Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:11 pm BST

PDB ID	:	1UYT
Title	:	Acetyl-CoA carboxylase carboxyltransferase domain
Authors	:	Zhang, H.; Tweel, B.; Tong, L.
Deposited on	:	2004-03-02
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

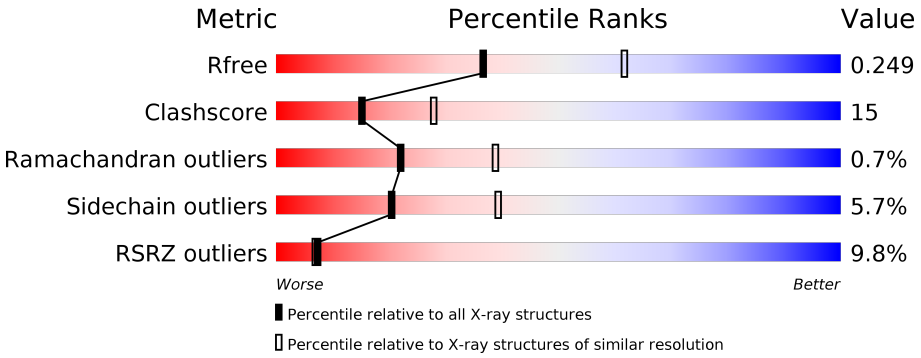
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	9% 65% 26% • 7%
1	B	737	9% 66% 24% • 8%
1	C	737	9% 62% 25% • 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16369 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	682	Total	C	N	O	S	0	0	1
			5425	3459	931	1016	19			
1	B	676	Total	C	N	O	S	0	0	1
			5377	3427	924	1007	19			
1	C	666	Total	C	N	O	S	0	0	1
			5299	3374	913	993	19			

- Molecule 2 is water.

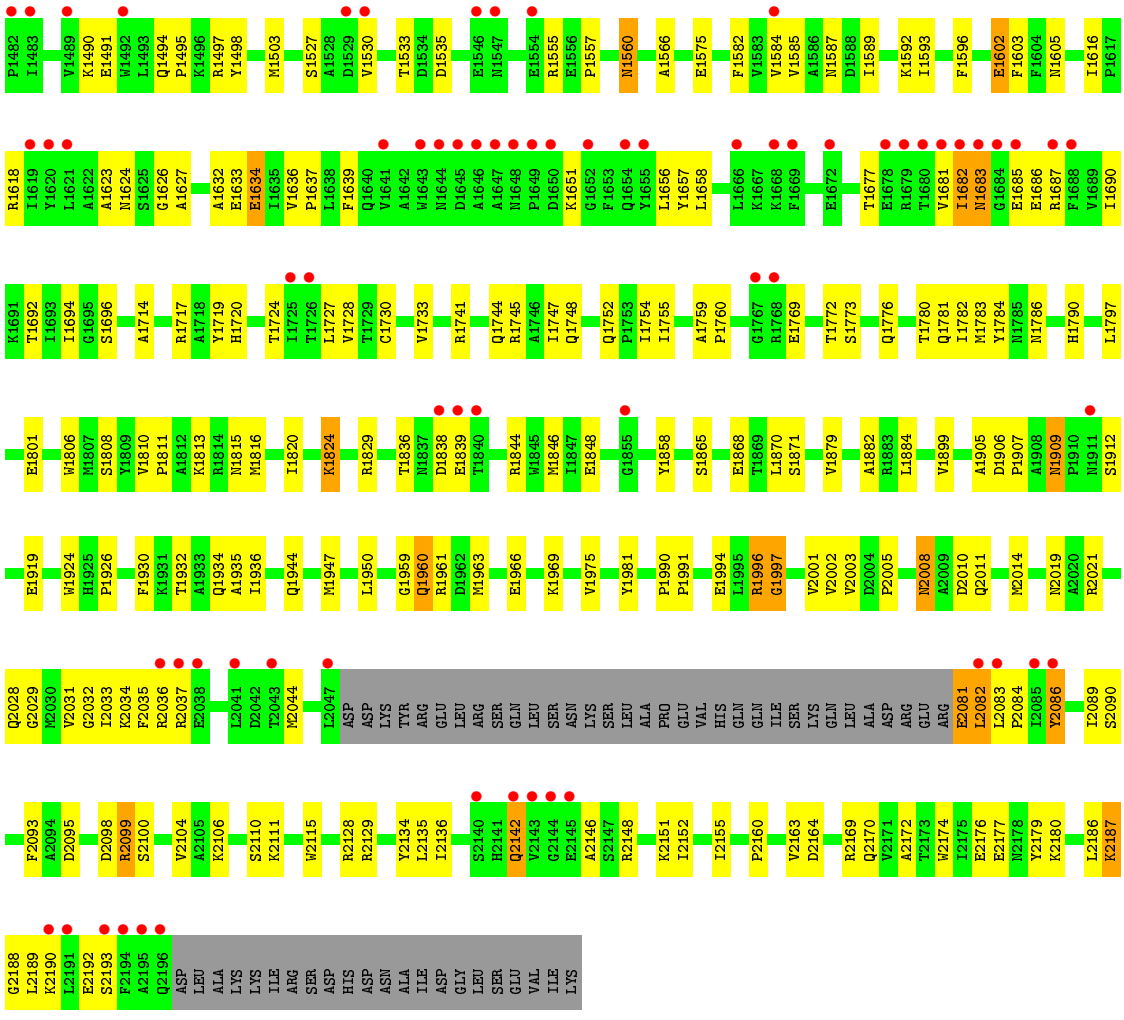
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	97	Total	O	0	0
			97	97		
2	B	99	Total	O	0	0
			99	99		
2	C	72	Total	O	0	0
			72	72		

3 Residue-property plots (i)

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

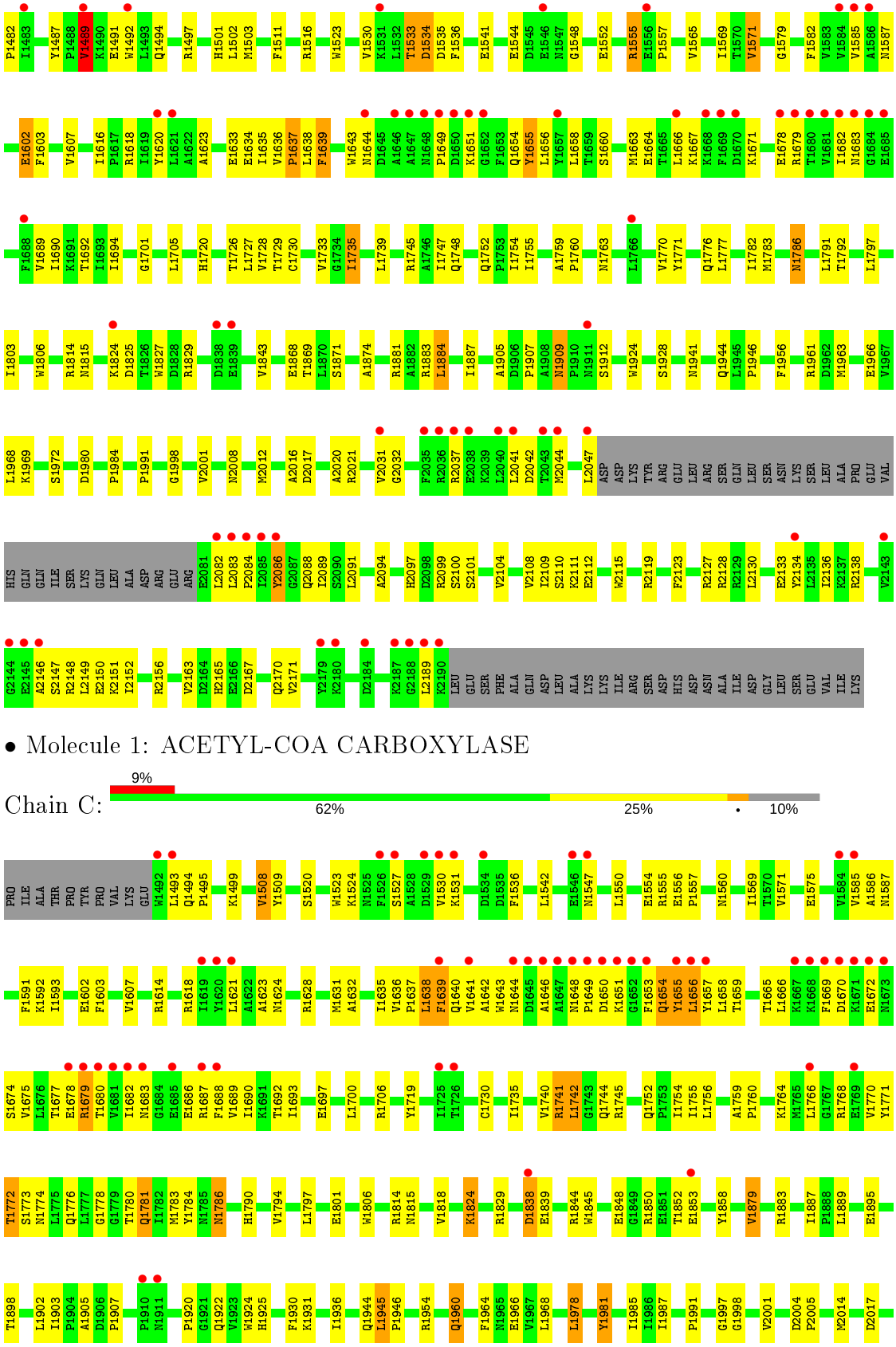
- Molecule 1: ACETYL-COA CARBOXYLASE

Chain A:



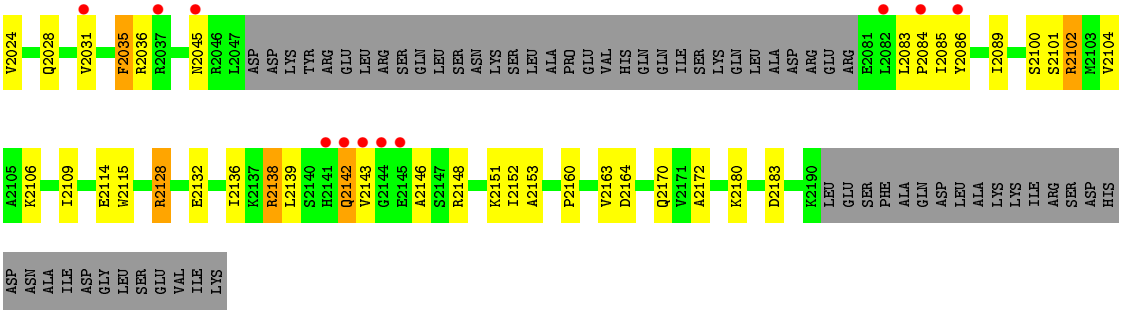
- Molecule 1: ACETYL-COA CARBOXYLASE

Chain B:



• Molecule 1: ACETYL-COA CARBOXYLASE

Chain C:


V2024 Q2028 V2031 F2035 R2036 R2037 N2045 R2046 L2047 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 E2081 L2082 L2083 P2084 I2085 Y2086 I2089 S2100 S2101 R2102 M2103 V2104
A2105 K2106 I2109 E2114 W2115 R2128 E2132 I2136 K2137 R2138 L2139 S2140 H2141 Q2142 V2143 G2144 E2145 A2146 S2147 R2148 K2151 I2152 A2153 P2160 V2163 D2164 Q2170 V2171 A2172 K2180 D2183 K2190 LEU GLU SER PHE ALA GLN ASP LEU ALA LYS LYS 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	246.80Å 125.21Å 145.50Å 90.00° 94.06° 90.00°	Depositor
Resolution (Å)	27.62 – 2.50 29.98 – 2.49	Depositor EDS
% Data completeness (in resolution range)	85.6 (27.62-2.50) 89.3 (29.98-2.49)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.52 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.250 0.219 , 0.249	Depositor DCC
R_{free} test set	14225 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å^2)	42.9	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	16369	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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	0.39	0/5547	0.60	0/7516
1	B	0.39	0/5498	0.60	0/7451
1	C	0.40	0/5416	0.58	0/7337
All	All	0.39	0/16461	0.59	0/22304

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	5425	0	5365	171	0
1	B	5377	0	5316	154	0
1	C	5299	0	5234	187	0
2	A	97	0	0	9	0
2	B	99	0	0	4	0
2	C	72	0	0	4	0
All	All	16369	0	15915	481	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 15.

All (481) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.07	1.08
1:B:2082:LEU:HA	1:C:1650:ASP:HB3	1.40	1.03
1:C:1772:THR:H	1:C:1776:GLN:HE22	1.06	0.93
1:B:1658:LEU:HD13	1:B:1690:ILE:HD11	1.49	0.92
1:A:1813:LYS:HG2	1:A:1816:MET:HE3	1.48	0.92
1:B:1815:ASN:H	1:B:1944:GLN:HE22	0.99	0.90
1:B:2147:SER:HB3	1:B:2150:GLU:HG3	1.54	0.88
1:A:1494:GLN:HE22	1:A:1557:PRO:HB2	1.41	0.86
1:C:1824:LYS:HE2	1:C:1824:LYS:H	1.40	0.86
1:A:1682:ILE:HD13	1:A:1682:ILE:H	1.38	0.85
1:B:1730:CYS:HA	1:B:1752:GLN:NE2	1.90	0.85
1:A:1813:LYS:HG2	1:A:1816:MET:CE	2.06	0.85
1:C:1648:ASN:HB2	1:C:1651:LYS:HB2	1.60	0.84
1:A:1582:PHE:HA	1:A:1616:ILE:HG23	1.60	0.83
1:A:1813:LYS:HE2	1:A:1816:MET:HE2	1.60	0.83
1:A:2135:LEU:HB3	1:A:2155:ILE:HD13	1.59	0.82
1:A:1936:ILE:HG12	1:A:1947:MET:HE1	1.62	0.82
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	1.95	0.81
1:C:1772:THR:H	1:C:1776:GLN:NE2	1.76	0.81
1:A:1772:THR:H	1:A:1776:GLN:HE22	1.30	0.80
1:A:2142:GLN:NE2	1:A:2192:GLU:HG2	1.98	0.79
1:C:1759:ALA:H	1:C:1774:ASN:HD21	1.31	0.79
1:B:2031:VAL:HG21	1:B:2091:LEU:HD23	1.65	0.78
1:A:2142:GLN:HE22	1:A:2192:GLU:HG2	1.50	0.77
1:B:1638:LEU:HD23	1:B:1638:LEU:H	1.51	0.76
1:C:1783:MET:HA	1:C:1786:ASN:HB2	1.64	0.76
1:B:1745:ARG:HG2	1:B:1806:TRP:CZ2	2.20	0.76
1:C:1646:ALA:HB3	1:C:1651:LYS:HG2	1.66	0.76
1:A:2031:VAL:HG23	1:A:2035:PHE:HB3	1.68	0.75
1:B:1786:ASN:ND2	1:C:1966:GLU:HG3	2.01	0.75
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.33	0.75
1:A:1836:THR:HB	1:A:1839:GLU:HB2	1.70	0.74
1:B:1582:PHE:HA	1:B:1616:ILE:HG23	1.68	0.74
1:A:1717:ARG:HA	2:A:3021:HOH:O	1.88	0.73
1:A:1494:GLN:NE2	1:A:1557:PRO:HB2	2.04	0.72
1:C:1635:ILE:O	1:C:1639:PHE:HB3	1.90	0.70
1:A:1824:LYS:HE2	1:A:1824:LYS:H	1.56	0.70
1:B:2008:ASN:N	1:B:2012:MET:HE3	2.07	0.70
1:B:2008:ASN:HB3	1:B:2012:MET:CE	2.21	0.69
1:A:1773:SER:H	1:A:1776:GLN:NE2	1.88	0.69
1:C:1844:ARG:HG3	1:C:1844:ARG:HH11	1.55	0.69
1:A:1681:VAL:HG12	1:A:1686:GLU:HA	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1815:ASN:H	1:B:1944:GLN:NE2	1.83	0.69
1:B:1511:PHE:CZ	1:B:1729:THR:HG21	2.28	0.69
1:A:1905:ALA:O	1:A:1907:PRO:HD3	1.92	0.69
1:B:2089:ILE:HD13	1:C:1641:VAL:HG21	1.74	0.68
1:A:1560:ASN:HD22	1:A:1560:ASN:H	1.39	0.68
1:C:1991:PRO:HG2	1:C:2115:TRP:HB2	1.76	0.68
1:A:1909:ASN:HB3	1:A:1912:SER:HB3	1.75	0.68
1:C:1772:THR:HG23	1:C:1776:GLN:HE22	1.57	0.68
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.91	0.66
1:C:1677:THR:HB	1:C:1688:PHE:HB3	1.76	0.66
1:C:1773:SER:H	1:C:1776:GLN:HE21	1.44	0.66
1:C:1772:THR:N	1:C:1776:GLN:HE22	1.88	0.66
1:A:1741:ARG:NH1	2:A:3030:HOH:O	2.27	0.66
1:C:1797:LEU:O	1:C:1801:GLU:HG3	1.95	0.65
1:A:1975:VAL:HG23	1:A:2002:VAL:HG23	1.78	0.65
1:C:1658:LEU:HD11	1:C:1690:ILE:HD11	1.77	0.65
1:A:1497:ARG:HB2	1:A:1497:ARG:NH1	2.10	0.65
1:C:1678:GLU:HB3	1:C:1689:VAL:HB	1.78	0.65
1:A:1991:PRO:HG3	1:A:2115:TRP:HB2	1.77	0.65
1:B:1884:LEU:HD13	1:B:2123:PHE:HA	1.78	0.65
1:B:2008:ASN:HB3	1:B:2012:MET:HE2	1.77	0.65
1:C:1682:ILE:HG21	1:C:1687:ARG:NH1	2.10	0.65
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.44	0.65
1:C:1773:SER:H	1:C:1776:GLN:NE2	1.95	0.65
1:B:1511:PHE:HZ	1:B:1729:THR:HG21	1.62	0.64
1:B:1782:ILE:O	1:B:1786:ASN:HB2	1.98	0.64
1:A:1906:ASP:H	1:A:1912:SER:HB2	1.62	0.64
1:C:1657:TYR:CD2	1:C:1687:ARG:HG2	2.33	0.64
1:B:1735:ILE:HD13	1:B:1739:LEU:HG	1.80	0.63
1:A:1935:ALA:HB2	2:A:3059:HOH:O	1.98	0.63
1:B:1694:ILE:HA	1:C:2102:ARG:HD3	1.80	0.63
1:C:1640:GLN:HG3	1:C:1659:THR:HG23	1.80	0.63
1:A:2003:VAL:O	1:A:2003:VAL:HG12	1.98	0.63
1:A:1815:ASN:ND2	1:A:1944:GLN:HE22	1.97	0.63
1:B:1660:SER:O	1:B:1664:GLU:HG2	1.98	0.63
1:B:1726:THR:HG21	2:B:3042:HOH:O	1.99	0.62
1:A:1634:GLU:OE1	1:A:1696:SER:HB3	2.00	0.62
1:B:1972:SER:HB3	1:C:1742:LEU:HD13	1.81	0.62
1:B:1533:THR:HB	1:B:1535:ASP:OD1	1.99	0.62
1:A:1991:PRO:O	1:A:2019:ASN:O	2.16	0.62
1:B:1827:TRP:HA	1:B:2119:ARG:HH11	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1773:SER:N	1:C:1776:GLN:HE21	1.97	0.62
1:A:2033:ILE:HA	1:A:2036:ARG:NH1	2.14	0.62
1:A:1724:THR:H	1:A:1745:ARG:HH21	1.48	0.61
1:C:2031:VAL:HG23	1:C:2035:PHE:HB3	1.82	0.61
1:A:1719:TYR:CE2	1:A:1744:GLN:HG3	2.36	0.61
1:C:2139:LEU:O	1:C:2142:GLN:HG2	2.01	0.61
1:B:1634:GLU:O	1:B:1638:LEU:HD21	2.01	0.61
1:A:1966:GLU:HB3	1:A:1969:LYS:HD2	1.83	0.60
1:B:1827:TRP:HA	1:B:2119:ARG:NH1	2.15	0.60
1:A:1836:THR:HG22	1:A:1838:ASP:H	1.66	0.60
1:A:1815:ASN:HD22	1:A:1944:GLN:HE22	1.50	0.60
1:C:2160:PRO:HD2	1:C:2163:VAL:HG21	1.83	0.60
1:B:1829:ARG:NH2	1:B:2119:ARG:HE	2.00	0.60
1:A:1677:THR:HG22	1:A:1690:ILE:HG22	1.84	0.60
1:A:2005:PRO:HG3	1:A:2014:MET:HB2	1.84	0.60
1:A:1582:PHE:HA	1:A:1616:ILE:CG2	2.31	0.59
1:B:1663:MET:O	1:B:1667:LYS:HG3	2.01	0.59
1:C:2138:ARG:HH22	1:C:2183:ASP:CG	2.06	0.59
1:C:1824:LYS:CE	1:C:1824:LYS:H	2.13	0.59
1:A:1783:MET:HA	1:A:1786:ASN:HB2	1.86	0.58
1:C:1772:THR:HG23	1:C:1776:GLN:NE2	2.18	0.58
1:B:1620:TYR:HB3	1:B:1726:THR:HG22	1.85	0.58
1:C:1991:PRO:CG	1:C:2115:TRP:HB2	2.33	0.58
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.66	0.58
1:B:1791:LEU:HD21	1:B:1869:THR:HG22	1.84	0.58
1:A:1533:THR:HB	1:A:1535:ASP:OD1	2.03	0.57
1:B:2094:ALA:HA	1:B:2097:HIS:HD2	1.69	0.57
1:A:1959:GLY:O	1:A:1963:MET:HB2	2.04	0.57
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.51	0.57
1:B:1909:ASN:HB3	1:B:1912:SER:HB3	1.86	0.57
1:C:1644:ASN:ND2	1:C:1682:ILE:HD13	2.20	0.57
1:C:1794:VAL:HG23	2:C:3026:HOH:O	2.05	0.57
1:B:2149:LEU:HD13	1:B:2149:LEU:O	2.05	0.57
1:C:1903:ILE:N	1:C:1903:ILE:HD12	2.19	0.57
1:A:1633:GLU:O	1:A:1636:VAL:HG12	2.05	0.57
1:B:1634:GLU:HG3	1:B:1671:LYS:HD3	1.87	0.57
1:C:1844:ARG:HG3	1:C:1844:ARG:NH1	2.19	0.56
1:A:2008:ASN:C	1:A:2008:ASN:HD22	2.08	0.56
1:A:2044:MET:HA	1:A:2086:TYR:CE2	2.40	0.56
1:B:2097:HIS:CE1	1:C:1632:ALA:H	2.23	0.56
1:C:1898:THR:HG22	1:C:1920:PRO:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1497:ARG:HB2	1:A:1497:ARG:HH11	1.71	0.56
1:B:1868:GLU:HG2	1:B:1871:SER:HB3	1.87	0.56
1:A:2033:ILE:HA	1:A:2036:ARG:HH12	1.70	0.56
1:C:2031:VAL:CG2	1:C:2035:PHE:HB3	2.35	0.56
1:A:2146:ALA:O	1:A:2151:LYS:HE3	2.06	0.56
1:C:1656:LEU:O	1:C:1690:ILE:HB	2.05	0.56
1:C:1815:ASN:ND2	1:C:1944:GLN:HE22	2.03	0.56
1:A:1772:THR:H	1:A:1776:GLN:NE2	2.02	0.56
1:A:1782:ILE:O	1:A:1786:ASN:HB2	2.06	0.56
1:B:1776:GLN:O	1:B:1782:ILE:HD11	2.05	0.56
1:A:1575:GLU:H	1:A:1575:GLU:CD	2.08	0.55
1:A:1624:ASN:HD22	1:A:1626:GLY:H	1.54	0.55
1:C:1642:ALA:HB1	1:C:1644:ASN:OD1	2.06	0.55
1:A:1724:THR:H	1:A:1745:ARG:NH2	2.04	0.55
1:A:2160:PRO:HD2	1:A:2163:VAL:HG21	1.89	0.55
1:C:2036:ARG:NH1	1:C:2036:ARG:HB3	2.20	0.55
1:A:1657:TYR:CE2	1:A:1687:ARG:HD2	2.41	0.55
1:B:2097:HIS:NE2	1:C:1631:MET:HG3	2.20	0.55
1:C:2136:ILE:HD11	1:C:2152:ILE:HG22	1.89	0.55
1:B:2008:ASN:HB3	1:B:2012:MET:HE3	1.89	0.55
1:B:2148:ARG:O	1:B:2152:ILE:HG13	2.07	0.55
1:A:1868:GLU:HG2	1:A:1871:SER:HB3	1.89	0.55
1:C:1569:ILE:HG22	1:C:1571:VAL:HG23	1.89	0.55
1:C:1638:LEU:HD22	1:C:1665:THR:HG21	1.88	0.55
1:C:1991:PRO:HG3	1:C:2017:ASP:CG	2.27	0.55
1:A:1926:PRO:HG2	2:A:3058:HOH:O	2.07	0.54
1:A:2083:LEU:HB3	1:A:2084:PRO:HD3	1.89	0.54
1:C:1675:VAL:HG12	1:C:1693:ILE:HA	1.89	0.54
1:B:1905:ALA:O	1:B:1907:PRO:HD3	2.06	0.54
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.04	0.54
1:A:2106:LYS:HA	1:A:2106:LYS:HE2	1.88	0.54
1:A:2186:LEU:C	1:A:2188:GLY:H	2.11	0.54
1:A:1790:HIS:HA	1:A:1870:LEU:HD23	1.89	0.54
1:A:1975:VAL:CG2	1:A:2002:VAL:HG23	2.36	0.54
1:C:2036:ARG:HB3	1:C:2036:ARG:HH11	1.73	0.54
1:A:2081:GLU:OE1	1:A:2081:GLU:N	2.41	0.54
1:B:2100:SER:O	1:B:2104:VAL:HG23	2.08	0.54
1:C:1642:ALA:HB3	1:C:1655:TYR:CB	2.37	0.54
1:B:1730:CYS:CA	1:B:1752:GLN:HE21	1.99	0.54
1:A:1491:GLU:O	1:A:1495:PRO:HA	2.08	0.54
1:B:1638:LEU:HD11	1:B:1666:LEU:CD1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1509:TYR:HE1	1:C:1560:ASN:ND2	2.05	0.54
1:B:1701:GLY:H	1:C:2102:ARG:HH22	1.56	0.54
1:A:1656:LEU:O	1:A:1690:ILE:HG12	2.08	0.53
1:A:1657:TYR:CZ	1:A:1687:ARG:HD2	2.43	0.53
1:C:1587:ASN:HB2	1:C:1623:ALA:O	2.08	0.53
1:C:1682:ILE:HG21	1:C:1687:ARG:HH11	1.72	0.53
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	2.06	0.53
1:B:1571:VAL:O	1:B:1579:GLY:HA2	2.08	0.53
1:B:2108:VAL:HG23	1:B:2109:ILE:HG23	1.91	0.53
1:B:1956:PHE:HB2	1:C:1756:LEU:HD13	1.91	0.53
1:B:1786:ASN:HD21	1:C:1966:GLU:HG3	1.74	0.53
1:B:1705:LEU:HD21	1:C:1997:GLY:HA2	1.89	0.53
1:B:2136:ILE:HD11	1:B:2152:ILE:HG12	1.90	0.53
1:B:1692:THR:HG21	1:C:2101:SER:HB2	1.91	0.53
1:A:2136:ILE:HD11	1:A:2152:ILE:HD13	1.91	0.53
1:C:1603:PHE:O	1:C:1607:VAL:HG23	2.08	0.53
1:C:1682:ILE:HG22	1:C:1687:ARG:HD2	1.90	0.53
1:C:1981:TYR:CG	1:C:1985:ILE:HD11	2.44	0.53
1:B:1644:ASN:OD1	1:B:1654:GLN:HG2	2.09	0.53
1:C:1527:SER:O	1:C:1530:VAL:HG22	2.08	0.53
1:B:1763:ASN:ND2	1:B:1770:VAL:H	2.08	0.52
1:C:1925:HIS:HE1	2:C:3042:HOH:O	1.93	0.52
1:C:2164:ASP:H	1:C:2170:GLN:HE22	1.57	0.52
1:B:1946:PRO:HG3	1:B:2130:LEU:HD21	1.92	0.52
1:C:1555:ARG:HH22	1:C:1560:ASN:HA	1.74	0.52
1:B:1786:ASN:ND2	1:C:1964:PHE:O	2.42	0.52
1:C:1587:ASN:ND2	1:C:1624:ASN:HD22	2.07	0.52
1:A:1497:ARG:HH11	1:A:1497:ARG:CB	2.22	0.52
1:A:1681:VAL:HG12	1:A:1686:GLU:CA	2.39	0.52
1:A:1720:HIS:HD2	2:A:3021:HOH:O	1.92	0.52
1:C:1642:ALA:HB3	1:C:1655:TYR:HB3	1.92	0.52
1:A:1773:SER:H	1:A:1776:GLN:HE21	1.55	0.52
1:B:1494:GLN:HB3	1:B:1497:ARG:HH21	1.75	0.52
1:B:1655:TYR:O	1:B:1656:LEU:HD23	2.10	0.52
1:B:1998:GLY:O	1:B:2001:VAL:HG12	2.10	0.51
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.58	0.51
1:A:2135:LEU:HB3	1:A:2155:ILE:CD1	2.37	0.51
1:B:2041:LEU:HA	1:B:2044:MET:HB2	1.92	0.51
1:C:1741:ARG:NH1	1:C:1744:GLN:HE22	2.08	0.51
1:C:2028:GLN:O	1:C:2031:VAL:HG12	2.10	0.51
1:A:2029:GLY:O	1:A:2033:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1730:CYS:HA	1:C:1752:GLN:OE1	2.10	0.51
1:C:2100:SER:O	1:C:2104:VAL:HG23	2.11	0.51
1:B:1541:GLU:OE1	1:B:1555:ARG:HD3	2.10	0.51
1:C:1586:ALA:HB2	1:C:1621:LEU:HB2	1.92	0.51
1:C:1922:GLN:HB2	1:C:1954:ARG:NH1	2.24	0.51
1:B:1733:VAL:HA	1:B:1755:ILE:O	2.11	0.51
1:A:1651:LYS:HB3	1:A:1651:LYS:HZ2	1.75	0.50
1:B:2101:SER:HB2	1:C:1692:THR:HG21	1.94	0.50
1:C:2152:ILE:HG13	1:C:2153:ALA:N	2.26	0.50
1:A:2190:LYS:C	1:A:2192:GLU:H	2.12	0.50
1:A:1759:ALA:HB3	1:A:1760:PRO:HD3	1.93	0.50
1:B:1633:GLU:HA	1:B:1636:VAL:HG23	1.93	0.50
1:C:1523:TRP:HB3	1:C:1530:VAL:HG21	1.93	0.50
1:A:1503:MET:HG2	1:A:1589:ILE:HG12	1.93	0.50
1:A:1838:ASP:O	1:A:1839:GLU:HG3	2.12	0.50
1:A:1991:PRO:CG	1:A:2115:TRP:HB2	2.42	0.50
1:B:2167:ASP:O	1:B:2171:VAL:HG23	2.11	0.50
1:A:2187:LYS:HA	1:A:2190:LYS:HE3	1.94	0.50
1:C:1790:HIS:HD2	2:C:3033:HOH:O	1.94	0.50
1:B:2031:VAL:CG2	1:B:2091:LEU:HD23	2.41	0.50
1:B:1829:ARG:CZ	1:B:2119:ARG:HE	2.25	0.50
1:C:1550:LEU:HD21	1:C:1607:VAL:HG22	1.94	0.50
1:C:1666:LEU:HB3	1:C:1672:GLU:HA	1.93	0.50
1:B:1523:TRP:HB3	1:B:1530:VAL:HG11	1.94	0.49
1:C:1936:ILE:HD13	1:C:1978:LEU:HD13	1.93	0.49
1:C:1998:GLY:O	1:C:2001:VAL:HG12	2.12	0.49
1:A:1682:ILE:H	1:A:1682:ILE:CD1	2.19	0.49
1:A:1683:ASN:HD22	1:A:1683:ASN:C	2.16	0.49
1:A:1870:LEU:HD12	2:A:3059:HOH:O	2.13	0.49
1:A:2010:ASP:OD2	1:A:2148:ARG:HD2	2.11	0.49
1:B:1489:VAL:HG23	1:B:1492:TRP:HB3	1.94	0.49
1:C:1575:GLU:CD	1:C:1575:GLU:H	2.15	0.49
1:B:1735:ILE:O	1:B:1735:ILE:HD13	2.13	0.49
1:A:1566:ALA:HA	1:A:1584:VAL:O	2.12	0.49
1:A:1720:HIS:CD2	2:A:3021:HOH:O	2.65	0.49
1:A:1936:ILE:HG12	1:A:1947:MET:CE	2.38	0.49
1:B:2146:ALA:O	1:B:2151:LYS:HE3	2.13	0.49
1:C:1683:ASN:HD22	1:C:1683:ASN:N	2.10	0.49
1:C:1686:GLU:HA	1:C:1686:GLU:OE1	2.12	0.49
1:A:1820:ILE:HD13	1:B:1487:TYR:CZ	2.48	0.49
1:A:1932:THR:O	1:A:1936:ILE:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2032:GLY:O	1:A:2033:ILE:HD13	2.12	0.49
1:B:1991:PRO:HG3	1:B:2017:ASP:OD2	2.12	0.49
1:C:1741:ARG:O	1:C:1741:ARG:HD3	2.12	0.49
1:C:1998:GLY:HA3	2:C:3052:HOH:O	2.11	0.48
1:B:1991:PRO:CG	1:B:2115:TRP:HB2	2.43	0.48
1:B:2134:TYR:O	1:B:2138:ARG:HG3	2.14	0.48
1:C:1883:ARG:HA	1:C:1887:ILE:O	2.12	0.48
1:B:1587:ASN:HB2	1:B:1623:ALA:O	2.13	0.48
1:B:1635:ILE:O	1:B:1639:PHE:HB3	2.13	0.48
1:B:1705:LEU:CD2	1:C:1997:GLY:HA2	2.42	0.48
1:C:1509:TYR:HE1	1:C:1560:ASN:HD22	1.60	0.48
1:C:1781:GLN:H	1:C:1781:GLN:HE21	1.61	0.48
1:C:2132:GLU:O	1:C:2136:ILE:HG13	2.13	0.48
1:A:1694:ILE:HD12	1:A:1694:ILE:N	2.29	0.48
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	1.94	0.48
1:B:2037:ARG:O	1:B:2041:LEU:HD23	2.14	0.48
1:C:1554:GLU:O	1:C:1554:GLU:HG3	2.13	0.48
1:A:1587:ASN:HB2	1:A:1623:ALA:O	2.14	0.48
1:B:1966:GLU:HB3	1:B:1969:LYS:HD2	1.95	0.48
1:C:1555:ARG:NH2	1:C:1560:ASN:HA	2.29	0.48
1:C:1754:ILE:O	1:C:1778:GLY:HA3	2.14	0.48
1:C:1879:VAL:HG13	1:C:1931:LYS:HE2	1.95	0.48
1:A:1682:ILE:HD13	1:A:1682:ILE:N	2.17	0.48
1:C:1852:THR:HG22	1:C:1853:GLU:H	1.78	0.48
1:B:1991:PRO:HG2	1:B:2115:TRP:HB2	1.95	0.47
1:B:1815:ASN:N	1:B:1944:GLN:HE22	1.85	0.47
1:A:1636:VAL:N	1:A:1637:PRO:CD	2.77	0.47
1:A:1997:GLY:O	1:A:2001:VAL:HG23	2.14	0.47
1:C:1586:ALA:CB	1:C:1621:LEU:HB2	2.44	0.47
1:B:2008:ASN:H	1:B:2012:MET:HE3	1.79	0.47
1:B:2163:VAL:HG13	1:B:2170:GLN:HG2	1.96	0.47
1:C:1766:LEU:HD12	1:C:1770:VAL:HG11	1.95	0.47
1:B:1966:GLU:OE2	1:B:1969:LYS:HD2	2.15	0.47
1:C:1493:LEU:N	1:C:1493:LEU:HD12	2.29	0.47
1:B:1783:MET:HA	1:B:1786:ASN:HB2	1.97	0.47
1:B:2083:LEU:HB3	1:B:2084:PRO:HD3	1.97	0.47
1:B:1984:PRO:HD3	1:B:2133:GLU:HG3	1.96	0.47
1:C:1527:SER:O	1:C:1530:VAL:HG13	2.15	0.47
1:B:1969:LYS:HG2	1:C:1741:ARG:CZ	2.45	0.47
1:C:1818:VAL:HG11	1:C:1946:PRO:HD3	1.95	0.47
1:C:1844:ARG:O	1:C:1848:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2102:ARG:O	1:C:2106:LYS:HG2	2.15	0.47
1:A:1745:ARG:HG2	1:A:1806:TRP:CZ2	2.50	0.47
1:A:1772:THR:N	1:A:1776:GLN:HE22	2.07	0.47
1:C:1493:LEU:HD21	1:C:1557:PRO:HB2	1.96	0.47
1:B:1636:VAL:N	1:B:1637:PRO:HD2	2.30	0.47
1:B:1555:ARG:NH2	2:B:3011:HOH:O	2.48	0.46
1:A:2011:GLN:HA	1:A:2129:ARG:HH22	1.81	0.46
1:C:1655:TYR:O	1:C:1656:LEU:HB2	2.15	0.46
1:A:1692:THR:HG22	1:A:1694:ILE:HD12	1.98	0.46
1:B:1678:GLU:O	1:B:1689:VAL:HG12	2.15	0.46
1:C:1639:PHE:HE1	1:C:1641:VAL:HG23	1.80	0.46
1:C:1679:ARG:HH11	1:C:1679:ARG:HG3	1.79	0.46
1:C:1614:ARG:HG3	1:C:1614:ARG:HH11	1.80	0.46
1:A:1596:PHE:HB2	1:A:1627:ALA:HA	1.96	0.46
1:B:1649:PRO:C	1:B:1651:LYS:H	2.19	0.46
1:C:1683:ASN:HD22	1:C:1683:ASN:H	1.64	0.46
1:A:2002:VAL:HG13	1:A:2003:VAL:HG23	1.98	0.46
1:B:1569:ILE:HG22	1:B:1571:VAL:HG22	1.97	0.46
1:B:1972:SER:HB3	1:C:1742:LEU:CD1	2.46	0.46
1:C:2083:LEU:N	1:C:2084:PRO:CD	2.78	0.46
1:B:1747:ILE:HD12	1:B:1803:ILE:HG13	1.97	0.46
1:C:1642:ALA:HB2	1:C:1657:TYR:CE1	2.50	0.46
1:C:2128:ARG:HE	1:C:2132:GLU:CD	2.18	0.46
1:A:1560:ASN:HD22	1:A:1560:ASN:N	2.10	0.46
1:C:1697:GLU:O	1:C:1700:LEU:HD13	2.16	0.46
1:B:1643:TRP:CE3	1:B:1649:PRO:HB2	2.51	0.46
1:B:2104:VAL:HG22	1:B:2109:ILE:HD11	1.96	0.46
1:C:1760:PRO:O	1:C:1764:LYS:HD3	2.15	0.46
1:A:2164:ASP:H	1:A:2170:GLN:NE2	2.14	0.46
1:A:2172:ALA:O	1:A:2176:GLU:HG3	2.16	0.46
1:C:1556:GLU:HG3	1:C:1557:PRO:HD2	1.97	0.46
1:C:2160:PRO:HB2	1:C:2163:VAL:HG23	1.98	0.46
1:A:1592:LYS:O	1:A:1593:ILE:HG12	2.16	0.45
1:B:1602:GLU:HG3	1:B:1603:PHE:N	2.31	0.45
1:C:1768:ARG:HG2	1:C:1768:ARG:HH11	1.81	0.45
1:C:1770:VAL:HG13	1:C:1771:TYR:N	2.30	0.45
1:C:1998:GLY:O	1:C:2001:VAL:CG1	2.64	0.45
1:C:1674:SER:O	1:C:1675:VAL:HG13	2.17	0.45
1:A:2090:SER:O	1:A:2093:PHE:HB3	2.16	0.45
1:A:2180:LYS:HD3	1:B:1482:PRO:HD3	1.98	0.45
1:C:1669:PHE:O	1:C:1670:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1883:ARG:HA	1:B:1887:ILE:O	2.17	0.45
1:C:1814:ARG:O	1:C:1815:ASN:HB2	2.17	0.45
1:A:1996:ARG:HG3	1:A:1996:ARG:HH11	1.82	0.45
1:A:1844:ARG:O	1:A:1848:GLU:HG2	2.17	0.45
1:C:1643:TRP:HA	1:C:1653:PHE:HA	1.99	0.45
1:A:1844:ARG:HH11	1:A:1844:ARG:HG3	1.81	0.45
1:A:2135:LEU:HD23	1:A:2155:ILE:HG23	1.99	0.45
1:C:1527:SER:HB3	1:C:1530:VAL:HG13	1.97	0.45
1:C:1677:THR:HA	1:C:1689:VAL:O	2.17	0.45
1:A:1632:ALA:HB1	1:A:1634:GLU:OE2	2.17	0.45
1:A:1899:VAL:HB	1:A:1919:GLU:HB2	1.98	0.45
1:B:1494:GLN:HB3	1:B:1497:ARG:NH2	2.32	0.45
1:B:1679:ARG:HG3	1:B:1679:ARG:O	2.17	0.45
1:B:1792:THR:HG23	2:B:3048:HOH:O	2.16	0.45
1:C:1845:TRP:CE2	1:C:1850:ARG:HD3	2.51	0.45
1:A:1527:SER:O	1:A:1530:VAL:HG22	2.16	0.45
1:A:2086:TYR:HA	1:A:2089:ILE:HD12	1.98	0.45
1:B:1682:ILE:HG22	1:B:1683:ASN:ND2	2.32	0.45
1:B:1874:ALA:HB1	1:B:1928:SER:HA	1.99	0.45
1:C:1818:VAL:CG1	1:C:1945:LEU:HD12	2.47	0.45
1:C:1829:ARG:CZ	1:C:1858:TYR:HB3	2.47	0.44
1:A:2110:SER:O	1:A:2111:LYS:HG3	2.16	0.44
1:C:1592:LYS:HD3	1:C:1628:ARG:CZ	2.47	0.44
1:C:1644:ASN:HD21	1:C:1687:ARG:HH12	1.64	0.44
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.64	0.44
1:C:1639:PHE:CE1	1:C:1641:VAL:HG23	2.52	0.44
1:C:1780:THR:O	1:C:1784:TYR:HB3	2.16	0.44
1:C:1889:LEU:HA	1:C:1945:LEU:HG	1.98	0.44
1:A:1587:ASN:ND2	1:A:1623:ALA:H	2.15	0.44
1:A:2134:TYR:CD2	1:A:2135:LEU:HD12	2.53	0.44
1:B:1638:LEU:CD2	1:B:1638:LEU:H	2.26	0.44
1:B:2016:ALA:O	1:B:2112:GLU:HA	2.18	0.44
1:B:2044:MET:HA	1:B:2086:TYR:HE2	1.82	0.44
1:C:1905:ALA:O	1:C:1907:PRO:HD3	2.17	0.44
1:B:2152:ILE:HG22	1:B:2156:ARG:HD2	1.99	0.44
1:C:1773:SER:N	1:C:1776:GLN:NE2	2.60	0.44
1:A:1491:GLU:HB3	1:A:1498:TYR:HB2	2.00	0.44
1:A:1681:VAL:HG12	1:A:1686:GLU:HB3	2.00	0.44
1:B:1829:ARG:CZ	1:B:2119:ARG:NE	2.81	0.44
1:B:2021:ARG:NH2	1:B:2099:ARG:NE	2.66	0.44
1:A:1780:THR:O	1:A:1784:TYR:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1813:LYS:HG2	1:A:1816:MET:HE2	1.92	0.43
1:A:2028:GLN:O	1:A:2031:VAL:HG12	2.19	0.43
1:B:1824:LYS:HG3	1:B:1825:ASP:N	2.32	0.43
1:B:2082:LEU:HD23	1:B:2082:LEU:H	1.83	0.43
1:A:2164:ASP:H	1:A:2170:GLN:HE22	1.65	0.43
1:A:1555:ARG:HH22	1:A:1560:ASN:HA	1.83	0.43
1:A:1639:PHE:HA	1:A:1658:LEU:HD23	1.99	0.43
1:A:1690:ILE:O	1:A:1690:ILE:HG13	2.18	0.43
1:A:1728:VAL:HG21	1:A:1754:ILE:HD11	2.00	0.43
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.83	0.43
1:A:2189:LEU:O	1:A:2192:GLU:HB3	2.19	0.43
1:C:1635:ILE:O	1:C:1635:ILE:HG22	2.18	0.43
1:B:1701:GLY:N	1:C:2102:ARG:HH22	2.17	0.43
1:C:1838:ASP:O	1:C:1839:GLU:HB2	2.18	0.43
1:C:2180:LYS:NZ	1:C:2180:LYS:HB3	2.33	0.43
1:A:1560:ASN:ND2	1:A:1560:ASN:N	2.67	0.43
1:A:1936:ILE:HA	1:A:1947:MET:HE3	2.00	0.43
1:A:2177:GLU:O	1:B:1501:HIS:HE1	2.02	0.43
1:C:1759:ALA:HB3	1:C:1760:PRO:HD3	2.00	0.43
1:C:1745:ARG:HG2	1:C:1806:TRP:CZ2	2.54	0.43
1:C:1719:TYR:CE2	1:C:1744:GLN:HG3	2.54	0.43
1:A:1797:LEU:O	1:A:1801:GLU:HG3	2.18	0.43
1:B:1643:TRP:CZ3	1:B:1649:PRO:HB2	2.54	0.43
1:C:2014:MET:HG2	1:C:2109:ILE:HG22	2.01	0.43
1:C:2148:ARG:HH11	1:C:2148:ARG:HG2	1.84	0.43
1:A:1906:ASP:H	1:A:1912:SER:CB	2.28	0.42
1:B:1637:PRO:HG2	1:B:1638:LEU:H	1.84	0.42
1:B:1728:VAL:HG21	1:B:1754:ILE:HD11	2.01	0.42
1:C:1852:THR:HG22	1:C:1853:GLU:N	2.33	0.42
1:C:1987:ILE:HG21	1:C:2014:MET:CE	2.49	0.42
1:C:1636:VAL:N	1:C:1637:PRO:HD2	2.34	0.42
1:A:1727:LEU:HD12	1:A:1747:ILE:O	2.18	0.42
1:C:1818:VAL:HG11	1:C:1945:LEU:HD12	2.00	0.42
1:B:1786:ASN:HA	1:B:1786:ASN:HD22	1.58	0.42
1:B:2008:ASN:CB	1:B:2012:MET:HE3	2.48	0.42
1:B:1701:GLY:HA2	1:C:2024:VAL:HG23	2.02	0.42
1:C:1683:ASN:ND2	1:C:1683:ASN:N	2.66	0.42
1:B:1776:GLN:O	1:C:1960:GLN:NE2	2.52	0.42
1:A:1636:VAL:HG13	1:A:1637:PRO:HD3	2.02	0.42
1:C:1637:PRO:HG2	1:C:1638:LEU:HD23	2.00	0.42
1:C:2085:ILE:O	1:C:2089:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1636:VAL:N	1:A:1637:PRO:HD2	2.34	0.42
1:B:2147:SER:HB3	1:B:2150:GLU:CG	2.37	0.42
1:A:1636:VAL:CG1	1:A:1637:PRO:HD3	2.49	0.42
1:A:1733:VAL:HA	1:A:1755:ILE:O	2.20	0.42
1:B:1544:GLU:HB3	1:B:1548:GLY:HA2	2.02	0.42
1:B:1881:ARG:HH11	1:B:1881:ARG:HG2	1.85	0.42
1:C:1494:GLN:N	1:C:1495:PRO:HD2	2.34	0.42
1:A:1490:LYS:HD3	1:A:1497:ARG:NE	2.34	0.42
1:A:1605:ASN:ND2	1:A:1714:ALA:HB2	2.35	0.42
1:C:1632:ALA:O	1:C:1636:VAL:HG23	2.20	0.42
1:C:2146:ALA:O	1:C:2151:LYS:HE3	2.20	0.42
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.50	0.41
1:A:1879:VAL:HG21	2:A:3059:HOH:O	2.19	0.41
1:A:2100:SER:O	1:A:2104:VAL:HG23	2.20	0.41
1:B:1776:GLN:O	1:B:1782:ILE:CD1	2.68	0.41
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.84	0.41
1:B:1792:THR:HG22	2:B:3056:HOH:O	2.20	0.41
1:B:2020:ALA:O	1:B:2021:ARG:HD2	2.20	0.41
1:A:1592:LYS:O	1:A:1593:ILE:CG1	2.67	0.41
1:B:2110:SER:O	1:B:2111:LYS:HG3	2.20	0.41
1:B:2088:GLN:HB2	1:C:1653:PHE:HE2	1.85	0.41
1:C:1677:THR:CB	1:C:1688:PHE:HB3	2.48	0.41
1:A:1865:SER:O	1:A:1882:ALA:HA	2.21	0.41
1:B:2134:TYR:CE1	1:B:2138:ARG:HD2	2.55	0.41
1:A:2095:ASP:O	1:A:2099:ARG:HD3	2.20	0.41
1:A:2179:TYR:HD1	1:B:1489:VAL:HA	1.85	0.41
1:C:1680:THR:O	1:C:1687:ARG:HB2	2.20	0.41
1:C:2004:ASP:HA	1:C:2005:PRO:HD3	1.95	0.41
1:B:1541:GLU:O	1:B:1552:GLU:HA	2.20	0.41
1:B:2088:GLN:HB2	1:C:1653:PHE:CE2	2.55	0.41
1:C:1783:MET:CA	1:C:1786:ASN:HB2	2.42	0.41
1:A:1994:GLU:HA	1:A:2021:ARG:O	2.21	0.41
1:A:2081:GLU:HB2	1:A:2082:LEU:H	1.50	0.41
1:A:2180:LYS:N	1:B:1491:GLU:OE1	2.50	0.41
1:B:1533:THR:HB	1:B:1534:ASP:H	1.51	0.41
1:C:1542:LEU:HD23	1:C:1550:LEU:HD23	2.02	0.41
1:C:1682:ILE:CG2	1:C:1687:ARG:HD2	2.51	0.41
1:C:1735:ILE:O	1:C:1735:ILE:HG13	2.20	0.41
1:C:1774:ASN:HD22	1:C:1774:ASN:HA	1.70	0.41
1:B:2083:LEU:N	1:B:2084:PRO:CD	2.84	0.41
1:A:2190:LYS:C	1:A:2192:GLU:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1509:TYR:OH	1:C:1560:ASN:HB3	2.19	0.41
1:C:1591:PHE:CD2	1:C:1591:PHE:C	2.94	0.41
1:C:1741:ARG:C	1:C:1741:ARG:HD3	2.41	0.41
1:A:1682:ILE:HD13	1:A:1685:GLU:O	2.21	0.41
1:A:1810:VAL:HG13	1:A:1811:PRO:HD2	2.03	0.40
1:A:2190:LYS:O	1:A:2193:SER:N	2.54	0.40
1:B:1720:HIS:ND1	1:B:1941:ASN:ND2	2.68	0.40
1:C:1587:ASN:HD21	1:C:1624:ASN:HD22	1.67	0.40
1:C:1772:THR:N	1:C:1776:GLN:NE2	2.56	0.40
1:A:1960:GLN:HE21	1:A:1961:ARG:N	2.19	0.40
1:A:2008:ASN:C	1:A:2008:ASN:ND2	2.74	0.40
1:C:2128:ARG:HA	1:C:2172:ALA:HB2	2.02	0.40
1:A:1790:HIS:CE1	2:A:3066:HOH:O	2.74	0.40
1:A:1836:THR:HG21	1:A:1839:GLU:OE2	2.22	0.40
1:A:2083:LEU:N	1:A:2084:PRO:CD	2.85	0.40
1:A:2160:PRO:HD3	1:A:2174:TRP:CE2	2.56	0.40
1:B:1603:PHE:O	1:B:1607:VAL:HG23	2.21	0.40
1:B:2097:HIS:HE1	1:C:1632:ALA:H	1.68	0.40
1:A:1602:GLU:HG3	1:A:1603:PHE:N	2.33	0.40
1:A:1575:GLU:HG2	1:A:1808:SER:O	2.21	0.40
1:B:1727:LEU:HB2	1:B:1803:ILE:HD11	2.03	0.40
1:B:1963:MET:CE	1:C:1755:ILE:HA	2.51	0.40
1:C:1592:LYS:O	1:C:1593:ILE:CG1	2.70	0.40
1:C:2086:TYR:HA	1:C:2089:ILE:HD12	2.04	0.40
1:A:1846:MET:HE1	1:A:1990:PRO:HB3	2.03	0.40
1:A:2169:ARG:HD3	1:B:1516:ARG:NH2	2.37	0.40
1:B:1814:ARG:O	1:B:1815:ASN:HB2	2.21	0.40
1:B:2008:ASN:CB	1:B:2012:MET:CE	2.95	0.40
1:B:1968:LEU:HD21	1:C:1756:LEU:HD21	2.02	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	678/737 (92%)	627 (92%)	48 (7%)	3 (0%)	34	54
1	B	672/737 (91%)	617 (92%)	49 (7%)	6 (1%)	17	31
1	C	662/737 (90%)	601 (91%)	56 (8%)	5 (1%)	19	35
All	All	2012/2211 (91%)	1845 (92%)	153 (8%)	14 (1%)	22	39

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1997	GLY
1	C	1649	PRO
1	C	1656	LEU
1	B	2189	LEU
1	A	2142	GLN
1	C	1654	GLN
1	B	1557	PRO
1	C	1508	VAL
1	B	1655	TYR
1	C	2143	VAL
1	A	2187	LYS
1	B	1637	PRO
1	B	2032	GLY
1	B	1489	VAL

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	577/628 (92%)	550 (95%)	27 (5%)	26	49
1	B	572/628 (91%)	543 (95%)	29 (5%)	24	45
1	C	563/628 (90%)	522 (93%)	41 (7%)	14	27
All	All	1712/1884 (91%)	1615 (94%)	97 (6%)	20	39

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1560	ASN
1	A	1585	VAL
1	A	1602	GLU
1	A	1618	ARG
1	A	1634	GLU
1	A	1682	ILE
1	A	1683	ASN
1	A	1769	GLU
1	A	1781	GLN
1	A	1824	LYS
1	A	1884	LEU
1	A	1909	ASN
1	A	1924	TRP
1	A	1930	PHE
1	A	1950	LEU
1	A	1960	GLN
1	A	1981	TYR
1	A	1996	ARG
1	A	2008	ASN
1	A	2034	LYS
1	A	2037	ARG
1	A	2081	GLU
1	A	2082	LEU
1	A	2086	TYR
1	A	2098	ASP
1	A	2099	ARG
1	A	2128	ARG
1	B	1489	VAL
1	B	1502	LEU
1	B	1503	MET
1	B	1533	THR
1	B	1534	ASP
1	B	1536	PHE
1	B	1555	ARG
1	B	1565	VAL
1	B	1571	VAL
1	B	1585	VAL
1	B	1602	GLU
1	B	1618	ARG
1	B	1639	PHE
1	B	1735	ILE
1	B	1777	LEU
1	B	1786	ASN

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Mol	Chain	Res	Type
1	B	1797	LEU
1	B	1843	VAL
1	B	1884	LEU
1	B	1909	ASN
1	B	1924	TRP
1	B	1961	ARG
1	B	1980	ASP
1	B	2042	ASP
1	B	2047	LEU
1	B	2086	TYR
1	B	2127	ARG
1	B	2128	ARG
1	B	2165	HIS
1	C	1499	LYS
1	C	1508	VAL
1	C	1520	SER
1	C	1524	LYS
1	C	1531	LYS
1	C	1536	PHE
1	C	1547	ASN
1	C	1585	VAL
1	C	1602	GLU
1	C	1618	ARG
1	C	1638	LEU
1	C	1639	PHE
1	C	1654	GLN
1	C	1655	TYR
1	C	1679	ARG
1	C	1706	ARG
1	C	1740	VAL
1	C	1741	ARG
1	C	1742	LEU
1	C	1772	THR
1	C	1781	GLN
1	C	1786	ASN
1	C	1824	LYS
1	C	1838	ASP
1	C	1879	VAL
1	C	1895	GLU
1	C	1902	LEU
1	C	1924	TRP
1	C	1930	PHE

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Mol	Chain	Res	Type
1	C	1945	LEU
1	C	1960	GLN
1	C	1968	LEU
1	C	1978	LEU
1	C	1981	TYR
1	C	2035	PHE
1	C	2045	ASN
1	C	2102	ARG
1	C	2114	GLU
1	C	2128	ARG
1	C	2138	ARG
1	C	2142	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
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	1640	GLN
1	A	1683	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
1	A	1934	GLN
1	A	1960	GLN
1	A	2008	ASN
1	A	2088	GLN
1	A	2092	GLN
1	A	2131	ASN
1	A	2142	GLN
1	A	2170	GLN
1	B	1494	GLN
1	B	1517	GLN
1	B	1525	ASN
1	B	1587	ASN

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Mol	Chain	Res	Type
1	B	1605	ASN
1	B	1624	ASN
1	B	1648	ASN
1	B	1683	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	1934	GLN
1	B	1941	ASN
1	B	1944	GLN
1	B	1983	GLN
1	B	2097	HIS
1	B	2131	ASN
1	C	1517	GLN
1	C	1522	GLN
1	C	1560	ASN
1	C	1587	ASN
1	C	1605	ASN
1	C	1640	GLN
1	C	1654	GLN
1	C	1683	ASN
1	C	1744	GLN
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	1922	GLN
1	C	1925	HIS
1	C	1934	GLN
1	C	1941	ASN
1	C	1960	GLN
1	C	2011	GLN
1	C	2092	GLN
1	C	2142	GLN

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Mol	Chain	Res	Type
1	C	2170	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 carbohydrates 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	682/737 (92%)	0.36	69 (10%) 7 6	22, 43, 99, 100	0
1	B	676/737 (91%)	0.40	65 (9%) 8 7	20, 44, 99, 100	0
1	C	666/737 (90%)	0.33	65 (9%) 7 7	19, 46, 100, 100	0
All	All	2024/2211 (91%)	0.36	199 (9%) 7 7	19, 45, 99, 100	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1649	PRO	10.5
1	B	2082	LEU	9.6
1	C	1644	ASN	7.8
1	C	2143	VAL	7.3
1	B	1680	THR	6.8
1	C	1685	GLU	6.5
1	A	2143	VAL	6.4
1	B	1492	TRP	6.4
1	A	2083	LEU	6.1
1	A	2047	LEU	6.1
1	C	1650	ASP	6.0
1	A	2144	GLY	5.9
1	C	2144	GLY	5.8
1	A	2037	ARG	5.8
1	A	2191	LEU	5.8
1	A	1492	TRP	5.7
1	C	1681	VAL	5.6
1	C	1647	ALA	5.6
1	A	1483	ILE	5.6
1	B	1649	PRO	5.5
1	B	1669	PHE	5.5
1	A	1682	ILE	5.4
1	B	2144	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	1683	ASN	5.3
1	A	1646	ALA	5.2
1	C	1648	ASN	5.2
1	A	1647	ALA	5.1
1	B	1483	ILE	5.0
1	B	1648	ASN	5.0
1	A	2145	GLU	4.9
1	B	2187	LYS	4.9
1	C	2141	HIS	4.9
1	C	1669	PHE	4.9
1	B	2043	THR	4.8
1	B	2190	LYS	4.8
1	A	2082	LEU	4.7
1	B	2041	LEU	4.7
1	B	1681	VAL	4.6
1	B	2189	LEU	4.6
1	B	1647	ALA	4.6
1	C	1655	TYR	4.6
1	A	1669	PHE	4.6
1	C	2142	GLN	4.5
1	B	2085	ILE	4.5
1	B	1679	ARG	4.5
1	B	2083	LEU	4.5
1	A	1649	PRO	4.4
1	C	1653	PHE	4.4
1	B	2143	VAL	4.3
1	A	2196	GLN	4.3
1	A	1685	GLU	4.2
1	C	1680	THR	4.2
1	B	1682	ILE	4.2
1	C	1678	GLU	4.2
1	B	2145	GLU	4.2
1	B	1683	ASN	4.2
1	C	2037	ARG	4.1
1	A	2194	PHE	4.1
1	B	2086	TYR	4.1
1	A	1645	ASP	4.1
1	B	1838	ASP	4.0
1	C	1646	ALA	4.0
1	A	1687	ARG	3.9
1	B	1651	LYS	3.9
1	C	1679	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	1679	ARG	3.8
1	A	2195	ALA	3.8
1	A	1855	GLY	3.8
1	A	1482	PRO	3.8
1	A	2142	GLN	3.8
1	B	2044	MET	3.7
1	A	1681	VAL	3.7
1	B	2037	ARG	3.7
1	C	1911	ASN	3.7
1	B	1684	GLY	3.7
1	C	1645	ASP	3.7
1	B	2084	PRO	3.5
1	A	1767	GLY	3.5
1	C	1682	ILE	3.5
1	A	1650	ASP	3.5
1	B	1678	GLU	3.5
1	B	1668	LYS	3.5
1	A	1652	GLY	3.4
1	A	1666	LEU	3.4
1	B	1685	GLU	3.4
1	C	1534	ASP	3.4
1	B	1911	ASN	3.4
1	C	1526	PHE	3.3
1	A	1680	THR	3.3
1	B	1584	VAL	3.3
1	A	2036	ARG	3.3
1	A	1648	ASN	3.2
1	B	1556	GLU	3.2
1	A	1688	PHE	3.2
1	C	1838	ASP	3.2
1	C	1641	VAL	3.2
1	C	1493	LEU	3.1
1	C	2082	LEU	3.1
1	A	2041	LEU	3.1
1	A	1838	ASP	3.0
1	A	1489	VAL	3.0
1	C	1530	VAL	3.0
1	C	1529	ASP	2.9
1	C	1547	ASN	2.9
1	C	1688	PHE	2.9
1	A	2086	TYR	2.9
1	C	1652	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	2180	LYS	2.8
1	C	1853	GLU	2.7
1	A	1547	ASN	2.7
1	B	1585	VAL	2.7
1	C	1668	LYS	2.7
1	C	2086	TYR	2.7
1	C	1683	ASN	2.7
1	B	1621	LEU	2.7
1	B	2036	ARG	2.7
1	B	2035	PHE	2.6
1	A	1554	GLU	2.6
1	A	1911	ASN	2.6
1	B	1839	GLU	2.6
1	B	2184	ASP	2.6
1	A	1768	ARG	2.6
1	A	1672	GLU	2.6
1	B	1586	ALA	2.6
1	C	1546	GLU	2.6
1	A	1668	LYS	2.6
1	B	1824	LYS	2.6
1	C	1531	LYS	2.6
1	B	1489	VAL	2.5
1	B	2146	ALA	2.5
1	A	1654	GLN	2.5
1	C	1651	LYS	2.5
1	A	2043	THR	2.5
1	A	1584	VAL	2.5
1	B	1646	ALA	2.5
1	B	1657	TYR	2.5
1	A	2190	LYS	2.5
1	B	1650	ASP	2.5
1	C	1656	LEU	2.4
1	A	1546	GLU	2.4
1	C	1725	ILE	2.4
1	B	1644	ASN	2.4
1	C	2031	VAL	2.4
1	B	2038	GLU	2.4
1	A	2085	ILE	2.4
1	B	1652	GLY	2.4
1	C	1910	PRO	2.4
1	C	1667	LYS	2.4
1	A	1839	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	1527	SER	2.4
1	A	1655	TYR	2.3
1	A	2193	SER	2.3
1	C	1621	LEU	2.3
1	A	1529	ASP	2.3
1	A	2038	GLU	2.3
1	C	1672	GLU	2.3
1	C	1620	TYR	2.3
1	B	1688	PHE	2.3
1	A	1644	ASN	2.3
1	B	2031	VAL	2.3
1	C	1639	PHE	2.3
1	A	1619	ILE	2.3
1	C	1585	VAL	2.3
1	C	1673	ASN	2.2
1	B	2188	GLY	2.2
1	C	1671	LYS	2.2
1	C	1670	ASP	2.2
1	B	2047	LEU	2.2
1	A	1643	TRP	2.2
1	C	2145	GLU	2.2
1	B	2134	TYR	2.2
1	B	1546	GLU	2.2
1	B	1531	LYS	2.2
1	B	2179	TYR	2.2
1	C	1492	TRP	2.2
1	A	1621	LEU	2.2
1	B	1620	TYR	2.2
1	C	1584	VAL	2.2
1	C	1619	ILE	2.1
1	C	2045	ASN	2.1
1	A	1530	VAL	2.1
1	C	1766	LEU	2.1
1	A	1684	GLY	2.1
1	A	1620	TYR	2.1
1	C	1769	GLU	2.1
1	A	1678	GLU	2.1
1	A	1840	THR	2.1
1	B	1766	LEU	2.1
1	A	1726	THR	2.1
1	B	1670	ASP	2.1
1	C	1687	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2140	SER	2.0
1	C	1657	TYR	2.0
1	B	1666	LEU	2.0
1	B	2040	LEU	2.0
1	A	1641	VAL	2.0
1	C	1726	THR	2.0
1	A	1725	ILE	2.0
1	C	2084	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.