Full wwPDB X-ray Structure Validation Report

Jun 14, 2020 – 08:09 am BST

PDB ID	:	1UYS
Title	:	Acetyl-CoA carboxylase carboxyltransferase domain in complex with inhibitor haloxyfop
Authors	:	Zhang, H.; Tweel, B.; Tong, L.
Deposited on	:	2004-03-02
Resolution	:	2.80 Å(reported)

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

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

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

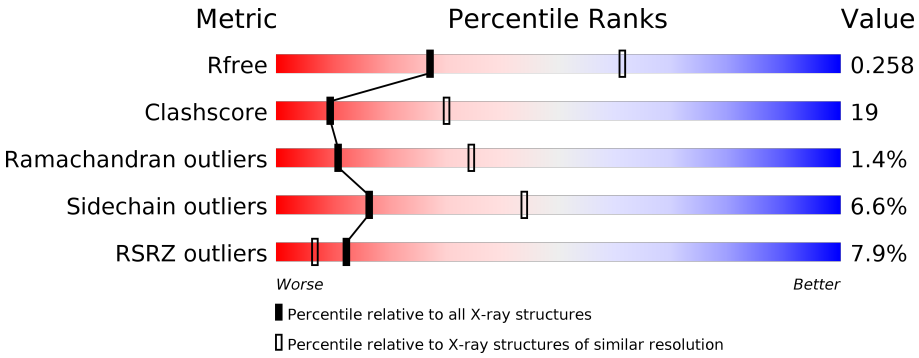
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	6% 56% 32% • 9%
1	B	737	8% 54% 33% • 9%
1	C	737	7% 53% 33% • 10%

2 Entry composition

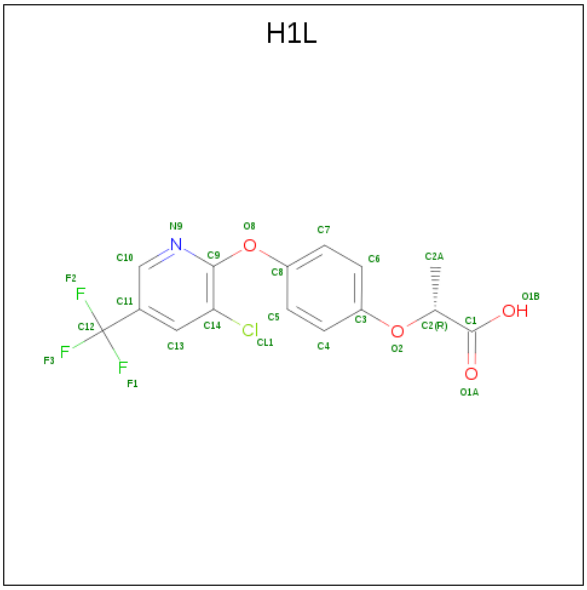
There are 3 unique types of molecules in this entry. The entry contains 16130 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	670	Total	C	N	O	S	Se	0	0	1
			5326	3396	914	998	2	16			
1	B	670	Total	C	N	O	S	Se	0	0	1
			5326	3396	914	998	2	16			
1	C	660	Total	C	N	O	S	Se	0	0	1
			5248	3343	903	984	2	16			

- Molecule 2 is (2R)-2-(4-{[3-chloro-5-(trifluoromethyl)pyridin-2-yl]oxy}phenoxy)propanoic acid (three-letter code: H1L) (formula: $C_{15}H_{11}ClF_3NO_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			24	15	1	3	1	4		
2	B	1	Total	C	Cl	F	N	O	0	0
			24	15	1	3	1	4		
2	C	1	Total	C	Cl	F	N	O	0	0
			24	15	1	3	1	4		

- Molecule 3 is water.

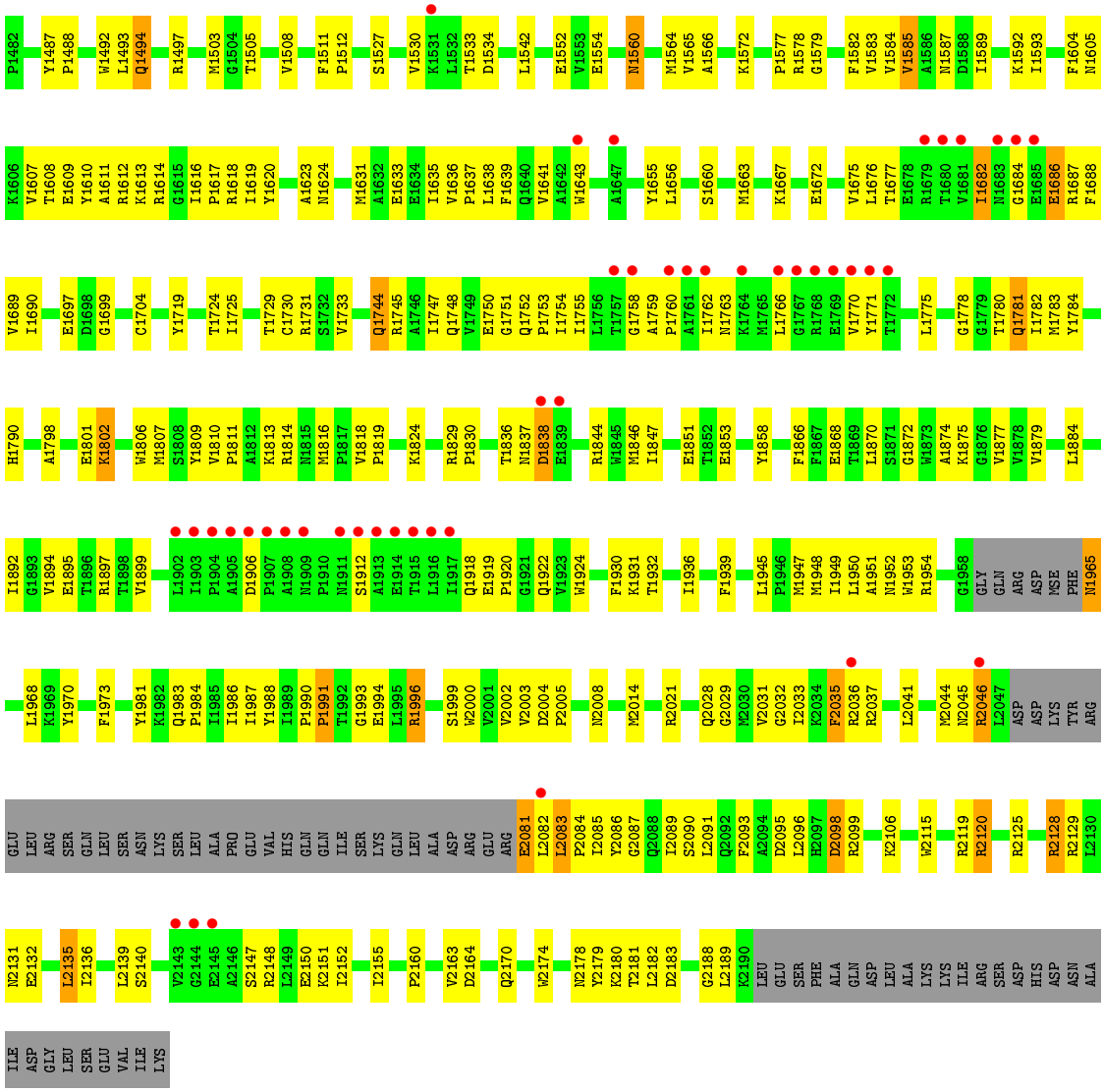
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	69	Total O 69 69	0	0
3	B	50	Total O 50 50	0	0
3	C	39	Total O 39 39	0	0

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.

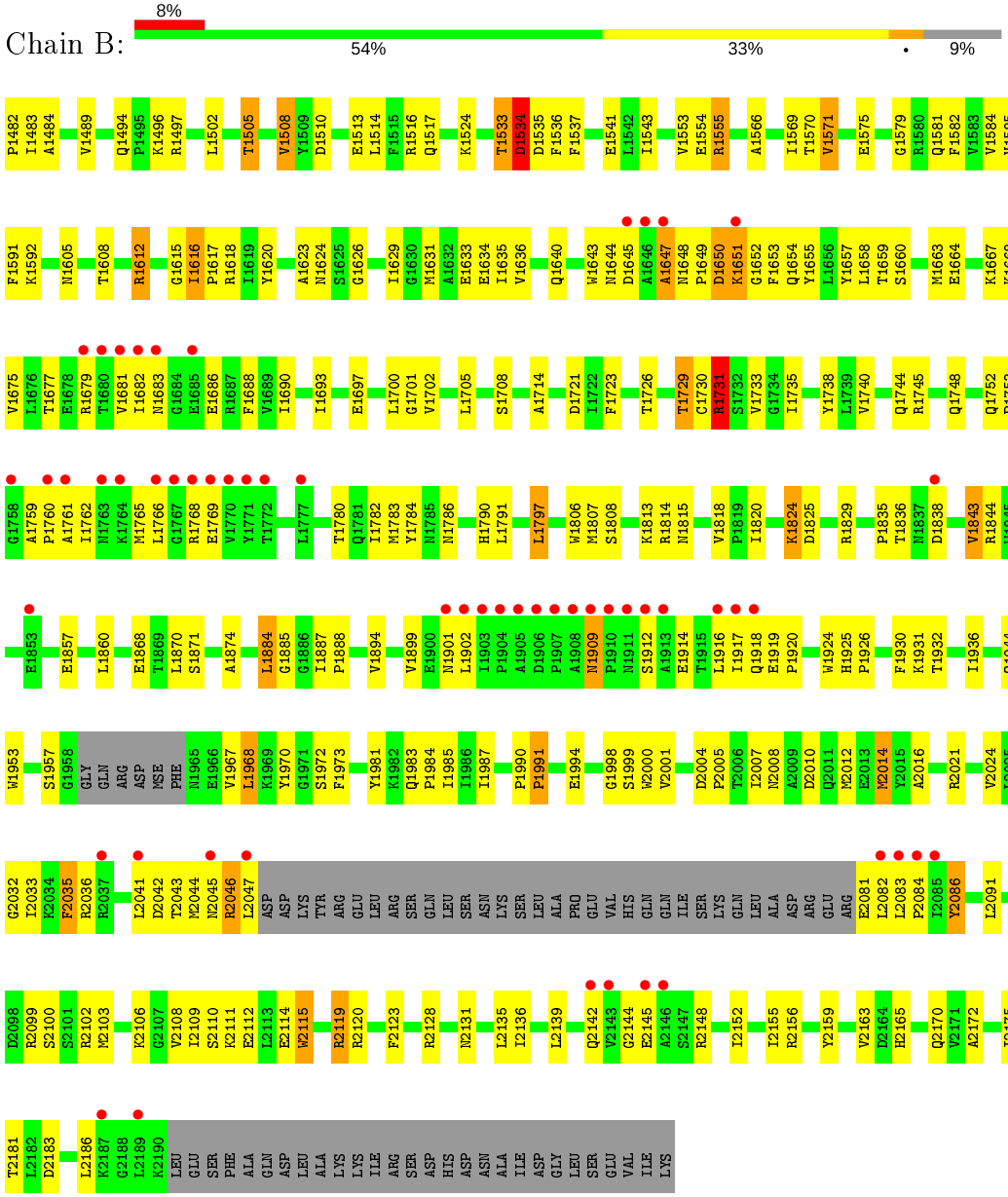
- Molecule 1: ACETYL-COA CARBOXYLASE

Chain A:



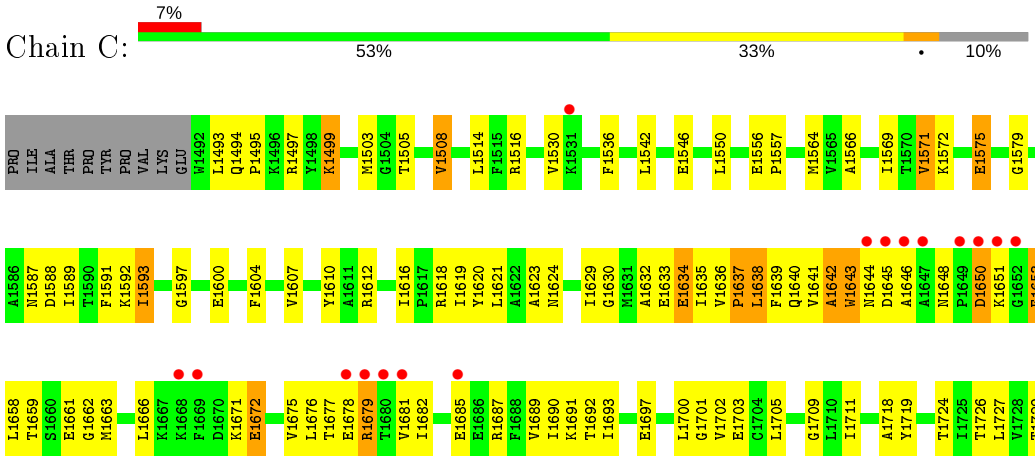
- Molecule 1: ACETYL-COA CARBOXYLASE

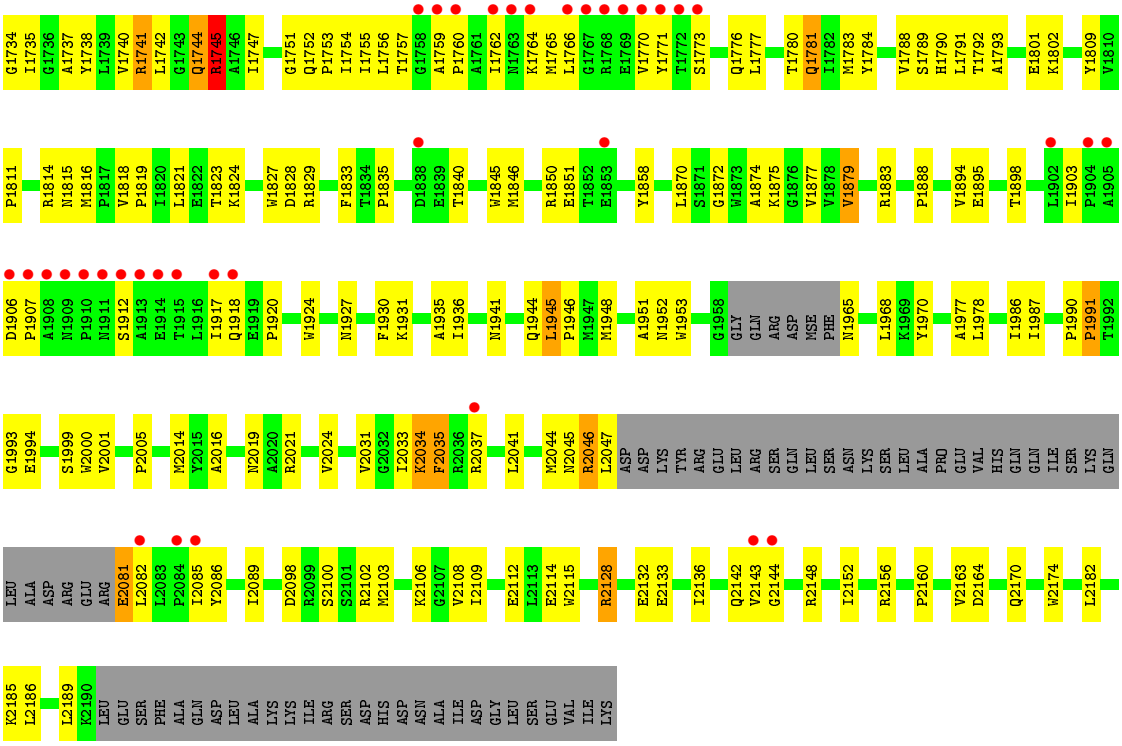
Chain B:



• Molecule 1: ACETYL-COA CARBOXYLASE

Chain C:




G1734 I1735 G1736 A1737 Y1738 L1739 V1740 R1741 L1742 G1743 Q1744 R1745 A1746 I1747 G1751 Q1752 P1753 I1754 I1755 L1756 T1757 G1758 A1759 P1760 A1761 I1762 N1763 K1764 M1765 L1766 G1767 R1768 E1769 V1770 Y1771 T1772 S1773 Q1776 L1777 T1780 Q1781 I1782 M1783 Y1784 V1788 S1789 H1790 L1791 T1792 A1793 E1801 K1802 Y1809 V1810
P1811 R1814 N1815 M1816 P1817 V1818 P1819 I1820 L1821 E1822 T1823 K1824 W1827 D1828 R1829 F1833 T1834 P1835 D1838 E1939 T1840 W1845 M1846 R1850 E1851 T1852 E1853 Y1858 L1870 S1871 G1872 W1873 A1874 K1875 G1876 V1877 V1878 V1879 R1883 P1888 V1894 E1895 T1898 L1902 I1903 P1904 A1905
D1906 P1907 A1908 N1909 P1910 N1911 S1912 A1913 E1914 T1915 L1916 I1917 Q1918 E1919 P1920 W1924 N1927 F1930 K1931 A1935 I1936 N1941 Q1944 L1945 P1946 M1947 M1948 A1951 N1952 W1953 G1958 GLY GLN ARG ASP MSE PHE N1965 L1968 K1969 Y1970 A1977 L1978 I1986 I1987 P1990 P1991 T1992
G1993 E1994 S1999 W2000 V2001 P2005 M2014 Y2015 A2016 N2019 A2020 R2021 V2024 V2031 G2032 I2033 K2034 F2035 R2036 R2037 L2041 M2044 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 D2098 R2099 S2100 S2101 R2102 M2103 K2106 G2107 V2108 I2109 E2112 L2113 E2114 W2115 R2128 E2132 E2133 I2136 Q2142 V2143 G2144 R2148 I2152 R2156 P2160 V2163 D2164 Q2170 W2174 L2182
K2185 L2186 L2189 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	246.21Å 125.58Å 146.88Å 90.00° 94.08° 90.00°	Depositor
Resolution (Å)	27.42 – 2.80 29.68 – 2.79	Depositor EDS
% Data completeness (in resolution range)	87.6 (27.42-2.80) 93.9 (29.68-2.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.252 0.225 , 0.258	Depositor DCC
R_{free} test set	10734 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.3	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	0.90	EDS
Total number of atoms	16130	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: H1L

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	0.51	0/5429	0.67	4/7332 (0.1%)
1	B	0.47	0/5429	0.61	0/7332
1	C	0.46	0/5347	0.63	3/7218 (0.0%)
All	All	0.48	0/16205	0.64	7/21882 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1745	ARG	NE-CZ-NH1	-12.57	114.02	120.30
1	C	1745	ARG	NE-CZ-NH2	11.36	125.98	120.30
1	A	1618	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	C	1745	ARG	CD-NE-CZ	-5.82	115.46	123.60
1	A	1618	ARG	NH1-CZ-NH2	-5.23	113.65	119.40
1	A	2174	TRP	CG-CD2-CE3	5.21	138.59	133.90
1	A	2120	ARG	NE-CZ-NH1	5.17	122.89	120.30

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	5326	0	5269	199	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5326	0	5269	215	0
1	C	5248	0	5187	231	0
2	A	24	0	10	0	0
2	B	24	0	10	4	0
2	C	24	0	10	6	0
3	A	69	0	0	4	0
3	B	50	0	0	3	0
3	C	39	0	0	4	0
All	All	16130	0	15755	618	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (618) 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:1618:ARG:HG2	1:C:1618:ARG:HH11	1.25	1.01
1:C:1637:PRO:HG2	1:C:1638:LEU:HD23	1.40	1.00
1:C:1823:THR:HG22	1:C:1824:LYS:H	1.33	0.93
1:A:2045:ASN:HB2	1:A:2046:ARG:CZ	1.99	0.92
1:A:1582:PHE:HA	1:A:1616:ILE:HG23	1.54	0.90
1:C:1754:ILE:HD12	1:C:1783:MSE:HG2	1.54	0.88
1:A:2135:LEU:HB3	1:A:2155:ILE:HD13	1.57	0.87
1:A:1624:ASN:ND2	1:A:1733:VAL:H	1.74	0.86
1:A:2045:ASN:HB2	1:A:2046:ARG:NH2	1.90	0.86
1:B:1899:VAL:HB	1:B:1919:GLU:HB2	1.58	0.85
1:B:2031:VAL:HG21	1:B:2091:LEU:HD23	1.59	0.85
1:A:1874:ALA:HB3	1:A:1931:LYS:HD2	1.60	0.84
1:B:1508:VAL:HG21	1:B:1588:ASP:HA	1.61	0.82
1:C:2045:ASN:HB2	1:C:2046:ARG:NH2	1.95	0.81
1:B:1708:SER:HB3	1:B:1735:ILE:HD13	1.63	0.81
1:C:1493:LEU:HB2	1:C:1497:ARG:NH1	1.96	0.80
1:A:1948:MSE:HE2	1:A:1950:LEU:CD1	2.11	0.79
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.32	0.78
1:A:2183:ASP:HB2	1:B:1482:PRO:HG3	1.67	0.77
1:C:1754:ILE:HB	1:C:1783:MSE:HE3	1.65	0.77
1:B:1756:LEU:HD21	1:C:1968:LEU:HD13	1.66	0.77
1:C:1737:ALA:O	1:C:1740:VAL:HG22	1.85	0.77
1:C:2081:GLU:HG2	1:C:2082:LEU:H	1.49	0.76
1:B:1677:THR:HG22	1:B:1690:ILE:HA	1.68	0.76
1:A:1965:ASN:N	1:A:1965:ASN:HD22	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2031:VAL:HG23	1:A:2035:PHE:HB3	1.68	0.75
1:C:1618:ARG:HG2	1:C:1618:ARG:NH1	1.93	0.75
1:A:2140:SER:OG	1:A:2151:LYS:HE2	1.88	0.74
1:B:1730:CYS:HA	1:B:1752:GLN:HG3	1.67	0.74
1:B:1702:VAL:HA	1:B:1705:LEU:HD12	1.68	0.74
1:A:1899:VAL:HB	1:A:1919:GLU:HB2	1.71	0.73
1:B:1733:VAL:HG12	1:B:1755:ILE:HB	1.71	0.73
1:A:1750:GLU:HA	1:A:1780:THR:HG21	1.71	0.73
1:A:1948:MSE:HE2	1:A:1950:LEU:HD13	1.69	0.73
1:A:1939:PHE:CD1	1:A:1947:MSE:HE3	2.24	0.73
1:C:2047:LEU:HD13	1:C:2082:LEU:HD11	1.70	0.73
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.52	0.72
1:B:2135:LEU:HB3	1:B:2155:ILE:HD13	1.70	0.72
1:C:2031:VAL:HG23	1:C:2035:PHE:HB3	1.72	0.72
1:B:1679:ARG:HH21	1:B:1681:VAL:HG21	1.54	0.71
1:C:1658:LEU:HG	1:C:1690:ILE:HD11	1.71	0.71
1:C:1676:LEU:HD12	1:C:1692:THR:HB	1.72	0.71
1:A:1906:ASP:HB3	1:A:1912:SER:OG	1.90	0.71
1:B:1681:VAL:HA	1:B:1686:GLU:HA	1.73	0.70
1:C:1638:LEU:H	1:C:1638:LEU:HD23	1.56	0.70
1:C:1672:GLU:H	1:C:1672:GLU:CD	1.95	0.70
1:C:1991:PRO:HG3	1:C:2115:TRP:HB2	1.72	0.70
1:B:1640:GLN:HG3	1:B:1659:THR:HG23	1.73	0.70
1:C:1759:ALA:HB3	1:C:1760:PRO:HD3	1.74	0.70
1:C:2148:ARG:CZ	1:C:2152:ILE:HD11	2.22	0.70
1:B:1968:LEU:HA	2:C:3000:H1L:CL1	2.29	0.70
1:A:1682:ILE:HD13	1:A:1682:ILE:H	1.56	0.69
1:B:1623:ALA:HB2	1:B:1729:THR:HG23	1.74	0.69
2:B:3000:H1L:CL1	1:C:1968:LEU:HA	2.30	0.69
1:C:2045:ASN:HB2	1:C:2046:ARG:CZ	2.22	0.69
1:B:1762:ILE:HG22	1:B:1766:LEU:HD12	1.75	0.69
1:C:1592:LYS:C	1:C:1593:ILE:HG13	2.12	0.68
1:B:2024:VAL:HG23	1:C:1701:GLY:HA2	1.75	0.68
1:B:1644:ASN:HB3	1:B:1654:GLN:HE21	1.58	0.68
1:C:1747:ILE:HD13	1:C:1802:LYS:HB2	1.75	0.68
1:A:1560:ASN:HD22	1:A:1560:ASN:H	1.40	0.67
1:A:1936:ILE:HG12	1:A:1947:MSE:HE1	1.76	0.67
1:A:1766:LEU:CD2	1:A:1770:VAL:HG11	2.25	0.67
1:A:1948:MSE:HE3	1:A:1988:TYR:HB3	1.75	0.67
1:A:2086:TYR:HA	1:A:2089:ILE:HD12	1.78	0.66
1:C:1651:LYS:HD2	1:C:1651:LYS:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1656:LEU:HB2	1:A:1690:ILE:HD11	1.77	0.66
1:A:1560:ASN:ND2	1:A:1560:ASN:H	1.94	0.66
1:B:1582:PHE:HA	1:B:1616:ILE:HG23	1.77	0.66
1:A:1846:MSE:HE1	1:A:1991:PRO:HD2	1.76	0.66
1:B:1790:HIS:HA	1:B:1870:LEU:HD23	1.77	0.66
1:A:1936:ILE:HA	1:A:1947:MSE:HE1	1.78	0.66
1:B:1663:MSE:O	1:B:1667:LYS:HG3	1.95	0.66
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.44	0.66
1:A:1766:LEU:HD22	1:A:1770:VAL:HG11	1.78	0.66
1:A:1572:LYS:HA	1:A:1579:GLY:HA2	1.78	0.66
1:B:2108:VAL:HG23	1:B:2109:ILE:HG23	1.77	0.66
1:B:2082:LEU:HD23	1:B:2082:LEU:H	1.60	0.65
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.44	0.65
1:A:1939:PHE:HD1	1:A:1947:MSE:HE3	1.60	0.65
1:B:1843:VAL:HG21	1:B:1894:VAL:O	1.97	0.65
1:C:1493:LEU:HD12	1:C:1497:ARG:HH12	1.62	0.65
1:B:2045:ASN:HB2	1:B:2046:ARG:CZ	2.27	0.65
1:A:1614:ARG:HH11	1:A:1614:ARG:HG3	1.63	0.64
1:A:1682:ILE:HG12	1:A:1684:GLY:H	1.63	0.64
1:C:1846:MSE:HE1	1:C:1990:PRO:HB3	1.79	0.64
1:A:2037:ARG:HB2	1:A:2037:ARG:NH1	2.12	0.64
1:B:1643:TRP:HA	1:B:1653:PHE:HA	1.79	0.64
1:B:1730:CYS:CA	1:B:1752:GLN:HG3	2.26	0.64
1:A:1623:ALA:HB2	1:A:1729:THR:CG2	2.27	0.63
1:C:1877:VAL:HG23	1:C:1931:LYS:HE2	1.79	0.63
1:C:1636:VAL:N	1:C:1637:PRO:HD2	2.13	0.63
1:B:1617:PRO:HB3	1:B:1723:PHE:HB3	1.80	0.63
1:C:1726:THR:HG21	1:C:1740:VAL:HG12	1.81	0.63
1:B:1970:TYR:O	1:B:1973:PHE:HB2	1.99	0.62
1:B:1998:GLY:HA2	1:B:2001:VAL:HG12	1.79	0.62
1:C:2148:ARG:NH1	1:C:2152:ILE:HD11	2.14	0.62
1:C:1637:PRO:HG2	1:C:1638:LEU:H	1.65	0.62
1:B:1902:LEU:HD12	1:B:1916:LEU:HD13	1.82	0.62
1:C:1783:MSE:HG3	1:C:1788:VAL:HB	1.81	0.62
1:A:1605:ASN:O	1:A:1609:GLU:HG2	2.00	0.62
1:A:1748:GLN:HE22	1:A:1783:MSE:HB2	1.65	0.62
1:B:1868:GLU:HG2	1:B:1871:SER:HB3	1.81	0.62
1:C:1793:ALA:HA	3:C:4012:HOH:O	1.99	0.62
1:B:2094:ALA:HA	1:B:2097:HIS:HD2	1.64	0.61
1:A:1530:VAL:HG23	1:A:1530:VAL:O	2.01	0.61
1:B:1483:ILE:HD12	1:B:1484:ALA:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1818:VAL:HG12	1:C:1945:LEU:HD12	1.82	0.61
1:A:1948:MSE:HE2	1:A:1950:LEU:HD11	1.81	0.61
1:B:1645:ASP:OD2	1:B:1651:LYS:HB2	2.00	0.61
1:B:2001:VAL:HG11	2:C:3000:H1L:C6	2.30	0.61
1:A:2028:GLN:HE21	1:A:2091:LEU:HD21	1.65	0.61
1:B:1884:LEU:HD13	1:B:2123:PHE:HA	1.82	0.61
1:A:2180:LYS:HA	1:B:1482:PRO:HD3	1.82	0.61
1:C:2182:LEU:O	1:C:2186:LEU:HD23	2.00	0.61
1:B:1829:ARG:HH11	1:B:1829:ARG:HG3	1.66	0.61
1:B:1814:ARG:HA	1:B:1944:GLN:HE22	1.65	0.61
1:A:1578:ARG:N	1:A:1578:ARG:HD2	2.16	0.60
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	2.16	0.60
1:C:1682:ILE:HG21	1:C:1687:ARG:HD2	1.82	0.60
1:A:2095:ASP:O	1:A:2099:ARG:NH1	2.34	0.60
1:C:2108:VAL:HG23	1:C:2109:ILE:HG23	1.84	0.60
1:C:1508:VAL:HG21	1:C:1588:ASP:HA	1.84	0.60
1:A:1759:ALA:HB3	1:A:1760:PRO:HD3	1.83	0.60
1:C:1874:ALA:HB3	1:C:1931:LYS:HD3	1.83	0.59
1:C:1818:VAL:HG11	1:C:1946:PRO:HD3	1.83	0.59
1:C:1757:THR:HB	1:C:1762:ILE:HD11	1.83	0.59
1:A:2180:LYS:HG2	1:B:1482:PRO:HD3	1.84	0.59
1:B:1745:ARG:HG2	1:B:1806:TRP:CZ2	2.38	0.58
1:A:2044:MSE:SE	1:A:2082:LEU:HD11	2.53	0.58
1:B:2036:ARG:HG2	1:B:2036:ARG:HH11	1.68	0.58
1:A:1682:ILE:HD12	1:A:1687:ARG:HG3	1.86	0.58
1:A:1811:PRO:HG3	1:A:1818:VAL:HA	1.85	0.58
1:C:1898:THR:HG22	1:C:1920:PRO:HA	1.84	0.58
1:A:1623:ALA:HB2	1:A:1729:THR:HG23	1.84	0.58
1:A:1724:THR:H	1:A:1745:ARG:HH21	1.50	0.58
1:A:2028:GLN:NE2	1:A:2091:LEU:HD21	2.19	0.58
1:B:1790:HIS:HD2	3:B:4039:HOH:O	1.85	0.58
1:A:2164:ASP:H	1:A:2170:GLN:HE22	1.49	0.58
1:B:1733:VAL:HA	1:B:1755:ILE:O	2.04	0.58
1:A:1809:TYR:O	1:A:1945:LEU:HD21	2.04	0.58
1:C:1737:ALA:HB3	1:C:1756:LEU:HD12	1.86	0.58
1:A:1996:ARG:HG3	1:A:1996:ARG:HH11	1.69	0.57
1:C:1823:THR:HB	3:C:4016:HOH:O	2.04	0.57
1:B:1679:ARG:HH21	1:B:1681:VAL:CG2	2.17	0.57
1:B:2031:VAL:HG13	1:B:2035:PHE:HB3	1.85	0.57
1:C:1823:THR:HG22	1:C:1824:LYS:N	2.12	0.57
1:B:2142:GLN:HG3	1:B:2186:LEU:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1572:LYS:HA	1:C:1579:GLY:HA2	1.87	0.57
1:B:1608:THR:O	1:B:1612:ARG:HG2	2.04	0.57
1:B:2096:LEU:HB3	1:C:1693:ILE:HG13	1.87	0.57
1:A:1894:VAL:HG11	1:A:1952:ASN:O	2.05	0.57
1:A:2136:ILE:HD11	1:A:2152:ILE:HD13	1.87	0.57
1:A:1846:MSE:HE2	1:A:2115:TRP:CH2	2.40	0.57
1:C:2160:PRO:HD2	1:C:2163:VAL:HG21	1.85	0.57
1:A:1582:PHE:HA	1:A:1616:ILE:CG2	2.33	0.57
1:B:2136:ILE:HD11	1:B:2152:ILE:HG12	1.87	0.56
1:A:1922:GLN:HB3	1:A:1954:ARG:HG3	1.87	0.56
1:B:1874:ALA:HB3	1:B:1931:LYS:HD3	1.86	0.56
1:B:1582:PHE:CB	1:B:1617:PRO:HG2	2.35	0.56
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	1.88	0.56
1:B:1846:MSE:HE1	1:B:1990:PRO:HB2	1.87	0.56
1:A:1624:ASN:HD21	1:A:1733:VAL:N	2.00	0.56
1:B:1748:GLN:HE22	1:B:1783:MSE:HB2	1.70	0.56
1:B:1874:ALA:HB3	1:B:1931:LYS:CD	2.36	0.56
1:B:1782:ILE:HG22	1:B:1783:MSE:HE2	1.87	0.56
1:C:1623:ALA:HB2	1:C:1729:THR:HG23	1.87	0.56
1:C:1677:THR:HG22	1:C:1690:ILE:HD13	1.88	0.56
1:C:1612:ARG:HD3	1:C:1718:ALA:HA	1.88	0.56
1:A:2147:SER:HB3	1:A:2150:GLU:HG3	1.88	0.56
1:A:1592:LYS:O	1:A:1593:ILE:HG12	2.06	0.55
1:B:1730:CYS:O	1:B:1731:ARG:C	2.45	0.55
1:A:1747:ILE:HD13	1:A:1802:LYS:HB3	1.89	0.55
1:C:2086:TYR:HA	1:C:2089:ILE:HD12	1.89	0.55
1:B:1605:ASN:ND2	1:B:1714:ALA:HB2	2.22	0.55
1:B:1768:ARG:HG2	1:B:1768:ARG:HH11	1.71	0.55
1:B:1991:PRO:HG3	1:B:2115:TRP:HB2	1.87	0.55
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.54	0.55
1:B:2001:VAL:HG11	2:C:3000:H1L:H6	1.89	0.55
1:B:2156:ARG:HD3	1:B:2159:TYR:HE1	1.72	0.55
1:C:1724:THR:O	1:C:1745:ARG:HG2	2.06	0.55
1:B:1582:PHE:HB3	1:B:1617:PRO:HG2	1.89	0.55
1:A:1948:MSE:HE3	1:A:1988:TYR:CB	2.37	0.55
1:B:1824:LYS:HE2	1:B:1825:ASP:N	2.22	0.55
1:B:1987:ILE:HG22	1:B:2014:MSE:HE3	1.89	0.55
1:A:1585:VAL:HG13	1:A:1607:VAL:HG11	1.89	0.55
1:C:1505:THR:HB	1:C:1730:CYS:HB2	1.90	0.54
1:A:1508:VAL:HG23	3:A:4018:HOH:O	2.05	0.54
1:A:2106:LYS:HA	1:A:2106:LYS:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2102:ARG:O	1:B:2106:LYS:HG2	2.06	0.54
1:C:1681:VAL:HG13	1:C:1685:GLU:O	2.08	0.54
1:A:1790:HIS:HA	1:A:1870:LEU:HD23	1.88	0.54
1:A:1970:TYR:O	1:A:1973:PHE:HB2	2.07	0.54
1:A:1948:MSE:CE	1:A:1988:TYR:HD1	2.20	0.54
1:B:1968:LEU:HD22	1:C:1741:ARG:HG3	1.90	0.54
1:A:1758:GLY:O	1:A:1762:ILE:HG13	2.07	0.54
1:C:2041:LEU:HD23	1:C:2044:MSE:HE3	1.89	0.54
1:A:2029:GLY:O	1:A:2033:ILE:HG12	2.07	0.54
1:B:1651:LYS:HE3	1:B:1651:LYS:HA	1.90	0.54
1:C:1874:ALA:HA	1:C:1927:ASN:HD22	1.73	0.54
1:B:1947:MSE:HE2	1:B:1985:ILE:HG12	1.90	0.54
1:B:2047:LEU:HD22	1:B:2082:LEU:HD22	1.90	0.54
1:B:1860:LEU:O	1:B:2119:ARG:HG3	2.07	0.54
1:C:1618:ARG:NH1	1:C:1620:TYR:HB2	2.22	0.54
1:C:1630:GLY:HA3	1:C:1700:LEU:HA	1.89	0.54
1:B:1824:LYS:HZ3	1:B:1825:ASP:H	1.56	0.54
1:B:1987:ILE:CG2	1:B:2014:MSE:HE3	2.38	0.54
1:B:2081:GLU:HB3	1:B:2083:LEU:HD13	1.88	0.54
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	2.09	0.53
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.56	0.53
1:A:1633:GLU:O	1:A:1636:VAL:HG12	2.07	0.53
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.71	0.53
1:B:1820:ILE:HD12	1:B:1887:ILE:HG12	1.90	0.53
1:B:1566:ALA:HA	1:B:1584:VAL:O	2.08	0.53
1:B:1629:ILE:HG22	1:C:2024:VAL:HG11	1.90	0.53
1:B:1972:SER:HB3	1:C:1742:LEU:HD12	1.90	0.53
1:C:1765:MSE:HE2	1:C:1766:LEU:HG	1.91	0.53
1:A:2002:VAL:HG13	1:A:2003:VAL:HG13	1.89	0.53
1:A:2085:ILE:HG23	1:A:2086:TYR:N	2.24	0.53
1:B:1681:VAL:HG22	1:B:1686:GLU:HB2	1.90	0.53
1:C:2016:ALA:O	1:C:2112:GLU:HA	2.07	0.53
1:A:1965:ASN:N	1:A:1965:ASN:ND2	2.56	0.53
1:C:1645:ASP:OD2	1:C:1651:LYS:HB2	2.08	0.53
1:C:1755:ILE:N	1:C:1755:ILE:HD12	2.23	0.53
1:A:2032:GLY:O	1:A:2033:ILE:HD13	2.09	0.53
1:B:1721:ASP:OD2	1:B:1814:ARG:NH1	2.41	0.53
1:B:1909:ASN:HB3	1:B:1912:SER:OG	2.09	0.53
1:C:1918:GLN:O	1:C:1920:PRO:HD3	2.08	0.53
1:A:1667:LYS:HG3	1:A:1672:GLU:OE2	2.09	0.53
1:C:1991:PRO:O	1:C:2019:ASN:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1733:VAL:HA	1:A:1755:ILE:O	2.09	0.53
1:A:1635:ILE:O	1:A:1639:PHE:HB3	2.08	0.52
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.58	0.52
1:B:1655:TYR:HE1	1:B:1657:TYR:HB3	1.74	0.52
1:A:1780:THR:O	1:A:1784:TYR:HB3	2.09	0.52
1:C:1569:ILE:HG22	1:C:1571:VAL:HG22	1.92	0.52
1:C:1894:VAL:HG11	1:C:1952:ASN:O	2.08	0.52
1:C:1702:VAL:HA	1:C:1705:LEU:HD12	1.90	0.52
1:C:1823:THR:CG2	1:C:1824:LYS:H	2.14	0.52
1:B:1932:THR:O	1:B:1936:ILE:HG13	2.09	0.52
1:C:1642:ALA:HB2	1:C:1657:TYR:CE1	2.45	0.52
1:C:1638:LEU:O	1:C:1658:LEU:HD21	2.10	0.52
1:A:1807:MSE:O	1:A:1810:VAL:HG22	2.09	0.52
1:C:1781:GLN:H	1:C:1781:GLN:NE2	2.06	0.52
1:A:2119:ARG:HB3	3:A:4041:HOH:O	2.09	0.52
1:B:1902:LEU:HD21	1:B:1914:GLU:CG	2.39	0.52
1:B:2001:VAL:HG23	1:C:1709:GLY:N	2.25	0.52
1:A:1614:ARG:NH1	1:A:1614:ARG:HG3	2.24	0.51
1:B:1664:GLU:O	1:B:1668:LYS:HG3	2.10	0.51
1:A:1836:THR:HG22	1:A:1838:ASP:H	1.75	0.51
1:A:2164:ASP:H	1:A:2170:GLN:NE2	2.09	0.51
1:B:1605:ASN:HD22	1:B:1714:ALA:HB2	1.74	0.51
1:C:2081:GLU:CD	1:C:2081:GLU:N	2.64	0.51
1:C:2100:SER:HA	1:C:2103:MSE:HE3	1.93	0.51
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.40	0.51
1:A:1948:MSE:HE1	1:A:1988:TYR:HD1	1.75	0.51
1:B:1738:TYR:CG	2:B:3000:H1L:H7	2.46	0.51
1:B:1860:LEU:HD21	1:B:1948:MSE:HE1	1.92	0.51
1:A:1751:GLY:O	1:A:1775:LEU:HD21	2.11	0.51
1:B:2008:ASN:HB3	1:B:2012:MSE:HG3	1.91	0.51
1:B:2156:ARG:HD3	1:B:2159:TYR:CE1	2.46	0.51
1:B:1660:SER:O	1:B:1664:GLU:HG2	2.11	0.50
1:C:1633:GLU:C	1:C:1635:ILE:H	2.14	0.50
1:B:1494:GLN:NE2	1:B:1496:LYS:HG2	2.26	0.50
1:C:1883:ARG:HH11	1:C:1883:ARG:HG3	1.75	0.50
1:C:1809:TYR:O	1:C:1945:LEU:HD11	2.10	0.50
1:A:1608:THR:O	1:A:1612:ARG:HG3	2.12	0.50
1:A:1918:GLN:O	1:A:1920:PRO:HD3	2.11	0.50
1:A:2005:PRO:HG3	1:A:2014:MSE:HB2	1.93	0.50
1:B:1605:ASN:HD22	1:B:1714:ALA:CB	2.24	0.50
1:C:1814:ARG:O	1:C:1815:ASN:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2160:PRO:HB2	1:C:2163:VAL:HG23	1.92	0.50
1:A:2179:TYR:HD1	1:B:1489:VAL:HA	1.75	0.50
1:B:1649:PRO:O	1:B:1651:LYS:N	2.44	0.50
1:B:1981:TYR:CG	1:B:1985:ILE:HD11	2.47	0.50
1:C:1835:PRO:HG2	1:C:1991:PRO:HB2	1.93	0.50
1:C:1818:VAL:HB	1:C:1888:PRO:HG2	1.93	0.50
1:B:1705:LEU:HB3	1:C:2000:TRP:CD1	2.45	0.50
1:A:1936:ILE:HA	1:A:1947:MSE:CE	2.42	0.50
1:B:1753:PRO:HB2	1:B:1755:ILE:HD11	1.93	0.50
1:B:1733:VAL:CG1	1:B:1755:ILE:HB	2.39	0.50
1:C:1987:ILE:HB	1:C:2014:MSE:HG3	1.93	0.50
1:C:1719:TYR:CE2	1:C:1744:GLN:HG3	2.46	0.50
1:A:2093:PHE:HA	1:A:2096:LEU:HD12	1.94	0.50
1:B:1634:GLU:HG3	1:B:1671:LYS:HD3	1.93	0.50
1:B:1697:GLU:O	1:B:1700:LEU:HD13	2.12	0.50
1:C:1493:LEU:HB2	1:C:1497:ARG:HH11	1.73	0.50
1:C:1621:LEU:HD22	1:C:1727:LEU:HD23	1.94	0.50
1:C:1659:THR:OG1	1:C:1661:GLU:HG3	2.12	0.50
1:C:1737:ALA:CB	1:C:1756:LEU:HD12	2.42	0.50
1:C:1780:THR:O	1:C:1784:TYR:HB3	2.12	0.50
1:C:1582:PHE:CD1	1:C:1619:ILE:HD13	2.47	0.50
1:C:1629:ILE:HG13	1:C:1629:ILE:O	2.09	0.50
1:A:1719:TYR:CE2	1:A:1744:GLN:HG3	2.47	0.49
1:A:2037:ARG:HB2	1:A:2037:ARG:CZ	2.42	0.49
1:B:1570:THR:HG23	1:B:1581:GLN:HG2	1.93	0.49
1:B:1918:GLN:O	1:B:1920:PRO:HD3	2.12	0.49
1:B:2031:VAL:C	1:B:2033:ILE:H	2.16	0.49
1:A:1564:MSE:HE3	1:A:1604:PHE:HB2	1.93	0.49
1:A:1636:VAL:N	1:A:1637:PRO:HD2	2.27	0.49
1:B:2045:ASN:HB2	1:B:2046:ARG:NH2	2.27	0.49
1:C:2021:ARG:HA	1:C:2098:ASP:O	2.12	0.49
1:A:1636:VAL:CG1	1:A:1637:PRO:HD3	2.42	0.49
1:C:1493:LEU:HD12	1:C:1497:ARG:NH1	2.28	0.49
1:C:1697:GLU:HB3	1:C:1700:LEU:HD11	1.94	0.49
1:B:1569:ILE:HG22	1:B:1571:VAL:HG22	1.93	0.49
1:B:1998:GLY:O	1:B:2001:VAL:HG12	2.12	0.49
1:B:2100:SER:HA	1:B:2103:MSE:HE3	1.94	0.49
1:A:1619:ILE:N	1:A:1619:ILE:HD12	2.27	0.49
1:B:1983:GLN:HB3	1:B:1984:PRO:HD2	1.94	0.49
1:B:1652:GLY:HA2	1:C:2085:ILE:HD11	1.94	0.49
1:B:2001:VAL:HG23	1:C:1709:GLY:CA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2099:ARG:HB2	1:C:1692:THR:HG23	1.95	0.49
1:A:1636:VAL:N	1:A:1637:PRO:CD	2.76	0.49
1:A:2041:LEU:O	1:A:2044:MSE:HB2	2.13	0.49
1:C:1811:PRO:HA	1:C:1819:PRO:HD3	1.95	0.49
1:A:2170:GLN:HG3	1:B:1517:GLN:NE2	2.28	0.49
1:B:1533:THR:OG1	1:B:1534:ASP:N	2.46	0.49
1:A:2135:LEU:HB3	1:A:2155:ILE:CD1	2.37	0.49
1:A:1572:LYS:HG2	1:A:1577:PRO:O	2.13	0.48
1:A:1660:SER:HB2	1:A:1686:GLU:OE2	2.12	0.48
1:B:1686:GLU:O	1:B:1686:GLU:HG3	2.12	0.48
1:B:1780:THR:O	1:B:1784:TYR:HB3	2.13	0.48
1:B:2103:MSE:HG2	1:C:1702:VAL:HG11	1.95	0.48
1:C:1641:VAL:HG12	1:C:1653:PHE:HB3	1.94	0.48
1:C:1655:TYR:C	1:C:1656:LEU:HD12	2.33	0.48
1:A:1487:TYR:HB3	1:A:1488:PRO:HD2	1.95	0.48
1:A:2044:MSE:HG3	1:A:2086:TYR:CE2	2.48	0.48
1:B:1631:MSE:HE2	1:C:2034:LYS:HB3	1.96	0.48
1:B:2120:ARG:HG3	3:B:4035:HOH:O	2.11	0.48
1:C:1592:LYS:O	1:C:1593:ILE:HG13	2.12	0.48
1:C:1550:LEU:HD11	1:C:1607:VAL:HA	1.95	0.48
1:C:1651:LYS:HD2	1:C:1651:LYS:N	2.26	0.48
1:A:1948:MSE:HA	1:A:1986:ILE:O	2.14	0.48
1:C:1951:ALA:O	1:C:1990:PRO:HD2	2.12	0.48
1:C:2133:GLU:HA	1:C:2136:ILE:HD12	1.93	0.48
1:C:2142:GLN:O	1:C:2144:GLY:N	2.46	0.48
1:A:1754:ILE:HD12	1:A:1783:MSE:HG3	1.95	0.48
1:A:1994:GLU:HA	1:A:2021:ARG:O	2.13	0.48
1:A:2005:PRO:CG	1:A:2014:MSE:HB2	2.43	0.48
1:B:2036:ARG:NH1	1:B:2036:ARG:HG2	2.28	0.48
1:A:1987:ILE:HB	1:A:2014:MSE:HG3	1.96	0.48
1:B:1829:ARG:HG3	1:B:1829:ARG:NH1	2.27	0.48
1:C:2164:ASP:H	1:C:2170:GLN:HE22	1.60	0.48
1:C:1879:VAL:CG1	1:C:1931:LYS:HE3	2.43	0.48
1:B:1755:ILE:N	1:B:1755:ILE:HD12	2.28	0.48
1:C:2081:GLU:OE1	1:C:2081:GLU:N	2.47	0.48
1:A:1503:MSE:HB3	1:A:1505:THR:HG22	1.95	0.48
1:B:2044:MSE:HA	1:B:2086:TYR:CE2	2.49	0.48
1:C:1650:ASP:HB2	1:C:1651:LYS:HD2	1.96	0.48
1:C:2185:LYS:O	1:C:2189:LEU:HD13	2.13	0.48
1:A:1798:ALA:O	1:A:1802:LYS:HD3	2.13	0.48
1:B:1994:GLU:HA	1:B:2021:ARG:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1499:LYS:O	1:C:1503:MSE:HG2	2.14	0.48
1:C:1643:TRP:C	1:C:1645:ASP:H	2.16	0.47
1:C:1948:MSE:HA	1:C:1986:ILE:O	2.13	0.47
1:C:1784:TYR:HA	1:C:1789:SER:HB2	1.95	0.47
1:C:2044:MSE:HG2	1:C:2086:TYR:CE2	2.49	0.47
1:A:1682:ILE:HD13	1:A:1682:ILE:N	2.25	0.47
1:A:1932:THR:O	1:A:1936:ILE:HG13	2.14	0.47
1:A:2000:TRP:C	1:A:2000:TRP:CD1	2.86	0.47
1:B:2131:ASN:HB3	1:B:2175:ILE:HG21	1.96	0.47
1:A:1830:PRO:HG3	1:A:2120:ARG:HH12	1.79	0.47
1:B:2001:VAL:O	1:B:2007:ILE:HD11	2.14	0.47
1:C:1546:GLU:CD	1:C:1546:GLU:H	2.18	0.47
1:A:2085:ILE:O	1:A:2089:ILE:HG13	2.14	0.47
1:A:2178:ASN:HB3	1:A:2181:THR:HB	1.96	0.47
2:B:3000:H1L:H2A1	1:C:2001:VAL:CG2	2.45	0.47
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.80	0.47
1:B:1868:GLU:CG	1:B:1871:SER:HB3	2.45	0.47
1:B:1925:HIS:CE1	1:B:1957:SER:HB3	2.49	0.47
1:C:1566:ALA:HA	1:C:1584:VAL:O	2.15	0.47
1:C:1738:TYR:CG	2:C:3000:H1L:H7	2.49	0.47
1:B:1682:ILE:HG22	1:B:1683:ASN:H	1.80	0.47
1:B:1846:MSE:HE1	1:B:1990:PRO:CB	2.44	0.47
1:C:1636:VAL:N	1:C:1637:PRO:CD	2.77	0.47
1:C:1681:VAL:HG22	1:C:1685:GLU:O	2.14	0.47
1:C:2152:ILE:O	1:C:2156:ARG:HG3	2.15	0.47
1:A:1844:ARG:HA	1:A:1847:ILE:HD12	1.96	0.47
1:B:1635:ILE:O	1:B:1635:ILE:HG22	2.14	0.47
1:B:2001:VAL:HG23	1:C:1709:GLY:HA2	1.95	0.47
1:C:1623:ALA:HB2	1:C:1729:THR:CG2	2.44	0.47
1:A:1582:PHE:CD1	1:A:1619:ILE:HD13	2.50	0.47
1:A:1875:LYS:HB2	1:A:1899:VAL:CG1	2.45	0.47
1:A:2179:TYR:HB2	1:B:1489:VAL:HG13	1.97	0.47
1:A:2135:LEU:HD21	1:A:2182:LEU:HD13	1.97	0.47
1:B:1786:ASN:OD1	1:C:1965:ASN:HB3	2.15	0.47
1:C:1790:HIS:HA	1:C:1870:LEU:HD23	1.97	0.47
1:B:1681:VAL:O	1:B:1682:ILE:HD13	2.14	0.46
1:B:1759:ALA:HA	1:B:1762:ILE:HD12	1.97	0.46
1:B:1991:PRO:CG	1:B:2115:TRP:HB2	2.45	0.46
1:C:2160:PRO:HD3	1:C:2174:TRP:CE2	2.49	0.46
1:A:1894:VAL:HG11	1:A:1922:GLN:HA	1.97	0.46
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1542:LEU:CD2	1:A:1552:GLU:HG2	2.46	0.46
1:B:1663:MSE:HG3	1:B:1688:PHE:CD2	2.49	0.46
1:C:1906:ASP:HB2	1:C:1912:SER:HB3	1.97	0.46
1:B:2163:VAL:HG13	1:B:2170:GLN:HG2	1.98	0.46
1:C:1827:TRP:CD2	1:C:1828:ASP:N	2.83	0.46
1:B:1835:PRO:HG2	1:B:1846:MSE:SE	2.65	0.46
1:C:1672:GLU:N	1:C:1672:GLU:CD	2.66	0.46
1:C:1872:GLY:HA2	1:C:1875:LYS:HE3	1.97	0.46
1:B:1658:LEU:O	1:B:1688:PHE:HB2	2.15	0.46
1:C:2148:ARG:O	1:C:2152:ILE:HG13	2.15	0.46
1:B:1624:ASN:ND2	1:B:1733:VAL:H	2.13	0.46
1:B:1768:ARG:NH1	1:B:1768:ARG:HG2	2.31	0.46
1:A:1675:VAL:HG22	1:A:1676:LEU:N	2.31	0.46
1:A:1583:VAL:HG21	1:A:1611:ALA:HB2	1.98	0.45
1:A:1990:PRO:HG2	1:A:1993:GLY:HA3	1.98	0.45
1:B:1571:VAL:O	1:B:1579:GLY:HA2	2.16	0.45
1:B:2000:TRP:CD1	1:C:1705:LEU:HB3	2.51	0.45
1:A:1760:PRO:HA	1:A:1763:ASN:HD22	1.81	0.45
1:A:2160:PRO:HD2	1:A:2163:VAL:HG21	1.97	0.45
2:B:3000:H1L:CL1	1:C:1968:LEU:HD12	2.53	0.45
1:C:1733:VAL:HA	1:C:1755:ILE:O	2.16	0.45
1:A:1494:GLN:HG3	1:A:1497:ARG:NH1	2.31	0.45
1:A:1801:GLU:HG2	3:A:4006:HOH:O	2.16	0.45
1:A:1813:LYS:HA	3:A:4033:HOH:O	2.15	0.45
1:A:2021:ARG:HA	1:A:2098:ASP:O	2.16	0.45
1:B:1616:ILE:HG13	1:B:1617:PRO:HD2	1.97	0.45
1:B:1759:ALA:N	1:B:1760:PRO:CD	2.79	0.45
1:B:1514:LEU:HD22	1:B:1797:LEU:HG	1.99	0.45
1:B:2024:VAL:HG11	1:C:1629:ILE:HG22	1.98	0.45
1:C:1550:LEU:HD12	1:C:1610:TYR:HB2	1.98	0.45
1:A:1770:VAL:HG13	1:A:1771:TYR:CD1	2.51	0.45
1:A:1745:ARG:HG2	1:A:1806:TRP:CZ2	2.51	0.45
1:A:1872:GLY:HA2	1:A:1875:LYS:HE2	1.98	0.45
1:A:2188:GLY:O	1:A:2189:LEU:HD12	2.17	0.45
1:B:1885:GLY:HA3	1:B:2123:PHE:CE1	2.52	0.45
1:C:1642:ALA:HB2	1:C:1657:TYR:CD1	2.51	0.45
1:C:1730:CYS:O	1:C:1731:ARG:C	2.55	0.45
1:C:2102:ARG:O	1:C:2106:LYS:HG2	2.16	0.45
1:B:1647:ALA:C	1:B:1649:PRO:HD3	2.37	0.45
1:B:1682:ILE:HG22	1:B:1683:ASN:N	2.31	0.45
1:B:2046:ARG:HD2	1:B:2046:ARG:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2110:SER:O	1:B:2111:LYS:HB3	2.17	0.45
1:C:1766:LEU:HD13	1:C:1770:VAL:HG11	1.99	0.45
1:C:1883:ARG:HG3	1:C:1883:ARG:NH1	2.32	0.45
1:B:1761:ALA:O	1:B:1765:MSE:HG3	2.16	0.45
1:B:1797:LEU:HB2	3:B:4029:HOH:O	2.17	0.45
1:B:2094:ALA:HA	1:B:2097:HIS:CD2	2.49	0.45
1:C:1591:PHE:CD2	1:C:1592:LYS:HG3	2.52	0.45
1:C:2082:LEU:O	1:C:2086:TYR:HB2	2.16	0.45
1:A:1527:SER:O	1:A:1530:VAL:HG22	2.16	0.45
1:B:1494:GLN:NE2	1:B:1496:LYS:H	2.12	0.45
1:B:1615:GLY:HA2	1:B:1814:ARG:NH1	2.32	0.45
1:B:1675:VAL:HG12	1:B:1693:ILE:HA	1.98	0.45
1:C:1875:LYS:O	1:C:1895:GLU:HG3	2.17	0.45
1:B:2179:TYR:HB2	1:B:2180:LYS:NZ	2.31	0.45
1:C:1682:ILE:CG2	1:C:1687:ARG:HD2	2.46	0.45
1:B:1534:ASP:C	1:B:1536:PHE:H	2.20	0.45
1:C:1564:MSE:HE3	1:C:1604:PHE:HB2	1.98	0.45
1:A:1750:GLU:HA	1:A:1780:THR:CG2	2.45	0.44
1:A:2081:GLU:N	1:A:2081:GLU:OE1	2.50	0.44
1:B:1633:GLU:HA	1:B:1636:VAL:HG23	1.99	0.44
1:C:1663:MSE:HE3	1:C:1666:LEU:HD12	1.99	0.44
1:A:1578:ARG:HD2	1:A:1578:ARG:H	1.83	0.44
1:B:1541:GLU:CD	1:B:1555:ARG:HH11	2.21	0.44
1:C:1879:VAL:HG12	1:C:1931:LYS:HE3	1.99	0.44
1:C:1990:PRO:HG2	1:C:1993:GLY:HA3	1.98	0.44
1:C:2031:VAL:CG2	1:C:2035:PHE:HB3	2.45	0.44
1:A:1492:TRP:CE3	1:A:1493:LEU:HD23	2.53	0.44
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.82	0.44
1:B:1901:ASN:ND2	1:B:1917:ILE:HD12	2.33	0.44
1:C:1655:TYR:O	1:C:1656:LEU:HD12	2.18	0.44
1:A:1875:LYS:HB2	1:A:1899:VAL:HG11	1.99	0.44
1:B:1649:PRO:C	1:B:1651:LYS:H	2.21	0.44
1:B:1731:ARG:HA	1:B:1753:PRO:O	2.18	0.44
1:B:1953:TRP:HB2	1:B:1999:SER:HB3	2.00	0.44
1:B:2083:LEU:N	1:B:2084:PRO:CD	2.81	0.44
1:A:1503:MSE:HG2	1:A:1589:ILE:HG12	1.98	0.44
1:A:2125:ARG:O	1:A:2129:ARG:HG3	2.17	0.44
1:B:1582:PHE:CD2	1:B:1807:MSE:HE1	2.52	0.44
1:C:1493:LEU:HB2	1:C:1497:ARG:HH12	1.78	0.44
1:C:1730:CYS:SG	1:C:1731:ARG:N	2.90	0.44
1:C:1903:ILE:HD13	1:C:1917:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1656:LEU:CB	1:A:1690:ILE:HD11	2.47	0.44
1:A:1892:ILE:CD1	1:A:1947:MSE:HE2	2.48	0.44
1:C:1655:TYR:OH	1:C:1687:ARG:NH1	2.51	0.44
1:C:1675:VAL:HG12	1:C:1693:ILE:HG23	1.99	0.44
1:C:1729:THR:O	1:C:1752:GLN:HG3	2.18	0.44
1:C:1745:ARG:HH11	1:C:1745:ARG:HD2	1.31	0.44
1:B:1824:LYS:HE2	1:B:1825:ASP:H	1.83	0.44
1:B:2004:ASP:CG	1:B:2005:PRO:HD2	2.38	0.44
1:C:1619:ILE:HD12	1:C:1619:ILE:N	2.33	0.44
1:C:1703:GLU:N	1:C:1703:GLU:OE1	2.45	0.44
1:C:2128:ARG:HE	1:C:2132:GLU:CD	2.22	0.44
1:A:1690:ILE:O	1:A:1690:ILE:HG13	2.17	0.43
1:C:1583:VAL:HG13	1:C:1616:ILE:HD11	1.98	0.43
1:A:2132:GLU:O	1:A:2136:ILE:HG13	2.18	0.43
1:B:1505:THR:HB	1:B:1730:CYS:HB2	2.00	0.43
1:B:1780:THR:C	1:B:1782:ILE:H	2.22	0.43
1:A:1778:GLY:HA2	1:A:1783:MSE:HE3	2.00	0.43
1:A:1641:VAL:HG13	1:A:1643:TRP:NE1	2.34	0.43
1:A:1663:MSE:HG3	1:A:1688:PHE:CD1	2.54	0.43
1:A:1699:GLY:HA2	1:A:1704:CYS:SG	2.59	0.43
1:B:2172:ALA:O	1:B:2176:GLU:HG3	2.18	0.43
1:C:1494:GLN:HB3	1:C:1495:PRO:CD	2.48	0.43
1:C:1879:VAL:HG12	1:C:1931:LYS:CE	2.49	0.43
1:A:1655:TYR:CE1	1:A:1689:VAL:HG22	2.54	0.43
1:A:1983:GLN:HB3	1:A:1984:PRO:HD2	2.00	0.43
1:C:1640:GLN:HB2	1:C:1657:TYR:CE1	2.54	0.43
1:C:1936:ILE:CG2	1:C:1977:ALA:HB1	2.48	0.43
1:B:1643:TRP:CZ3	1:B:1649:PRO:HB3	2.53	0.43
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	2.00	0.43
1:B:1970:TYR:HH	1:C:1970:TYR:HH	1.66	0.43
1:C:1607:VAL:O	1:C:1610:TYR:HB3	2.19	0.43
1:C:1738:TYR:HB2	2:C:3000:H1L:C7	2.49	0.43
1:A:1892:ILE:HD11	1:A:1947:MSE:HE2	2.00	0.43
1:B:1815:ASN:H	1:B:1944:GLN:HE22	1.65	0.43
1:C:1644:ASN:N	1:C:1644:ASN:HD22	2.16	0.43
1:A:1677:THR:HA	1:A:1689:VAL:O	2.19	0.43
1:B:1844:ARG:HA	1:B:1847:ILE:HD12	2.01	0.43
1:A:1584:VAL:HA	1:A:1619:ILE:O	2.19	0.42
1:A:1879:VAL:HG13	1:A:1931:LYS:HE2	2.00	0.42
1:C:1811:PRO:HB2	1:C:1816:MSE:HB2	2.01	0.42
1:C:1827:TRP:CG	1:C:1828:ASP:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1846:MSE:CE	1:A:1991:PRO:HD2	2.45	0.42
1:A:2128:ARG:C	1:A:2128:ARG:HD3	2.39	0.42
1:A:2180:LYS:HG2	1:B:1482:PRO:CD	2.48	0.42
1:C:1677:THR:HA	1:C:1689:VAL:O	2.20	0.42
1:A:2180:LYS:CA	1:B:1482:PRO:HD3	2.49	0.42
1:C:1597:GLY:H	1:C:1600:GLU:HB2	1.84	0.42
1:A:1619:ILE:HG13	1:A:1725:ILE:CG2	2.49	0.42
1:A:1844:ARG:HG3	1:A:1844:ARG:HH11	1.83	0.42
1:B:1582:PHE:HB2	1:B:1617:PRO:HG2	2.01	0.42
1:B:1726:THR:HG21	1:B:1740:VAL:HG22	2.02	0.42
1:B:1926:PRO:HG3	1:B:1967:VAL:HG23	2.00	0.42
1:C:1634:GLU:HG3	1:C:1671:LYS:HD3	2.01	0.42
1:C:1646:ALA:C	1:C:1648:ASN:H	2.22	0.42
1:C:2037:ARG:O	1:C:2041:LEU:HG	2.19	0.42
1:A:1996:ARG:O	1:A:1999:SER:HB2	2.19	0.42
1:B:2102:ARG:NH1	1:B:2106:LYS:HG3	2.35	0.42
1:C:1756:LEU:HD21	2:C:3000:H1L:CL1	2.57	0.42
1:C:1773:SER:HB3	1:C:1776:GLN:HG3	2.02	0.42
1:C:1833:PHE:CZ	1:C:1845:TRP:HE3	2.38	0.42
1:A:1953:TRP:HB2	1:A:1999:SER:HB3	2.02	0.42
1:A:2087:GLY:O	1:A:2090:SER:HB2	2.18	0.42
1:B:1543:ILE:HD11	1:B:1553:VAL:HG11	2.01	0.42
1:B:1585:VAL:O	1:B:1620:TYR:HA	2.19	0.42
1:C:1790:HIS:HD2	3:C:4018:HOH:O	2.02	0.42
1:A:1866:PHE:CE1	1:A:1868:GLU:HB2	2.54	0.42
1:A:1877:VAL:CG2	1:A:1931:LYS:HD3	2.50	0.42
1:C:1792:THR:CG2	1:C:1793:ALA:N	2.83	0.42
1:B:1701:GLY:HA2	1:C:2024:VAL:HG23	2.01	0.42
1:A:1753:PRO:HA	1:A:1778:GLY:O	2.20	0.42
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.68	0.42
1:B:2010:ASP:OD2	1:B:2148:ARG:HD3	2.20	0.42
1:B:2156:ARG:HG3	1:B:2156:ARG:HH11	1.84	0.42
1:C:1751:GLY:O	1:C:1753:PRO:HD3	2.19	0.42
1:C:1829:ARG:CZ	1:C:1858:TYR:HB3	2.49	0.42
1:A:1565:VAL:HG12	1:A:1566:ALA:N	2.34	0.42
1:B:1818:VAL:HB	1:B:1888:PRO:CG	2.48	0.42
1:B:1850:ARG:NH1	1:B:1857:GLU:OE2	2.52	0.42
1:B:2114:GLU:O	1:B:2115:TRP:C	2.57	0.42
1:C:1711:ILE:HD11	1:C:1735:ILE:HG12	2.02	0.42
1:C:1790:HIS:O	1:C:1791:LEU:HD23	2.20	0.42
1:A:1585:VAL:O	1:A:1620:TYR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1505:THR:HB	1:A:1730:CYS:HB2	2.02	0.41
1:A:2083:LEU:N	1:A:2084:PRO:CD	2.82	0.41
1:A:2095:ASP:C	1:A:2099:ARG:NH1	2.73	0.41
1:B:1494:GLN:NE2	1:B:1496:LYS:CG	2.83	0.41
1:B:1537:PHE:CD2	1:B:1571:VAL:HG13	2.55	0.41
1:A:1807:MSE:HA	1:A:1810:VAL:HG22	2.02	0.41
1:B:2027:PRO:O	1:B:2031:VAL:HG23	2.19	0.41
1:C:1753:PRO:CG	1:C:1755:ILE:HD11	2.50	0.41
1:A:1616:ILE:HA	1:A:1617:PRO:HD3	1.91	0.41
1:B:2016:ALA:O	1:B:2112:GLU:HA	2.19	0.41
1:C:1585:VAL:O	1:C:1620:TYR:HA	2.20	0.41
1:C:1678:GLU:OE2	1:C:1691:LYS:HD2	2.20	0.41
1:A:1655:TYR:CD1	1:A:1689:VAL:HG13	2.55	0.41
1:A:1781:GLN:O	1:A:1782:ILE:HD13	2.20	0.41
1:B:1543:ILE:HD13	1:B:1553:VAL:HG21	2.02	0.41
1:C:1587:ASN:ND2	1:C:1623:ALA:H	2.18	0.41
1:C:1759:ALA:HB2	1:C:1777:LEU:HD12	2.02	0.41
1:C:1850:ARG:HG2	1:C:1851:GLU:N	2.35	0.41
1:C:2033:ILE:HG22	1:C:2034:LYS:HD2	2.02	0.41
1:A:1542:LEU:HD21	1:A:1552:GLU:HG2	2.02	0.41
1:B:1648:ASN:ND2	1:B:1650:ASP:OD2	2.53	0.41
1:C:1530:VAL:O	1:C:1530:VAL:HG23	2.21	0.41
1:C:1589:ILE:HA	1:C:1589:ILE:HD12	1.95	0.41
1:C:2081:GLU:CG	1:C:2082:LEU:H	2.23	0.41
1:C:1587:ASN:ND2	1:C:1624:ASN:HD22	2.18	0.41
1:C:1733:VAL:HG12	1:C:1734:GLY:N	2.35	0.41
1:C:1770:VAL:HG13	1:C:1771:TYR:H	1.85	0.41
1:A:1607:VAL:O	1:A:1610:TYR:HB3	2.21	0.41
1:B:1524:LYS:HE2	1:B:1524:LYS:HA	2.03	0.41
1:B:1591:PHE:O	1:B:1592:LYS:C	2.57	0.41
1:C:1661:GLU:HG3	1:C:1662:GLY:N	2.35	0.41
1:C:1679:ARG:HH11	1:C:1679:ARG:HB2	1.85	0.41
1:C:2005:PRO:HG3	1:C:2014:MSE:HB2	2.03	0.41
1:C:1753:PRO:HG2	1:C:1755:ILE:HD11	2.02	0.41
1:A:1951:ALA:O	1:A:1990:PRO:HD2	2.21	0.41
1:C:1569:ILE:CG2	1:C:1571:VAL:HG22	2.51	0.41
1:C:1719:TYR:O	1:C:1941:ASN:HB3	2.21	0.41
1:C:1764:LYS:HD2	1:C:1764:LYS:N	2.36	0.41
1:C:1818:VAL:CG1	1:C:1945:LEU:HD12	2.50	0.41
1:A:1813:LYS:O	1:A:1816:MSE:HB2	2.21	0.40
1:B:1497:ARG:HD3	1:B:1510:ASP:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1636:VAL:HG12	1:A:1637:PRO:HD3	2.03	0.40
1:A:1682:ILE:C	1:A:1684:GLY:N	2.73	0.40
1:A:2131:ASN:ND2	1:A:2179:TYR:OH	2.54	0.40
1:B:2139:LEU:HD22	1:B:2155:ILE:HG13	2.03	0.40
1:C:1575:GLU:OE1	1:C:1821:LEU:HD22	2.21	0.40
1:C:1792:THR:HG22	1:C:1793:ALA:N	2.36	0.40
1:C:2148:ARG:HH11	1:C:2148:ARG:HG2	1.85	0.40
1:A:2004:ASP:HA	1:A:2005:PRO:HD3	1.98	0.40
1:C:1556:GLU:HA	1:C:1557:PRO:HD3	1.92	0.40
1:C:1754:ILE:HB	1:C:1783:MSE:CE	2.45	0.40
1:C:1935:ALA:HA	3:C:4024:HOH:O	2.22	0.40
1:C:1666:LEU:HB3	1:C:1671:LYS:O	2.21	0.40
1:C:1505:THR:CB	1:C:1730:CYS:HB2	2.51	0.40
1:C:1953:TRP:HB2	1:C:1999:SER:HB3	2.04	0.40
1:A:1511:PHE:N	1:A:1512:PRO:CD	2.84	0.40
1:A:1762:ILE:O	1:A:1766:LEU:HD13	2.22	0.40
1:A:1949:ILE:HD12	1:A:1987:ILE:CD1	2.52	0.40
1:B:1575:GLU:OE1	1:B:1808:SER:HB2	2.22	0.40
1:C:1994:GLU:HA	1:C:2021:ARG:O	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1970:TYR:OH	1:A:1970:TYR:OH[2_555]	2.19	0.01

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	664/737 (90%)	602 (91%)	57 (9%)	5 (1%)	19 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	664/737 (90%)	597 (90%)	57 (9%)	10 (2%)	10 33
1	C	654/737 (89%)	576 (88%)	66 (10%)	12 (2%)	8 28
All	All	1982/2211 (90%)	1775 (90%)	180 (9%)	27 (1%)	11 34

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1991	PRO
1	B	1534	ASP
1	B	1650	ASP
1	B	1731	ARG
1	C	1632	ALA
1	C	2143	VAL
1	A	2036	ARG
1	B	1744	GLN
1	C	1642	ALA
1	C	1744	GLN
1	C	1907	PRO
1	A	1731	ARG
1	A	1744	GLN
1	B	1533	THR
1	C	1634	GLU
1	C	1637	PRO
1	C	1731	ARG
1	A	1819	PRO
1	B	1991	PRO
1	B	2115	TRP
1	C	1508	VAL
1	C	1653	PHE
1	B	1647	ALA
1	B	2144	GLY
1	C	1650	ASP
1	B	2032	GLY
1	C	1991	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	567/611 (93%)	530 (94%)	37 (6%)	17 44
1	B	567/611 (93%)	523 (92%)	44 (8%)	12 35
1	C	558/611 (91%)	527 (94%)	31 (6%)	21 51
All	All	1692/1833 (92%)	1580 (93%)	112 (7%)	16 44

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1494	GLN
1	A	1533	THR
1	A	1534	ASP
1	A	1554	GLU
1	A	1560	ASN
1	A	1585	VAL
1	A	1613	LYS
1	A	1631	MSE
1	A	1638	LEU
1	A	1682	ILE
1	A	1686	GLU
1	A	1697	GLU
1	A	1781	GLN
1	A	1802	LYS
1	A	1814	ARG
1	A	1824	LYS
1	A	1837	ASN
1	A	1838	ASP
1	A	1851	GLU
1	A	1853	GLU
1	A	1884	LEU
1	A	1924	TRP
1	A	1930	PHE
1	A	1965	ASN
1	A	1968	LEU
1	A	1981	TYR
1	A	1996	ARG
1	A	2008	ASN
1	A	2035	PHE
1	A	2046	ARG
1	A	2081	GLU

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Mol	Chain	Res	Type
1	A	2083	LEU
1	A	2098	ASP
1	A	2128	ARG
1	A	2135	LEU
1	A	2139	LEU
1	A	2148	ARG
1	B	1502	LEU
1	B	1505	THR
1	B	1508	VAL
1	B	1513	GLU
1	B	1516	ARG
1	B	1534	ASP
1	B	1535	ASP
1	B	1554	GLU
1	B	1555	ARG
1	B	1571	VAL
1	B	1612	ARG
1	B	1616	ILE
1	B	1618	ARG
1	B	1651	LYS
1	B	1729	THR
1	B	1731	ARG
1	B	1769	GLU
1	B	1791	LEU
1	B	1797	LEU
1	B	1813	LYS
1	B	1824	LYS
1	B	1843	VAL
1	B	1850	ARG
1	B	1884	LEU
1	B	1909	ASN
1	B	1924	TRP
1	B	1930	PHE
1	B	1968	LEU
1	B	2014	MSE
1	B	2026	GLU
1	B	2027	PRO
1	B	2035	PHE
1	B	2041	LEU
1	B	2042	ASP
1	B	2043	THR
1	B	2046	ARG

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Mol	Chain	Res	Type
1	B	2086	TYR
1	B	2119	ARG
1	B	2128	ARG
1	B	2145	GLU
1	B	2165	HIS
1	B	2179	TYR
1	B	2181	THR
1	B	2183	ASP
1	C	1499	LYS
1	C	1514	LEU
1	C	1516	ARG
1	C	1536	PHE
1	C	1542	LEU
1	C	1571	VAL
1	C	1575	GLU
1	C	1585	VAL
1	C	1593	ILE
1	C	1638	LEU
1	C	1639	PHE
1	C	1643	TRP
1	C	1672	GLU
1	C	1679	ARG
1	C	1732	SER
1	C	1741	ARG
1	C	1745	ARG
1	C	1781	GLN
1	C	1801	GLU
1	C	1840	THR
1	C	1879	VAL
1	C	1924	TRP
1	C	1930	PHE
1	C	1945	LEU
1	C	1978	LEU
1	C	2034	LYS
1	C	2035	PHE
1	C	2046	ARG
1	C	2081	GLU
1	C	2114	GLU
1	C	2128	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1522	GLN
1	A	1525	ASN
1	A	1540	ASN
1	A	1547	ASN
1	A	1560	ASN
1	A	1587	ASN
1	A	1605	ASN
1	A	1624	ASN
1	A	1644	ASN
1	A	1744	GLN
1	A	1748	GLN
1	A	1752	GLN
1	A	1815	ASN
1	A	2008	ASN
1	A	2028	GLN
1	A	2045	ASN
1	A	2092	GLN
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	1654	GLN
1	B	1720	HIS
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1790	HIS
1	B	1815	ASN
1	B	1901	ASN
1	B	1909	ASN
1	B	1941	ASN
1	B	1944	GLN
1	B	2019	ASN
1	B	2045	ASN
1	B	2097	HIS
1	B	2178	ASN
1	C	1517	GLN
1	C	1522	GLN
1	C	1560	ASN

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Mol	Chain	Res	Type
1	C	1587	ASN
1	C	1605	ASN
1	C	1640	GLN
1	C	1644	ASN
1	C	1654	GLN
1	C	1683	ASN
1	C	1748	GLN
1	C	1774	ASN
1	C	1781	GLN
1	C	1786	ASN
1	C	1790	HIS
1	C	1815	ASN
1	C	1922	GLN
1	C	1934	GLN
1	C	2011	GLN
1	C	2092	GLN
1	C	2142	GLN
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

3 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	H1L	C	3000	-	21,25,25	0.95	0	28,36,36	1.57	7 (25%)
2	H1L	B	3000	-	21,25,25	1.33	3 (14%)	28,36,36	1.77	8 (28%)
2	H1L	A	3000	-	21,25,25	1.05	1 (4%)	28,36,36	1.62	8 (28%)

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	H1L	C	3000	-	-	5/14/18/18	0/2/2/2
2	H1L	B	3000	-	-	3/14/18/18	0/2/2/2
2	H1L	A	3000	-	-	4/14/18/18	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3000	H1L	C7-C6	2.48	1.43	1.38
2	B	3000	H1L	C12-C11	2.26	1.54	1.49
2	B	3000	H1L	C5-C8	2.24	1.43	1.38
2	A	3000	H1L	O2-C3	-2.11	1.34	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3000	H1L	C11-C10-N9	-3.78	119.73	123.34
2	B	3000	H1L	C13-C11-C10	3.65	121.07	118.99
2	B	3000	H1L	C11-C10-N9	-3.33	120.16	123.34
2	A	3000	H1L	C3-O2-C2	-3.30	114.25	118.57
2	C	3000	H1L	C11-C10-N9	-3.19	120.29	123.34
2	B	3000	H1L	C2A-C2-C1	-3.08	109.37	113.35
2	C	3000	H1L	O8-C9-N9	3.08	123.56	119.49
2	B	3000	H1L	C8-O8-C9	-3.04	112.14	118.16
2	C	3000	H1L	C3-O2-C2	-3.00	114.64	118.57
2	A	3000	H1L	C13-C11-C10	2.80	120.58	118.99
2	B	3000	H1L	F3-C12-C11	-2.76	106.86	112.93
2	C	3000	H1L	C2A-C2-C1	-2.66	109.91	113.35
2	B	3000	H1L	C3-O2-C2	-2.64	115.11	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3000	H1L	C10-N9-C9	2.60	122.96	116.27
2	C	3000	H1L	C8-O8-C9	-2.52	113.16	118.16
2	A	3000	H1L	C10-N9-C9	2.26	122.08	116.27
2	B	3000	H1L	O8-C9-N9	2.24	122.45	119.49
2	A	3000	H1L	C8-O8-C9	-2.19	113.83	118.16
2	A	3000	H1L	F2-C12-C11	-2.17	108.16	112.93
2	A	3000	H1L	C13-C14-CL1	2.11	121.90	118.49
2	C	3000	H1L	O2-C2-C2A	2.06	109.73	105.53
2	B	3000	H1L	C14-C13-C11	-2.02	117.05	119.43
2	A	3000	H1L	C2A-C2-C1	-2.01	110.75	113.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3000	H1L	C1-C2-O2-C3
2	C	3000	H1L	C2A-C2-O2-C3
2	B	3000	H1L	C1-C2-O2-C3
2	B	3000	H1L	C2A-C2-O2-C3
2	A	3000	H1L	C1-C2-O2-C3
2	A	3000	H1L	C2A-C2-O2-C3
2	A	3000	H1L	C4-C3-O2-C2
2	C	3000	H1L	C4-C3-O2-C2
2	A	3000	H1L	C6-C3-O2-C2
2	B	3000	H1L	C14-C9-O8-C8
2	C	3000	H1L	C10-C11-C12-F1
2	C	3000	H1L	C10-C11-C12-F2

There are no ring outliers.

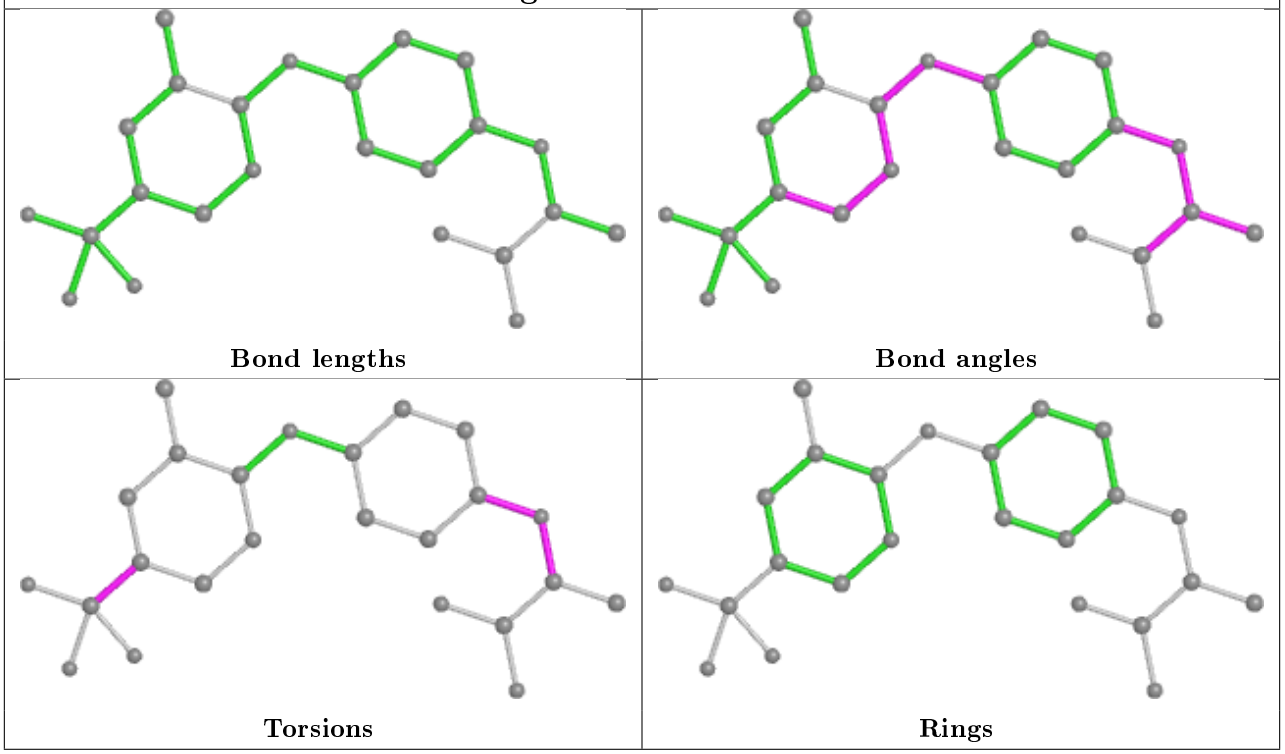
2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3000	H1L	6	0
2	B	3000	H1L	4	0

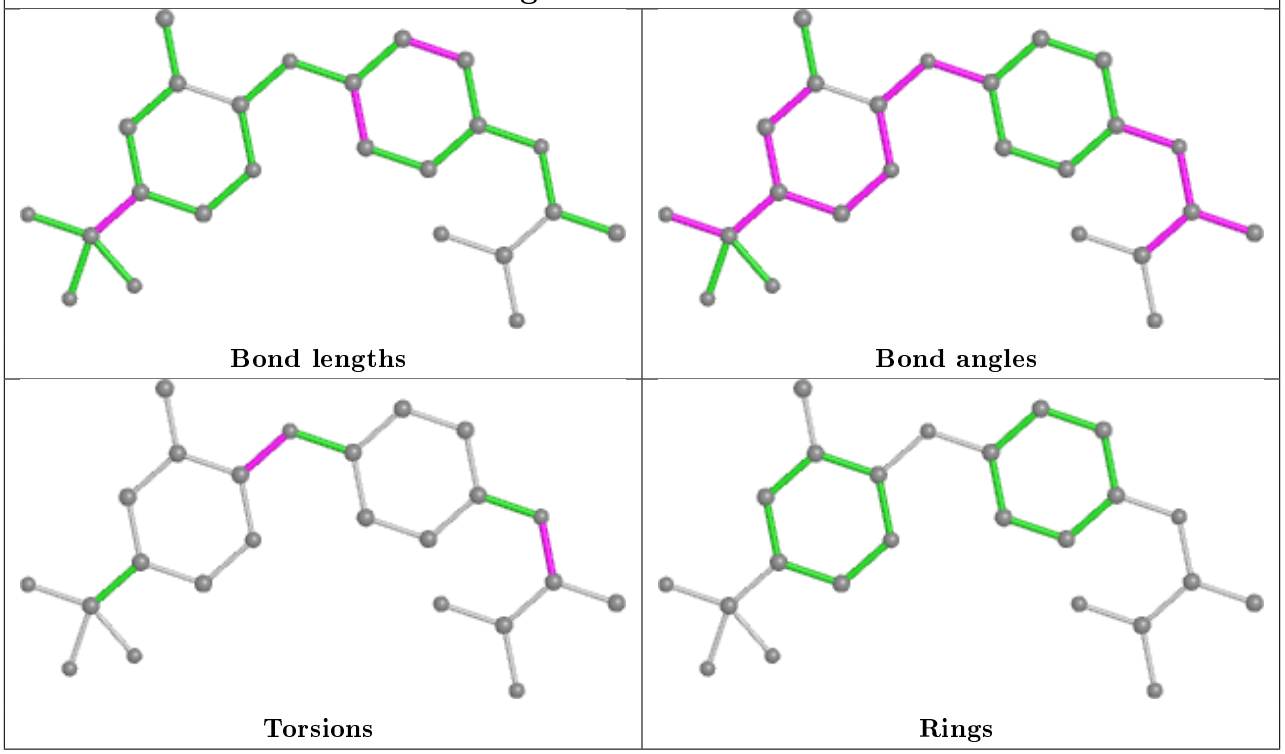
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

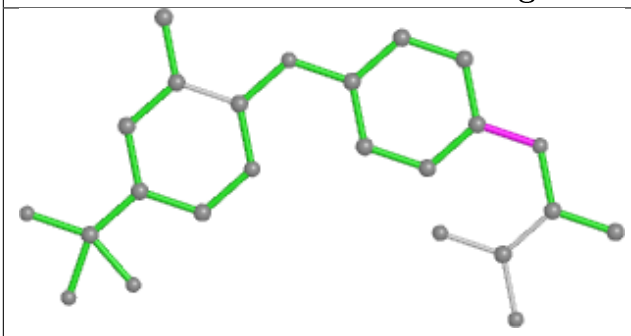
Ligand H1L C 3000



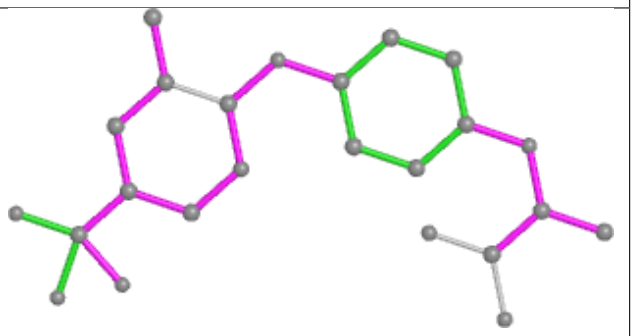
Ligand H1L B 3000



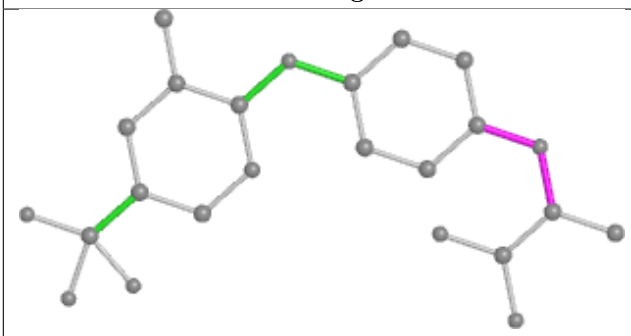
Ligand H1L A 3000



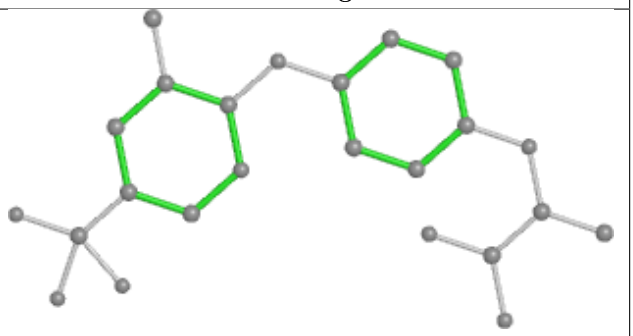
Bond lengths



Bond angles



Torsions



Rings

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	654/737 (88%)	-0.06	45 (6%)	16 10	13, 32, 98, 100	0
1	B	654/737 (88%)	0.02	56 (8%)	10 5	15, 37, 99, 100	0
1	C	644/737 (87%)	-0.01	53 (8%)	11 6	14, 37, 100, 100	0
All	All	1952/2211 (88%)	-0.02	154 (7%)	12 7	13, 36, 100, 100	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1685	GLU	6.7
1	B	1911	ASN	6.3
1	B	1904	PRO	6.3
1	B	2082	LEU	5.9
1	C	1908	ALA	5.7
1	A	1771	TYR	5.6
1	C	1770	VAL	5.4
1	A	1770	VAL	5.3
1	A	1766	LEU	5.3
1	C	1681	VAL	5.3
1	C	1758	GLY	5.1
1	B	1770	VAL	5.1
1	B	1910	PRO	5.1
1	A	2145	GLU	4.8
1	A	1838	ASP	4.8
1	C	1772	THR	4.7
1	A	1911	ASN	4.7
1	A	1907	PRO	4.6
1	A	1905	ALA	4.5
1	C	1771	TYR	4.5
1	C	1766	LEU	4.4
1	C	1913	ALA	4.4
1	B	1903	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	2143	VAL	4.3
1	B	1905	ALA	4.2
1	B	1766	LEU	4.1
1	B	1908	ALA	4.1
1	B	1680	THR	4.1
1	C	1906	ASP	4.1
1	C	1909	ASN	4.1
1	C	1838	ASP	4.0
1	B	1761	ALA	4.0
1	C	1907	PRO	4.0
1	B	1907	PRO	4.0
1	A	1768	ARG	4.0
1	C	1767	GLY	4.0
1	B	1912	SER	4.0
1	A	1758	GLY	4.0
1	A	1913	ALA	3.9
1	C	1769	GLU	3.9
1	C	1904	PRO	3.9
1	C	1669	PHE	3.8
1	A	1683	ASN	3.8
1	C	1762	ILE	3.8
1	B	1647	ALA	3.8
1	B	1838	ASP	3.8
1	B	2145	GLU	3.7
1	C	1645	ASP	3.7
1	B	1683	ASN	3.6
1	B	1768	ARG	3.6
1	A	1904	PRO	3.6
1	C	2144	GLY	3.6
1	C	1759	ALA	3.6
1	C	1911	ASN	3.5
1	A	1912	SER	3.5
1	C	1679	ARG	3.5
1	C	1651	LYS	3.5
1	A	1915	THR	3.5
1	B	2037	ARG	3.5
1	C	1768	ARG	3.5
1	C	1644	ASN	3.4
1	A	2143	VAL	3.4
1	A	1681	VAL	3.4
1	B	1909	ASN	3.4
1	B	1902	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	1679	ARG	3.3
1	B	1760	PRO	3.3
1	A	1767	GLY	3.3
1	B	1682	ILE	3.3
1	C	1764	LYS	3.3
1	C	1912	SER	3.3
1	C	1760	PRO	3.3
1	A	1769	GLU	3.2
1	C	1680	THR	3.2
1	A	1916	LEU	3.2
1	B	1681	VAL	3.2
1	B	2084	PRO	3.2
1	B	2146	ALA	3.2
1	A	1772	THR	3.2
1	B	1917	ILE	3.1
1	C	1650	ASP	3.1
1	B	2085	ILE	3.1
1	C	1914	GLU	3.0
1	A	1647	ALA	3.0
1	C	1902	LEU	3.0
1	B	2187	LYS	3.0
1	C	1905	ALA	3.0
1	A	2082	LEU	3.0
1	B	1913	ALA	2.9
1	A	1685	GLU	2.9
1	A	1760	PRO	2.9
1	A	1908	ALA	2.9
1	C	1531	LYS	2.9
1	C	1646	ALA	2.9
1	A	1906	ASP	2.8
1	B	1906	ASP	2.8
1	C	1763	ASN	2.8
1	B	1669	PHE	2.8
1	B	1772	THR	2.8
1	B	1646	ALA	2.7
1	B	1771	TYR	2.7
1	B	1769	GLU	2.7
1	A	1761	ALA	2.7
1	C	1915	THR	2.7
1	B	2041	LEU	2.7
1	C	1917	ILE	2.7
1	A	1684	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1679	ARG	2.7
1	A	2036	ARG	2.7
1	C	2037	ARG	2.7
1	B	1916	LEU	2.6
1	B	1767	GLY	2.6
1	B	1918	GLN	2.6
1	B	1853	GLU	2.6
1	C	1647	ALA	2.6
1	B	1758	GLY	2.6
1	C	1853	GLU	2.6
1	C	1668	LYS	2.5
1	B	1764	LYS	2.5
1	B	2143	VAL	2.4
1	C	1652	GLY	2.4
1	B	2142	GLN	2.4
1	A	2046	ARG	2.4
1	B	1777	LEU	2.4
1	A	1909	ASN	2.4
1	B	2045	ASN	2.4
1	A	1903	ILE	2.4
1	A	2144	GLY	2.3
1	B	2083	LEU	2.3
1	C	2085	ILE	2.3
1	A	1531	LYS	2.3
1	A	1680	THR	2.3
1	C	1910	PRO	2.3
1	A	1917	ILE	2.3
1	B	1685	GLU	2.3
1	C	2084	PRO	2.2
1	A	1762	ILE	2.2
1	C	1649	PRO	2.2
1	A	1643	TRP	2.2
1	B	2189	LEU	2.2
1	C	1773	SER	2.2
1	B	1645	ASP	2.2
1	A	1914	GLU	2.2
1	C	1918	GLN	2.1
1	B	2047	LEU	2.1
1	B	1763	ASN	2.1
1	B	1651	LYS	2.1
1	B	1901	ASN	2.1
1	A	1757	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1902	LEU	2.1
1	A	1839	GLU	2.1
1	C	1678	GLU	2.1
1	A	1764	LYS	2.0
1	C	2082	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 carbohydrates in this entry.

6.4 Ligands (i)

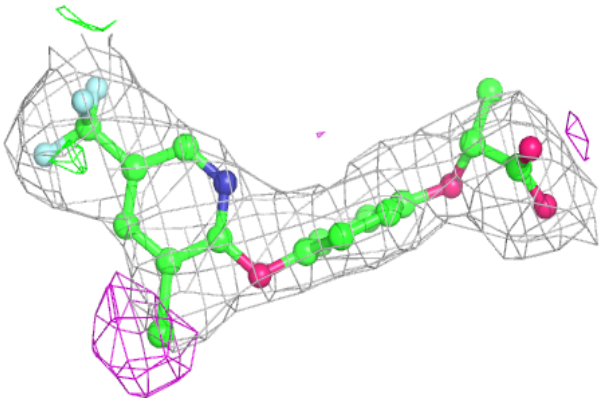
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

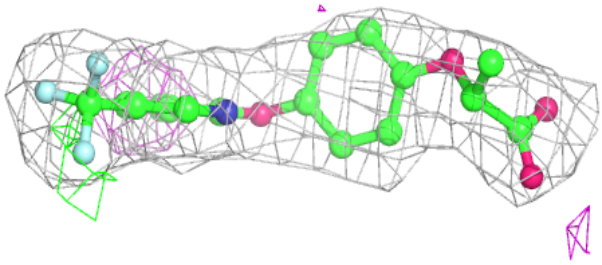
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	H1L	C	3000	24/24	0.92	0.21	52,55,60,71	0
2	H1L	B	3000	24/24	0.92	0.22	44,49,59,71	0
2	H1L	A	3000	24/24	0.93	0.20	29,38,45,54	0

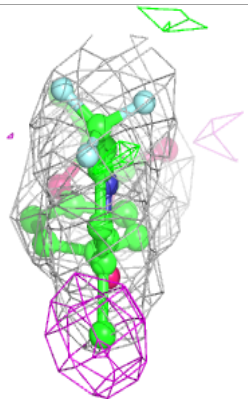
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around H1L C 3000:

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

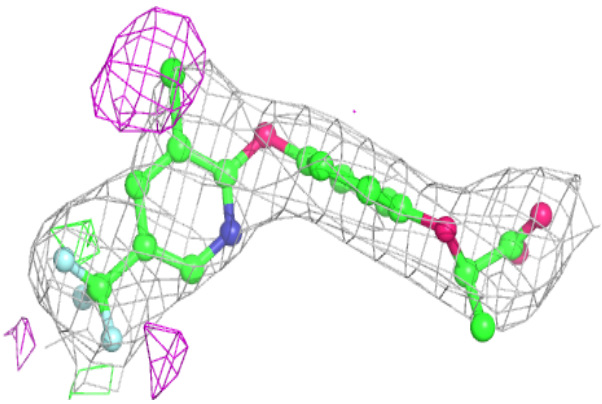


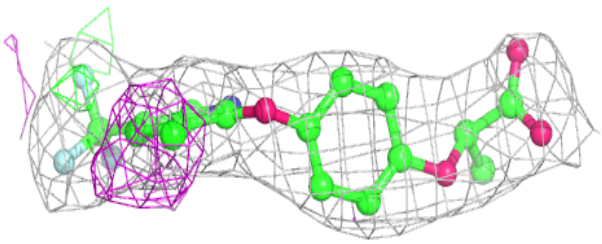


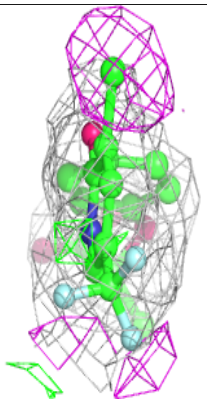


Electron density around H1L B 3000:

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

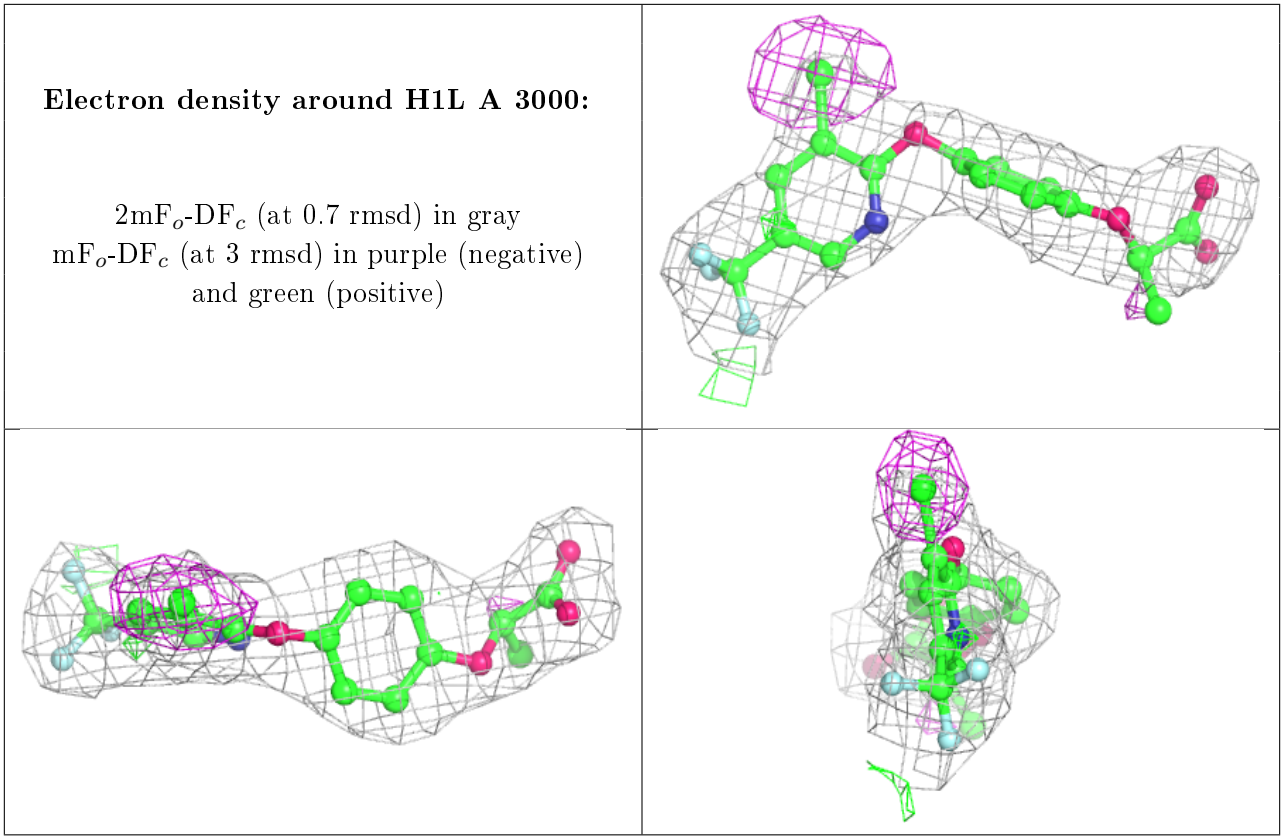






Electron density around H1L A 3000:

$2mF_o$-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.