Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 10:03 pm BST

PDB ID	:	1UYR
Title	:	Acetyl-CoA Carboxylase Carboxyltransferase Domain in complex with inhibitor Diclofop
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 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:

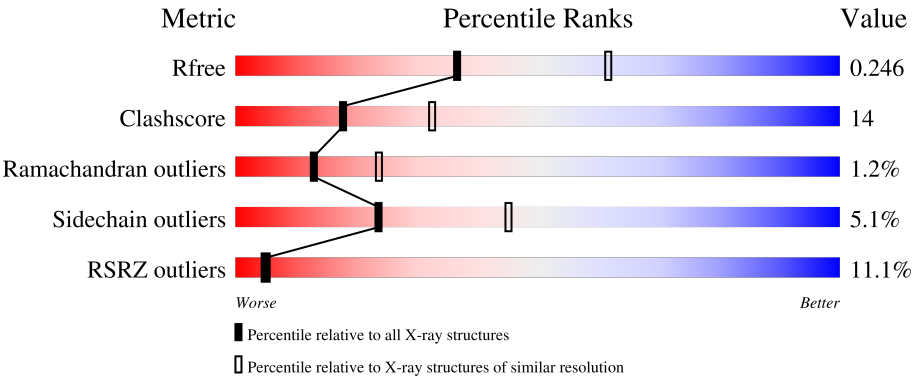
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.50 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 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	11% 69% 23% • 5%
1	B	737	10% 66% 26% • 6%

2 Entry composition

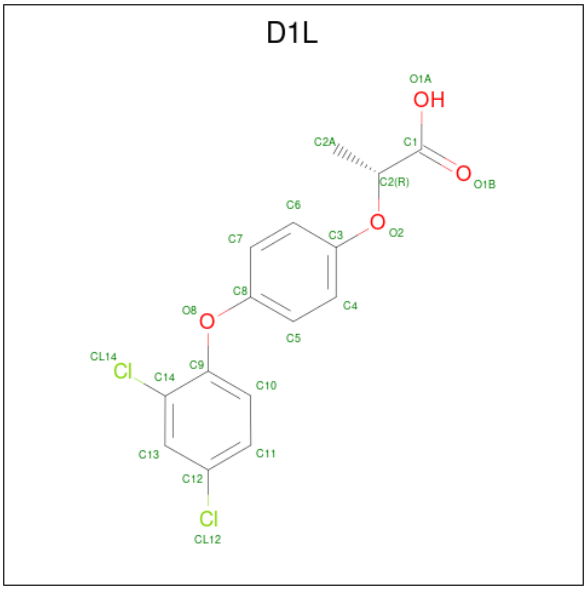
There are 3 unique types of molecules in this entry. The entry contains 11229 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	698	Total	C	N	O	S	0	0	0
			5515	3514	949	1034	18			
1	B	695	Total	C	N	O	S	0	0	0
			5495	3498	947	1032	18			

- Molecule 2 is 2-[4-(2,4-DICHLOROPHENOXY)PHENOXY]PROPANOIC ACID (three-letter code: D1L) (formula: $C_{15}H_{12}Cl_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	O	0	0
			21	15	2	4		
2	B	1	Total	C	Cl	O	0	0
			21	15	2	4		

- Molecule 3 is water.

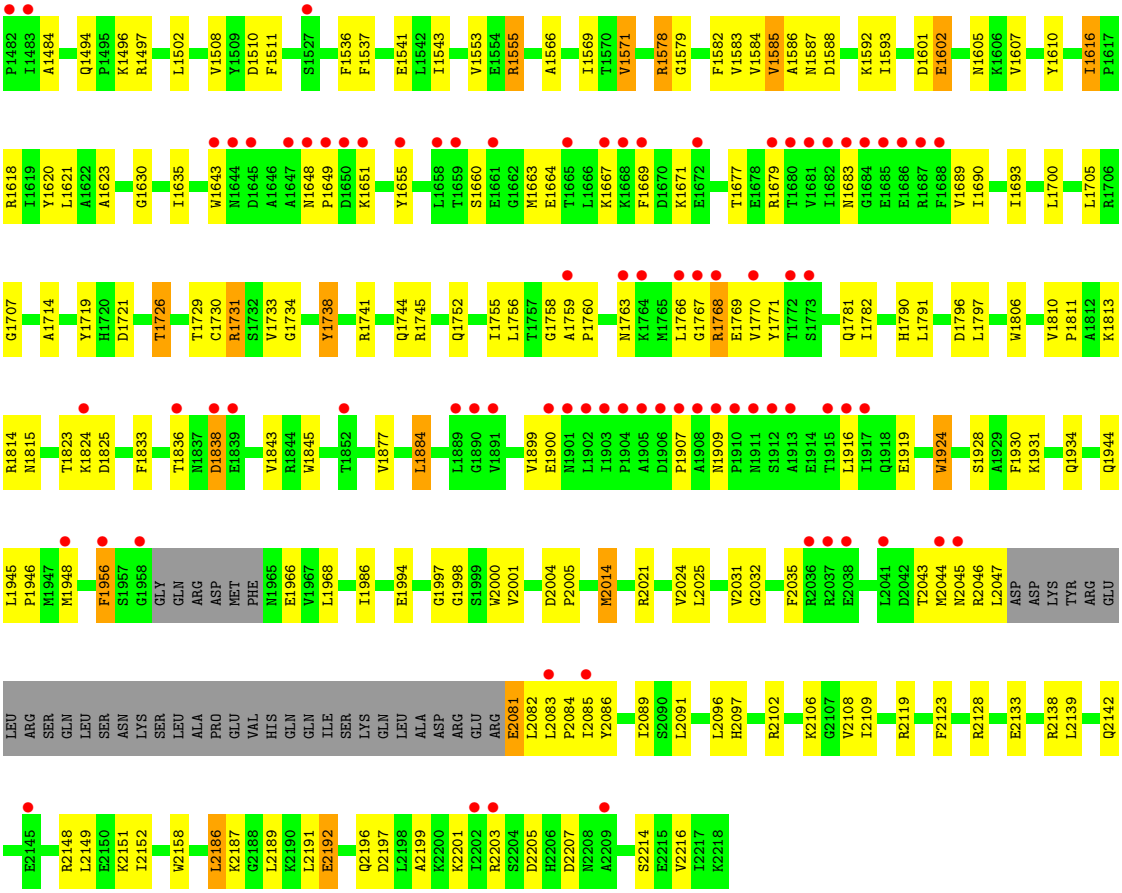
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	92	Total O 92 92	0	0
3	B	85	Total O 85 85	0	0

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.

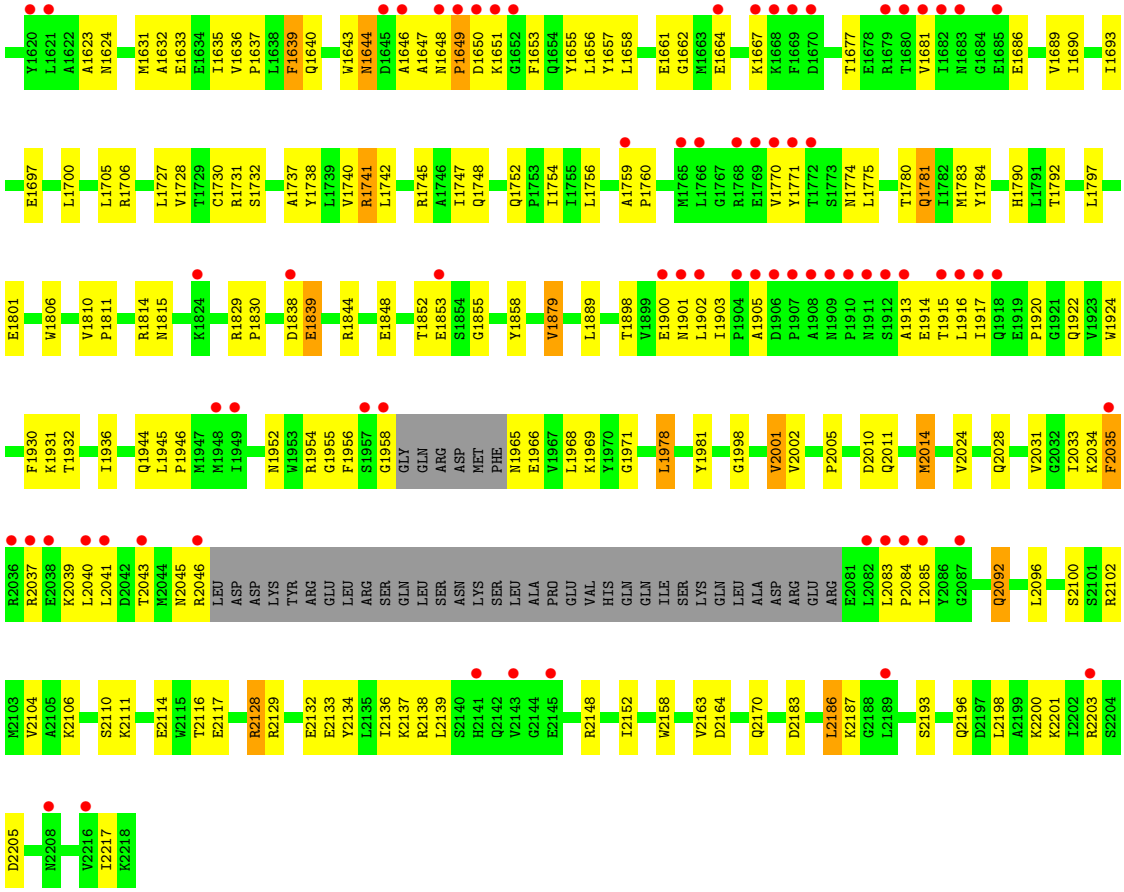
• Molecule 1: ACETYL-COA CARBOXYLASE

Chain A:



• Molecule 1: ACETYL-COA CARBOXYLASE

Chain B:


Y1620 L1621 A1622 A1623 N1624
M1631 A1632 E1633 E1634 I1635 V1636 P1637 L1638 F1639 Q1640
W1643 N1644 D1645 A1646 A1647 N1648 P1649 D1650 K1651 G1652 F1653 Q1654 Y1655 L1656 Y1657 L1658
E1661 G1662 M1663 E1664
K1667 K1668 F1669 D1670
T1677 E1678 R1679 T1680 V1681 I1682 N1683 G1684 E1685 E1686
V1689 I1690
I1693
E1697
L1700
L1705 R1706
L1727 V1728 T1729 C1730 R1731 S1732
A1737 Y1738 L1739 V1740 R1741 L1742
R1745 A1746 I1747 Q1748
Q1752 P1753 I1754 I1755 L1756
A1759 P1760
M1765 L1766 G1767 R1768 E1769 V1770 Y1771 T1772 S1773
N1774 L1775
T1780 Q1781 I1782 M1783 Y1784
H1790 L1791 T1792
L1797
E1801 W1806 V1810 P1811 R1814 N1815 K1824 R1829 P1830 D1838 E1839 R1844 E1848 T1852 E1853 S1854 G1855 Y1858 V1879 L1889 T1898 V1899 E1900 N1901 L1902 I1903 P1904 A1905 D1906 P1907 A1908 N1909 P1910 N1911 S1912 A1913 E1914 T1915 L1916 I1917 Q1918 E1919 P1920 G1921 Q1922 V1923 W1924
F1930 K1931 T1932 I1936 Q1944 L1945 P1946 M1947 M1948 I1949 N1952 W1953 R1954 G1955 F1956 S1957 G1958 GLY GLN ARG ASP MET PHE N1965 E1966 V1967 L1968 K1969 Y1970 G1971 L1978 Y1981 G1998 V2001 V2002 P2005 D2010 Q2011 M2014 V2024 Q2028 V2031 G2032 I2033 K2034 F2035
R2036 R2037 E2038 K2039 L2040 L2041 D2042 T2043 M2044 N2045 R2046 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 E2061 L2082 L2083 P2084 I2085 Y2086 G2087 Q2092 L2096 S2100 S2101 R2102
M2103 V2104 A2105 K2106 S2110 K2111 E2114 W2115 T2116 E2117 R2128 R2129 E2132 E2133 Y2134 L2135 I2136 K2137 R2138 L2139 S2140 H2141 Q2142 V2143 G2144 E2145 R2148 I2152 W2158 V2163 D2164 Q2170 D2183 L2186 K2187 G2188 L2189 S2193 Q2196 D2197 L2198 A2199 K2200 K2201 I2202 R2203 S2204
D2205 N2208 W2216 I2217 K2218

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	136.78Å 136.78Å 244.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.58 – 2.50 29.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.58-2.50) 98.5 (29.84-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.30 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.248 0.215 , 0.246	Depositor DCC
R_{free} test set	9060 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11229	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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

Bond lengths and bond angles in the following residue types are not validated in this section: D1L

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	0.37	0/5635	0.59	0/7634
1	B	0.37	0/5614	0.60	1/7605 (0.0%)
All	All	0.37	0/11249	0.59	1/15239 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1647	ALA	N-CA-C	-5.36	96.54	111.00

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	5515	0	5430	141	0
1	B	5495	0	5404	168	0
2	A	21	0	11	6	0
2	B	21	0	11	6	0
3	A	92	0	0	3	0
3	B	85	0	0	5	0
All	All	11229	0	10856	297	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 (297) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1494:GLN:HE21	1:A:1496:LYS:H	1.11	0.98
1:A:2014:MET:HG2	1:A:2109:ILE:HG22	1.45	0.98
1:A:1815:ASN:H	1:A:1944:GLN:HE22	1.06	0.97
1:B:1681:VAL:HA	1:B:1686:GLU:HA	1.51	0.90
1:A:2082:LEU:HD23	1:A:2082:LEU:H	1.38	0.88
1:B:1759:ALA:H	1:B:1774:ASN:HD21	1.20	0.87
1:B:1646:ALA:HB1	1:B:1648:ASN:O	1.77	0.85
1:A:2031:VAL:HG21	1:A:2091:LEU:HD23	1.60	0.84
2:A:3219:D1L:H13	1:B:1971:GLY:HA3	1.59	0.83
1:A:1585:VAL:HG13	1:A:1607:VAL:HG11	1.60	0.83
1:A:1660:SER:O	1:A:1664:GLU:HG2	1.79	0.83
1:A:1781:GLN:HE21	1:A:1782:ILE:HG13	1.46	0.81
1:B:1658:LEU:HG	1:B:1690:ILE:HD11	1.64	0.80
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.29	0.79
1:A:1836:THR:HG22	1:A:1838:ASP:H	1.48	0.79
1:A:1677:THR:HG22	1:A:1690:ILE:HA	1.66	0.78
1:B:2164:ASP:H	1:B:2170:GLN:NE2	1.82	0.77
1:B:1560:ASN:HD22	1:B:1560:ASN:H	1.34	0.76
1:A:1508:VAL:HG21	1:A:1588:ASP:HA	1.68	0.75
1:B:1681:VAL:HG22	1:B:1686:GLU:HB3	1.69	0.74
1:B:2037:ARG:NH1	1:B:2041:LEU:HD22	2.04	0.72
1:B:2183:ASP:OD1	1:B:2187:LYS:HE3	1.89	0.72
1:A:1738:TYR:CD1	2:A:3219:D1L:H5	2.24	0.72
1:B:1759:ALA:H	1:B:1774:ASN:ND2	1.89	0.71
1:B:1954:ARG:HG3	1:B:1955:GLY:H	1.56	0.70
2:A:3219:D1L:CL14	1:B:1968:LEU:HD12	2.28	0.70
1:A:1738:TYR:OH	1:B:2002:VAL:HG12	1.91	0.70
1:B:2028:GLN:O	1:B:2031:VAL:HG12	1.90	0.70
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.57	0.70
1:B:1697:GLU:O	1:B:1700:LEU:HD13	1.92	0.68
1:A:2085:ILE:O	1:A:2089:ILE:HG13	1.94	0.67
1:B:2164:ASP:H	1:B:2170:GLN:HE22	1.41	0.67
1:B:1737:ALA:O	1:B:1740:VAL:HG22	1.95	0.67
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	1.93	0.66
1:B:1745:ARG:NH2	3:B:4037:HOH:O	2.29	0.66
1:B:1730:CYS:HA	1:B:1752:GLN:OE1	1.96	0.66
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.44	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2197:ASP:OD2	1:A:2201:LYS:HE2	1.96	0.66
1:A:1663:MET:O	1:A:1667:LYS:HG3	1.97	0.64
1:A:2001:VAL:HG21	2:B:3219:D1L:H4	1.79	0.64
1:B:2137:LYS:HE3	3:B:4079:HOH:O	1.97	0.63
1:A:1745:ARG:NH2	3:A:4038:HOH:O	2.31	0.62
1:A:1768:ARG:H	1:A:1768:ARG:HD3	1.65	0.62
1:A:1968:LEU:HD23	2:B:3219:D1L:CL14	2.36	0.62
1:B:2083:LEU:HB3	1:B:2084:PRO:HD3	1.82	0.62
1:A:2083:LEU:HB3	1:A:2084:PRO:HD3	1.82	0.62
1:A:1511:PHE:HZ	1:A:1729:THR:HG21	1.64	0.62
1:A:1956:PHE:CE1	1:A:1998:GLY:HA3	2.34	0.61
1:A:1956:PHE:HE1	1:A:1998:GLY:HA3	1.65	0.61
1:A:2192:GLU:O	1:A:2196:GLN:HG2	2.01	0.61
1:B:1781:GLN:H	1:B:1781:GLN:HE21	1.47	0.60
1:A:2046:ARG:NH1	1:A:2047:LEU:HD11	2.17	0.59
1:B:1902:LEU:HD12	1:B:1915:THR:O	2.02	0.59
1:B:2033:ILE:HG22	1:B:2034:LYS:HD2	1.83	0.59
1:B:1527:SER:O	1:B:1530:VAL:HG22	2.01	0.59
1:A:1571:VAL:O	1:A:1579:GLY:HA2	2.03	0.59
1:B:2110:SER:O	1:B:2111:LYS:HB3	2.02	0.58
1:B:2102:ARG:NH1	1:B:2106:LYS:HG3	2.18	0.58
2:A:3219:D1L:CL14	1:B:1968:LEU:HA	2.40	0.58
1:B:1792:THR:HG23	3:B:4038:HOH:O	2.03	0.58
1:B:1681:VAL:HG22	1:B:1686:GLU:CB	2.34	0.58
1:B:1745:ARG:HG2	1:B:1806:TRP:CZ2	2.39	0.58
2:A:3219:D1L:C4	1:B:2001:VAL:HG11	2.34	0.57
1:A:2046:ARG:C	1:A:2047:LEU:HD12	2.24	0.57
1:B:1901:ASN:HB3	1:B:1917:ILE:HB	1.85	0.57
1:A:1586:ALA:HB2	1:A:1621:LEU:HB2	1.86	0.57
1:B:2136:ILE:HD11	1:B:2152:ILE:HG12	1.84	0.57
1:B:1898:THR:HG22	1:B:1920:PRO:HA	1.85	0.57
1:A:1537:PHE:HD2	1:A:1571:VAL:HG13	1.70	0.57
1:A:2148:ARG:HG3	1:A:2148:ARG:HH11	1.69	0.57
1:B:1838:ASP:O	1:B:1839:GLU:HB2	2.05	0.57
1:B:1905:ALA:HB2	1:B:1913:ALA:C	2.25	0.57
1:B:1560:ASN:H	1:B:1560:ASN:ND2	2.01	0.56
1:A:2001:VAL:HG21	2:B:3219:D1L:C4	2.34	0.56
1:A:2082:LEU:HD23	1:A:2082:LEU:N	2.15	0.56
1:A:1719:TYR:CE2	1:A:1744:GLN:HG3	2.41	0.56
1:A:1763:ASN:HD21	1:A:1771:TYR:H	1.53	0.56
1:B:1569:ILE:HG22	1:B:1571:VAL:HG23	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1815:ASN:ND2	1:B:1944:GLN:HE22	2.02	0.56
1:A:2097:HIS:NE2	1:B:1631:MET:HG3	2.21	0.56
1:B:1902:LEU:HD11	1:B:1914:GLU:OE1	2.06	0.56
1:A:2086:TYR:HA	1:A:2089:ILE:HD12	1.87	0.55
1:A:2097:HIS:CE1	1:B:1632:ALA:H	2.25	0.55
1:A:1884:LEU:HD13	1:A:2123:PHE:HA	1.89	0.55
1:A:2142:GLN:NE2	1:A:2151:LYS:HE2	2.22	0.55
1:B:2033:ILE:HG22	1:B:2034:LYS:CD	2.36	0.55
1:B:2100:SER:O	1:B:2104:VAL:HG23	2.06	0.55
1:A:1729:THR:HG22	1:A:1796:ASP:OD1	2.07	0.55
1:B:1903:ILE:HD12	1:B:1903:ILE:N	2.21	0.55
1:B:1966:GLU:HA	1:B:1966:GLU:OE1	2.05	0.54
1:B:1643:TRP:HA	1:B:1653:PHE:HA	1.89	0.54
1:A:1541:GLU:OE1	1:A:1555:ARG:HD3	2.07	0.54
1:A:1756:LEU:HD21	1:B:1968:LEU:HD13	1.90	0.54
1:B:1797:LEU:O	1:B:1801:GLU:HG3	2.08	0.54
1:A:1630:GLY:O	1:A:1700:LEU:HD22	2.08	0.53
1:A:1815:ASN:H	1:A:1944:GLN:NE2	1.90	0.53
1:B:1661:GLU:HG3	1:B:1662:GLY:N	2.23	0.53
1:B:1756:LEU:HD22	2:B:3219:D1L:H7	1.91	0.53
1:B:2193:SER:HA	1:B:2196:GLN:HB2	1.90	0.53
1:A:1630:GLY:C	1:A:1700:LEU:HD22	2.29	0.53
1:B:1922:GLN:HG2	1:B:1952:ASN:O	2.09	0.53
1:A:1630:GLY:O	1:A:1700:LEU:HB3	2.09	0.52
1:B:1900:GLU:OE1	1:B:1916:LEU:HD21	2.10	0.52
1:B:1741:ARG:O	1:B:1741:ARG:HD3	2.09	0.51
1:A:1494:GLN:NE2	1:A:1496:LYS:H	1.94	0.51
1:A:2043:THR:O	1:A:2047:LEU:HD13	2.10	0.51
1:A:2148:ARG:HG3	1:A:2148:ARG:NH1	2.26	0.51
1:A:2139:LEU:HD21	1:A:2189:LEU:HD23	1.93	0.51
1:B:1781:GLN:H	1:B:1781:GLN:NE2	2.08	0.51
1:A:1578:ARG:HG2	1:A:1578:ARG:HH11	1.75	0.51
1:A:1810:VAL:HG13	1:A:1811:PRO:HD2	1.92	0.51
1:B:1589:ILE:HG13	1:B:1589:ILE:O	2.11	0.51
1:B:2010:ASP:OD1	1:B:2148:ARG:HD3	2.11	0.51
1:B:1958:GLY:O	1:B:1965:ASN:ND2	2.44	0.51
1:B:2031:VAL:HG23	1:B:2035:PHE:HB3	1.93	0.51
1:A:1586:ALA:CB	1:A:1621:LEU:HB2	2.41	0.50
1:B:1661:GLU:HG3	1:B:1662:GLY:H	1.76	0.50
1:A:1968:LEU:HA	2:B:3219:D1L:CL14	2.48	0.50
1:A:2024:VAL:HG12	1:A:2025:LEU:HD13	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1643:TRP:CE2	1:B:1649:PRO:HG3	2.47	0.50
1:B:2128:ARG:HE	1:B:2132:GLU:CD	2.15	0.50
1:A:1824:LYS:HG3	1:A:1825:ASP:N	2.26	0.50
1:B:1635:ILE:O	1:B:1639:PHE:HB3	2.10	0.50
1:B:1998:GLY:HA2	1:B:2001:VAL:CG1	2.41	0.50
1:A:1648:ASN:HB3	1:A:1651:LYS:HG2	1.93	0.50
1:A:1768:ARG:H	1:A:1768:ARG:CD	2.24	0.50
1:A:1781:GLN:NE2	1:A:1782:ILE:HG13	2.23	0.50
1:A:1605:ASN:ND2	1:A:1714:ALA:HB2	2.27	0.50
1:B:2136:ILE:CD1	1:B:2152:ILE:HG12	2.42	0.50
1:B:2133:GLU:O	1:B:2137:LYS:HG2	2.11	0.49
1:B:1587:ASN:ND2	1:B:1624:ASN:HD22	2.10	0.49
1:B:2005:PRO:HD3	1:B:2014:MET:HG3	1.93	0.49
1:B:1790:HIS:HD2	3:B:4057:HOH:O	1.96	0.49
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	2.24	0.49
1:B:2045:ASN:HD22	1:B:2046:ARG:NH1	2.10	0.49
1:A:2047:LEU:HD12	1:A:2047:LEU:N	2.27	0.49
1:A:2148:ARG:O	1:A:2152:ILE:HG13	2.12	0.49
1:B:1646:ALA:HB1	1:B:1648:ASN:C	2.33	0.49
1:B:1844:ARG:O	1:B:1848:GLU:HG2	2.13	0.49
1:B:1492:TRP:HZ2	1:B:1556:GLU:CG	2.26	0.49
1:A:1602:GLU:HG3	3:A:4023:HOH:O	2.13	0.48
1:B:1544:GLU:OE2	1:B:1602:GLU:OE2	2.31	0.48
1:B:1636:VAL:N	1:B:1637:PRO:HD2	2.28	0.48
1:A:1900:GLU:HB3	1:A:1916:LEU:HD11	1.94	0.48
1:A:2133:GLU:OE2	1:A:2148:ARG:NH2	2.45	0.48
1:B:1727:LEU:HD12	1:B:1747:ILE:O	2.14	0.48
1:B:1741:ARG:HD3	1:B:1741:ARG:C	2.34	0.48
1:A:1705:LEU:HD21	1:B:2024:VAL:HG22	1.95	0.48
1:A:2031:VAL:CG2	1:A:2091:LEU:HD23	2.39	0.48
1:A:1664:GLU:OE2	1:A:1667:LYS:HD2	2.13	0.48
1:B:2043:THR:HG23	1:B:2046:ARG:CZ	2.43	0.48
1:B:1815:ASN:HD22	1:B:1944:GLN:HE22	1.62	0.48
1:A:2046:ARG:CZ	1:A:2047:LEU:HD11	2.44	0.47
1:A:2086:TYR:HA	1:A:2089:ILE:CD1	2.44	0.47
1:A:1635:ILE:HG22	1:A:1635:ILE:O	2.14	0.47
1:B:1646:ALA:C	1:B:1648:ASN:H	2.12	0.47
1:B:1830:PRO:HB2	1:B:2116:THR:HG23	1.95	0.47
1:B:1503:MET:CE	1:B:1731:ARG:HH21	2.28	0.47
1:A:2158:TRP:CZ3	1:A:2186:LEU:HD13	2.50	0.47
1:A:2000:TRP:HB3	1:B:1705:LEU:HD13	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1677:THR:CG2	1:B:1690:ILE:HD13	2.44	0.47
1:B:2198:LEU:O	1:B:2201:LYS:HB2	2.15	0.47
1:B:1508:VAL:HG21	1:B:1588:ASP:HA	1.96	0.47
1:B:1664:GLU:O	1:B:1667:LYS:HB2	2.14	0.47
1:A:1497:ARG:HD3	1:A:1510:ASP:OD1	2.14	0.47
1:B:1612:ARG:O	1:B:1814:ARG:NH2	2.48	0.47
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	1.97	0.47
1:B:2043:THR:O	1:B:2043:THR:HG22	2.15	0.47
1:B:2046:ARG:HD2	1:B:2046:ARG:N	2.29	0.47
1:A:1741:ARG:NH2	1:A:1934:GLN:NE2	2.63	0.47
1:B:2035:PHE:HE1	1:B:2040:LEU:HA	1.80	0.47
1:A:1745:ARG:HG2	1:A:1806:TRP:CZ2	2.50	0.47
1:A:2004:ASP:OD1	1:B:1706:ARG:HA	2.15	0.46
1:A:2082:LEU:H	1:A:2082:LEU:CD2	2.20	0.46
1:B:2200:LYS:HG3	1:B:2203:ARG:NH2	2.30	0.46
1:A:1592:LYS:O	1:A:1593:ILE:HG12	2.14	0.46
1:A:2001:VAL:HG11	2:B:3219:D1L:H4	1.97	0.46
1:A:2149:LEU:C	1:A:2149:LEU:HD13	2.35	0.46
1:B:1489:VAL:CG1	1:B:1497:ARG:HH12	2.28	0.46
1:B:1494:GLN:HB3	1:B:1495:PRO:CD	2.44	0.46
1:A:1578:ARG:HG2	1:A:1578:ARG:NH1	2.30	0.46
1:A:1620:TYR:HB3	1:A:1726:THR:HB	1.97	0.46
1:B:1602:GLU:HG3	3:B:4017:HOH:O	2.15	0.46
1:B:1646:ALA:C	1:B:1648:ASN:N	2.66	0.46
1:A:1733:VAL:HA	1:A:1755:ILE:O	2.16	0.46
2:A:3219:D1L:C13	1:B:1971:GLY:HA3	2.39	0.46
1:B:1640:GLN:HB3	1:B:1657:TYR:CZ	2.51	0.46
1:B:1852:THR:HG23	1:B:1855:GLY:N	2.31	0.46
1:A:1836:THR:HG22	1:A:1838:ASP:HB2	1.98	0.45
1:A:1511:PHE:CZ	1:A:1729:THR:HG21	2.48	0.45
1:A:1616:ILE:HD12	1:A:1813:LYS:HB3	1.98	0.45
1:B:1491:GLU:HG2	1:B:1492:TRP:HE3	1.81	0.45
1:B:1915:THR:HG22	1:B:1916:LEU:N	2.31	0.45
1:A:1833:PHE:CZ	1:A:1845:TRP:HE3	2.34	0.45
1:A:2149:LEU:HD13	1:A:2149:LEU:O	2.15	0.45
1:B:1546:GLU:H	1:B:1546:GLU:CD	2.19	0.45
1:B:1633:GLU:HA	1:B:1636:VAL:HG23	1.96	0.45
1:B:2092:GLN:HE22	1:B:2096:LEU:HG	1.81	0.45
1:B:2035:PHE:HA	1:B:2039:LYS:HD2	1.98	0.45
1:A:1543:ILE:HD11	1:A:1553:VAL:HG11	1.98	0.45
1:B:1810:VAL:HG13	1:B:1811:PRO:HD2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1994:GLU:HA	1:A:2021:ARG:O	2.17	0.45
1:A:2097:HIS:HE1	1:B:1632:ALA:H	1.64	0.45
1:B:1643:TRP:CD1	1:B:1649:PRO:HA	2.51	0.45
1:B:1780:THR:O	1:B:1784:TYR:HB3	2.16	0.45
1:A:1966:GLU:OE1	1:A:1966:GLU:HA	2.16	0.45
1:B:1853:GLU:CD	1:B:1853:GLU:H	2.20	0.45
1:B:2045:ASN:HB2	1:B:2046:ARG:NH1	2.31	0.45
1:A:1669:PHE:C	1:A:1671:LYS:H	2.20	0.45
1:B:1770:VAL:HG13	1:B:1771:TYR:CD1	2.52	0.45
1:B:1605:ASN:O	1:B:1609:GLU:HG3	2.17	0.45
1:B:2045:ASN:HD22	1:B:2046:ARG:HH12	1.65	0.45
1:B:2158:TRP:HZ3	1:B:2186:LEU:HD13	1.81	0.45
1:B:1494:GLN:HB3	1:B:1495:PRO:HD3	1.98	0.44
1:A:1730:CYS:O	1:A:1731:ARG:C	2.55	0.44
1:A:1566:ALA:HA	1:A:1584:VAL:O	2.17	0.44
1:A:1924:TRP:HD1	1:A:1928:SER:HB2	1.82	0.44
1:A:2096:LEU:HB3	1:B:1693:ILE:HG13	2.00	0.44
1:B:1537:PHE:CD2	1:B:1571:VAL:HG22	2.52	0.44
1:B:1487:TYR:CD2	1:B:1488:PRO:HD2	2.52	0.44
1:B:1491:GLU:HG2	1:B:1492:TRP:CE3	2.53	0.44
1:B:1664:GLU:CD	1:B:1667:LYS:HD3	2.38	0.44
1:B:2045:ASN:HB2	1:B:2046:ARG:HH11	1.83	0.44
1:A:1770:VAL:HG13	1:A:1907:PRO:O	2.18	0.44
1:B:1492:TRP:CZ2	1:B:1556:GLU:CG	3.01	0.44
1:A:1583:VAL:HG11	1:A:1607:VAL:CG1	2.48	0.44
1:B:1492:TRP:CZ2	1:B:1556:GLU:HG2	2.53	0.44
1:B:1635:ILE:O	1:B:1635:ILE:HG22	2.17	0.44
1:A:2187:LYS:O	1:A:2191:LEU:HG	2.18	0.43
1:B:1655:TYR:C	1:B:1656:LEU:HD12	2.38	0.43
1:A:1663:MET:HB3	1:A:1667:LYS:HE2	2.00	0.43
1:A:2214:SER:C	1:A:2216:VAL:N	2.72	0.43
1:B:1643:TRP:NE1	1:B:1649:PRO:HB3	2.32	0.43
1:A:1679:ARG:HG3	1:A:1679:ARG:O	2.18	0.43
1:A:2214:SER:C	1:A:2216:VAL:H	2.22	0.43
1:B:2011:GLN:O	1:B:2129:ARG:NH2	2.51	0.43
1:B:2158:TRP:CZ3	1:B:2186:LEU:HD13	2.54	0.43
1:A:1649:PRO:O	1:B:2085:ILE:HG12	2.19	0.43
1:A:1677:THR:HG22	1:A:1689:VAL:O	2.19	0.43
1:A:1759:ALA:N	1:A:1760:PRO:CD	2.81	0.43
1:A:2108:VAL:HG23	1:A:2109:ILE:HG23	2.00	0.43
1:B:1508:VAL:CG2	1:B:1588:ASP:HA	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1899:VAL:HB	1:A:1919:GLU:HB2	2.01	0.43
1:B:1487:TYR:HA	1:B:1488:PRO:HD3	1.88	0.43
1:B:1677:THR:HA	1:B:1689:VAL:O	2.17	0.43
1:B:2139:LEU:N	1:B:2139:LEU:HD12	2.33	0.43
1:A:1693:ILE:HG13	1:B:2096:LEU:HB3	2.00	0.43
1:A:1877:VAL:CG1	1:A:1931:LYS:HD3	2.48	0.43
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.84	0.43
1:A:2081:GLU:OE1	1:A:2082:LEU:HD23	2.19	0.42
1:B:1728:VAL:HG21	1:B:1754:ILE:HD11	2.01	0.42
1:B:2005:PRO:HG2	1:B:2014:MET:HB2	2.01	0.42
1:B:1879:VAL:HG13	1:B:1931:LYS:HE2	2.01	0.42
1:B:1889:LEU:HA	1:B:1946:PRO:HD2	2.01	0.42
1:A:2199:ALA:O	1:A:2203:ARG:HG2	2.19	0.42
1:B:1533:THR:HG1	1:B:1535:ASP:CG	2.23	0.42
1:B:2045:ASN:C	1:B:2046:ARG:HD2	2.39	0.42
1:A:1537:PHE:CD2	1:A:1571:VAL:HG13	2.52	0.42
1:B:1852:THR:HG23	1:B:1855:GLY:H	1.83	0.42
1:A:1755:ILE:HD12	1:A:1758:GLY:HA2	2.02	0.42
1:B:1639:PHE:CD1	1:B:1639:PHE:C	2.91	0.42
1:B:1644:ASN:C	1:B:1646:ALA:H	2.23	0.42
1:A:1587:ASN:HB2	1:A:1623:ALA:O	2.20	0.42
1:A:1814:ARG:O	1:A:1815:ASN:HB2	2.20	0.42
1:B:1560:ASN:ND2	1:B:1560:ASN:N	2.68	0.42
1:B:1954:ARG:HG3	1:B:1955:GLY:N	2.30	0.42
1:A:1790:HIS:HD2	3:A:4053:HOH:O	2.03	0.42
1:A:2102:ARG:O	1:A:2106:LYS:HG2	2.20	0.42
1:B:1829:ARG:CZ	1:B:1858:TYR:HB3	2.49	0.42
1:B:1901:ASN:O	1:B:1917:ILE:N	2.53	0.42
1:A:1582:PHE:HA	1:A:1616:ILE:HG23	2.02	0.41
1:A:1945:LEU:HA	1:A:1946:PRO:HD3	1.88	0.41
1:B:1775:LEU:HD12	1:B:1775:LEU:N	2.34	0.41
1:A:2005:PRO:HG3	1:A:2014:MET:HB2	2.01	0.41
1:B:1677:THR:HG22	1:B:1689:VAL:O	2.20	0.41
1:A:1569:ILE:HG22	1:A:1571:VAL:HG22	2.02	0.41
1:A:1733:VAL:HG12	1:A:1734:GLY:N	2.34	0.41
1:A:1810:VAL:HA	1:A:1811:PRO:HD3	1.94	0.41
1:A:1948:MET:HA	1:A:1986:ILE:O	2.20	0.41
1:B:2163:VAL:HG13	1:B:2170:GLN:HE21	1.86	0.41
1:A:2000:TRP:CD1	1:A:2000:TRP:C	2.94	0.41
1:B:1664:GLU:OE1	1:B:1667:LYS:HD3	2.20	0.41
1:A:2045:ASN:C	1:A:2047:LEU:N	2.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1655:TYR:CD1	1:A:1689:VAL:HG23	2.56	0.41
1:B:1936:ILE:HD13	1:B:1978:LEU:HD13	2.02	0.41
1:A:1601:ASP:OD1	1:A:1707:GLY:HA3	2.21	0.41
1:A:1605:ASN:HD22	1:A:1714:ALA:HB2	1.85	0.40
1:A:1643:TRP:CZ3	1:A:1649:PRO:HB3	2.56	0.40
1:A:2044:MET:HA	1:A:2086:TYR:CE2	2.56	0.40
1:B:1527:SER:O	1:B:1530:VAL:HG13	2.21	0.40
1:A:1741:ARG:CZ	1:B:1969:LYS:HG2	2.51	0.40
1:B:1649:PRO:O	1:B:1651:LYS:N	2.54	0.40
1:B:2116:THR:HG22	1:B:2117:GLU:OE2	2.20	0.40
1:B:1932:THR:O	1:B:1936:ILE:HG13	2.22	0.40
1:A:1607:VAL:O	1:A:1610:TYR:HB3	2.22	0.40
1:B:1697:GLU:OE2	1:B:1697:GLU:HA	2.21	0.40
1:B:2134:TYR:O	1:B:2138:ARG:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	692/737 (94%)	628 (91%)	54 (8%)	10 (1%)	11	20
1	B	689/737 (94%)	619 (90%)	63 (9%)	7 (1%)	15	28
All	All	1381/1474 (94%)	1247 (90%)	117 (8%)	17 (1%)	13	24

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1766	LEU
1	A	2205	ASP
1	A	1683	ASN
1	A	1731	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1997	GLY
1	A	2207	ASP
1	B	1644	ASN
1	B	1650	ASP
1	B	1839	GLU
1	A	1484	ALA
1	B	1534	ASP
1	A	1838	ASP
1	B	1649	PRO
1	B	2205	ASP
1	A	2032	GLY
1	B	2217	ILE
1	A	1767	GLY

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	579/628 (92%)	548 (95%)	31 (5%)	22	42
1	B	577/628 (92%)	549 (95%)	28 (5%)	25	47
All	All	1156/1256 (92%)	1097 (95%)	59 (5%)	24	45

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1502	LEU
1	A	1536	PHE
1	A	1555	ARG
1	A	1571	VAL
1	A	1578	ARG
1	A	1585	VAL
1	A	1602	GLU
1	A	1616	ILE
1	A	1618	ARG
1	A	1721	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1726	THR
1	A	1738	TYR
1	A	1768	ARG
1	A	1769	GLU
1	A	1791	LEU
1	A	1797	LEU
1	A	1823	THR
1	A	1843	VAL
1	A	1884	LEU
1	A	1909	ASN
1	A	1924	TRP
1	A	1930	PHE
1	A	1956	PHE
1	A	2014	MET
1	A	2035	PHE
1	A	2081	GLU
1	A	2119	ARG
1	A	2128	ARG
1	A	2138	ARG
1	A	2186	LEU
1	A	2192	GLU
1	B	1490	LYS
1	B	1508	VAL
1	B	1536	PHE
1	B	1542	LEU
1	B	1550	LEU
1	B	1560	ASN
1	B	1585	VAL
1	B	1602	GLU
1	B	1639	PHE
1	B	1732	SER
1	B	1738	TYR
1	B	1741	ARG
1	B	1742	LEU
1	B	1781	GLN
1	B	1879	VAL
1	B	1924	TRP
1	B	1930	PHE
1	B	1945	LEU
1	B	1956	PHE
1	B	1978	LEU
1	B	1981	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2001	VAL
1	B	2014	MET
1	B	2035	PHE
1	B	2092	GLN
1	B	2114	GLU
1	B	2128	ARG
1	B	2186	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1494	GLN
1	A	1517	GLN
1	A	1525	ASN
1	A	1587	ASN
1	A	1605	ASN
1	A	1624	ASN
1	A	1683	ASN
1	A	1748	GLN
1	A	1752	GLN
1	A	1763	ASN
1	A	1781	GLN
1	A	1790	HIS
1	A	1815	ASN
1	A	1909	ASN
1	A	1911	ASN
1	A	1934	GLN
1	A	1944	GLN
1	A	2097	HIS
1	A	2131	ASN
1	A	2142	GLN
1	A	2196	GLN
1	B	1517	GLN
1	B	1522	GLN
1	B	1560	ASN
1	B	1587	ASN
1	B	1605	ASN
1	B	1640	GLN
1	B	1644	ASN
1	B	1648	ASN
1	B	1748	GLN
1	B	1774	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1781	GLN
1	B	1785	ASN
1	B	1790	HIS
1	B	1815	ASN
1	B	1918	GLN
1	B	2011	GLN
1	B	2045	ASN
1	B	2092	GLN
1	B	2142	GLN
1	B	2170	GLN
1	B	2178	ASN
1	B	2208	ASN

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

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	D1L	A	3219	-	22,22,22	0.79	1 (4%)	30,30,30	0.96	1 (3%)
2	D1L	B	3219	-	22,22,22	0.80	1 (4%)	30,30,30	0.95	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D1L	A	3219	-	-	4/12/12/12	0/2/2/2
2	D1L	B	3219	-	-	2/12/12/12	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3219	D1L	O1A-C1	-2.20	1.23	1.30
2	A	3219	D1L	O1A-C1	-2.12	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3219	D1L	O2-C2-C1	-3.10	107.36	111.34
2	A	3219	D1L	O2-C2-C1	-2.84	107.70	111.34

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3219	D1L	C1-C2-O2-C3
2	B	3219	D1L	C1-C2-O2-C3
2	A	3219	D1L	O1A-C1-C2-O2
2	A	3219	D1L	C2A-C2-O2-C3
2	B	3219	D1L	C2A-C2-O2-C3
2	A	3219	D1L	O1B-C1-C2-O2

There are no ring outliers.

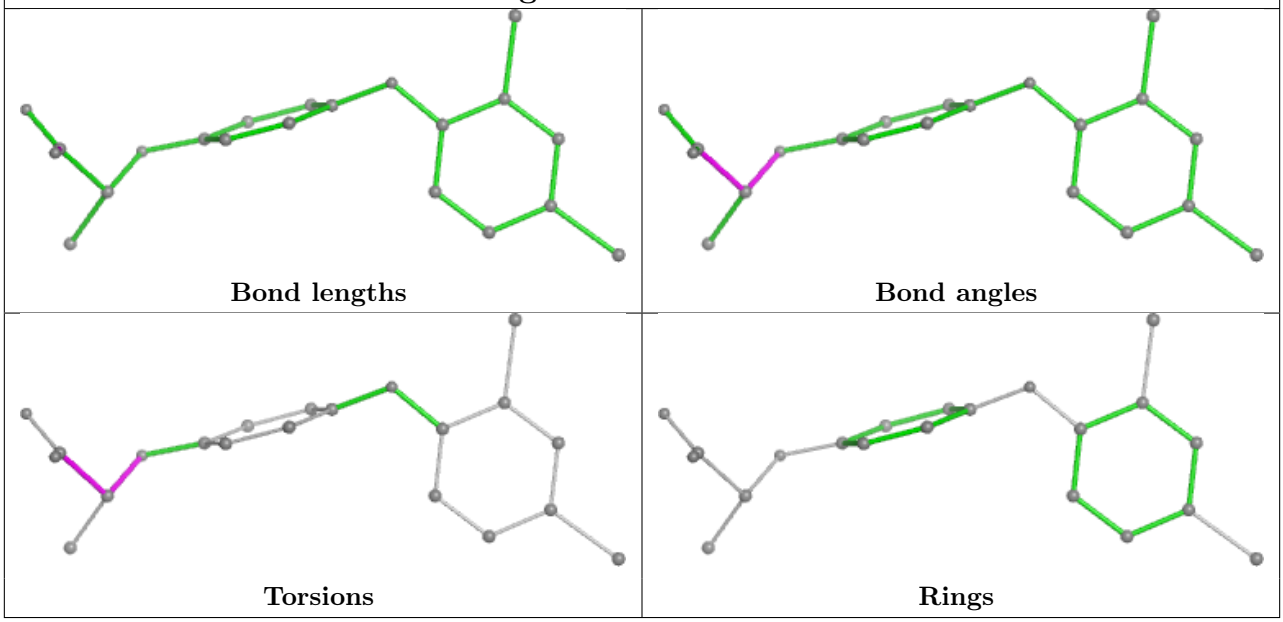
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3219	D1L	6	0
2	B	3219	D1L	6	0

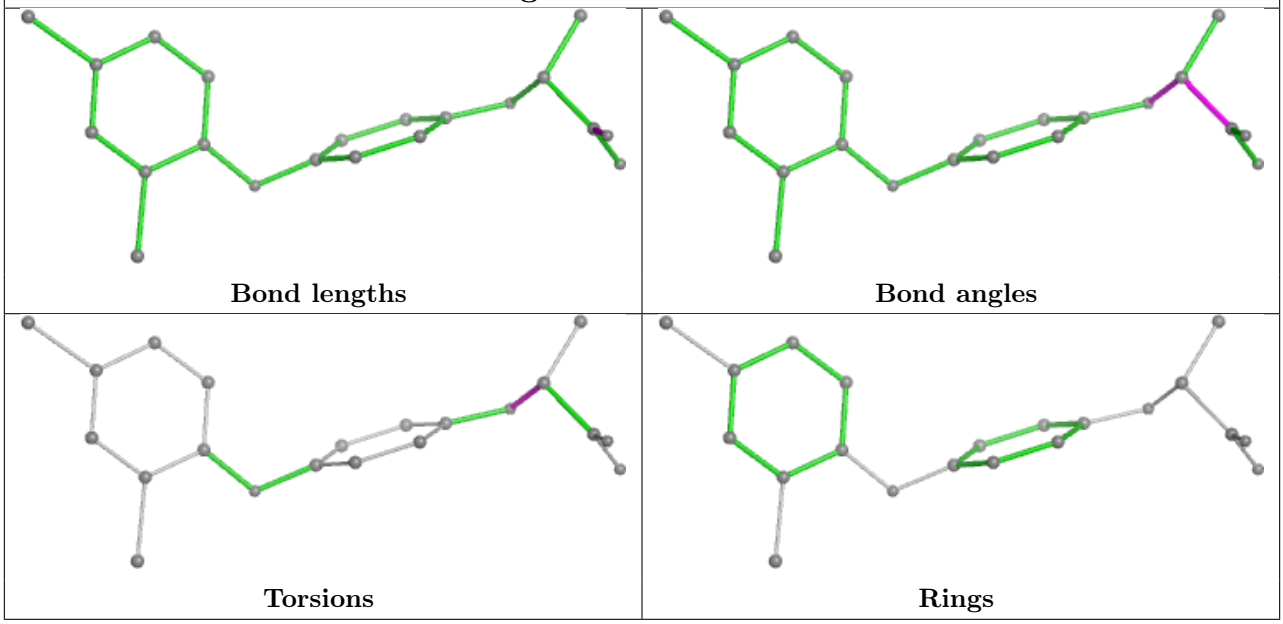
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand D1L A 3219



Ligand D1L B 3219



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, 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	698/737 (94%)	0.37	79 (11%)	5 4	21, 43, 100, 100	0
1	B	695/737 (94%)	0.38	76 (10%)	5 5	21, 44, 100, 100	0
All	All	1393/1474 (94%)	0.37	155 (11%)	5 5	21, 43, 100, 100	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1682	ILE	9.9
1	B	2083	LEU	7.2
1	B	1645	ASP	6.7
1	A	1648	ASN	6.5
1	A	1683	ASN	6.4
1	B	1766	LEU	6.2
1	B	1907	PRO	6.2
1	A	1647	ALA	6.1
1	A	1910	PRO	6.0
1	B	1912	SER	5.9
1	B	1681	VAL	5.6
1	A	1669	PHE	5.5
1	B	1913	ALA	5.4
1	B	1916	LEU	5.2
1	B	1911	ASN	5.1
1	B	1910	PRO	5.1
1	A	1681	VAL	5.1
1	A	1684	GLY	4.9
1	A	1644	ASN	4.8
1	A	2203	ARG	4.8
1	A	1651	LYS	4.6
1	A	1679	ARG	4.6
1	A	1909	ASN	4.6
1	B	1908	ALA	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1650	ASP	4.5
1	A	1905	ALA	4.5
1	A	1685	GLU	4.5
1	A	2037	ARG	4.4
1	A	1911	ASN	4.4
1	A	1908	ALA	4.4
1	B	1769	GLU	4.3
1	B	1905	ALA	4.2
1	B	1651	LYS	4.1
1	B	1648	ASN	4.1
1	B	2041	LEU	4.1
1	B	1669	PHE	4.1
1	B	2084	PRO	4.0
1	B	2145	GLU	4.0
1	A	1680	THR	3.9
1	B	2037	ARG	3.9
1	B	1685	GLU	3.9
1	A	1912	SER	3.8
1	A	1958	GLY	3.8
1	B	1909	ASN	3.8
1	A	1902	LEU	3.8
1	A	1916	LEU	3.8
1	B	1650	ASP	3.8
1	B	2036	ARG	3.7
1	A	1838	ASP	3.7
1	B	1838	ASP	3.7
1	A	1913	ALA	3.7
1	B	1680	THR	3.6
1	B	2038	GLU	3.6
1	B	2203	ARG	3.6
1	A	1904	PRO	3.6
1	B	1649	PRO	3.6
1	A	1645	ASP	3.5
1	A	2045	ASN	3.5
1	A	1773	SER	3.5
1	B	1770	VAL	3.5
1	B	2085	ILE	3.5
1	B	1900	GLU	3.4
1	A	1658	LEU	3.4
1	B	2082	LEU	3.4
1	B	1918	GLN	3.4
1	A	1767	GLY	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1902	LEU	3.4
1	A	1667	LYS	3.3
1	B	1652	GLY	3.3
1	B	1679	ARG	3.3
1	B	1904	PRO	3.2
1	B	1901	ASN	3.2
1	A	2085	ILE	3.2
1	B	1682	ILE	3.1
1	A	1665	THR	3.1
1	A	1900	GLU	3.1
1	B	1957	SER	3.1
1	A	1668	LYS	3.1
1	A	2202	ILE	3.0
1	B	1824	LYS	3.0
1	A	1907	PRO	3.0
1	A	1482	PRO	3.0
1	B	2040	LEU	3.0
1	B	2035	PHE	2.9
1	A	1643	TRP	2.9
1	A	1917	ILE	2.9
1	A	1688	PHE	2.9
1	A	1483	ILE	2.9
1	B	1853	GLU	2.8
1	B	1646	ALA	2.8
1	B	1492	TRP	2.8
1	A	1903	ILE	2.8
1	A	2083	LEU	2.8
1	A	1836	THR	2.8
1	B	2141	HIS	2.7
1	B	1765	MET	2.7
1	A	1915	THR	2.7
1	A	1686	GLU	2.7
1	B	1621	LEU	2.6
1	B	2208	ASN	2.6
1	A	1649	PRO	2.6
1	A	2038	GLU	2.6
1	A	1770	VAL	2.6
1	B	1584	VAL	2.5
1	B	1906	ASP	2.5
1	A	2044	MET	2.5
1	A	1672	GLU	2.5
1	A	1764	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2087	GLY	2.5
1	A	1766	LEU	2.5
1	B	2046	ARG	2.5
1	A	1824	LYS	2.5
1	B	1772	THR	2.4
1	A	2041	LEU	2.4
1	A	1661	GLU	2.4
1	A	1906	ASP	2.4
1	B	1668	LYS	2.4
1	B	2216	VAL	2.4
1	A	1839	GLU	2.4
1	B	1915	THR	2.4
1	A	1889	LEU	2.4
1	B	1667	LYS	2.3
1	A	2209	ALA	2.3
1	A	1687	ARG	2.3
1	A	1759	ALA	2.3
1	A	1901	ASN	2.3
1	B	1670	ASP	2.3
1	A	1772	THR	2.3
1	A	1852	THR	2.3
1	B	2043	THR	2.2
1	B	2189	LEU	2.2
1	A	2145	GLU	2.2
1	B	1917	ILE	2.2
1	B	1958	GLY	2.2
1	B	1768	ARG	2.2
1	B	1494	GLN	2.2
1	B	1683	ASN	2.2
1	A	2036	ARG	2.2
1	A	1527	SER	2.2
1	A	1655	TYR	2.2
1	B	1949	ILE	2.2
1	A	1891	VAL	2.1
1	B	2143	VAL	2.1
1	A	1659	THR	2.1
1	B	1948	MET	2.1
1	B	1759	ALA	2.1
1	A	1768	ARG	2.1
1	B	1585	VAL	2.1
1	A	1890	GLY	2.1
1	B	1620	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1948	MET	2.0
1	B	1771	TYR	2.0
1	A	1763	ASN	2.0
1	A	1956	PHE	2.0
1	B	1664	GLU	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)

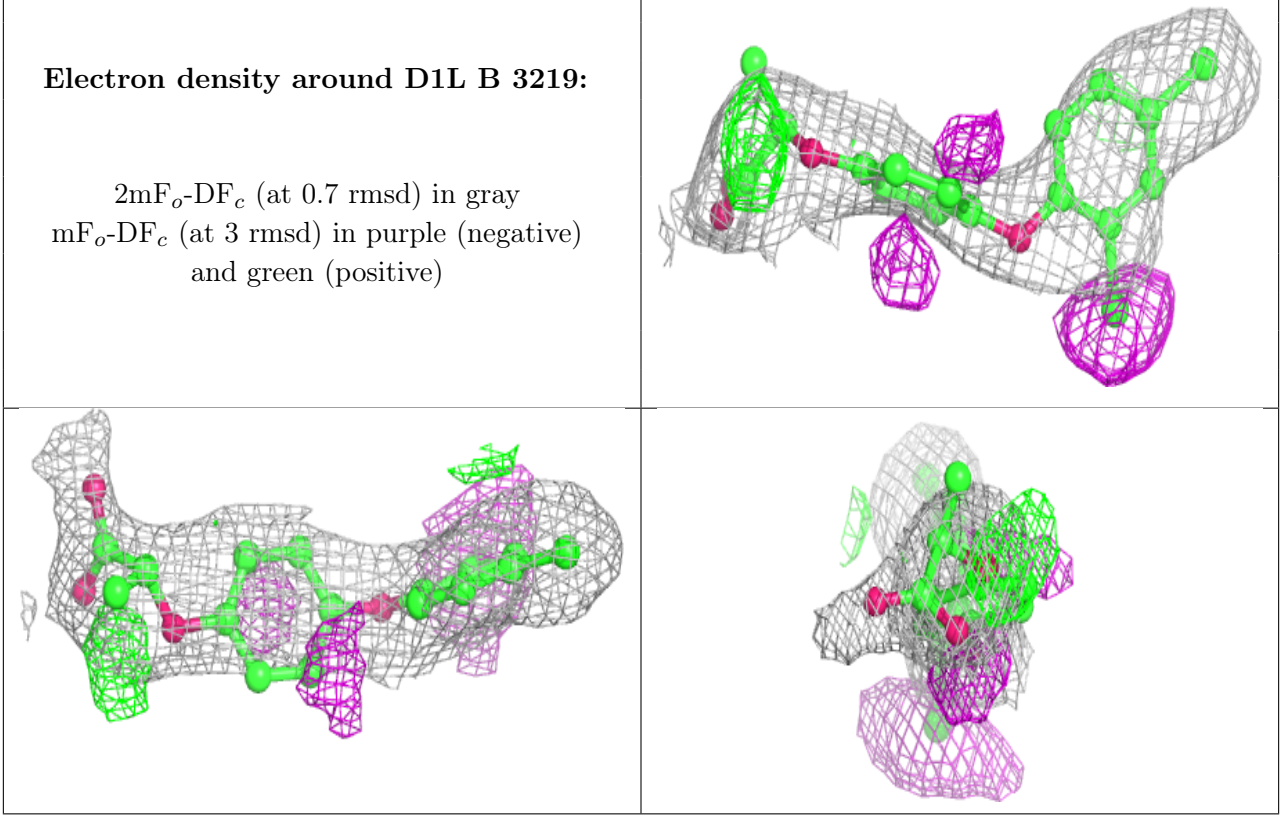
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	D1L	B	3219	21/21	0.81	0.27	73,78,80,89	0
2	D1L	A	3219	21/21	0.84	0.24	74,79,80,88	0

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

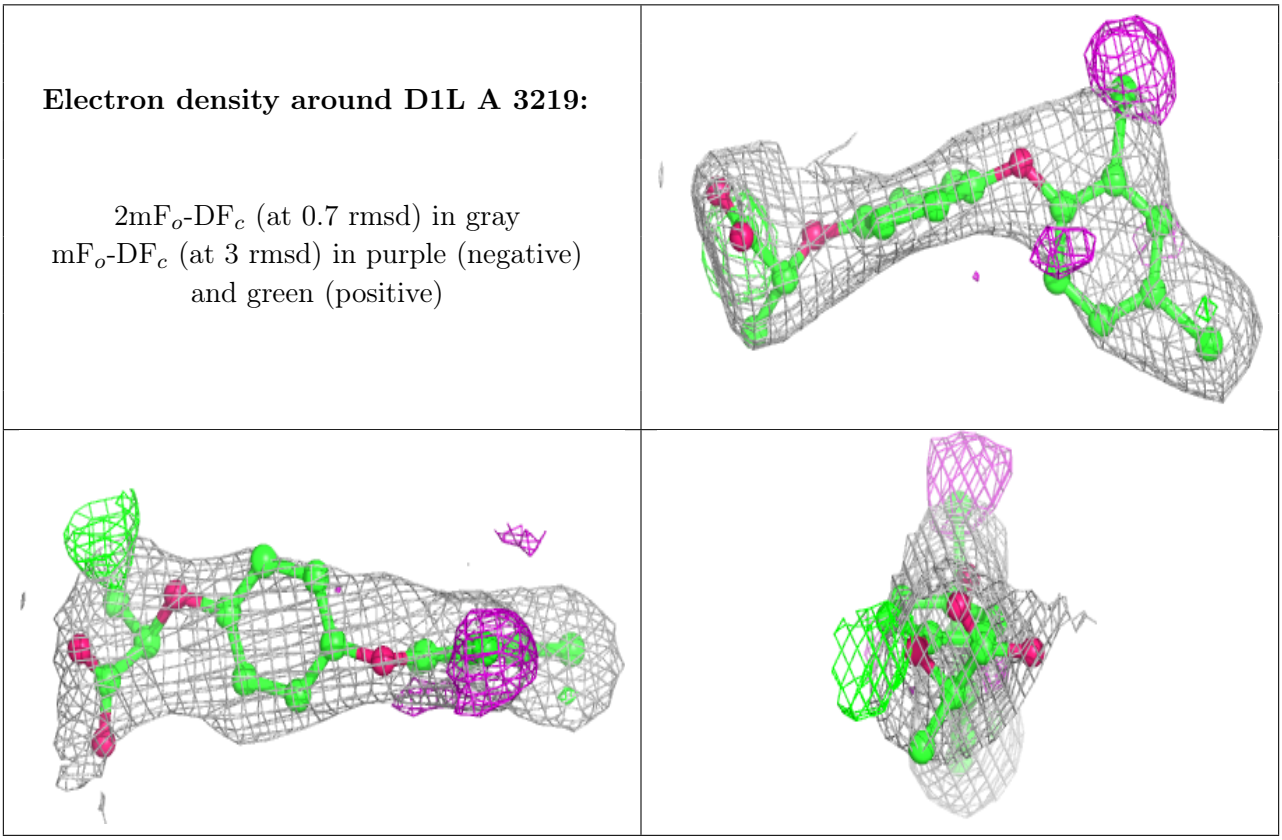
Electron density around D1L B 3219:

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



Electron density around D1L A 3219:

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



6.5 Other polymers (i)

There are no such residues in this entry.