Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 12:28 pm GMT

PDB ID	:	7BAM
EMDB ID	:	EMD-12124
Title	:	human Teneurin4 WT C2
Authors	:	Meijer, D.H.; Janssen, B.J.C.
Deposited on	:	2020-12-16
Resolution	:	3.50 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

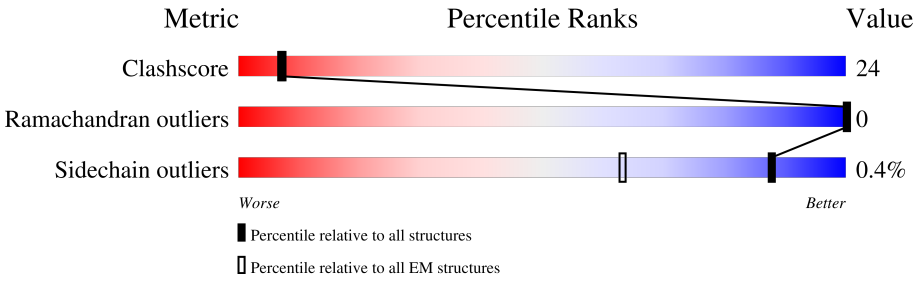
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



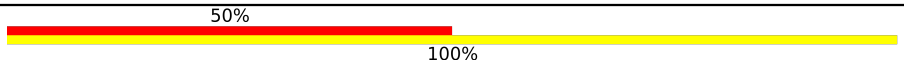
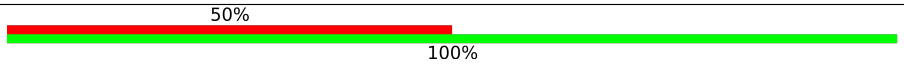
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1932	16% 64% 35% ·
1	B	1932	16% 63% 35% ·
2	C	2	50% 50% 50%
2	D	2	50% 50%
2	E	2	50% 100%
2	F	2	50% 100%
2	G	2	50% 50% 50%
2	H	2	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	2	
2	J	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30612 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

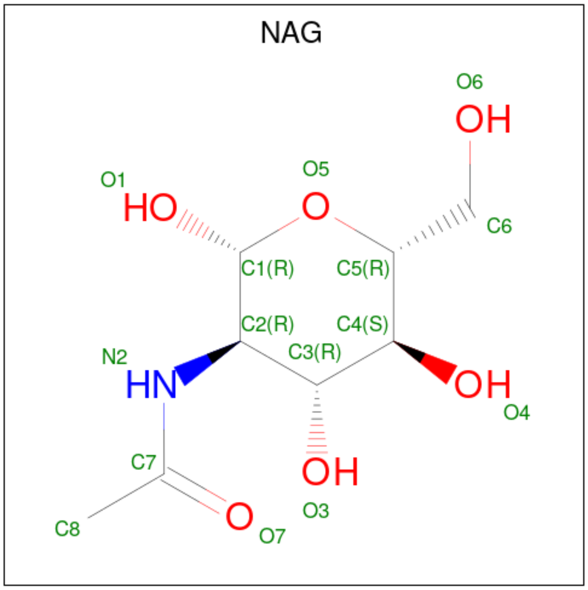
- Molecule 1 is a protein called Teneurin-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1904	Total	C	N	O	S	0	0
			15093	9515	2625	2880	73		
1	B	1904	Total	C	N	O	S	0	0
			15093	9515	2625	2880	73		

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	A	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

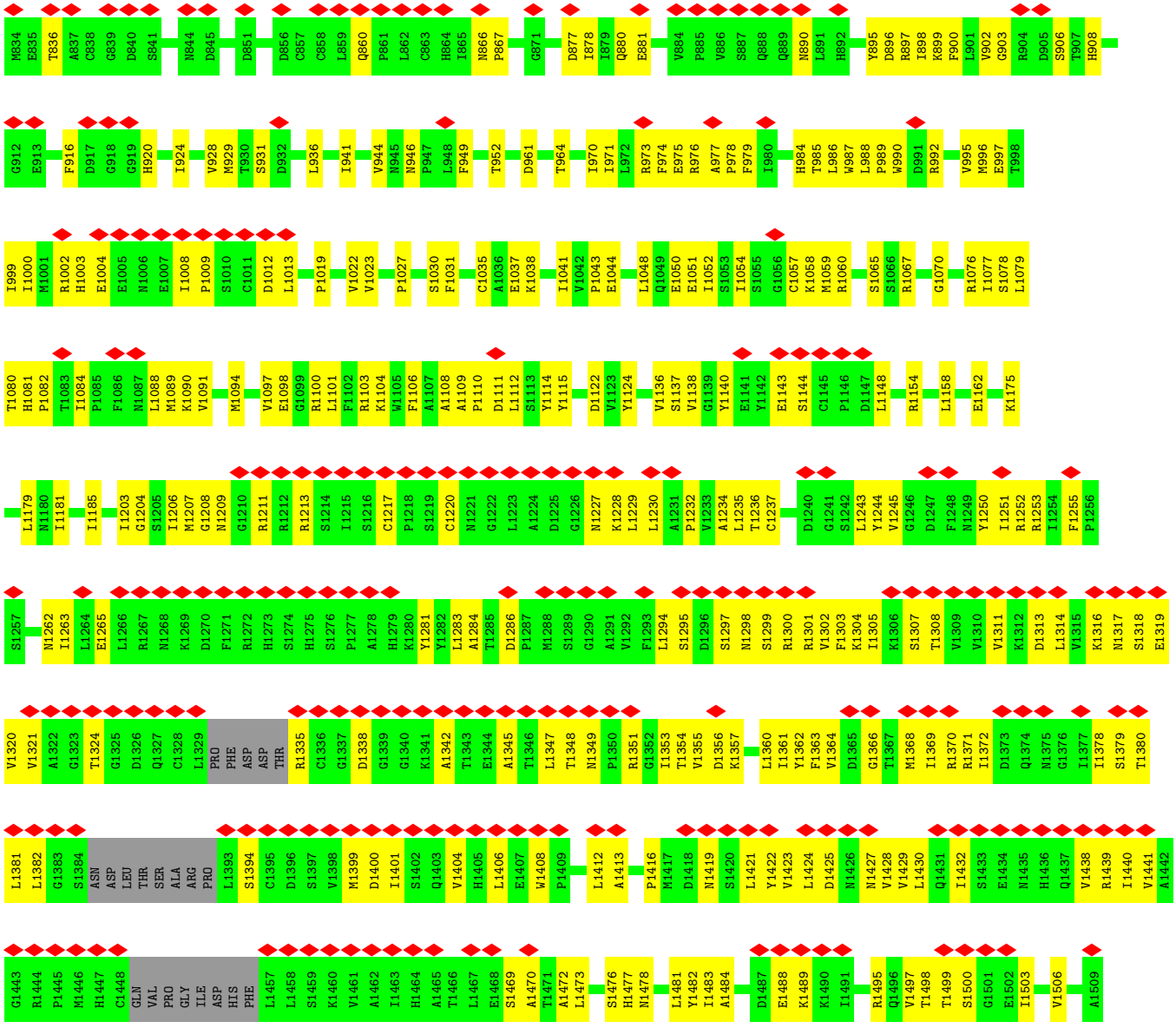
Mol	Chain	Residues	Atoms	AltConf
4	A	3	Total Ca 3 3	0
4	B	3	Total Ca 3 3	0

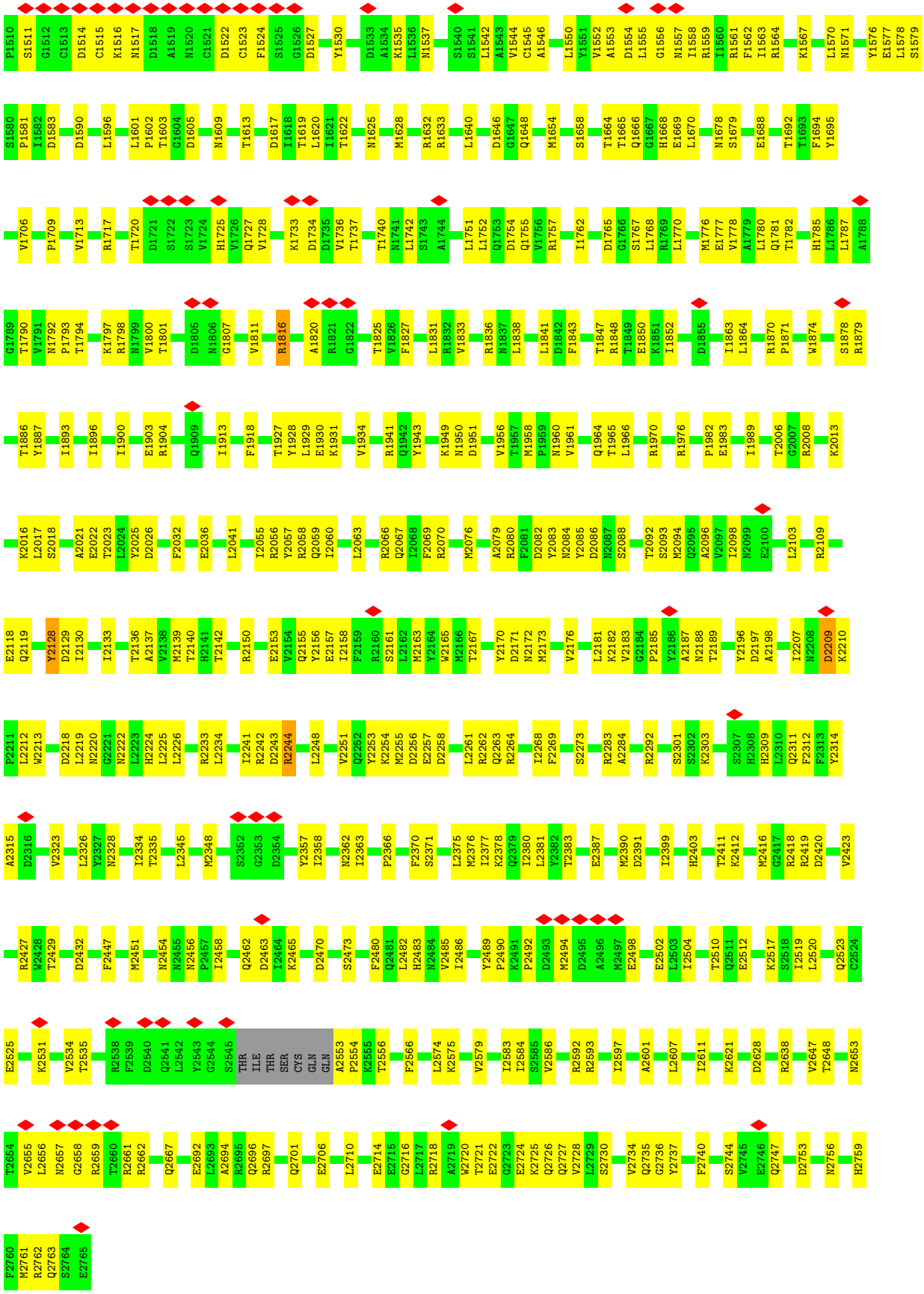
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Teneurin-4

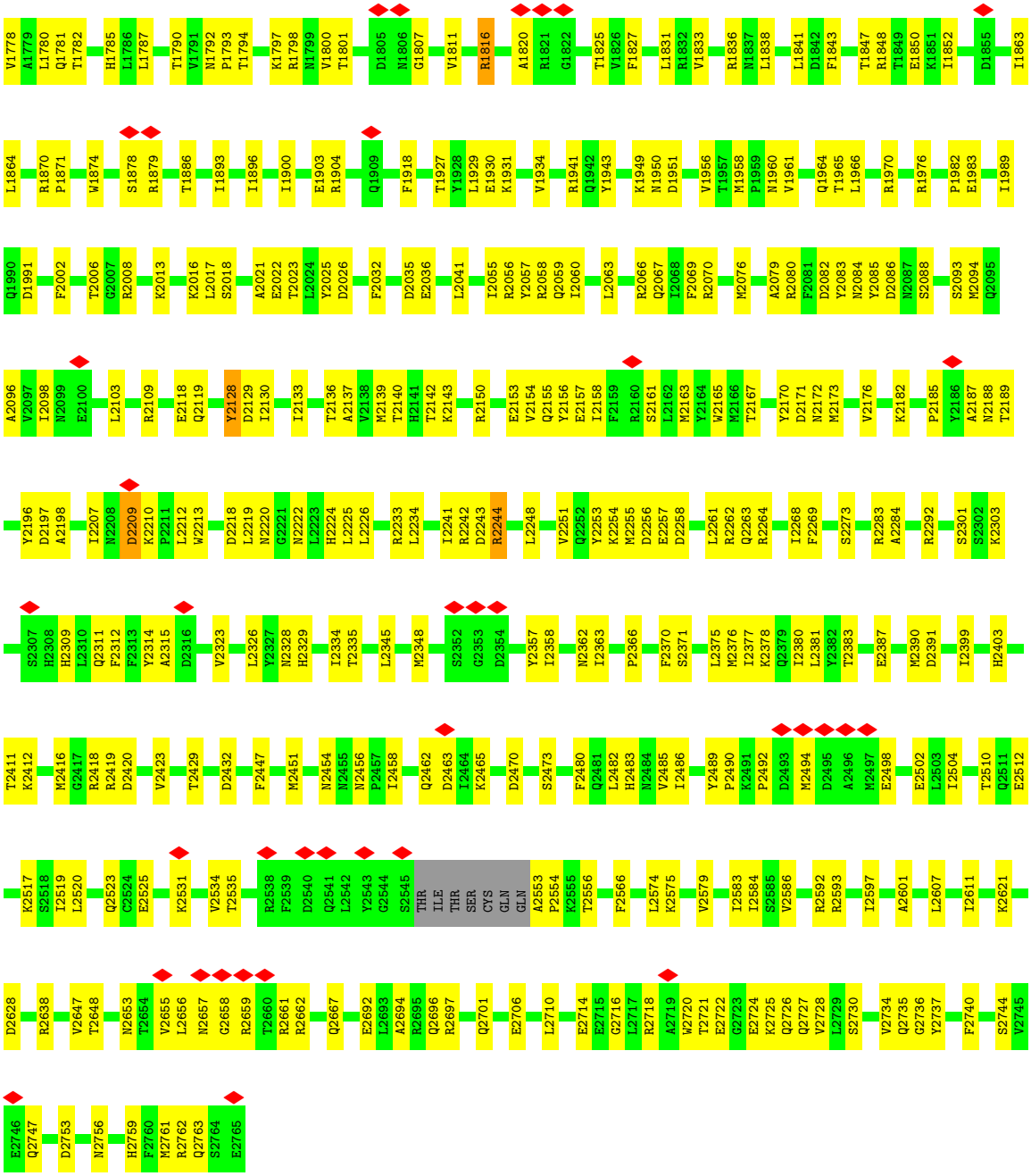
Chain A:




P1510 S1511 G1512 C1513 D1514 C1515 K1516 N1517 D1518 A1519 N1520 C1521 D1522 C1523 F1524 S1525 G1526 D1527 Y1530 D1533 A1534 K1535 L1536 N1537 S1540 S1541 L1542 A1543 V1544 C1545 A1546 L1550 Y1551 V1552 A1553 D1554 L1555 G1556 N1557 I1558 R1559 I1560 R1561 F1562 I1563 R1564 K1567 L1570 N1571 Y1576 E1577 L1578 S1579
S1580 P1581 I1582 D1583 D1590 L1596 L1601 P1602 T1603 G1604 D1605 N1609 T1613 D1617 I1618 T1619 L1620 I1621 T1622 N1625 M1628 R1632 R1633 L1640 D1646 G1647 Q1648 M1654 S1658 T1664 T1665 Q1666 G1667 H1668 E1669 L1670 N1678 S1679 E1688 T1692 F1693 F1694 Y1695
V1706 P1709 V1713 R1717 T1720 D1721 S1722 S1723 V1724 H1725 V1726 Q1727 V1728 K1733 D1734 D1735 V1736 T1737 T1740 N1741 L1742 S1743 A1744 L1751 L1752 Q1753 D1754 Q1755 V1756 R1757 I1762 D1765 G1766 S1767 L1768 R1769 L1770 M1776 E1777 V1778 A1779 L1780 Q1781 T1782 H1785 L1786 L1787 A1788
G1789 T1790 V1791 N1792 P1793 T1794 K1797 R1798 N1799 V1800 T1801 D1805 N1806 G1807 V1811 R1816 A1820 R1821 G1822 T1825 V1826 F1827 L1831 R1832 V1833 R1836 N1837 L1838 L1841 D1842 F1843 T1847 R1848 T1849 E1850 K1851 I1852 D1855 I1863 L1864 R1870 P1871 W1874 S1878 R1879
T1886 Y1887 I1893 I1896 I1900 E1903 R1904 Q1909 I1913 F1918 T1927 Y1928 L1929 E1930 K1931 V1934 R1941 Q1942 Y1943 K1949 N1950 D1951 V1956 T1957 M1958 P1959 N1960 V1961 Q1964 T1965 L1966 R1970 R1976 P1982 E1983 I1989 T2006 G2007 R2008 K2013
K2016 L2017 S2018 A2021 E2022 T2023 L2024 Y2025 D2026 F2032 E2036 L2041 I2055 R2056 Y2057 R2058 Q2059 I2060 L2063 R2066 Q2067 I2068 F2069 R2070 M2076 A2079 R2080 F2081 D2082 Y2083 N2084 Y2085 D2086 N2087 S2088 T2092 S2093 M2094 Q2095 A2096 V2097 I2098 N2099 E2100 L2103 R2109
E2118 Q2119 Y2128 D2129 I2130 I2133 T2136 A2137 Y2138 M2139 T2140 H2141 T2142 R2150 E2153 Y2154 Q2155 Y2156 E2157 I2158 F2159 R2160 S2161 L2162 M2163 Y2164 W2165 M2166 T2167 Y2170 D2171 N2172 M2173 V2176 L2181 K2182 V2183 G2184 P2185 Y2186 A2187 N2188 T2189 Y2196 D2197 A2198 I2207 W2208 D2209 K2210
P2211 L2212 W2213 D2218 L2219 N2220 G2221 N2222 L2223 H2224 L2225 L2226 R2233 L2234 I2241 R2242 D2243 R2244 L2248 V2251 Q2252 Y2253 K2254 M2255 D2256 E2257 D2258 L2261 R2262 Q2263 R2264 I2268 F2269 S2273 R2283 A2284 R2292 S2301 S2302 K2303 S2307 H2308 H2309 L2310 Q2311 F2312 F2313 Y2314
A2315 D2316 V2323 L2326 Y2327 N2328 I2334 T2335 L2345 M2348 S2352 G2353 D2354 Y2357 I2358 N2362 I2363 P2366 F2370 S2371 L2375 M2376 I2377 K2378 Q2379 I2380 L2381 Y2382 T2383 E2387 M2390 D2391 I2399 H2403 T2411 K2412 M2416 G2417 R2418 R2419 D2420 V2423
R2427 W2428 T2429 D2432 F2447 M2451 N2454 N2455 N2456 P2457 I2458 Q2462 D2463 I2464 K2465 D2470 S2473 F2480 Q2481 L2482 H2483 N2484 V2485 I2486 Y2489 P2490 K2491 P2492 D2493 M2494 D2495 A2496 M2497 E2498 E2502 L2503 I2504 T2510 Q2511 E2512 K2517 S2518 I2519 L2520 Q2523 C2524
E2525 K2531 V2534 T2535 R2538 F2539 D2540 Q2541 L2542 Y2543 G2544 S2545 THR ILE THR SER CYS GLN GLN A2553 P2554 K2555 T2556 F2566 L2574 K2575 V2579 I2583 I2584 S2585 V2586 R2592 R2593 I2597 A2601 L2607 I2611 K2621 D2628 R2638 V2647 T2648 N2653
T2654 V2655 L2656 N2657 G2658 R2659 T2660 R2661 R2662 Q2667 E2692 L2693 A2694 R2695 Q2696 R2697 Q2701 E2706 L2710 E2714 E2715 G2716 L2717 R2718 A2719 W2720 T2721 E2722 G2723 E2724 K2725 Q2726 Q2727 V2728 L2729 S2730 V2734 Q2735 G2736 Y2737 F2740 S2744 Y2745 E2746 Q2747 D2753 N2756 H2759
F2760 M2761 R2762 Q2763 S2764 E2765

• Molecule 1: Teneurin-4

Chain B:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

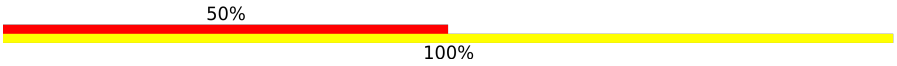
Chain C:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

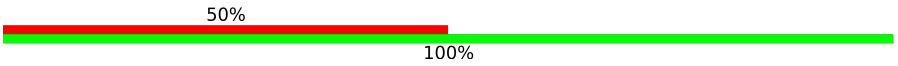
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

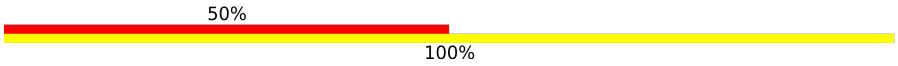
Chain G:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

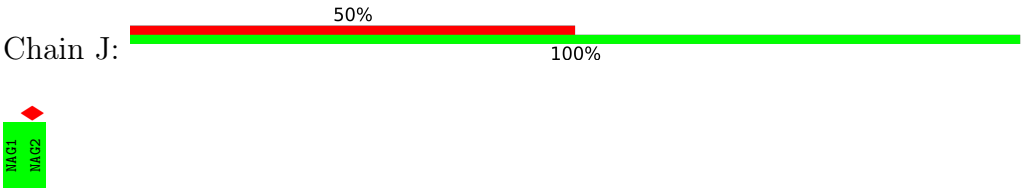
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	35929	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.358	Depositor
Minimum map value	-0.177	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	273.936, 273.936, 273.936	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.878, 0.878, 0.878	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.40	0/15425	0.53	0/20912
1	B	0.40	0/15425	0.53	0/20912
All	All	0.40	0/30850	0.53	0/41824

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2025	TYR	Peptide
1	B	2025	TYR	Peptide

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	15093	0	14710	704	0
1	B	15093	0	14710	708	0
2	C	28	0	25	1	0
2	D	28	0	25	1	0
2	E	28	0	25	4	0
2	F	28	0	25	0	0
2	G	28	0	25	1	0
2	H	28	0	25	1	0
2	I	28	0	25	4	0
2	J	28	0	25	0	0
3	A	98	0	91	7	0
3	B	98	0	91	6	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
All	All	30612	0	29802	1425	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 24.

All (1425) 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:2485:VAL:HG23	1:A:2486:ILE:HD12	1.25	1.13
1:A:1816:ARG:HG2	1:A:1816:ARG:HH11	1.13	1.10
1:B:2485:VAL:HG23	1:B:2486:ILE:HD12	1.25	1.09
1:B:1816:ARG:HG2	1:B:1816:ARG:HH11	1.13	1.06
1:A:2489:TYR:CD1	1:A:2490:PRO:HD2	1.94	1.02
1:B:2489:TYR:CD1	1:B:2490:PRO:HD2	1.94	1.01
3:B:2803:NAG:H3	3:B:2803:NAG:H83	1.44	0.99
3:A:2803:NAG:H3	3:A:2803:NAG:H83	1.44	0.98
1:A:1770:LEU:HD21	1:A:1778:VAL:HB	1.47	0.97
1:B:1770:LEU:HD21	1:B:1778:VAL:HB	1.47	0.96
1:A:2403:HIS:HB3	1:A:2416:MET:HE1	1.46	0.95
1:B:2403:HIS:HB3	1:B:2416:MET:HE1	1.46	0.94
1:B:1051:GLU:OE2	1:B:1060:ARG:HD3	1.69	0.93
1:A:985:THR:OG1	1:A:1357:LYS:NZ	2.02	0.93
1:B:985:THR:OG1	1:B:1357:LYS:NZ	2.02	0.93
1:A:1051:GLU:OE2	1:A:1060:ARG:HD3	1.69	0.91
1:B:2470:ASP:OD1	1:B:2473:SER:OG	1.87	0.91
1:B:2489:TYR:HD1	1:B:2490:PRO:HD2	1.34	0.90
1:A:2470:ASP:OD1	1:A:2473:SER:OG	1.87	0.90
1:A:896:ASP:HA	1:A:899:LYS:HZ3	1.36	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2140:THR:HB	1:B:2157:GLU:HB3	1.55	0.89
1:B:2726:GLN:NE2	1:B:2730:SER:OG	2.06	0.88
1:A:2726:GLN:NE2	1:A:2730:SER:OG	2.06	0.88
1:B:2638:ARG:HG3	1:B:2648:THR:HG22	1.55	0.88
1:B:896:ASP:HA	1:B:899:LYS:HZ3	1.38	0.88
1:A:2638:ARG:HG3	1:A:2648:THR:HG22	1.55	0.87
1:A:1579:SER:OG	1:A:1792:ASN:ND2	2.08	0.87
1:A:2262:ARG:HH12	1:A:2268:ILE:HG23	1.39	0.87
1:A:2489:TYR:HD1	1:A:2490:PRO:HD2	1.34	0.87
1:A:2140:THR:HB	1:A:2157:GLU:HB3	1.55	0.87
1:A:2268:ILE:HD11	1:A:2283:ARG:HH21	1.40	0.87
1:B:1579:SER:OG	1:B:1792:ASN:ND2	2.08	0.86
1:A:1019:PRO:HA	1:A:1140:TYR:HE2	1.41	0.86
1:B:2006:THR:OG1	1:B:2258:ASP:OD2	1.94	0.85
1:B:2262:ARG:HH12	1:B:2268:ILE:HG23	1.39	0.84
1:B:1019:PRO:HA	1:B:1140:TYR:HE2	1.41	0.84
1:B:974:PHE:HE2	1:B:984:HIS:HD1	1.25	0.84
1:A:974:PHE:HE2	1:A:984:HIS:HD1	1.25	0.84
1:A:1362:TYR:HE1	1:A:1371:ARG:HG3	1.41	0.84
1:A:1816:ARG:HG2	1:A:1816:ARG:NH1	1.88	0.84
1:A:2006:THR:OG1	1:A:2258:ASP:OD2	1.94	0.84
1:B:1665:THR:HG22	1:B:1666:GLN:H	1.43	0.84
1:B:1300:ARG:NH1	1:B:1348:THR:O	2.11	0.84
1:A:929:MET:N	1:A:999:ILE:O	2.10	0.84
1:B:929:MET:N	1:B:999:ILE:O	2.10	0.84
1:A:1665:THR:HG22	1:A:1666:GLN:H	1.43	0.83
1:B:1362:TYR:HE1	1:B:1371:ARG:HG3	1.41	0.83
1:B:2268:ILE:HD11	1:B:2283:ARG:HH21	1.40	0.83
1:A:2583:ILE:HD13	1:A:2592:ARG:HG2	1.61	0.83
1:A:1300:ARG:NH1	1:A:1348:THR:O	2.11	0.83
1:B:1300:ARG:NH1	1:B:1349:ASN:OD1	2.12	0.82
1:B:2583:ILE:HD13	1:B:2592:ARG:HG2	1.61	0.82
1:A:1412:LEU:HD11	1:A:1421:LEU:HD11	1.62	0.82
1:B:1412:LEU:HD11	1:B:1421:LEU:HD11	1.62	0.82
1:B:2128:TYR:HD1	1:B:2129:ASP:H	1.28	0.81
1:A:1300:ARG:NH1	1:A:1349:ASN:OD1	2.12	0.81
1:A:2371:SER:HB3	1:A:2377:ILE:HD11	1.63	0.81
1:B:2371:SER:HB3	1:B:2377:ILE:HD11	1.63	0.81
1:B:2378:LYS:HE3	1:B:2380:ILE:HD11	1.63	0.81
1:B:2658:GLY:O	1:B:2659:ARG:HD3	1.81	0.81
1:A:1263:ILE:HD11	1:A:1308:THR:HA	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1263:ILE:HD11	1:B:1308:THR:HA	1.64	0.80
1:B:2451:MET:SD	1:B:2454:ASN:HA	2.22	0.80
1:A:2451:MET:SD	1:A:2454:ASN:HA	2.22	0.79
1:A:1481:LEU:HD22	1:A:1483:ILE:HD11	1.63	0.79
1:B:1816:ARG:HG2	1:B:1816:ARG:NH1	1.88	0.79
1:A:2378:LYS:HE3	1:A:2380:ILE:HD11	1.63	0.79
1:B:2041:LEU:HB2	1:B:2510:THR:HG21	1.65	0.79
1:A:2658:GLY:O	1:A:2659:ARG:HD3	1.81	0.79
1:B:1564:ARG:HH11	1:B:1567:LYS:HE3	1.47	0.78
1:A:1213:ARG:HH11	1:A:1229:LEU:HA	1.48	0.78
1:A:1970:ARG:NH2	1:A:2566:PHE:HB2	1.98	0.78
1:B:1481:LEU:HD22	1:B:1483:ILE:HD11	1.63	0.78
1:A:1524:PHE:HB3	1:A:1557:ASN:ND2	1.98	0.78
1:B:1524:PHE:HB3	1:B:1557:ASN:ND2	1.98	0.78
1:B:1088:LEU:HD11	1:B:1140:TYR:CD1	2.18	0.78
1:B:2207:ILE:HD13	1:B:2212:LEU:HD12	1.66	0.78
1:B:1213:ARG:HH11	1:B:1229:LEU:HA	1.48	0.78
1:B:1970:ARG:NH2	1:B:2566:PHE:HB2	1.98	0.78
1:A:1564:ARG:HH11	1:A:1567:LYS:HE3	1.47	0.78
1:A:1088:LEU:HD11	1:A:1140:TYR:CD1	2.18	0.77
1:A:2207:ILE:HD13	1:A:2212:LEU:HD12	1.66	0.77
1:B:2136:THR:HG22	1:B:2137:ALA:H	1.50	0.77
1:A:1088:LEU:HD11	1:A:1140:TYR:HD1	1.49	0.77
1:A:1421:LEU:HB3	1:A:1432:ILE:HB	1.65	0.77
1:A:2041:LEU:HB2	1:A:2510:THR:HG21	1.65	0.77
1:B:1253:ARG:HE	1:B:1255:PHE:HE1	1.33	0.77
1:A:1527:ASP:OD1	1:A:1561:ARG:NH2	2.17	0.77
1:A:2136:THR:HG22	1:A:2137:ALA:H	1.50	0.77
1:A:2418:ARG:HD2	1:A:2418:ARG:O	1.85	0.77
1:B:2262:ARG:HH12	1:B:2268:ILE:CG2	1.98	0.77
1:A:1472:ALA:O	1:A:1473:LEU:HD12	1.85	0.76
1:B:2418:ARG:HD2	1:B:2418:ARG:O	1.85	0.76
1:A:2262:ARG:HH12	1:A:2268:ILE:CG2	1.98	0.76
1:B:1527:ASP:OD1	1:B:1561:ARG:NH2	2.17	0.76
1:B:1421:LEU:HB3	1:B:1432:ILE:HB	1.65	0.76
1:B:1472:ALA:O	1:B:1473:LEU:HD12	1.85	0.76
1:A:2165:TRP:CZ3	1:A:2167:THR:HG23	2.21	0.75
1:B:1090:LYS:HG3	1:B:1106:PHE:O	1.86	0.75
1:B:2165:TRP:CZ3	1:B:2167:THR:HG23	2.21	0.75
1:A:1090:LYS:HG3	1:A:1106:PHE:O	1.86	0.75
1:A:2128:TYR:HD1	1:A:2129:ASP:H	1.28	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1213:ARG:HB2	1:B:1230:LEU:HD21	1.68	0.74
1:A:1250:TYR:HB3	1:A:1262:ASN:HD21	1.52	0.74
1:B:1081:HIS:HB3	1:B:1082:PRO:HD2	1.69	0.74
1:A:1253:ARG:HE	1:A:1255:PHE:HE1	1.33	0.74
1:A:2023:THR:HG21	1:A:2502:GLU:OE2	1.88	0.74
1:A:1213:ARG:HB2	1:A:1230:LEU:HD21	1.69	0.74
1:A:1430:LEU:HD13	1:A:1440:ILE:HD13	1.69	0.74
1:A:1605:ASP:OD2	1:A:1848:ARG:NH2	2.21	0.74
1:A:2207:ILE:HD11	1:A:2213:TRP:HZ3	1.52	0.74
1:B:2207:ILE:HD11	1:B:2213:TRP:HZ3	1.52	0.74
1:A:1372:ILE:HD13	1:A:1378:ILE:HG22	1.70	0.74
1:B:2023:THR:HG21	1:B:2502:GLU:OE2	1.88	0.74
1:B:1605:ASP:OD2	1:B:1848:ARG:NH2	2.21	0.73
1:A:2722:GLU:HA	1:A:2725:LYS:HG2	1.70	0.73
1:B:1088:LEU:HD11	1:B:1140:TYR:HD1	1.49	0.73
1:B:2722:GLU:HA	1:B:2725:LYS:HG2	1.70	0.73
1:B:961:ASP:OD2	1:B:1124:TYR:OH	2.07	0.73
1:A:1562:PHE:HE2	1:A:1564:ARG:HE	1.37	0.73
1:A:1970:ARG:HH21	1:A:2566:PHE:HB2	1.54	0.72
1:B:1250:TYR:HB3	1:B:1262:ASN:HD21	1.52	0.72
1:B:1298:ASN:OD1	1:B:1299:SER:N	2.23	0.72
1:B:2156:TYR:OH	1:B:2357:TYR:HB3	1.90	0.72
1:B:2597:ILE:HG22	1:B:2628:ASP:HB3	1.71	0.72
1:A:1081:HIS:HB3	1:A:1082:PRO:HD2	1.69	0.72
1:A:2597:ILE:HG22	1:A:2628:ASP:HB3	1.71	0.72
1:B:1970:ARG:HH21	1:B:2566:PHE:HB2	1.54	0.72
1:A:2165:TRP:HZ3	1:A:2167:THR:HG23	1.55	0.72
1:B:1562:PHE:HE2	1:B:1564:ARG:HE	1.37	0.72
1:A:1031:PHE:CE2	1:A:2525:GLU:HG2	2.25	0.72
1:B:1430:LEU:HD13	1:B:1440:ILE:HD13	1.69	0.72
3:B:2803:NAG:H3	3:B:2803:NAG:C8	2.19	0.72
1:B:1372:ILE:HD13	1:B:1378:ILE:HG22	1.70	0.72
1:A:2163:MET:SD	1:A:2185:PRO:HD3	2.30	0.72
1:A:2156:TYR:OH	1:A:2357:TYR:HB3	1.90	0.71
1:B:1362:TYR:CE1	1:B:1371:ARG:HG3	2.25	0.71
1:A:1298:ASN:OD1	1:A:1299:SER:N	2.23	0.71
1:B:1625:ASN:OD1	1:B:1870:ARG:NH1	2.21	0.71
1:A:961:ASP:OD2	1:A:1124:TYR:OH	2.07	0.71
1:A:2128:TYR:HD1	1:A:2129:ASP:N	1.88	0.71
1:B:1031:PHE:CE2	1:B:2525:GLU:HG2	2.25	0.71
1:B:2656:LEU:HB3	1:B:2659:ARG:HH21	1.56	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2128:TYR:CD1	1:B:2129:ASP:N	2.58	0.71
1:B:2163:MET:SD	1:B:2185:PRO:HD3	2.30	0.71
1:A:1785:HIS:HB2	1:A:1794:THR:HG23	1.72	0.71
1:B:2656:LEU:HB2	1:B:2659:ARG:HB2	1.71	0.71
1:B:2710:LEU:HD21	1:B:2725:LYS:HB2	1.73	0.71
1:B:1688:GLU:HG3	1:B:1950:ASN:ND2	2.06	0.71
1:A:2656:LEU:HB2	1:A:2659:ARG:HB2	1.71	0.71
1:B:1785:HIS:HB2	1:B:1794:THR:HG23	1.72	0.71
1:A:1688:GLU:HG3	1:A:1950:ASN:ND2	2.06	0.70
1:B:2128:TYR:HD1	1:B:2129:ASP:N	1.88	0.70
1:A:2656:LEU:HB3	1:A:2659:ARG:HH21	1.56	0.70
1:B:1351:ARG:HB2	1:B:1364:VAL:HB	1.73	0.70
1:B:1785:HIS:CD2	1:B:1794:THR:HG21	2.27	0.70
1:B:1785:HIS:HD2	1:B:1794:THR:HG21	1.57	0.70
1:A:1785:HIS:HD2	1:A:1794:THR:HG21	1.57	0.70
1:B:2483:HIS:CD2	1:B:2492:PRO:HD3	2.27	0.70
1:A:2248:LEU:HD12	1:A:2248:LEU:O	1.92	0.70
1:B:1368:MET:HG3	1:B:1370:ARG:HD3	1.73	0.70
1:B:2165:TRP:HZ3	1:B:2167:THR:HG23	1.55	0.70
1:A:1351:ARG:HB2	1:A:1364:VAL:HB	1.73	0.70
3:A:2803:NAG:H3	3:A:2803:NAG:C8	2.19	0.70
1:A:1514:ASP:HB2	1:A:1517:ASN:HB2	1.74	0.70
1:A:1770:LEU:CD2	1:A:1778:VAL:HB	2.21	0.70
1:B:908:HIS:HA	1:B:952:THR:HG22	1.74	0.70
1:A:2128:TYR:CD1	1:A:2129:ASP:N	2.58	0.70
1:A:1581:PRO:CB	1:A:1794:THR:HG22	2.22	0.70
1:B:1514:ASP:HB2	1:B:1517:ASN:HB2	1.74	0.70
1:B:1581:PRO:CB	1:B:1794:THR:HG22	2.22	0.70
1:A:1115:TYR:OH	1:A:1720:THR:OG1	2.09	0.69
1:A:1368:MET:HG3	1:A:1370:ARG:HD3	1.73	0.69
1:A:1625:ASN:OD1	1:A:1870:ARG:NH1	2.21	0.69
1:A:1976:ARG:HD2	1:A:1989:ILE:HG23	1.73	0.69
1:B:1976:ARG:HD2	1:B:1989:ILE:HG23	1.73	0.69
1:A:1785:HIS:CD2	1:A:1794:THR:HG21	2.27	0.69
1:A:2483:HIS:CD2	1:A:2492:PRO:HD3	2.27	0.69
1:A:1362:TYR:CE1	1:A:1371:ARG:HG3	2.25	0.69
1:A:2710:LEU:HD21	1:A:2725:LYS:HB2	1.73	0.69
1:B:1956:VAL:HG11	1:B:2447:PHE:HZ	1.56	0.69
1:B:1770:LEU:CD2	1:B:1778:VAL:HB	2.21	0.69
1:A:2096:ALA:HB3	1:A:2103:LEU:HD12	1.74	0.69
1:A:2375:LEU:HD12	1:A:2376:MET:H	1.56	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2657:ASN:HB2	1:A:2659:ARG:HH12	1.57	0.69
1:B:2096:ALA:HB3	1:B:2103:LEU:HD12	1.74	0.69
1:A:1209:ASN:OD1	1:A:1211:ARG:HG2	1.92	0.69
1:A:1956:VAL:HG11	1:A:2447:PHE:HZ	1.56	0.69
1:A:1109:ALA:HB3	1:A:1112:LEU:HD21	1.75	0.69
1:B:2248:LEU:HD12	1:B:2248:LEU:O	1.92	0.69
1:B:2657:ASN:HB2	1:B:2659:ARG:HH12	1.57	0.69
1:B:2375:LEU:HD12	1:B:2376:MET:H	1.56	0.69
1:B:1115:TYR:OH	1:B:1720:THR:OG1	2.09	0.68
1:B:2656:LEU:HB3	1:B:2659:ARG:NH2	2.08	0.68
1:A:908:HIS:HA	1:A:952:THR:HG22	1.74	0.68
1:A:1550:LEU:HD22	1:A:1563:ILE:HD13	1.75	0.68
1:A:1524:PHE:HB3	1:A:1557:ASN:HD22	1.58	0.68
1:A:1665:THR:HG22	1:A:1666:GLN:OE1	1.93	0.68
1:B:1412:LEU:HD11	1:B:1421:LEU:HD21	1.75	0.68
1:B:1524:PHE:HB3	1:B:1557:ASN:HD22	1.58	0.68
1:B:1209:ASN:OD1	1:B:1211:ARG:HG2	1.92	0.68
1:A:2657:ASN:HB2	1:A:2659:ARG:NH1	2.09	0.68
1:A:2656:LEU:HB3	1:A:2659:ARG:NH2	2.08	0.68
1:B:1181:ILE:HD11	1:B:1576:TYR:CZ	2.29	0.68
1:B:1360:LEU:HD23	1:B:1361:ILE:N	2.09	0.68
1:A:2520:LEU:HD23	1:A:2523:GLN:HE21	1.59	0.67
1:B:1976:ARG:CD	1:B:1989:ILE:HG23	2.25	0.67
1:A:1181:ILE:HD11	1:A:1576:TYR:CZ	2.29	0.67
1:A:1360:LEU:HD23	1:A:1361:ILE:N	2.09	0.67
1:A:1976:ARG:CD	1:A:1989:ILE:HG23	2.24	0.67
1:A:2209:ASP:O	1:A:2210:LYS:HD2	1.94	0.67
1:B:1550:LEU:HD22	1:B:1563:ILE:HD13	1.75	0.67
1:B:2176:VAL:O	1:B:2196:TYR:OH	2.07	0.67
1:B:1109:ALA:HB3	1:B:1112:LEU:HD21	1.75	0.67
1:A:2744:SER:OG	1:A:2747:GLN:OE1	2.12	0.67
1:B:1665:THR:HG22	1:B:1666:GLN:OE1	1.93	0.67
1:B:2156:TYR:CE2	1:B:2158:ILE:HD11	2.30	0.67
1:B:2657:ASN:HB2	1:B:2659:ARG:NH1	2.09	0.67
1:B:1294:LEU:HD12	1:B:1295:SER:N	2.10	0.67
1:B:1412:LEU:CD1	1:B:1421:LEU:HD21	2.25	0.67
1:B:2063:LEU:HB3	1:B:2085:TYR:CE2	2.30	0.67
1:B:2520:LEU:HD23	1:B:2523:GLN:HE21	1.59	0.67
1:A:996:MET:CE	1:A:997:GLU:HG3	2.25	0.67
1:A:1412:LEU:HD11	1:A:1421:LEU:HD21	1.75	0.67
1:A:1577:GLU:O	1:A:1578:LEU:HD22	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2176:VAL:O	1:A:2196:TYR:OH	2.07	0.67
1:A:1294:LEU:HD12	1:A:1295:SER:N	2.10	0.67
1:A:1961:VAL:HG12	1:A:1961:VAL:O	1.94	0.67
1:B:2188:ASN:ND2	3:B:2807:NAG:O7	2.28	0.67
1:A:1213:ARG:HB2	1:A:1230:LEU:CD2	2.25	0.66
1:B:1424:LEU:HD22	1:B:1473:LEU:HD11	1.77	0.66
1:B:2013:LYS:HB2	1:B:2022:GLU:HB2	1.77	0.66
1:B:2485:VAL:HG23	1:B:2486:ILE:CD1	2.16	0.66
1:A:2156:TYR:CE2	1:A:2158:ILE:HD11	2.30	0.66
1:A:2188:ASN:ND2	3:A:2807:NAG:O7	2.28	0.66
1:A:1091:VAL:CG2	1:A:1106:PHE:HB2	2.26	0.66
1:B:1091:VAL:CG2	1:B:1106:PHE:HB2	2.26	0.66
1:B:1356:ASP:OD1	1:B:1357:LYS:N	2.28	0.66
1:B:1421:LEU:HD23	1:B:1422:TYR:N	2.11	0.66
1:B:1577:GLU:O	1:B:1578:LEU:HD22	1.95	0.66
1:B:2209:ASP:O	1:B:2210:LYS:HD2	1.94	0.66
1:A:1421:LEU:HD23	1:A:1422:TYR:N	2.11	0.66
1:B:1929:LEU:O	1:B:1930:GLU:HG3	1.96	0.66
1:A:1929:LEU:O	1:A:1930:GLU:HG3	1.96	0.66
1:A:1811:VAL:HG22	1:A:1833:VAL:HG12	1.78	0.66
1:B:996:MET:CE	1:B:997:GLU:HG3	2.25	0.66
1:B:2335:THR:HG21	1:B:2348:MET:CE	2.26	0.66
1:A:2063:LEU:HB3	1:A:2085:TYR:CE2	2.30	0.66
1:A:1019:PRO:HG3	1:A:1140:TYR:CD2	2.31	0.66
1:A:2058:ARG:HD3	1:A:2066:ARG:HH21	1.61	0.66
1:B:1961:VAL:HG12	1:B:1961:VAL:O	1.95	0.66
1:A:2262:ARG:NH1	1:A:2268:ILE:HG23	2.11	0.65
1:A:1023:VAL:HG11	1:A:1136:VAL:HG11	1.77	0.65
1:A:1956:VAL:HG11	1:A:2447:PHE:CZ	2.31	0.65
1:A:1424:LEU:HD22	1:A:1473:LEU:HD11	1.77	0.65
1:A:2013:LYS:HB2	1:A:2022:GLU:HB2	1.77	0.65
1:A:2182:LYS:HE3	1:A:2187:ALA:O	1.96	0.65
1:A:1356:ASP:OD1	1:A:1357:LYS:N	2.28	0.65
1:B:1213:ARG:HH21	1:B:1217:CYS:HB2	1.62	0.65
1:A:1484:ALA:HB2	1:A:1542:LEU:HD11	1.77	0.65
1:B:903:GLY:O	1:B:906:SER:HB2	1.97	0.65
1:B:1213:ARG:HB2	1:B:1230:LEU:CD2	2.25	0.65
1:B:1484:ALA:HB2	1:B:1542:LEU:HD11	1.77	0.65
1:A:979:PHE:CE1	1:A:1002:ARG:HA	2.32	0.65
1:B:1956:VAL:HG11	1:B:2447:PHE:CZ	2.31	0.65
1:B:2182:LYS:HE3	1:B:2187:ALA:O	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:PRO:HA	1:A:1140:TYR:CE2	2.29	0.65
1:A:1412:LEU:CD1	1:A:1421:LEU:HD21	2.25	0.65
1:B:1019:PRO:HG3	1:B:1140:TYR:CD2	2.31	0.65
1:A:2335:THR:HG21	1:A:2348:MET:CE	2.26	0.65
1:B:2224:HIS:O	1:B:2225:LEU:HD23	1.97	0.64
1:B:979:PHE:CE1	1:B:1002:ARG:HA	2.32	0.64
1:A:903:GLY:O	1:A:906:SER:HB2	1.97	0.64
1:B:1816:ARG:HH11	1:B:1816:ARG:CG	1.99	0.64
1:A:2224:HIS:O	1:A:2225:LEU:HD23	1.97	0.64
1:B:1811:VAL:HG22	1:B:1833:VAL:HG12	1.78	0.64
1:A:877:ASP:O	1:A:880:GLN:HG2	1.98	0.64
1:B:2058:ARG:HD3	1:B:2066:ARG:HH21	1.61	0.64
1:A:1013:LEU:HD11	1:A:1144:SER:HB2	1.80	0.64
1:A:1564:ARG:NH1	1:A:1567:LYS:HE3	2.13	0.64
1:B:1023:VAL:HG11	1:B:1136:VAL:HG11	1.77	0.64
1:B:1564:ARG:NH1	1:B:1567:LYS:HE3	2.13	0.64
1:B:1013:LEU:HD11	1:B:1144:SER:HB2	1.80	0.64
1:A:1581:PRO:CG	1:A:1794:THR:HG22	2.28	0.64
1:A:2248:LEU:O	1:A:2251:VAL:HG22	1.98	0.64
1:A:1089:MET:HE2	1:A:1143:GLU:CG	2.28	0.64
1:B:1089:MET:HE2	1:B:1143:GLU:CG	2.28	0.64
1:B:1472:ALA:C	1:B:1473:LEU:HD12	2.17	0.64
1:B:2692:GLU:OE1	1:B:2692:GLU:HA	1.98	0.64
1:A:1577:GLU:OE2	1:A:1790:THR:HG23	1.99	0.63
1:B:877:ASP:O	1:B:880:GLN:HG2	1.98	0.63
1:B:1577:GLU:C	1:B:1578:LEU:HD22	2.19	0.63
1:B:1581:PRO:CG	1:B:1794:THR:HG22	2.28	0.63
1:B:2744:SER:OG	1:B:2747:GLN:OE1	2.12	0.63
1:A:1472:ALA:C	1:A:1473:LEU:HD12	2.17	0.63
1:A:1717:ARG:NH2	1:A:1727:GLN:HG3	2.14	0.63
1:A:2718:ARG:HD3	1:A:2720:TRP:NE1	2.13	0.63
1:B:1213:ARG:HA	1:B:1228:LYS:HZ1	1.62	0.63
1:A:1737:THR:OG1	1:A:1752:LEU:HB3	1.99	0.63
1:A:941:ILE:HD12	1:A:974:PHE:CD1	2.34	0.63
1:B:1234:ALA:HB1	1:B:1283:LEU:HD23	1.81	0.63
1:B:1019:PRO:HA	1:B:1140:TYR:CE2	2.29	0.63
1:A:1094:MET:HE1	1:A:1103:ARG:HH12	1.64	0.63
1:A:1213:ARG:HH21	1:A:1217:CYS:HB2	1.62	0.63
1:A:1577:GLU:C	1:A:1578:LEU:HD22	2.19	0.63
1:B:941:ILE:HD12	1:B:974:PHE:CD1	2.34	0.63
1:A:944:VAL:HG22	1:A:971:ILE:CG2	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1737:THR:OG1	1:B:1752:LEU:HB3	1.98	0.63
1:B:1371:ARG:NH2	1:B:1379:SER:HB3	2.14	0.62
1:B:1717:ARG:NH2	1:B:1727:GLN:HG3	2.14	0.62
1:B:944:VAL:HG22	1:B:971:ILE:CG2	2.29	0.62
1:B:2248:LEU:O	1:B:2251:VAL:HG22	1.98	0.62
1:B:2456:ASN:OD1	1:B:2458:ILE:HG22	1.99	0.62
1:B:1688:GLU:HG3	1:B:1950:ASN:HD22	1.64	0.62
1:A:1008:ILE:CG1	1:A:1009:PRO:HD3	2.30	0.62
1:A:1603:THR:HG23	1:A:1843:PHE:CZ	2.35	0.62
1:A:2692:GLU:OE1	1:A:2692:GLU:HA	1.98	0.62
1:A:1213:ARG:HA	1:A:1228:LYS:HZ1	1.64	0.62
1:A:1234:ALA:HB1	1:A:1283:LEU:HD23	1.81	0.62
1:A:1688:GLU:HG3	1:A:1950:ASN:HD22	1.64	0.62
1:A:2017:LEU:O	1:A:2018:SER:OG	2.12	0.62
1:B:1603:THR:HG23	1:B:1843:PHE:CZ	2.35	0.62
1:B:2718:ARG:HD3	1:B:2720:TRP:NE1	2.13	0.62
1:A:2737:TYR:CE1	1:A:2762:ARG:HG2	2.35	0.62
1:B:1577:GLU:OE2	1:B:1790:THR:HG23	1.99	0.62
1:B:2498:GLU:OE2	1:B:2504:ILE:HD11	1.99	0.62
1:B:2737:TYR:CE1	1:B:2762:ARG:HG2	2.35	0.62
1:A:2098:ILE:HB	1:A:2334:ILE:CD1	2.29	0.62
1:B:987:TRP:CE3	1:B:1416:PRO:HB3	2.35	0.62
1:A:1476:SER:HA	1:A:1544:VAL:HG11	1.82	0.61
1:B:924:ILE:HD11	1:B:988:LEU:HD21	1.83	0.61
1:B:2098:ILE:HB	1:B:2334:ILE:CD1	2.29	0.61
1:A:987:TRP:CE3	1:A:1416:PRO:HB3	2.35	0.61
1:A:1371:ARG:NH2	1:A:1379:SER:HB3	2.14	0.61
1:A:1511:SER:HB3	1:A:1535:LYS:NZ	2.16	0.61
1:A:2083:TYR:CE2	1:A:2094:MET:HG3	2.36	0.61
1:B:996:MET:HE2	1:B:997:GLU:HG3	1.82	0.61
1:B:1008:ILE:CG1	1:B:1009:PRO:HD3	2.30	0.61
1:A:1755:GLN:OE1	1:A:1755:GLN:N	2.33	0.61
1:A:1918:PHE:HB3	1:A:2173:MET:HE2	1.82	0.61
1:A:2456:ASN:OD1	1:A:2458:ILE:HG22	1.99	0.61
1:A:1097:VAL:O	1:A:1100:ARG:HG2	2.01	0.61
1:A:1976:ARG:HD2	1:A:1989:ILE:CG2	2.31	0.61
1:B:1476:SER:HA	1:B:1544:VAL:HG11	1.82	0.61
1:B:1755:GLN:N	1:B:1755:GLN:OE1	2.33	0.61
1:B:2017:LEU:O	1:B:2018:SER:OG	2.12	0.61
1:B:2066:ARG:HG2	1:B:2082:ASP:OD1	2.00	0.61
1:A:2498:GLU:OE2	1:A:2504:ILE:HD11	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1294:LEU:HD12	1:B:1295:SER:H	1.65	0.61
1:B:1620:LEU:HD21	1:B:1622:THR:HG23	1.83	0.61
1:A:924:ILE:HD11	1:A:988:LEU:HD21	1.83	0.61
1:A:1091:VAL:HG23	1:A:1106:PHE:HB2	1.83	0.61
1:A:2086:ASP:O	1:A:2088:SER:N	2.34	0.61
1:A:2209:ASP:C	1:A:2210:LYS:HD2	2.21	0.61
1:B:1000:ILE:O	1:B:1000:ILE:HG13	1.99	0.61
1:B:1511:SER:HB3	1:B:1535:LYS:NZ	2.15	0.61
1:B:2358:ILE:HG21	1:B:2366:PRO:HB3	1.83	0.61
1:A:2485:VAL:HG23	1:A:2486:ILE:CD1	2.16	0.61
1:B:1976:ARG:HD2	1:B:1989:ILE:CG2	2.31	0.61
1:A:1000:ILE:O	1:A:1000:ILE:HG13	1.99	0.61
1:A:2066:ARG:HG2	1:A:2082:ASP:OD1	2.00	0.61
1:B:1089:MET:HE2	1:B:1143:GLU:HG2	1.82	0.61
1:B:2083:TYR:CE2	1:B:2094:MET:HG3	2.35	0.61
1:B:2209:ASP:C	1:B:2210:LYS:HD2	2.21	0.61
1:A:1620:LEU:HD21	1:A:1622:THR:HG23	1.83	0.60
1:A:1816:ARG:HH11	1:A:1816:ARG:CG	1.99	0.60
1:A:1368:MET:CE	1:A:1380:THR:HB	2.31	0.60
1:A:1762:ILE:HG13	1:A:1762:ILE:O	2.01	0.60
1:A:977:ALA:HB3	1:A:978:PRO:HD3	1.83	0.60
1:B:1097:VAL:O	1:B:1100:ARG:HG2	2.01	0.60
1:A:2358:ILE:HG21	1:A:2366:PRO:HB3	1.83	0.60
1:B:1091:VAL:HG23	1:B:1106:PHE:HB2	1.83	0.60
1:B:1929:LEU:C	1:B:1930:GLU:HG3	2.22	0.60
1:B:2658:GLY:C	1:B:2659:ARG:HD3	2.22	0.60
1:A:1929:LEU:C	1:A:1930:GLU:HG3	2.22	0.60
1:B:977:ALA:HB3	1:B:978:PRO:HD3	1.83	0.60
1:B:1665:THR:HG22	1:B:1666:GLN:N	2.17	0.60
1:B:2086:ASP:O	1:B:2088:SER:N	2.34	0.60
1:A:2658:GLY:C	1:A:2659:ARG:HD3	2.22	0.60
1:B:1368:MET:CE	1:B:1380:THR:HB	2.31	0.60
1:A:1002:ARG:NH1	1:A:1003:HIS:HB3	2.17	0.60
1:A:1294:LEU:HD12	1:A:1295:SER:H	1.65	0.60
1:B:1931:LYS:NZ	1:B:1951:ASP:OD1	2.20	0.60
1:B:2021:ALA:O	1:B:2022:GLU:HG2	2.02	0.60
1:A:1089:MET:HE2	1:A:1143:GLU:HG2	1.84	0.59
1:B:1762:ILE:HG13	1:B:1762:ILE:O	2.01	0.59
1:A:1307:SER:HB2	1:A:1317:ASN:ND2	2.18	0.59
1:B:2262:ARG:NH1	1:B:2268:ILE:HG23	2.11	0.59
1:A:1918:PHE:HB3	1:A:2173:MET:CE	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2171:ASP:OD1	1:B:2172:ASN:N	2.35	0.59
1:A:1234:ALA:CB	1:A:1283:LEU:HD23	2.33	0.59
1:A:2130:ILE:HG22	1:A:2130:ILE:O	2.03	0.59
1:B:944:VAL:HG22	1:B:971:ILE:HG23	1.84	0.59
1:B:1094:MET:CE	1:B:1103:ARG:HH12	2.16	0.59
1:A:2021:ALA:O	1:A:2022:GLU:HG2	2.02	0.59
1:B:1002:ARG:NH1	1:B:1003:HIS:HB3	2.17	0.59
1:B:1307:SER:HB2	1:B:1317:ASN:ND2	2.18	0.59
1:B:2130:ILE:HG22	1:B:2130:ILE:O	2.03	0.59
1:B:2726:GLN:NE2	1:B:2730:SER:HG	2.00	0.59
1:A:944:VAL:HG22	1:A:971:ILE:HG23	1.84	0.59
1:B:1801:THR:HA	1:B:1807:GLY:O	2.02	0.58
1:A:1203:ILE:HG13	1:A:1204:GLY:H	1.68	0.58
1:B:979:PHE:CD1	1:B:1002:ARG:HA	2.39	0.58
1:B:1234:ALA:CB	1:B:1283:LEU:HD23	2.33	0.58
1:A:1424:LEU:HD22	1:A:1473:LEU:CD1	2.33	0.58
1:A:1094:MET:CE	1:A:1103:ARG:HH12	2.16	0.58
1:B:1709:PRO:HB3	1:B:1970:ARG:HH11	1.68	0.58
1:B:1918:PHE:HB3	1:B:2173:MET:CE	2.33	0.58
1:B:2657:ASN:H	1:B:2659:ARG:NH2	2.01	0.58
1:A:1801:THR:HA	1:A:1807:GLY:O	2.02	0.58
1:A:2726:GLN:NE2	1:A:2730:SER:HG	2.00	0.58
1:A:2312:PHE:CD1	1:A:2326:LEU:HD21	2.39	0.58
1:B:1785:HIS:HB2	1:B:1794:THR:CG2	2.33	0.58
1:A:2657:ASN:H	1:A:2659:ARG:NH2	2.01	0.58
1:B:1424:LEU:HD22	1:B:1473:LEU:CD1	2.33	0.58
1:A:989:PRO:HB3	1:A:1477:HIS:ND1	2.19	0.58
1:A:1820:ALA:HB2	1:A:1825:THR:HG23	1.86	0.58
1:A:1781:GLN:HB2	1:A:1797:LYS:HB2	1.86	0.57
1:B:1203:ILE:HG13	1:B:1204:GLY:H	1.68	0.57
1:B:1668:HIS:CE1	1:B:1949:LYS:HE2	2.39	0.57
1:A:897:ARG:NH2	1:A:1122:ASP:OD2	2.37	0.57
1:A:1213:ARG:HD3	1:A:1252:ARG:HH22	1.69	0.57
1:A:1785:HIS:HB2	1:A:1794:THR:CG2	2.33	0.57
1:A:2257:GLU:OE1	1:A:2257:GLU:N	2.30	0.57
1:B:897:ARG:NH2	1:B:1122:ASP:OD2	2.37	0.57
1:A:2207:ILE:HD11	1:A:2213:TRP:CZ3	2.38	0.57
1:A:2233:ARG:NH1	1:A:2233:ARG:HB3	2.19	0.57
1:B:1213:ARG:HD3	1:B:1252:ARG:HH22	1.69	0.57
1:B:1313:ASP:HB2	1:B:1316:LYS:HB2	1.87	0.57
1:A:1098:GLU:HA	1:A:1098:GLU:OE1	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1286:ASP:HA	1:A:1355:VAL:HG11	1.87	0.57
1:A:2171:ASP:OD1	1:A:2172:ASN:N	2.35	0.57
1:B:2593:ARG:O	1:B:2597:ILE:HG12	2.05	0.57
1:B:1927:THR:HB	1:B:1934:VAL:CG1	2.35	0.57
1:B:2722:GLU:HA	1:B:2725:LYS:NZ	2.19	0.57
1:A:902:VAL:HG22	1:A:902:VAL:O	2.05	0.57
1:A:979:PHE:CD1	1:A:1002:ARG:HA	2.39	0.57
1:A:1044:GLU:OE2	1:A:1740:THR:OG1	2.23	0.57
1:A:1253:ARG:NE	1:A:1255:PHE:HE1	2.03	0.57
1:A:1751:LEU:HD11	1:A:2519:ILE:HD11	1.86	0.57
1:B:902:VAL:HG22	1:B:902:VAL:O	2.05	0.57
1:B:1244:TYR:CE1	1:B:1253:ARG:HD3	2.40	0.57
1:B:2233:ARG:HB3	1:B:2233:ARG:NH1	2.19	0.57
1:A:1213:ARG:HH12	1:A:1230:LEU:HG	1.70	0.57
1:A:1931:LYS:NZ	1:A:1951:ASP:OD1	2.20	0.57
1:A:2375:LEU:HD12	1:A:2376:MET:N	2.20	0.57
1:A:2722:GLU:HA	1:A:2725:LYS:NZ	2.19	0.57
1:B:2312:PHE:CD1	1:B:2326:LEU:HD21	2.39	0.57
1:A:1244:TYR:CE1	1:A:1253:ARG:HD3	2.40	0.57
1:B:1054:ILE:HG13	1:B:1054:ILE:O	2.05	0.57
1:A:1368:MET:HE1	1:A:1380:THR:HB	1.87	0.56
1:A:1495:ARG:HB3	1:A:1503:ILE:HD11	1.87	0.56
1:B:989:PRO:HB3	1:B:1477:HIS:ND1	2.19	0.56
1:B:1349:ASN:HB2	1:B:1366:GLY:CA	2.35	0.56
1:B:1751:LEU:HD11	1:B:2519:ILE:HD11	1.86	0.56
1:A:1472:ALA:HB3	1:A:1484:ALA:HB3	1.86	0.56
1:A:1488:GLU:HB3	1:A:1516:LYS:HD2	1.87	0.56
1:A:1668:HIS:CE1	1:A:1949:LYS:HE2	2.39	0.56
1:A:1927:THR:HB	1:A:1934:VAL:CG1	2.35	0.56
1:B:1820:ALA:HB2	1:B:1825:THR:HG23	1.86	0.56
1:B:2375:LEU:HD12	1:B:2376:MET:N	2.20	0.56
1:A:996:MET:HE3	1:A:997:GLU:HG3	1.88	0.56
1:A:1251:ILE:O	1:A:1263:ILE:HG22	2.06	0.56
1:A:1688:GLU:OE2	1:A:1950:ASN:ND2	2.38	0.56
1:A:1709:PRO:HB3	1:A:1970:ARG:HH11	1.68	0.56
1:A:2026:ASP:OD1	1:A:2756:ASN:HB3	2.06	0.56
1:B:970:ILE:HG22	1:B:971:ILE:N	2.21	0.56
1:B:1495:ARG:HB3	1:B:1503:ILE:HD11	1.87	0.56
1:B:1733:LYS:HG2	1:B:1734:ASP:N	2.19	0.56
1:B:1781:GLN:HB2	1:B:1797:LYS:HB2	1.86	0.56
1:A:970:ILE:HG22	1:A:971:ILE:N	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1430:LEU:HD13	1:B:1440:ILE:CD1	2.35	0.56
1:B:1780:LEU:HD21	1:B:1798:ARG:HG3	1.88	0.56
1:B:2257:GLU:OE1	1:B:2257:GLU:N	2.30	0.56
1:B:2371:SER:HB3	1:B:2377:ILE:CD1	2.33	0.56
1:A:1054:ILE:HG13	1:A:1054:ILE:O	2.05	0.56
1:A:1244:TYR:HE1	1:A:1253:ARG:HD3	1.71	0.56
1:A:1665:THR:HG22	1:A:1666:GLN:N	2.17	0.56
1:A:2593:ARG:O	1:A:2597:ILE:HG12	2.05	0.56
1:B:1098:GLU:OE1	1:B:1098:GLU:HA	2.04	0.56
1:B:1251:ILE:O	1:B:1263:ILE:HG22	2.05	0.56
1:B:1780:LEU:CD2	1:B:1798:ARG:HG3	2.35	0.56
1:A:1008:ILE:HG13	1:A:1009:PRO:HD3	1.87	0.56
1:A:1733:LYS:HG2	1:A:1734:ASP:N	2.19	0.56
1:A:1780:LEU:CD2	1:A:1798:ARG:HG3	2.35	0.56
1:B:1570:LEU:HD12	1:B:1576:TYR:CZ	2.41	0.56
1:B:2026:ASP:OD1	1:B:2756:ASN:HB3	2.06	0.56
1:B:2378:LYS:HE3	1:B:2380:ILE:CD1	2.35	0.56
3:B:2803:NAG:H83	3:B:2803:NAG:C3	2.28	0.56
1:B:1488:GLU:HB3	1:B:1516:LYS:HD2	1.87	0.56
1:A:1304:LYS:N	1:A:1319:GLU:O	2.39	0.56
1:A:1349:ASN:HB2	1:A:1366:GLY:CA	2.35	0.56
1:A:1777:GLU:HB3	1:A:1801:THR:HG22	1.87	0.56
1:A:1780:LEU:HD21	1:A:1798:ARG:HG3	1.87	0.56
1:A:2292:ARG:HB2	1:A:2301:SER:OG	2.06	0.56
1:B:1213:ARG:HH12	1:B:1230:LEU:HG	1.70	0.56
1:B:979:PHE:HE1	1:B:1002:ARG:HD2	1.71	0.56
1:B:1286:ASP:HA	1:B:1355:VAL:HG11	1.87	0.56
1:A:929:MET:O	1:A:1000:ILE:HA	2.06	0.56
1:A:1357:LYS:HD3	1:A:1419:ASN:HD21	1.71	0.56
1:A:2218:ASP:OD1	1:A:2219:LEU:N	2.31	0.56
1:B:1304:LYS:N	1:B:1319:GLU:O	2.39	0.56
1:A:979:PHE:CE1	1:A:1002:ARG:HD2	2.41	0.55
1:A:996:MET:HE2	1:A:997:GLU:HG3	1.87	0.55
1:A:1430:LEU:HD13	1:A:1440:ILE:CD1	2.36	0.55
1:B:929:MET:O	1:B:1000:ILE:HA	2.07	0.55
1:B:1013:LEU:HD23	1:B:1148:LEU:HD11	1.88	0.55
1:B:1357:LYS:HD3	1:B:1419:ASN:HD21	1.71	0.55
1:A:1313:ASP:HB2	1:A:1316:LYS:HB2	1.87	0.55
1:A:1570:LEU:HD12	1:A:1576:TYR:CZ	2.41	0.55
1:A:1965:THR:C	1:A:1966:LEU:HD22	2.27	0.55
1:A:2058:ARG:HD3	1:A:2066:ARG:NH2	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2083:TYR:OH	1:A:2315:ALA:O	2.19	0.55
1:A:2378:LYS:HE3	1:A:2380:ILE:CD1	2.35	0.55
1:B:979:PHE:CE1	1:B:1002:ARG:HD2	2.41	0.55
1:B:1044:GLU:OE2	1:B:1740:THR:OG1	2.23	0.55
1:B:1728:VAL:HB	1:B:1736:VAL:CG2	2.36	0.55
1:B:1777:GLU:HB3	1:B:1801:THR:HG22	1.87	0.55
1:B:1960:ASN:OD1	1:B:2220:ASN:ND2	2.38	0.55
2:E:1:NAG:H61	2:E:2:NAG:N2	2.22	0.55
1:A:1035:CYS:HB3	1:A:1038:LYS:HG2	1.88	0.55
1:A:1213:ARG:NH1	1:A:1230:LEU:HG	2.21	0.55
1:A:1400:ASP:OD1	1:A:1401:ILE:N	2.37	0.55
1:B:1213:ARG:HA	1:B:1228:LYS:NZ	2.22	0.55
1:B:1472:ALA:HB3	1:B:1484:ALA:HB3	1.86	0.55
1:A:973:ARG:HD2	1:A:975:GLU:OE2	2.07	0.55
1:B:1213:ARG:NH1	1:B:1230:LEU:HG	2.21	0.55
2:I:1:NAG:H61	2:I:2:NAG:N2	2.22	0.55
1:B:1244:TYR:HE1	1:B:1253:ARG:HD3	1.71	0.55
1:A:1213:ARG:HA	1:A:1228:LYS:NZ	2.22	0.55
1:B:1013:LEU:HB2	1:B:1148:LEU:HD11	1.88	0.55
1:B:1263:ILE:CD1	1:B:1308:THR:HA	2.34	0.55
1:B:1342:ALA:HB3	1:B:1378:ILE:HG23	1.89	0.55
1:B:2058:ARG:HD3	1:B:2066:ARG:NH2	2.21	0.55
1:B:2136:THR:HG22	1:B:2137:ALA:N	2.20	0.55
1:B:2335:THR:HG21	1:B:2348:MET:HE3	1.87	0.55
1:A:979:PHE:HE1	1:A:1002:ARG:HD2	1.71	0.55
1:A:1371:ARG:HH11	1:A:1381:LEU:HB2	1.72	0.55
1:B:1008:ILE:HG13	1:B:1009:PRO:HD3	1.87	0.55
1:B:1360:LEU:HD21	1:B:1371:ARG:HG3	1.88	0.55
1:B:1368:MET:HE1	1:B:1380:THR:HB	1.89	0.55
1:B:1965:THR:C	1:B:1966:LEU:HD22	2.27	0.55
1:A:1960:ASN:OD1	1:A:2220:ASN:ND2	2.38	0.55
1:A:2371:SER:HB3	1:A:2377:ILE:CD1	2.33	0.55
1:B:2218:ASP:OD1	1:B:2219:LEU:N	2.31	0.55
1:B:2292:ARG:HB2	1:B:2301:SER:OG	2.06	0.55
1:A:1342:ALA:HB3	1:A:1378:ILE:HG23	1.89	0.55
1:A:2727:GLN:NE2	1:A:2735:GLN:OE1	2.40	0.55
1:B:2016:LYS:NZ	1:B:2032:PHE:O	2.40	0.55
1:B:2207:ILE:HD11	1:B:2213:TRP:CZ3	2.38	0.55
1:A:1013:LEU:HD23	1:A:1148:LEU:HD11	1.88	0.55
1:A:941:ILE:HD12	1:A:974:PHE:HD1	1.72	0.54
1:A:1013:LEU:HB2	1:A:1148:LEU:HD11	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1368:MET:HG3	1:A:1370:ARG:CD	2.37	0.54
1:A:2736:GLY:O	1:A:2762:ARG:HD2	2.07	0.54
1:B:1811:VAL:HG13	1:B:1833:VAL:CG1	2.38	0.54
1:B:2727:GLN:NE2	1:B:2735:GLN:OE1	2.40	0.54
1:B:973:ARG:HD2	1:B:975:GLU:OE2	2.07	0.54
1:B:1035:CYS:HB3	1:B:1038:LYS:HG2	1.88	0.54
1:A:1236:THR:O	1:A:1243:LEU:HD12	2.08	0.54
1:A:2016:LYS:NZ	1:A:2032:PHE:O	2.40	0.54
1:B:1523:CYS:SG	1:B:1537:ASN:ND2	2.81	0.54
1:A:1307:SER:O	1:A:1317:ASN:ND2	2.37	0.54
1:A:2136:THR:HG22	1:A:2137:ALA:N	2.20	0.54
1:B:2656:LEU:CD1	1:B:2661:ARG:HB2	2.38	0.54
1:A:1523:CYS:SG	1:A:1537:ASN:ND2	2.81	0.54
1:B:1425:ASP:O	1:B:1428:VAL:HG12	2.08	0.54
1:B:2736:GLY:O	1:B:2762:ARG:HD2	2.07	0.54
1:A:1811:VAL:HG13	1:A:1833:VAL:CG1	2.38	0.54
1:A:1109:ALA:O	1:A:1112:LEU:HD23	2.08	0.54
1:A:1263:ILE:CD1	1:A:1308:THR:HA	2.34	0.54
1:A:1368:MET:CG	1:A:1370:ARG:HD3	2.37	0.54
1:A:1728:VAL:HB	1:A:1736:VAL:CG2	2.36	0.54
1:B:1008:ILE:HG13	1:B:1009:PRO:CD	2.38	0.54
1:B:1236:THR:O	1:B:1243:LEU:HD12	2.08	0.54
1:B:1688:GLU:OE2	1:B:1950:ASN:ND2	2.38	0.54
1:B:2714:GLU:N	1:B:2714:GLU:OE1	2.41	0.54
1:A:2109:ARG:NE	1:A:2119:GLN:OE1	2.39	0.53
1:A:2656:LEU:CD1	1:A:2661:ARG:HB2	2.38	0.53
1:B:1351:ARG:O	1:B:1353:ILE:HG23	2.09	0.53
1:B:1371:ARG:HH11	1:B:1381:LEU:HB2	1.72	0.53
1:B:1412:LEU:HD11	1:B:1421:LEU:CD1	2.37	0.53
1:B:2253:TYR:CE1	1:B:2264:ARG:HG3	2.43	0.53
1:B:2403:HIS:CB	1:B:2416:MET:HE1	2.30	0.53
1:A:1057:CYS:SG	1:A:1059:MET:HG2	2.48	0.53
1:A:2335:THR:HG21	1:A:2348:MET:HE3	1.90	0.53
1:B:836:THR:O	1:B:860:GLN:NE2	2.33	0.53
1:B:1400:ASP:OD1	1:B:1401:ILE:N	2.37	0.53
1:B:2556:THR:HG23	1:B:2556:THR:O	2.09	0.53
1:A:1360:LEU:HD21	1:A:1371:ARG:HG3	1.88	0.53
1:A:1778:VAL:HG13	1:A:1800:VAL:HG12	1.91	0.53
1:B:1811:VAL:HG13	1:B:1833:VAL:HG12	1.90	0.53
1:B:2611:ILE:HD12	1:B:2697:ARG:CZ	2.39	0.53
1:A:2253:TYR:CE1	1:A:2264:ARG:HG3	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1057:CYS:SG	1:B:1059:MET:HG2	2.48	0.53
1:B:1785:HIS:CE1	1:B:1787:LEU:HB2	2.43	0.53
1:A:1008:ILE:HG13	1:A:1009:PRO:CD	2.38	0.53
1:B:1357:LYS:HD3	1:B:1419:ASN:OD1	2.08	0.53
1:B:1713:VAL:HG11	1:B:2575:LYS:HD3	1.91	0.53
1:B:2153:GLU:HG3	1:B:2167:THR:HG22	1.91	0.53
1:A:1019:PRO:HG3	1:A:1140:TYR:HD2	1.74	0.53
1:A:2153:GLU:HG3	1:A:2167:THR:HG22	1.91	0.53
1:A:2520:LEU:CD2	1:A:2523:GLN:HG3	2.38	0.53
1:A:2556:THR:O	1:A:2556:THR:HG23	2.09	0.53
1:B:1620:LEU:HD21	1:B:1622:THR:CG2	2.39	0.53
1:B:2520:LEU:CD2	1:B:2523:GLN:HG3	2.38	0.53
1:A:2714:GLU:OE1	1:A:2714:GLU:N	2.41	0.53
1:B:1084:ILE:HD11	1:B:1110:PRO:HB3	1.91	0.53
1:B:2163:MET:HG3	1:B:2370:PHE:CE1	2.44	0.53
1:A:1030:SER:HB3	1:A:1031:PHE:HD1	1.74	0.53
1:A:1620:LEU:HD21	1:A:1622:THR:CG2	2.39	0.53
1:A:1983:GLU:HB2	1:A:2241:ILE:HD11	1.91	0.53
1:B:1077:ILE:HG13	1:B:1077:ILE:O	2.09	0.53
1:B:880:GLN:HG3	1:B:881:GLU:HG3	1.91	0.53
1:B:1900:ILE:HG22	1:B:1900:ILE:O	2.09	0.53
1:B:1983:GLU:HB2	1:B:2241:ILE:HD11	1.91	0.53
1:A:1425:ASP:O	1:A:1428:VAL:HG12	2.08	0.52
1:A:1785:HIS:CE1	1:A:1787:LEU:HB2	2.43	0.52
1:B:1109:ALA:O	1:B:1112:LEU:HD23	2.08	0.52
1:B:1253:ARG:NE	1:B:1255:PHE:HE1	2.03	0.52
1:A:880:GLN:HG3	1:A:881:GLU:HG3	1.91	0.52
1:A:1357:LYS:HD3	1:A:1419:ASN:OD1	2.08	0.52
1:A:1811:VAL:HG13	1:A:1833:VAL:HG12	1.90	0.52
1:A:2118:GLU:O	1:A:2118:GLU:HG3	2.09	0.52
1:B:1488:GLU:HB3	1:B:1516:LYS:CD	2.40	0.52
1:B:1778:VAL:HG13	1:B:1800:VAL:HG12	1.91	0.52
1:A:1713:VAL:HG11	1:A:2575:LYS:HD3	1.91	0.52
1:B:1368:MET:CG	1:B:1370:ARG:HD3	2.37	0.52
1:A:1089:MET:CE	1:A:1143:GLU:HA	2.39	0.52
1:A:2163:MET:HG3	1:A:2370:PHE:CE1	2.44	0.52
1:B:1019:PRO:HG3	1:B:1140:TYR:HD2	1.74	0.52
1:B:1207:MET:HE3	1:B:1229:LEU:HB3	1.92	0.52
1:B:1646:ASP:OD1	1:B:1648:GLN:N	2.42	0.52
1:B:2109:ARG:NE	1:B:2119:GLN:OE1	2.39	0.52
1:B:2118:GLU:HG3	1:B:2118:GLU:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1900:ILE:HG22	1:A:1900:ILE:O	2.09	0.52
1:A:2377:ILE:O	1:A:2377:ILE:HG22	2.10	0.52
1:A:2638:ARG:NH2	2:E:1:NAG:O5	2.43	0.52
3:A:2807:NAG:O7	3:A:2807:NAG:C1	2.58	0.52
1:A:1070:GLY:HA3	1:A:1679:SER:OG	2.10	0.52
1:A:1077:ILE:O	1:A:1077:ILE:HG13	2.09	0.52
1:A:1351:ARG:O	1:A:1353:ILE:HG23	2.09	0.52
1:A:1581:PRO:HG2	1:A:1794:THR:HG22	1.91	0.52
1:B:1581:PRO:HG2	1:B:1794:THR:HG22	1.91	0.52
1:B:896:ASP:OD1	1:B:897:ARG:N	2.43	0.52
1:B:941:ILE:HD12	1:B:974:PHE:HD1	1.72	0.52
1:B:1013:LEU:HD11	1:B:1144:SER:CB	2.40	0.52
1:A:1583:ASP:OD1	1:A:1583:ASP:O	2.28	0.52
1:A:2086:ASP:C	1:A:2088:SER:H	2.10	0.52
1:A:896:ASP:OD1	1:A:897:ARG:N	2.43	0.52
1:A:1524:PHE:HA	1:A:1535:LYS:O	2.09	0.52
1:A:1646:ASP:OD1	1:A:1648:GLN:N	2.42	0.52
1:A:2244:ARG:HB3	1:A:2255:MET:HG3	1.91	0.52
1:B:1031:PHE:CD2	1:B:2525:GLU:HG2	2.45	0.52
1:B:1368:MET:HG3	1:B:1370:ARG:CD	2.38	0.52
1:B:1570:LEU:HD23	1:B:1571:ASN:O	2.10	0.52
1:A:1370:ARG:NH1	1:A:1378:ILE:HD12	2.25	0.52
1:A:1871:PRO:O	1:A:1887:TYR:OH	2.17	0.52
1:A:2303:LYS:HD2	1:A:2309:HIS:NE2	2.25	0.52
1:B:2638:ARG:NH2	2:I:1:NAG:O5	2.43	0.52
1:A:1422:TYR:HE1	1:A:1441:VAL:HG21	1.75	0.51
1:A:2611:ILE:HD12	1:A:2697:ARG:CZ	2.39	0.51
1:B:2083:TYR:OH	1:B:2315:ALA:O	2.19	0.51
1:B:2244:ARG:HB3	1:B:2255:MET:HG3	1.91	0.51
1:A:1041:ILE:HD11	1:A:1706:VAL:HG11	1.92	0.51
1:A:1488:GLU:HB3	1:A:1516:LYS:CD	2.40	0.51
1:A:1871:PRO:HB2	1:A:1874:TRP:CH2	2.45	0.51
1:A:2058:ARG:HH11	1:A:2058:ARG:HG2	1.76	0.51
1:B:1089:MET:CE	1:B:1143:GLU:HA	2.39	0.51
1:B:1524:PHE:HA	1:B:1535:LYS:O	2.09	0.51
1:B:2312:PHE:HE1	1:B:2399:ILE:HG12	1.75	0.51
1:B:2377:ILE:HG22	1:B:2377:ILE:O	2.10	0.51
1:A:1013:LEU:HD11	1:A:1144:SER:CB	2.40	0.51
1:A:2722:GLU:HA	1:A:2725:LYS:HZ2	1.74	0.51
1:B:1048:LEU:H	1:B:1065:SER:HB3	1.75	0.51
1:B:1422:TYR:HE1	1:B:1441:VAL:HG21	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2056:ARG:HE	1:B:2070:ARG:HH12	1.58	0.51
1:B:2303:LYS:HD2	1:B:2309:HIS:NE2	2.24	0.51
1:A:1050:GLU:OE2	1:A:1695:TYR:OH	2.24	0.51
1:A:1976:ARG:CD	1:A:1989:ILE:CG2	2.88	0.51
1:A:2740:PHE:HB2	1:A:2759:HIS:CE1	2.45	0.51
1:B:1041:ILE:HD11	1:B:1706:VAL:HG11	1.92	0.51
1:B:1094:MET:HB2	1:B:1137:SER:HB2	1.92	0.51
1:B:1713:VAL:CG1	1:B:2575:LYS:HD3	2.40	0.51
1:B:2086:ASP:C	1:B:2088:SER:H	2.10	0.51
1:A:1031:PHE:CD2	1:A:2525:GLU:HG2	2.45	0.51
1:A:1084:ILE:HD11	1:A:1110:PRO:HB3	1.91	0.51
1:A:1713:VAL:CG1	1:A:2575:LYS:HD3	2.40	0.51
1:A:2056:ARG:HE	1:A:2070:ARG:HH12	1.59	0.51
1:B:1070:GLY:HA3	1:B:1679:SER:OG	2.10	0.51
1:B:1370:ARG:NH1	1:B:1378:ILE:HD12	2.25	0.51
1:B:1976:ARG:CD	1:B:1989:ILE:CG2	2.88	0.51
1:A:944:VAL:HG12	1:A:973:ARG:HB2	1.93	0.51
1:A:1203:ILE:HG13	1:A:1204:GLY:N	2.26	0.51
1:A:2520:LEU:HD23	1:A:2523:GLN:NE2	2.26	0.51
1:B:931:SER:HB3	1:B:1002:ARG:HG2	1.92	0.51
1:B:1104:LYS:NZ	1:B:1106:PHE:CZ	2.79	0.51
1:A:920:HIS:ND1	1:A:990:TRP:HZ3	2.09	0.51
1:A:1048:LEU:H	1:A:1065:SER:HB3	1.75	0.51
1:A:1357:LYS:HD3	1:A:1419:ASN:ND2	2.26	0.51
1:A:2055:ILE:HG12	1:A:2069:PHE:CD1	2.46	0.51
1:B:1357:LYS:HD3	1:B:1419:ASN:ND2	2.26	0.51
1:B:1871:PRO:HB2	1:B:1874:TRP:CH2	2.45	0.51
1:B:2055:ILE:HG12	1:B:2069:PHE:CD1	2.46	0.51
1:A:1770:LEU:HD23	1:A:1770:LEU:H	1.76	0.51
1:B:996:MET:HE3	1:B:997:GLU:HG3	1.92	0.51
1:B:2722:GLU:HA	1:B:2725:LYS:HZ2	1.75	0.51
1:A:836:THR:O	1:A:860:GLN:NE2	2.33	0.51
1:A:1104:LYS:NZ	1:A:1106:PHE:CZ	2.79	0.51
1:A:2057:TYR:HE1	1:A:2067:GLN:HE21	1.58	0.51
1:A:2157:GLU:OE2	1:A:2161:SER:N	2.44	0.51
1:B:944:VAL:HG12	1:B:973:ARG:HB2	1.93	0.51
1:B:1303:PHE:HD2	1:B:1318:SER:OG	1.94	0.51
1:B:1583:ASP:OD1	1:B:1583:ASP:O	2.28	0.51
1:A:1284:ALA:HB2	1:A:1353:ILE:HG13	1.91	0.51
1:A:1570:LEU:HD23	1:A:1571:ASN:O	2.10	0.51
1:A:2312:PHE:HE1	1:A:2399:ILE:HG12	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1530:TYR:HE2	1:B:1765:ASP:HB2	1.76	0.51
1:B:2057:TYR:HE1	1:B:2067:GLN:HE21	1.58	0.51
1:A:2463:ASP:OD2	1:A:2465:LYS:HB2	2.11	0.50
1:B:2041:LEU:CB	1:B:2510:THR:HG21	2.40	0.50
1:B:2058:ARG:HG2	1:B:2058:ARG:HH11	1.76	0.50
1:A:1303:PHE:HD2	1:A:1318:SER:OG	1.94	0.50
1:B:1030:SER:HB3	1:B:1031:PHE:HD1	1.75	0.50
1:B:1203:ILE:HG13	1:B:1204:GLY:N	2.26	0.50
1:B:2268:ILE:HD11	1:B:2283:ARG:NH2	2.19	0.50
1:B:1481:LEU:HD22	1:B:1483:ILE:CD1	2.39	0.50
1:B:1841:LEU:HD13	1:B:1852:ILE:HG13	1.94	0.50
1:B:2740:PHE:HB2	1:B:2759:HIS:CE1	2.45	0.50
3:B:2807:NAG:O7	3:B:2807:NAG:C1	2.58	0.50
1:A:1207:MET:HE3	1:A:1229:LEU:HB3	1.93	0.50
1:A:1530:TYR:HE2	1:A:1765:ASP:HB2	1.76	0.50
1:B:986:LEU:HD11	1:B:996:MET:SD	2.52	0.50
1:B:1284:ALA:HB2	1:B:1353:ILE:HG13	1.92	0.50
1:B:1751:LEU:CD1	1:B:2519:ILE:HD11	2.41	0.50
1:B:1770:LEU:HD23	1:B:1770:LEU:H	1.76	0.50
1:B:2098:ILE:HB	1:B:2334:ILE:HD13	1.93	0.50
1:A:986:LEU:HD11	1:A:996:MET:SD	2.52	0.50
1:A:995:VAL:HG21	1:A:1101:LEU:HB2	1.94	0.50
1:B:898:ILE:HG22	1:B:898:ILE:O	2.12	0.50
1:B:1427:ASN:OD1	1:B:1469:SER:N	2.44	0.50
1:A:1300:ARG:HH12	1:A:1349:ASN:HA	1.76	0.50
1:A:2383:THR:HG23	1:A:2387:GLU:O	2.12	0.50
1:A:931:SER:HB3	1:A:1002:ARG:HG2	1.92	0.50
1:A:1762:ILE:HG22	1:A:1768:LEU:CD1	2.42	0.50
1:A:1841:LEU:HD13	1:A:1852:ILE:HG13	1.94	0.50
1:B:1498:THR:HG22	1:B:1500:SER:H	1.77	0.50
1:A:1031:PHE:HD2	1:A:2525:GLU:CB	2.25	0.50
1:A:1094:MET:HB2	1:A:1137:SER:HB2	1.92	0.50
1:A:1590:ASP:HB3	1:A:1596:LEU:HD12	1.94	0.50
1:A:1751:LEU:CD1	1:A:2519:ILE:HD11	2.41	0.50
1:A:1755:GLN:HG2	1:A:2036:GLU:O	2.11	0.50
1:B:1878:SER:O	1:B:1879:ARG:HG2	2.12	0.50
1:B:2021:ALA:C	1:B:2022:GLU:HG2	2.33	0.50
1:A:1235:LEU:HD11	1:A:1553:ALA:HB2	1.94	0.50
1:B:1235:LEU:HD11	1:B:1553:ALA:HB2	1.93	0.50
1:B:1300:ARG:NH1	1:B:1349:ASN:HA	2.27	0.50
1:B:1755:GLN:HG2	1:B:2036:GLU:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1427:ASN:OD1	1:A:1469:SER:N	2.44	0.49
1:A:1767:SER:C	1:A:1768:LEU:HD22	2.33	0.49
1:A:2021:ALA:C	1:A:2022:GLU:HG2	2.33	0.49
1:A:2647:VAL:HA	1:A:2667:GLN:O	2.12	0.49
1:B:1050:GLU:OE2	1:B:1695:TYR:OH	2.24	0.49
1:B:1590:ASP:HB3	1:B:1596:LEU:HD12	1.94	0.49
1:B:1664:THR:HG22	1:B:1665:THR:O	2.12	0.49
1:B:2129:ASP:OD1	1:B:2130:ILE:N	2.40	0.49
1:B:2697:ARG:O	1:B:2701:GLN:OE1	2.30	0.49
1:A:2098:ILE:HB	1:A:2334:ILE:HD13	1.93	0.49
1:A:2482:LEU:HB2	1:A:2489:TYR:HE2	1.78	0.49
1:A:2584:ILE:HG13	1:A:2586:VAL:HG12	1.94	0.49
1:B:1031:PHE:HD2	1:B:2525:GLU:CB	2.25	0.49
1:B:2312:PHE:CE1	1:B:2326:LEU:HD21	2.47	0.49
1:B:2463:ASP:OD2	1:B:2465:LYS:HB2	2.11	0.49
1:B:2482:LEU:HB2	1:B:2489:TYR:HE2	1.78	0.49
1:A:1603:THR:HG23	1:A:1843:PHE:HZ	1.74	0.49
1:A:2026:ASP:OD2	1:A:2273:SER:OG	2.30	0.49
1:A:2312:PHE:CE1	1:A:2326:LEU:HD21	2.47	0.49
1:B:877:ASP:HA	1:B:880:GLN:HG2	1.95	0.49
1:B:2647:VAL:HA	1:B:2667:GLN:O	2.12	0.49
1:B:920:HIS:ND1	1:B:990:TRP:HZ3	2.09	0.49
1:B:989:PRO:HG3	1:B:992:ARG:NH2	2.27	0.49
1:B:1094:MET:HE1	1:B:1103:ARG:HH12	1.78	0.49
1:B:1762:ILE:HG22	1:B:1768:LEU:CD1	2.42	0.49
1:A:1498:THR:HG22	1:A:1500:SER:H	1.77	0.49
1:A:1664:THR:HG22	1:A:1665:THR:O	2.12	0.49
1:A:2076:MET:SD	1:A:2311:GLN:NE2	2.85	0.49
1:A:898:ILE:O	1:A:898:ILE:HG22	2.12	0.49
1:A:989:PRO:HG3	1:A:992:ARG:NH2	2.27	0.49
1:A:1878:SER:O	1:A:1879:ARG:HG2	2.12	0.49
1:B:2157:GLU:OE2	1:B:2161:SER:N	2.44	0.49
1:B:2383:THR:HG23	1:B:2387:GLU:O	2.12	0.49
1:A:1300:ARG:NH1	1:A:1349:ASN:HA	2.27	0.49
1:A:2736:GLY:C	1:A:2763:GLN:HE22	2.16	0.49
1:B:1603:THR:HG23	1:B:1843:PHE:HZ	1.74	0.49
1:B:2520:LEU:HD23	1:B:2520:LEU:H	1.78	0.49
1:A:2008:ARG:NH2	1:A:2256:ASP:OD2	2.45	0.49
1:A:2096:ALA:CB	1:A:2103:LEU:HD12	2.41	0.49
1:B:2055:ILE:HG12	1:B:2069:PHE:HD1	1.77	0.49
1:B:2233:ARG:HB3	1:B:2233:ARG:CZ	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:990:TRP:HE1	1:A:1546:ALA:HB3	1.78	0.49
1:A:1581:PRO:HB3	1:A:1794:THR:HG22	1.94	0.49
1:B:990:TRP:HE1	1:B:1546:ALA:HB3	1.78	0.49
1:B:995:VAL:HG21	1:B:1101:LEU:HB2	1.94	0.49
1:B:2736:GLY:C	1:B:2763:GLN:HE22	2.16	0.49
1:A:877:ASP:HA	1:A:880:GLN:HG2	1.95	0.49
1:A:1043:PRO:HD2	1:A:2520:LEU:HA	1.95	0.49
1:A:1601:LEU:HB3	1:A:1602:PRO:HD3	1.95	0.49
1:B:1213:ARG:HG2	1:B:1228:LYS:HG3	1.95	0.49
1:B:1349:ASN:HB2	1:B:1366:GLY:HA2	1.94	0.49
1:B:1767:SER:C	1:B:1768:LEU:HD22	2.33	0.49
1:B:2026:ASP:OD2	1:B:2273:SER:OG	2.30	0.49
1:A:1148:LEU:HD12	1:A:1148:LEU:O	2.13	0.48
1:A:1349:ASN:HB2	1:A:1366:GLY:HA2	1.94	0.48
1:A:2653:ASN:OD1	1:A:2662:ARG:HB3	2.13	0.48
1:B:2086:ASP:O	1:B:2086:ASP:OD1	2.31	0.48
1:A:1913:ILE:O	1:A:1928:TYR:OH	2.26	0.48
1:B:1043:PRO:HD2	1:B:2520:LEU:HA	1.95	0.48
1:A:1511:SER:HB3	1:A:1535:LYS:HZ2	1.78	0.48
1:A:2694:ALA:HB1	1:A:2753:ASP:HB3	1.96	0.48
1:B:916:PHE:CE1	1:B:964:THR:HA	2.49	0.48
1:B:1777:GLU:HB3	1:B:1801:THR:CG2	2.43	0.48
1:A:916:PHE:CE1	1:A:964:THR:HA	2.49	0.48
1:A:1360:LEU:HD21	1:A:1362:TYR:CE1	2.49	0.48
1:A:2520:LEU:HD23	1:A:2520:LEU:H	1.78	0.48
1:B:2008:ARG:NH2	1:B:2256:ASP:OD2	2.45	0.48
1:A:2697:ARG:O	1:A:2701:GLN:OE1	2.30	0.48
1:B:1148:LEU:HD12	1:B:1148:LEU:O	2.13	0.48
1:B:2314:TYR:CZ	1:B:2323:VAL:HG12	2.49	0.48
1:B:2653:ASN:OD1	1:B:2662:ARG:HB3	2.13	0.48
1:A:1012:ASP:C	1:A:1013:LEU:HD22	2.34	0.48
1:A:1213:ARG:HG2	1:A:1228:LYS:HG3	1.95	0.48
1:A:1537:ASN:ND2	1:A:1556:GLY:HA3	2.29	0.48
1:A:1632:ARG:O	1:A:1640:LEU:HB2	2.14	0.48
1:A:2086:ASP:O	1:A:2086:ASP:OD1	2.31	0.48
1:B:1103:ARG:O	1:B:1103:ARG:HG3	2.14	0.48
1:B:1300:ARG:HH12	1:B:1349:ASN:HA	1.76	0.48
1:B:1552:VAL:CG1	1:B:1561:ARG:HB2	2.44	0.48
1:B:2008:ARG:NH2	1:B:2258:ASP:OD2	2.42	0.48
1:A:964:THR:HB	1:A:970:ILE:CD1	2.44	0.48
1:A:1432:ILE:HD13	1:A:1438:VAL:HG12	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1537:ASN:ND2	1:B:1556:GLY:HA3	2.29	0.48
1:A:1777:GLU:HB3	1:A:1801:THR:CG2	2.43	0.48
1:A:2759:HIS:NE2	1:A:2761:MET:CE	2.77	0.48
1:A:1204:GLY:HA3	1:A:1562:PHE:CZ	2.49	0.48
1:A:2197:ASP:OD1	1:A:2198:ALA:N	2.43	0.48
1:B:1918:PHE:HB3	1:B:2173:MET:HE2	1.94	0.48
1:B:2759:HIS:NE2	1:B:2761:MET:CE	2.77	0.48
1:A:1335:ARG:HB3	1:A:1338:ASP:HB3	1.95	0.47
1:A:1079:LEU:CD1	1:A:1106:PHE:CE2	2.97	0.47
1:A:1481:LEU:HD22	1:A:1483:ILE:CD1	2.39	0.47
1:A:2150:ARG:HG3	1:A:2150:ARG:HH11	1.80	0.47
1:A:2150:ARG:NH1	1:A:2170:TYR:CD1	2.82	0.47
1:A:2233:ARG:HB3	1:A:2233:ARG:CZ	2.43	0.47
1:A:2314:TYR:CZ	1:A:2323:VAL:HG12	2.49	0.47
1:A:2378:LYS:CE	1:A:2380:ILE:HD11	2.41	0.47
1:B:2096:ALA:CB	1:B:2103:LEU:HD12	2.41	0.47
1:B:2150:ARG:HG3	1:B:2150:ARG:HH11	1.80	0.47
1:B:2694:ALA:HB1	1:B:2753:ASP:HB3	1.96	0.47
1:A:979:PHE:HE1	1:A:1002:ARG:HA	1.79	0.47
1:B:970:ILE:HG22	1:B:971:ILE:H	1.79	0.47
1:B:979:PHE:HE1	1:B:1002:ARG:HA	1.79	0.47
1:B:1511:SER:HB3	1:B:1535:LYS:HZ1	1.78	0.47
1:B:2150:ARG:NH1	1:B:2170:TYR:CD1	2.82	0.47
1:A:1498:THR:HG22	1:A:1499:THR:N	2.30	0.47
1:A:1552:VAL:CG1	1:A:1561:ARG:HB2	2.44	0.47
1:A:2016:LYS:H	1:A:2016:LYS:HD2	1.79	0.47
1:B:1012:ASP:C	1:B:1013:LEU:HD22	2.34	0.47
1:B:1432:ILE:HD13	1:B:1438:VAL:HG12	1.96	0.47
1:B:1831:LEU:HD23	1:B:1838:LEU:HD23	1.97	0.47
1:A:880:GLN:HG3	1:A:881:GLU:N	2.29	0.47
1:A:1265:GLU:N	1:A:1314:LEU:O	2.47	0.47
1:A:1620:LEU:CD2	1:A:1622:THR:HG23	2.44	0.47
1:A:1831:LEU:HD23	1:A:1838:LEU:HD23	1.97	0.47
1:B:1601:LEU:HB3	1:B:1602:PRO:HD3	1.95	0.47
1:B:1632:ARG:O	1:B:1640:LEU:HB2	2.14	0.47
1:A:1027:PRO:HA	1:A:1742:LEU:HD21	1.95	0.47
1:A:2335:THR:HG21	1:A:2348:MET:HE2	1.94	0.47
1:B:1204:GLY:HA3	1:B:1562:PHE:CZ	2.50	0.47
1:B:1311:VAL:HG22	1:B:1313:ASP:H	1.79	0.47
1:B:1360:LEU:HD21	1:B:1362:TYR:CE1	2.49	0.47
1:B:2534:VAL:HG22	1:B:2534:VAL:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2584:ILE:HG13	1:B:2586:VAL:HG12	1.94	0.47
1:A:1008:ILE:N	1:A:1009:PRO:CD	2.78	0.47
1:A:1103:ARG:HG3	1:A:1103:ARG:O	2.14	0.47
1:A:1412:LEU:HD11	1:A:1421:LEU:CD1	2.37	0.47
1:A:1613:THR:HG22	1:A:1617:ASP:H	1.79	0.47
1:A:2055:ILE:HG12	1:A:2069:PHE:HD1	1.77	0.47
1:A:2362:ASN:OD1	1:A:2363:ILE:HG23	2.15	0.47
1:A:2403:HIS:CB	1:A:2416:MET:HE1	2.32	0.47
1:A:2553:ALA:N	1:A:2554:PRO:HD2	2.30	0.47
1:B:880:GLN:HG3	1:B:881:GLU:N	2.29	0.47
1:B:964:THR:HB	1:B:970:ILE:CD1	2.44	0.47
1:B:1307:SER:O	1:B:1317:ASN:ND2	2.37	0.47
1:B:1335:ARG:HB3	1:B:1338:ASP:HB3	1.95	0.47
1:B:2076:MET:SD	1:B:2311:GLN:NE2	2.85	0.47
1:B:2520:LEU:HD23	1:B:2523:GLN:NE2	2.26	0.47
1:A:970:ILE:HG22	1:A:971:ILE:H	1.79	0.47
1:B:1027:PRO:HA	1:B:1742:LEU:HD21	1.95	0.47
1:B:2358:ILE:CG2	1:B:2366:PRO:HB3	2.45	0.47
1:B:2362:ASN:OD1	1:B:2363:ILE:HG23	2.15	0.47
1:B:2574:LEU:CD2	1:B:2579:VAL:HG22	2.45	0.47
1:A:1237:CYS:SG	1:A:1545:CYS:N	2.88	0.47
1:A:1311:VAL:HG22	1:A:1313:ASP:H	1.79	0.47
1:B:1079:LEU:CD1	1:B:1106:PHE:CE2	2.97	0.47
1:B:2016:LYS:H	1:B:2016:LYS:HD2	1.80	0.47
1:B:2084:ASN:HB2	1:B:2093:SER:OG	2.15	0.47
1:A:1037:GLU:CD	1:A:1037:GLU:H	2.18	0.47
1:A:1054:ILE:HD11	1:A:1059:MET:HB2	1.95	0.47
1:A:1207:MET:HG2	1:A:1208:GLY:N	2.30	0.47
1:A:2156:TYR:CD2	1:A:2158:ILE:HD11	2.49	0.47
1:A:2419:ARG:NH1	1:A:2432:ASP:HB2	2.30	0.47
1:A:2534:VAL:O	1:A:2534:VAL:HG22	2.15	0.47
1:B:1613:THR:HG22	1:B:1617:ASP:H	1.79	0.47
1:B:1770:LEU:HD23	1:B:1770:LEU:N	2.30	0.47
1:B:2036:GLU:OE1	1:B:2036:GLU:HA	2.15	0.47
1:A:941:ILE:CD1	1:A:974:PHE:HD1	2.28	0.46
1:A:1482:TYR:CE2	1:A:1506:VAL:HG21	2.51	0.46
3:A:2803:NAG:H83	3:A:2803:NAG:C3	2.28	0.46
1:B:1054:ILE:HD11	1:B:1059:MET:HB2	1.96	0.46
1:B:1076:ARG:HG3	1:B:1720:THR:HG21	1.98	0.46
1:B:1620:LEU:CD2	1:B:1622:THR:HG23	2.44	0.46
1:B:1725:HIS:NE2	1:B:1727:GLN:NE2	2.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2056:ARG:NE	1:B:2070:ARG:HH12	2.13	0.46
1:B:2419:ARG:NH1	1:B:2432:ASP:HB2	2.30	0.46
1:A:1349:ASN:O	1:A:1366:GLY:N	2.48	0.46
1:A:1394:SER:HB3	1:A:1399:MET:SD	2.55	0.46
1:A:2036:GLU:HA	1:A:2036:GLU:OE1	2.15	0.46
1:B:1622:THR:HG22	1:B:1628:MET:HG2	1.97	0.46
1:A:2008:ARG:NH2	1:A:2258:ASP:OD2	2.42	0.46
1:A:2728:VAL:HG22	1:A:2734:VAL:HG23	1.97	0.46
1:B:941:ILE:CD1	1:B:974:PHE:HD1	2.28	0.46
1:B:1080:THR:HG1	1:B:1112:LEU:H	1.62	0.46
1:B:2222:ASN:ND2	1:B:2243:ASP:OD2	2.45	0.46
1:A:1058:LYS:HE2	1:A:1175:LYS:HZ1	1.81	0.46
1:A:2531:LYS:O	1:A:2535:THR:HG23	2.15	0.46
1:B:1037:GLU:H	1:B:1037:GLU:CD	2.18	0.46
1:B:1302:VAL:HG23	1:B:1321:VAL:HG12	1.98	0.46
1:B:1394:SER:HB3	1:B:1399:MET:SD	2.55	0.46
1:B:2156:TYR:CD2	1:B:2158:ILE:HD11	2.49	0.46
2:I:1:NAG:O7	2:I:1:NAG:O3	2.30	0.46
1:A:1297:SER:C	1:A:1300:ARG:HH21	2.19	0.46
1:A:1622:THR:HG22	1:A:1628:MET:HG2	1.97	0.46
1:A:1770:LEU:HD23	1:A:1770:LEU:N	2.30	0.46
1:A:2129:ASP:OD1	1:A:2130:ILE:N	2.40	0.46
1:B:2553:ALA:N	1:B:2554:PRO:HD2	2.30	0.46
1:A:1302:VAL:HG23	1:A:1321:VAL:HG12	1.98	0.46
1:A:1646:ASP:OD1	1:A:1648:GLN:HB2	2.15	0.46
1:A:2718:ARG:HD3	1:A:2720:TRP:HE1	1.80	0.46
1:B:1067:ARG:HG2	1:B:1162:GLU:CD	2.36	0.46
1:B:1237:CYS:SG	1:B:1545:CYS:N	2.88	0.46
1:B:1498:THR:HG22	1:B:1499:THR:N	2.30	0.46
1:B:1864:LEU:C	1:B:1864:LEU:HD23	2.36	0.46
2:E:1:NAG:O7	2:E:1:NAG:O3	2.30	0.46
1:A:1762:ILE:HG22	1:A:1768:LEU:HD13	1.97	0.46
1:A:1941:ARG:NH2	1:A:1943:TYR:OH	2.47	0.46
1:A:2056:ARG:NE	1:A:2070:ARG:HH12	2.13	0.46
1:A:2084:ASN:HB2	1:A:2093:SER:OG	2.15	0.46
1:B:1297:SER:C	1:B:1300:ARG:HH21	2.18	0.46
1:B:2655:VAL:HG23	1:B:2659:ARG:O	2.16	0.46
1:A:2574:LEU:CD2	1:A:2579:VAL:HG22	2.45	0.46
1:B:1008:ILE:N	1:B:1009:PRO:CD	2.78	0.46
1:A:1080:THR:O	1:A:1111:ASP:HA	2.16	0.46
1:A:1401:ILE:O	1:A:1404:VAL:HG22	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1207:MET:HG2	1:B:1208:GLY:N	2.30	0.46
1:A:1022:VAL:HB	1:A:1078:SER:OG	2.16	0.46
1:A:1077:ILE:HD11	1:A:1114:TYR:HB3	1.98	0.46
1:A:1207:MET:CE	1:A:1229:LEU:HD13	2.46	0.46
1:B:1581:PRO:HB3	1:B:1794:THR:HG22	1.94	0.46
1:B:2254:LYS:HB3	1:B:2263:GLN:HB3	1.98	0.46
1:B:2378:LYS:CE	1:B:2380:ILE:HD11	2.41	0.46
1:A:1067:ARG:HG2	1:A:1162:GLU:CD	2.36	0.45
1:B:1265:GLU:N	1:B:1314:LEU:O	2.47	0.45
1:B:1595:HIS:O	1:B:1612:TYR:OH	2.28	0.45
1:B:1646:ASP:OD1	1:B:1648:GLN:HB2	2.15	0.45
1:B:2721:THR:C	1:B:2725:LYS:HZ2	2.20	0.45
1:A:1725:HIS:NE2	1:A:1727:GLN:NE2	2.64	0.45
1:A:1864:LEU:C	1:A:1864:LEU:HD23	2.36	0.45
1:A:2391:ASP:OD1	1:A:2391:ASP:O	2.34	0.45
1:A:2655:VAL:HG23	1:A:2659:ARG:O	2.16	0.45
1:B:1080:THR:O	1:B:1111:ASP:HA	2.16	0.45
1:B:1207:MET:CE	1:B:1229:LEU:HD13	2.46	0.45
1:A:1031:PHE:HE2	1:A:2525:GLU:HG2	1.80	0.45
1:B:976:ARG:HB3	1:B:979:PHE:HB2	1.97	0.45
1:B:1203:ILE:CD1	1:B:1563:ILE:HG13	2.46	0.45
1:B:1850:GLU:HB3	1:B:1863:ILE:HB	1.99	0.45
1:A:1203:ILE:CD1	1:A:1563:ILE:HG13	2.46	0.45
1:A:2133:ILE:HG23	1:A:2142:THR:HG22	1.98	0.45
1:A:2268:ILE:HD11	1:A:2283:ARG:NH2	2.19	0.45
1:B:1762:ILE:HG22	1:B:1768:LEU:HD13	1.97	0.45
1:B:2133:ILE:HG23	1:B:2142:THR:HG22	1.98	0.45
1:B:2391:ASP:OD1	1:B:2391:ASP:O	2.34	0.45
1:B:2531:LYS:O	1:B:2535:THR:HG23	2.15	0.45
1:A:976:ARG:HB3	1:A:979:PHE:HB2	1.97	0.45
1:A:1076:ARG:HG3	1:A:1720:THR:HG21	1.98	0.45
1:A:1483:ILE:HD13	1:A:1497:VAL:HG23	1.99	0.45
1:A:2254:LYS:HB3	1:A:2263:GLN:HB3	1.98	0.45
1:B:1012:ASP:O	1:B:1013:LEU:HD22	2.17	0.45
1:B:1181:ILE:HD11	1:B:1576:TYR:OH	2.16	0.45
1:B:1401:ILE:O	1:B:1404:VAL:HG22	2.16	0.45
1:B:1725:HIS:HE1	1:B:1737:THR:CG2	2.30	0.45
1:A:1012:ASP:O	1:A:1013:LEU:HD22	2.17	0.45
1:A:1181:ILE:HD11	1:A:1576:TYR:OH	2.16	0.45
1:B:1022:VAL:HB	1:B:1078:SER:OG	2.16	0.45
1:B:1482:TYR:CE2	1:B:1506:VAL:HG21	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2728:VAL:HG22	1:B:2734:VAL:HG23	1.97	0.45
1:A:990:TRP:NE1	1:A:1546:ALA:HB3	2.32	0.45
1:A:1058:LYS:HE2	1:A:1175:LYS:NZ	2.32	0.45
1:A:2358:ILE:CG2	1:A:2366:PRO:HB3	2.45	0.45
1:B:1079:LEU:HD22	1:B:1138:VAL:HG21	1.99	0.45
1:B:1489:LYS:O	1:B:1514:ASP:OD1	2.35	0.45
1:B:1941:ARG:NH2	1:B:1943:TYR:OH	2.47	0.45
1:A:1037:GLU:OE1	1:A:1037:GLU:N	2.50	0.45
1:A:1927:THR:HB	1:A:1934:VAL:HG12	1.99	0.45
1:B:1077:ILE:HD11	1:B:1114:TYR:HB3	1.98	0.45
1:B:1483:ILE:HD13	1:B:1497:VAL:HG23	1.99	0.45
1:B:1964:GLN:HG3	1:B:1982:PRO:HD3	1.99	0.45
1:B:2189:THR:O	1:B:2189:THR:HG23	2.17	0.45
1:A:1207:MET:HG3	1:A:1227:ASN:HB3	1.99	0.45
1:A:1489:LYS:O	1:A:1514:ASP:OD1	2.35	0.45
1:A:1495:ARG:NH2	1:A:1503:ILE:HG12	2.32	0.45
1:B:989:PRO:HB3	1:B:1477:HIS:CE1	2.52	0.45
1:B:1058:LYS:HE2	1:B:1175:LYS:NZ	2.32	0.45
1:A:1079:LEU:HD22	1:A:1138:VAL:HG21	1.99	0.45
1:A:1372:ILE:HD13	1:A:1378:ILE:CG2	2.45	0.45
1:A:1725:HIS:HE1	1:A:1737:THR:CG2	2.30	0.45
1:A:2462:GLN:OE1	1:A:2462:GLN:N	2.48	0.45
1:A:1850:GLU:HB3	1:A:1863:ILE:HB	1.99	0.44
1:B:1495:ARG:NH2	1:B:1503:ILE:HG12	2.32	0.44
1:B:2098:ILE:HB	1:B:2334:ILE:HD11	1.99	0.44
1:A:896:ASP:CA	1:A:899:LYS:HZ3	2.20	0.44
1:A:989:PRO:HB3	1:A:1477:HIS:CE1	2.52	0.44
1:B:1037:GLU:N	1:B:1037:GLU:OE1	2.50	0.44
1:B:1058:LYS:HE2	1:B:1175:LYS:HZ1	1.83	0.44
1:B:1349:ASN:O	1:B:1366:GLY:N	2.48	0.44
1:B:1678:ASN:OD1	1:B:1678:ASN:C	2.56	0.44
1:A:1088:LEU:HD23	1:A:1108:ALA:HB2	1.99	0.44
1:A:1903:GLU:HG3	1:A:1904:ARG:N	2.32	0.44
1:A:2079:ALA:CB	1:A:2098:ILE:HG12	2.48	0.44
1:A:2222:ASN:ND2	1:A:2243:ASP:OD2	2.45	0.44
1:B:1217:CYS:O	1:B:1220:CYS:SG	2.76	0.44
1:B:1836:ARG:HH11	1:B:1836:ARG:HB2	1.82	0.44
1:B:2079:ALA:CB	1:B:2098:ILE:HG12	2.48	0.44
1:A:1031:PHE:CD1	1:A:1031:PHE:N	2.84	0.44
1:A:2041:LEU:CB	1:A:2510:THR:HG21	2.40	0.44
1:A:2494:MET:O	1:A:2494:MET:SD	2.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1713:VAL:HG13	1:B:1713:VAL:O	2.17	0.44
1:B:2018:SER:OG	1:B:2517:LYS:CE	2.66	0.44
1:B:2026:ASP:OD1	1:B:2756:ASN:CB	2.65	0.44
1:B:2066:ARG:HD3	1:B:2080:ARG:NH2	2.32	0.44
1:B:2718:ARG:HD3	1:B:2720:TRP:HE1	1.80	0.44
1:A:1030:SER:HB3	1:A:1031:PHE:CD1	2.53	0.44
1:A:1136:VAL:CG1	1:A:1154:ARG:HB2	2.47	0.44
1:A:1668:HIS:CD2	1:A:1949:LYS:HD2	2.53	0.44
1:A:1678:ASN:C	1:A:1678:ASN:OD1	2.56	0.44
1:A:2139:MET:HG2	1:A:2140:THR:H	1.83	0.44
1:A:2269:PHE:HE2	1:A:2411:THR:HB	1.83	0.44
1:B:1088:LEU:HD23	1:B:1108:ALA:HB2	1.99	0.44
1:B:1368:MET:SD	1:B:1369:ILE:N	2.91	0.44
1:B:1554:ASP:HB3	1:B:1557:ASN:OD1	2.17	0.44
1:B:2269:PHE:HE2	1:B:2411:THR:HB	1.83	0.44
1:A:1550:LEU:HD23	1:A:1550:LEU:C	2.38	0.44
1:A:2066:ARG:HD3	1:A:2080:ARG:NH2	2.32	0.44
1:A:2079:ALA:HB1	1:A:2098:ILE:HG12	2.00	0.44
1:A:2165:TRP:CE3	1:A:2167:THR:HG23	2.52	0.44
1:A:2721:THR:C	1:A:2725:LYS:HZ2	2.20	0.44
1:B:1031:PHE:N	1:B:1031:PHE:CD1	2.84	0.44
1:B:1207:MET:HG3	1:B:1227:ASN:HB3	1.99	0.44
1:B:2165:TRP:CE3	1:B:2167:THR:HG23	2.52	0.44
1:A:1360:LEU:CD2	1:A:1362:TYR:CE1	3.01	0.44
1:A:1368:MET:SD	1:A:1369:ILE:N	2.91	0.44
1:A:1382:LEU:HD21	1:A:1406:LEU:HD23	2.00	0.44
1:A:1522:ASP:OD1	1:A:1523:CYS:N	2.51	0.44
1:A:1554:ASP:HB3	1:A:1557:ASN:OD1	2.17	0.44
1:A:1752:LEU:HD13	1:A:1757:ARG:HB2	2.00	0.44
1:A:2058:ARG:HG2	1:A:2058:ARG:NH1	2.33	0.44
1:A:2098:ILE:HB	1:A:2334:ILE:HD11	1.99	0.44
1:A:2657:ASN:H	1:A:2659:ARG:CZ	2.31	0.44
1:B:990:TRP:NE1	1:B:1546:ALA:HB3	2.32	0.44
1:B:1903:GLU:HG3	1:B:1904:ARG:N	2.32	0.44
1:B:2197:ASP:OD1	1:B:2198:ALA:N	2.43	0.44
1:B:2512:GLU:OE1	1:B:2512:GLU:HA	2.18	0.44
1:A:1008:ILE:HG12	1:A:1009:PRO:HD3	2.00	0.44
1:A:1052:ILE:HG23	1:A:1670:LEU:CD2	2.48	0.44
1:B:1836:ARG:NH1	1:B:1836:ARG:CB	2.81	0.44
1:B:2736:GLY:HA3	1:B:2762:ARG:NH1	2.33	0.44
1:A:1217:CYS:O	1:A:1220:CYS:SG	2.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1245:VAL:CG1	1:A:1252:ARG:HB2	2.48	0.44
1:A:1695:TYR:HD1	1:A:1706:VAL:HG12	1.83	0.44
1:A:1964:GLN:HG3	1:A:1982:PRO:HD3	1.99	0.44
1:A:2189:THR:HG23	1:A:2189:THR:O	2.17	0.44
1:A:2482:LEU:HB3	1:A:2489:TYR:CD2	2.53	0.44
1:B:941:ILE:HD12	1:B:974:PHE:CE1	2.53	0.44
1:B:1008:ILE:HG12	1:B:1009:PRO:HD3	2.00	0.44
1:B:1031:PHE:HE2	1:B:2525:GLU:HG2	1.80	0.44
1:B:1158:LEU:HD23	1:B:1158:LEU:HA	1.79	0.44
1:B:1511:SER:HB3	1:B:1535:LYS:HZ2	1.83	0.44
1:B:1522:ASP:OD1	1:B:1523:CYS:N	2.51	0.44
1:B:1558:ILE:HG13	1:B:1558:ILE:O	2.18	0.44
1:B:1752:LEU:HD13	1:B:1757:ARG:HB2	2.00	0.44
1:B:2060:ILE:HG13	1:B:2060:ILE:O	2.18	0.44
1:B:2079:ALA:HB1	1:B:2098:ILE:HG12	2.00	0.44
1:A:1692:THR:HG23	1:A:1694:PHE:HE1	1.83	0.43
1:A:1836:ARG:HH11	1:A:1836:ARG:HB2	1.82	0.43
1:B:2058:ARG:HG2	1:B:2058:ARG:NH1	2.33	0.43
1:B:2234:LEU:HD23	1:B:2234:LEU:H	1.83	0.43
1:B:2243:ASP:OD1	1:B:2243:ASP:O	2.36	0.43
1:B:2412:LYS:O	1:B:2423:VAL:HG12	2.18	0.43
1:B:2607:LEU:HD23	1:B:2607:LEU:HA	1.79	0.43
1:A:976:ARG:HD3	1:A:979:PHE:CD2	2.54	0.43
1:A:1669:GLU:O	1:A:1669:GLU:HG3	2.18	0.43
1:B:1245:VAL:CG1	1:B:1252:ARG:HB2	2.48	0.43
1:B:1372:ILE:HD13	1:B:1378:ILE:CG2	2.45	0.43
1:B:1754:ASP:C	1:B:1755:GLN:OE1	2.57	0.43
1:B:2482:LEU:HB3	1:B:2489:TYR:CD2	2.53	0.43
1:B:2494:MET:O	1:B:2494:MET:SD	2.76	0.43
1:A:2026:ASP:OD1	1:A:2756:ASN:CB	2.65	0.43
1:B:1668:HIS:CD2	1:B:1949:LYS:HD2	2.53	0.43
1:B:2381:LEU:HD12	1:B:2390:MET:CE	2.49	0.43
1:A:866:ASN:OD1	1:A:867:PRO:HD2	2.18	0.43
1:A:1557:ASN:O	1:A:1559:ARG:HG2	2.18	0.43
1:A:2253:TYR:CZ	1:A:2264:ARG:HG3	2.54	0.43
1:B:1002:ARG:O	1:B:1004:GLU:HG2	2.18	0.43
1:B:1052:ILE:HG23	1:B:1670:LEU:CD2	2.48	0.43
1:B:1136:VAL:CG1	1:B:1154:ARG:HB2	2.47	0.43
1:B:1424:LEU:HD21	1:B:1470:ALA:O	2.19	0.43
1:B:1552:VAL:HG12	1:B:1561:ARG:HB2	2.01	0.43
1:B:1918:PHE:HB3	1:B:2173:MET:HE1	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1976:ARG:HD3	1:B:1989:ILE:HG23	2.01	0.43
1:A:1058:LYS:HB2	1:A:1058:LYS:HE3	1.81	0.43
1:A:1080:THR:HG1	1:A:1112:LEU:H	1.60	0.43
1:A:1354:THR:HG21	1:A:1413:ALA:HA	2.00	0.43
1:A:1371:ARG:NH1	1:A:1381:LEU:CA	2.82	0.43
1:A:2234:LEU:H	1:A:2234:LEU:HD23	1.83	0.43
1:A:2412:LYS:O	1:A:2423:VAL:HG12	2.18	0.43
1:B:1430:LEU:HD12	1:B:1439:ARG:C	2.39	0.43
1:B:1927:THR:HB	1:B:1934:VAL:HG12	1.99	0.43
1:B:2056:ARG:CD	1:B:2070:ARG:HH12	2.32	0.43
1:A:1013:LEU:HD23	1:A:1148:LEU:HD21	2.01	0.43
1:A:1097:VAL:O	1:A:1097:VAL:HG23	2.19	0.43
1:A:1515:CYS:HB3	1:A:1523:CYS:HB3	1.71	0.43
1:A:1754:ASP:HB3	1:A:1755:GLN:OE1	2.19	0.43
1:A:1836:ARG:NH1	1:A:1836:ARG:CB	2.81	0.43
1:A:2283:ARG:HG3	1:A:2284:ALA:N	2.34	0.43
1:A:2381:LEU:HD12	1:A:2390:MET:CE	2.49	0.43
1:A:2736:GLY:HA3	1:A:2762:ARG:NH1	2.33	0.43
1:B:920:HIS:HB2	1:B:990:TRP:CZ3	2.54	0.43
1:B:990:TRP:CD1	1:B:1546:ALA:C	2.92	0.43
1:B:1550:LEU:C	1:B:1550:LEU:HD23	2.38	0.43
1:B:2139:MET:HG2	1:B:2140:THR:H	1.83	0.43
1:B:2283:ARG:HG3	1:B:2284:ALA:N	2.34	0.43
1:A:1301:ARG:HD3	1:A:1320:VAL:HG11	2.00	0.43
1:A:2056:ARG:CD	1:A:2070:ARG:HH12	2.32	0.43
1:B:1357:LYS:CG	1:B:1419:ASN:HD21	2.32	0.43
1:B:1961:VAL:O	1:B:1961:VAL:CG1	2.65	0.43
1:B:2248:LEU:HD12	1:B:2248:LEU:C	2.38	0.43
1:B:2335:THR:HG21	1:B:2348:MET:HE2	1.97	0.43
1:B:2657:ASN:H	1:B:2659:ARG:CZ	2.31	0.43
1:A:920:HIS:HB2	1:A:990:TRP:CZ3	2.53	0.43
1:A:929:MET:HB3	1:A:1000:ILE:HG22	2.01	0.43
1:A:990:TRP:CD1	1:A:1546:ALA:C	2.92	0.43
1:A:1044:GLU:HA	1:A:1044:GLU:OE1	2.18	0.43
1:A:1430:LEU:HD12	1:A:1439:ARG:C	2.39	0.43
1:A:1619:THR:HG22	1:A:1633:ARG:HE	1.84	0.43
1:A:2060:ILE:HG13	1:A:2060:ILE:O	2.18	0.43
1:B:929:MET:HB3	1:B:1000:ILE:HG22	2.01	0.43
1:B:1354:THR:HG21	1:B:1413:ALA:HA	2.00	0.43
1:B:1371:ARG:NH1	1:B:1381:LEU:CA	2.82	0.43
1:B:1654:MET:HE2	1:B:1658:SER:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1695:TYR:HD1	1:B:1706:VAL:HG12	1.83	0.43
1:A:989:PRO:N	1:A:1477:HIS:HE1	2.17	0.43
1:A:1002:ARG:O	1:A:1004:GLU:HG2	2.18	0.43
1:A:1371:ARG:NH1	1:A:1381:LEU:HA	2.34	0.43
1:A:1713:VAL:HG13	1:A:1713:VAL:O	2.18	0.43
1:A:2018:SER:OG	1:A:2517:LYS:CE	2.66	0.43
1:A:2512:GLU:OE1	1:A:2512:GLU:HA	2.18	0.43
1:B:1081:HIS:HB3	1:B:1082:PRO:CD	2.44	0.43
1:B:1557:ASN:O	1:B:1559:ARG:HG2	2.18	0.43
1:B:1613:THR:CG2	1:B:1617:ASP:HB2	2.48	0.43
1:B:1976:ARG:NE	1:B:1991:ASP:OD1	2.52	0.43
1:A:941:ILE:HD12	1:A:974:PHE:CE1	2.53	0.43
1:A:1179:LEU:HD12	1:A:1185:ILE:O	2.19	0.43
1:A:1360:LEU:HD11	1:A:1371:ARG:HG2	2.01	0.43
1:A:2248:LEU:HD12	1:A:2248:LEU:C	2.38	0.43
1:B:985:THR:HG1	1:B:1357:LYS:NZ	2.11	0.43
1:B:1058:LYS:HB2	1:B:1058:LYS:HE3	1.81	0.43
1:B:1301:ARG:HD3	1:B:1320:VAL:HG11	2.00	0.43
1:B:1893:ILE:HD12	1:B:1893:ILE:H	1.84	0.43
1:A:1115:TYR:OH	1:A:1720:THR:CB	2.67	0.42
1:A:1158:LEU:HA	1:A:1158:LEU:HD23	1.79	0.42
1:A:1338:ASP:OD1	1:A:1378:ILE:HG13	2.19	0.42
1:A:1558:ILE:HG13	1:A:1558:ILE:O	2.18	0.42
1:A:1893:ILE:HG21	1:A:1896:ILE:HD11	2.01	0.42
1:A:2656:LEU:HB2	1:A:2659:ARG:NE	2.34	0.42
1:B:866:ASN:OD1	1:B:867:PRO:HD2	2.18	0.42
1:B:976:ARG:HD3	1:B:979:PHE:CD2	2.53	0.42
1:B:976:ARG:HD3	1:B:979:PHE:HD2	1.83	0.42
1:B:989:PRO:N	1:B:1477:HIS:HE1	2.16	0.42
1:B:1044:GLU:OE1	1:B:1044:GLU:HA	2.18	0.42
1:B:1089:MET:O	1:B:1108:ALA:N	2.49	0.42
1:B:1353:ILE:HG22	1:B:1363:PHE:CB	2.49	0.42
1:B:1360:LEU:CD2	1:B:1362:TYR:CE1	3.01	0.42
1:B:1692:THR:HG23	1:B:1694:PHE:HE1	1.83	0.42
1:B:1728:VAL:HB	1:B:1736:VAL:HG22	2.01	0.42
1:B:1893:ILE:HG21	1:B:1896:ILE:HD11	2.01	0.42
1:B:2207:ILE:CD1	1:B:2212:LEU:HD12	2.43	0.42
1:A:1357:LYS:CG	1:A:1419:ASN:HD21	2.32	0.42
1:A:1424:LEU:HD21	1:A:1470:ALA:O	2.19	0.42
1:A:1613:THR:CG2	1:A:1617:ASP:HB2	2.49	0.42
1:A:2059:GLN:HG3	1:A:2063:LEU:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2163:MET:CG	1:A:2370:PHE:CE1	3.02	0.42
1:A:2243:ASP:OD1	1:A:2427:ARG:NH2	2.46	0.42
1:A:2692:GLU:O	1:A:2696:GLN:HG2	2.19	0.42
1:B:985:THR:OG1	1:B:1358:PHE:CE1	2.72	0.42
1:B:1179:LEU:HD12	1:B:1185:ILE:O	2.19	0.42
1:B:1669:GLU:O	1:B:1669:GLU:HG3	2.18	0.42
1:B:1754:ASP:HB3	1:B:1755:GLN:OE1	2.19	0.42
1:B:1976:ARG:NH1	1:B:1989:ILE:HD13	2.35	0.42
1:B:2056:ARG:HD2	1:B:2070:ARG:HH12	1.84	0.42
1:B:2253:TYR:CZ	1:B:2264:ARG:HG3	2.54	0.42
1:B:2531:LYS:HE2	1:B:2531:LYS:HA	2.01	0.42
1:B:2655:VAL:HG22	1:B:2656:LEU:O	2.19	0.42
1:A:2243:ASP:OD1	1:A:2243:ASP:O	2.36	0.42
1:A:2706:GLU:OE2	1:A:2716:GLY:HA3	2.19	0.42
1:B:928:VAL:O	1:B:928:VAL:HG13	2.19	0.42
1:B:1338:ASP:OD1	1:B:1378:ILE:HG13	2.19	0.42
1:A:1067:ARG:HG2	1:A:1162:GLU:OE2	2.19	0.42
1:A:1324:THR:HG23	1:A:1345:ALA:O	2.19	0.42
1:A:1613:THR:HG22	1:A:1617:ASP:HB2	2.01	0.42
1:A:1893:ILE:HD12	1:A:1893:ILE:H	1.84	0.42
1:A:2724:GLU:O	1:A:2728:VAL:HG23	2.19	0.42
1:B:1301:ARG:HA	1:B:1347:LEU:HD21	2.01	0.42
1:B:1412:LEU:HD11	1:B:1421:LEU:CD2	2.46	0.42
1:B:1755:GLN:CG	1:B:2036:GLU:O	2.67	0.42
1:B:2233:ARG:NH1	1:B:2233:ARG:CB	2.82	0.42
1:B:2656:LEU:HB2	1:B:2659:ARG:NE	2.34	0.42
1:B:2706:GLU:OE2	1:B:2716:GLY:HA3	2.19	0.42
1:A:2226:LEU:HD12	1:A:2226:LEU:C	2.40	0.42
1:A:2345:LEU:CD2	1:A:2358:ILE:HD12	2.50	0.42
1:A:2586:VAL:O	1:A:2586:VAL:HG22	2.20	0.42
1:A:2655:VAL:HG22	1:A:2656:LEU:O	2.19	0.42
1:B:1030:SER:HB3	1:B:1031:PHE:CD1	2.53	0.42
1:B:1097:VAL:O	1:B:1097:VAL:HG23	2.19	0.42
1:B:1360:LEU:HD11	1:B:1371:ARG:HG2	2.01	0.42
1:B:1371:ARG:NH1	1:B:1381:LEU:HA	2.34	0.42
1:B:1400:ASP:O	1:B:1404:VAL:HG13	2.20	0.42
1:B:2059:GLN:HG3	1:B:2063:LEU:O	2.19	0.42
1:B:2692:GLU:OE1	1:B:2692:GLU:CA	2.67	0.42
1:A:1961:VAL:O	1:A:1961:VAL:CG1	2.65	0.42
1:A:2601:ALA:HB2	1:A:2621:LYS:HD3	2.02	0.42
1:B:1232:PRO:HD2	1:B:1555:LEU:HD23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1281:TYR:CD2	1:B:1294:LEU:HD11	2.55	0.42
1:B:1613:THR:HG22	1:B:1617:ASP:HB2	2.01	0.42
1:A:944:VAL:HG22	1:A:971:ILE:HG21	2.01	0.42
1:A:1552:VAL:HG12	1:A:1561:ARG:HB2	2.01	0.42
1:A:1976:ARG:NH1	1:A:1989:ILE:HD13	2.35	0.42
1:A:2378:LYS:HG2	1:A:2380:ILE:HD11	2.02	0.42
1:B:1175:LYS:HA	1:B:1175:LYS:HD3	1.81	0.42
1:B:1203:ILE:HD12	1:B:1563:ILE:HG13	2.02	0.42
1:B:1338:ASP:OD2	1:B:1370:ARG:NH1	2.53	0.42
1:B:2724:GLU:O	1:B:2728:VAL:HG23	2.19	0.42
1:A:895:TYR:O	1:A:899:LYS:NZ	2.52	0.42
1:A:1089:MET:HE3	1:A:1143:GLU:HA	2.02	0.42
1:A:1755:GLN:CG	1:A:2036:GLU:O	2.67	0.42
1:B:1305:ILE:H	1:B:1305:ILE:HD12	1.85	0.42
1:B:1382:LEU:HD21	1:B:1406:LEU:HD23	2.00	0.42
1:B:2026:ASP:OD2	1:B:2273:SER:N	2.53	0.42
1:B:2601:ALA:HB2	1:B:2621:LYS:HD3	2.02	0.42
1:A:1084:ILE:HD11	1:A:1110:PRO:CA	2.50	0.42
1:A:1097:VAL:HG23	1:A:1100:ARG:CG	2.50	0.42
1:A:1305:ILE:HD12	1:A:1305:ILE:H	1.85	0.42
1:A:1353:ILE:HG22	1:A:1363:PHE:CB	2.49	0.42
1:A:1515:CYS:SG	1:A:1537:ASN:ND2	2.93	0.42
1:A:1558:ILE:O	1:A:1559:ARG:HG2	2.20	0.42
1:A:1754:ASP:C	1:A:1755:GLN:OE1	2.57	0.42
1:A:1787:LEU:HD11	1:A:1827:PHE:CG	2.55	0.42
1:B:895:TYR:O	1:B:899:LYS:NZ	2.52	0.42
1:B:1091:VAL:HG23	1:B:1106:PHE:HD2	1.85	0.42
1:B:1097:VAL:HG23	1:B:1100:ARG:CG	2.50	0.42
1:B:1324:THR:HG23	1:B:1345:ALA:O	2.19	0.42
1:B:1619:THR:HG22	1:B:1633:ARG:HE	1.84	0.42
1:B:1665:THR:HG22	1:B:1666:GLN:CD	2.40	0.42
1:A:928:VAL:O	1:A:928:VAL:HG13	2.19	0.42
1:A:976:ARG:HD3	1:A:979:PHE:HD2	1.84	0.42
1:A:1054:ILE:HD11	1:A:1059:MET:CB	2.50	0.42
1:A:1281:TYR:CD2	1:A:1294:LEU:HD11	2.55	0.42
1:A:1976:ARG:HD3	1:A:1989:ILE:HG23	2.00	0.42
1:B:1013:LEU:HD23	1:B:1148:LEU:HD21	2.01	0.42
1:B:1067:ARG:HG2	1:B:1162:GLU:OE2	2.19	0.42
1:B:1342:ALA:HB2	1:B:1378:ILE:HG12	2.02	0.42
1:B:1646:ASP:OD1	1:B:1646:ASP:C	2.58	0.42
1:B:2142:THR:OG1	1:B:2155:GLN:HB3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2345:LEU:CD2	1:B:2358:ILE:HD12	2.50	0.42
1:B:2378:LYS:HG2	1:B:2380:ILE:HD11	2.02	0.42
1:A:881:GLU:HA	1:B:2662:ARG:HG2	2.01	0.41
1:A:1362:TYR:HD2	1:A:1421:LEU:HD12	1.85	0.41
1:A:1400:ASP:O	1:A:1404:VAL:HG13	2.20	0.41
1:A:1688:GLU:OE1	1:A:1688:GLU:N	2.37	0.41
1:A:2142:THR:OG1	1:A:2155:GLN:HB3	2.20	0.41
1:A:2233:ARG:NH1	1:A:2233:ARG:CB	2.82	0.41
1:A:2736:GLY:O	1:A:2763:GLN:NE2	2.53	0.41
1:B:1084:ILE:HD11	1:B:1110:PRO:CA	2.50	0.41
1:B:2163:MET:CG	1:B:2370:PHE:CE1	3.03	0.41
1:A:936:LEU:HD21	1:A:976:ARG:HD2	2.02	0.41
1:A:1301:ARG:HA	1:A:1347:LEU:HD21	2.01	0.41
1:A:1646:ASP:OD1	1:A:1646:ASP:C	2.58	0.41
1:A:2607:LEU:HA	1:A:2607:LEU:HD23	1.79	0.41
1:B:1423:VAL:O	1:B:1429:VAL:HA	2.20	0.41
1:B:2420:ASP:O	1:B:2429:THR:HG23	2.20	0.41
1:B:2480:PHE:HB3	1:B:2482:LEU:CD1	2.50	0.41
1:A:985:THR:HG1	1:A:1357:LYS:NZ	2.12	0.41
1:A:1232:PRO:HD2	1:A:1555:LEU:HD23	2.02	0.41
1:A:1782:THR:HB	1:A:1793:PRO:HB2	2.02	0.41
1:A:1785:HIS:HE1	1:A:1787:LEU:HB2	1.84	0.41
1:A:2656:LEU:CB	1:A:2659:ARG:HE	2.33	0.41
1:B:1787:LEU:HD11	1:B:1827:PHE:CG	2.55	0.41
1:B:2586:VAL:HG22	1:B:2586:VAL:O	2.20	0.41
1:B:2692:GLU:O	1:B:2696:GLN:HG2	2.19	0.41
1:A:1338:ASP:OD2	1:A:1370:ARG:NH1	2.53	0.41
1:A:2692:GLU:OE1	1:A:2692:GLU:CA	2.67	0.41
1:A:2759:HIS:NE2	1:A:2761:MET:HE1	2.35	0.41
1:B:989:PRO:HG3	1:B:992:ARG:CZ	2.51	0.41
1:B:1115:TYR:OH	1:B:1720:THR:CB	2.67	0.41
1:B:1931:LYS:HB3	1:B:1931:LYS:HE3	1.93	0.41
1:B:2226:LEU:C	1:B:2226:LEU:HD12	2.40	0.41
1:A:1886:THR:HG1	3:A:2803:NAG:C7	2.34	0.41
1:A:2056:ARG:HD2	1:A:2070:ARG:HH12	1.84	0.41
1:A:2139:MET:HG2	1:A:2140:THR:N	2.35	0.41
1:A:2480:PHE:HB3	1:A:2482:LEU:CD1	2.50	0.41
1:A:2520:LEU:HD21	1:A:2523:GLN:HG3	2.03	0.41
1:B:936:LEU:HD21	1:B:976:ARG:HD2	2.02	0.41
1:B:1041:ILE:HD11	1:B:1706:VAL:HG21	2.03	0.41
1:B:1307:SER:HB2	1:B:1317:ASN:HD21	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1515:CYS:SG	1:B:1537:ASN:ND2	2.93	0.41
1:B:1558:ILE:O	1:B:1559:ARG:HG2	2.20	0.41
1:B:1886:THR:HG1	3:B:2803:NAG:C7	2.34	0.41
1:B:2139:MET:HG2	1:B:2140:THR:N	2.35	0.41
1:B:1609:ASN:HD22	2:G:1:NAG:H83	1.85	0.41
1:B:1660:LEU:HD12	1:B:1660:LEU:HA	1.80	0.41
1:B:1958:MET:O	1:B:1960:ASN:N	2.53	0.41
2:E:1:NAG:H61	2:E:2:NAG:C7	2.50	0.41
1:A:878:ILE:HG22	1:A:900:PHE:HD2	1.86	0.41
1:A:1089:MET:HE2	1:A:1143:GLU:CB	2.50	0.41
1:A:2482:LEU:HB2	1:A:2489:TYR:CE2	2.55	0.41
1:B:944:VAL:HG22	1:B:971:ILE:HG21	2.01	0.41
1:B:1054:ILE:HD11	1:B:1059:MET:CB	2.50	0.41
1:B:1878:SER:C	1:B:1879:ARG:HG2	2.41	0.41
1:B:2143:LYS:HD3	1:B:2154:VAL:HG22	2.03	0.41
1:B:2326:LEU:HA	1:B:2326:LEU:HD23	1.85	0.41
1:B:2656:LEU:CB	1:B:2659:ARG:HE	2.33	0.41
2:I:1:NAG:H61	2:I:2:NAG:C7	2.50	0.41
1:A:1609:ASN:HD22	2:C:1:NAG:H83	1.85	0.41
1:A:2662:ARG:HG2	1:B:881:GLU:HA	2.02	0.41
1:B:1515:CYS:HB3	1:B:1523:CYS:HB3	1.71	0.41
1:B:1704:THR:HG22	1:B:1705:ASN:ND2	2.36	0.41
1:B:2759:HIS:NE2	1:B:2761:MET:HE2	2.35	0.41
1:A:890:ASN:HD21	1:A:1181:ILE:HG22	1.85	0.41
1:A:903:GLY:O	1:A:906:SER:CB	2.67	0.41
1:A:946:ASN:ND2	1:A:949:PHE:CE1	2.89	0.41
1:A:1206:ILE:HG23	1:A:1562:PHE:CD1	2.56	0.41
1:A:1412:LEU:HD11	1:A:1421:LEU:CD2	2.46	0.41
1:A:1423:VAL:O	1:A:1429:VAL:HA	2.20	0.41
1:A:1511:SER:HB3	1:A:1535:LYS:HZ1	1.83	0.41
1:A:1958:MET:O	1:A:1960:ASN:N	2.53	0.41
1:A:2531:LYS:HE2	1:A:2531:LYS:HA	2.01	0.41
1:B:878:ILE:HG22	1:B:900:PHE:HD2	1.86	0.41
1:B:890:ASN:HD21	1:B:1181:ILE:HG22	1.85	0.41
1:B:1362:TYR:HD2	1:B:1421:LEU:HD12	1.85	0.41
1:B:1847:THR:O	1:B:1847:THR:HG22	2.21	0.41
1:B:2309:HIS:H	1:B:2329:HIS:HB3	1.86	0.41
1:B:2328:ASN:ND2	2:H:1:NAG:O7	2.54	0.41
1:A:1203:ILE:HD12	1:A:1563:ILE:HG13	2.02	0.41
1:A:1654:MET:HE2	1:A:1658:SER:HA	2.02	0.41
1:A:1878:SER:C	1:A:1879:ARG:HG2	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2158:ILE:O	1:A:2161:SER:OG	2.36	0.41
1:B:1206:ILE:HG23	1:B:1562:PHE:CD1	2.56	0.41
1:B:1357:LYS:CD	1:B:1419:ASN:HD21	2.34	0.41
1:B:2242:ARG:HB2	1:B:2244:ARG:HD3	2.02	0.41
1:B:2462:GLN:OE1	1:B:2462:GLN:N	2.48	0.41
1:A:1031:PHE:HD2	1:A:2525:GLU:HB2	1.86	0.40
1:B:1229:LEU:HD23	1:B:1229:LEU:N	2.36	0.40
1:A:970:ILE:CG2	1:A:971:ILE:N	2.84	0.40
1:A:1089:MET:O	1:A:1108:ALA:N	2.49	0.40
1:A:1203:ILE:HD12	1:A:1562:PHE:O	2.21	0.40
1:A:1342:ALA:HB2	1:A:1378:ILE:HG12	2.02	0.40
1:A:1362:TYR:HE1	1:A:1371:ARG:CG	2.23	0.40
1:A:1725:HIS:HE1	1:A:1737:THR:HB	1.87	0.40
1:A:1931:LYS:HB3	1:A:1931:LYS:HE3	1.93	0.40
1:A:2084:ASN:O	1:A:2092:THR:HG22	2.21	0.40
1:A:2242:ARG:HB2	1:A:2244:ARG:HD3	2.02	0.40
1:A:2420:ASP:O	1:A:2429:THR:HG23	2.20	0.40
1:B:946:ASN:ND2	1:B:949:PHE:CE1	2.89	0.40
1:B:1203:ILE:HD12	1:B:1562:PHE:O	2.21	0.40
1:B:1424:LEU:HB2	1:B:1473:LEU:HD21	2.04	0.40
1:B:1782:THR:HB	1:B:1793:PRO:HB2	2.02	0.40
1:B:1934:VAL:O	1:B:1934:VAL:HG13	2.21	0.40
1:A:1213:ARG:HD3	1:A:1228:LYS:O	2.21	0.40
1:A:1351:ARG:HH12	1:A:1408:TRP:HE1	1.68	0.40
1:A:1424:LEU:HB2	1:A:1473:LEU:HD21	2.03	0.40
1:A:1665:THR:HG22	1:A:1666:GLN:CD	2.40	0.40
1:A:2255:MET:SD	1:A:2261:LEU:HA	2.61	0.40
1:A:2378:LYS:HE3	1:A:2380:ILE:CG1	2.52	0.40
3:A:2803:NAG:H82	3:A:2803:NAG:C1	2.52	0.40
1:B:1301:ARG:HD3	1:B:1320:VAL:CG1	2.51	0.40
1:B:1351:ARG:HH12	1:B:1408:TRP:HE1	1.68	0.40
1:B:2158:ILE:O	1:B:2161:SER:OG	2.36	0.40
1:B:2255:MET:SD	1:B:2261:LEU:HA	2.61	0.40
1:B:2736:GLY:O	1:B:2763:GLN:NE2	2.53	0.40
1:A:989:PRO:HG3	1:A:992:ARG:CZ	2.51	0.40
1:A:1012:ASP:O	1:A:1012:ASP:OD1	2.39	0.40
1:A:1094:MET:N	1:A:1137:SER:O	2.44	0.40
1:A:1934:VAL:O	1:A:1934:VAL:HG13	2.21	0.40
1:A:2163:MET:HG3	1:A:2370:PHE:CZ	2.57	0.40
1:A:2181:LEU:HD13	1:A:2183:VAL:HG23	2.04	0.40
1:A:2328:ASN:ND2	2:D:1:NAG:O7	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:884:VAL:HB	1:B:885:PRO:HD2	2.04	0.40
1:B:1031:PHE:HD2	1:B:2525:GLU:HB2	1.86	0.40
1:B:1048:LEU:HB3	1:B:1065:SER:HB2	2.04	0.40
1:B:1668:HIS:HE1	1:B:1688:GLU:O	2.04	0.40
1:B:2035:ASP:OD1	1:B:2036:GLU:N	2.55	0.40
1:A:1605:ASP:CG	1:A:1848:ARG:HH22	2.25	0.40
1:A:1847:THR:HG22	1:A:1847:THR:O	2.21	0.40
1:A:2656:LEU:HB2	1:A:2659:ARG:HE	1.87	0.40
1:B:1295:SER:OG	1:B:1353:ILE:HG21	2.22	0.40
1:B:1688:GLU:OE1	1:B:1688:GLU:N	2.37	0.40
1:B:1989:ILE:HB	1:B:2002:PHE:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1894/1932 (98%)	1785 (94%)	109 (6%)	0	100	100
1	B	1894/1932 (98%)	1785 (94%)	109 (6%)	0	100	100
All	All	3788/3864 (98%)	3570 (94%)	218 (6%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	1663/1689 (98%)	1657 (100%)	6 (0%)	89 95
1	B	1663/1689 (98%)	1657 (100%)	6 (0%)	89 95
All	All	3326/3378 (98%)	3314 (100%)	12 (0%)	88 95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1478	ASN
1	A	1776	MET
1	A	1816	ARG
1	A	2128	TYR
1	A	2209	ASP
1	A	2244	ARG
1	B	1478	ASN
1	B	1776	MET
1	B	1816	ARG
1	B	2128	TYR
1	B	2209	ASP
1	B	2244	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1477	HIS
1	A	1785	HIS
1	A	1792	ASN
1	A	2224	HIS
1	A	2483	HIS
1	A	2523	GLN
1	A	2726	GLN
1	B	1477	HIS
1	B	1792	ASN
1	B	2224	HIS
1	B	2483	HIS
1	B	2523	GLN
1	B	2726	GLN

5.3.3 RNA

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)

16 monosaccharides 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	NAG	C	1	2,1	14,14,15	0.22	0	17,19,21	0.47	0
2	NAG	C	2	2	14,14,15	0.33	0	17,19,21	0.43	0
2	NAG	D	1	2,1	14,14,15	0.35	0	17,19,21	0.55	0
2	NAG	D	2	2	14,14,15	0.30	0	17,19,21	0.48	0
2	NAG	E	1	2,1	14,14,15	0.46	0	17,19,21	0.46	0
2	NAG	E	2	2	14,14,15	0.17	0	17,19,21	0.43	0
2	NAG	F	1	2,1	14,14,15	0.40	0	17,19,21	0.46	0
2	NAG	F	2	2	14,14,15	0.30	0	17,19,21	0.42	0
2	NAG	G	1	2,1	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	G	2	2	14,14,15	0.33	0	17,19,21	0.44	0
2	NAG	H	1	2,1	14,14,15	0.35	0	17,19,21	0.55	0
2	NAG	H	2	2	14,14,15	0.30	0	17,19,21	0.48	0
2	NAG	I	1	2,1	14,14,15	0.46	0	17,19,21	0.47	0
2	NAG	I	2	2	14,14,15	0.18	0	17,19,21	0.43	0
2	NAG	J	1	2,1	14,14,15	0.39	0	17,19,21	0.45	0
2	NAG	J	2	2	14,14,15	0.30	0	17,19,21	0.42	0

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	NAG	C	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C1-C2-N2-C7
2	I	1	NAG	C1-C2-N2-C7
2	D	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C3-C2-N2-C7
2	I	1	NAG	C3-C2-N2-C7

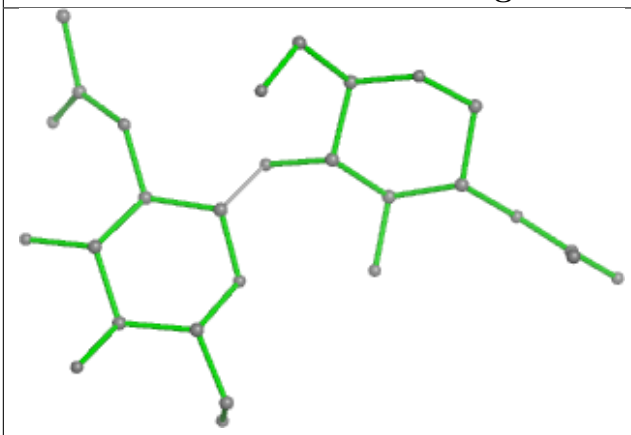
There are no ring outliers.

8 monomers are involved in 12 short contacts:

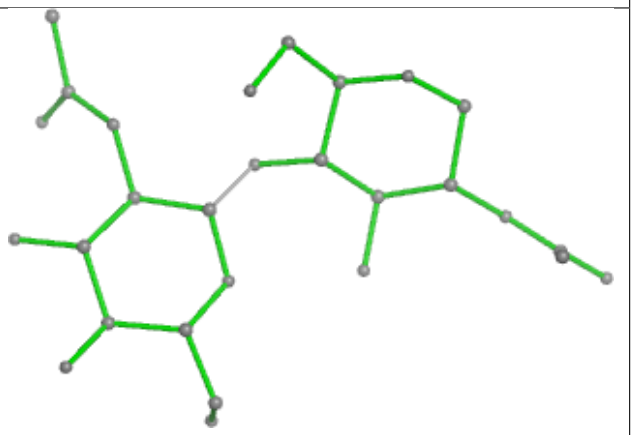
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
2	I	2	NAG	2	0
2	D	1	NAG	1	0
2	E	1	NAG	4	0
2	I	1	NAG	4	0
2	H	1	NAG	1	0
2	E	2	NAG	2	0
2	G	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

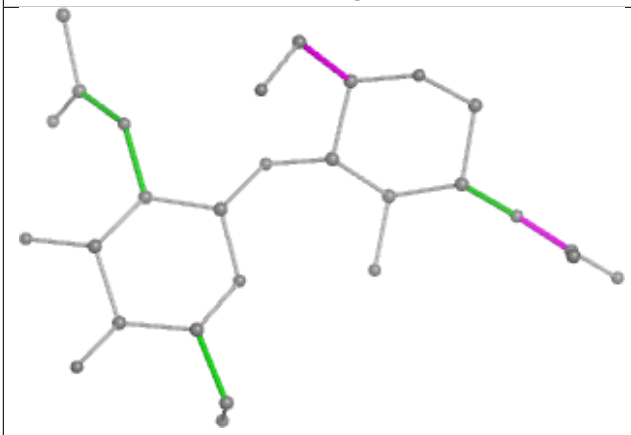
Oligosaccharide Chain C



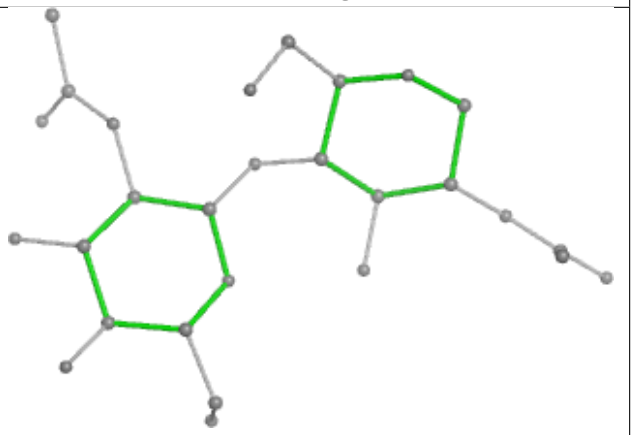
Bond lengths



Bond angles

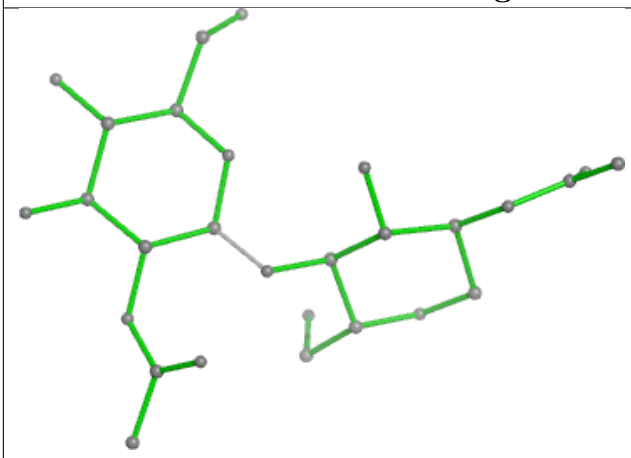


Torsions

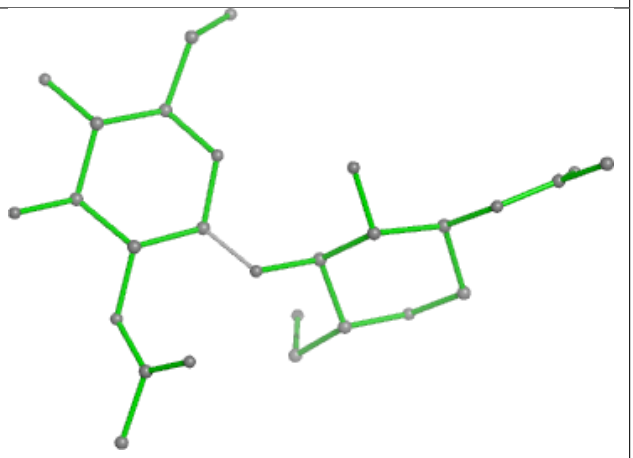


Rings

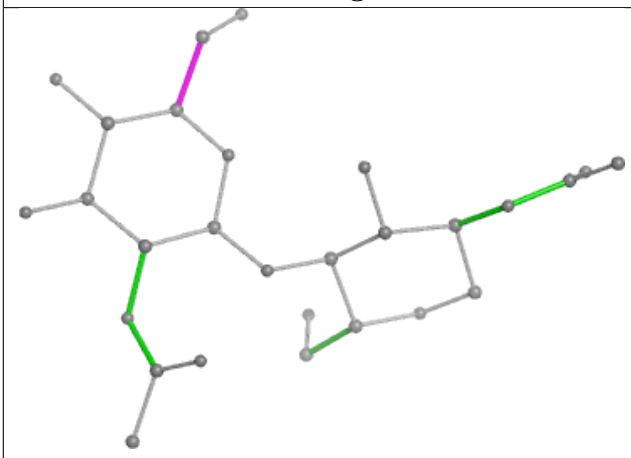
Oligosaccharide Chain D



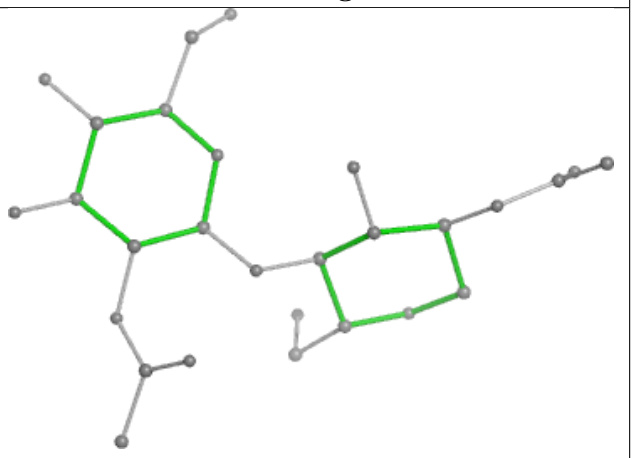
Bond lengths



Bond angles

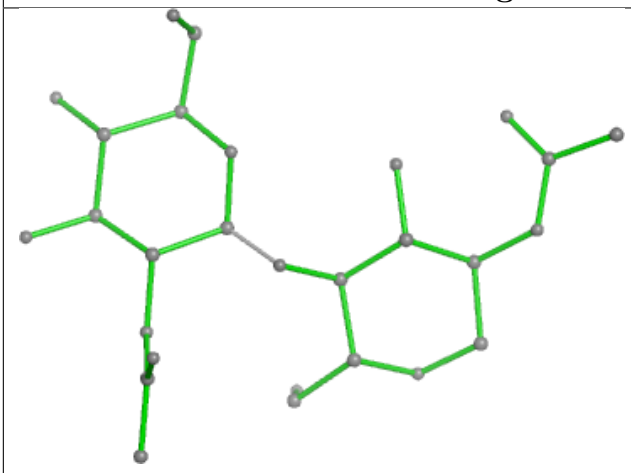


Torsions

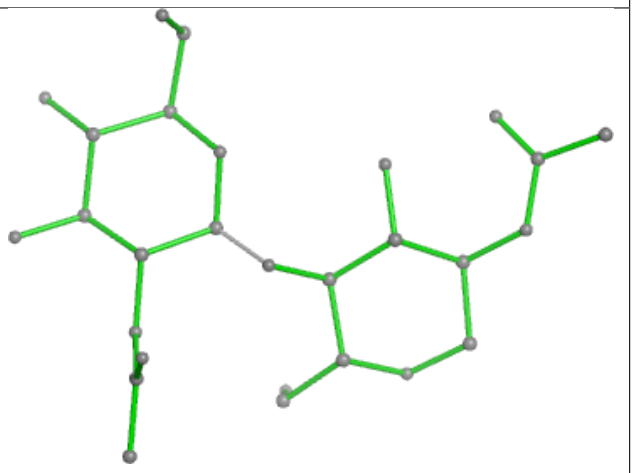


Rings

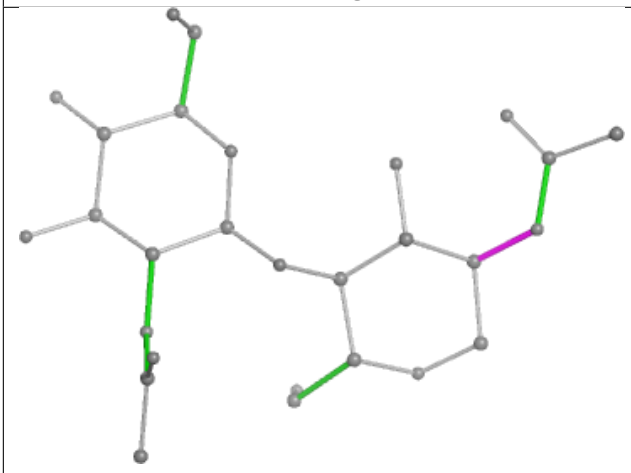
Oligosaccharide Chain E



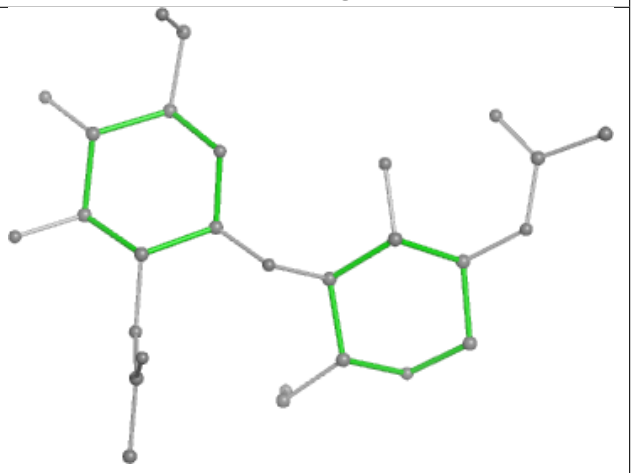
Bond lengths



Bond angles

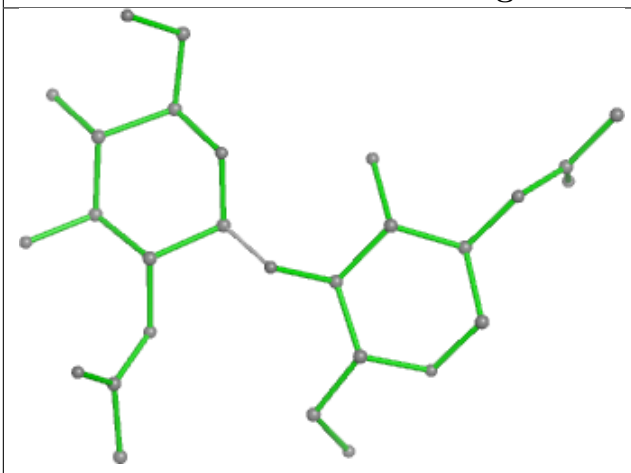


Torsions

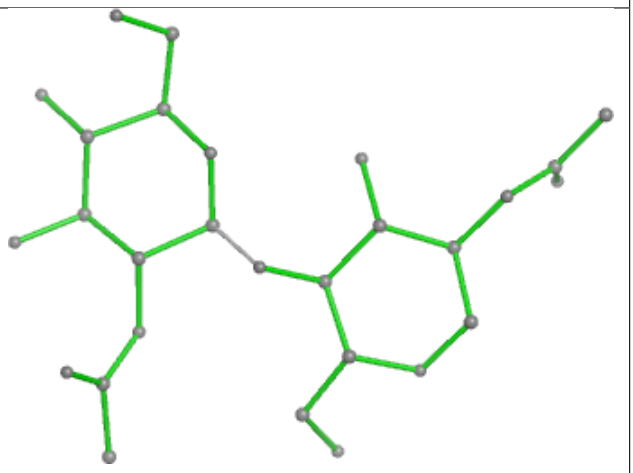


Rings

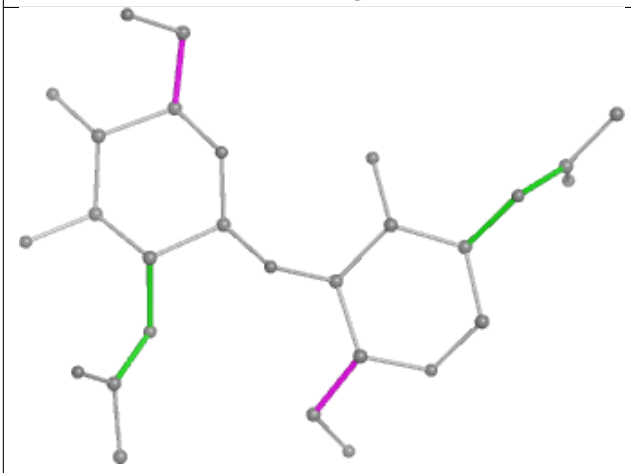
Oligosaccharide Chain F



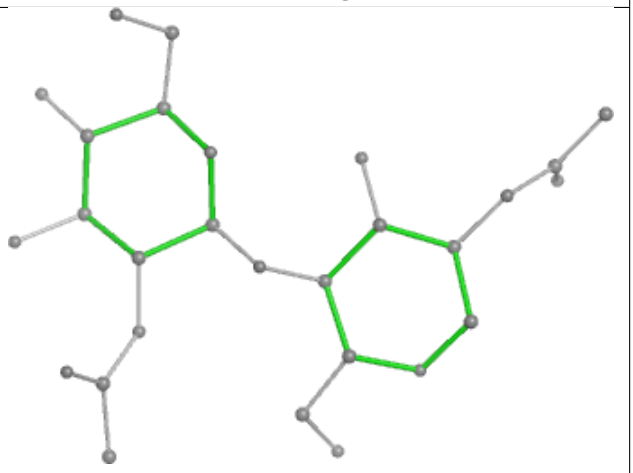
Bond lengths



Bond angles

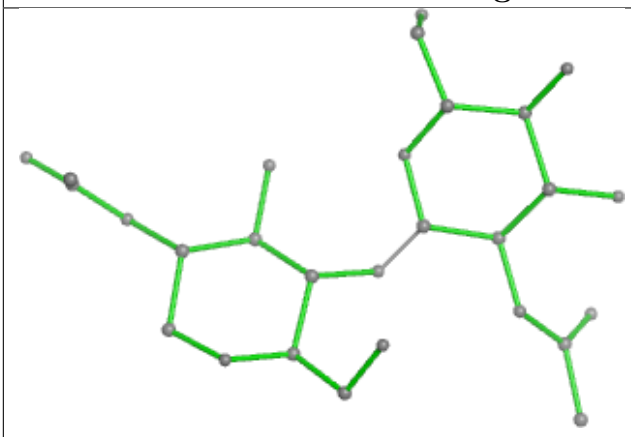


Torsions

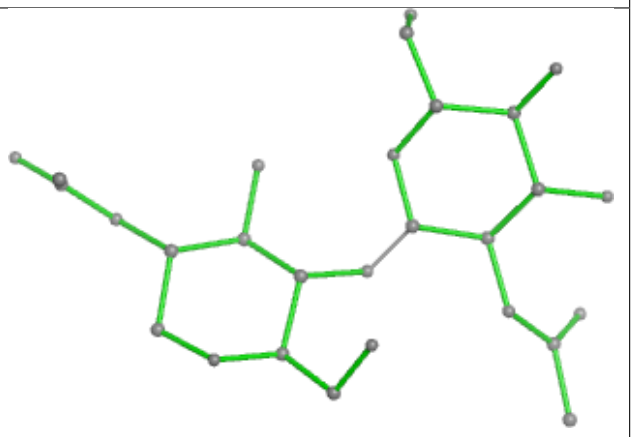


Rings

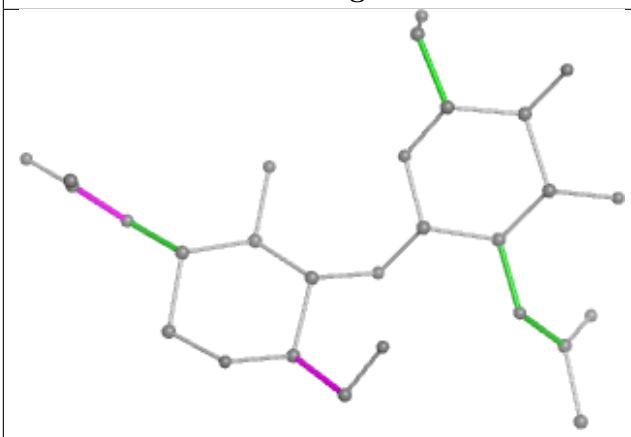
Oligosaccharide Chain G



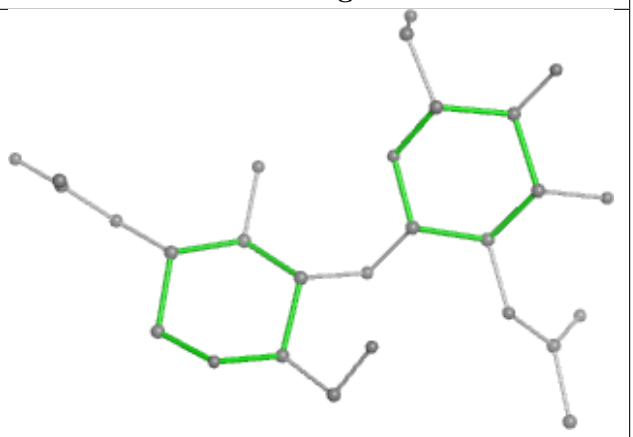
Bond lengths



Bond angles

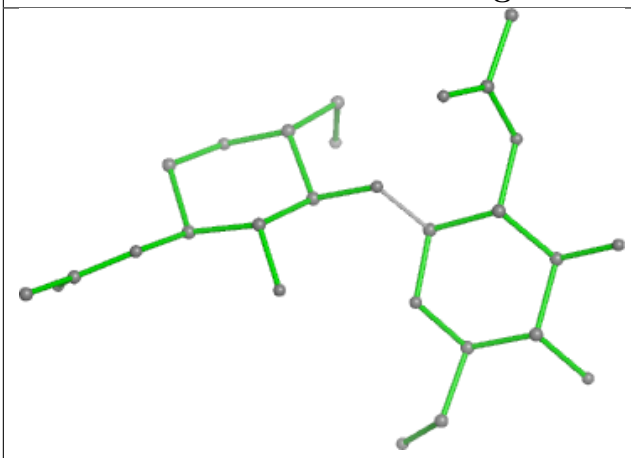


Torsions

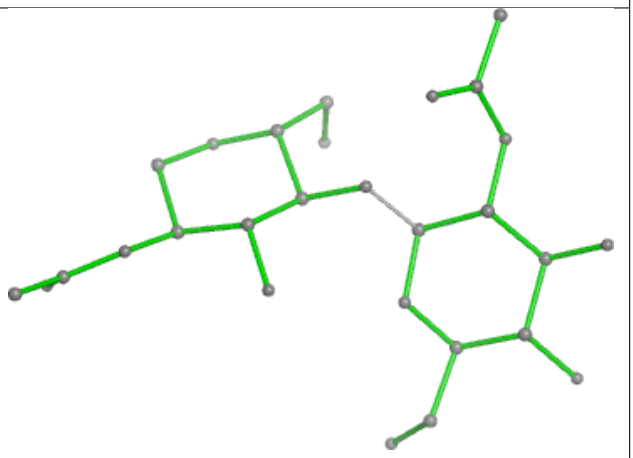


Rings

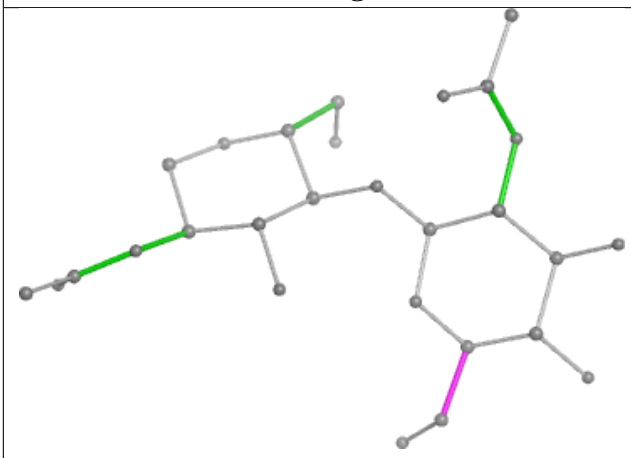
Oligosaccharide Chain H



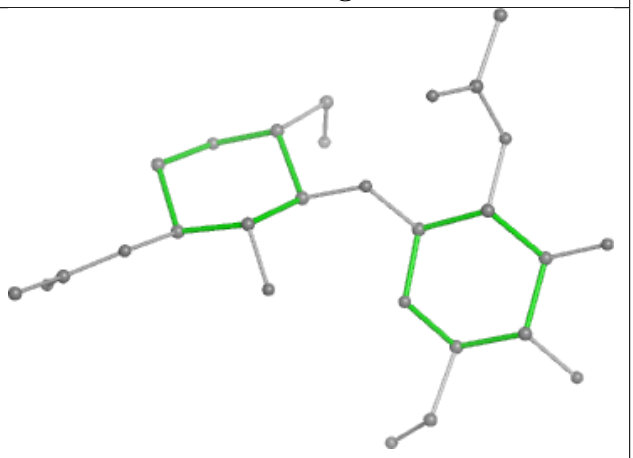
Bond lengths



Bond angles

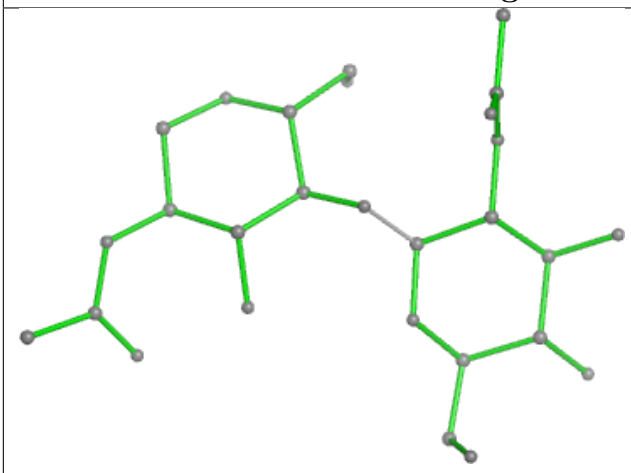


Torsions

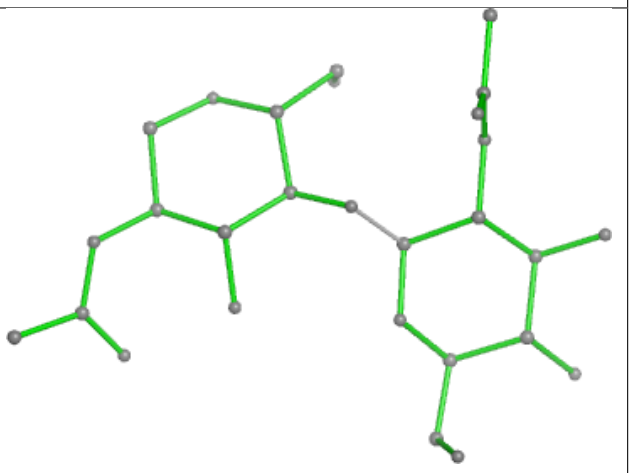


Rings

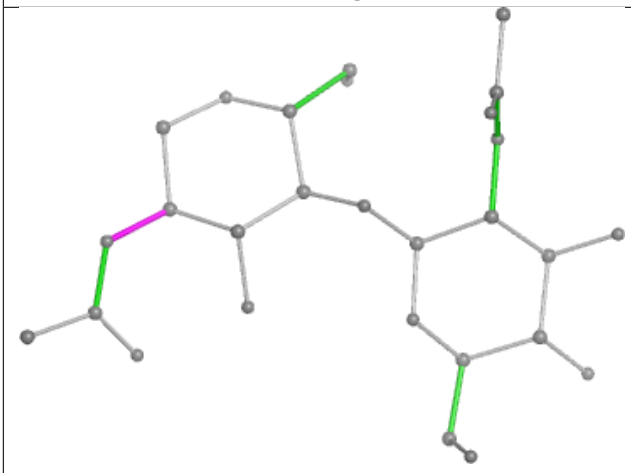
Oligosaccharide Chain I



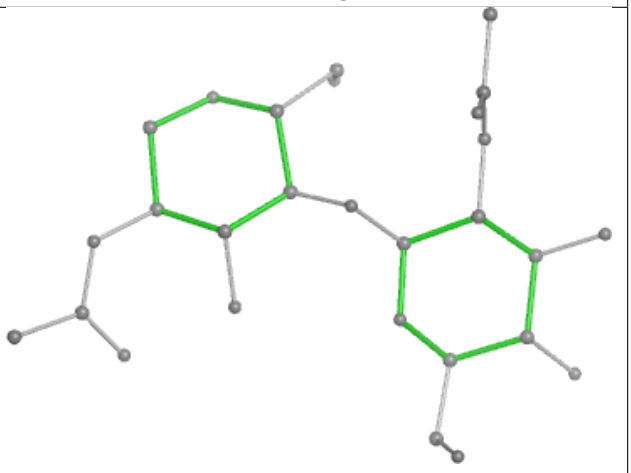
Bond lengths



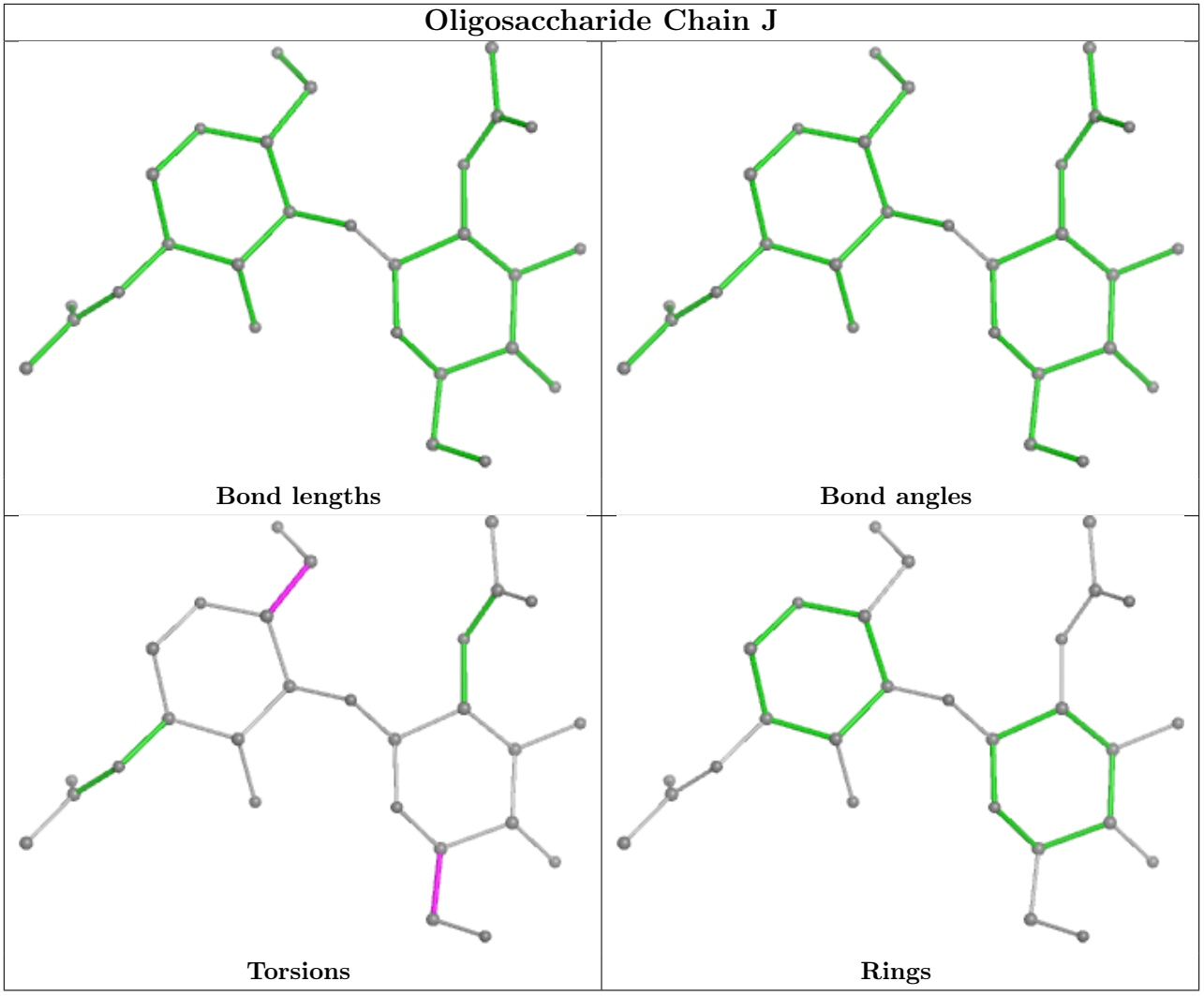
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 for Mogul analysis.

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	$\#\|Z\|>2$
3	NAG	A	2804	1	14,14,15	0.28	0	17,19,21	0.49	0
3	NAG	A	2805	1	14,14,15	0.29	0	17,19,21	0.37	0
3	NAG	A	2807	1	14,14,15	0.62	0	17,19,21	0.79	0
3	NAG	B	2803	1	14,14,15	0.32	0	17,19,21	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	2807	1	14,14,15	0.63	0	17,19,21	0.79	1 (5%)
3	NAG	B	2802	1	14,14,15	0.26	0	17,19,21	0.48	0
3	NAG	B	2801	1	14,14,15	0.30	0	17,19,21	0.40	0
3	NAG	B	2805	1	14,14,15	0.29	0	17,19,21	0.37	0
3	NAG	A	2801	1	14,14,15	0.30	0	17,19,21	0.40	0
3	NAG	B	2804	1	14,14,15	0.29	0	17,19,21	0.49	0
3	NAG	B	2806	1	14,14,15	0.36	0	17,19,21	0.47	0
3	NAG	A	2803	1	14,14,15	0.33	0	17,19,21	0.92	1 (5%)
3	NAG	A	2802	1	14,14,15	0.26	0	17,19,21	0.48	0
3	NAG	A	2806	1	14,14,15	0.34	0	17,19,21	0.47	0

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
3	NAG	A	2804	1	-	4/6/23/26	0/1/1/1
3	NAG	A	2805	1	-	4/6/23/26	0/1/1/1
3	NAG	A	2807	1	-	3/6/23/26	0/1/1/1
3	NAG	B	2803	1	-	5/6/23/26	0/1/1/1
3	NAG	B	2807	1	-	3/6/23/26	0/1/1/1
3	NAG	B	2802	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2801	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2805	1	-	4/6/23/26	0/1/1/1
3	NAG	A	2801	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2804	1	-	4/6/23/26	0/1/1/1
3	NAG	B	2806	1	-	4/6/23/26	0/1/1/1
3	NAG	A	2803	1	-	5/6/23/26	0/1/1/1
3	NAG	A	2802	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2806	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2803	NAG	C1-O5-C5	3.09	116.38	112.19
3	B	2803	NAG	C1-O5-C5	3.05	116.33	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2807	NAG	C1-C2-N2	2.01	113.92	110.49

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2807	NAG	C1-C2-N2-C7
3	B	2807	NAG	C1-C2-N2-C7
3	A	2806	NAG	O5-C5-C6-O6
3	A	2807	NAG	O5-C5-C6-O6
3	B	2806	NAG	O5-C5-C6-O6
3	B	2807	NAG	O5-C5-C6-O6
3	A	2804	NAG	C4-C5-C6-O6
3	B	2804	NAG	C4-C5-C6-O6
3	A	2802	NAG	O5-C5-C6-O6
3	B	2802	NAG	O5-C5-C6-O6
3	A	2806	NAG	C4-C5-C6-O6
3	B	2806	NAG	C4-C5-C6-O6
3	A	2807	NAG	C4-C5-C6-O6
3	B	2807	NAG	C4-C5-C6-O6
3	B	2803	NAG	O5-C5-C6-O6
3	A	2803	NAG	C8-C7-N2-C2
3	A	2803	NAG	O7-C7-N2-C2
3	A	2804	NAG	C8-C7-N2-C2
3	A	2804	NAG	O7-C7-N2-C2
3	A	2806	NAG	C8-C7-N2-C2
3	A	2806	NAG	O7-C7-N2-C2
3	B	2803	NAG	C8-C7-N2-C2
3	B	2803	NAG	O7-C7-N2-C2
3	B	2804	NAG	C8-C7-N2-C2
3	B	2804	NAG	O7-C7-N2-C2
3	B	2806	NAG	C8-C7-N2-C2
3	B	2806	NAG	O7-C7-N2-C2
3	A	2803	NAG	O5-C5-C6-O6
3	A	2803	NAG	C4-C5-C6-O6
3	B	2803	NAG	C4-C5-C6-O6
3	A	2804	NAG	O5-C5-C6-O6
3	B	2804	NAG	O5-C5-C6-O6
3	A	2805	NAG	C1-C2-N2-C7
3	B	2805	NAG	C1-C2-N2-C7
3	B	2805	NAG	O5-C5-C6-O6
3	A	2805	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	2802	NAG	C4-C5-C6-O6
3	A	2805	NAG	C4-C5-C6-O6
3	B	2802	NAG	C4-C5-C6-O6
3	B	2805	NAG	C4-C5-C6-O6
3	A	2801	NAG	O5-C5-C6-O6
3	B	2801	NAG	O5-C5-C6-O6
3	A	2801	NAG	C4-C5-C6-O6
3	B	2801	NAG	C4-C5-C6-O6
3	A	2803	NAG	C3-C2-N2-C7
3	B	2803	NAG	C3-C2-N2-C7
3	A	2805	NAG	C3-C2-N2-C7
3	B	2805	NAG	C3-C2-N2-C7

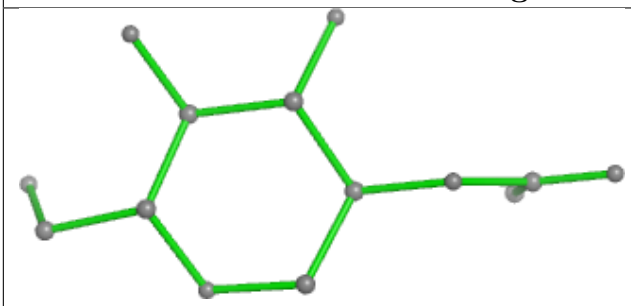
There are no ring outliers.

4 monomers are involved in 13 short contacts:

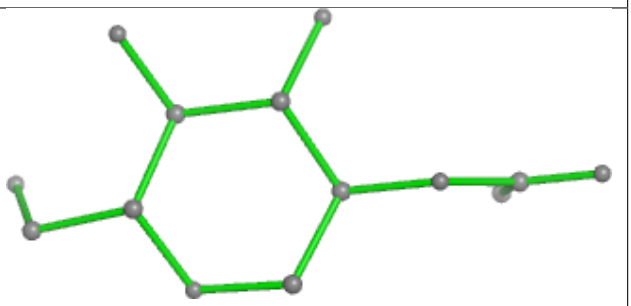
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2807	NAG	2	0
3	B	2803	NAG	4	0
3	B	2807	NAG	2	0
3	A	2803	NAG	5	0

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.

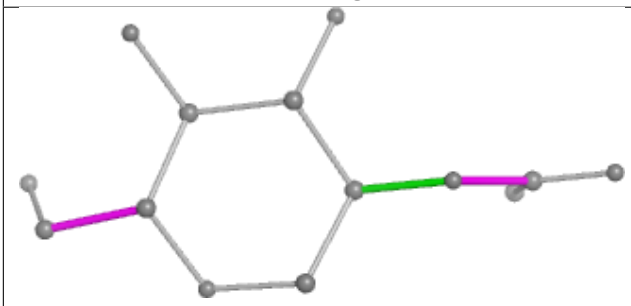
Ligand NAG A 2804



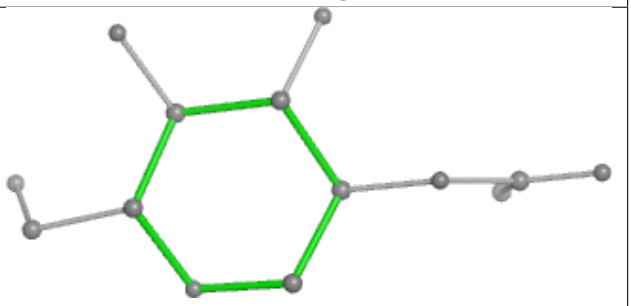
Bond lengths



Bond angles

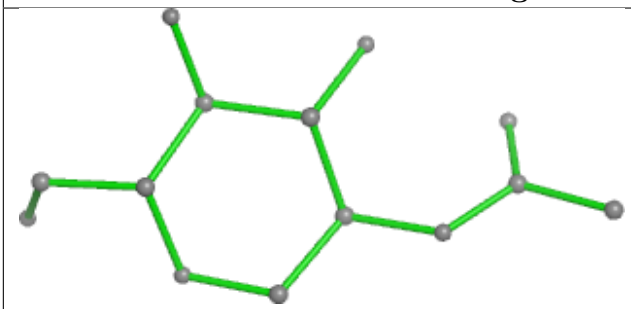


Torsions

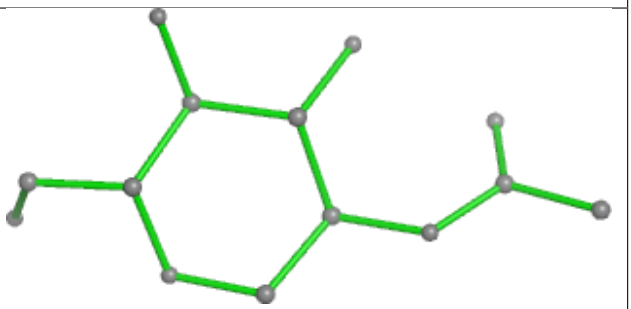


Rings

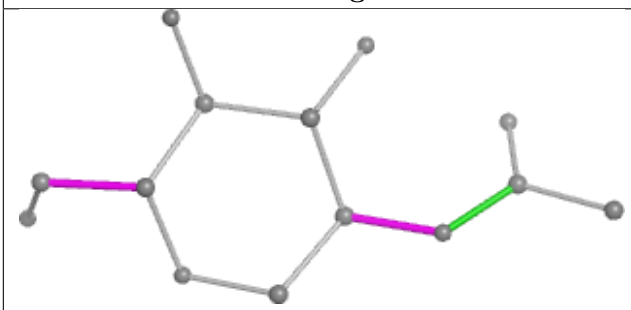
Ligand NAG A 2805



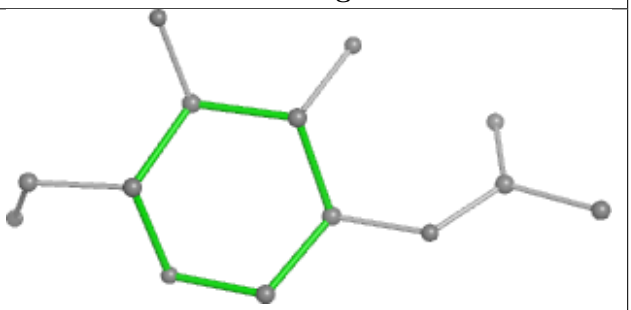
Bond lengths



Bond angles

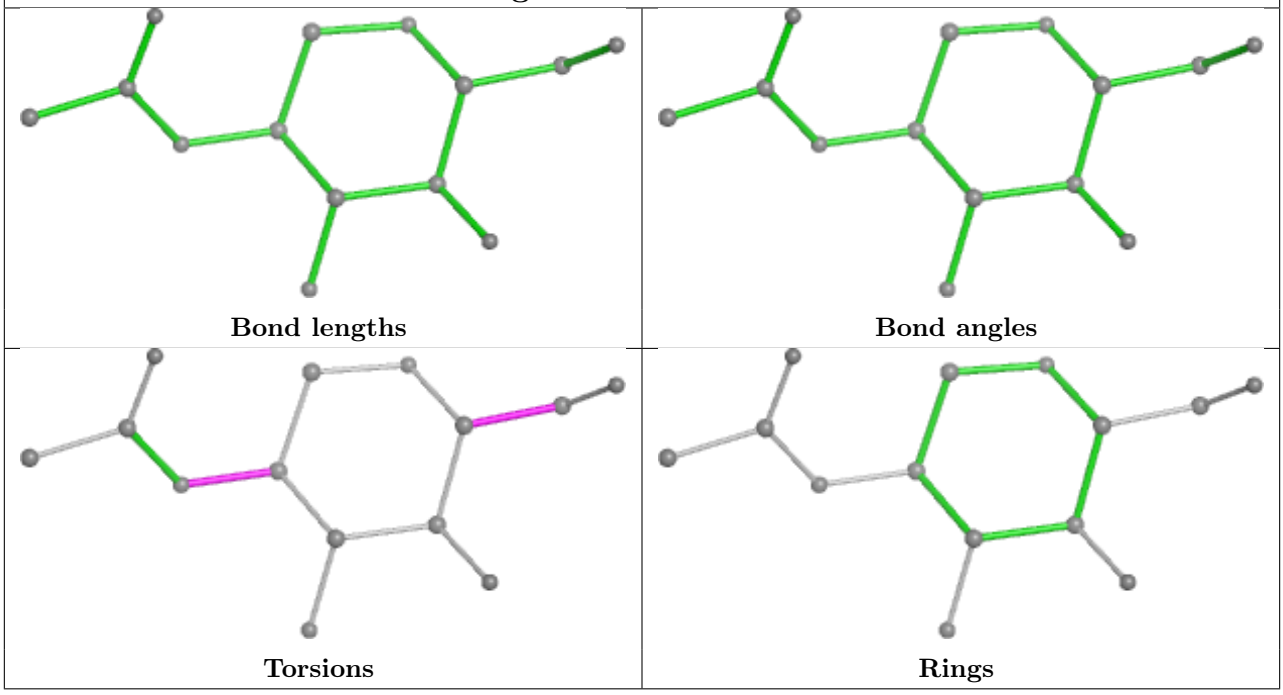


Torsions

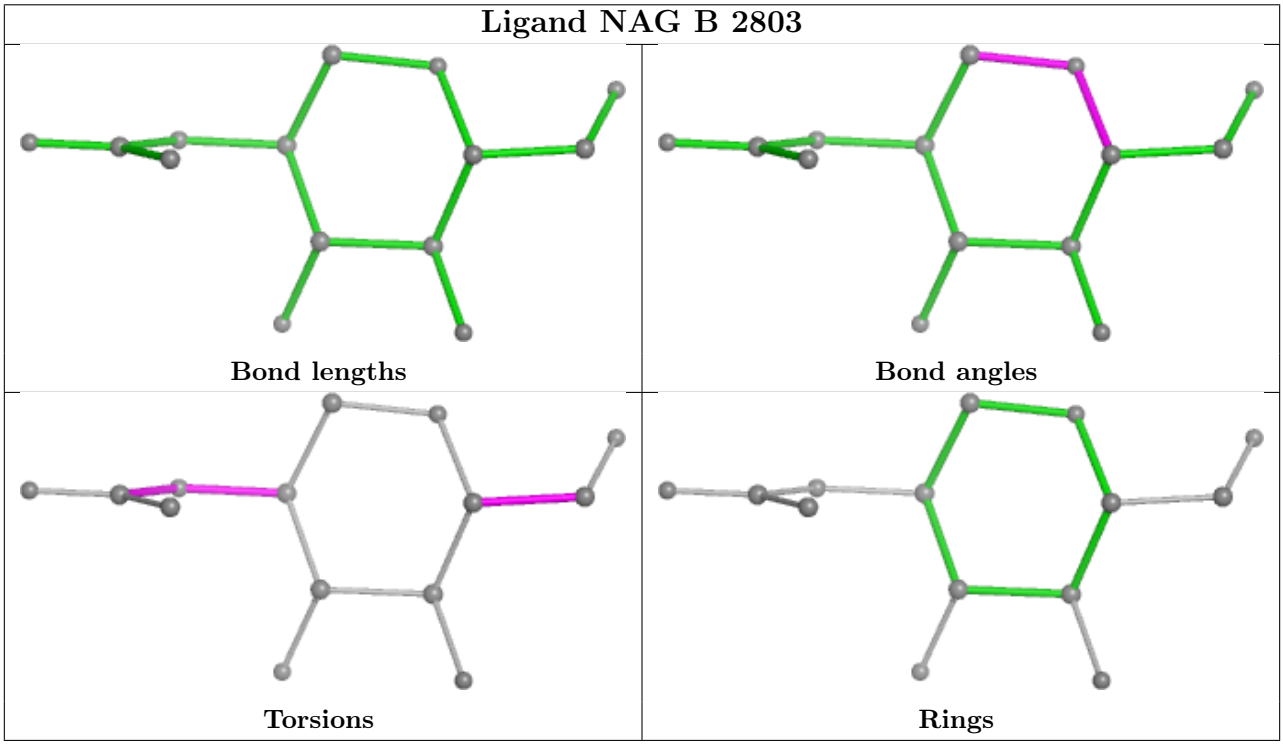


Rings

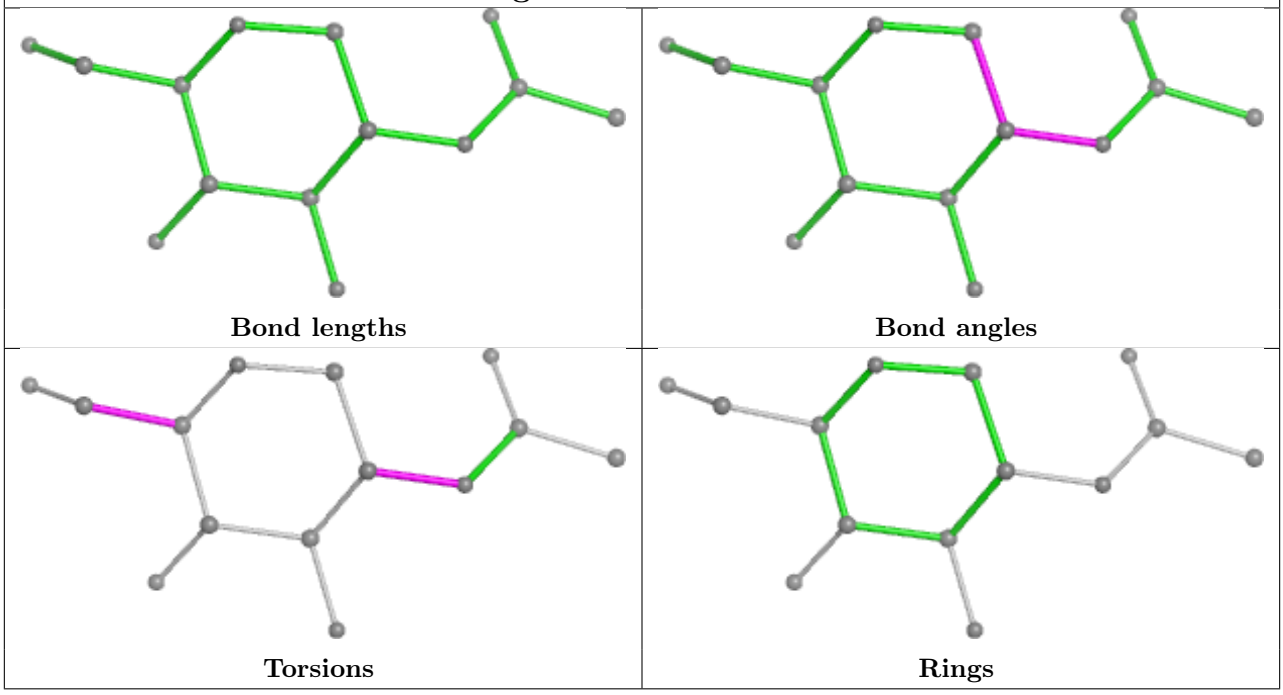
Ligand NAG A 2807



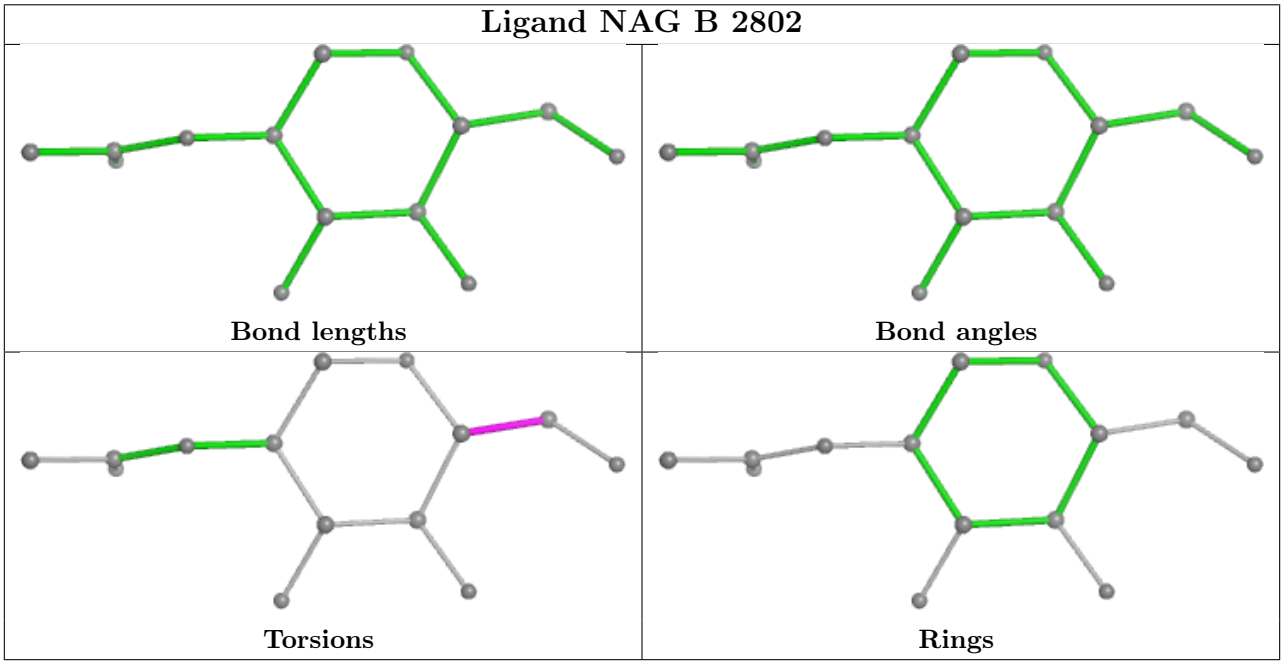
Ligand NAG B 2803



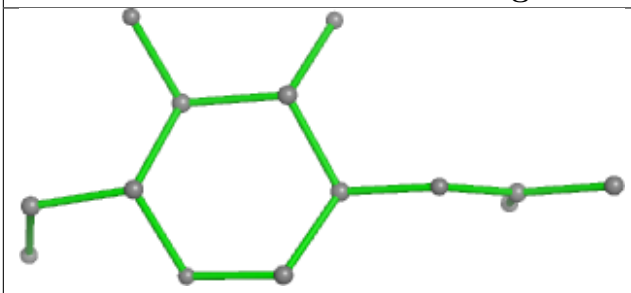
Ligand NAG B 2807



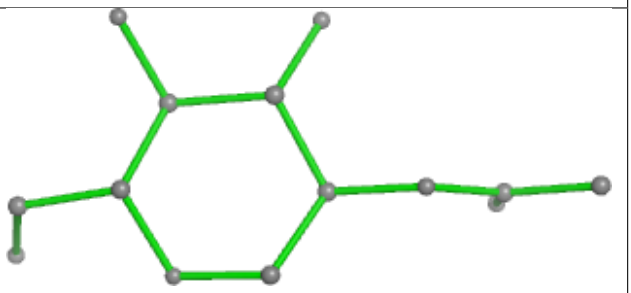
Ligand NAG B 2802



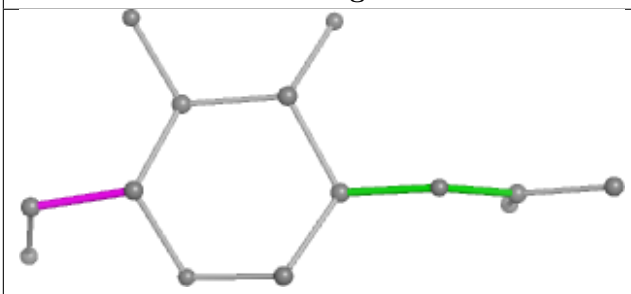
Ligand NAG B 2801



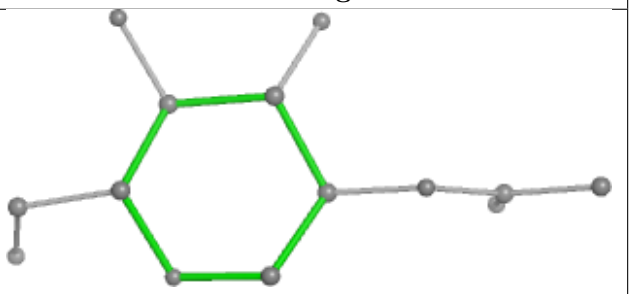
Bond lengths



Bond angles

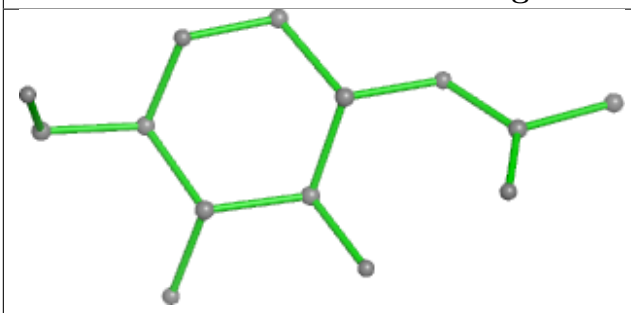


Torsions

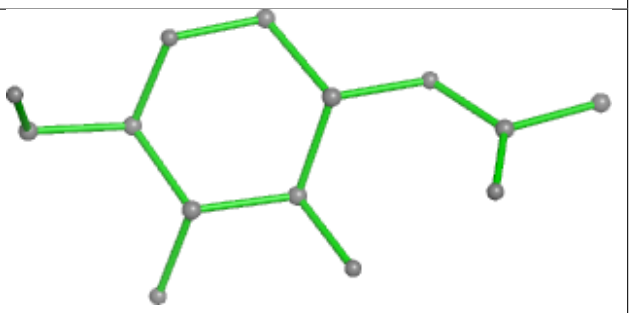


Rings

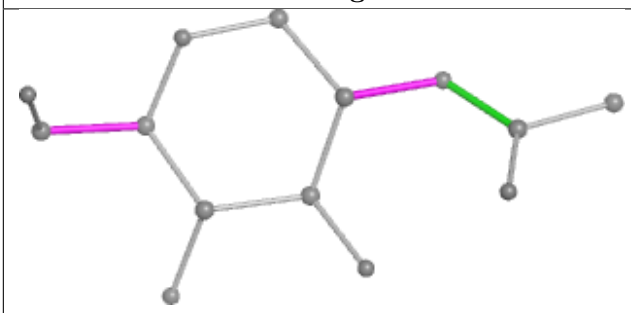
Ligand NAG B 2805



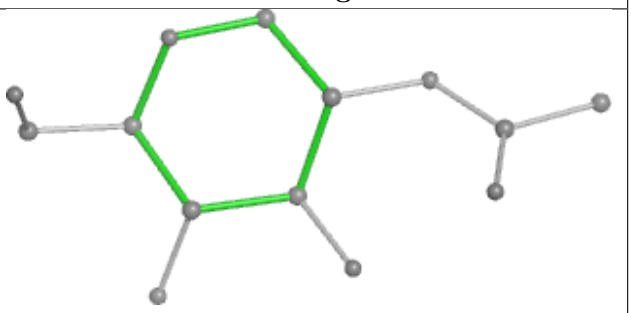
Bond lengths



Bond angles

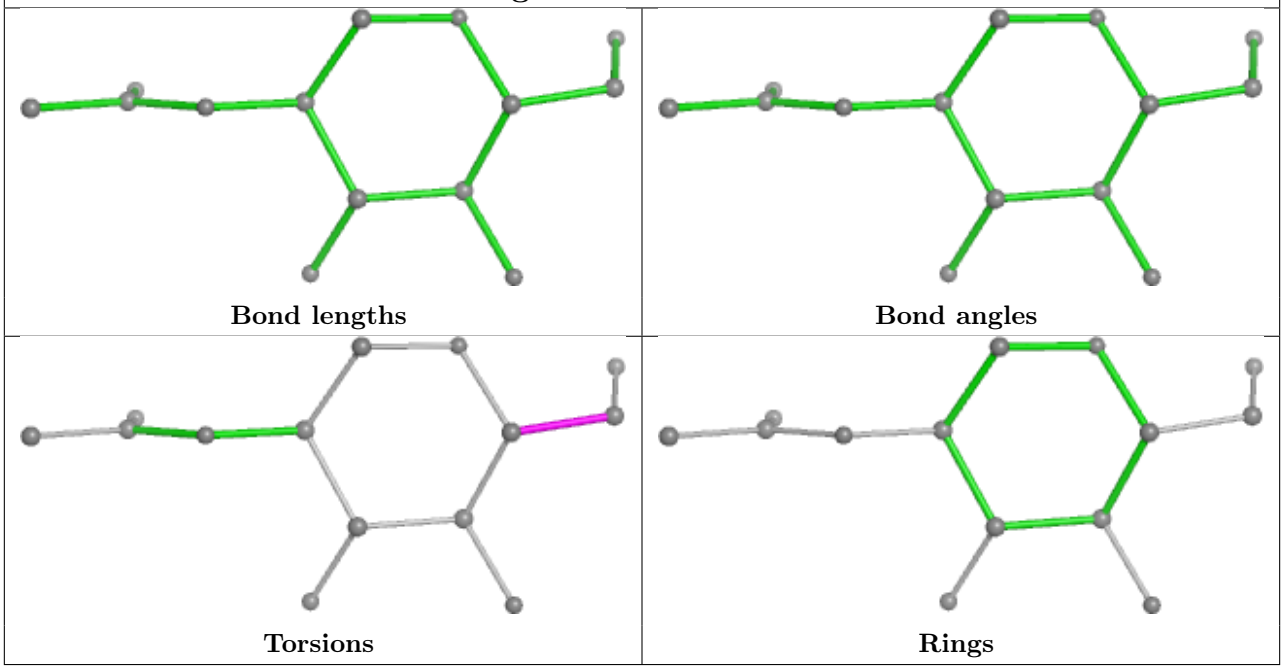


Torsions

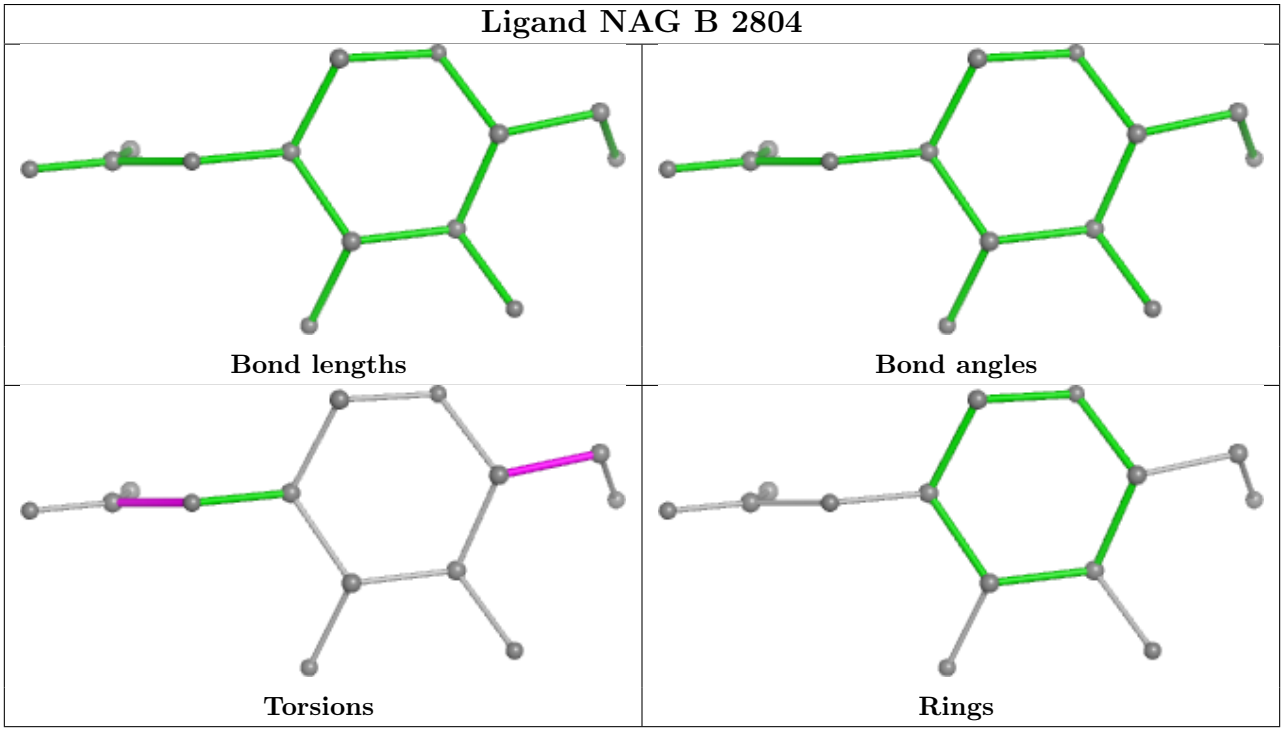


Rings

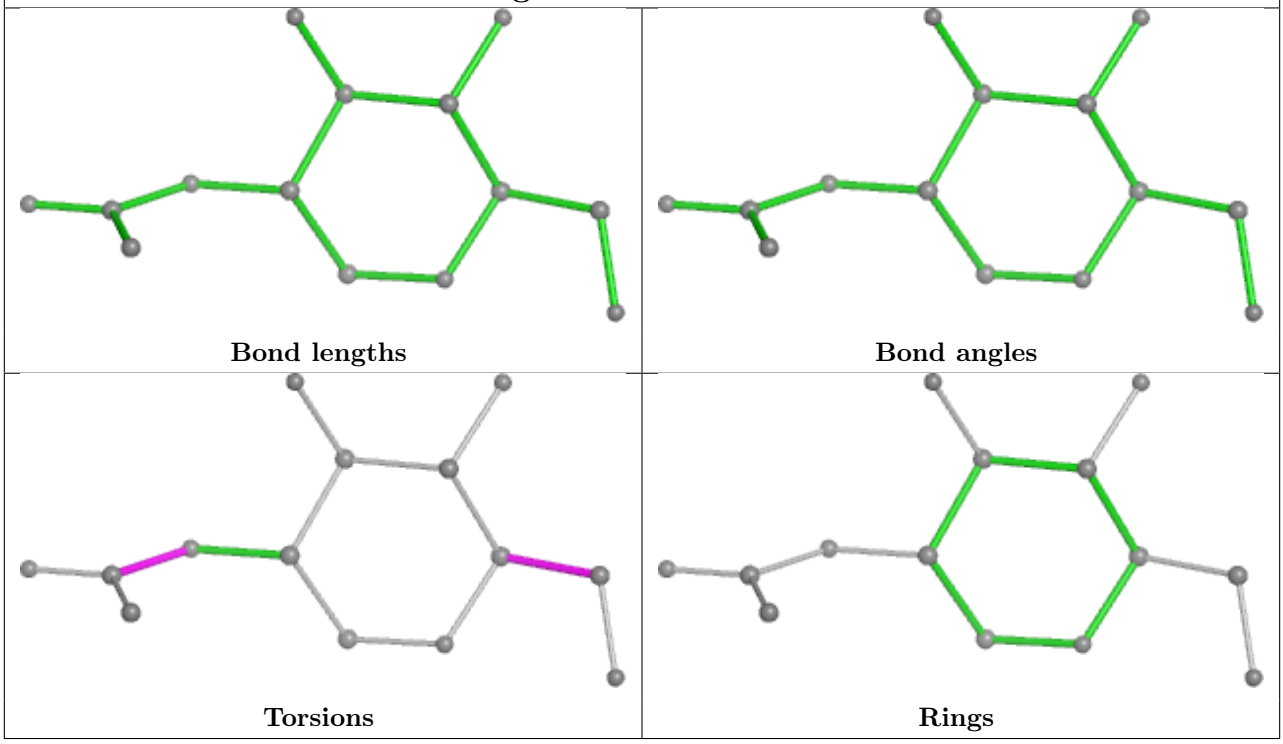
Ligand NAG A 2801



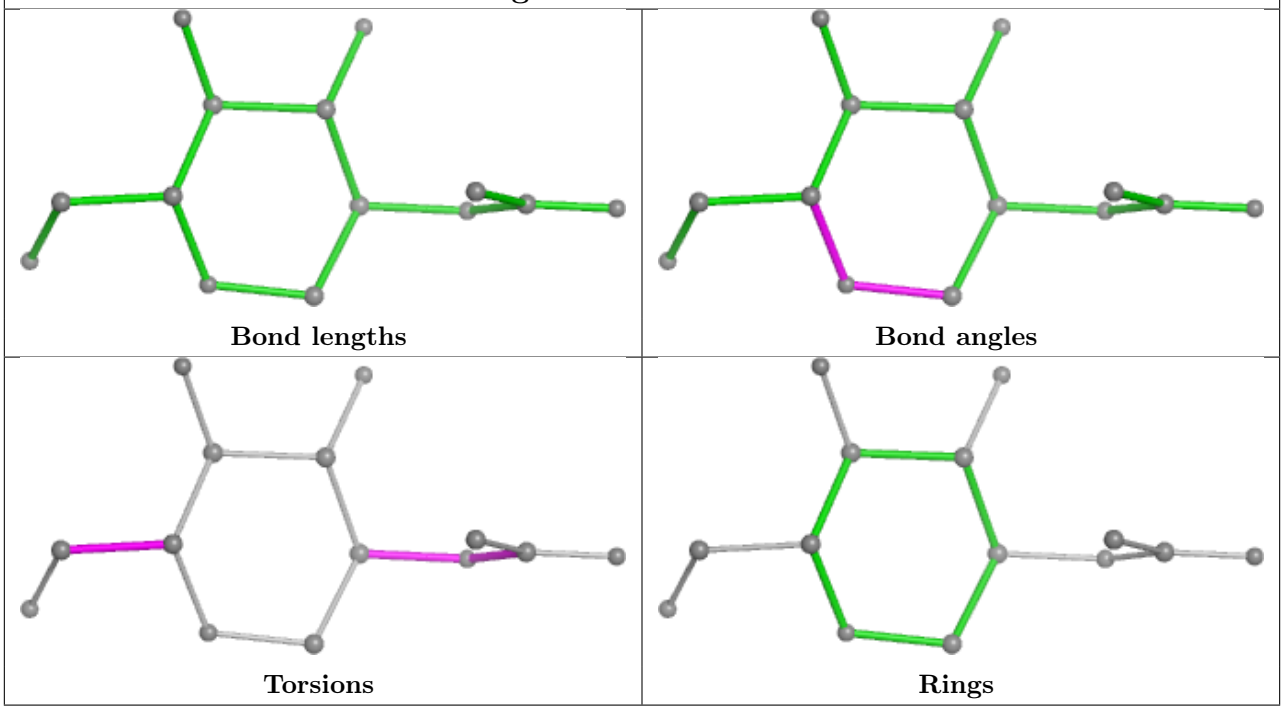
Ligand NAG B 2804



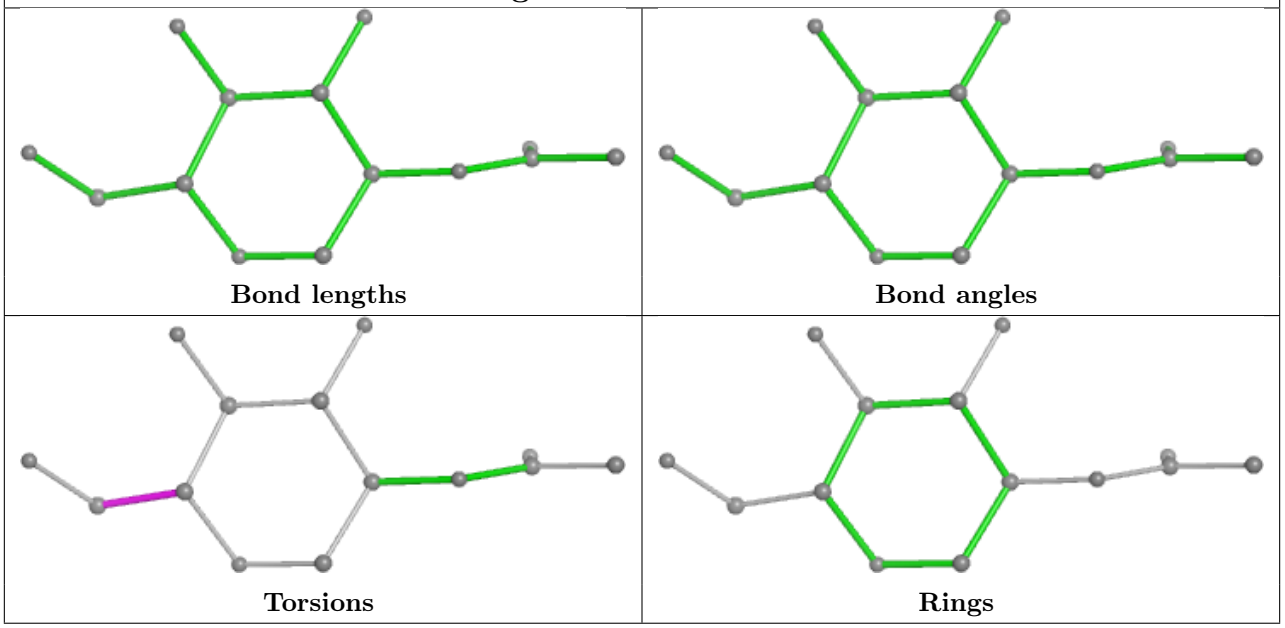
Ligand NAG B 2806



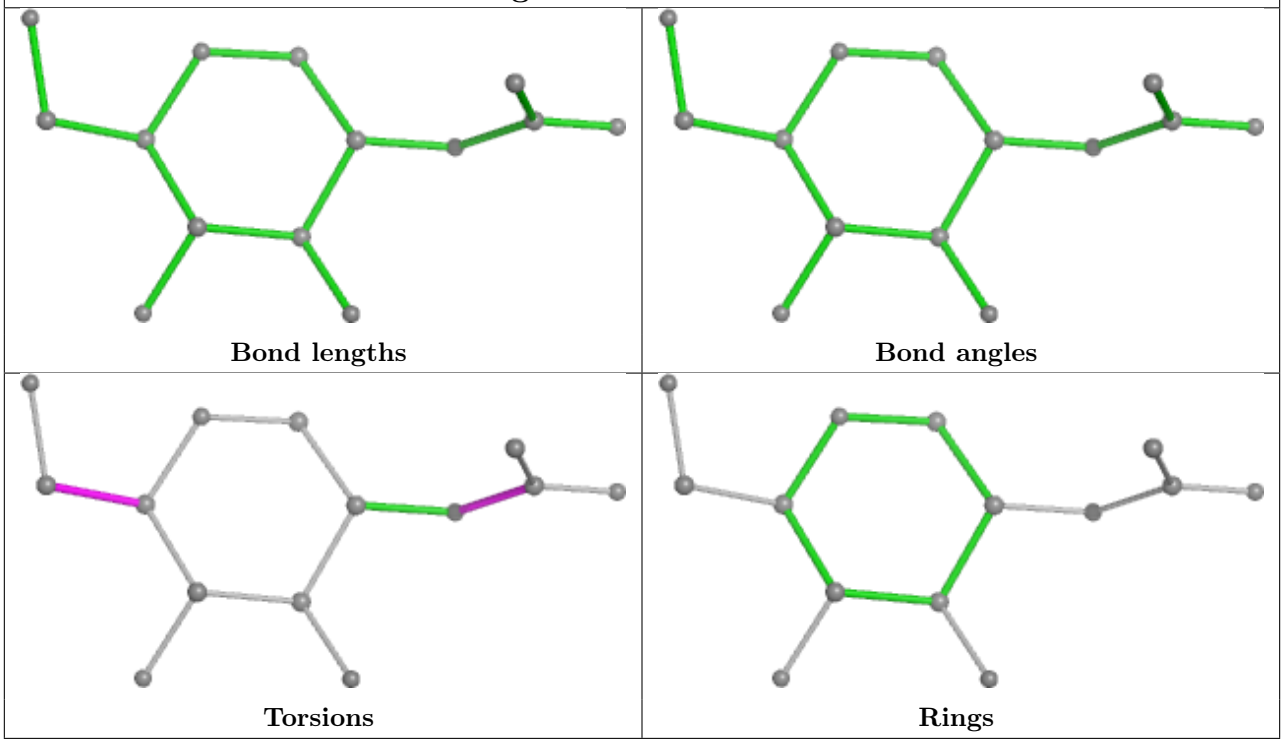
Ligand NAG A 2803



Ligand NAG A 2802



Ligand NAG A 2806



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.

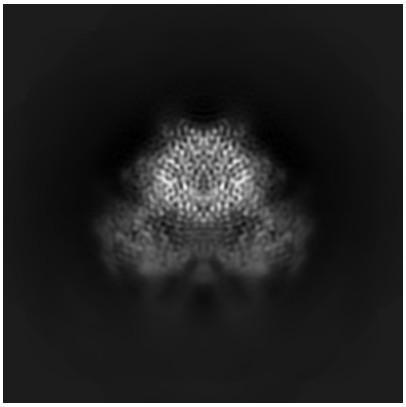
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12124. These allow visual inspection of the internal detail of the map and identification of artifacts.

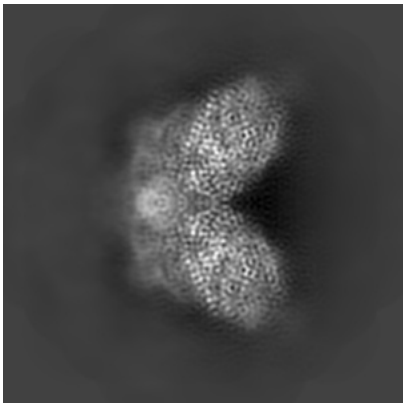
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

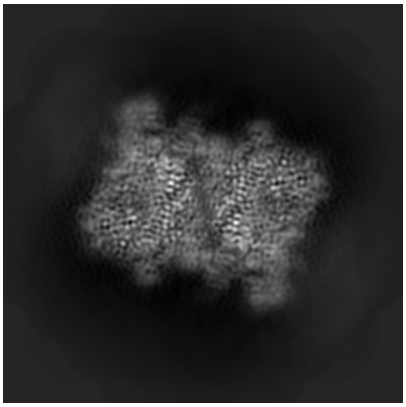
6.1.1 Primary map



X



Y

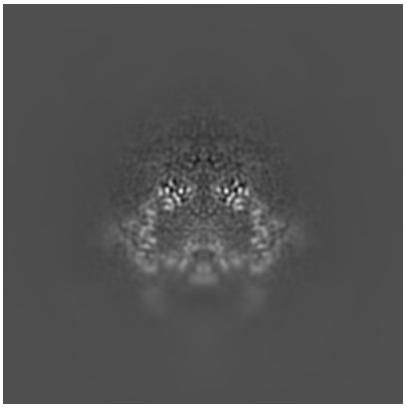


Z

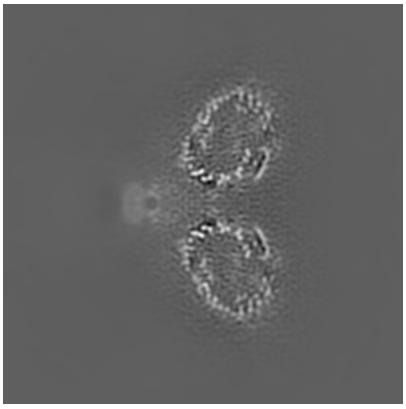
The images above show the map projected in three orthogonal directions.

6.2 Central slices

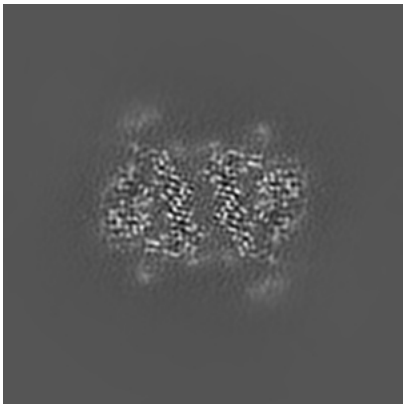
6.2.1 Primary map



X Index: 156



Y Index: 156

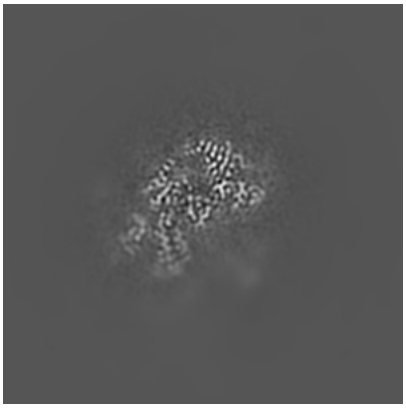


Z Index: 156

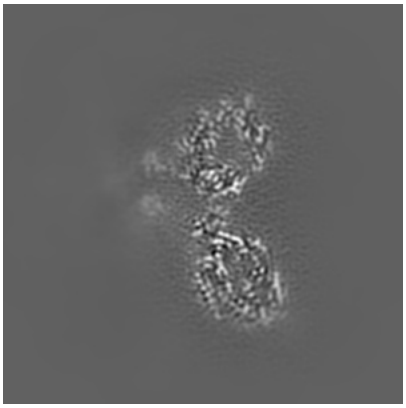
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

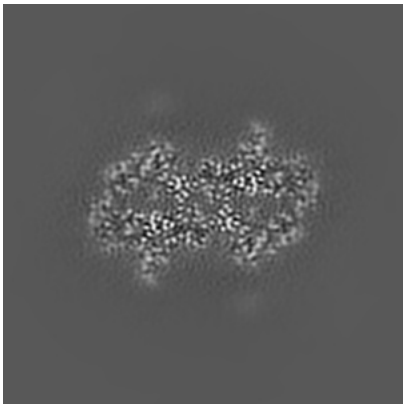
6.3.1 Primary map



X Index: 185



Y Index: 142

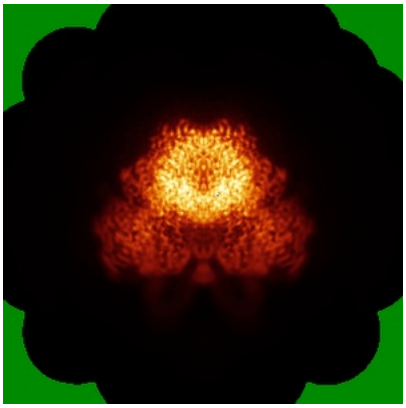


Z Index: 166

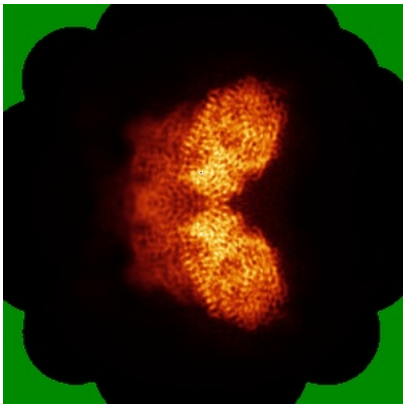
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

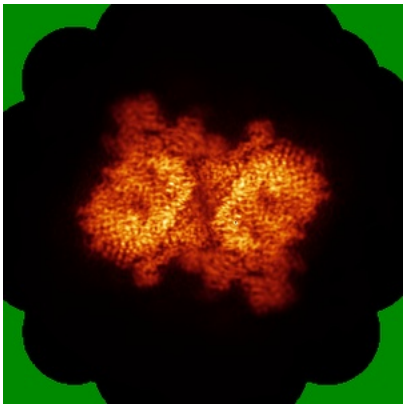
6.4.1 Primary map



X



Y

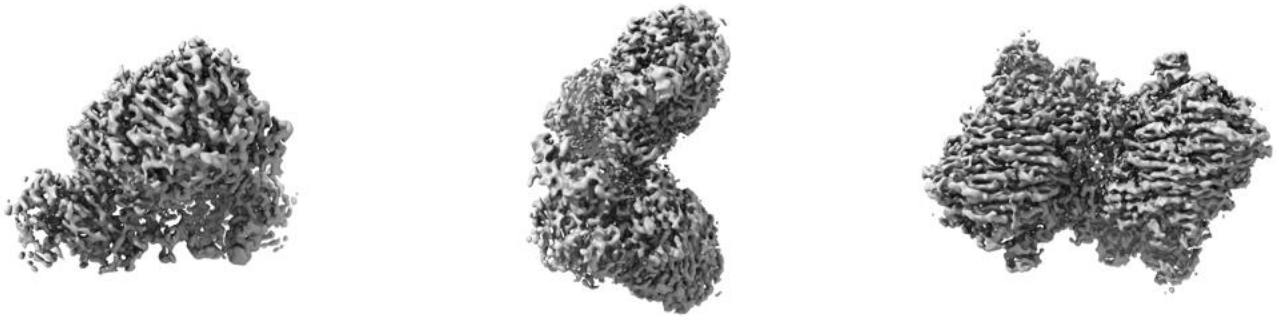


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

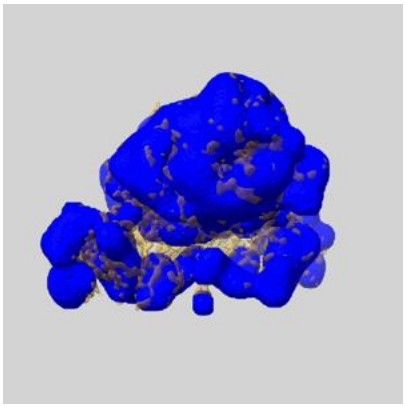
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

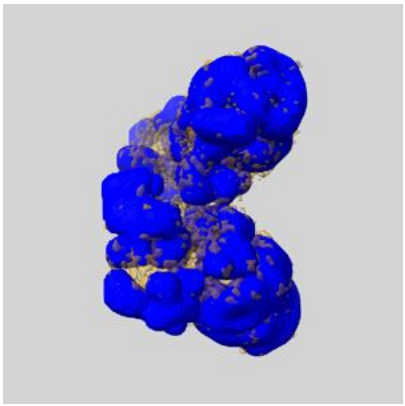
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

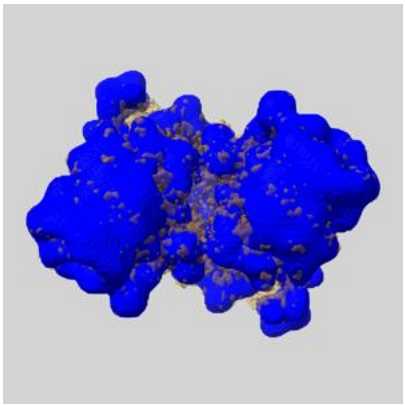
6.6.1 emd_12124_msk_1.map



X



Y

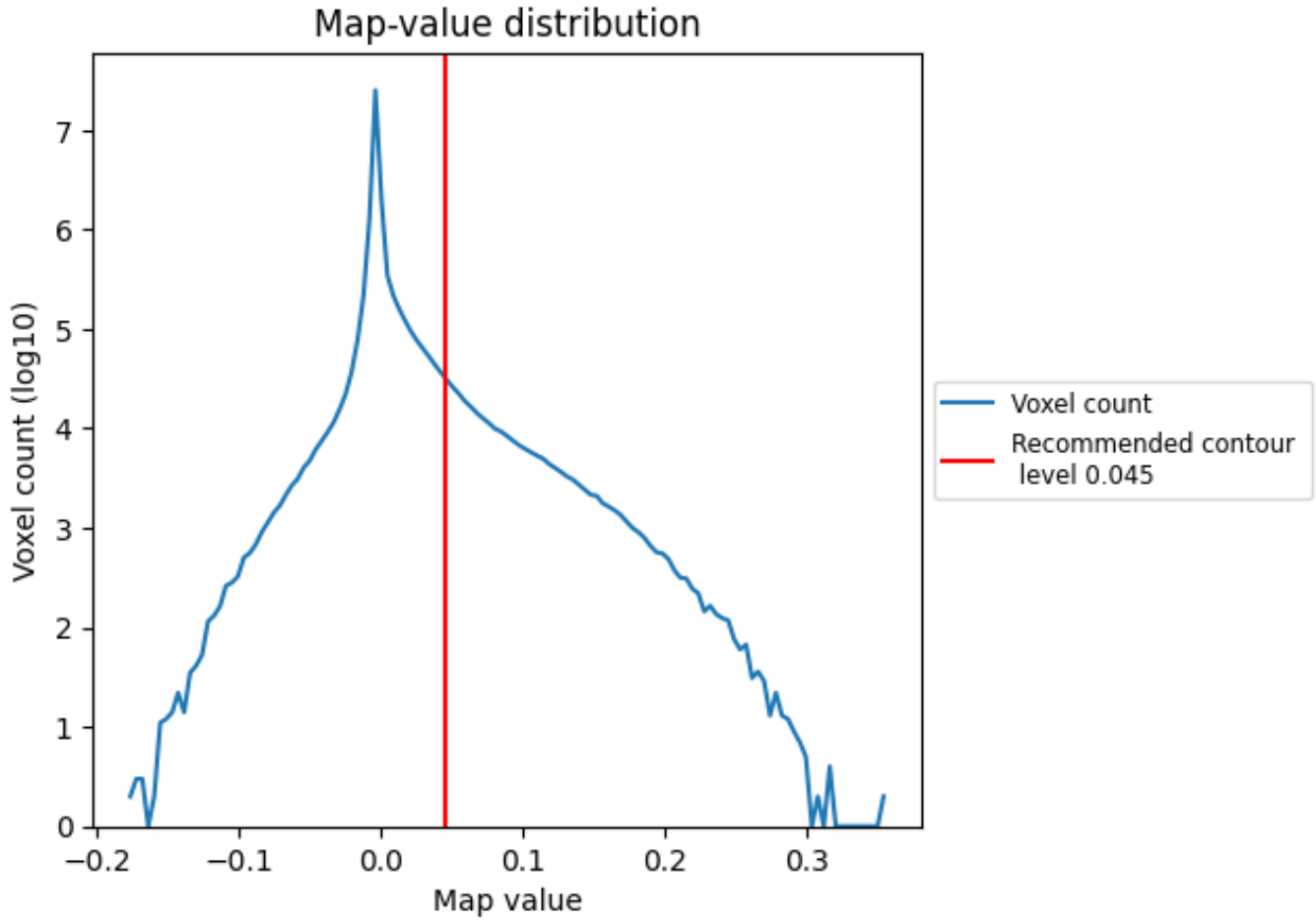


Z

7 Map analysis

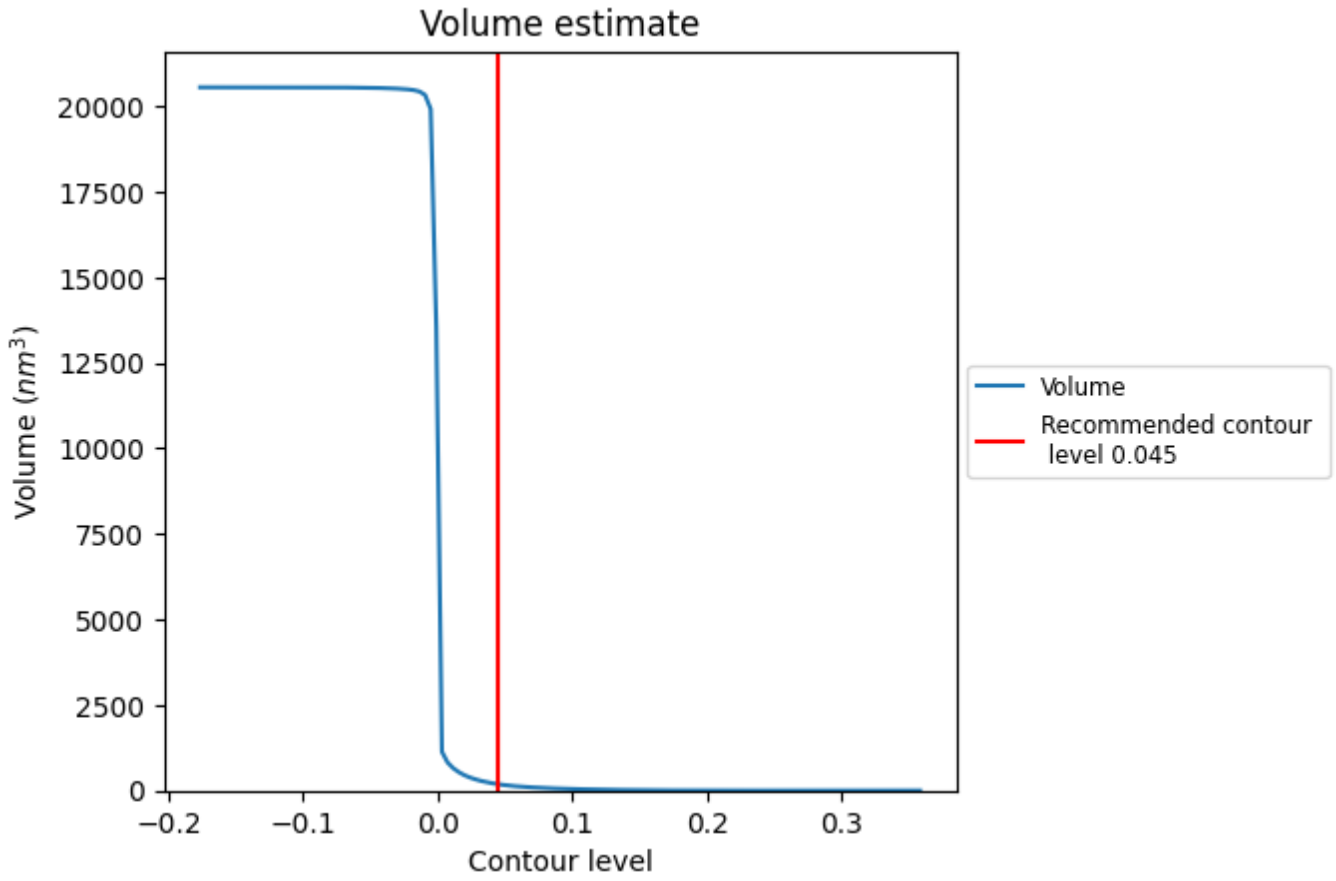
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

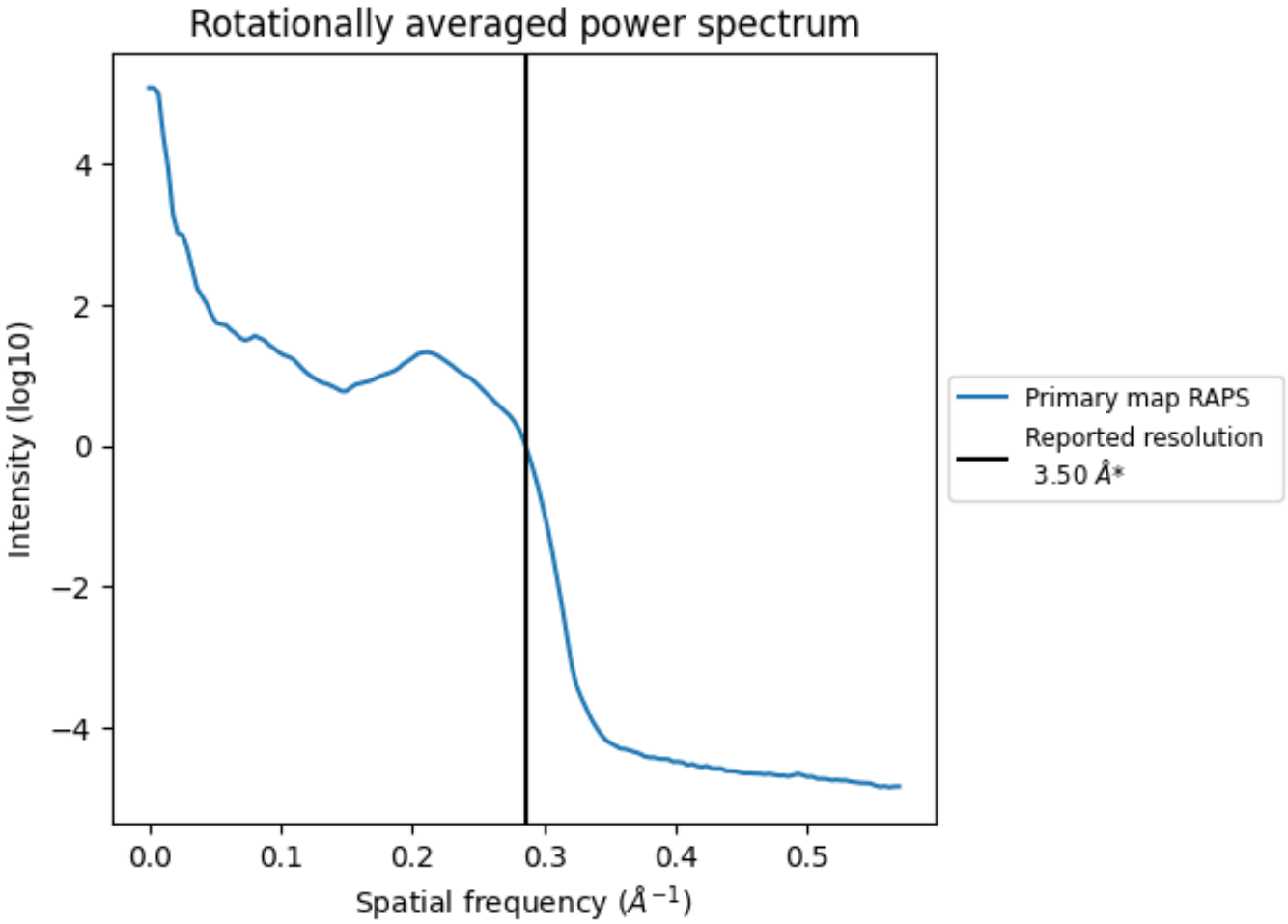
7.2 Volume estimate



The volume at the recommended contour level is 184 nm^3; this corresponds to an approximate mass of 167 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

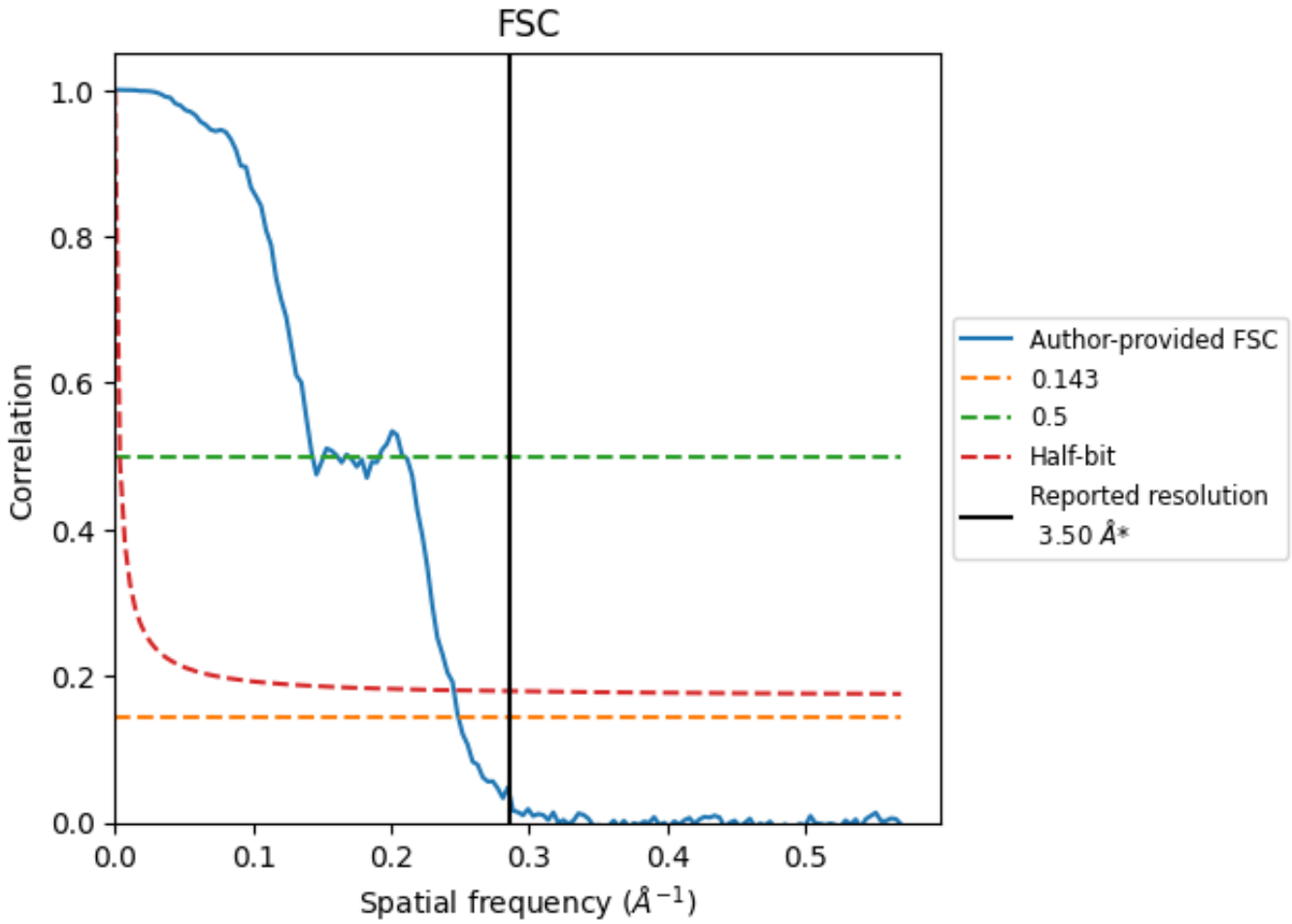


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

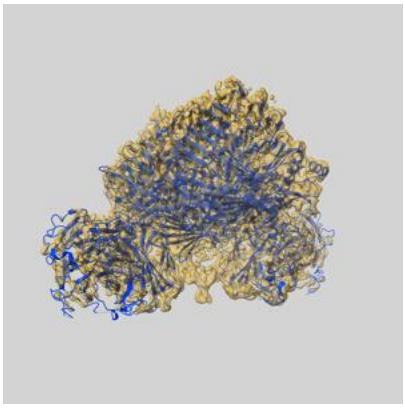
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	4.02	6.99	4.07
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 3.5 by more than 10 %

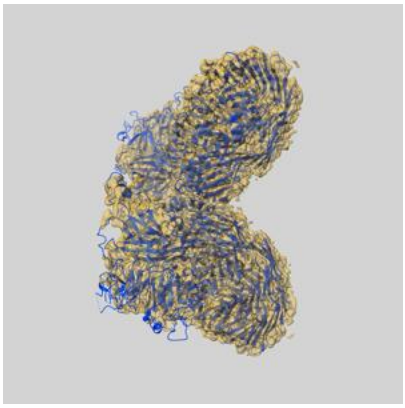
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12124 and PDB model 7BAM. Per-residue inclusion information can be found in section 3 on page 7.

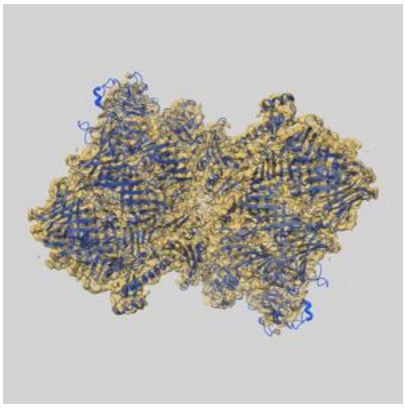
9.1 Map-model overlay



X



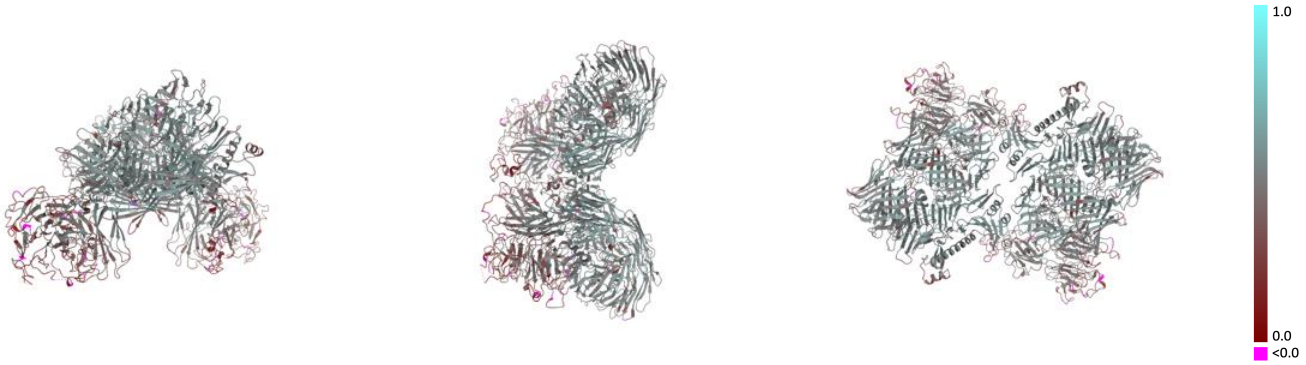
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

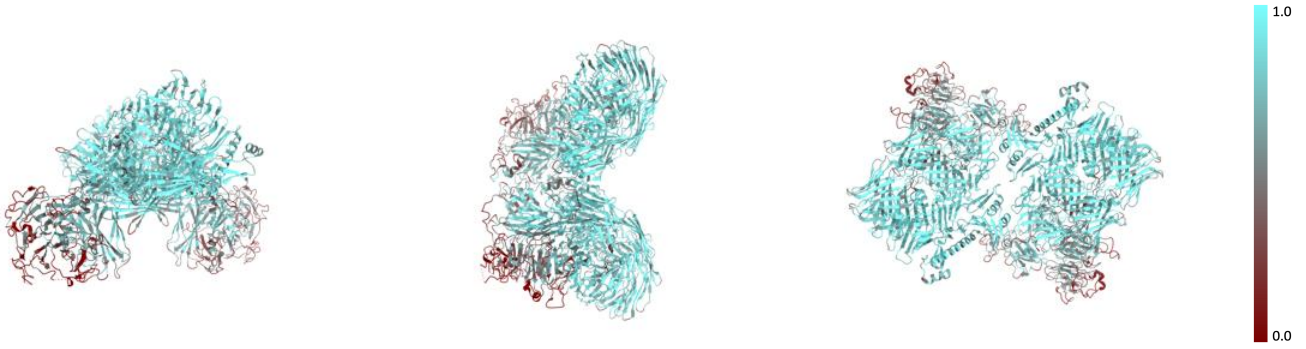
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

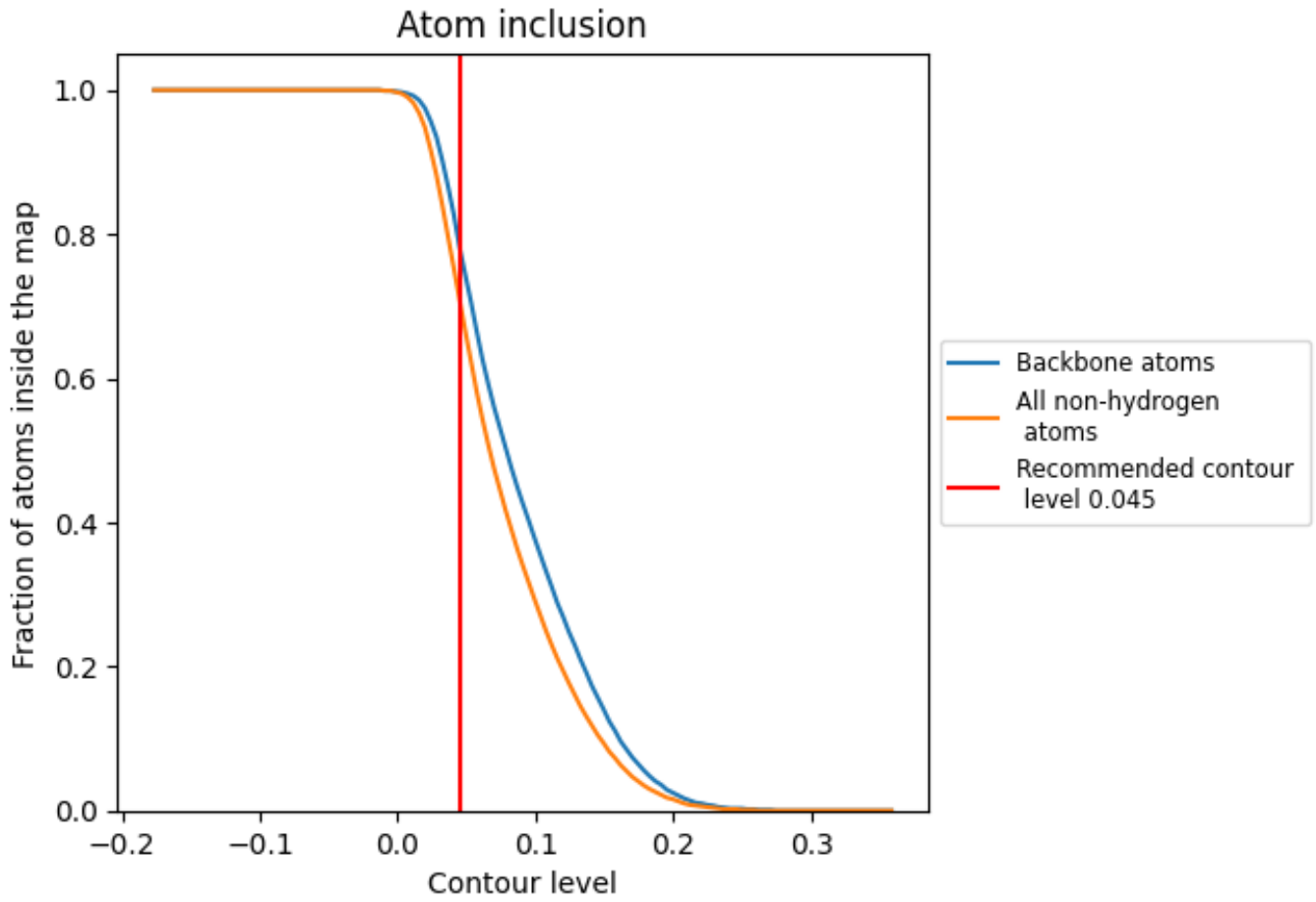
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7070	0.4520
A	0.7080	0.4520
B	0.7070	0.4530
C	0.6790	0.3910
D	0.7140	0.4890
E	0.6790	0.4900
F	0.4290	0.3800
G	0.6790	0.3820
H	0.7140	0.4780
I	0.6790	0.4710
J	0.4290	0.3960