Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2024 – 08:15 PM EDT

PDB ID	:	3H0J
Title	:	Crystal structure of the carboxyltransferase domain of acetyl-coenzyme A carboxylase in complex with compound 2
Authors	:	Zhang, H.; Tong, L.
Deposited on	:	2009-04-09
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 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:

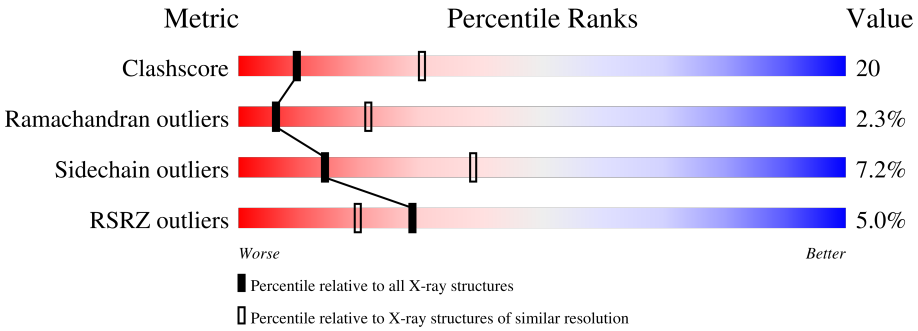
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 2.80 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))
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 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	769	4% 57% 28% · 11%
1	B	769	5% 50% 33% · 12%
1	C	769	5% 55% 27% · 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16200 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	681	Total	C	N	O	S	0	0	0
			5424	3459	930	1016	19			
1	B	675	Total	C	N	O	S	0	0	0
			5376	3427	923	1007	19			
1	C	665	Total	C	N	O	S	0	0	0
			5298	3374	912	993	19			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1473	MET	-	expression tag	UNP Q00955
A	1474	ALA	-	expression tag	UNP Q00955
A	1475	SER	-	expression tag	UNP Q00955
A	2234	LEU	-	expression tag	UNP Q00955
A	2235	GLU	-	expression tag	UNP Q00955
A	2236	HIS	-	expression tag	UNP Q00955
A	2237	HIS	-	expression tag	UNP Q00955
A	2238	HIS	-	expression tag	UNP Q00955
A	2239	HIS	-	expression tag	UNP Q00955
A	2240	HIS	-	expression tag	UNP Q00955
A	2241	HIS	-	expression tag	UNP Q00955
B	1473	MET	-	expression tag	UNP Q00955
B	1474	ALA	-	expression tag	UNP Q00955
B	1475	SER	-	expression tag	UNP Q00955
B	2234	LEU	-	expression tag	UNP Q00955
B	2235	GLU	-	expression tag	UNP Q00955
B	2236	HIS	-	expression tag	UNP Q00955
B	2237	HIS	-	expression tag	UNP Q00955
B	2238	HIS	-	expression tag	UNP Q00955
B	2239	HIS	-	expression tag	UNP Q00955
B	2240	HIS	-	expression tag	UNP Q00955
B	2241	HIS	-	expression tag	UNP Q00955
C	1473	MET	-	expression tag	UNP Q00955

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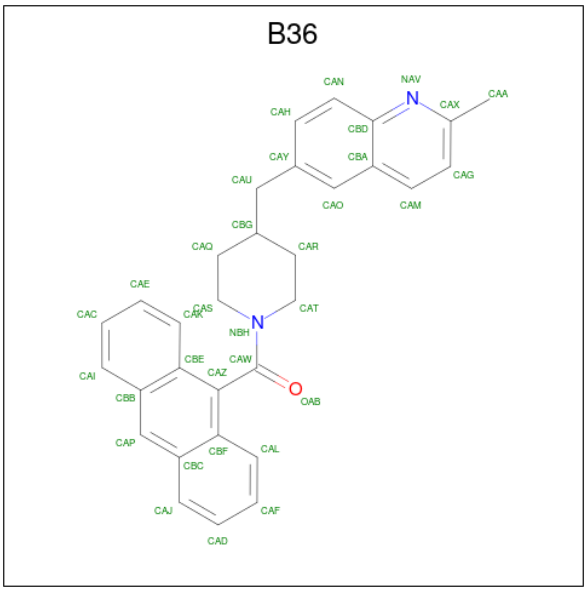
Chain	Residue	Modelled	Actual	Comment	Reference
C	1474	ALA	-	expression tag	UNP Q00955
C	1475	SER	-	expression tag	UNP Q00955
C	2234	LEU	-	expression tag	UNP Q00955
C	2235	GLU	-	expression tag	UNP Q00955
C	2236	HIS	-	expression tag	UNP Q00955
C	2237	HIS	-	expression tag	UNP Q00955
C	2238	HIS	-	expression tag	UNP Q00955
C	2239	HIS	-	expression tag	UNP Q00955
C	2240	HIS	-	expression tag	UNP Q00955
C	2241	HIS	-	expression tag	UNP Q00955

- Molecule 2 is 6-{[1-(anthracen-9-ylcarbonyl)piperidin-4-yl]methyl}-2-methylquinoline (three-letter code: B36) (formula: $C_{31}H_{28}N_2O$).

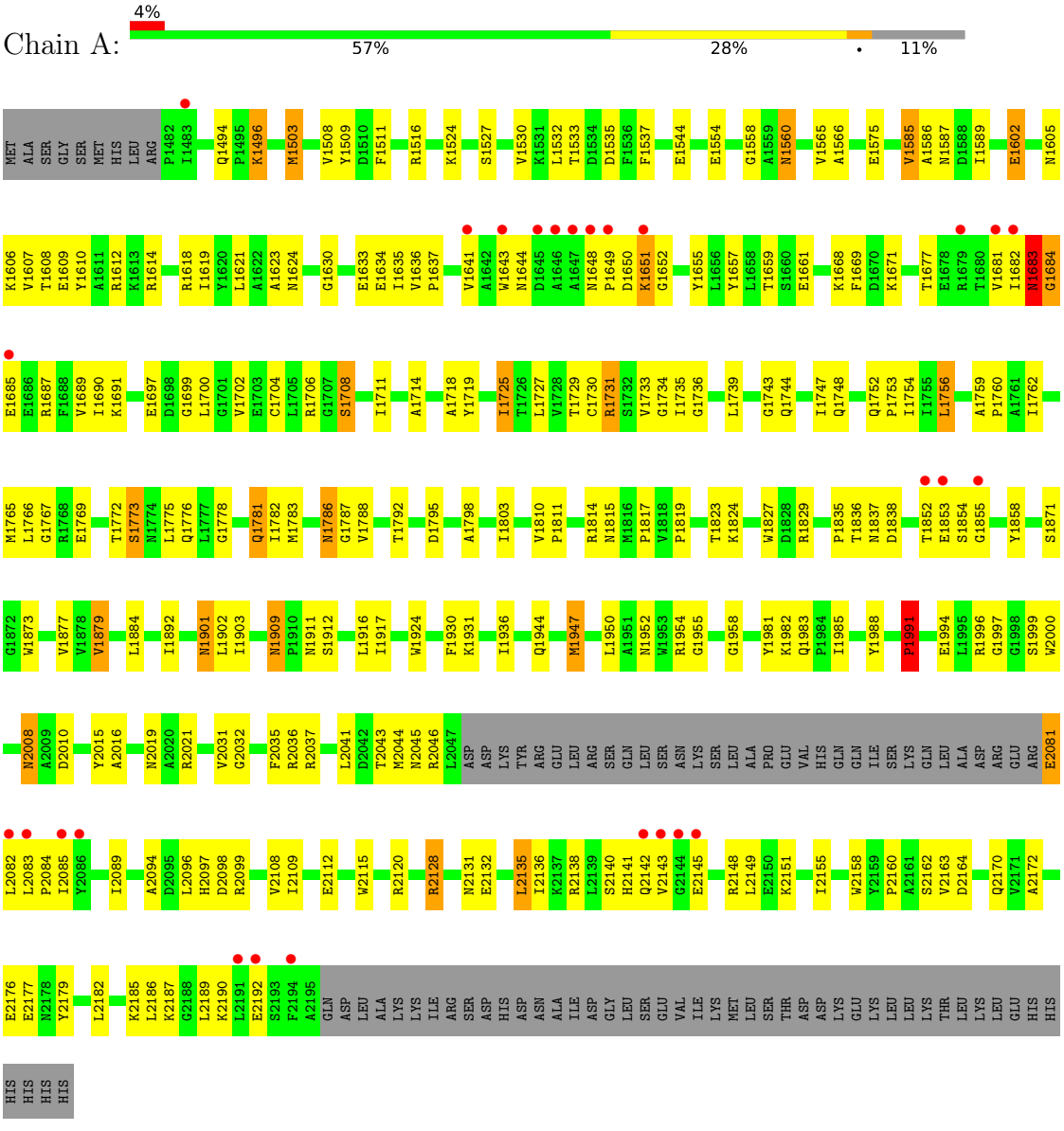


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	31	2	1		
2	B	1	Total	C	N	O	0	0
			34	31	2	1		
2	C	1	Total	C	N	O	0	0
			34	31	2	1		

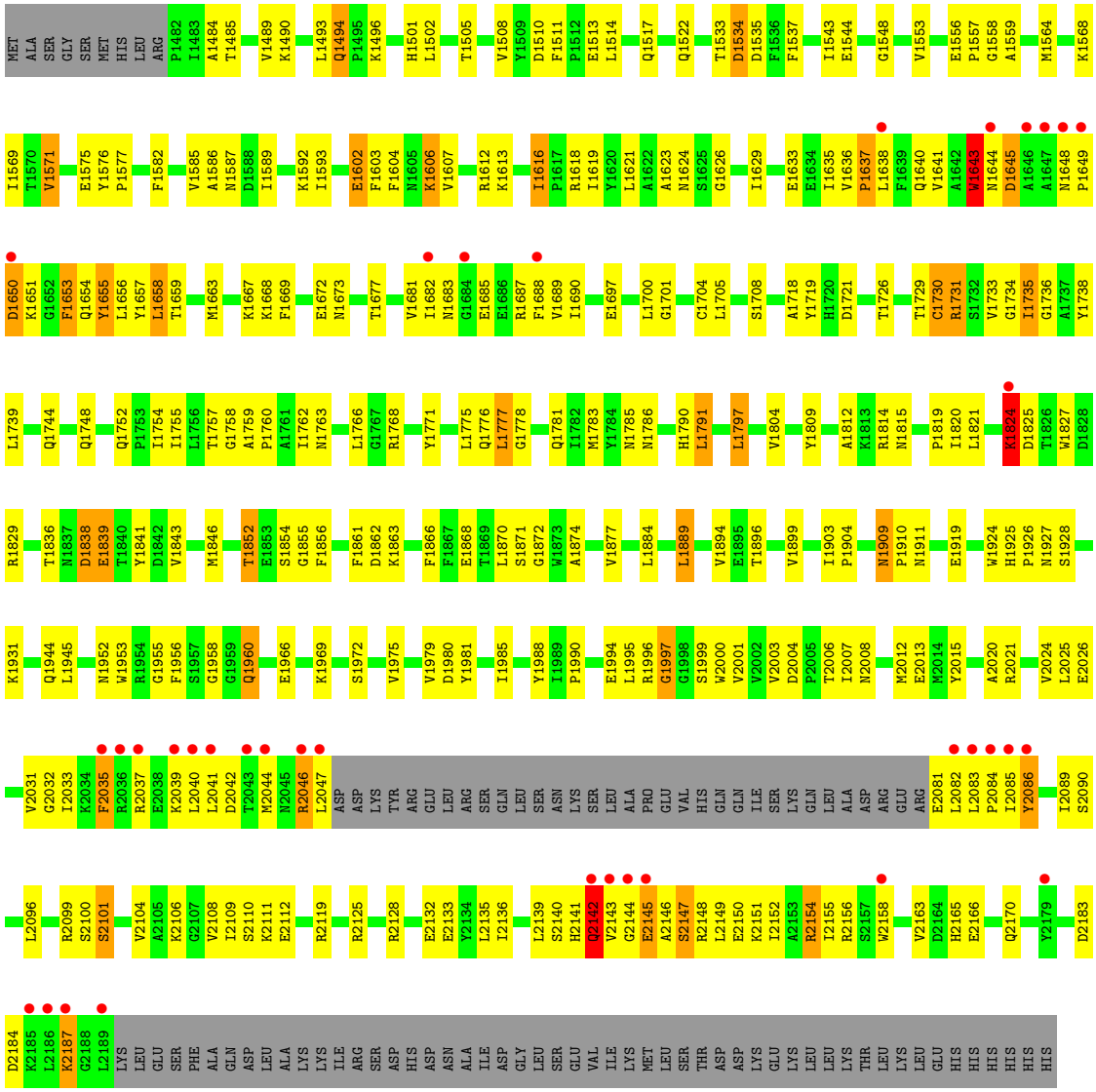
3 Residue-property plots (i)

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

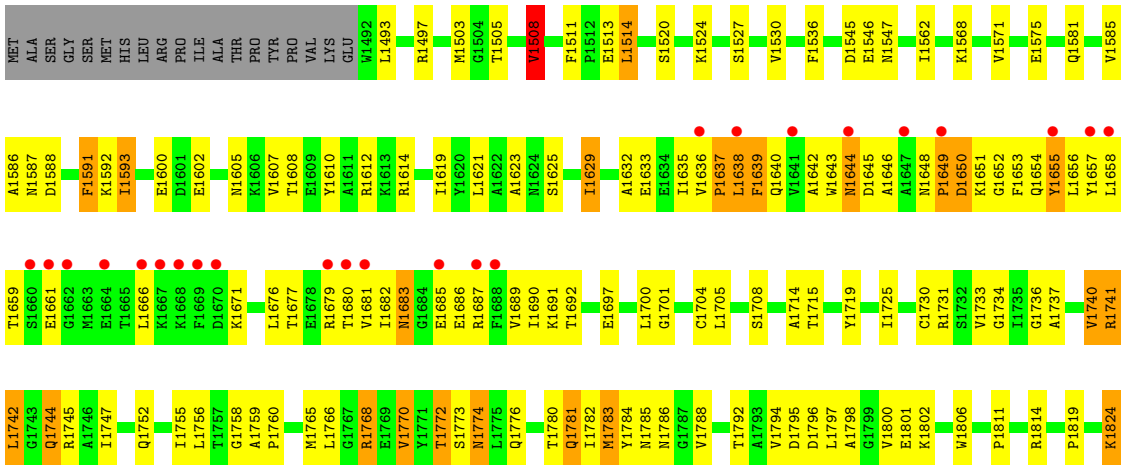


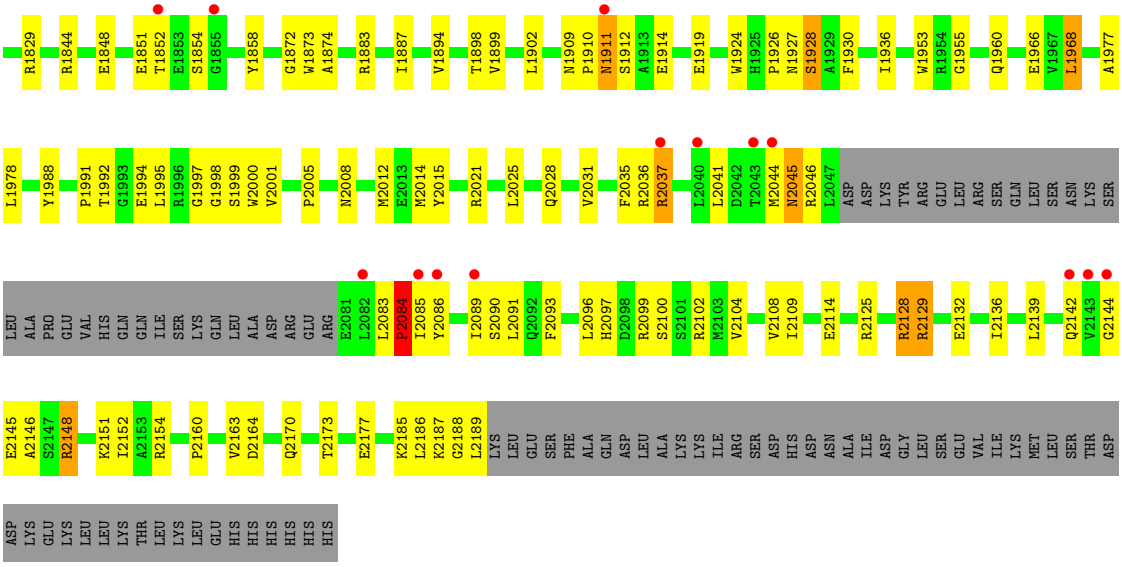
• Molecule 1: Acetyl-CoA carboxylase



• Molecule 1: Acetyl-CoA carboxylase

Chain C:




R1829 R1844 E1848 E1851 T1852 E1853 S1854 G1855 Y1858 G1872 W1873 A1874 R1883 I1887 V1894 T1898 V1899 L1902 N1909 P1910 N1911 S1912 A1913 E1914 E1919 W1924 H1925 P1926 N1927 S1928 A1929 F1930 I1936 W1953 R1954 G1955 Q1960 E1966 V1967 L1968 A1977
L1978 Y1988 P1991 T1992 G1993 E1994 L1995 R1996 G1997 G1998 S1999 W2000 V2001 P2005 N2008 M2012 E2013 M2014 Y2015 R2021 L2025 Q2028 V2031 F2035 R2036 R2037 L2040 L2041 D2042 T2043 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 S2090 L2091 Q2092 F2093 L2096 H2097 D2098 R2099 S2100 S2101 R2102 M2103 V2104 V2108 I2109 E2114 R2125 R2128 R2129 E2132 I2136 L2139 Q2142 V2143 G2144
E2145 A2146 S2147 R2148 K2151 I2152 A2153 R2154 P2160 V2163 D2164 Q2170 T2173 E2177 K2185 L2186 K2187 G2188 L2189 LYS 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 MET LEU SER THR ASP
ASP LYS GLU LYS LEU LEU LYS THR LEU LYS LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	246.74Å 122.86Å 145.88Å 90.00° 93.92° 90.00°	Depositor
Resolution (Å)	51.25 – 2.80 51.25 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (51.25-2.80) 99.3 (51.25-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.90 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.257 0.222 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.3	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	0.92	EDS
Total number of atoms	16200	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 2.87% 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: B36

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	0.38	0/5546	0.66	0/7514
1	B	0.36	0/5497	0.65	1/7449 (0.0%)
1	C	0.36	0/5415	0.64	0/7335
All	All	0.37	0/16458	0.65	1/22298 (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	1791	LEU	CA-CB-CG	5.60	128.17	115.30

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	5424	0	5365	211	0
1	B	5376	0	5316	222	0
1	C	5298	0	5234	220	0
2	A	34	0	28	1	0
2	B	34	0	28	2	0
2	C	34	0	28	1	0
All	All	16200	0	15999	628	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 20.

All (628) 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:HA	1:A:1496:LYS:HE3	1.39	0.99
1:A:2135:LEU:HB3	1:A:2155:ILE:HD13	1.43	0.99
1:A:1772:THR:H	1:A:1776:GLN:NE2	1.61	0.97
1:C:1773:SER:H	1:C:1776:GLN:HE21	1.04	0.97
1:C:1772:THR:H	1:C:1776:GLN:HE22	1.00	0.95
1:C:1638:LEU:H	1:C:1638:LEU:HD23	1.28	0.95
1:A:1772:THR:H	1:A:1776:GLN:HE22	1.07	0.94
1:A:1824:LYS:HZ3	1:A:1824:LYS:H	1.12	0.93
1:C:1781:GLN:H	1:C:1781:GLN:HE21	1.17	0.92
1:C:1759:ALA:H	1:C:1774:ASN:HD21	1.12	0.91
1:B:2154:ARG:NH1	1:B:2158:TRP:HE1	1.69	0.91
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.33	0.90
1:A:1683:ASN:ND2	1:A:1684:GLY:H	1.71	0.89
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.37	0.89
1:C:1781:GLN:H	1:C:1781:GLN:NE2	1.71	0.88
1:B:1815:ASN:H	1:B:1944:GLN:HE22	1.21	0.87
1:A:2135:LEU:HD21	1:A:2182:LEU:HD13	1.58	0.84
1:A:1494:GLN:CA	1:A:1496:LYS:HE3	2.06	0.84
1:A:1824:LYS:H	1:A:1824:LYS:NZ	1.77	0.83
1:A:1496:LYS:H	1:A:1496:LYS:HD3	1.43	0.83
1:C:1773:SER:H	1:C:1776:GLN:NE2	1.76	0.82
1:C:1629:ILE:HD13	1:C:1629:ILE:H	1.45	0.82
1:C:1642:ALA:HB1	1:C:1644:ASN:HD22	1.46	0.81
1:A:1852:THR:HG22	1:A:1854:SER:H	1.45	0.80
1:B:2083:LEU:HB3	1:B:2084:PRO:HD3	1.64	0.80
1:A:1657:TYR:CE2	1:A:1687:ARG:HD2	2.17	0.79
1:C:1772:THR:H	1:C:1776:GLN:NE2	1.80	0.79
1:B:1815:ASN:H	1:B:1944:GLN:NE2	1.81	0.78
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.30	0.78
1:B:2183:ASP:O	1:B:2187:LYS:HE3	1.84	0.78
1:B:2044:MET:SD	1:B:2082:LEU:HD21	2.24	0.77
1:C:1737:ALA:O	1:C:1740:VAL:HG13	1.85	0.77
1:B:1730:CYS:CA	1:B:1752:GLN:HE21	1.99	0.75
1:C:1642:ALA:HB1	1:C:1644:ASN:ND2	2.02	0.75
1:C:1772:THR:N	1:C:1776:GLN:HE22	1.79	0.75
1:C:1682:ILE:HG21	1:C:1687:ARG:CZ	2.17	0.75
1:C:2160:PRO:HG2	1:C:2163:VAL:HG23	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1729:THR:O	1:B:1730:CYS:HB3	1.85	0.75
1:C:1658:LEU:HG	1:C:1690:ILE:HD11	1.67	0.75
1:B:1658:LEU:HD13	1:B:1690:ILE:HD11	1.68	0.74
1:A:1524:LYS:HB2	1:A:1524:LYS:NZ	2.02	0.74
1:B:1852:THR:HG22	1:B:1855:GLY:O	1.88	0.74
1:B:1735:ILE:HD13	1:B:1735:ILE:O	1.88	0.74
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.87	0.73
1:C:2100:SER:O	1:C:2104:VAL:HG23	1.88	0.72
1:B:2007:ILE:HB	1:B:2012:MET:HE3	1.71	0.72
1:C:2129:ARG:NH1	1:C:2129:ARG:HB3	2.05	0.72
1:B:2154:ARG:HH11	1:B:2158:TRP:HE1	1.36	0.72
1:A:1836:THR:HG22	1:A:1838:ASP:H	1.53	0.72
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.38	0.72
1:C:1773:SER:N	1:C:1776:GLN:HE21	1.85	0.72
1:B:1667:LYS:HG2	1:B:1672:GLU:HG2	1.72	0.71
1:B:1815:ASN:N	1:B:1944:GLN:HE22	1.87	0.71
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.38	0.71
1:B:1824:LYS:HG3	1:B:1825:ASP:H	1.54	0.71
1:C:2185:LYS:O	1:C:2189:LEU:HD13	1.91	0.71
1:C:2045:ASN:C	1:C:2045:ASN:HD22	1.94	0.71
1:B:1663:MET:HG3	1:B:1688:PHE:CD2	2.27	0.70
1:C:1824:LYS:HZ3	1:C:1824:LYS:HB2	1.55	0.70
1:A:2041:LEU:O	1:A:2044:MET:HB2	1.91	0.70
1:C:1493:LEU:HD12	1:C:1497:ARG:HH21	1.55	0.70
1:B:2008:ASN:HB3	1:B:2012:MET:HE2	1.72	0.69
1:C:1911:ASN:HD22	1:C:1911:ASN:N	1.91	0.69
1:A:1533:THR:HB	1:A:1535:ASP:OD1	1.92	0.69
1:A:1817:PRO:HD3	1:B:1484:ALA:HB1	1.73	0.69
1:A:2189:LEU:O	1:A:2192:GLU:HB2	1.92	0.69
1:C:1824:LYS:HB2	1:C:1824:LYS:NZ	2.08	0.69
1:B:1730:CYS:HA	1:B:1752:GLN:NE2	2.08	0.68
1:B:1612:ARG:HD3	1:B:1718:ALA:HA	1.75	0.68
1:C:1796:ASP:O	1:C:1800:VAL:HG23	1.93	0.68
1:C:2104:VAL:HG22	1:C:2109:ILE:HD11	1.74	0.68
1:C:1638:LEU:HD23	1:C:1638:LEU:N	2.08	0.67
1:C:1824:LYS:H	1:C:1824:LYS:HZ2	1.42	0.67
1:B:2110:SER:O	1:B:2111:LYS:HG3	1.93	0.67
1:A:1762:ILE:O	1:A:1766:LEU:HD13	1.95	0.67
1:C:1797:LEU:O	1:C:1801:GLU:HG3	1.94	0.67
1:B:1824:LYS:HG3	1:B:1825:ASP:N	2.08	0.67
1:B:2163:VAL:HA	1:B:2170:GLN:NE2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1683:ASN:HD22	1:A:1684:GLY:H	1.42	0.67
1:A:2164:ASP:H	1:A:2170:GLN:HE22	1.41	0.66
1:A:1759:ALA:HB3	1:A:1760:PRO:HD3	1.77	0.66
1:B:1643:TRP:HA	1:B:1653:PHE:HA	1.77	0.66
1:B:1775:LEU:O	1:B:1781:GLN:NE2	2.29	0.66
1:B:2046:ARG:HG2	1:C:1643:TRP:HH2	1.60	0.66
1:A:2143:VAL:HG22	1:A:2145:GLU:H	1.60	0.66
1:B:2146:ALA:O	1:B:2151:LYS:HE2	1.95	0.65
1:A:2041:LEU:HA	1:A:2044:MET:CG	2.26	0.65
1:A:1683:ASN:HD22	1:A:1684:GLY:N	1.94	0.65
1:A:1560:ASN:H	1:A:1560:ASN:HD22	1.44	0.65
1:A:1681:VAL:HG23	1:A:1685:GLU:O	1.96	0.65
1:C:1629:ILE:H	1:C:1629:ILE:CD1	2.08	0.65
1:C:1759:ALA:N	1:C:1774:ASN:HD21	1.89	0.65
1:B:2037:ARG:O	1:B:2041:LEU:HD13	1.97	0.64
1:B:1730:CYS:H	1:B:1752:GLN:HG3	1.62	0.64
1:A:1677:THR:HG22	1:A:1690:ILE:HA	1.79	0.64
1:A:1683:ASN:ND2	1:A:1684:GLY:N	2.45	0.64
1:B:1641:VAL:HG21	1:C:2089:ILE:HD13	1.80	0.64
1:C:1527:SER:O	1:C:1530:VAL:HG22	1.97	0.64
1:C:2148:ARG:HG3	1:C:2148:ARG:HH11	1.62	0.64
1:A:1954:ARG:O	1:A:1996:ARG:HB2	1.97	0.64
1:A:1624:ASN:ND2	1:A:1733:VAL:H	1.95	0.63
1:B:2156:ARG:HG3	1:B:2156:ARG:HH11	1.63	0.63
1:A:1643:TRP:CZ3	1:A:1649:PRO:HB3	2.32	0.63
1:A:1824:LYS:HZ3	1:A:1824:LYS:N	1.91	0.63
1:A:2082:LEU:HD23	1:A:2082:LEU:H	1.62	0.63
1:B:2040:LEU:HD11	1:B:2086:TYR:O	1.98	0.62
1:A:1527:SER:O	1:A:1530:VAL:HG22	1.99	0.62
1:A:1633:GLU:O	1:A:1636:VAL:HG12	1.97	0.62
1:B:1677:THR:HG22	1:B:1690:ILE:HA	1.81	0.62
1:A:1903:ILE:N	1:A:1903:ILE:HD12	2.14	0.62
1:C:2108:VAL:HG23	1:C:2109:ILE:HG23	1.81	0.62
1:C:2041:LEU:O	1:C:2044:MET:HB2	1.99	0.62
1:B:1543:ILE:HD11	1:B:1553:VAL:HG11	1.79	0.62
1:A:1852:THR:HB	1:A:1855:GLY:O	1.99	0.62
1:C:1654:GLN:O	1:C:1655:TYR:HB3	2.00	0.62
1:C:2041:LEU:HA	1:C:2044:MET:HG3	1.81	0.62
1:C:2129:ARG:HB3	1:C:2129:ARG:CZ	2.28	0.62
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.64	0.62
1:B:1969:LYS:HG2	1:C:1741:ARG:CZ	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1636:VAL:HB	1:C:1637:PRO:HD3	1.82	0.61
1:C:1644:ASN:HD21	1:C:1687:ARG:NH1	1.97	0.61
1:B:1786:ASN:OD1	1:C:1966:GLU:HG3	1.99	0.61
1:B:2085:ILE:HG13	1:C:1650:ASP:HA	1.82	0.61
1:B:2135:LEU:HB3	1:B:2155:ILE:HD13	1.83	0.61
1:B:1668:LYS:HD2	1:B:1669:PHE:CE2	2.36	0.61
1:B:1548:GLY:O	1:B:1606:LYS:HE2	2.00	0.61
1:C:1648:ASN:ND2	1:C:1651:LYS:HE2	2.16	0.61
1:A:1634:GLU:O	1:A:1634:GLU:HG2	2.01	0.61
1:A:1677:THR:CG2	1:A:1690:ILE:HG22	2.31	0.61
1:C:1681:VAL:HG22	1:C:1686:GLU:HA	1.82	0.61
1:A:1511:PHE:HZ	1:A:1729:THR:HG21	1.65	0.60
1:A:1677:THR:HG22	1:A:1690:ILE:HG22	1.83	0.60
1:C:1783:MET:HA	1:C:1786:ASN:HB2	1.84	0.60
1:A:1783:MET:HA	1:A:1786:ASN:HB2	1.81	0.60
1:C:1638:LEU:H	1:C:1638:LEU:CD2	2.05	0.60
1:A:1944:GLN:HA	1:A:1983:GLN:NE2	2.17	0.60
1:C:1625:SER:HB3	1:C:1731:ARG:NH2	2.17	0.60
1:C:2148:ARG:HH12	1:C:2152:ILE:HD13	1.66	0.60
1:B:1657:TYR:CE2	1:B:1687:ARG:HG2	2.37	0.60
1:B:1966:GLU:HG2	1:C:1786:ASN:OD1	2.02	0.60
1:A:2143:VAL:HB	1:A:2192:GLU:OE1	2.02	0.59
1:A:1823:THR:HB	1:A:1824:LYS:HZ3	1.66	0.59
1:A:1852:THR:HG22	1:A:1853:GLU:N	2.16	0.59
1:C:2045:ASN:C	1:C:2045:ASN:ND2	2.56	0.59
1:A:2170:GLN:HG3	1:B:1517:GLN:NE2	2.17	0.59
1:C:1586:ALA:HB2	1:C:1621:LEU:HB2	1.85	0.59
1:C:1794:VAL:HG23	1:C:1795:ASP:OD1	2.03	0.59
1:A:1955:GLY:HA2	1:A:1999:SER:OG	2.02	0.58
1:B:2139:LEU:HD23	1:B:2151:LYS:HG2	1.85	0.58
1:B:1648:ASN:N	1:B:1649:PRO:HD3	2.18	0.58
1:B:2140:SER:O	1:B:2144:GLY:HA3	2.03	0.58
1:B:1790:HIS:HA	1:B:1870:LEU:HD23	1.85	0.58
1:A:1586:ALA:HB2	1:A:1621:LEU:HB2	1.86	0.58
1:B:2031:VAL:HG13	1:B:2035:PHE:HB3	1.85	0.57
1:B:1899:VAL:HB	1:B:1919:GLU:HB2	1.86	0.57
1:B:2000:TRP:CD1	1:C:1705:LEU:HB3	2.38	0.57
1:A:1524:LYS:HB2	1:A:1524:LYS:HZ2	1.69	0.57
1:B:2041:LEU:HA	1:B:2044:MET:HB2	1.86	0.57
1:C:1715:THR:HG22	1:C:1742:LEU:HB3	1.87	0.57
1:C:2041:LEU:HA	1:C:2044:MET:CG	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1496:LYS:HD3	1:A:1496:LYS:N	2.15	0.57
1:A:1936:ILE:HG12	1:A:1947:MET:CE	2.34	0.57
1:A:1991:PRO:O	1:A:2019:ASN:O	2.22	0.57
1:B:1735:ILE:HD13	1:B:1739:LEU:HG	1.87	0.57
1:B:1643:TRP:CZ3	1:B:1649:PRO:HB3	2.40	0.57
1:A:1877:VAL:HG23	1:A:1931:LYS:HD3	1.87	0.57
1:A:1901:ASN:HB3	1:A:1917:ILE:HB	1.87	0.56
1:C:1637:PRO:HB2	1:C:1638:LEU:HD23	1.85	0.56
1:A:1909:ASN:ND2	1:A:1911:ASN:H	2.03	0.56
1:C:2031:VAL:HG21	1:C:2091:LEU:HD23	1.87	0.56
1:C:2188:GLY:C	1:C:2189:LEU:HD12	2.25	0.56
1:A:1648:ASN:HB2	1:A:1651:LYS:HG2	1.85	0.56
1:B:2154:ARG:NH1	1:B:2158:TRP:NE1	2.47	0.56
1:C:1612:ARG:O	1:C:1814:ARG:NH2	2.38	0.56
1:A:2190:LYS:C	1:A:2192:GLU:H	2.08	0.56
1:C:1909:ASN:HD22	1:C:1912:SER:HB2	1.69	0.56
1:C:1629:ILE:HD13	1:C:1629:ILE:N	2.19	0.56
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	1.88	0.56
1:C:1781:GLN:HE21	1:C:1781:GLN:N	1.95	0.56
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.36	0.56
1:C:1607:VAL:O	1:C:1610:TYR:HB3	2.06	0.56
1:B:1738:TYR:CE1	1:C:1968:LEU:HD12	2.41	0.55
1:B:1783:MET:HA	1:B:1786:ASN:HB2	1.88	0.55
1:C:1844:ARG:HH11	1:C:1844:ARG:HG3	1.72	0.55
1:B:2184:ASP:HA	1:B:2187:LYS:HB2	1.88	0.55
1:A:2158:TRP:CE2	1:A:2185:LYS:HD3	2.42	0.55
1:A:1772:THR:N	1:A:1776:GLN:NE2	2.44	0.55
1:C:1782:ILE:O	1:C:1786:ASN:HB2	2.06	0.55
1:C:1911:ASN:N	1:C:1911:ASN:ND2	2.55	0.55
1:B:1866:PHE:CE1	1:B:1868:GLU:HB2	2.42	0.55
1:C:1568:LYS:HE2	1:C:1581:GLN:NE2	2.21	0.55
1:A:1725:ILE:HD12	1:A:1803:ILE:HG12	1.88	0.55
1:B:1814:ARG:O	1:B:1815:ASN:HB2	2.06	0.55
1:A:1994:GLU:HA	1:A:2021:ARG:O	2.07	0.54
1:A:2140:SER:OG	1:A:2151:LYS:HE3	2.07	0.54
1:A:2179:TYR:HD1	1:B:1489:VAL:HA	1.73	0.54
1:B:1644:ASN:O	1:B:1645:ASP:HB2	2.07	0.54
1:A:2008:ASN:C	1:A:2008:ASN:HD22	2.10	0.54
1:A:2041:LEU:HA	1:A:2044:MET:HG2	1.89	0.54
1:B:2132:GLU:O	1:B:2136:ILE:HG13	2.07	0.54
1:C:1508:VAL:HG21	1:C:1588:ASP:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2148:ARG:NH1	1:C:2152:ILE:HD13	2.22	0.54
1:A:1733:VAL:HG12	1:A:1734:GLY:N	2.21	0.54
1:B:1633:GLU:HA	1:B:1636:VAL:HG23	1.88	0.54
1:C:1655:TYR:O	1:C:1656:LEU:HD12	2.07	0.54
1:C:1747:ILE:HD13	1:C:1802:LYS:HB2	1.88	0.54
1:A:1565:VAL:HG12	1:A:1566:ALA:N	2.21	0.54
1:A:1614:ARG:HG3	1:A:1614:ARG:HH11	1.71	0.54
1:A:1815:ASN:ND2	1:A:1944:GLN:HE22	2.05	0.54
1:B:1681:VAL:HG13	1:B:1685:GLU:O	2.06	0.54
1:C:1643:TRP:O	1:C:1645:ASP:N	2.40	0.54
1:A:2132:GLU:O	1:A:2136:ILE:HG13	2.08	0.54
1:A:2164:ASP:H	1:A:2170:GLN:NE2	2.05	0.54
1:C:1783:MET:SD	1:C:1786:ASN:ND2	2.80	0.54
1:A:1708:SER:OG	1:A:1735:ILE:HB	2.08	0.54
1:C:1530:VAL:O	1:C:1530:VAL:HG23	2.08	0.54
1:C:1851:GLU:OE1	1:C:1851:GLU:HA	2.08	0.54
1:A:2083:LEU:HB2	1:A:2084:PRO:HD3	1.90	0.54
1:C:1585:VAL:HG22	1:C:1607:VAL:HG11	1.90	0.54
1:B:2044:MET:HA	1:B:2086:TYR:CE2	2.43	0.53
1:A:1605:ASN:HD22	1:A:1714:ALA:HB2	1.73	0.53
1:B:2008:ASN:HB3	1:B:2012:MET:CE	2.38	0.53
1:A:1648:ASN:O	1:A:1651:LYS:HG2	2.09	0.53
1:B:1544:GLU:OE1	1:B:1602:GLU:OE1	2.25	0.53
1:A:1544:GLU:OE1	1:A:1602:GLU:OE2	2.27	0.53
1:A:1560:ASN:HD22	1:A:1560:ASN:N	2.06	0.53
1:B:1956:PHE:HB2	1:C:1756:LEU:HD13	1.91	0.53
1:B:1755:ILE:HD12	1:B:1758:GLY:HA2	1.90	0.53
1:C:1736:GLY:O	1:C:1740:VAL:HG12	2.09	0.53
1:B:1877:VAL:HG13	1:B:1931:LYS:HD3	1.90	0.52
1:B:2089:ILE:HD13	1:C:1653:PHE:CE2	2.43	0.52
1:C:2173:THR:O	1:C:2177:GLU:HB2	2.09	0.52
1:A:1753:PRO:HB3	1:A:1775:LEU:HD23	1.91	0.52
1:A:1766:LEU:N	1:A:1766:LEU:HD12	2.24	0.52
1:B:2024:VAL:HG12	1:B:2025:LEU:HD13	1.91	0.52
1:B:1762:ILE:HD12	1:B:1777:LEU:HD21	1.91	0.52
1:B:2031:VAL:O	1:B:2033:ILE:N	2.42	0.52
1:C:1719:TYR:CE2	1:C:1744:GLN:HG3	2.44	0.52
1:C:1902:LEU:HD11	1:C:1914:GLU:OE2	2.09	0.52
1:A:1682:ILE:C	1:A:1683:ASN:HD22	2.12	0.52
1:A:2108:VAL:HG23	1:A:2109:ILE:HG23	1.90	0.52
1:B:1586:ALA:HB2	1:B:1621:LEU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1679:ARG:NH2	1:C:1686:GLU:HG2	2.24	0.52
1:C:2083:LEU:HB2	1:C:2084:PRO:HD3	1.89	0.52
1:A:2187:LYS:O	1:A:2190:LYS:HG2	2.10	0.52
1:B:1790:HIS:O	1:B:1791:LEU:HD13	2.09	0.52
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.58	0.52
1:B:1730:CYS:H	1:B:1752:GLN:CG	2.23	0.52
1:B:1809:TYR:O	1:B:1945:LEU:HD21	2.10	0.52
1:B:2046:ARG:HG2	1:C:1643:TRP:CH2	2.44	0.52
1:B:1624:ASN:ND2	1:B:1733:VAL:H	2.07	0.52
1:B:1852:THR:HG23	1:B:1854:SER:H	1.75	0.52
1:C:1829:ARG:CZ	1:C:1858:TYR:HB3	2.40	0.52
1:C:2128:ARG:HE	1:C:2132:GLU:CD	2.13	0.52
1:A:2128:ARG:HE	1:A:2132:GLU:CD	2.12	0.52
1:C:1657:TYR:CD2	1:C:1687:ARG:HG3	2.44	0.52
1:A:1511:PHE:CZ	1:A:1729:THR:HG21	2.45	0.51
1:A:1648:ASN:HB2	1:A:1651:LYS:CG	2.40	0.51
1:B:1505:THR:HB	1:B:1730:CYS:HB2	1.91	0.51
1:A:1634:GLU:OE2	1:A:1634:GLU:N	2.40	0.51
1:C:2142:GLN:HG3	1:C:2142:GLN:O	2.11	0.51
1:B:2046:ARG:HB3	1:B:2086:TYR:OH	2.11	0.51
1:A:1766:LEU:N	1:A:1766:LEU:CD1	2.73	0.51
1:B:1958:GLY:H	2:B:1:B36:CAM	2.23	0.51
1:C:1844:ARG:O	1:C:1848:GLU:HG2	2.10	0.51
1:C:2090:SER:O	1:C:2093:PHE:HB3	2.11	0.51
1:B:1576:TYR:N	1:B:1577:PRO:HD3	2.26	0.51
1:C:1681:VAL:HG13	1:C:1685:GLU:O	2.10	0.51
1:A:1981:TYR:CG	1:A:1985:ILE:HD11	2.45	0.51
1:B:1708:SER:CB	1:B:1735:ILE:HG13	2.41	0.51
1:B:1975:VAL:O	1:B:1979:VAL:HG23	2.11	0.51
1:B:1981:TYR:CG	1:B:1985:ILE:HD11	2.46	0.51
1:C:1575:GLU:CD	1:C:1575:GLU:H	2.15	0.51
1:A:1605:ASN:O	1:A:1609:GLU:HG3	2.10	0.51
1:C:1883:ARG:HA	1:C:1887:ILE:O	2.10	0.51
1:C:1955:GLY:HA2	1:C:1999:SER:HB3	1.93	0.51
1:A:1852:THR:CG2	1:A:1853:GLU:N	2.74	0.51
1:C:1682:ILE:HG23	1:C:1682:ILE:O	2.11	0.51
1:A:1981:TYR:CD2	1:A:1985:ILE:HD11	2.45	0.50
1:B:1757:THR:HG22	1:B:1762:ILE:HG13	1.93	0.50
1:A:1503:MET:CE	1:A:1589:ILE:HG13	2.40	0.50
1:B:1650:ASP:HA	1:C:2085:ILE:HB	1.94	0.50
1:C:1998:GLY:O	1:C:2001:VAL:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2187:LYS:C	1:C:2189:LEU:H	2.14	0.50
1:A:1786:ASN:HB3	1:A:1788:VAL:HG23	1.93	0.50
1:C:1680:THR:O	1:C:1687:ARG:HB3	2.11	0.50
1:A:1608:THR:O	1:A:1612:ARG:HG2	2.12	0.50
1:A:2085:ILE:O	1:A:2089:ILE:HG13	2.12	0.50
1:B:1556:GLU:HG3	1:B:1559:ALA:HB2	1.94	0.50
1:B:1729:THR:O	1:B:1730:CYS:CB	2.56	0.50
1:B:1776:GLN:O	1:C:1960:GLN:HG3	2.12	0.50
1:B:2148:ARG:O	1:B:2152:ILE:HG13	2.12	0.50
1:C:1772:THR:N	1:C:1776:GLN:NE2	2.49	0.50
1:C:2146:ALA:O	1:C:2151:LYS:HE3	2.12	0.50
1:B:1582:PHE:HA	1:B:1616:ILE:HG23	1.94	0.50
1:B:1909:ASN:C	1:B:1909:ASN:HD22	2.14	0.50
1:A:2041:LEU:HA	1:A:2044:MET:HG3	1.93	0.49
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.59	0.49
1:C:2096:LEU:HD23	1:C:2099:ARG:NH2	2.27	0.49
1:A:1909:ASN:ND2	1:A:1909:ASN:C	2.66	0.49
1:C:1591:PHE:C	1:C:1591:PHE:CD2	2.86	0.49
1:C:1733:VAL:HG12	1:C:1734:GLY:N	2.25	0.49
1:A:1711:ILE:HD12	1:A:1739:LEU:HD11	1.94	0.49
1:C:2008:ASN:HB3	1:C:2012:MET:HG3	1.93	0.49
1:A:1612:ARG:CD	1:A:1718:ALA:HA	2.42	0.49
1:A:1636:VAL:N	1:A:1637:PRO:CD	2.75	0.49
1:A:1814:ARG:O	1:A:1815:ASN:HB2	2.12	0.49
1:B:1861:PHE:CE2	1:B:1889:LEU:HD21	2.48	0.49
1:B:2108:VAL:HG23	1:B:2109:ILE:HG23	1.94	0.49
1:A:1636:VAL:N	1:A:1637:PRO:HD2	2.27	0.49
1:B:1785:ASN:HA	1:B:1872:GLY:O	2.12	0.49
1:A:2149:LEU:HD12	1:A:2149:LEU:O	2.13	0.49
1:B:1569:ILE:HG22	1:B:1571:VAL:HG22	1.94	0.49
1:B:1909:ASN:HD21	1:B:1911:ASN:CG	2.16	0.49
1:B:2082:LEU:HD23	1:B:2082:LEU:H	1.76	0.49
1:C:1852:THR:HG22	1:C:1854:SER:H	1.78	0.49
1:A:1496:LYS:HZ3	1:A:1558:GLY:HA3	1.78	0.49
1:B:1697:GLU:O	1:B:1700:LEU:HD13	2.12	0.49
1:C:2136:ILE:HD11	1:C:2152:ILE:CG2	2.43	0.49
1:A:2031:VAL:HG23	1:A:2032:GLY:N	2.28	0.49
1:A:2160:PRO:HD2	1:A:2163:VAL:HG21	1.94	0.49
1:B:2148:ARG:HG3	1:B:2148:ARG:HH11	1.78	0.49
1:C:2044:MET:C	1:C:2046:ARG:H	2.16	0.49
1:B:1543:ILE:CD1	1:B:1553:VAL:HG11	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1589:ILE:HG13	1:B:1589:ILE:O	2.13	0.48
1:B:2096:LEU:HD23	1:B:2099:ARG:NH2	2.27	0.48
1:C:1505:THR:HB	1:C:1730:CYS:HB2	1.94	0.48
1:B:1705:LEU:HB3	1:C:2000:TRP:CD1	2.47	0.48
1:B:2110:SER:O	1:B:2111:LYS:CG	2.61	0.48
1:B:2148:ARG:HG3	1:B:2148:ARG:NH1	2.28	0.48
1:C:1759:ALA:N	1:C:1760:PRO:HD2	2.28	0.48
1:A:1958:GLY:H	2:A:1:B36:CAM	2.27	0.48
1:A:1815:ASN:HD22	1:A:1944:GLN:HE22	1.61	0.48
1:B:2152:ILE:O	1:B:2156:ARG:HG2	2.13	0.48
1:C:1644:ASN:HD21	1:C:1687:ARG:HH12	1.60	0.48
1:B:1576:TYR:CE2	1:B:1812:ALA:HB2	2.49	0.48
1:B:1644:ASN:HD21	1:B:1654:GLN:HE21	1.60	0.48
1:C:1619:ILE:HD13	1:C:1619:ILE:N	2.29	0.48
1:C:2036:ARG:HB3	1:C:2036:ARG:NH1	2.28	0.48
1:B:1576:TYR:CZ	1:B:1812:ALA:HB2	2.49	0.48
1:B:1733:VAL:HG12	1:B:1734:GLY:N	2.28	0.48
1:B:1827:TRP:HA	1:B:2119:ARG:NH1	2.29	0.48
1:C:1677:THR:HA	1:C:1689:VAL:O	2.13	0.48
1:C:1786:ASN:HB3	1:C:1788:VAL:H	1.79	0.48
1:A:2043:THR:C	1:A:2045:ASN:H	2.15	0.48
1:B:1754:ILE:O	1:B:1778:GLY:HA3	2.13	0.48
1:B:2104:VAL:HG21	1:B:2112:GLU:HG2	1.96	0.48
1:A:1524:LYS:HB2	1:A:1524:LYS:HZ3	1.79	0.48
1:B:1653:PHE:CD1	1:B:1653:PHE:N	2.82	0.48
1:C:1697:GLU:O	1:C:1700:LEU:HD13	2.14	0.48
1:A:1795:ASP:O	1:A:1798:ALA:HB3	2.14	0.47
1:A:1892:ILE:HD12	1:A:1947:MET:HE1	1.95	0.47
1:B:1768:ARG:CB	1:B:1768:ARG:HH11	2.26	0.47
1:C:2045:ASN:ND2	1:C:2045:ASN:O	2.47	0.47
1:A:1773:SER:H	1:A:1776:GLN:HE21	1.63	0.47
1:C:1586:ALA:CB	1:C:1621:LEU:HB2	2.44	0.47
1:B:2147:SER:HB3	1:B:2150:GLU:OE2	2.14	0.47
1:C:1730:CYS:HA	1:C:1752:GLN:OE1	2.14	0.47
1:A:1936:ILE:HG12	1:A:1947:MET:HE1	1.96	0.47
1:B:1636:VAL:N	1:B:1637:PRO:HD2	2.29	0.47
1:C:1619:ILE:HD12	1:C:1725:ILE:HG22	1.96	0.47
1:C:2125:ARG:O	1:C:2129:ARG:HG2	2.14	0.47
1:A:1575:GLU:HB3	1:A:1819:PRO:HB2	1.96	0.47
1:A:1682:ILE:O	1:A:1683:ASN:C	2.53	0.47
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.63	0.47
1:B:1836:THR:HG22	1:B:1838:ASP:OD2	2.14	0.47
1:B:1996:ARG:NE	1:B:2026:GLU:HG2	2.30	0.47
1:A:1668:LYS:O	1:A:1668:LYS:HG2	2.14	0.47
1:A:2045:ASN:O	1:A:2046:ARG:HD2	2.15	0.47
1:C:1909:ASN:ND2	1:C:1912:SER:HB2	2.30	0.47
1:A:1659:THR:OG1	1:A:1661:GLU:HB3	2.14	0.47
1:B:2156:ARG:HG3	1:B:2156:ARG:NH1	2.28	0.47
1:C:1755:ILE:HD12	1:C:1758:GLY:HA2	1.95	0.47
1:C:1785:ASN:HA	1:C:1872:GLY:O	2.15	0.47
1:A:1605:ASN:ND2	1:A:1714:ALA:HB2	2.29	0.47
1:A:1748:GLN:O	1:A:1792:THR:HA	2.15	0.47
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.61	0.47
1:C:1493:LEU:CD1	1:C:1497:ARG:HH21	2.25	0.47
1:C:2005:PRO:HG3	1:C:2014:MET:HB2	1.96	0.47
1:A:2096:LEU:HA	1:A:2099:ARG:NH1	2.30	0.46
1:B:2096:LEU:HD23	1:B:2099:ARG:CZ	2.46	0.46
1:C:2085:ILE:O	1:C:2089:ILE:HG13	2.15	0.46
1:A:2140:SER:C	1:A:2142:GLN:H	2.18	0.46
1:C:2148:ARG:HH11	1:C:2148:ARG:CG	2.27	0.46
1:B:1603:PHE:O	1:B:1607:VAL:HG23	2.15	0.46
1:C:1666:LEU:HD22	1:C:1671:LYS:O	2.15	0.46
1:C:1766:LEU:O	1:C:1768:ARG:N	2.46	0.46
1:B:1721:ASP:OD2	1:B:1814:ARG:NH1	2.48	0.46
1:C:2139:LEU:HD21	1:C:2154:ARG:HD2	1.97	0.46
1:A:1619:ILE:HD12	1:A:1619:ILE:N	2.29	0.46
1:A:1754:ILE:O	1:A:1778:GLY:HA3	2.14	0.46
1:B:1592:LYS:O	1:B:1593:ILE:HG12	2.16	0.46
1:B:1838:ASP:O	1:B:1839:GLU:HB2	2.15	0.46
1:B:1909:ASN:ND2	1:B:1911:ASN:H	2.13	0.46
1:C:1766:LEU:HD13	1:C:1770:VAL:HG11	1.97	0.46
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.13	0.46
1:C:1605:ASN:HD22	1:C:1714:ALA:HB2	1.81	0.46
1:B:2046:ARG:NH1	1:C:1639:PHE:O	2.48	0.46
1:C:1654:GLN:O	1:C:1655:TYR:CB	2.63	0.46
1:A:1619:ILE:HG13	1:A:1725:ILE:CG2	2.46	0.46
1:A:1982:LYS:HB2	1:A:1983:GLN:OE1	2.16	0.46
1:C:1643:TRP:O	1:C:1644:ASN:C	2.55	0.46
1:A:2008:ASN:C	1:A:2008:ASN:ND2	2.69	0.46
1:A:2138:ARG:HB3	1:A:2186:LEU:HD13	1.97	0.46
1:B:1649:PRO:C	1:B:1651:LYS:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1909:ASN:C	1:B:1909:ASN:ND2	2.68	0.46
1:A:1823:THR:HB	1:A:1824:LYS:NZ	2.31	0.46
1:B:1629:ILE:HD13	1:C:2025:LEU:HD11	1.98	0.46
1:B:1682:ILE:CG1	1:B:1687:ARG:HD2	2.46	0.46
1:B:1874:ALA:HB2	1:B:1927:ASN:HB2	1.98	0.46
1:A:1619:ILE:HG13	1:A:1725:ILE:HG22	1.97	0.45
1:A:2135:LEU:HD23	1:A:2155:ILE:CG2	2.46	0.45
1:B:1649:PRO:O	1:B:1651:LYS:N	2.46	0.45
1:B:2020:ALA:O	1:B:2021:ARG:HD2	2.16	0.45
1:C:1899:VAL:HB	1:C:1919:GLU:HB2	1.99	0.45
1:C:2154:ARG:HG3	1:C:2154:ARG:HH11	1.80	0.45
1:A:1607:VAL:O	1:A:1610:TYR:HB3	2.16	0.45
1:B:1927:ASN:OD1	1:B:1928:SER:N	2.48	0.45
1:C:1546:GLU:CD	1:C:1546:GLU:H	2.19	0.45
1:A:1496:LYS:H	1:A:1496:LYS:CD	2.07	0.45
1:A:1766:LEU:CD1	1:A:1766:LEU:H	2.29	0.45
1:B:1640:GLN:OE1	1:B:1659:THR:HG23	2.16	0.45
1:B:1829:ARG:HG3	1:B:1829:ARG:HH11	1.82	0.45
1:B:1909:ASN:HD22	1:B:1910:PRO:N	2.15	0.45
1:B:2101:SER:HB2	1:C:1692:THR:HG21	1.98	0.45
1:C:1592:LYS:O	1:C:1593:ILE:CG1	2.65	0.45
1:C:1682:ILE:O	1:C:1683:ASN:C	2.54	0.45
1:C:1844:ARG:HG3	1:C:1844:ARG:NH1	2.28	0.45
1:A:2000:TRP:CD1	1:A:2000:TRP:C	2.89	0.45
1:B:1925:HIS:O	1:B:1926:PRO:C	2.54	0.45
1:A:1649:PRO:O	1:A:1651:LYS:N	2.49	0.45
1:A:2135:LEU:HD23	1:A:2155:ILE:HG23	1.97	0.45
1:C:2025:LEU:HD22	2:C:1:B36:HAK	1.98	0.45
1:B:2035:PHE:HD2	1:B:2090:SER:CB	2.30	0.45
1:A:2000:TRP:CD1	1:A:2000:TRP:O	2.69	0.45
1:B:1537:PHE:CD2	1:B:1571:VAL:HG13	2.52	0.45
1:B:1972:SER:HB3	1:C:1742:LEU:CD1	2.47	0.45
1:B:2100:SER:O	1:B:2104:VAL:HG23	2.17	0.45
1:C:1783:MET:HG3	1:C:1788:VAL:HB	1.98	0.45
1:A:1879:VAL:HG13	1:A:1931:LYS:HE2	1.99	0.45
1:A:2190:LYS:O	1:A:2192:GLU:N	2.41	0.45
1:B:1510:ASP:O	1:B:1513:GLU:HB3	2.15	0.45
1:B:1708:SER:HB3	1:B:1735:ILE:HG13	1.99	0.45
1:B:1966:GLU:HB3	1:B:1969:LYS:HD2	1.98	0.45
1:B:1997:GLY:HA2	1:C:1705:LEU:CD2	2.47	0.45
1:C:2000:TRP:CD1	1:C:2000:TRP:C	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2097:HIS:O	1:C:2102:ARG:HD3	2.17	0.45
1:A:1655:TYR:CE1	1:A:1689:VAL:HG22	2.52	0.45
1:A:2081:GLU:CD	1:A:2081:GLU:N	2.70	0.45
1:B:1575:GLU:H	1:B:1575:GLU:CD	2.21	0.45
1:B:2013:GLU:OE1	1:B:2125:ARG:NH2	2.38	0.45
1:A:1727:LEU:HD12	1:A:1747:ILE:O	2.17	0.44
1:A:1835:PRO:HG2	1:A:1991:PRO:HB2	1.99	0.44
1:B:2133:GLU:OE1	1:B:2148:ARG:NH2	2.49	0.44
1:C:1587:ASN:HB2	1:C:1623:ALA:O	2.17	0.44
1:C:1873:TRP:O	1:C:1874:ALA:C	2.54	0.44
1:A:1909:ASN:C	1:A:1909:ASN:HD22	2.20	0.44
1:A:2190:LYS:C	1:A:2192:GLU:N	2.69	0.44
1:B:1629:ILE:CD1	1:C:2025:LEU:HD11	2.46	0.44
1:B:1952:ASN:HA	1:B:1994:GLU:O	2.17	0.44
1:C:1608:THR:O	1:C:1612:ARG:HG3	2.16	0.44
1:A:1508:VAL:HG13	1:A:1509:TYR:N	2.32	0.44
1:A:1649:PRO:C	1:A:1651:LYS:H	2.21	0.44
1:A:1787:GLY:HA3	1:A:1873:TRP:CE3	2.52	0.44
1:A:2094:ALA:O	1:A:2097:HIS:HB2	2.17	0.44
1:A:2162:SER:HB3	1:B:1797:LEU:HB3	2.00	0.44
1:B:1856:PHE:CZ	1:B:1863:LYS:HG3	2.52	0.44
1:B:2106:LYS:HE2	1:B:2106:LYS:HA	1.99	0.44
1:A:1733:VAL:O	1:A:1736:GLY:N	2.48	0.44
1:B:1877:VAL:CG1	1:B:1931:LYS:HD3	2.48	0.44
1:C:1591:PHE:C	1:C:1591:PHE:HD2	2.20	0.44
1:B:1846:MET:HE1	1:B:1990:PRO:HB2	2.00	0.44
1:C:1909:ASN:HA	1:C:1910:PRO:HD3	1.79	0.44
1:A:1810:VAL:HG13	1:A:1811:PRO:HD2	1.99	0.44
1:A:1575:GLU:CD	1:A:1575:GLU:H	2.21	0.44
1:A:1605:ASN:HD22	1:A:1714:ALA:CB	2.30	0.44
1:A:1756:LEU:HD12	1:A:1756:LEU:HA	1.77	0.44
1:A:2037:ARG:HG3	1:A:2037:ARG:HH11	1.83	0.44
1:B:1955:GLY:HA2	1:B:1999:SER:HB3	1.98	0.44
1:B:1836:THR:HB	1:B:1839:GLU:HB3	2.00	0.44
1:C:1811:PRO:HA	1:C:1819:PRO:HD3	1.98	0.44
1:C:1902:LEU:C	1:C:1902:LEU:HD13	2.38	0.44
1:B:1663:MET:O	1:B:1667:LYS:HG3	2.18	0.43
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.82	0.43
1:B:1841:TYR:CZ	1:B:1896:THR:HG21	2.52	0.43
1:B:1868:GLU:HG2	1:B:1871:SER:HB3	2.00	0.43
1:C:1648:ASN:HD21	1:C:1651:LYS:HE2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1781:GLN:NE2	1:C:1781:GLN:N	2.51	0.43
1:A:2143:VAL:HG22	1:A:2145:GLU:N	2.30	0.43
1:B:1635:ILE:O	1:B:1635:ILE:HG22	2.19	0.43
1:B:2035:PHE:CD1	1:B:2039:LYS:HD2	2.54	0.43
1:C:1682:ILE:HD13	1:C:1687:ARG:NH1	2.33	0.43
1:A:1743:GLY:O	1:A:1744:GLN:HB2	2.18	0.43
1:B:1587:ASN:HB2	1:B:1623:ALA:O	2.18	0.43
1:A:1614:ARG:HG3	1:A:1614:ARG:NH1	2.33	0.43
1:C:1715:THR:CG2	1:C:1742:LEU:HB3	2.48	0.43
1:C:2085:ILE:HG23	1:C:2086:TYR:HD1	1.83	0.43
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.83	0.43
1:A:2083:LEU:N	1:A:2084:PRO:CD	2.82	0.43
1:C:1633:GLU:HA	1:C:1636:VAL:HG23	2.00	0.43
1:C:1619:ILE:HD12	1:C:1725:ILE:CG2	2.49	0.43
1:A:1503:MET:HE2	1:A:1589:ILE:HG13	2.00	0.43
1:A:1636:VAL:CG1	1:A:1637:PRO:HD3	2.48	0.43
1:B:1981:TYR:CB	1:B:1985:ILE:HD11	2.48	0.43
1:C:1991:PRO:C	1:C:1992:THR:HG23	2.39	0.43
1:A:1827:TRP:CZ3	1:A:2120:ARG:HG2	2.54	0.43
1:A:2172:ALA:O	1:A:2176:GLU:HG3	2.19	0.43
1:B:1575:GLU:C	1:B:1577:PRO:HD3	2.39	0.43
1:B:1862:ASP:OD1	1:B:2119:ARG:NH2	2.52	0.43
1:B:1995:LEU:HD12	1:B:1995:LEU:HA	1.89	0.43
1:C:1745:ARG:HG2	1:C:1806:TRP:CZ2	2.54	0.43
1:C:2160:PRO:HG2	1:C:2163:VAL:CG2	2.44	0.43
1:C:1508:VAL:CG2	1:C:1588:ASP:HA	2.48	0.43
1:C:1798:ALA:O	1:C:1802:LYS:HG2	2.18	0.43
1:B:1533:THR:HB	1:B:1535:ASP:OD2	2.19	0.43
1:C:1646:ALA:HB1	1:C:1648:ASN:OD1	2.19	0.43
1:C:1994:GLU:HA	1:C:2021:ARG:O	2.18	0.43
1:A:1892:ILE:CD1	1:A:1947:MET:HE1	2.48	0.42
1:A:1902:LEU:HD13	1:A:1916:LEU:HD13	2.00	0.42
1:A:2021:ARG:HD2	1:A:2098:ASP:HB2	2.01	0.42
1:A:2043:THR:C	1:A:2045:ASN:N	2.72	0.42
1:B:1514:LEU:HD22	1:B:1797:LEU:HG	2.00	0.42
1:B:1735:ILE:O	1:B:1739:LEU:HG	2.17	0.42
1:C:1585:VAL:CG2	1:C:1607:VAL:HG11	2.49	0.42
1:A:1503:MET:HE3	1:A:1589:ILE:HG13	2.01	0.42
1:B:1619:ILE:N	1:B:1619:ILE:HD12	2.33	0.42
1:B:2047:LEU:HD13	1:B:2047:LEU:C	2.40	0.42
1:C:1545:ASP:OD1	1:C:1547:ASN:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1592:LYS:C	1:C:1593:ILE:HG12	2.40	0.42
1:C:1936:ILE:CG2	1:C:1977:ALA:HB1	2.49	0.42
1:C:2154:ARG:HG3	1:C:2154:ARG:NH1	2.34	0.42
1:A:1586:ALA:CB	1:A:1621:LEU:HB2	2.49	0.42
1:C:1511:PHE:HA	1:C:1514:LEU:HD22	2.00	0.42
1:C:1643:TRP:HA	1:C:1653:PHE:HA	2.00	0.42
1:C:1648:ASN:HA	1:C:1649:PRO:HD3	1.78	0.42
1:A:2148:ARG:HE	1:A:2148:ARG:HB2	1.67	0.42
1:B:1624:ASN:HD22	1:B:1626:GLY:N	2.17	0.42
1:B:1701:GLY:O	1:B:1704:CYS:HB2	2.20	0.42
1:B:1719:TYR:CE2	1:B:1744:GLN:HG3	2.54	0.42
1:B:1960:GLN:HE21	1:B:1960:GLN:C	2.21	0.42
1:C:1503:MET:HB2	1:C:1505:THR:HG22	2.01	0.42
1:C:1635:ILE:HG22	1:C:1635:ILE:O	2.19	0.42
1:C:1655:TYR:C	1:C:1656:LEU:HD12	2.39	0.42
1:A:1988:TYR:HA	1:A:2015:TYR:O	2.20	0.42
1:A:2008:ASN:HD21	1:A:2010:ASP:HB2	1.84	0.42
1:A:2082:LEU:H	1:A:2082:LEU:CD2	2.31	0.42
1:B:1852:THR:HG23	1:B:1854:SER:N	2.35	0.42
1:B:1903:ILE:HA	1:B:1904:PRO:HD3	1.79	0.42
1:B:1996:ARG:O	1:B:1997:GLY:C	2.57	0.42
1:C:2187:LYS:C	1:C:2189:LEU:N	2.73	0.42
1:A:1606:LYS:HD2	1:A:1606:LYS:HA	1.83	0.42
1:A:1669:PHE:O	1:A:1671:LYS:HG3	2.20	0.42
1:A:1730:CYS:O	1:A:1731:ARG:C	2.56	0.42
1:A:2131:ASN:ND2	1:A:2179:TYR:OH	2.53	0.42
1:B:1820:ILE:HG22	1:B:1821:LEU:N	2.35	0.42
1:B:2139:LEU:CD2	1:B:2151:LYS:HG2	2.50	0.42
1:B:1739:LEU:HD23	1:B:1739:LEU:HA	1.79	0.42
1:C:1824:LYS:NZ	1:C:1824:LYS:CB	2.80	0.42
1:A:1769:GLU:HG3	1:A:1769:GLU:O	2.20	0.42
1:A:1991:PRO:HG3	1:A:2115:TRP:HB2	2.01	0.42
1:B:1586:ALA:CB	1:B:1621:LEU:HB2	2.50	0.42
1:B:1705:LEU:HA	1:B:1705:LEU:HD23	1.78	0.42
1:B:2183:ASP:O	1:B:2187:LYS:HB2	2.19	0.42
1:C:1639:PHE:CD1	1:C:1639:PHE:C	2.94	0.42
1:C:1927:ASN:OD1	1:C:1928:SER:N	2.53	0.42
1:A:1772:THR:N	1:A:1776:GLN:HE22	1.92	0.42
1:A:1781:GLN:CD	1:A:1781:GLN:H	2.21	0.42
1:A:1782:ILE:O	1:A:1786:ASN:HB2	2.19	0.42
1:A:1952:ASN:HA	1:A:1994:GLU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1494:GLN:OE1	1:B:1496:LYS:HB2	2.20	0.42
1:B:1522:GLN:OE1	1:B:1804:VAL:HG13	2.20	0.42
1:B:2142:GLN:HB3	1:B:2143:VAL:H	1.57	0.41
1:C:1995:LEU:HD12	1:C:1995:LEU:HA	1.90	0.41
1:A:1516:ARG:HA	1:A:1537:PHE:CD2	2.55	0.41
1:A:1699:GLY:HA2	1:A:1704:CYS:SG	2.61	0.41
1:A:1691:LYS:HA	1:A:1691:LYS:HD3	1.88	0.41
1:A:2016:ALA:O	1:A:2112:GLU:HA	2.20	0.41
1:B:1564:MET:CE	1:B:1604:PHE:HD1	2.33	0.41
1:A:1697:GLU:OE2	1:A:1697:GLU:HA	2.19	0.41
1:A:1733:VAL:CG1	1:A:1734:GLY:N	2.82	0.41
1:C:1894:VAL:HG22	1:C:1953:TRP:CZ2	2.55	0.41
1:A:1630:GLY:C	1:A:1700:LEU:HD22	2.41	0.41
1:B:1655:TYR:C	1:B:1656:LEU:HD12	2.40	0.41
1:C:1562:ILE:HB	1:C:1600:GLU:OE2	2.21	0.41
1:C:1592:LYS:O	1:C:1593:ILE:HG12	2.21	0.41
1:C:1610:TYR:CE1	1:C:1614:ARG:CZ	3.04	0.41
1:C:1701:GLY:O	1:C:1704:CYS:HB2	2.21	0.41
1:A:1719:TYR:CE2	1:A:1744:GLN:HG3	2.56	0.41
1:A:1903:ILE:N	1:A:1903:ILE:CD1	2.81	0.41
1:B:1655:TYR:O	1:B:1656:LEU:HD12	2.21	0.41
2:B:1:B36:HARA	1:C:1765:MET:SD	2.60	0.41
1:C:1650:ASP:C	1:C:1652:GLY:H	2.23	0.41
1:C:1691:LYS:HA	1:C:1691:LYS:HE2	2.01	0.41
1:A:1587:ASN:HB2	1:A:1623:ALA:O	2.21	0.41
1:A:2177:GLU:O	1:B:1501:HIS:HE1	2.03	0.41
1:B:1988:TYR:HA	1:B:2015:TYR:O	2.21	0.41
1:C:1514:LEU:HD12	1:C:1514:LEU:HA	1.88	0.41
1:C:1640:GLN:HG3	1:C:1659:THR:HG23	2.03	0.41
1:C:1645:ASP:O	1:C:1646:ALA:HB2	2.21	0.41
1:C:1991:PRO:O	1:C:1992:THR:HG23	2.20	0.41
1:A:1585:VAL:HG22	1:A:1607:VAL:HG11	2.03	0.41
1:B:1533:THR:HG22	1:B:1534:ASP:N	2.35	0.41
1:B:1556:GLU:CG	1:B:1559:ALA:HB2	2.50	0.41
1:B:1824:LYS:HB2	1:B:1824:LYS:NZ	2.36	0.41
1:C:1705:LEU:O	1:C:1708:SER:HB2	2.21	0.41
1:C:1988:TYR:HA	1:C:2015:TYR:O	2.21	0.41
1:B:1730:CYS:O	1:B:1731:ARG:O	2.38	0.41
1:B:2149:LEU:HD13	1:B:2149:LEU:O	2.20	0.41
1:C:1784:TYR:CE2	1:C:1872:GLY:HA3	2.56	0.41
1:C:1780:THR:O	1:C:1784:TYR:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2164:ASP:H	1:C:2170:GLN:HE22	1.69	0.40
1:A:1634:GLU:O	1:A:1634:GLU:CG	2.70	0.40
1:B:1576:TYR:CE1	1:B:1819:PRO:HB3	2.57	0.40
1:C:1520:SER:O	1:C:1524:LYS:HG2	2.20	0.40
1:C:1648:ASN:ND2	1:C:1651:LYS:HG2	2.37	0.40
1:C:2036:ARG:HB3	1:C:2036:ARG:HH11	1.86	0.40
1:A:1644:ASN:ND2	1:A:1652:GLY:C	2.75	0.40
1:A:1719:TYR:O	1:A:1719:TYR:CG	2.73	0.40
1:A:1765:MET:C	1:A:1767:GLY:H	2.24	0.40
1:A:2021:ARG:HH11	1:A:2021:ARG:HG2	1.86	0.40
1:B:1511:PHE:CD1	1:B:1621:LEU:HD13	2.57	0.40
1:B:1733:VAL:O	1:B:1736:GLY:N	2.50	0.40
1:B:1894:VAL:HG22	1:B:1953:TRP:CE2	2.57	0.40
1:A:1560:ASN:N	1:A:1560:ASN:ND2	2.70	0.40
1:B:1648:ASN:N	1:B:1649:PRO:CD	2.83	0.40
1:C:1644:ASN:ND2	1:C:1687:ARG:HH12	2.19	0.40
1:B:2004:ASP:OD2	1:B:2006:THR:HG23	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	677/769 (88%)	608 (90%)	58 (9%)	11 (2%)	9 31
1	B	671/769 (87%)	589 (88%)	63 (9%)	19 (3%)	5 17
1	C	661/769 (86%)	585 (88%)	60 (9%)	16 (2%)	6 20
All	All	2009/2307 (87%)	1782 (89%)	181 (9%)	46 (2%)	6 21

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1683	ASN
1	B	1643	TRP
1	B	1731	ARG
1	B	1839	GLU
1	B	2142	GLN
1	B	2145	GLU
1	C	1644	ASN
1	C	1655	TYR
1	A	1650	ASP
1	A	1684	GLY
1	A	1997	GLY
1	B	1645	ASP
1	B	1650	ASP
1	B	1766	LEU
1	B	1997	GLY
1	B	2032	GLY
1	C	1650	ASP
1	C	1768	ARG
1	C	1997	GLY
1	C	2037	ARG
1	A	1731	ARG
1	A	1991	PRO
1	A	2141	HIS
1	B	1683	ASN
1	B	2046	ARG
1	C	1632	ALA
1	C	2145	GLU
1	A	1912	SER
1	A	2036	ARG
1	B	1824	LYS
1	B	2147	SER
1	C	1683	ASN
1	C	1744	GLN
1	C	2144	GLY
1	B	1655	TYR
1	B	1730	CYS
1	A	1635	ILE
1	B	1557	PRO
1	C	1508	VAL
1	C	1637	PRO
1	C	1649	PRO
1	B	1558	GLY
1	C	2084	PRO

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Mol	Chain	Res	Type
1	A	1702	VAL
1	B	1637	PRO
1	C	1593	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	577/658 (88%)	543 (94%)	34 (6%)	19	49
1	B	572/658 (87%)	522 (91%)	50 (9%)	10	30
1	C	563/658 (86%)	523 (93%)	40 (7%)	14	39
All	All	1712/1974 (87%)	1588 (93%)	124 (7%)	14	38

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1496	LYS
1	A	1503	MET
1	A	1532	LEU
1	A	1554	GLU
1	A	1560	ASN
1	A	1585	VAL
1	A	1602	GLU
1	A	1618	ARG
1	A	1641	VAL
1	A	1651	LYS
1	A	1683	ASN
1	A	1706	ARG
1	A	1708	SER
1	A	1725	ILE
1	A	1756	LEU
1	A	1773	SER
1	A	1781	GLN
1	A	1786	ASN
1	A	1837	ASN

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Mol	Chain	Res	Type
1	A	1871	SER
1	A	1879	VAL
1	A	1884	LEU
1	A	1901	ASN
1	A	1909	ASN
1	A	1924	TRP
1	A	1930	PHE
1	A	1947	MET
1	A	1950	LEU
1	A	1991	PRO
1	A	2008	ASN
1	A	2035	PHE
1	A	2081	GLU
1	A	2128	ARG
1	A	2135	LEU
1	B	1485	THR
1	B	1490	LYS
1	B	1493	LEU
1	B	1494	GLN
1	B	1502	LEU
1	B	1508	VAL
1	B	1534	ASP
1	B	1568	LYS
1	B	1571	VAL
1	B	1585	VAL
1	B	1602	GLU
1	B	1606	LYS
1	B	1613	LYS
1	B	1616	ILE
1	B	1618	ARG
1	B	1638	LEU
1	B	1643	TRP
1	B	1653	PHE
1	B	1658	LEU
1	B	1673	ASN
1	B	1689	VAL
1	B	1726	THR
1	B	1735	ILE
1	B	1777	LEU
1	B	1797	LEU
1	B	1824	LYS
1	B	1838	ASP

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Mol	Chain	Res	Type
1	B	1843	VAL
1	B	1852	THR
1	B	1884	LEU
1	B	1889	LEU
1	B	1909	ASN
1	B	1924	TRP
1	B	1960	GLN
1	B	1980	ASP
1	B	2001	VAL
1	B	2003	VAL
1	B	2035	PHE
1	B	2042	ASP
1	B	2081	GLU
1	B	2086	TYR
1	B	2101	SER
1	B	2128	ARG
1	B	2141	HIS
1	B	2142	GLN
1	B	2145	GLU
1	B	2154	ARG
1	B	2165	HIS
1	B	2166	GLU
1	B	2187	LYS
1	C	1508	VAL
1	C	1513	GLU
1	C	1514	LEU
1	C	1536	PHE
1	C	1571	VAL
1	C	1591	PHE
1	C	1602	GLU
1	C	1629	ILE
1	C	1638	LEU
1	C	1639	PHE
1	C	1661	GLU
1	C	1676	LEU
1	C	1740	VAL
1	C	1741	ARG
1	C	1742	LEU
1	C	1770	VAL
1	C	1772	THR
1	C	1774	ASN
1	C	1781	GLN

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Mol	Chain	Res	Type
1	C	1783	MET
1	C	1792	THR
1	C	1824	LYS
1	C	1898	THR
1	C	1911	ASN
1	C	1924	TRP
1	C	1926	PRO
1	C	1928	SER
1	C	1930	PHE
1	C	1968	LEU
1	C	1978	LEU
1	C	2028	GLN
1	C	2035	PHE
1	C	2037	ARG
1	C	2045	ASN
1	C	2084	PRO
1	C	2114	GLU
1	C	2128	ARG
1	C	2129	ARG
1	C	2148	ARG
1	C	2186	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1522	GLN
1	A	1547	ASN
1	A	1560	ASN
1	A	1587	ASN
1	A	1605	ASN
1	A	1624	ASN
1	A	1644	ASN
1	A	1683	ASN
1	A	1748	GLN
1	A	1752	GLN
1	A	1776	GLN
1	A	1786	ASN
1	A	1815	ASN
1	A	1901	ASN
1	A	1909	ASN
1	A	1922	GLN
1	A	1934	GLN

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Mol	Chain	Res	Type
1	A	2008	ASN
1	A	2028	GLN
1	A	2092	GLN
1	A	2097	HIS
1	A	2131	ASN
1	A	2170	GLN
1	B	1517	GLN
1	B	1525	ASN
1	B	1587	ASN
1	B	1605	ASN
1	B	1624	ASN
1	B	1644	ASN
1	B	1683	ASN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1815	ASN
1	B	1909	ASN
1	B	1934	GLN
1	B	1941	ASN
1	B	1944	GLN
1	B	1960	GLN
1	B	2088	GLN
1	B	2097	HIS
1	B	2131	ASN
1	C	1517	GLN
1	C	1522	GLN
1	C	1525	ASN
1	C	1560	ASN
1	C	1581	GLN
1	C	1587	ASN
1	C	1605	ASN
1	C	1640	GLN
1	C	1644	ASN
1	C	1654	GLN
1	C	1748	GLN
1	C	1774	ASN
1	C	1776	GLN
1	C	1781	GLN
1	C	1815	ASN
1	C	1909	ASN
1	C	1911	ASN

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Mol	Chain	Res	Type
1	C	1934	GLN
1	C	1937	ASN
1	C	1941	ASN
1	C	2011	GLN
1	C	2045	ASN
1	C	2092	GLN
1	C	2142	GLN
1	C	2170	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B36	C	1	-	39,39,39	3.51	27 (69%)	56,56,56	1.32	6 (10%)
2	B36	A	1	-	39,39,39	2.78	23 (58%)	56,56,56	1.46	9 (16%)
2	B36	B	1	-	39,39,39	3.72	30 (76%)	56,56,56	1.27	4 (7%)

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	B36	C	1	-	-	4/12/22/22	0/6/6/6
2	B36	A	1	-	-	2/12/22/22	0/6/6/6
2	B36	B	1	-	-	2/12/22/22	0/6/6/6

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	B36	CAZ-CBE	7.14	1.50	1.41
2	C	1	B36	CAZ-CBF	7.13	1.50	1.41
2	A	1	B36	CAZ-CBE	6.50	1.50	1.41
2	B	1	B36	CAZ-CBF	6.11	1.49	1.41
2	C	1	B36	CBA-CBD	6.07	1.51	1.42
2	C	1	B36	CAX-NAV	5.99	1.45	1.33
2	A	1	B36	CAZ-CBF	5.81	1.49	1.41
2	B	1	B36	CBE-CBB	5.67	1.53	1.43
2	B	1	B36	CAZ-CAW	5.42	1.55	1.50
2	B	1	B36	CAX-NAV	5.38	1.43	1.33
2	B	1	B36	CAP-CBC	5.14	1.49	1.39
2	C	1	B36	CAZ-CBE	5.14	1.48	1.41
2	B	1	B36	CAN-CAH	4.76	1.46	1.36
2	C	1	B36	CAF-CAL	4.70	1.47	1.36
2	B	1	B36	CBF-CBC	4.66	1.51	1.43
2	C	1	B36	CAZ-CAW	4.65	1.54	1.50
2	C	1	B36	CAN-CAH	4.53	1.46	1.36
2	B	1	B36	CAC-CAI	4.53	1.47	1.36
2	C	1	B36	CAE-CAK	4.49	1.46	1.36
2	B	1	B36	CAF-CAL	4.45	1.46	1.36
2	B	1	B36	CAE-CAK	4.41	1.46	1.36
2	B	1	B36	CAP-CBB	4.34	1.47	1.39
2	C	1	B36	CBE-CBB	4.29	1.50	1.43
2	C	1	B36	CAD-CAJ	4.25	1.46	1.36
2	C	1	B36	CAW-NBH	4.14	1.43	1.34
2	A	1	B36	CBA-CBD	3.95	1.48	1.42
2	B	1	B36	CBA-CBD	3.95	1.48	1.42
2	A	1	B36	CAZ-CAW	3.95	1.53	1.50
2	B	1	B36	CAM-CAG	3.93	1.44	1.36
2	C	1	B36	CAM-CAG	3.89	1.44	1.36
2	C	1	B36	CBF-CBC	3.87	1.50	1.43
2	B	1	B36	CBD-NAV	3.87	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	B36	CBE-CBB	3.78	1.49	1.43
2	C	1	B36	CAL-CBF	3.76	1.50	1.42
2	A	1	B36	CAW-NBH	3.73	1.43	1.34
2	B	1	B36	CAD-CAJ	3.69	1.45	1.36
2	B	1	B36	CAO-CAY	3.66	1.46	1.37
2	C	1	B36	CAP-CBB	3.62	1.46	1.39
2	B	1	B36	CAW-NBH	3.62	1.42	1.34
2	A	1	B36	CBF-CBC	3.54	1.49	1.43
2	C	1	B36	CAH-CAY	3.53	1.46	1.38
2	B	1	B36	CAH-CAY	3.52	1.46	1.38
2	A	1	B36	CAO-CAY	3.48	1.45	1.37
2	C	1	B36	CAC-CAI	3.47	1.44	1.36
2	C	1	B36	CBD-NAV	3.36	1.43	1.37
2	A	1	B36	CAS-NBH	3.34	1.53	1.47
2	C	1	B36	CAP-CBC	3.31	1.45	1.39
2	B	1	B36	CAC-CAE	3.27	1.46	1.38
2	C	1	B36	CAG-CAX	3.26	1.46	1.39
2	A	1	B36	CAN-CAH	3.24	1.43	1.36
2	A	1	B36	CAE-CAK	3.23	1.44	1.36
2	A	1	B36	CAM-CAG	3.21	1.43	1.36
2	B	1	B36	CAK-CBE	3.13	1.48	1.42
2	A	1	B36	CAX-NAV	3.09	1.39	1.33
2	B	1	B36	CAS-NBH	3.04	1.52	1.47
2	A	1	B36	CAF-CAL	3.04	1.43	1.36
2	C	1	B36	CAO-CAY	3.00	1.44	1.37
2	C	1	B36	CAS-NBH	2.94	1.52	1.47
2	B	1	B36	CAT-NBH	2.86	1.52	1.47
2	A	1	B36	CAD-CAJ	2.86	1.43	1.36
2	A	1	B36	CAC-CAI	2.82	1.43	1.36
2	C	1	B36	CAF-CAD	2.75	1.45	1.38
2	B	1	B36	CAL-CBF	2.73	1.47	1.42
2	A	1	B36	CAH-CAY	2.67	1.44	1.38
2	B	1	B36	CAF-CAD	2.59	1.44	1.38
2	C	1	B36	CAC-CAE	2.57	1.44	1.38
2	B	1	B36	CAR-CBG	2.54	1.59	1.52
2	B	1	B36	CAQ-CAS	2.53	1.59	1.52
2	B	1	B36	CAQ-CBG	2.51	1.59	1.52
2	B	1	B36	CAN-CBD	2.41	1.46	1.41
2	C	1	B36	OAB-CAW	2.39	1.27	1.22
2	C	1	B36	CAU-CBG	2.38	1.61	1.53
2	A	1	B36	CBD-NAV	2.35	1.41	1.37
2	B	1	B36	CAJ-CBC	2.29	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	B36	CAP-CBC	2.27	1.43	1.39
2	A	1	B36	CAC-CAE	2.22	1.43	1.38
2	A	1	B36	CAP-CBB	2.22	1.43	1.39
2	A	1	B36	CAF-CAD	2.18	1.43	1.38
2	C	1	B36	CAQ-CBG	2.11	1.58	1.52
2	A	1	B36	CAL-CBF	2.01	1.46	1.42

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	B36	CAN-CBD-NAV	3.84	124.55	118.69
2	A	1	B36	CBE-CAZ-CAW	3.83	122.87	119.28
2	B	1	B36	CBA-CBD-NAV	-3.40	117.21	122.26
2	C	1	B36	CBE-CAZ-CAW	3.33	122.40	119.28
2	C	1	B36	CAN-CBD-NAV	3.32	123.75	118.69
2	A	1	B36	CAN-CBD-NAV	3.27	123.67	118.69
2	A	1	B36	CBA-CBD-NAV	-3.17	117.55	122.26
2	A	1	B36	OAB-CAW-CAZ	-2.99	118.70	121.59
2	A	1	B36	CBF-CAZ-CBE	-2.95	117.27	120.94
2	A	1	B36	CAZ-CAW-NBH	2.91	121.13	117.86
2	C	1	B36	CBA-CBD-NAV	-2.68	118.27	122.26
2	A	1	B36	CAI-CBB-CAP	-2.49	117.92	122.00
2	A	1	B36	CAJ-CBC-CAP	-2.39	118.09	122.00
2	C	1	B36	CAI-CBB-CAP	-2.22	118.36	122.00
2	C	1	B36	CAM-CBA-CAO	-2.14	118.24	122.02
2	B	1	B36	CAO-CBA-CBD	2.07	120.97	118.27
2	B	1	B36	CAR-CAT-NBH	-2.06	107.69	110.82
2	C	1	B36	CBF-CAZ-CBE	-2.04	118.40	120.94
2	A	1	B36	CAP-CBC-CBF	2.02	121.42	119.26

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	B36	CBG-CAU-CAY-CAO
2	C	1	B36	CBG-CAU-CAY-CAO
2	B	1	B36	CBG-CAU-CAY-CAH
2	C	1	B36	CBG-CAU-CAY-CAH
2	C	1	B36	NBH-CAW-CAZ-CBE
2	C	1	B36	NBH-CAW-CAZ-CBF
2	A	1	B36	CBG-CAU-CAY-CAO
2	A	1	B36	CBG-CAU-CAY-CAH

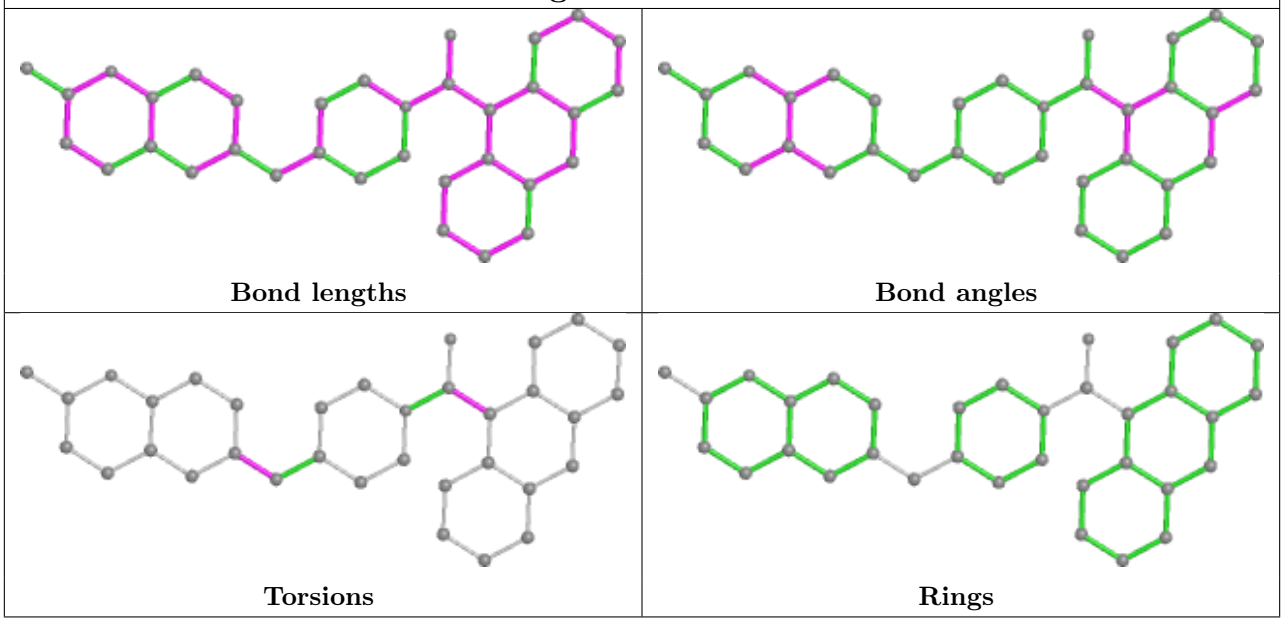
There are no ring outliers.

3 monomers are involved in 4 short contacts:

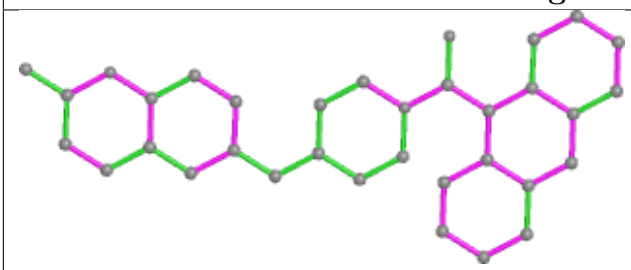
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	B36	1	0
2	A	1	B36	1	0
2	B	1	B36	2	0

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.

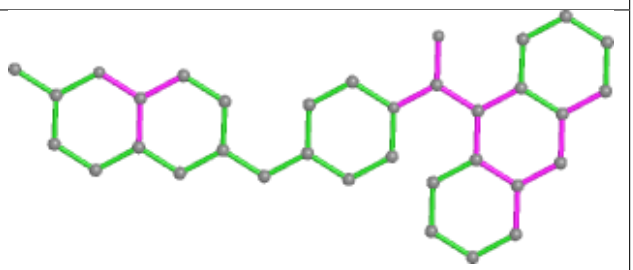
Ligand B36 C 1



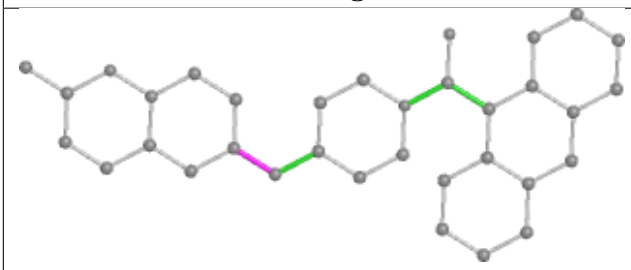
Ligand B36 A 1



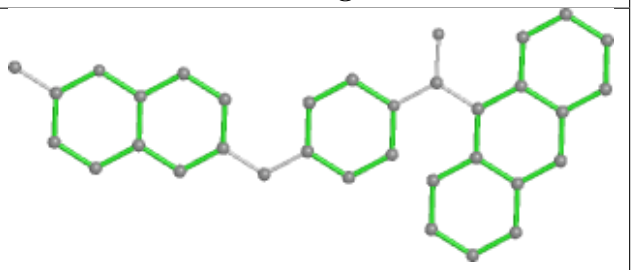
Bond lengths



Bond angles

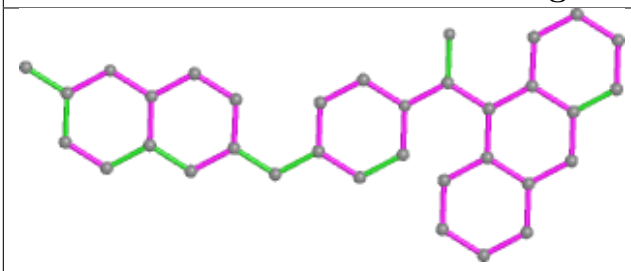


Torsions

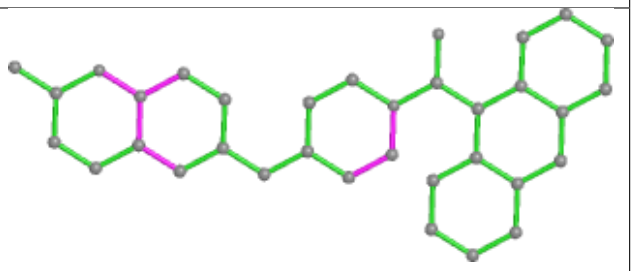


Rings

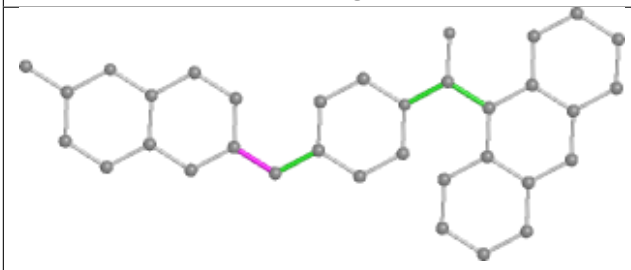
Ligand B36 B 1



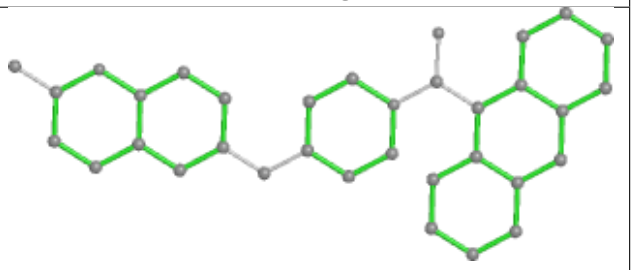
Bond lengths



Bond angles



Torsions



Rings

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	681/769 (88%)	-0.04	27 (3%)	38	28	24, 43, 89, 107	0
1	B	675/769 (87%)	0.07	36 (5%)	26	17	22, 46, 102, 119	0
1	C	665/769 (86%)	0.09	38 (5%)	23	15	23, 46, 111, 132	0
All	All	2021/2307 (87%)	0.04	101 (4%)	28	19	22, 45, 99, 132	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2037	ARG	5.8
1	C	2082	LEU	5.4
1	B	2082	LEU	5.2
1	B	2143	VAL	5.2
1	C	1679	ARG	5.0
1	B	2086	TYR	4.9
1	B	2189	LEU	4.8
1	C	2085	ILE	4.5
1	C	1685	GLU	4.5
1	C	2143	VAL	4.5
1	B	1646	ALA	4.5
1	A	1647	ALA	4.3
1	C	1657	TYR	4.0
1	B	2186	LEU	4.0
1	A	1685	GLU	4.0
1	C	1681	VAL	3.9
1	A	1643	TRP	3.9
1	A	2082	LEU	3.8
1	B	2043	THR	3.8
1	B	2145	GLU	3.8
1	A	2086	TYR	3.7
1	B	2085	ILE	3.7
1	B	2144	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	1644	ASN	3.4
1	C	1649	PRO	3.4
1	B	2142	GLN	3.4
1	C	1662	GLY	3.4
1	C	2043	THR	3.4
1	C	2044	MET	3.3
1	A	2144	GLY	3.3
1	B	1647	ALA	3.2
1	A	2085	ILE	3.2
1	B	2041	LEU	3.1
1	C	2086	TYR	3.1
1	C	1688	PHE	3.1
1	B	1682	ILE	3.1
1	A	1679	ARG	3.1
1	B	2044	MET	3.1
1	C	1636	VAL	3.1
1	B	2185	LYS	3.0
1	B	2187	LYS	3.0
1	A	1682	ILE	3.0
1	A	2143	VAL	2.9
1	C	1647	ALA	2.9
1	C	1669	PHE	2.9
1	C	1911	ASN	2.9
1	B	2158	TRP	2.8
1	C	1668	LYS	2.7
1	A	1648	ASN	2.7
1	B	1638	LEU	2.7
1	C	1641	VAL	2.7
1	A	1483	ILE	2.6
1	B	2036	ARG	2.6
1	C	1666	LEU	2.6
1	C	2037	ARG	2.6
1	A	2192	GLU	2.6
1	C	1664	GLU	2.6
1	B	1644	ASN	2.6
1	C	2142	GLN	2.5
1	A	2083	LEU	2.5
1	A	1646	ALA	2.5
1	A	1852	THR	2.5
1	B	2040	LEU	2.5
1	C	1638	LEU	2.5
1	A	1645	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1649	PRO	2.4
1	A	1641	VAL	2.4
1	B	1688	PHE	2.4
1	C	1855	GLY	2.4
1	C	1687	ARG	2.4
1	C	1660	SER	2.4
1	C	2144	GLY	2.4
1	A	2142	GLN	2.4
1	A	2194	PHE	2.4
1	B	1684	GLY	2.4
1	B	1649	PRO	2.4
1	C	1670	ASP	2.4
1	A	2191	LEU	2.4
1	C	1655	TYR	2.3
1	C	1658	LEU	2.3
1	A	2145	GLU	2.3
1	B	1824	LYS	2.3
1	B	2083	LEU	2.3
1	B	2084	PRO	2.3
1	C	2040	LEU	2.2
1	C	1852	THR	2.2
1	C	1667	LYS	2.2
1	C	1680	THR	2.2
1	A	1853	GLU	2.2
1	A	1681	VAL	2.2
1	A	1855	GLY	2.1
1	A	1651	LYS	2.1
1	B	1648	ASN	2.1
1	B	2035	PHE	2.1
1	B	2046	ARG	2.1
1	B	2047	LEU	2.1
1	B	1650	ASP	2.1
1	B	2039	LYS	2.1
1	C	1661	GLU	2.0
1	C	2089	ILE	2.0
1	B	2179	TYR	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)

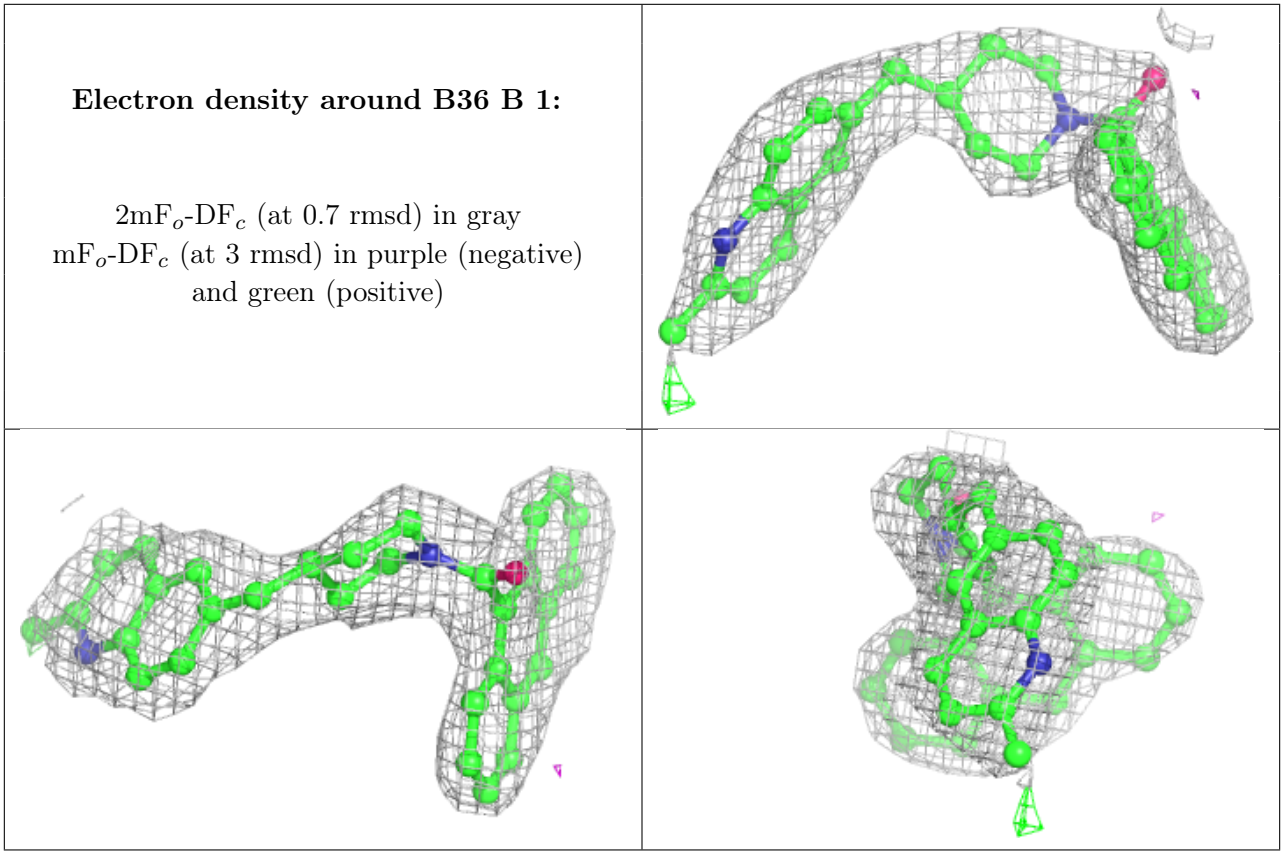
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	B36	B	1	34/34	0.89	0.23	63,68,71,72	0
2	B36	A	1	34/34	0.90	0.25	65,70,74,74	0
2	B36	C	1	34/34	0.93	0.24	59,61,63,64	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.

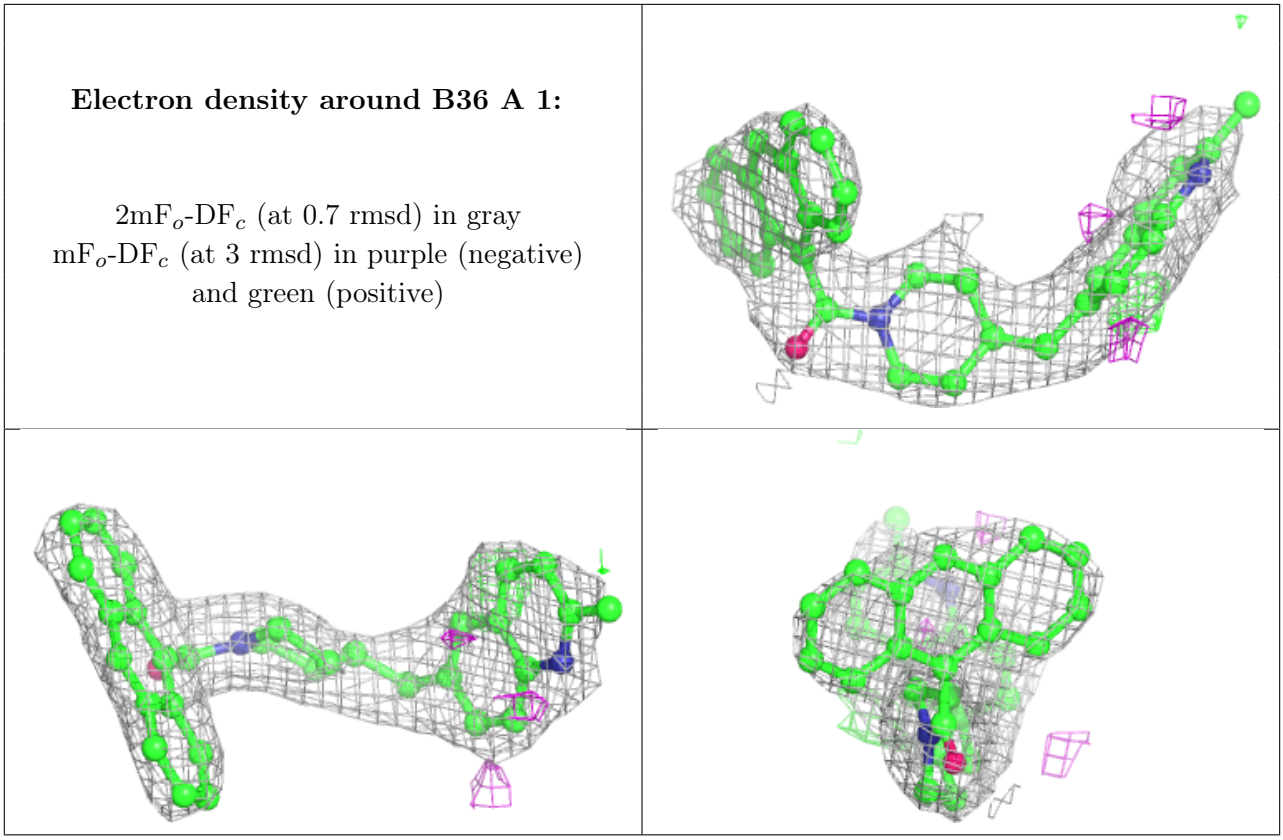
Electron density around B36 B 1:

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



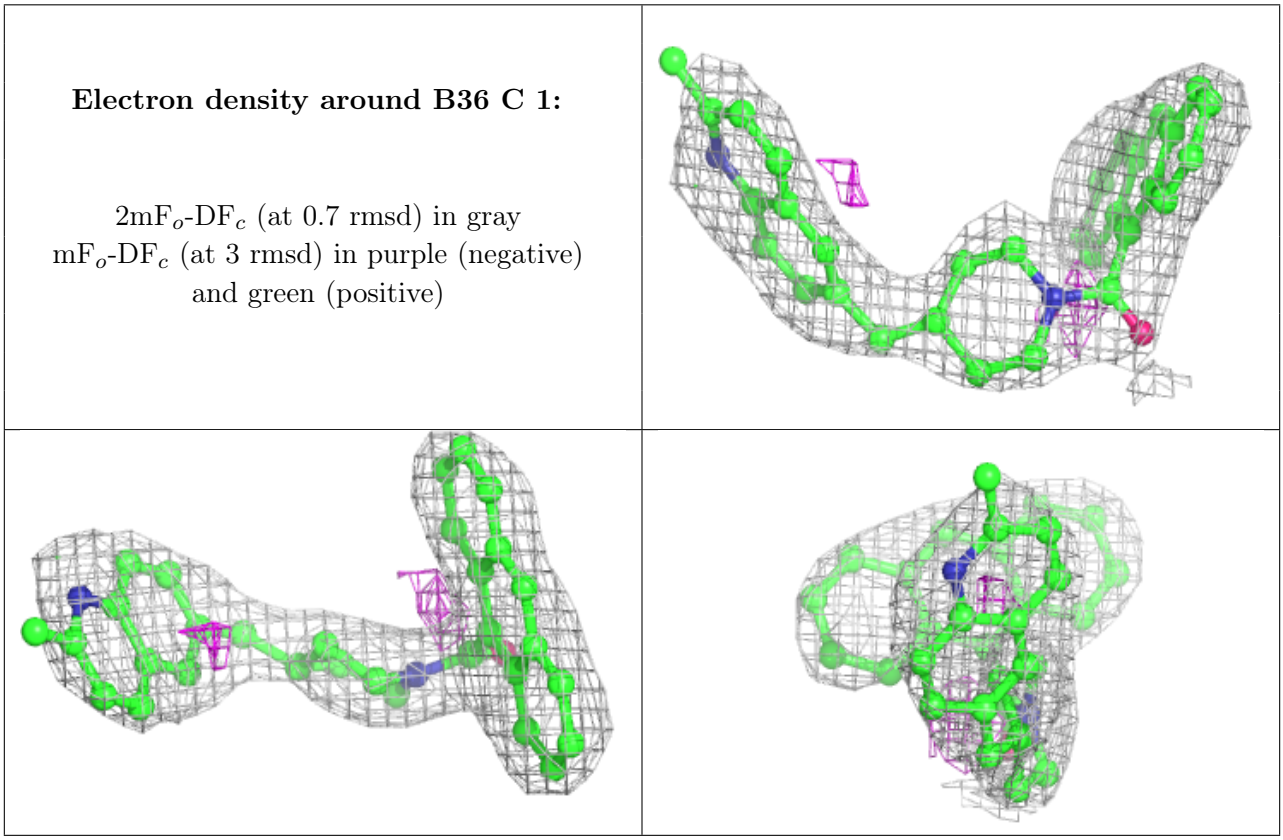
Electron density around B36 A 1:

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



Electron density around B36 C 1:

$2mF_o$-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.