733:VAL:HA	1:B:1755:ILE:O	2.10	0.51
1:C:1952:ASN:OD1	1:C:1993:GLY:HA2	2.09	0.51
1:C:1607:VAL:O	1:C:1610:TYR:HB3	2.09	0.51
1:A:1560:ASN:H	1:A:1560:ASN:ND2	2.08	0.51
1:C:1829:ARG:CZ	1:C:1858:TYR:HB3	2.41	0.51
1:A:1497:ARG:HB2	1:A:1497:ARG:NH1	2.21	0.50
1:A:2160:PRO:HD2	1:A:2163:VAL:HG21	1.93	0.50
1:C:2111:LYS:HG2	1:C:2112:GLU:N	2.27	0.50
1:A:1711:ILE:HD12	1:A:1739:LEU:HD11	1.93	0.50
1:C:2148:ARG:HG2	1:C:2148:ARG:HH11	1.76	0.50
1:A:1909:ASN:ND2	1:A:1911:ASN:H	2.09	0.50
1:B:1489:VAL:HG23	1:B:1492:TRP:HB3	1.93	0.50
1:B:1954:ARG:HG2	1:B:1994:GLU:OE2	2.11	0.50
1:C:1845:TRP:CD2	1:C:1850:ARG:HD3	2.47	0.50
1:C:2138:ARG:HB3	1:C:2138:ARG:NH1	2.27	0.50
1:A:2100:SER:O	1:A:2104:VAL:HG23	2.11	0.49
1:B:1494:GLN:CD	1:B:1496:LYS:HD2	2.32	0.49
1:B:2015:TYR:HB3	1:B:2113:LEU:HD21	1.94	0.49
1:C:1528:ALA:O	1:C:1530:VAL:HG22	2.11	0.49
1:A:1721:ASP:OD2	1:A:1814:ARG:NH1	2.46	0.49
1:B:1780:THR:O	1:B:1784:TYR:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2007:ILE:HB	1:B:2012:MET:CE	2.43	0.49
1:B:2187:LYS:C	1:B:2189:LEU:H	2.16	0.49
1:C:1994:GLU:HA	1:C:2021:ARG:O	2.13	0.49
1:C:2004:ASP:OD2	1:C:2005:PRO:HD2	2.13	0.49
1:A:1817:PRO:HD3	1:B:1484:ALA:HB1	1.94	0.49
1:A:1881:ARG:CZ	1:A:1939:PHE:HE2	2.26	0.48
1:B:1866:PHE:CE1	1:B:1868:GLU:HB2	2.48	0.48
1:C:1899:VAL:HB	1:C:1919:GLU:HB2	1.94	0.48
1:B:1981:TYR:CG	1:B:1985:ILE:HD11	2.48	0.48
1:A:1820:ILE:HD13	1:B:1487:TYR:CZ	2.48	0.48
1:A:2021:ARG:HB3	1:A:2021:ARG:CZ	2.43	0.48
1:C:1773:SER:N	1:C:1776:GLN:HE22	2.11	0.48
1:C:2196:GLN:HE22	1:C:2200:LYS:HD3	1.78	0.48
1:C:1730:CYS:O	1:C:1731:ARG:C	2.51	0.48
1:A:1544:GLU:HB3	1:A:1548:GLY:HA2	1.96	0.48
1:A:2146:ALA:O	1:A:2151:LYS:HE3	2.12	0.48
1:C:1754:ILE:O	1:C:1778:GLY:HA3	2.14	0.48
1:A:1489:VAL:O	1:A:1493:LEU:HG	2.14	0.47
1:A:1527:SER:OG	1:A:1530:VAL:HG13	2.14	0.47
1:C:1943:GLU:O	1:C:1945:LEU:HD13	2.14	0.47
1:C:2111:LYS:HG2	1:C:2112:GLU:O	2.13	0.47
1:B:1491:GLU:HG2	1:B:1498:TYR:HB2	1.95	0.47
1:B:1814:ARG:O	1:B:1815:ASN:HB2	2.13	0.47
1:A:1733:VAL:HA	1:A:1755:ILE:O	2.14	0.47
1:C:1626:GLY:N	1:C:1733:VAL:HB	2.29	0.47
1:C:1991:PRO:CG	1:C:2115:TRP:HB2	2.44	0.47
1:A:1824:LYS:HE2	1:A:1824:LYS:H	1.78	0.47
1:B:1820:ILE:HD13	1:B:1887:ILE:HA	1.97	0.47
1:B:1927:ASN:OD1	1:B:1928:SER:N	2.48	0.47
1:B:2000:TRP:CE2	1:C:1705:ILE:HG23	2.49	0.47
1:C:2136:ILE:HD11	1:C:2152:ILE:CG2	2.44	0.47
1:A:1619:ILE:HG13	1:A:1725:ILE:CG2	2.45	0.47
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	2.12	0.47
1:A:1884:LEU:HD13	1:A:2123:PHE:HA	1.97	0.47
1:B:1768:ARG:HG2	1:B:1768:ARG:HH11	1.79	0.47
1:B:2148:ARG:O	1:B:2152:ILE:HG13	2.14	0.47
1:C:2148:ARG:HG2	1:C:2148:ARG:NH1	2.30	0.47
1:C:1509:TYR:HE1	1:C:1560:ASN:ND2	2.12	0.47
1:C:1619:ILE:HD12	1:C:1619:ILE:N	2.29	0.47
1:C:1838:ASP:O	1:C:1839:GLU:HB2	2.14	0.47
1:A:1759:ALA:HB3	1:A:1760:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1575:GLU:CD	1:A:1575:GLU:H	2.18	0.47
1:B:2129:ARG:HG3	1:B:2129:ARG:HH11	1.79	0.47
1:C:2022:ALA:HB3	1:C:2103:MET:SD	2.55	0.46
1:A:1836:THR:HB	1:A:1839:GLU:HB2	1.97	0.46
1:C:2021:ARG:NH2	1:C:2099:ARG:HE	2.14	0.46
1:C:1818:VAL:HB	1:C:1888:PRO:HG2	1.97	0.46
1:C:1759:ALA:HB3	1:C:1760:PRO:HD3	1.97	0.46
1:A:1730:CYS:O	1:A:1731:ARG:HB2	2.16	0.46
1:C:1713:GLY:O	1:C:1717:ARG:HG3	2.15	0.46
1:C:1727:LEU:HB2	1:C:1803:ILE:HD11	1.97	0.46
1:C:1809:TYR:O	1:C:1945:LEU:HD11	2.15	0.46
1:A:1936:ILE:HA	1:A:1947:MET:HE2	1.97	0.46
1:B:1756:LEU:HD21	1:C:1968:LEU:HD11	1.96	0.46
1:B:2113:LEU:HD23	1:B:2113:LEU:N	2.31	0.46
1:C:1603:PHE:O	1:C:1607:VAL:HG23	2.16	0.46
1:C:1780:THR:O	1:C:1784:TYR:HB3	2.15	0.46
1:B:1727:LEU:HB2	1:B:1803:ILE:HD11	1.96	0.46
1:B:1983:GLN:HB3	1:B:1984:PRO:HD2	1.98	0.46
1:A:1566:ALA:HA	1:A:1584:VAL:O	2.15	0.46
1:B:1491:GLU:O	1:B:1495:PRO:HA	2.16	0.46
1:C:1569:ILE:HG22	1:C:1571:VAL:HG23	1.97	0.46
1:B:1490:LYS:HE2	1:B:1497:ARG:CZ	2.45	0.45
1:B:1587:ASN:HB2	1:B:1623:ALA:O	2.16	0.45
1:C:1991:PRO:HG2	1:C:2115:TRP:HB2	1.98	0.45
1:A:2131:ASN:ND2	1:A:2179:TYR:OH	2.49	0.45
1:C:1546:GLU:CD	1:C:1546:GLU:H	2.18	0.45
1:C:2180:LYS:HE2	1:C:2180:LYS:HA	1.98	0.45
1:A:2005:PRO:HG3	1:A:2014:MET:HB2	1.97	0.45
1:A:2140:SER:O	1:A:2144:GLY:HA2	2.17	0.45
1:A:2177:GLU:O	1:B:1501:HIS:HE1	1.99	0.45
1:B:1918:GLN:O	1:B:1920:PRO:HD3	2.16	0.45
1:C:1797:LEU:O	1:C:1801:GLU:HG3	2.17	0.45
1:A:1745:ARG:NH1	1:A:1943:GLU:HG3	2.32	0.45
1:A:2016:ALA:O	1:A:2112:GLU:HA	2.17	0.45
1:C:1792:THR:O	1:C:1802:LYS:HE3	2.16	0.45
1:A:1845:TRP:CE2	1:A:1850:ARG:HD3	2.51	0.45
1:C:1898:THR:HG22	1:C:1920:PRO:HA	1.99	0.45
1:C:1903:ILE:N	1:C:1903:ILE:HD12	2.31	0.45
1:B:1550:LEU:HD12	1:B:1610:TYR:HB2	1.99	0.45
1:B:1792:THR:O	1:B:1802:LYS:HE3	2.17	0.45
1:B:2134:TYR:O	1:B:2138:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2004:ASP:O	1:C:2007:ILE:HG13	2.17	0.45
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	2.17	0.45
1:A:2008:ASN:C	1:A:2008:ASN:HD22	2.20	0.45
1:B:1494:GLN:HB3	1:B:1497:ARG:HH21	1.81	0.45
1:B:1578:ARG:HH11	1:B:1578:ARG:HG2	1.81	0.45
1:B:1996:ARG:HA	1:B:1996:ARG:HD3	1.82	0.45
1:B:1530:VAL:O	1:B:1530:VAL:HG13	2.16	0.45
1:C:1507:TYR:HB3	1:C:1510:ASP:OD2	2.17	0.45
1:C:1741:ARG:HD3	1:C:1741:ARG:C	2.37	0.45
1:C:1940:ASN:HB2	1:C:1981:TYR:CE1	2.52	0.45
1:A:1936:ILE:HA	1:A:1947:MET:CE	2.47	0.45
1:B:1494:GLN:HB3	1:B:1497:ARG:NH2	2.32	0.45
1:A:1505:THR:HB	1:A:1730:CYS:HB2	1.99	0.44
1:A:1865:SER:O	1:A:1882:ALA:HA	2.18	0.44
1:A:1936:ILE:HG12	1:A:1947:MET:CE	2.46	0.44
1:B:2151:LYS:O	1:B:2155:ILE:HG13	2.17	0.44
1:B:1873:TRP:O	1:B:1874:ALA:C	2.55	0.44
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.47	0.44
1:A:1575:GLU:HB3	1:A:1819:PRO:HB2	2.00	0.44
1:A:1790:HIS:HA	1:A:1870:LEU:HD23	1.99	0.44
1:A:1873:TRP:O	1:A:1874:ALA:C	2.56	0.44
1:C:1733:VAL:HA	1:C:1755:ILE:O	2.18	0.44
1:C:1781:GLN:H	1:C:1781:GLN:NE2	2.10	0.44
1:B:1843:VAL:CG1	1:B:1894:VAL:O	2.57	0.44
1:C:1824:LYS:H	1:C:1824:LYS:CE	2.29	0.44
1:A:2143:VAL:HB	1:A:2192:GLU:OE1	2.17	0.44
1:C:2148:ARG:O	1:C:2152:ILE:HG12	2.18	0.44
1:A:2014:MET:HG2	1:A:2015:TYR:N	2.33	0.44
1:B:1605:ASN:HD22	1:B:1714:ALA:HB2	1.82	0.44
1:B:1735:ILE:HD13	1:B:1739:LEU:HG	1.99	0.44
1:B:1762:ILE:HD12	1:B:1777:LEU:HD21	1.99	0.44
1:B:1991:PRO:HG3	1:B:2017:ASP:CG	2.38	0.44
1:C:1811:PRO:HA	1:C:1819:PRO:HD3	2.00	0.44
1:B:1963:MET:HE2	1:C:1755:ILE:HA	2.00	0.44
1:B:1607:VAL:O	1:B:1610:TYR:HB3	2.18	0.43
1:C:1954:ARG:HG3	1:C:1954:ARG:HH11	1.82	0.43
1:A:2190:LYS:C	1:A:2192:GLU:N	2.71	0.43
1:B:1602:GLU:HG3	1:B:1603:PHE:N	2.31	0.43
1:B:1969:LYS:HG2	1:C:1741:ARG:CZ	2.48	0.43
1:A:1490:LYS:HE3	1:A:1497:ARG:NH2	2.33	0.43
1:B:1578:ARG:HG2	1:B:1578:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1894:VAL:HG11	1:B:1922:GLN:HA	1.99	0.43
1:C:1818:VAL:HG11	1:C:1946:PRO:HD3	2.01	0.43
1:A:1780:THR:O	1:A:1784:TYR:HB3	2.19	0.43
1:A:2102:ARG:O	1:A:2106:LYS:HG2	2.19	0.43
1:B:1582:PHE:CD1	1:B:1619:ILE:HD13	2.53	0.43
1:C:1836:THR:HB	1:C:1839:GLU:HB3	2.01	0.43
1:A:1624:ASN:ND2	1:A:1733:VAL:H	2.15	0.43
1:B:2004:ASP:OD1	1:B:2005:PRO:HD2	2.19	0.43
1:C:1493:LEU:HB2	1:C:1497:ARG:HH12	1.82	0.43
1:B:1829:ARG:CZ	1:B:1858:TYR:HB3	2.48	0.43
1:B:1972:SER:HB3	1:C:1742:LEU:HD13	1.99	0.43
1:C:1741:ARG:HD3	1:C:1741:ARG:O	2.19	0.43
1:C:2135:LEU:HD13	1:C:2155:ILE:HG23	1.99	0.43
1:B:1821:LEU:O	1:B:1886:GLY:HA2	2.19	0.43
1:B:1766:LEU:HD23	1:B:1766:LEU:O	2.19	0.43
1:B:1951:ALA:HB1	1:B:1995:LEU:HD13	2.01	0.43
1:C:1704:CYS:SG	1:C:1705:ILE:N	2.91	0.43
1:C:1850:ARG:HG2	1:C:1851:GLU:N	2.34	0.43
1:C:2142:GLN:CB	1:C:2190:LYS:HG2	2.46	0.43
1:C:2195:ALA:C	1:C:2199:ALA:HB3	2.39	0.43
1:B:1511:PHE:CD2	1:B:1514:LEU:HD12	2.53	0.43
1:B:2002:VAL:HG23	1:B:2003:VAL:HG13	2.01	0.43
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.66	0.42
1:B:1730:CYS:O	1:B:1731:ARG:HB3	2.19	0.42
1:B:1742:LEU:HD23	1:C:1972:SER:HB3	2.01	0.42
1:B:1964:PHE:O	1:C:1786:ASN:ND2	2.52	0.42
1:B:1991:PRO:O	1:B:1992:THR:OG1	2.31	0.42
1:C:2102:ARG:NH1	1:C:2106:LYS:HE2	2.35	0.42
1:A:1947:MET:HG2	1:A:1948:MET:N	2.34	0.42
1:A:2135:LEU:HB3	1:A:2155:ILE:CD1	2.39	0.42
1:B:2004:ASP:HB3	1:C:1709:GLY:HA3	2.00	0.42
1:C:2023:GLY:HA3	1:C:2098:ASP:OD1	2.19	0.42
1:A:1772:THR:HB	1:A:1776:GLN:NE2	2.35	0.42
1:B:1592:LYS:O	1:B:1593:ILE:CG1	2.67	0.42
1:C:1852:THR:HG22	1:C:1853:GLU:N	2.34	0.42
1:C:1987:ILE:HG21	1:C:2014:MET:CE	2.50	0.42
1:C:2104:VAL:CG2	1:C:2109:ILE:HD11	2.47	0.42
1:A:1626:GLY:N	1:A:1733:VAL:HB	2.34	0.42
1:B:1508:VAL:HG23	1:B:1509:TYR:H	1.83	0.42
1:B:1513:GLU:OE1	1:B:1516:ARG:NH1	2.53	0.42
1:C:1719:TYR:O	1:C:1941:ASN:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1719:TYR:CE2	1:B:1744:GLN:HG3	2.54	0.42
1:B:2008:ASN:CB	1:B:2012:MET:HE2	2.43	0.42
1:A:1996:ARG:NH2	1:A:2026:GLU:HG2	2.35	0.42
1:A:1997:GLY:O	1:A:2001:VAL:HG23	2.20	0.42
1:B:1776:GLN:O	1:B:1782:ILE:HD11	2.20	0.42
1:C:1748:GLN:HE22	1:C:1783:MET:HB2	1.85	0.42
1:C:2021:ARG:NH2	1:C:2099:ARG:HH21	2.18	0.42
1:C:2100:SER:HA	1:C:2103:MET:HE3	2.02	0.42
1:C:2160:PRO:HD2	1:C:2163:VAL:HG21	2.01	0.42
1:B:1837:ASN:HA	1:B:2021:ARG:HH21	1.83	0.41
1:C:2108:VAL:HG23	1:C:2109:ILE:HG23	2.02	0.41
1:A:1730:CYS:CA	1:A:1752:GLN:HE21	2.29	0.41
1:A:1905:ALA:O	1:A:1907:PRO:HD3	2.20	0.41
1:A:2018:VAL:HG12	1:A:2112:GLU:OE1	2.19	0.41
1:C:2001:VAL:HG13	1:C:2002:VAL:HG13	2.02	0.41
1:A:1727:LEU:HB2	1:A:1803:ILE:HD11	2.02	0.41
1:B:1571:VAL:O	1:B:1579:GLY:HA2	2.19	0.41
1:B:1924:TRP:HZ3	1:B:1999:SER:HB2	1.86	0.41
1:C:1545:ASP:HB2	1:C:1546:GLU:OE2	2.20	0.41
1:A:1565:VAL:HG12	1:A:1566:ALA:N	2.36	0.41
1:B:1586:ALA:HB2	1:B:1621:LEU:HB2	2.01	0.41
1:B:1843:VAL:HG13	2:B:3045:HOH:O	2.20	0.41
1:B:1948:MET:HA	1:B:1986:ILE:O	2.20	0.41
1:C:1575:GLU:CD	1:C:1575:GLU:H	2.23	0.41
1:A:1824:LYS:H	1:A:1824:LYS:CE	2.33	0.41
1:C:1770:VAL:HG21	1:C:1908:ALA:HA	2.01	0.41
1:A:1846:MET:CE	1:A:1990:PRO:HB3	2.51	0.41
1:B:1991:PRO:HG3	1:B:2115:TRP:HB2	2.02	0.41
1:A:2186:LEU:C	1:A:2188:GLY:H	2.23	0.41
1:C:2160:PRO:HB2	1:C:2163:VAL:HG23	2.02	0.41
1:A:1616:ILE:HA	1:A:1617:PRO:HD3	1.94	0.41
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.69	0.41
1:A:1844:ARG:HG3	1:A:1844:ARG:NH1	2.34	0.41
1:B:2132:GLU:O	1:B:2136:ILE:HG13	2.21	0.41
1:C:1814:ARG:O	1:C:1815:ASN:HB2	2.21	0.41
1:B:1705:ILE:HG23	1:C:2024:VAL:HG22	2.03	0.41
1:B:1768:ARG:HG2	1:B:1768:ARG:NH1	2.36	0.41
1:B:1874:ALA:HB2	1:B:1927:ASN:HB2	2.03	0.41
1:C:1731:ARG:CB	1:C:1731:ARG:HH11	2.34	0.41
1:A:1719:TYR:CE2	1:A:1744:GLN:HG3	2.57	0.40
1:A:2148:ARG:O	1:A:2152:ILE:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1781:GLN:HE21	1:C:1781:GLN:N	2.09	0.40
1:A:1531:LYS:HA	1:A:1531:LYS:HE2	2.03	0.40
1:A:2180:LYS:O	1:A:2183:ASP:HB3	2.22	0.40
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	2.02	0.40
1:C:1810:VAL:HG13	1:C:1811:PRO:HD2	2.03	0.40
1:C:2190:LYS:C	1:C:2191:LEU:HD12	2.41	0.40
1:A:2167:ASP:O	1:A:2171:VAL:HG23	2.20	0.40
1:B:1790:HIS:HA	1:B:1870:LEU:HD23	2.03	0.40
1:B:2001:VAL:O	1:B:2007:ILE:HD11	2.21	0.40
1:C:1560:ASN:H	1:C:1560:ASN:HD22	1.69	0.40
1:A:1533:THR:HB	1:A:1535:ASP:OD1	2.22	0.40
1:B:1619:ILE:HD12	1:B:1619:ILE:N	2.37	0.40
1:A:1626:GLY:HA2	1:A:1733:VAL:O	2.20	0.40
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.86	0.40
1:A:1759:ALA:N	1:A:1760:PRO:CD	2.85	0.40
1:B:1820:ILE:HD12	1:B:1887:ILE:HG12	2.04	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	566/737 (77%)	527 (93%)	34 (6%)	5 (1%)	17	35
1	B	547/737 (74%)	507 (93%)	37 (7%)	3 (0%)	29	52
1	C	565/737 (77%)	521 (92%)	37 (6%)	7 (1%)	13	27
All	All	1678/2211 (76%)	1555 (93%)	108 (6%)	15 (1%)	17	35

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1529	ASP

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Mol	Chain	Res	Type
1	A	1731	ARG
1	A	2142	GLN
1	B	2142	GLN
1	C	2199	ALA
1	C	1744	GLN
1	B	1731	ARG
1	B	1744	GLN
1	C	1839	GLU
1	A	1744	GLN
1	A	2193	SER
1	C	1528	ALA
1	C	1508	VAL
1	C	1705	ILE
1	C	1904	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	480/628 (76%)	458 (95%)	22 (5%)	27 51
1	B	465/628 (74%)	440 (95%)	25 (5%)	22 44
1	C	479/628 (76%)	452 (94%)	27 (6%)	21 42
All	All	1424/1884 (76%)	1350 (95%)	74 (5%)	23 46

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1496	LYS
1	A	1497	ARG
1	A	1534	ASP
1	A	1536	PHE
1	A	1554	GLU
1	A	1560	ASN
1	A	1585	VAL
1	A	1602	GLU

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Mol	Chain	Res	Type
1	A	1732	SER
1	A	1765	MET
1	A	1884	LEU
1	A	1909	ASN
1	A	1924	TRP
1	A	1950	LEU
1	A	1960	GLN
1	A	1981	TYR
1	A	1996	ARG
1	A	2002	VAL
1	A	2008	ASN
1	A	2021	ARG
1	A	2128	ARG
1	A	2135	LEU
1	B	1489	VAL
1	B	1491	GLU
1	B	1516	ARG
1	B	1536	PHE
1	B	1555	ARG
1	B	1571	VAL
1	B	1602	GLU
1	B	1618	ARG
1	B	1705	ILE
1	B	1726	THR
1	B	1732	SER
1	B	1735	ILE
1	B	1777	LEU
1	B	1786	ASN
1	B	1791	LEU
1	B	1797	LEU
1	B	1884	LEU
1	B	1909	ASN
1	B	1924	TRP
1	B	1961	ARG
1	B	1983	GLN
1	B	2113	LEU
1	B	2128	ARG
1	B	2165	HIS
1	B	2179	TYR
1	C	1508	VAL
1	C	1511	PHE
1	C	1536	PHE

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Mol	Chain	Res	Type
1	C	1556	GLU
1	C	1560	ASN
1	C	1602	GLU
1	C	1618	ARG
1	C	1703	GLU
1	C	1705	ILE
1	C	1706	ARG
1	C	1731	ARG
1	C	1740	VAL
1	C	1741	ARG
1	C	1742	LEU
1	C	1781	GLN
1	C	1792	THR
1	C	1895	GLU
1	C	1924	TRP
1	C	1968	LEU
1	C	1978	LEU
1	C	1981	TYR
1	C	2006	THR
1	C	2114	GLU
1	C	2128	ARG
1	C	2138	ARG
1	C	2180	LYS
1	C	2189	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1494	GLN
1	A	1501	HIS
1	A	1522	GLN
1	A	1547	ASN
1	A	1560	ASN
1	A	1587	ASN
1	A	1605	ASN
1	A	1624	ASN
1	A	1748	GLN
1	A	1752	GLN
1	A	1776	GLN
1	A	1790	HIS
1	A	1815	ASN
1	A	1909	ASN

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Mol	Chain	Res	Type
1	A	1911	ASN
1	A	1918	GLN
1	A	1934	GLN
1	A	2008	ASN
1	A	2131	ASN
1	A	2170	GLN
1	B	1494	GLN
1	B	1517	GLN
1	B	1525	ASN
1	B	1587	ASN
1	B	1605	ASN
1	B	1624	ASN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1786	ASN
1	B	1815	ASN
1	B	1909	ASN
1	B	1918	GLN
1	B	1934	GLN
1	B	1941	ASN
1	B	1944	GLN
1	B	1960	GLN
1	B	1983	GLN
1	B	2131	ASN
1	C	1517	GLN
1	C	1522	GLN
1	C	1525	ASN
1	C	1560	ASN
1	C	1587	ASN
1	C	1605	ASN
1	C	1748	GLN
1	C	1774	ASN
1	C	1776	GLN
1	C	1781	GLN
1	C	1786	ASN
1	C	1790	HIS
1	C	1815	ASN
1	C	1911	ASN
1	C	1918	GLN
1	C	1934	GLN
1	C	1941	ASN

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Mol	Chain	Res	Type
1	C	2011	GLN
1	C	2142	GLN
1	C	2170	GLN
1	C	2196	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	572/737 (77%)	-0.18	35 (6%)	21	16	21, 41, 93, 100	0
1	B	553/737 (75%)	-0.24	27 (4%)	29	23	22, 42, 84, 100	0
1	C	571/737 (77%)	-0.07	46 (8%)	12	8	23, 45, 97, 100	0
All	All	1696/2211 (76%)	-0.17	108 (6%)	19	14	21, 43, 90, 100	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2027	PRO	6.9
1	C	2143	VAL	6.5
1	C	2197	ASP	6.2
1	A	1492	TRP	5.9
1	C	1702	VAL	5.7
1	A	1631	MET	5.4
1	B	1492	TRP	5.4
1	A	1489	VAL	5.2
1	C	2102	ARG	5.0
1	A	2025	LEU	4.9
1	C	2101	SER	4.8
1	C	2024	VAL	4.7
1	C	2025	LEU	4.5
1	C	1631	MET	4.5
1	C	2194	PHE	4.1
1	C	2104	VAL	4.0
1	A	1483	ILE	4.0
1	C	2105	ALA	3.9
1	C	2106	LYS	3.9
1	C	1630	GLY	3.9
1	A	2106	LYS	3.9
1	B	1630	GLY	3.8
1	A	2102	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	1997	GLY	3.6
1	A	2104	VAL	3.6
1	B	1855	GLY	3.5
1	B	1766	LEU	3.5
1	C	1706	ARG	3.5
1	A	2144	GLY	3.5
1	B	1489	VAL	3.5
1	C	1531	LYS	3.4
1	A	1632	ALA	3.4
1	C	2198	LEU	3.4
1	B	1482	PRO	3.4
1	B	1483	ILE	3.3
1	C	1629	ILE	3.3
1	A	2100	SER	3.3
1	C	1704	CYS	3.3
1	B	2188	GLY	3.2
1	A	2194	PHE	3.2
1	C	2141	HIS	3.2
1	B	1768	ARG	3.2
1	B	2134	TYR	3.1
1	A	1630	GLY	3.1
1	A	2103	MET	3.1
1	A	2020	ALA	3.0
1	B	2141	HIS	3.0
1	A	2105	ALA	2.9
1	B	2022	ALA	2.9
1	A	2143	VAL	2.9
1	C	1703	GLU	2.9
1	C	1701	GLY	2.9
1	C	2190	LYS	2.9
1	C	2100	SER	2.8
1	B	2145	GLU	2.8
1	C	2144	GLY	2.8
1	A	2099	ARG	2.8
1	C	2196	GLN	2.7
1	B	1838	ASP	2.7
1	C	2098	ASP	2.7
1	A	2024	VAL	2.6
1	C	2189	LEU	2.6
1	C	2026	GLU	2.6
1	B	2187	LYS	2.6
1	C	2099	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1838	ASP	2.6
1	A	1490	LYS	2.6
1	C	1547	ASN	2.6
1	B	1996	ARG	2.6
1	C	1764	LYS	2.5
1	A	2195	ALA	2.5
1	C	1767	GLY	2.5
1	C	2023	GLY	2.5
1	B	1703	GLU	2.5
1	A	2023	GLY	2.5
1	B	1767	GLY	2.5
1	B	2144	GLY	2.4
1	C	1911	ASN	2.4
1	C	2199	ALA	2.4
1	C	1620	TYR	2.3
1	A	1529	ASP	2.3
1	A	1855	GLY	2.3
1	B	1854	SER	2.3
1	C	2103	MET	2.3
1	A	2145	GLU	2.2
1	B	1546	GLU	2.2
1	C	1853	GLU	2.2
1	B	2189	LEU	2.2
1	C	1621	LEU	2.2
1	C	1584	VAL	2.2
1	C	1529	ASP	2.2
1	A	2192	GLU	2.2
1	C	2192	GLU	2.2
1	C	1528	ALA	2.2
1	C	2145	GLU	2.1
1	A	1531	LYS	2.1
1	A	1911	ASN	2.1
1	B	2190	LYS	2.1
1	B	2021	ARG	2.1
1	A	1482	PRO	2.1
1	A	2026	GLU	2.1
1	A	1765	MET	2.1
1	B	1584	VAL	2.1
1	C	2193	SER	2.1
1	B	1488	PRO	2.0
1	A	1528	ALA	2.0
1	A	1546	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	2191	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.