Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 10:35 AM JST

PDB ID	:	7W9L
EMDB ID	:	EMD-32369
Title	:	Cryo-EM structure of human Nav1.7(E406K)-beta1-beta2 complex
Authors	:	Yan, N.; Huang, G.; Liu, D.; Wei, P.; Shen, H.
Deposited on	:	2021-12-10
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:

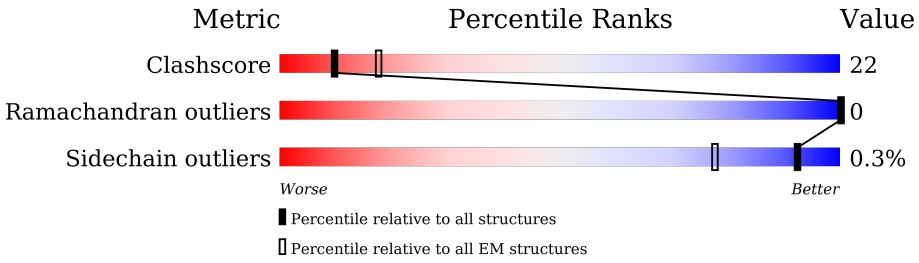
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2031	10% 44% 26% 30%
2	B	218	48% 31% • 21%
3	C	215	36% 48% 7% 45%
4	D	2	100%
4	E	2	100%
4	F	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PCW	A	2018	-	-	X	-
7	Y01	A	2005	-	-	X	-
8	9Z9	A	2006	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14915 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 Sodium channel protein type 9 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1420	11445	7554	1802	2004	85	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	expression tag	UNP Q15858
A	-41	ALA	-	expression tag	UNP Q15858
A	-40	SER	-	expression tag	UNP Q15858
A	-39	TRP	-	expression tag	UNP Q15858
A	-38	SER	-	expression tag	UNP Q15858
A	-37	HIS	-	expression tag	UNP Q15858
A	-36	PRO	-	expression tag	UNP Q15858
A	-35	GLN	-	expression tag	UNP Q15858
A	-34	PHE	-	expression tag	UNP Q15858
A	-33	GLU	-	expression tag	UNP Q15858
A	-32	LYS	-	expression tag	UNP Q15858
A	-31	GLY	-	expression tag	UNP Q15858
A	-30	GLY	-	expression tag	UNP Q15858
A	-29	GLY	-	expression tag	UNP Q15858
A	-28	ALA	-	expression tag	UNP Q15858
A	-27	ARG	-	expression tag	UNP Q15858
A	-26	GLY	-	expression tag	UNP Q15858
A	-25	GLY	-	expression tag	UNP Q15858
A	-24	SER	-	expression tag	UNP Q15858
A	-23	GLY	-	expression tag	UNP Q15858
A	-22	GLY	-	expression tag	UNP Q15858
A	-21	GLY	-	expression tag	UNP Q15858
A	-20	SER	-	expression tag	UNP Q15858
A	-19	TRP	-	expression tag	UNP Q15858
A	-18	SER	-	expression tag	UNP Q15858
A	-17	HIS	-	expression tag	UNP Q15858
A	-16	PRO	-	expression tag	UNP Q15858
A	-15	GLN	-	expression tag	UNP Q15858

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PHE	-	expression tag	UNP Q15858
A	-13	GLU	-	expression tag	UNP Q15858
A	-12	LYS	-	expression tag	UNP Q15858
A	-11	GLY	-	expression tag	UNP Q15858
A	-10	PHE	-	expression tag	UNP Q15858
A	-9	ASP	-	expression tag	UNP Q15858
A	-8	TYR	-	expression tag	UNP Q15858
A	-7	LYS	-	expression tag	UNP Q15858
A	-6	ASP	-	expression tag	UNP Q15858
A	-5	ASP	-	expression tag	UNP Q15858
A	-4	ASP	-	expression tag	UNP Q15858
A	-3	ASP	-	expression tag	UNP Q15858
A	-2	LYS	-	expression tag	UNP Q15858
A	-1	GLY	-	expression tag	UNP Q15858
A	0	THR	-	expression tag	UNP Q15858
A	406	LYS	GLU	engineered mutation	UNP Q15858

- Molecule 2 is a protein called Sodium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	173	Total	C	N	O	S	0	0
			1416	902	232	272	10		

- Molecule 3 is a protein called Sodium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	119	Total	C	N	O	S	4	0
			980	615	172	183	10		

- Molecule 4 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
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

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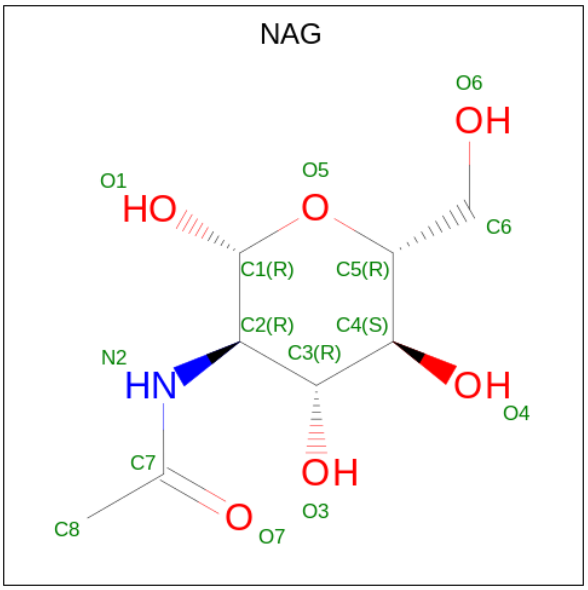
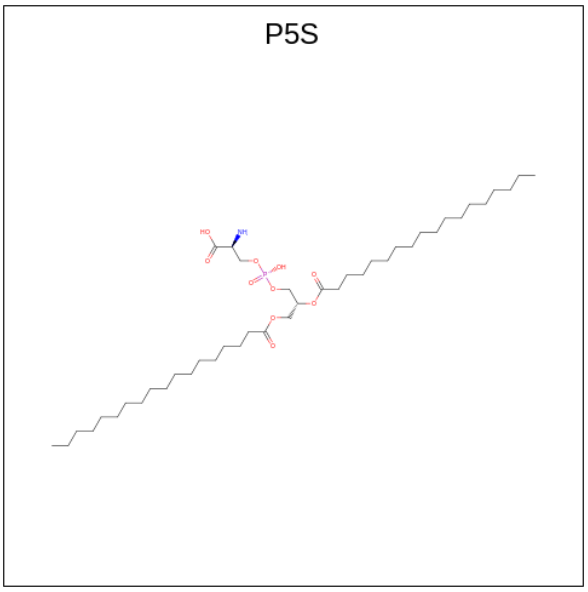
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 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).



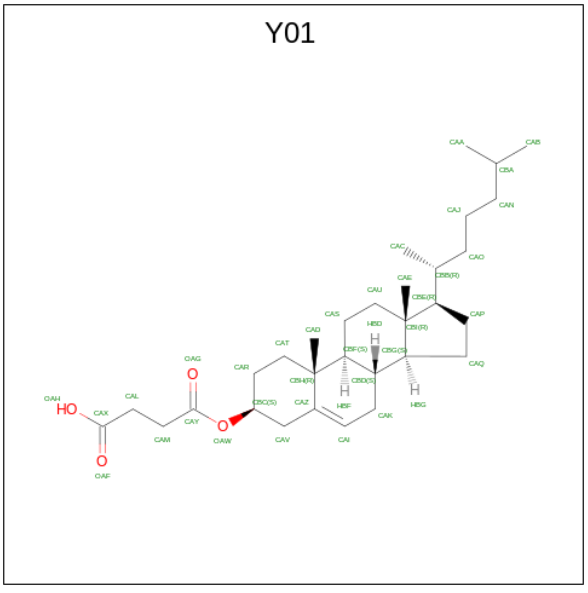
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			28	16	2	10	
5	A	1	Total	C	N	O	0
			28	16	2	10	
5	B	1	Total	C	N	O	0
			42	24	3	15	
5	B	1	Total	C	N	O	0
			42	24	3	15	
5	B	1	Total	C	N	O	0
			42	24	3	15	

- Molecule 6 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: $C_{42}H_{82}NO_{10}P$).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			110	77	3	27	3	
6	A	1	Total	C	N	O	P	0
			110	77	3	27	3	
6	A	1	Total	C	N	O	P	0
			110	77	3	27	3	

- Molecule 7 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			210	186	24	

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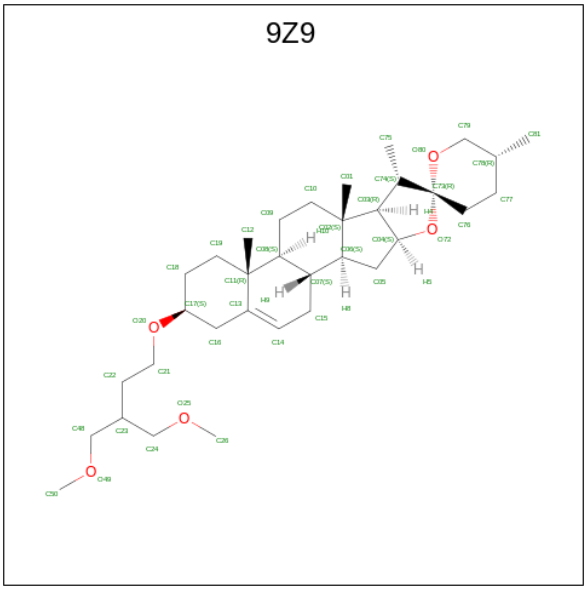
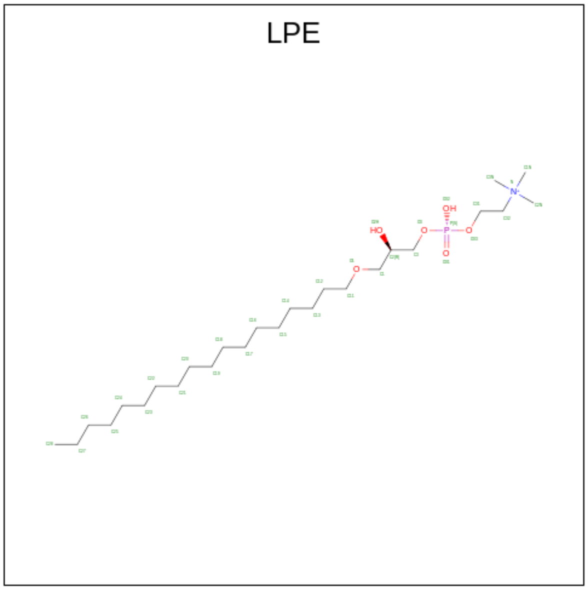
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			210	186	24	
7	A	1	Total	C	O	0
			210	186	24	
7	A	1	Total	C	O	0
			210	186	24	
7	A	1	Total	C	O	0
			210	186	24	
7	A	1	Total	C	O	0
			210	186	24	

- Molecule 8 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (three-letter code: 9Z9) (formula: $C_{34}H_{56}O_5$).



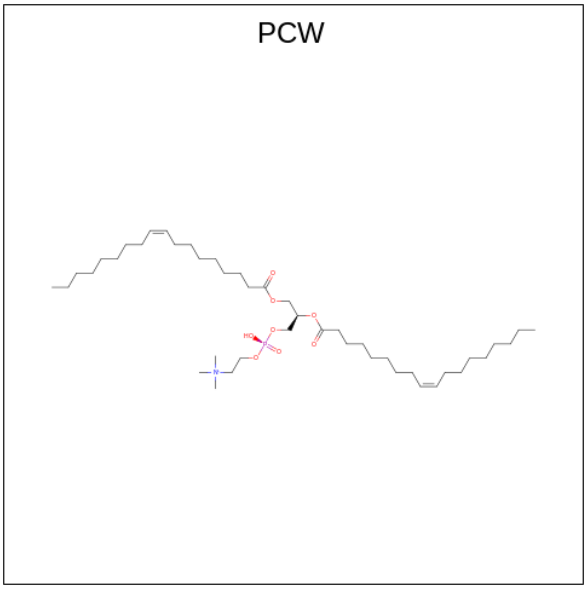
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			39	34	5	

- Molecule 9 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula: $C_{26}H_{57}NO_6P$).



Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C N O P 312 208 13 78 13	0
9	A	1	Total C N O P 312 208 13 78 13	0
9	A	1	Total C N O P 312 208 13 78 13	0
9	A	1	Total C N O P 312 208 13 78 13	0
9	A	1	Total C N O P 312 208 13 78 13	0
9	A	1	Total C N O P 312 208 13 78 13	0
9	A	1	Total C N O P 312 208 13 78 13	0
9	A	1	Total C N O P 312 208 13 78 13	0
9	A	1	Total C N O P 312 208 13 78 13	0
9	A	1	Total C N O P 312 208 13 78 13	0
9	A	1	Total C N O P 312 208 13 78 13	0
9	A	1	Total C N O P 312 208 13 78 13	0
9	A	1	Total C N O P 312 208 13 78 13	0
9	B	1	Total C N O P 17 9 1 6 1	0

- Molecule 10 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



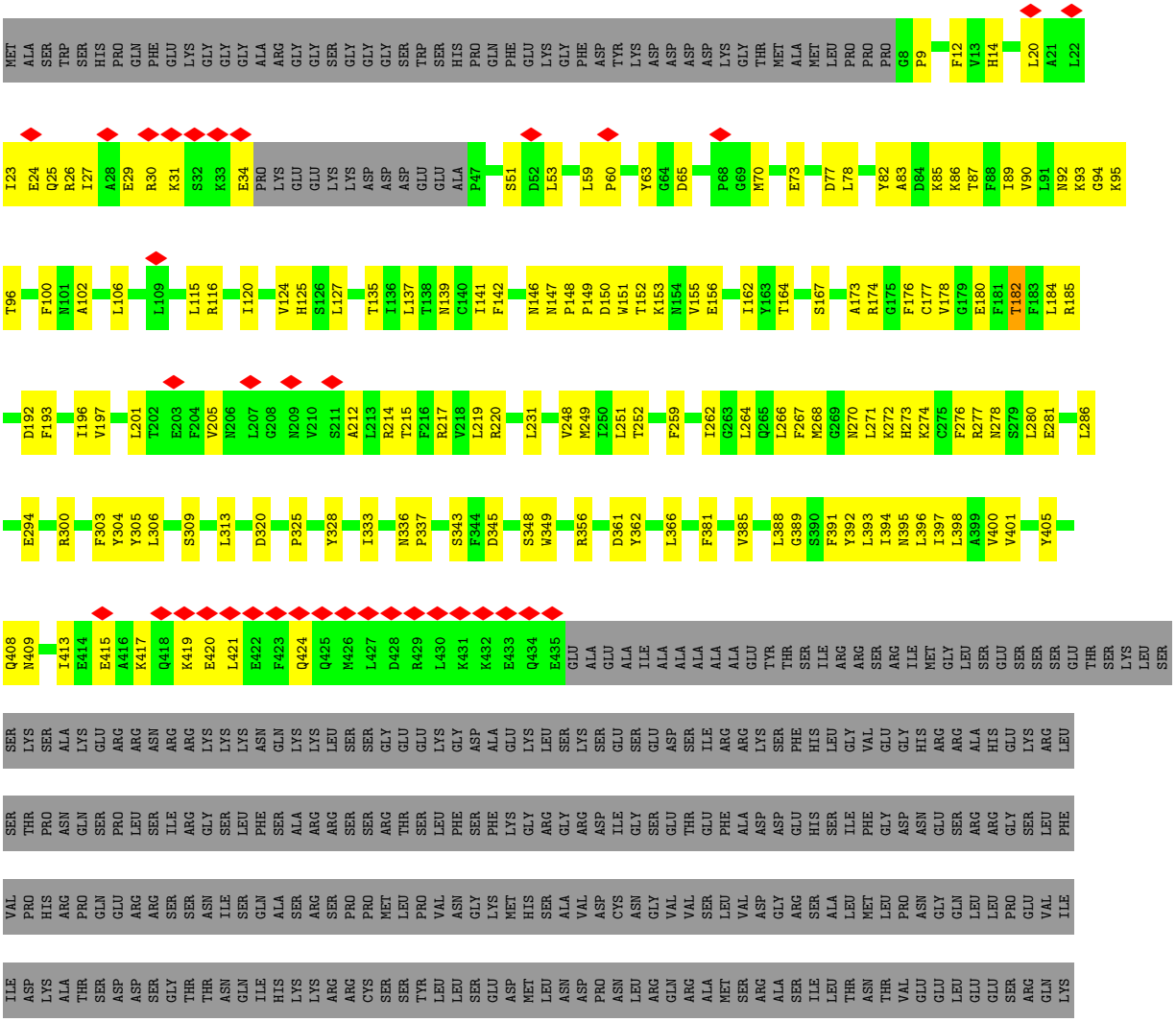
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
10	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
10	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
10	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
10	A	1	Total	C	N	O	P	0
			232	182	5	40	5	

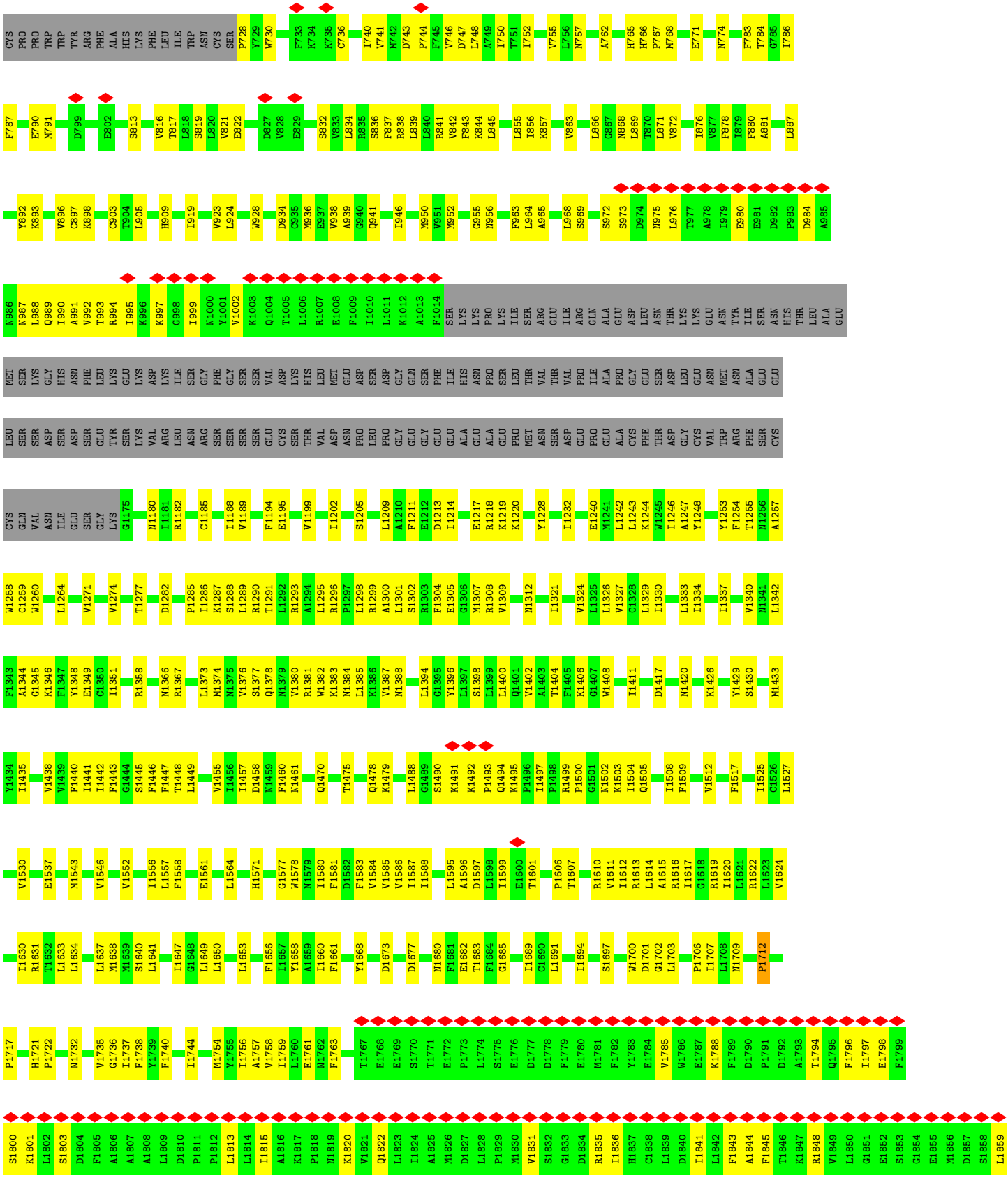
3 Residue-property plots (i)

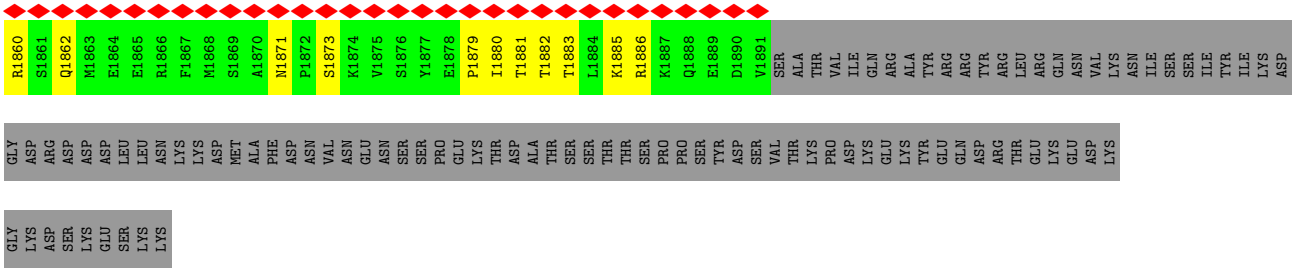
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Sodium channel protein type 9 subunit alpha

Chain A:

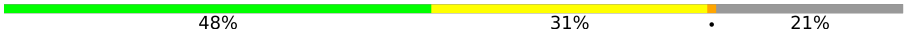


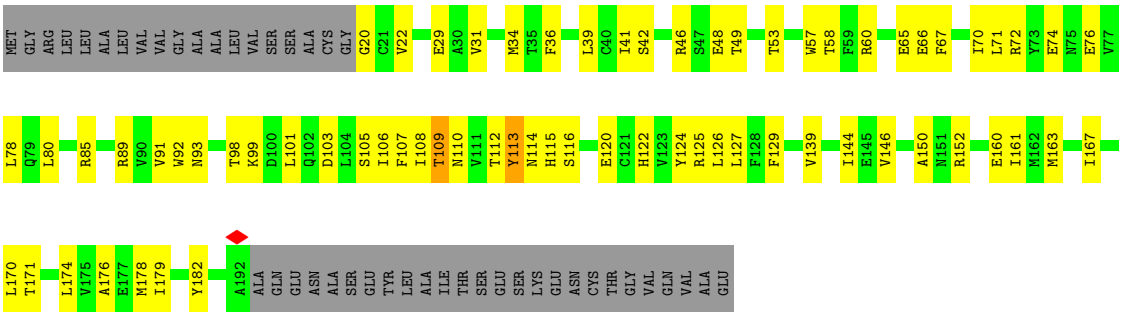

CYS PRO PRO TRP TRP TYR ARG PHE ALA HIS LYS PHE LEU ILE TRP ASN CYS SER P728 Y729 W730 F733 K734 K735 C736 I740 V741 M742 D743 P744 F745 V746 D747 L748 A749 I750 T751 I752 V755 L756 N757 A762 H765 H766 P767 M768 E771 N774 F783 T784 G785 I786
F787 E790 M791 D799 E802 S813 V816 T817 L818 S819 L820 V821 E822 D827 V828 E829 S832 W833 L834 R835 S836 F837 R838 L839 L840 R841 V842 F843 K844 L845 L855 I856 K857 V863 L866 G867 N868 L869 T870 L871 V872 I876 V877 F878 I879 F880 A881 L887
Y892 K893 V896 C897 K898 C903 T904 L905 H909 I919 V923 L924 W928 D934 C935 M936 E937 V938 A939 G940 Q941 I946 M950 V951 M952 G955 N956 F963 L964 A965 L968 S969 S972 S973 D974 N975 L976 T977 A978 I979 E980 E981 D982 P983 D984 A985
N986 N987 L988 Q989 I990 A991 V992 T993 R994 I995 K996 K997 G998 I999 N1000 Y1001 V1002 K1003 Q1004 T1005 L1006 R1007 E1008 F1009 I1010 L1011 K1012 A1013 F1014 SER LYS LYS PRO LYS ILE SER ARG GLU ILE ARG GLN ALA GLU ASP LEU ASN THR LYS LYS GLU ASN TYR ILE SER ASN HIS THR LEU ALA GLU
MET SER LYS GLY HIS ASN PHE LEU LYS GLU LYS ASP LYS ILE SER GLY PHE GLY SER SER VAL ASP LYS HIS LEU MET GLU ASP SER ASP GLY GLN SER PHE ILE HIS ASN PRO SER LEU THR VAL THR VAL PRO ILE ALA PRO GLY GLU SER ASP LEU GLU ASN MET ASN ALA GLU GLU
LEU SER SER ASP SER ASP SER GLU TYR SER LYS VAL ARG LEU ASN ARG SER SER SER GLU CYS SER THR VAL ASP ASN PRO LEU PRO GLY GLU GLY GLU GLU ALA GLU ALA GLU PRO MET ASN SER ASP GLU PRO GLU ALA CYS PHE THR ASP GLY CYS VAL TRP ARG PHE SER CYS
CYS GLN VAL ASN ILE GLU SER GLY LYS G1175 N1180 I1181 R1182 C1185 I1188 V1189 F1194 E1195 V1199 I1202 S1205 L1209 A1210 F1211 E1212 D1213 I1214 E1217 R1218 K1219 K1220 Y1228 I1232 E1240 M1241 L1242 L1243 K1244 W1245 I1246 A1247 Y1248 Y1253 F1254 T1255 N1256 A1257
W1258 C1259 W1260 L1264 V1271 V1274 T1277 D1282 P1285 I1286 K1287 S1288 L1289 R1290 T1291 L1292 R1293 A1294 L1295 R1296 P1297 L1298 R1299 A1300 L1301 S1302 R1303 F1304 E1305 G1306 M1307 R1308 V1309 N1312 I1321 V1324 L1325 L1326 V1327 C1328 L1329 I1330 L1333 I1334 I1337 V1340 N1341 L1342
F1343 A1344 G1345 K1346 F1347 Y1348 E1349 C1350 I1351 R1358 N1366 R1367 L1373 M1374 M1375 V1376 S1377 Q1378 N1379 V1380 R1381 W1382 K1383 N1384 L1385 K1386 V1387 N1388 L1394 G1395 Y1396 L1397 S1398 L1399 L1400 Q1401 V1402 A1403 T1404 F1405 K1406 G1407 W1408 I1411 D1417 N1420 K1426 Y1429 S1430 M1433
Y1434 I1435 V1438 V1439 F1440 I1441 I1442 F1443 G1444 S1445 F1446 F1447 T1448 L1449 V1455 T1456 I1457 D1458 N1459 F1460 N1461 Q1470 T1475 Q1478 K1479 L1488 G1489 S1490 K1491 K1492 P1493 Q1494 K1495 P1496 I1497 P1498 R1499 P1500 G1501 N1502 K1503 I1504 Q1505 I1508 F1509 V1512 F1517 I1525 C1526 L1527
V1530 E1537 M1543 V1546 V1552 I1556 L1557 F1558 E1561 L1564 H1571 G1577 W1578 N1579 I1580 F1581 D1582 F1583 V1584 V1585 V1586 I1587 I1588 L1595 A1596 D1597 L1598 I1599 E1600 T1601 P1606 T1607 R1610 V1611 I1612 R1613 L1614 A1615 R1616 I1617 G1618 R1619 I1620 L1621 R1622 L1623 V1624
I1630 R1631 T1632 L1633 L1634 L1637 M1638 M1639 S1640 L1641 I1647 G1648 L1649 L1650 L1653 F1656 I1657 Y1658 A1659 I1660 F1661 Y1668 D1673 D1677 N1680 F1681 E1682 T1683 F1684 G1685 I1689 C1690 L1691 I1694 S1697 W1700 D1701 G1702 L1703 P1706 I1707 L1708 N1709 P1712
P1717 H1721 P1722 N1732 V1735 G1736 I1737 F1738 Y1739 F1740 I1744 M1754 Y1755 I1756 A1757 V1758 I1759 L1760 E1761 N1762 F1763 T1767 E1768 E1769 S1770 T1771 E1772 P1773 L1774 S1775 E1776 D1777 D1778 F1779 E1780 M1781 F1782 Y1783 E1784 V1785 W1786 E1787 K1788 F1789 D1790 P1791 D1792 A1793 T1794 Q1795 F1796 I1797 E1798 F1799
S1800 K1801 L1802 S1803 D1804 F1805 A1806 A1807 A1808 L1809 D1810 P1811 P1812 L1813 L1814 I1815 A1816 K1817 P1818 N1819 K1820 V1821 Q1822 L1823 I1824 A1825 M1826 D1827 L1828 P1829 M1830 V1831 S1832 G1833 D1834 R1835 I1836 H1837 C1838 L1839 D1840 I1841 L1842 F1843 A1844 F1845 T1846 K1847 R1848 V1849 L1850 G1851 E1852 S1853 G1854 E1855 M1856 D1857 S1858 L1859



• Molecule 2: Sodium channel subunit beta-1

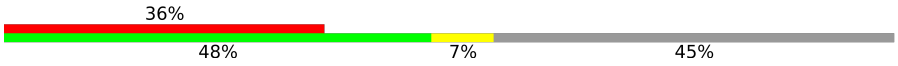
Chain B:

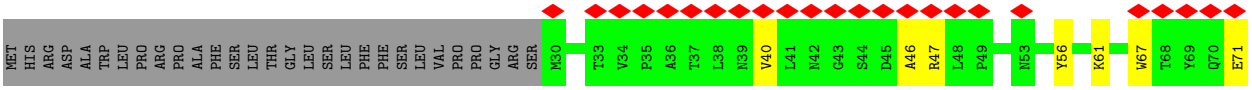


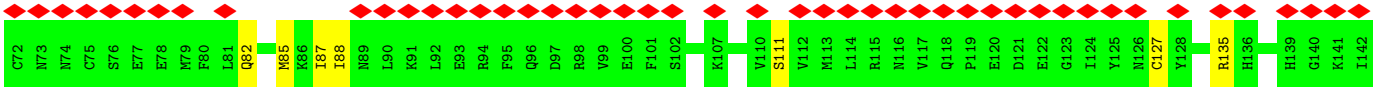


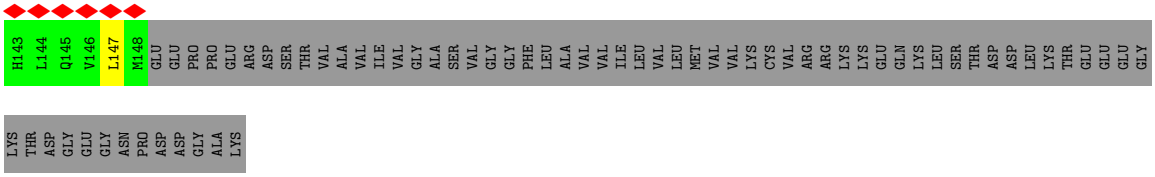
• Molecule 3: Sodium channel subunit beta-2

Chain C:



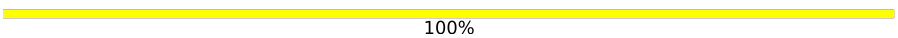






• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



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

Chain E:

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

Chain F:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1197096	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.345	Depositor
Minimum map value	-3.549	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.116	Depositor
Recommended contour level	0.43	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, LPE, 9Z9, PCW, P5S, Y01

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	0.48	0/11719	0.52	0/15869
2	B	0.53	0/1442	0.55	0/1949
3	C	0.36	0/1011	0.59	0/1367
All	All	0.48	0/14172	0.53	0/19185

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1712	PRO	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	11445	0	11662	539	0
2	B	1416	0	1379	78	0
3	C	980	0	935	17	0
4	D	28	0	25	1	0
4	E	28	0	25	5	0
4	F	28	0	25	6	0
5	A	28	0	26	0	0
5	B	42	0	39	6	0
6	A	110	0	130	24	0
7	A	210	0	294	74	0
8	A	39	0	0	33	0
9	A	312	0	426	58	0
9	B	17	0	19	9	0
10	A	232	0	323	50	0
All	All	14915	0	15308	666	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 22.

All (666) 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)
2:B:178:MET:CE	9:B:304:LPE:H12	1.51	1.41
1:A:1330:ILE:CD1	7:A:2005:Y01:HAB2	1.60	1.32
1:A:1653:LEU:HB3	9:A:2014:LPE:C16	1.60	1.29
1:A:398:LEU:HD23	8:A:2006:9Z9:C75	1.61	1.28
1:A:212:ALA:HB1	7:A:2007:Y01:OAG	1.31	1.27
1:A:950:MET:CE	10:A:2016:PCW:H251	1.68	1.23
1:A:964:LEU:HD22	8:A:2006:9Z9:C05	1.69	1.23
1:A:963:PHE:CE1	8:A:2006:9Z9:C81	2.26	1.18
1:A:1763:PHE:CE2	8:A:2006:9Z9:C19	2.27	1.16
1:A:1653:LEU:CB	9:A:2014:LPE:C16	2.21	1.16
1:A:963:PHE:CZ	8:A:2006:9Z9:C81	2.28	1.15
2:B:178:MET:HE3	9:B:304:LPE:C1	1.77	1.14
1:A:963:PHE:CE1	8:A:2006:9Z9:C77	2.31	1.13
2:B:178:MET:CE	9:B:304:LPE:C1	2.26	1.12
1:A:842:VAL:CG2	7:A:2005:Y01:HAA2	1.79	1.12
1:A:1330:ILE:HD12	7:A:2005:Y01:HAB2	1.16	1.11
1:A:1584:VAL:HG11	10:A:2018:PCW:H181	1.32	1.09
1:A:842:VAL:HG23	7:A:2005:Y01:HAA2	1.29	1.07
1:A:950:MET:HE1	10:A:2016:PCW:H251	1.11	1.07
1:A:398:LEU:CD2	8:A:2006:9Z9:C75	2.34	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1634:LEU:HD12	6:A:2017:P5S:H42	1.38	1.02
1:A:1759:ILE:HG21	8:A:2006:9Z9:C09	1.89	1.02
1:A:1759:ILE:HG21	8:A:2006:9Z9:C10	1.87	1.02
1:A:1634:LEU:CD1	6:A:2017:P5S:H42	1.89	1.01
1:A:963:PHE:HE1	8:A:2006:9Z9:C77	1.74	1.00
1:A:398:LEU:HD23	8:A:2006:9Z9:O80	1.61	0.99
1:A:1255:THR:O	7:A:2003:Y01:HAV1	1.64	0.98
1:A:1330:ILE:HD12	7:A:2005:Y01:CAB	1.94	0.95
1:A:1307:MET:HE1	9:A:2023:LPE:C19	1.97	0.95
1:A:876:ILE:HD11	7:A:2007:Y01:HAB1	1.48	0.94
1:A:964:LEU:CD2	8:A:2006:9Z9:C04	2.45	0.93
1:A:1307:MET:CE	9:A:2023:LPE:C19	2.47	0.93
1:A:950:MET:SD	10:A:2016:PCW:C26	2.57	0.93
1:A:1584:VAL:HG11	10:A:2018:PCW:C18	2.00	0.92
1:A:1218:ARG:NH1	9:A:2022:LPE:H3N3	1.83	0.91
1:A:946:ILE:HD13	10:A:2016:PCW:H181	1.52	0.90
1:A:963:PHE:CE1	8:A:2006:9Z9:C78	2.55	0.89
1:A:1254:PHE:CD2	7:A:2004:Y01:HAP2	2.07	0.88
1:A:1638:MET:HB3	6:A:2017:P5S:H44A	1.54	0.88
2:B:178:MET:HE1	9:B:304:LPE:C1	2.01	0.87
1:A:964:LEU:HD21	8:A:2006:9Z9:C04	2.03	0.87
1:A:1653:LEU:HB2	9:A:2014:LPE:C16	2.05	0.86
1:A:1763:PHE:CZ	8:A:2006:9Z9:C19	2.59	0.86
1:A:1683:THR:HG22	1:A:1685:GLY:H	1.39	0.85
1:A:897:CYS:HB2	3:C:56:TYR:CZ	2.11	0.85
2:B:126:LEU:HD21	4:F:1:NAG:H82	1.57	0.85
1:A:964:LEU:CD2	8:A:2006:9Z9:C05	2.56	0.84
1:A:212:ALA:CB	7:A:2007:Y01:HAL2	2.08	0.84
1:A:212:ALA:CB	7:A:2007:Y01:OAG	2.23	0.83
1:A:1301:LEU:HD13	9:A:2014:LPE:C15	2.08	0.83
1:A:898:LYS:HG3	3:C:56:TYR:CE1	2.14	0.82
1:A:950:MET:CE	10:A:2016:PCW:C25	2.54	0.82
1:A:398:LEU:CD2	8:A:2006:9Z9:O80	2.27	0.81
1:A:1329:LEU:HD11	10:A:2013:PCW:H441	1.62	0.81
2:B:178:MET:HE3	9:B:304:LPE:H12	0.82	0.81
1:A:1301:LEU:HD13	9:A:2014:LPE:H152	1.61	0.81
1:A:1584:VAL:CG1	10:A:2018:PCW:H181	2.11	0.80
1:A:1254:PHE:CE2	7:A:2004:Y01:HAP2	2.17	0.80
1:A:212:ALA:HB3	7:A:2007:Y01:HAL2	1.64	0.80
2:B:89:ARG:NH2	5:B:302:NAG:C8	2.45	0.80
2:B:89:ARG:HH22	5:B:302:NAG:C8	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1304:PHE:CE2	9:A:2023:LPE:C19	2.65	0.79
1:A:1330:ILE:HD11	7:A:2005:Y01:HAJ1	1.65	0.79
1:A:964:LEU:HD22	8:A:2006:9Z9:C04	2.08	0.79
1:A:1374:MET:HG2	1:A:1380:VAL:HG23	1.64	0.78
1:A:1759:ILE:HD13	8:A:2006:9Z9:C10	2.14	0.78
1:A:897:CYS:HB2	3:C:56:TYR:OH	1.84	0.77
1:A:963:PHE:CZ	8:A:2006:9Z9:C77	2.67	0.77
1:A:1722:PRO:HB3	2:B:103:ASP:HB2	1.67	0.77
1:A:903:CYS:CB	3:C:135:ARG:HE	1.98	0.76
1:A:1211:PHE:CE2	9:A:2023:LPE:H311	2.21	0.76
2:B:31:VAL:HG23	2:B:34:MET:HB2	1.69	0.75
1:A:1584:VAL:HG21	10:A:2018:PCW:H161	1.68	0.75
1:A:24:GLU:HA	1:A:27:ILE:HD12	1.69	0.74
4:E:1:NAG:H4	4:E:2:NAG:O7	1.87	0.74
1:A:249:MET:HA	1:A:252:THR:HG22	1.68	0.74
1:A:1330:ILE:HD11	7:A:2005:Y01:CAJ	2.17	0.74
1:A:1737:ILE:HD11	9:A:2011:LPE:O1	1.87	0.74
1:A:1330:ILE:HD11	7:A:2005:Y01:HAB2	1.65	0.74
1:A:398:LEU:HB3	8:A:2006:9Z9:C75	2.18	0.73
1:A:755:VAL:HG13	7:A:2005:Y01:CAN	2.18	0.73
1:A:968:LEU:HD11	8:A:2006:9Z9:C15	2.18	0.73
1:A:963:PHE:CD1	8:A:2006:9Z9:C81	2.71	0.73
1:A:1333:LEU:HD22	7:A:2030:Y01:HAA1	1.70	0.72
1:A:897:CYS:N	3:C:56:TYR:OH	2.23	0.72
1:A:1264:LEU:HD11	7:A:2003:Y01:HAA1	1.70	0.72
1:A:1499:ARG:NH2	1:A:1500:PRO:O	2.18	0.72
1:A:822:GLU:HB3	1:A:834:LEU:HD22	1.72	0.71
1:A:1218:ARG:HH12	9:A:2022:LPE:H3N3	1.55	0.71
1:A:389:GLY:HA2	1:A:393:LEU:HD23	1.71	0.71
1:A:135:THR:HG21	1:A:162:ILE:HG21	1.73	0.71
2:B:124:TYR:CE2	4:F:2:NAG:H82	2.25	0.70
1:A:903:CYS:HB3	3:C:135:ARG:HE	1.56	0.70
1:A:1185:CYS:HA	1:A:1188:ILE:HG22	1.74	0.70
1:A:1712:PRO:HB3	1:A:1717:PRO:HD3	1.74	0.70
1:A:1682:GLU:OE1	2:B:20:GLY:N	2.24	0.70
1:A:1254:PHE:HD2	7:A:2004:Y01:HAP2	1.58	0.69
1:A:963:PHE:CE2	8:A:2006:9Z9:C81	2.76	0.69
1:A:396:LEU:HD13	1:A:1633:LEU:HD13	1.75	0.68
1:A:1634:LEU:HD12	6:A:2017:P5S:C42	2.21	0.68
1:A:1321:ILE:HA	1:A:1324:VAL:HG22	1.75	0.68
1:A:1641:LEU:HD22	9:A:2019:LPE:H151	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:HA	1:A:23:ILE:HD12	1.76	0.68
1:A:1209:LEU:HD11	1:A:1296:ARG:HB3	1.76	0.68
1:A:1298:LEU:HD21	9:A:2015:LPE:H132	1.76	0.68
1:A:1307:MET:HE3	9:A:2023:LPE:C19	2.22	0.68
1:A:182:THR:HG22	1:A:185:ARG:HG2	1.76	0.68
1:A:1426:LYS:HB2	1:A:1429:TYR:HB2	1.74	0.67
1:A:845:LEU:HD21	7:A:2005:Y01:HAA1	1.77	0.67
1:A:1617:ILE:CG1	10:A:2018:PCW:H261	2.24	0.67
1:A:1738:PHE:CE2	9:A:2014:LPE:H1N2	2.30	0.67
1:A:1797:ILE:HD11	1:A:1801:LYS:HD2	1.76	0.66
1:A:1211:PHE:HE2	9:A:2023:LPE:H2N2	1.61	0.66
1:A:1505:GLN:HA	1:A:1508:ILE:HD12	1.76	0.66
1:A:1813:LEU:HD11	1:A:1845:PHE:HB3	1.76	0.65
1:A:787:PHE:O	1:A:791:MET:HG2	1.95	0.65
1:A:1295:LEU:HD11	9:A:2015:LPE:H192	1.78	0.65
1:A:1634:LEU:HD13	6:A:2017:P5S:H42	1.76	0.65
1:A:1258:TRP:CZ3	9:A:2015:LPE:H21	2.31	0.65
2:B:112:THR:H	2:B:115:HIS:CD2	2.14	0.65
6:A:2017:P5S:H22	10:A:2018:PCW:H131	1.79	0.65
1:A:1494:GLN:HE21	10:A:2018:PCW:H83	1.60	0.65
2:B:57:TRP:HB2	2:B:71:LEU:HG	1.77	0.65
1:A:259:PHE:HZ	1:A:388:LEU:HD13	1.62	0.64
1:A:276:PHE:HE2	1:A:280:LEU:HD11	1.62	0.64
1:A:212:ALA:HB3	7:A:2007:Y01:CAL	2.25	0.64
1:A:1205:SER:HB2	1:A:1296:ARG:HD3	1.79	0.64
1:A:1384:ASN:OD1	1:A:1388:ASN:ND2	2.30	0.64
2:B:108:ILE:HD11	2:B:115:HIS:CD2	2.32	0.64
1:A:177:CYS:HB2	1:A:184:LEU:HD12	1.80	0.63
2:B:124:TYR:CE2	4:F:2:NAG:C8	2.82	0.63
1:A:736:CYS:O	1:A:740:ILE:HG12	1.98	0.63
1:A:887:LEU:HD11	7:A:2007:Y01:HAT1	1.81	0.63
6:A:2002:P5S:H50	9:A:2025:LPE:H122	1.81	0.63
1:A:1182:ARG:NH1	1:A:1247:ALA:O	2.28	0.63
1:A:755:VAL:HG13	7:A:2005:Y01:HAN2	1.79	0.63
2:B:116:SER:HB2	2:B:146:VAL:HG12	1.80	0.63
1:A:845:LEU:CD2	7:A:2005:Y01:HAA1	2.29	0.62
1:A:1219:LYS:HZ1	9:A:2023:LPE:H3N2	1.63	0.62
1:A:1377:SER:OG	1:A:1378:GLN:N	2.32	0.62
1:A:1759:ILE:CG2	8:A:2006:9Z9:C10	2.73	0.62
1:A:212:ALA:CB	7:A:2007:Y01:CAL	2.78	0.62
1:A:839:LEU:HB3	1:A:1334:ILE:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1430:SER:OG	1:A:1433:MET:SD	2.57	0.62
1:A:1738:PHE:HD2	9:A:2014:LPE:H2N3	1.65	0.62
1:A:755:VAL:HG13	7:A:2005:Y01:HAN1	1.81	0.62
4:E:1:NAG:H4	4:E:2:NAG:C7	2.29	0.62
1:A:1494:GLN:NE2	10:A:2018:PCW:H83	2.14	0.62
1:A:281:GLU:OE2	1:A:281:GLU:N	2.31	0.61
1:A:1509:PHE:HA	1:A:1512:VAL:HG12	1.81	0.61
9:A:2010:LPE:H121	9:A:2012:LPE:O32	2.00	0.61
1:A:1398:SER:HB2	1:A:1411:ILE:HD13	1.81	0.61
1:A:1613:ARG:HH21	1:A:1616:ARG:HH12	1.48	0.61
1:A:750:ILE:HD11	1:A:790:GLU:HG3	1.82	0.61
1:A:941:GLN:HE22	10:A:2016:PCW:H52	1.66	0.60
1:A:897:CYS:CB	3:C:56:TYR:OH	2.49	0.60
1:A:1254:PHE:O	1:A:1260:TRP:NE1	2.32	0.60
1:A:1358:ARG:NH2	1:A:1417:ASP:OD2	2.35	0.60
1:A:1490:SER:HA	1:A:1492:LYS:HE2	1.82	0.60
1:A:1759:ILE:CG2	8:A:2006:9Z9:C09	2.74	0.60
7:A:2007:Y01:HAE2	7:A:2007:Y01:HAC1	1.84	0.60
2:B:76:GLU:OE2	2:B:99:LYS:N	2.34	0.60
1:A:248:VAL:HG22	1:A:1633:LEU:HD11	1.83	0.60
7:A:2004:Y01:HAC1	7:A:2004:Y01:HAE2	1.84	0.60
7:A:2009:Y01:HAC1	7:A:2009:Y01:HAE2	1.83	0.60
1:A:1218:ARG:CZ	9:A:2022:LPE:H3N3	2.31	0.60
2:B:72:ARG:NH2	2:B:74:GLU:OE1	2.33	0.60
2:B:29:GLU:N	2:B:29:GLU:OE1	2.34	0.60
1:A:1638:MET:HE3	9:A:2020:LPE:H131	1.84	0.60
9:A:2012:LPE:H112	7:A:2030:Y01:HAO1	1.84	0.60
1:A:1257:ALA:HB1	9:A:2015:LPE:H31	1.84	0.59
1:A:876:ILE:HD11	7:A:2007:Y01:CAB	2.27	0.59
1:A:1301:LEU:HD13	9:A:2014:LPE:H151	1.82	0.59
1:A:1348:TYR:HB3	1:A:1382:TRP:CE2	2.37	0.59
1:A:1396:TYR:HB3	10:A:2013:PCW:H181	1.83	0.59
7:A:2005:Y01:HAE2	7:A:2005:Y01:HAC1	1.84	0.59
1:A:1880:ILE:HG13	1:A:1881:THR:HG22	1.85	0.59
7:A:2003:Y01:HAE2	7:A:2003:Y01:HAC1	1.83	0.59
2:B:42:SER:O	2:B:125:ARG:NH2	2.36	0.59
1:A:90:VAL:HG21	1:A:120:ILE:HG21	1.83	0.59
1:A:903:CYS:HB2	3:C:135:ARG:HE	1.66	0.59
1:A:1219:LYS:NZ	9:A:2023:LPE:C3N	2.65	0.59
1:A:106:LEU:HA	1:A:178:VAL:HG11	1.84	0.59
1:A:149:PRO:O	1:A:152:THR:OG1	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1624:VAL:HG21	6:A:2017:P5S:H29A	1.84	0.59
1:A:843:PHE:CD1	1:A:856:ILE:HD11	2.37	0.59
1:A:1706:PRO:O	1:A:1709:ASN:ND2	2.37	0.58
1:A:264:LEU:O	1:A:268:MET:HB2	2.03	0.58
1:A:276:PHE:CE2	1:A:280:LEU:HD11	2.39	0.58
1:A:1763:PHE:CE2	8:A:2006:9Z9:C18	2.86	0.58
1:A:1301:LEU:CD1	9:A:2014:LPE:H152	2.32	0.58
1:A:1680:ASN:ND2	1:A:1682:GLU:OE2	2.37	0.58
2:B:53:THR:HB	2:B:101:LEU:H	1.69	0.58
1:A:878:PHE:O	1:A:881:ALA:HB3	2.04	0.58
1:A:1584:VAL:HG21	10:A:2018:PCW:C16	2.31	0.58
1:A:395:ASN:ND2	1:A:1758:VAL:HB	2.18	0.58
1:A:1333:LEU:HD22	7:A:2030:Y01:CAA	2.34	0.58
9:A:2010:LPE:C19	9:A:2012:LPE:H111	2.33	0.58
1:A:880:PHE:HE1	7:A:2007:Y01:HAC2	1.68	0.58
2:B:112:THR:H	2:B:115:HIS:HD2	1.49	0.58
1:A:866:LEU:HD23	1:A:965:ALA:HB1	1.86	0.58
1:A:219:LEU:HD21	7:A:2007:Y01:HAQ1	1.86	0.57
1:A:1219:LYS:NZ	9:A:2023:LPE:H3N2	2.20	0.57
1:A:1634:LEU:CD1	6:A:2017:P5S:C42	2.75	0.57
1:A:1700:TRP:CD2	1:A:1744:ILE:HD11	2.39	0.57
1:A:994:ARG:HA	1:A:997:LYS:HD2	1.84	0.57
1:A:1387:VAL:O	1:A:1398:SER:HB3	2.04	0.57
1:A:215:THR:HG22	7:A:2007:Y01:HAK2	1.85	0.57
1:A:950:MET:CE	10:A:2016:PCW:H222	2.34	0.57
2:B:178:MET:HE1	9:B:304:LPE:O1	2.04	0.57
1:A:1491:LYS:HB3	1:A:1493:PRO:HD3	1.87	0.57
6:A:2017:P5S:C35	6:A:2017:P5S:C46	2.83	0.57
2:B:178:MET:CE	9:B:304:LPE:C2	2.81	0.57
1:A:1653:LEU:HD21	9:A:2023:LPE:H182	1.86	0.57
1:A:388:LEU:HD11	6:A:2017:P5S:H34	1.87	0.57
9:A:2021:LPE:H3N1	9:A:2022:LPE:H32	1.87	0.57
1:A:356:ARG:NH2	1:A:362:TYR:O	2.38	0.57
1:A:841:ARG:HB3	1:A:844:LYS:HE3	1.86	0.57
1:A:1288:SER:O	1:A:1291:THR:OG1	2.23	0.57
1:A:271:LEU:HD12	1:A:343:SER:HA	1.87	0.56
1:A:923:VAL:HG23	1:A:928:TRP:HB3	1.85	0.56
1:A:1348:TYR:CE2	1:A:1384:ASN:HB2	2.40	0.56
1:A:1502:ASN:HD22	1:A:1505:GLN:HG3	1.70	0.56
3:C:61:LYS:HA	3:C:85:MET:HG2	1.87	0.56
1:A:259:PHE:CZ	1:A:388:LEU:HD13	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:ARG:NH2	5:B:302:NAG:H83	2.18	0.56
1:A:1377:SER:OG	4:D:1:NAG:H83	2.05	0.56
2:B:78:LEU:HD12	2:B:92:TRP:HB2	1.87	0.56
1:A:26:ARG:NH1	1:A:83:ALA:O	2.40	0.55
2:B:113:TYR:HA	2:B:146:VAL:HG11	1.89	0.55
1:A:1494:GLN:HE21	10:A:2018:PCW:C8	2.19	0.55
1:A:219:LEU:HD21	7:A:2007:Y01:CAQ	2.37	0.55
1:A:1253:TYR:CE2	1:A:1259:CYS:HB3	2.41	0.55
1:A:1367:ARG:HG3	1:A:1382:TRP:CD2	2.41	0.55
1:A:968:LEU:HD11	8:A:2006:9Z9:C14	2.37	0.55
1:A:1517:PHE:HZ	1:A:1561:GLU:HB2	1.71	0.55
1:A:876:ILE:CD1	7:A:2007:Y01:HAB1	2.30	0.54
1:A:1351:ILE:HD13	1:A:1383:LYS:HD3	1.89	0.54
2:B:178:MET:CE	9:B:304:LPE:O2H	2.55	0.54
2:B:152:ARG:NH1	2:B:160:GLU:OE1	2.37	0.54
1:A:1457:ILE:HG13	1:A:1458:ASP:N	2.21	0.54
1:A:266:LEU:O	1:A:1610:ARG:NH1	2.41	0.54
1:A:345:ASP:HB3	1:A:1537:GLU:HB3	1.89	0.54
1:A:1844:ALA:O	1:A:1848:ARG:NH1	2.40	0.54
1:A:842:VAL:HG23	7:A:2005:Y01:CAA	2.20	0.54
9:A:2021:LPE:H2N2	9:A:2022:LPE:H111	1.89	0.54
2:B:89:ARG:NH1	2:B:110:ASN:HB3	2.23	0.54
1:A:286:LEU:HD11	1:A:333:ILE:HG21	1.89	0.53
1:A:988:LEU:O	1:A:992:VAL:HG23	2.09	0.53
1:A:1304:PHE:CD2	9:A:2023:LPE:C19	2.90	0.53
1:A:1470:GLN:HB3	1:A:1479:LYS:NZ	2.24	0.53
1:A:1581:PHE:O	1:A:1585:VAL:HG23	2.08	0.53
1:A:300:ARG:HG2	1:A:305:TYR:HB2	1.89	0.53
1:A:336:ASN:HB3	1:A:337:PRO:HD2	1.90	0.53
1:A:784:THR:HG23	1:A:838:ARG:HH12	1.73	0.53
1:A:1381:ARG:HH12	1:A:1383:LYS:HD2	1.74	0.53
1:A:1558:PHE:O	1:A:1561:GLU:HG3	2.09	0.53
2:B:124:TYR:CZ	4:F:2:NAG:H82	2.43	0.53
1:A:146:ASN:OD1	1:A:147:ASN:N	2.42	0.53
2:B:66:GLU:OE2	2:B:67:PHE:N	2.42	0.53
1:A:819:SER:HA	1:A:834:LEU:HD21	1.90	0.53
1:A:1254:PHE:HD2	7:A:2004:Y01:CAP	2.22	0.53
1:A:973:SER:HA	1:A:976:LEU:HG	1.89	0.53
9:A:2022:LPE:H11	9:A:2023:LPE:H1N3	1.91	0.53
1:A:1366:ASN:HD22	4:E:1:NAG:C7	2.22	0.52
2:B:71:LEU:HB3	2:B:80:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:THR:HG22	1:A:196:ILE:HD11	1.92	0.52
1:A:14:HIS:CE1	1:A:70:MET:HG2	2.45	0.52
1:A:92:ASN:HB3	1:A:96:THR:HB	1.91	0.52
1:A:1254:PHE:CD2	7:A:2004:Y01:CAP	2.89	0.52
1:A:1584:VAL:HG11	10:A:2018:PCW:C16	2.40	0.52
1:A:1707:ILE:HD12	1:A:1740:PHE:HE2	1.74	0.52
1:A:1606:PRO:O	1:A:1610:ARG:HG2	2.09	0.52
1:A:771:GLU:HA	1:A:774:ASN:HD21	1.75	0.52
1:A:1298:LEU:CD1	9:A:2014:LPE:H151	2.40	0.52
1:A:1599:ILE:HD11	1:A:1612:ILE:HD12	1.90	0.52
1:A:25:GLN:O	1:A:29:GLU:HG2	2.10	0.52
1:A:139:ASN:ND2	1:A:220:ARG:HD3	2.24	0.52
1:A:393:LEU:O	1:A:397:ILE:HG12	2.09	0.52
1:A:1738:PHE:CD2	9:A:2014:LPE:H2N3	2.43	0.52
2:B:167:ILE:O	2:B:171:THR:HG23	2.09	0.52
1:A:1441:ILE:O	1:A:1445:SER:N	2.40	0.52
1:A:1577:GLY:H	10:A:2018:PCW:H51	1.75	0.52
1:A:176:PHE:CZ	1:A:184:LEU:HD11	2.45	0.52
1:A:928:TRP:CD1	1:A:952:MET:HE3	2.45	0.52
1:A:1803:SER:HB3	1:A:1820:LYS:HD3	1.92	0.52
3:C:67:TRP:CZ2	3:C:127:CYS:HB3	2.45	0.52
2:B:91:VAL:HG12	2:B:92:TRP:N	2.25	0.51
1:A:1443:PHE:O	1:A:1447:PHE:N	2.42	0.51
1:A:1607:THR:O	1:A:1611:VAL:HG23	2.09	0.51
1:A:1617:ILE:HD11	10:A:2018:PCW:C27	2.40	0.51
1:A:1640:SER:HB2	1:A:1761:GLU:HG3	1.91	0.51
1:A:1785:VAL:HG23	1:A:1788:LYS:HD3	1.92	0.51
3:C:47:ARG:NH2	3:C:111[B]:SER:OG	2.43	0.51
1:A:898:LYS:HG3	3:C:56:TYR:HE1	1.69	0.51
1:A:1219:LYS:HZ3	9:A:2023:LPE:C3N	2.23	0.51
1:A:1794:THR:HG23	1:A:1796:PHE:H	1.76	0.51
7:A:2009:Y01:HAE2	7:A:2009:Y01:CAC	2.41	0.51
1:A:1324:VAL:HG11	1:A:1455:VAL:HG21	1.93	0.51
2:B:39:LEU:HA	2:B:105:SER:HB2	1.93	0.51
1:A:106:LEU:H	1:A:178:VAL:HG21	1.76	0.51
1:A:1384:ASN:OD1	1:A:1385:LEU:N	2.44	0.51
1:A:919:ILE:O	1:A:923:VAL:HG12	2.11	0.50
1:A:391:PHE:CZ	1:A:1754:MET:HB3	2.45	0.50
1:A:1504:ILE:HG13	1:A:1505:GLN:N	2.26	0.50
4:E:1:NAG:C4	4:E:2:NAG:C7	2.89	0.50
1:A:1282:ASP:HA	1:A:1287:LYS:HE3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2012:LPE:H3N2	7:A:2030:Y01:HAV1	1.93	0.50
2:B:108:ILE:HD11	2:B:115:HIS:CG	2.46	0.50
1:A:248:VAL:HG21	1:A:400:VAL:HG11	1.93	0.50
1:A:325:PRO:HB2	2:B:129:PHE:HZ	1.76	0.50
1:A:398:LEU:HD23	8:A:2006:9Z9:C73	2.40	0.50
1:A:748:LEU:O	1:A:752:ILE:HG12	2.12	0.50
1:A:1502:ASN:HB3	1:A:1505:GLN:HB2	1.93	0.50
1:A:92:ASN:OD1	1:A:93:LYS:N	2.45	0.50
1:A:320:ASP:HB2	9:A:2021:LPE:H1N2	1.93	0.50
1:A:1497:ILE:HD12	1:A:1497:ILE:H	1.76	0.50
1:A:388:LEU:CD1	6:A:2017:P5S:H34	2.42	0.50
1:A:892:TYR:O	1:A:893:LYS:C	2.49	0.50
1:A:1588:ILE:HD11	10:A:2027:PCW:H242	1.94	0.50
1:A:1638:MET:CB	6:A:2017:P5S:H44A	2.33	0.50
1:A:86:LYS:HB3	1:A:102:ALA:HB3	1.93	0.50
1:A:897:CYS:HB2	3:C:56:TYR:CE1	2.46	0.50
1:A:969:SER:O	1:A:972:SER:OG	2.28	0.50
1:A:1242:LEU:HD23	6:A:2002:P5S:H56B	1.94	0.50
9:A:2010:LPE:O2H	7:A:2030:Y01:HAR2	2.12	0.50
1:A:82:TYR:HA	1:A:85:LYS:HE2	1.93	0.49
1:A:950:MET:SD	10:A:2016:PCW:C25	2.99	0.49
1:A:1217:GLU:O	1:A:1220:LYS:NZ	2.40	0.49
1:A:1502:ASN:OD1	1:A:1503:LYS:N	2.45	0.49
1:A:294:GLU:OE1	1:A:294:GLU:N	2.45	0.49
1:A:1653:LEU:CD1	9:A:2014:LPE:C16	2.90	0.49
7:A:2007:Y01:HAE2	7:A:2007:Y01:CAC	2.41	0.49
1:A:251:LEU:HB2	1:A:1630:ILE:HD12	1.94	0.49
1:A:394:ILE:O	1:A:398:LEU:HD13	2.12	0.49
1:A:1285:PRO:O	1:A:1289:LEU:N	2.42	0.49
6:A:2002:P5S:H42	9:A:2026:LPE:O32	2.12	0.49
1:A:1558:PHE:CD2	1:A:1619:ARG:HD2	2.46	0.49
1:A:1843:PHE:HE2	1:A:1859:LEU:HD23	1.78	0.49
1:A:963:PHE:CE1	8:A:2006:9Z9:C79	2.95	0.49
1:A:1330:ILE:HD11	7:A:2005:Y01:HAJ2	1.91	0.49
1:A:1442:ILE:O	1:A:1446:PHE:N	2.45	0.49
1:A:167:SER:OG	1:A:192:ASP:OD1	2.28	0.49
1:A:1290:ARG:O	1:A:1293:ARG:CB	2.61	0.49
1:A:1330:ILE:CD1	7:A:2005:Y01:HAJ1	2.40	0.49
1:A:989:GLN:O	1:A:993:THR:HG23	2.13	0.48
1:A:1302:SER:O	1:A:1308:ARG:NH1	2.45	0.48
1:A:277:ARG:O	1:A:278:ASN:ND2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:PHE:CE1	1:A:1754:MET:HB3	2.48	0.48
1:A:863:VAL:HG12	1:A:863:VAL:O	2.12	0.48
1:A:936:MET:HG2	1:A:941:GLN:HA	1.96	0.48
1:A:1402:VAL:HA	1:A:1408:TRP:HB3	1.95	0.48
2:B:36:PHE:HE2	2:B:144:ILE:HD12	1.76	0.48
2:B:78:LEU:CD1	2:B:92:TRP:HB2	2.43	0.48
1:A:139:ASN:HD21	1:A:220:ARG:HD3	1.77	0.48
7:A:2004:Y01:HAE2	7:A:2004:Y01:CAC	2.41	0.48
1:A:950:MET:SD	10:A:2016:PCW:H251	2.53	0.48
1:A:349:TRP:CZ3	10:A:2016:PCW:H321	2.48	0.48
1:A:766:HIS:CD2	1:A:1345:GLY:HA3	2.49	0.48
1:A:12:PHE:HB3	1:A:70:MET:SD	2.54	0.48
1:A:267:PHE:HA	1:A:270:ASN:HD22	1.78	0.48
1:A:272:LYS:O	1:A:274:LYS:HG3	2.14	0.48
1:A:755:VAL:HG22	7:A:2005:Y01:HAN2	1.95	0.48
1:A:1304:PHE:HE2	9:A:2023:LPE:C19	2.24	0.48
7:A:2009:Y01:HAC1	7:A:2009:Y01:HAU2	1.96	0.48
1:A:765:HIS:CE1	1:A:768:MET:HG2	2.49	0.48
1:A:1394:LEU:HD22	10:A:2013:PCW:H121	1.96	0.48
1:A:177:CYS:HA	1:A:182:THR:HG21	1.95	0.48
7:A:2003:Y01:HAC1	7:A:2003:Y01:HAU2	1.96	0.48
7:A:2007:Y01:HAC1	7:A:2007:Y01:HAU2	1.96	0.48
2:B:127:LEU:HB3	2:B:129:PHE:CE2	2.48	0.48
1:A:51:SER:O	1:A:51:SER:OG	2.30	0.48
1:A:1214:ILE:HG22	2:B:22:VAL:HG21	1.96	0.48
1:A:1578:TRP:CH2	6:A:2017:P5S:C26	2.97	0.48
1:A:1701:ASP:N	1:A:1701:ASP:OD1	2.45	0.48
1:A:1732:ASN:HB3	1:A:1735:VAL:HG12	1.96	0.48
7:A:2009:Y01:OAG	7:A:2009:Y01:HAV2	2.14	0.48
1:A:100:PHE:HE1	1:A:174:ARG:HG2	1.79	0.47
1:A:251:LEU:HD13	1:A:1630:ILE:HG23	1.96	0.47
1:A:1494:GLN:OE1	1:A:1495:LYS:N	2.47	0.47
10:A:2016:PCW:H42	10:A:2016:PCW:H83	1.62	0.47
1:A:1246:ILE:HD13	6:A:2002:P5S:H51	1.96	0.47
1:A:1661:PHE:CD2	9:A:2014:LPE:H311	2.49	0.47
2:B:126:LEU:CD2	4:F:1:NAG:H82	2.36	0.47
2:B:76:GLU:OE2	2:B:98:THR:N	2.46	0.47
1:A:300:ARG:NH2	1:A:309:SER:O	2.46	0.47
1:A:1307:MET:HE2	1:A:1649:LEU:HB3	1.96	0.47
1:A:1348:TYR:HB3	1:A:1382:TRP:CZ2	2.50	0.47
1:A:1404:THR:O	1:A:1406:LYS:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:999:ILE:HA	1:A:1002:VAL:HG22	1.96	0.47
1:A:1258:TRP:CZ3	9:A:2015:LPE:C2	2.98	0.47
1:A:1333:LEU:HB2	7:A:2030:Y01:HAA1	1.95	0.47
7:A:2004:Y01:HAC1	7:A:2004:Y01:HAU2	1.96	0.47
1:A:991:ALA:O	1:A:995:ILE:HG12	2.14	0.47
1:A:9:PRO:HA	1:A:63:TYR:HA	1.96	0.47
1:A:762:ALA:HB2	1:A:1337:ILE:HD11	1.96	0.47
1:A:1189:VAL:HA	1:A:1194:PHE:CD2	2.50	0.47
1:A:1195:GLU:O	1:A:1199:VAL:HG23	2.14	0.47
1:A:1624:VAL:HG12	1:A:1631:ARG:HG2	1.96	0.47
1:A:53:LEU:HD21	1:A:78:LEU:HG	1.96	0.47
1:A:1290:ARG:O	1:A:1293:ARG:HB3	2.15	0.47
1:A:1613:ARG:HE	1:A:1616:ARG:NH1	2.13	0.47
1:A:1617:ILE:HD11	10:A:2018:PCW:H261	1.97	0.47
1:A:1700:TRP:CG	1:A:1744:ILE:HD11	2.50	0.47
9:A:2010:LPE:HO21	7:A:2030:Y01:HAR2	1.79	0.47
7:A:2030:Y01:HAP1	7:A:2030:Y01:HAO2	1.36	0.47
1:A:834:LEU:O	1:A:836:SER:N	2.48	0.47
1:A:950:MET:HE1	10:A:2016:PCW:H222	1.96	0.47
1:A:1650:LEU:HD11	9:A:2014:LPE:H132	1.96	0.47
1:A:1578:TRP:CH2	6:A:2017:P5S:H26	2.50	0.47
1:A:1373:LEU:HA	1:A:1376:VAL:HG12	1.97	0.46
7:A:2003:Y01:HAE2	7:A:2003:Y01:CAC	2.41	0.46
7:A:2005:Y01:HAC1	7:A:2005:Y01:HAU2	1.96	0.46
1:A:786:ILE:O	1:A:790:GLU:HG2	2.15	0.46
1:A:1527:LEU:HA	1:A:1530:VAL:HG12	1.96	0.46
1:A:12:PHE:CE2	1:A:63:TYR:HB3	2.50	0.46
1:A:1340:VAL:O	1:A:1344:ALA:HB2	2.15	0.46
1:A:398:LEU:CB	8:A:2006:9Z9:C75	2.89	0.46
1:A:896:VAL:CG1	1:A:905:LEU:HD23	2.45	0.46
4:E:1:NAG:C4	4:E:2:NAG:O7	2.60	0.46
1:A:120:ILE:O	1:A:124:VAL:HG22	2.15	0.46
1:A:946:ILE:CD1	10:A:2016:PCW:H181	2.35	0.46
7:A:2005:Y01:HAE2	7:A:2005:Y01:CAC	2.41	0.46
10:A:2013:PCW:H242	10:A:2013:PCW:H283	1.96	0.46
6:A:2029:P5S:H20A	6:A:2029:P5S:H1A	1.74	0.46
1:A:73:GLU:H	1:A:90:VAL:HG13	1.81	0.46
1:A:115:LEU:HD12	1:A:115:LEU:H	1.81	0.46
1:A:417:LYS:O	1:A:421:LEU:HG	2.16	0.46
1:A:1232:ILE:HD11	2:B:163:MET:HA	1.98	0.46
1:A:1836:ILE:HG23	1:A:1841:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2005:Y01:HAV2	7:A:2005:Y01:OAG	2.14	0.46
1:A:100:PHE:CE1	1:A:174:ARG:HG2	2.51	0.46
1:A:1240:GLU:OE2	1:A:1244:LYS:HD2	2.15	0.46
1:A:1324:VAL:HA	1:A:1327:VAL:HG12	1.97	0.46
1:A:1656:PHE:O	1:A:1660:ILE:HG12	2.16	0.46
10:A:2027:PCW:H341	10:A:2027:PCW:H371	1.56	0.46
1:A:156:GLU:OE2	1:A:220:ARG:NH1	2.47	0.46
1:A:1491:LYS:C	1:A:1493:PRO:HD3	2.36	0.46
2:B:46:ARG:O	2:B:49:THR:HG22	2.15	0.46
2:B:112:THR:N	2:B:115:HIS:HD2	2.12	0.46
1:A:413:ILE:HG22	1:A:417:LYS:HZ3	1.80	0.46
1:A:1435:ILE:O	1:A:1438:VAL:HG22	2.16	0.46
1:A:1504:ILE:HG13	1:A:1505:GLN:H	1.81	0.46
1:A:1800:SER:O	1:A:1803:SER:OG	2.34	0.46
1:A:396:LEU:HD23	1:A:396:LEU:HA	1.75	0.45
1:A:743:ASP:HB3	1:A:987:ASN:HD21	1.80	0.45
1:A:1274:VAL:HA	1:A:1277:THR:HG22	1.98	0.45
1:A:1658:TYR:CE1	9:A:2014:LPE:H312	2.51	0.45
1:A:741:VAL:HG23	1:A:746:VAL:HG11	1.97	0.45
1:A:1488:LEU:HD11	10:A:2018:PCW:H12	1.98	0.45
1:A:1882:THR:HG23	1:A:1885:LYS:H	1.81	0.45
2:B:112:THR:HG23	2:B:114:ASN:H	1.81	0.45
2:B:178:MET:HE1	9:B:304:LPE:O2H	2.16	0.45
1:A:77:ASP:OD2	1:A:87:THR:OG1	2.28	0.45
1:A:834:LEU:O	1:A:837:PHE:N	2.48	0.45
1:A:1180:ASN:HB3	2:B:182:TYR:HE1	1.81	0.45
1:A:1218:ARG:CZ	9:A:2022:LPE:C3N	2.95	0.45
2:B:71:LEU:HD21	2:B:106:ILE:HG21	1.98	0.45
1:A:1346:LYS:HG2	1:A:1420:ASN:O	2.16	0.45
1:A:1543:MET:HA	1:A:1546:VAL:HG12	1.98	0.45
1:A:1597:ASP:O	1:A:1601:THR:HG23	2.17	0.45
1:A:1859:LEU:HD12	1:A:1862:GLN:HE21	1.81	0.45
10:A:2027:PCW:H42	10:A:2027:PCW:H63	1.59	0.45
2:B:89:ARG:HH22	5:B:302:NAG:H81	1.79	0.45
1:A:125:HIS:CE1	1:A:127:LEU:HD23	2.51	0.45
1:A:262:ILE:HG12	1:A:1614:LEU:HD11	1.98	0.45
1:A:325:PRO:HD3	2:B:46:ARG:HD3	1.97	0.45
1:A:1525:ILE:HD11	1:A:1622:ARG:HD3	1.99	0.45
10:A:2018:PCW:H31	10:A:2027:PCW:H31	1.98	0.45
2:B:89:ARG:HH22	5:B:302:NAG:H82	1.79	0.45
1:A:1243:LEU:HD11	2:B:174:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1228:TYR:CD1	2:B:163:MET:HE1	2.52	0.45
1:A:1615:ALA:HA	10:A:2018:PCW:H252	1.99	0.45
9:A:2014:LPE:H311	9:A:2014:LPE:H3N2	1.68	0.45
1:A:201:LEU:O	1:A:205:VAL:HG12	2.17	0.44
7:A:2030:Y01:HAS2	7:A:2030:Y01:HAE1	1.81	0.44
1:A:728:PRO:HG2	1:A:730:TRP:HB3	1.99	0.44
1:A:743:ASP:HB2	1:A:744:PRO:HD3	1.99	0.44
1:A:924:LEU:HD21	1:A:955:GLY:HA3	1.99	0.44
9:A:2021:LPE:C3N	9:A:2022:LPE:H32	2.48	0.44
1:A:952:MET:O	1:A:956:ASN:HB2	2.17	0.44
1:A:1508:ILE:HG23	1:A:1564:LEU:HD22	1.99	0.44
1:A:392:TYR:CZ	1:A:1637:LEU:HB2	2.52	0.44
1:A:1213:ASP:OD1	1:A:1683:THR:HG23	2.16	0.44
1:A:1296:ARG:HG3	1:A:1299:ARG:NH2	2.32	0.44
1:A:231:LEU:HA	1:A:231:LEU:HD23	1.65	0.44
1:A:304:TYR:HB2	1:A:328:TYR:CE2	2.53	0.44
1:A:1305:GLU:HG3	1:A:1308:ARG:HH21	1.82	0.44
1:A:1617:ILE:HD11	10:A:2018:PCW:C26	2.47	0.44
1:A:1691:LEU:HA	1:A:1691:LEU:HD23	1.74	0.44
2:B:93:ASN:HB2	2:B:107:PHE:HB2	1.99	0.44
1:A:215:THR:CG2	7:A:2007:Y01:HAK2	2.48	0.44
1:A:869:LEU:O	1:A:872:VAL:HG22	2.18	0.44
1:A:934:ASP:O	1:A:938:VAL:HG22	2.17	0.44
1:A:1202:ILE:HG21	1:A:1300:ALA:HB2	1.98	0.44
1:A:1460:PHE:HD2	1:A:1756:ILE:HG21	1.82	0.44
2:B:101:LEU:HD23	2:B:101:LEU:HA	1.74	0.44
1:A:270:ASN:O	1:A:272:LYS:N	2.44	0.44
1:A:747:ASP:OD1	1:A:987:ASN:HB3	2.17	0.44
1:A:1182:ARG:NH1	1:A:1248:TYR:O	2.51	0.44
1:A:1595:LEU:O	1:A:1599:ILE:HG13	2.18	0.44
1:A:395:ASN:HD21	1:A:1758:VAL:HB	1.83	0.44
1:A:952:MET:HB2	1:A:952:MET:HE2	1.68	0.44
1:A:963:PHE:HB2	1:A:1446:PHE:HE1	1.83	0.44
1:A:1286:ILE:HD12	1:A:1286:ILE:H	1.83	0.44
1:A:1440:PHE:O	1:A:1441:ILE:C	2.55	0.44
1:A:1552:VAL:O	1:A:1556:ILE:HG22	2.17	0.44
1:A:1583:PHE:HA	1:A:1586:VAL:HG12	2.00	0.44
1:A:150:ASP:HA	1:A:153:LYS:HE2	1.99	0.43
1:A:361:ASP:OD2	1:A:928:TRP:CD1	2.71	0.43
1:A:984:ASP:OD1	1:A:990:ILE:HD11	2.18	0.43
7:A:2005:Y01:HAN2	7:A:2005:Y01:HAC3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:TYR:CE1	1:A:78:LEU:HD21	2.53	0.43
1:A:137:LEU:O	1:A:141:ILE:HG12	2.18	0.43
1:A:1381:ARG:NH1	1:A:1383:LYS:HD2	2.32	0.43
2:B:46:ARG:NE	2:B:48:GLU:OE2	2.37	0.43
2:B:89:ARG:NH2	5:B:302:NAG:H81	2.30	0.43
7:A:2009:Y01:HAN2	7:A:2009:Y01:HAC3	2.00	0.43
1:A:1271:VAL:HA	1:A:1274:VAL:HG12	1.99	0.43
1:A:757:ASN:HA	1:A:783:PHE:CE2	2.53	0.43
1:A:1326:LEU:HD23	1:A:1326:LEU:HA	1.71	0.43
1:A:1580:ILE:HG22	10:A:2018:PCW:H121	2.00	0.43
1:A:1831:VAL:HA	1:A:1879:PRO:HA	2.00	0.43
1:A:1329:LEU:HD23	1:A:1329:LEU:HA	1.77	0.43
1:A:267:PHE:HA	1:A:270:ASN:ND2	2.34	0.43
1:A:832:SER:HB2	1:A:1342:LEU:HD21	1.99	0.43
1:A:1492:LYS:N	1:A:1493:PRO:HD3	2.33	0.43
1:A:65:ASP:HA	1:A:95:LYS:HZ1	1.84	0.43
1:A:146:ASN:O	1:A:148:PRO:HD3	2.19	0.43
1:A:180:GLU:HA	1:A:185:ARG:HH22	1.84	0.43
1:A:950:MET:HE2	10:A:2016:PCW:C22	2.49	0.43
1:A:980:GLU:H	1:A:980:GLU:CD	2.22	0.43
2:B:107:PHE:CE1	2:B:109:THR:HG22	2.53	0.43
1:A:12:PHE:HE2	1:A:63:TYR:HB3	1.84	0.43
1:A:755:VAL:HG21	7:A:2005:Y01:HAC3	2.00	0.43
1:A:1349:GLU:HG3	1:A:1351:ILE:HG23	2.00	0.43
1:A:1442:ILE:O	1:A:1443:PHE:C	2.58	0.43
1:A:817:THR:O	1:A:821:VAL:HG23	2.19	0.43
1:A:845:LEU:HD22	7:A:2005:Y01:CAA	2.49	0.43
1:A:905:LEU:HB3	1:A:909:HIS:ND1	2.33	0.43
1:A:924:LEU:HD23	1:A:924:LEU:HA	1.66	0.43
1:A:1189:VAL:HG11	1:A:1244:LYS:HG2	2.00	0.43
1:A:1798:GLU:HG3	1:A:1801:LYS:H	1.84	0.43
2:B:58:THR:CG2	2:B:120:GLU:HB2	2.49	0.43
3:C:87:ILE:HD13	3:C:87:ILE:HA	1.78	0.43
1:A:876:ILE:HD13	1:A:876:ILE:HA	1.87	0.42
1:A:1634:LEU:CD1	6:A:2017:P5S:H40	2.49	0.42
1:A:1673:ASP:N	1:A:1673:ASP:OD1	2.52	0.42
2:B:31:VAL:HG11	2:B:150:ALA:HB2	2.01	0.42
2:B:60:ARG:HD2	2:B:65:GLU:HA	2.00	0.42
1:A:30:ARG:HD2	1:A:31:LYS:HZ2	1.84	0.42
1:A:78:LEU:H	1:A:89:ILE:HD12	1.85	0.42
1:A:214:ARG:NH1	1:A:217:ARG:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:SER:HB2	10:A:2016:PCW:H332	2.01	0.42
1:A:415:GLU:HG3	1:A:419:LYS:HE2	2.01	0.42
1:A:972:SER:O	1:A:975:ASN:N	2.52	0.42
1:A:1653:LEU:HD13	9:A:2014:LPE:C16	2.49	0.42
1:A:1871:ASN:OD1	1:A:1873:SER:OG	2.29	0.42
3:C:82:GLN:O	3:C:88:ILE:HB	2.19	0.42
1:A:743:ASP:O	1:A:747:ASP:CB	2.68	0.42
1:A:857:LYS:HD3	1:A:857:LYS:HA	1.75	0.42
1:A:950:MET:HE2	10:A:2016:PCW:H251	1.82	0.42
1:A:1457:ILE:HG13	1:A:1458:ASP:H	1.85	0.42
1:A:1694:ILE:CG2	1:A:1703:LEU:HD12	2.50	0.42
2:B:91:VAL:CG1	2:B:92:TRP:N	2.83	0.42
1:A:938:VAL:HG23	1:A:939:ALA:N	2.34	0.42
1:A:938:VAL:HG23	1:A:939:ALA:H	1.84	0.42
1:A:1290:ARG:HH22	1:A:1293:ARG:NH2	2.18	0.42
1:A:1624:VAL:HG21	6:A:2017:P5S:C29	2.50	0.42
1:A:1701:ASP:OD1	1:A:1702:GLY:N	2.47	0.42
2:B:170:LEU:HD23	2:B:170:LEU:HA	1.72	0.42
1:A:73:GLU:N	1:A:90:VAL:HG13	2.34	0.42
1:A:193:PHE:O	1:A:197:VAL:HG22	2.20	0.42
1:A:845:LEU:CD2	7:A:2005:Y01:CAA	2.96	0.42
1:A:142:PHE:HE2	1:A:151:TRP:HZ3	1.68	0.42
1:A:1326:LEU:HD13	7:A:2005:Y01:HAQ2	2.00	0.42
1:A:1475:THR:HG23	1:A:1478:GLN:OE1	2.20	0.42
1:A:1571:HIS:CE1	6:A:2029:P5S:HN	2.38	0.42
1:A:1596:ALA:HA	1:A:1599:ILE:HD12	2.02	0.42
2:B:122:HIS:ND1	2:B:139:VAL:HG22	2.35	0.42
1:A:1189:VAL:HA	1:A:1194:PHE:HD2	1.85	0.42
1:A:1329:LEU:O	1:A:1396:TYR:OH	2.37	0.42
1:A:1668:TYR:HB3	1:A:1721:HIS:NE2	2.34	0.42
1:A:1860:ARG:HA	1:A:1860:ARG:HD2	1.91	0.42
1:A:1441:ILE:O	1:A:1442:ILE:C	2.58	0.42
1:A:1457:ILE:O	1:A:1461:ASN:N	2.51	0.42
1:A:1617:ILE:HG13	10:A:2018:PCW:H261	2.00	0.42
10:A:2028:PCW:H211	10:A:2028:PCW:H182	1.59	0.42
1:A:381:PHE:O	1:A:385:VAL:HG23	2.20	0.42
1:A:1677:ASP:OD1	2:B:46:ARG:NH2	2.49	0.42
1:A:408:GLN:O	1:A:409:ASN:C	2.58	0.41
1:A:420:GLU:OE2	1:A:424:GLN:NE2	2.53	0.41
1:A:903:CYS:HB3	3:C:135:ARG:NE	2.28	0.41
1:A:1785:VAL:O	1:A:1788:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:ASP:O	1:A:747:ASP:HB2	2.20	0.41
2:B:48:GLU:HG2	2:B:49:THR:N	2.35	0.41
1:A:748:LEU:HA	1:A:748:LEU:HD12	1.84	0.41
1:A:1330:ILE:HD13	1:A:1330:ILE:HA	1.91	0.41
1:A:1406:LYS:HG3	1:A:1697:SER:O	2.20	0.41
10:A:2018:PCW:H41	10:A:2018:PCW:H73	1.57	0.41
1:A:59:LEU:HD12	1:A:60:PRO:HD2	2.01	0.41
1:A:142:PHE:CZ	1:A:155:VAL:HG11	2.55	0.41
1:A:398:LEU:HD23	8:A:2006:9Z9:C74	2.41	0.41
1:A:1587:ILE:HD13	1:A:1587:ILE:HA	1.91	0.41
1:A:1647:ILE:HG21	1:A:1754:MET:HG3	2.02	0.41
1:A:1685:GLY:O	1:A:1689:ILE:HG12	2.21	0.41
1:A:1815:ILE:HG21	1:A:1822:GLN:NE2	2.35	0.41
1:A:1831:VAL:HG12	1:A:1835:ARG:O	2.21	0.41
1:A:1881:THR:OG1	1:A:1882:THR:N	2.54	0.41
2:B:70:ILE:HG13	2:B:71:LEU:N	2.35	0.41
3:C:40:VAL:HG11	3:C:46:ALA:HB2	2.03	0.41
1:A:92:ASN:CG	1:A:94:GLY:H	2.24	0.41
1:A:1617:ILE:HA	1:A:1620:ILE:HD13	2.03	0.41
7:A:2007:Y01:HAE1	7:A:2007:Y01:HAS2	1.81	0.41
10:A:2013:PCW:H222	10:A:2013:PCW:H251	1.76	0.41
2:B:176:ALA:O	2:B:179:ILE:HG22	2.20	0.41
1:A:274:LYS:HB3	1:A:303:PHE:HD2	1.86	0.41
9:A:2026:LPE:H3N2	9:A:2026:LPE:H312	1.72	0.41
1:A:397:ILE:O	1:A:401:VAL:HG22	2.20	0.41
1:A:1757:ALA:O	1:A:1761:GLU:HG2	2.20	0.41
1:A:313:LEU:HD12	1:A:313:LEU:HA	1.82	0.41
1:A:405:TYR:HE2	1:A:409:ASN:HD21	1.69	0.41
1:A:755:VAL:CG1	7:A:2005:Y01:HAN2	2.47	0.41
1:A:1289:LEU:HD12	1:A:1289:LEU:HA	1.94	0.41
7:A:2009:Y01:HAE1	7:A:2009:Y01:HAS2	1.81	0.41
2:B:72:ARG:HH21	2:B:74:GLU:CD	2.24	0.41
1:A:270:ASN:O	1:A:273:HIS:CD2	2.74	0.41
1:A:856:ILE:HD13	1:A:856:ILE:HA	1.79	0.41
1:A:1557:LEU:HD12	1:A:1557:LEU:HA	1.67	0.41
1:A:1617:ILE:CD1	10:A:2018:PCW:H261	2.50	0.41
1:A:1641:LEU:HA	1:A:1641:LEU:HD23	1.85	0.41
10:A:2013:PCW:H161	10:A:2013:PCW:H19	1.79	0.41
2:B:39:LEU:HD23	2:B:41:ILE:HD11	2.03	0.41
2:B:161:ILE:HD13	2:B:161:ILE:HA	1.93	0.41
1:A:366:LEU:HD12	1:A:366:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:ILE:HD13	1:A:786:ILE:HA	1.90	0.41
1:A:1246:ILE:HD11	6:A:2002:P5S:H56A	2.02	0.41
1:A:1381:ARG:O	1:A:1383:LYS:N	2.54	0.41
2:B:53:THR:CG2	2:B:101:LEU:HB2	2.51	0.41
1:A:1298:LEU:HD12	9:A:2014:LPE:H151	2.03	0.40
1:A:1578:TRP:CZ3	6:A:2017:P5S:H26	2.55	0.40
1:A:1703:LEU:HA	1:A:1703:LEU:HD23	1.86	0.40
1:A:1707:ILE:HG21	1:A:1736:GLY:HA3	2.03	0.40
1:A:116:ARG:NE	1:A:173:ALA:O	2.49	0.40
1:A:1502:ASN:ND2	1:A:1505:GLN:HG3	2.33	0.40
2:B:85:ARG:O	2:B:115:HIS:HE1	2.04	0.40
2:B:124:TYR:CE2	4:F:2:NAG:H81	2.55	0.40
1:A:30:ARG:O	1:A:34:GLU:HG2	2.22	0.40
1:A:306:LEU:HD23	1:A:306:LEU:HA	1.85	0.40
1:A:1309:VAL:HA	1:A:1312:ASN:ND2	2.36	0.40
1:A:1491:LYS:NZ	10:A:2027:PCW:H83	2.36	0.40
1:A:1883:THR:HA	1:A:1886:ARG:NH2	2.36	0.40
1:A:272:LYS:HG3	1:A:336:ASN:HD22	1.86	0.40
1:A:819:SER:HA	1:A:834:LEU:HD11	2.03	0.40
1:A:855:LEU:HA	1:A:855:LEU:HD12	1.83	0.40
1:A:868:ASN:O	1:A:871:LEU:HB3	2.22	0.40
1:A:1400:LEU:HD22	10:A:2013:PCW:H212	2.03	0.40
1:A:1470:GLN:HB3	1:A:1479:LYS:HZ1	1.86	0.40
1:A:1488:LEU:HA	1:A:1491:LYS:HE2	2.03	0.40
1:A:1638:MET:CE	9:A:2020:LPE:H131	2.50	0.40
1:A:1759:ILE:HD11	8:A:2006:9Z9:C75	2.50	0.40
1:A:766:HIS:HB3	1:A:767:PRO:HD3	2.04	0.40
1:A:813:SER:HA	1:A:816:VAL:HG12	2.03	0.40
1:A:928:TRP:NE1	1:A:952:MET:HE3	2.35	0.40
1:A:1448:THR:OG1	1:A:1449:LEU:N	2.55	0.40
1:A:1564:LEU:HD23	1:A:1564:LEU:HA	1.72	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	1412/2031 (70%)	1300 (92%)	112 (8%)	0	100	100
2	B	171/218 (78%)	153 (90%)	18 (10%)	0	100	100
3	C	120/215 (56%)	116 (97%)	4 (3%)	0	100	100
All	All	1703/2464 (69%)	1569 (92%)	134 (8%)	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	1268/1809 (70%)	1267 (100%)	1 (0%)	93	98
2	B	157/190 (83%)	155 (99%)	2 (1%)	69	86
3	C	114/193 (59%)	112 (98%)	2 (2%)	59	81
All	All	1539/2192 (70%)	1534 (100%)	5 (0%)	92	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	THR
2	B	109	THR
2	B	113	TYR
3	C	71	GLU
3	C	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	278	ASN

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Mol	Chain	Res	Type
1	A	336	ASN
1	A	365	ASN
1	A	368	GLN
1	A	425	GLN
1	A	780	ASN
1	A	941	GLN
1	A	1191	HIS
1	A	1341	ASN
1	A	1686	ASN
1	A	1693	GLN
1	A	1709	ASN
2	B	102	GLN
2	B	115	HIS
2	B	134	HIS
3	C	53	ASN
3	C	70	GLN
3	C	82	GLN
3	C	118	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

6 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	$\#\|Z\| > 2$
4	NAG	D	1	1,4	14,14,15	0.22	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	D	2	4	14,14,15	0.30	0	17,19,21	0.71	1 (5%)
4	NAG	E	1	1,4	14,14,15	0.31	0	17,19,21	0.89	1 (5%)
4	NAG	E	2	4	14,14,15	0.27	0	17,19,21	0.90	1 (5%)
4	NAG	F	1	2,4	14,14,15	0.57	0	17,19,21	1.19	2 (11%)
4	NAG	F	2	4	14,14,15	0.66	0	17,19,21	1.19	1 (5%)

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
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	NAG	F	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1	NAG	C4-C3-C2	-2.91	106.75	111.02
4	E	2	NAG	C4-C3-C2	-2.83	106.87	111.02
4	F	1	NAG	C1-O5-C5	2.73	115.89	112.19
4	F	1	NAG	C3-C4-C5	-2.63	105.55	110.24
4	F	2	NAG	C4-C3-C2	-2.40	107.50	111.02
4	D	2	NAG	O5-C1-C2	-2.03	108.09	111.29

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O7-C7-N2-C2
4	E	1	NAG	C8-C7-N2-C2
4	F	2	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6

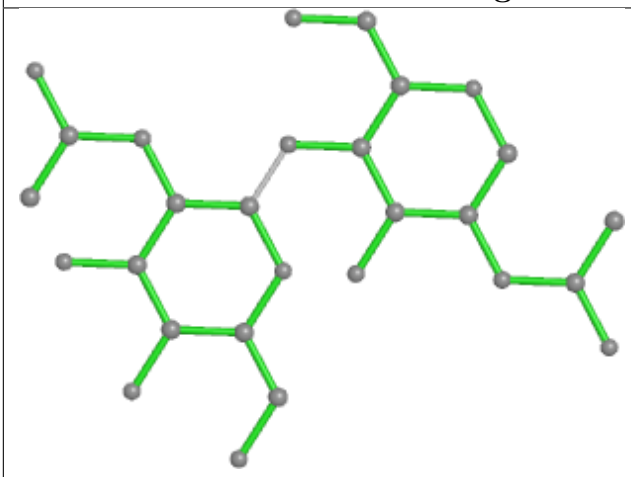
There are no ring outliers.

5 monomers are involved in 12 short contacts:

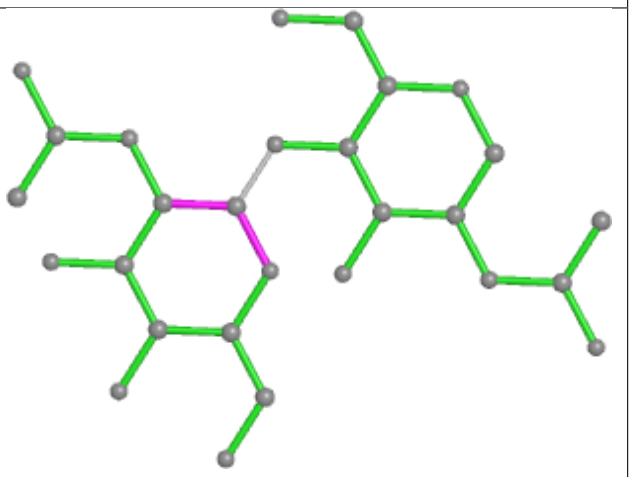
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	5	0
4	F	2	NAG	4	0
4	F	1	NAG	2	0
4	D	1	NAG	1	0
4	E	2	NAG	4	0

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

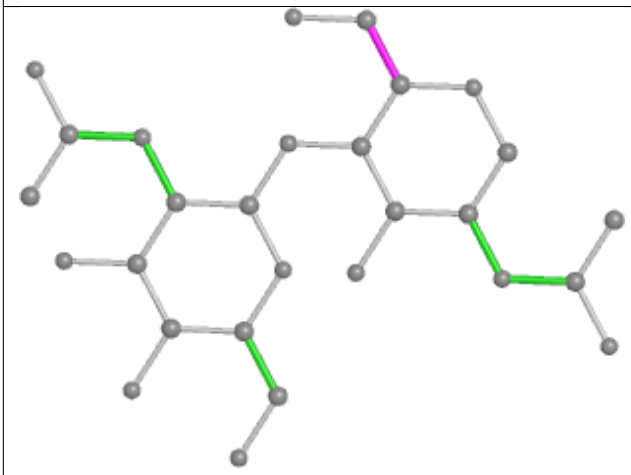
Oligosaccharide Chain D



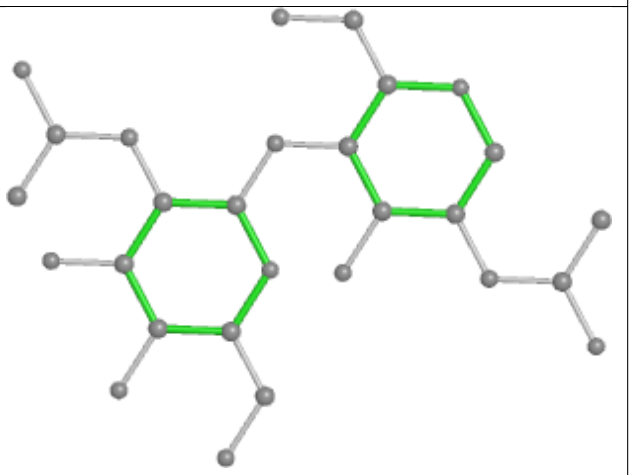
Bond lengths



Bond angles

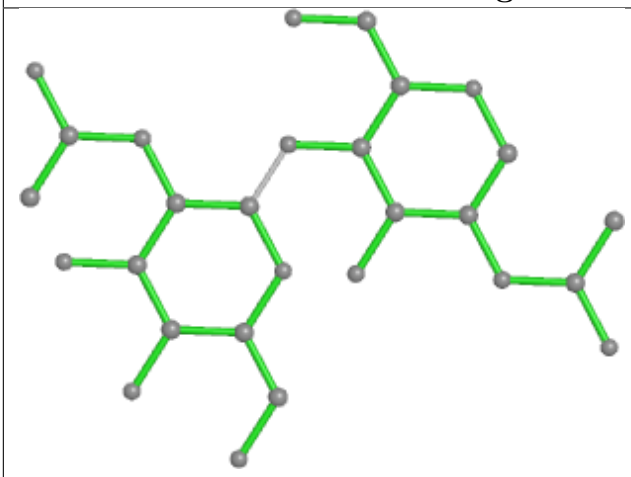


Torsions

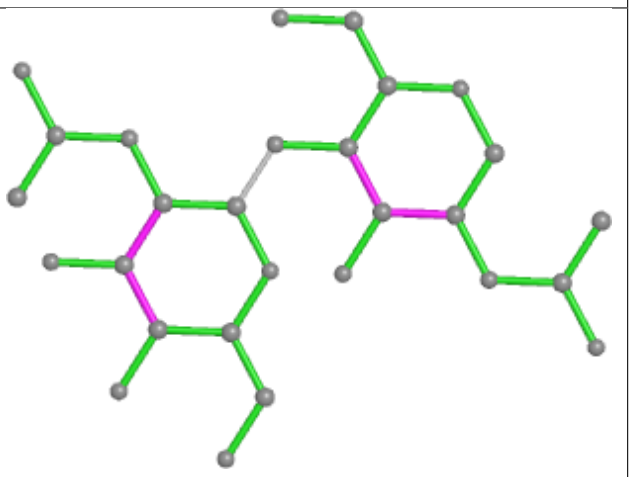


Rings

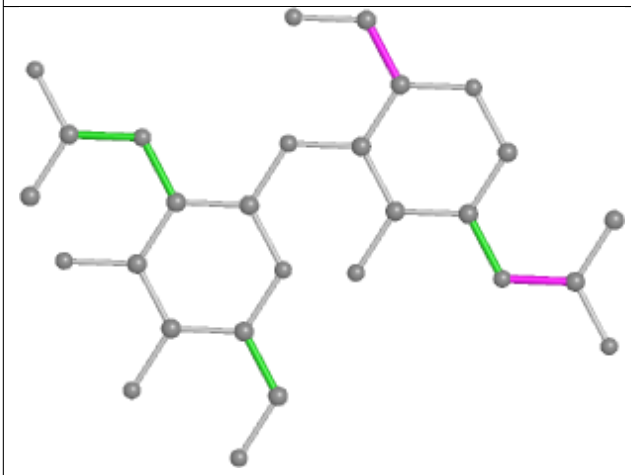
Oligosaccharide Chain E



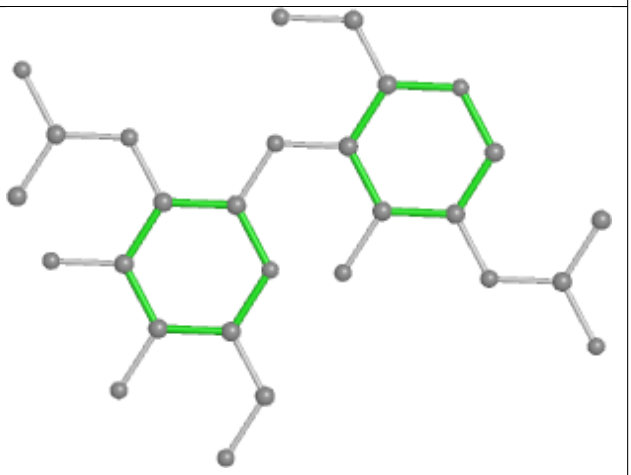
Bond lengths



Bond angles

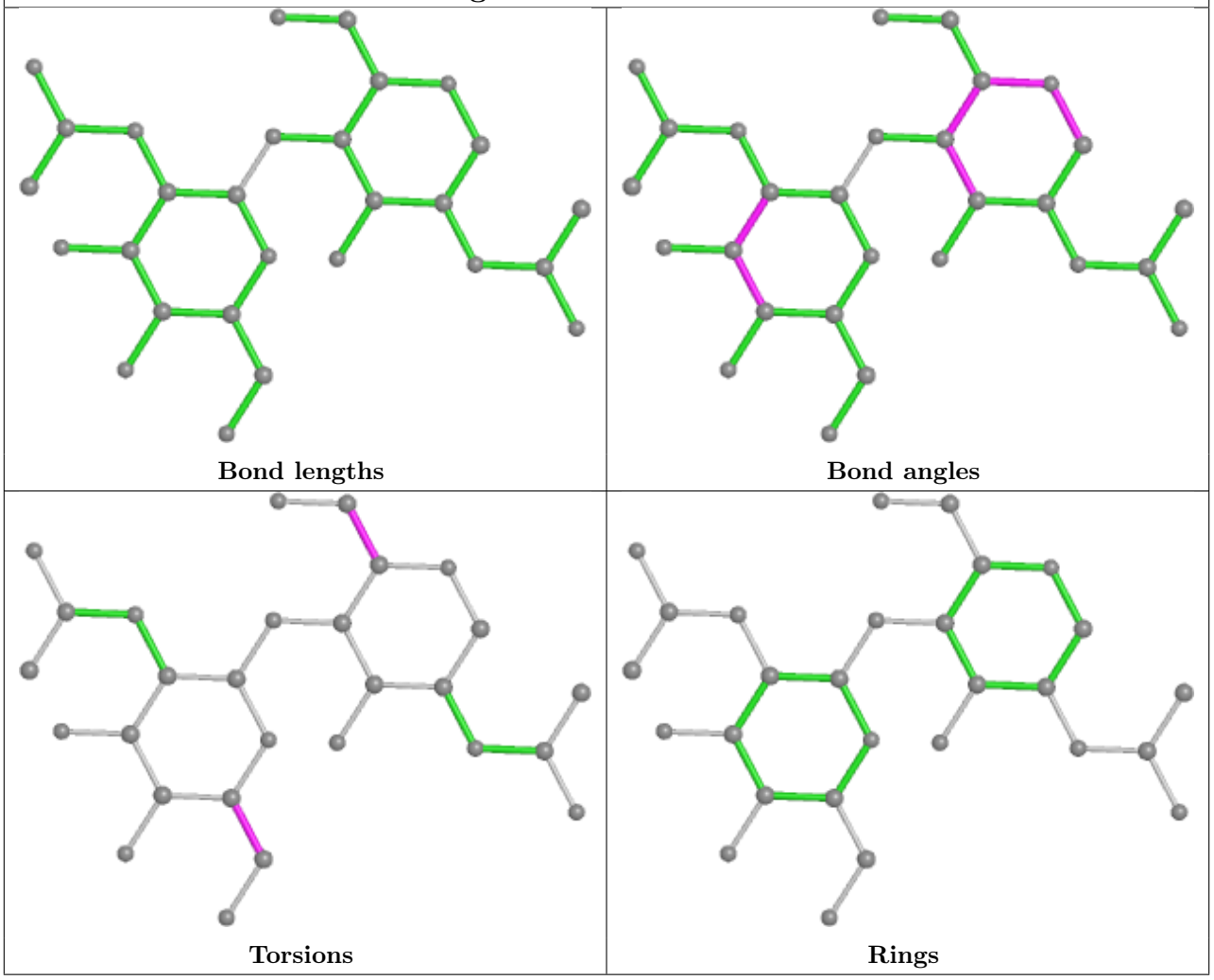


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

34 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	9Z9	A	2006	-	44,44,44	0.70	1 (2%)	66,68,68	1.45	12 (18%)
5	NAG	A	2008	1	14,14,15	0.29	0	17,19,21	1.04	1 (5%)
6	P5S	A	2017	-	40,40,53	1.13	3 (7%)	43,45,60	1.37	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	B	303	2	14,14,15	0.27	0	17,19,21	0.43	0
6	P5S	A	2029	-	32,33,53	1.16	4 (12%)	36,40,60	1.04	3 (8%)
7	Y01	A	2007	-	38,38,38	0.67	1 (2%)	57,57,57	1.79	11 (19%)
9	LPE	A	2026	-	16,16,33	0.69	0	20,22,39	0.67	0
10	PCW	A	2018	-	43,43,53	1.01	2 (4%)	49,51,61	1.12	5 (10%)
7	Y01	A	2003	-	38,38,38	0.66	1 (2%)	57,57,57	1.78	12 (21%)
9	LPE	A	2015	-	27,27,33	0.54	0	31,33,39	0.60	0
9	LPE	A	2019	-	24,24,33	0.57	0	28,30,39	0.67	0
10	PCW	A	2013	-	52,52,53	0.93	2 (3%)	58,60,61	1.03	3 (5%)
9	LPE	A	2021	-	24,24,33	0.60	0	28,30,39	0.87	0
9	LPE	A	2011	-	24,24,33	0.33	0	25,27,39	0.60	0
5	NAG	B	301	2	14,14,15	0.65	0	17,19,21	0.99	0
7	Y01	A	2004	-	38,38,38	0.65	1 (2%)	57,57,57	1.78	11 (19%)
9	LPE	A	2012	-	19,19,33	0.62	0	23,25,39	0.51	0
10	PCW	A	2016	-	46,46,53	0.99	3 (6%)	52,54,61	1.18	4 (7%)
10	PCW	A	2028	-	43,43,53	0.99	2 (4%)	49,51,61	2.91	7 (14%)
5	NAG	A	2001	1	14,14,15	0.35	0	17,19,21	0.44	0
9	LPE	A	2020	-	24,24,33	0.85	0	28,30,39	0.92	1 (3%)
9	LPE	A	2025	-	24,24,33	0.54	0	28,30,39	0.50	0
9	LPE	A	2023	-	24,24,33	0.53	0	28,30,39	0.54	0
7	Y01	A	2005	-	38,38,38	1.16	4 (10%)	57,57,57	1.74	11 (19%)
9	LPE	A	2024	-	24,24,33	0.51	0	28,30,39	0.62	0
9	LPE	A	2014	-	21,21,33	0.67	0	25,27,39	1.03	2 (8%)
7	Y01	A	2030	-	38,38,38	1.62	7 (18%)	57,57,57	1.63	10 (17%)
9	LPE	A	2022	-	24,24,33	0.53	0	28,30,39	0.64	0
6	P5S	A	2002	-	33,34,53	0.86	1 (3%)	36,40,60	1.66	5 (13%)
7	Y01	A	2009	-	38,38,38	1.15	4 (10%)	57,57,57	1.74	12 (21%)
5	NAG	B	302	2	14,14,15	0.37	0	17,19,21	0.96	1 (5%)
9	LPE	B	304	-	16,16,33	0.66	0	20,22,39	0.60	0
10	PCW	A	2027	-	43,43,53	1.03	2 (4%)	49,51,61	0.94	2 (4%)
9	LPE	A	2010	-	24,24,33	0.51	0	28,30,39	0.60	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
8	9Z9	A	2006	-	-	0/12/100/100	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	2008	1	-	2/6/23/26	0/1/1/1
6	P5S	A	2017	-	-	8/44/44/59	-
5	NAG	B	303	2	-	0/6/23/26	0/1/1/1
6	P5S	A	2029	-	-	16/39/39/59	-
7	Y01	A	2007	-	-	0/19/77/77	0/4/4/4
9	LPE	A	2026	-	-	7/17/17/34	-
10	PCW	A	2018	-	-	12/47/47/57	-
7	Y01	A	2003	-	-	0/19/77/77	0/4/4/4
9	LPE	A	2015	-	-	10/28/28/34	-
9	LPE	A	2019	-	-	5/25/25/34	-
10	PCW	A	2013	-	-	10/56/56/57	-
9	LPE	A	2021	-	-	3/25/25/34	-
9	LPE	A	2011	-	-	8/25/25/34	-
5	NAG	B	301	2	-	0/6/23/26	0/1/1/1
7	Y01	A	2004	-	-	0/19/77/77	0/4/4/4
9	LPE	A	2012	-	-	10/20/20/34	-
10	PCW	A	2016	-	-	13/50/50/57	-
10	PCW	A	2028	-	-	10/47/47/57	-
5	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
9	LPE	A	2020	-	-	12/25/25/34	-
9	LPE	A	2025	-	-	10/25/25/34	-
9	LPE	A	2023	-	-	8/25/25/34	-
7	Y01	A	2005	-	-	4/19/77/77	0/4/4/4
9	LPE	A	2024	-	-	6/25/25/34	-
9	LPE	A	2014	-	-	15/22/22/34	-
7	Y01	A	2030	-	-	7/19/77/77	0/4/4/4
9	LPE	A	2022	-	-	3/25/25/34	-
6	P5S	A	2002	-	-	7/39/39/59	-
7	Y01	A	2009	-	-	4/19/77/77	0/4/4/4
5	NAG	B	302	2	-	2/6/23/26	0/1/1/1
9	LPE	B	304	-	-	9/17/17/34	-
10	PCW	A	2027	-	-	16/47/47/57	-
9	LPE	A	2010	-	-	10/25/25/34	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2017	P5S	O37-C38	4.40	1.46	1.34
10	A	2027	PCW	O3-C11	4.39	1.46	1.33
7	A	2030	Y01	CBB-CBE	-4.36	1.46	1.54
6	A	2002	P5S	O37-C38	4.27	1.46	1.34
10	A	2028	PCW	O3-C11	4.25	1.45	1.33
10	A	2013	PCW	O3-C11	4.19	1.45	1.33
7	A	2030	Y01	CAR-CBC	-4.14	1.40	1.51
10	A	2028	PCW	O2-C31	4.09	1.45	1.34
10	A	2013	PCW	O2-C31	3.96	1.45	1.34
10	A	2018	PCW	O2-C31	3.93	1.45	1.34
6	A	2017	P5S	O19-C17	3.90	1.44	1.33
10	A	2018	PCW	O3-C11	3.88	1.44	1.33
10	A	2027	PCW	O2-C31	3.87	1.45	1.34
10	A	2016	PCW	O3-C11	3.87	1.44	1.33
7	A	2030	Y01	OAW-CAY	3.67	1.44	1.34
10	A	2016	PCW	O2-C31	3.64	1.44	1.34
7	A	2009	Y01	OAW-CAY	3.63	1.44	1.34
7	A	2005	Y01	OAW-CAY	3.61	1.44	1.34
6	A	2017	P5S	C28-C27	-3.34	1.32	1.51
7	A	2030	Y01	CAV-CBC	2.89	1.59	1.52
6	A	2029	P5S	O19-C17	2.71	1.41	1.33
6	A	2029	P5S	O37-C2	-2.48	1.40	1.46
7	A	2005	Y01	CAM-CAY	2.39	1.57	1.50
7	A	2030	Y01	CAM-CAY	2.38	1.57	1.50
7	A	2009	Y01	CAM-CAY	2.36	1.57	1.50
6	A	2029	P5S	O19-C1	-2.26	1.40	1.45
7	A	2005	Y01	CAL-CAX	2.26	1.55	1.50
6	A	2029	P5S	O37-C38	2.24	1.40	1.34
7	A	2009	Y01	CAL-CAX	2.24	1.55	1.50
7	A	2005	Y01	CBH-CBF	-2.20	1.52	1.56
7	A	2003	Y01	CBH-CBF	-2.20	1.52	1.56
8	A	2006	9Z9	C11-C08	-2.20	1.52	1.56
7	A	2030	Y01	CAL-CAX	2.18	1.55	1.50
7	A	2007	Y01	CBH-CBF	-2.17	1.52	1.56
7	A	2030	Y01	CBH-CBF	-2.17	1.52	1.56
7	A	2004	Y01	CBH-CBF	-2.13	1.52	1.56
7	A	2009	Y01	CBH-CBF	-2.11	1.52	1.56
10	A	2016	PCW	C6-N	-2.11	1.43	1.50

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	2028	PCW	C8-N-C6	-12.05	77.99	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	2028	PCW	C8-N-C7	-12.04	78.02	108.97
10	A	2028	PCW	C8-N-C5	-7.82	77.94	109.92
6	A	2002	P5S	O37-C38-C39	6.69	125.92	111.50
7	A	2009	Y01	CBI-CBE-CBB	-5.95	110.16	119.49
7	A	2005	Y01	CBI-CBE-CBB	-5.94	110.19	119.49
7	A	2007	Y01	CBI-CBE-CBB	-5.90	110.24	119.49
7	A	2004	Y01	CBI-CBE-CBB	-5.90	110.25	119.49
7	A	2003	Y01	CBI-CBE-CBB	-5.88	110.27	119.49
6	A	2017	P5S	O37-C38-C39	5.46	123.27	111.50
10	A	2016	PCW	O2-C31-C32	4.84	121.94	111.50
7	A	2004	Y01	CBI-CBG-CBD	-4.80	107.27	114.38
7	A	2007	Y01	CBI-CBG-CBD	-4.79	107.28	114.38
7	A	2003	Y01	CBI-CBG-CBD	-4.76	107.33	114.38
7	A	2005	Y01	CBI-CBG-CBD	-4.75	107.34	114.38
7	A	2030	Y01	CBI-CBG-CBD	-4.74	107.37	114.38
7	A	2009	Y01	CBI-CBG-CBD	-4.69	107.43	114.38
8	A	2006	9Z9	C02-C06-C07	-4.42	107.84	114.38
7	A	2030	Y01	CBI-CBE-CBB	-4.16	112.98	119.49
7	A	2004	Y01	OAW-CAY-CAM	3.97	120.06	111.50
7	A	2007	Y01	OAW-CAY-CAM	3.96	120.03	111.50
7	A	2003	Y01	OAW-CAY-CAM	3.96	120.03	111.50
9	A	2020	LPE	C3N-N-C2N	3.93	119.09	108.97
10	A	2028	PCW	O2-C31-C32	3.79	119.67	111.50
7	A	2009	Y01	OAW-CAY-CAM	3.76	119.60	111.50
7	A	2005	Y01	OAW-CAY-CAM	3.74	119.56	111.50
7	A	2030	Y01	OAW-CAY-CAM	3.59	119.23	111.50
8	A	2006	9Z9	C21-C22-C23	-3.47	109.48	113.88
6	A	2029	P5S	O37-C38-C39	3.44	118.91	111.50
7	A	2030	Y01	CAS-CAU-CBI	-3.33	107.07	112.78
7	A	2009	Y01	CAS-CAU-CBI	-3.33	107.07	112.78
7	A	2005	Y01	CAS-CAU-CBI	-3.31	107.11	112.78
7	A	2003	Y01	CAS-CAU-CBI	-3.30	107.12	112.78
8	A	2006	9Z9	C09-C10-C02	-3.30	107.12	112.78
7	A	2004	Y01	CAS-CAU-CBI	-3.29	107.14	112.78
7	A	2007	Y01	CAS-CAU-CBI	-3.29	107.14	112.78
8	A	2006	9Z9	C02-C03-C74	-3.24	109.53	120.56
10	A	2027	PCW	O2-C31-C32	3.24	118.48	111.50
6	A	2002	P5S	O37-C38-O47	-3.23	115.91	123.70
10	A	2013	PCW	C2-O2-C31	-3.13	110.09	117.79
10	A	2016	PCW	O3-C11-C12	3.07	121.53	111.91
10	A	2013	PCW	O2-C31-C32	3.02	118.00	111.50
7	A	2009	Y01	CAD-CBH-CBF	-2.95	108.17	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	2003	Y01	CAD-CBH-CBF	-2.95	108.17	111.68
7	A	2004	Y01	CAD-CBH-CBF	-2.92	108.20	111.68
5	A	2008	NAG	C4-C3-C2	-2.89	106.78	111.02
7	A	2007	Y01	CAD-CBH-CBF	-2.88	108.25	111.68
10	A	2018	PCW	C3-C2-C1	-2.88	104.98	111.79
8	A	2006	9Z9	C12-C11-C08	-2.87	108.26	111.68
7	A	2005	Y01	CAD-CBH-CBF	-2.87	108.26	111.68
7	A	2030	Y01	CAD-CBH-CBF	-2.86	108.27	111.68
9	A	2014	LPE	C3-C2-C1	-2.86	104.38	112.79
10	A	2018	PCW	O2-C31-C32	2.81	117.55	111.50
8	A	2006	9Z9	C76-C73-C74	-2.78	109.98	115.69
10	A	2028	PCW	O3-C11-C12	2.75	120.53	111.91
7	A	2007	Y01	CBG-CBI-CBE	2.74	103.32	100.07
7	A	2003	Y01	CBG-CBI-CBE	2.73	103.31	100.07
7	A	2009	Y01	CBG-CBI-CBE	2.73	103.31	100.07
7	A	2004	Y01	CBG-CBI-CBE	2.71	103.29	100.07
7	A	2030	Y01	CBG-CBI-CBE	2.70	103.28	100.07
7	A	2005	Y01	CBG-CBI-CBE	2.69	103.26	100.07
10	A	2028	PCW	C7-N-C6	2.62	115.71	108.97
7	A	2007	Y01	CAS-CBF-CBH	-2.58	109.68	113.08
9	A	2014	LPE	C31-C32-N	-2.55	107.27	115.78
7	A	2030	Y01	CAS-CBF-CBH	-2.55	109.73	113.08
8	A	2006	9Z9	C75-C74-C73	-2.53	110.30	114.92
7	A	2004	Y01	CAS-CBF-CBH	-2.52	109.76	113.08
7	A	2003	Y01	CAS-CBF-CBH	-2.52	109.77	113.08
7	A	2005	Y01	CAS-CBF-CBH	-2.51	109.78	113.08
6	A	2002	P5S	OXT-C-O	-2.51	118.40	124.09
7	A	2009	Y01	CAS-CBF-CBH	-2.51	109.78	113.08
10	A	2018	PCW	O3-C11-C12	2.50	119.75	111.91
7	A	2003	Y01	CBD-CAK-CAI	-2.47	109.19	112.73
7	A	2030	Y01	CBD-CAK-CAI	-2.47	109.19	112.73
7	A	2009	Y01	CBD-CAK-CAI	-2.46	109.19	112.73
7	A	2007	Y01	CBD-CAK-CAI	-2.44	109.22	112.73
8	A	2006	9Z9	C09-C08-C11	-2.44	109.86	113.08
6	A	2029	P5S	O19-C17-C20	2.43	119.54	111.91
7	A	2004	Y01	CBD-CAK-CAI	-2.42	109.25	112.73
7	A	2005	Y01	CBD-CAK-CAI	-2.42	109.26	112.73
8	A	2006	9Z9	C07-C15-C14	-2.40	109.28	112.73
6	A	2017	P5S	C41-C40-C39	-2.38	104.64	113.19
7	A	2003	Y01	CBF-CBH-CAZ	2.33	113.31	109.65
10	A	2027	PCW	O3-C11-C12	2.32	119.20	111.91
7	A	2005	Y01	CBF-CBH-CAZ	2.32	113.29	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	2009	Y01	CBF-CBH-CAZ	2.32	113.29	109.65
7	A	2007	Y01	CBF-CBH-CAZ	2.31	113.27	109.65
7	A	2030	Y01	CBF-CBH-CAZ	2.30	113.26	109.65
8	A	2006	9Z9	C08-C11-C13	2.28	113.23	109.65
7	A	2004	Y01	CBF-CBH-CAZ	2.28	113.22	109.65
7	A	2007	Y01	CAC-CBB-CBE	-2.27	109.44	112.92
6	A	2002	P5S	O37-C2-C1	2.26	116.48	108.36
7	A	2004	Y01	CAC-CBB-CBE	-2.24	109.48	112.92
10	A	2028	PCW	C2-O2-C31	-2.23	112.30	117.79
10	A	2013	PCW	O3-C11-C12	2.21	118.85	111.91
7	A	2003	Y01	CAC-CBB-CBE	-2.21	109.54	112.92
7	A	2009	Y01	CAC-CBB-CBE	-2.20	109.55	112.92
7	A	2005	Y01	CAC-CBB-CBE	-2.20	109.55	112.92
10	A	2018	PCW	C34-C33-C32	-2.17	105.40	113.19
6	A	2029	P5S	OXT-C-CA	2.12	120.61	113.38
6	A	2017	P5S	O15-P12-O13	2.11	122.65	112.24
10	A	2016	PCW	O2-C31-O31	-2.10	118.62	123.70
6	A	2002	P5S	C3-C2-C1	-2.08	106.93	111.80
5	B	302	NAG	C2-N2-C7	-2.08	119.94	122.90
10	A	2018	PCW	O3-C3-C2	2.08	114.49	108.43
10	A	2016	PCW	O3-C11-O11	-2.05	118.43	123.59
8	A	2006	9Z9	O80-C79-C78	-2.04	109.24	112.18
7	A	2004	Y01	CAQ-CBG-CBD	-2.04	115.71	119.08
7	A	2003	Y01	CAQ-CBG-CBD	-2.04	115.72	119.08
7	A	2005	Y01	CAQ-CBG-CBD	-2.04	115.73	119.08
8	A	2006	9Z9	C17-C16-C13	-2.03	108.36	111.52
7	A	2009	Y01	CAQ-CBG-CBD	-2.02	115.75	119.08
7	A	2030	Y01	CAQ-CBG-CBD	-2.02	115.76	119.08
7	A	2009	Y01	CBC-CAV-CAZ	-2.01	108.39	111.52
7	A	2007	Y01	CAQ-CBG-CBD	-2.00	115.78	119.08
7	A	2003	Y01	CBC-CAV-CAZ	-2.00	108.41	111.52

There are no chirality outliers.

All (229) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	302	NAG	C8-C7-N2-C2
5	B	302	NAG	O7-C7-N2-C2
6	A	2002	P5S	N-CA-CB-OG
6	A	2002	P5S	C39-C38-O37-C2
6	A	2002	P5S	O47-C38-O37-C2
6	A	2017	P5S	CB-OG-P12-O15

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Mol	Chain	Res	Type	Atoms
6	A	2017	P5S	C3-O16-P12-OG
6	A	2017	P5S	C3-O16-P12-O13
6	A	2017	P5S	C3-O16-P12-O15
6	A	2029	P5S	C3-O16-P12-O13
9	A	2010	LPE	C3-O3-P-O31
9	A	2011	LPE	C3-O3-P-O31
9	A	2012	LPE	C3-O3-P-O32
9	A	2012	LPE	C31-O33-P-O31
9	A	2014	LPE	O1-C1-C2-C3
9	A	2014	LPE	C3-O3-P-O32
9	A	2014	LPE	C31-O33-P-O3
9	A	2014	LPE	C31-O33-P-O31
9	A	2014	LPE	C32-C31-O33-P
9	A	2014	LPE	O33-C31-C32-N
9	A	2015	LPE	C3-O3-P-O32
9	A	2019	LPE	C31-O33-P-O31
9	A	2019	LPE	C31-O33-P-O32
9	A	2020	LPE	C31-O33-P-O31
9	A	2023	LPE	C31-O33-P-O32
9	A	2024	LPE	C31-O33-P-O31
9	A	2025	LPE	O1-C1-C2-C3
9	A	2025	LPE	C3-O3-P-O32
9	A	2025	LPE	C31-O33-P-O3
9	A	2025	LPE	C31-O33-P-O31
9	A	2025	LPE	C31-O33-P-O32
9	B	304	LPE	C3-O3-P-O31
9	B	304	LPE	C3-O3-P-O32
9	B	304	LPE	C3-O3-P-O33
10	A	2013	PCW	C1-O3P-P-O1P
10	A	2013	PCW	C1-O3P-P-O2P
10	A	2013	PCW	C1-O3P-P-O4P
10	A	2016	PCW	O4P-C4-C5-N
10	A	2018	PCW	C32-C31-O2-C2
10	A	2027	PCW	O4P-C4-C5-N
10	A	2027	PCW	C1-O3P-P-O2P
10	A	2028	PCW	C4-O4P-P-O2P
10	A	2028	PCW	C4-O4P-P-O3P
6	A	2029	P5S	O18-C17-O19-C1
6	A	2029	P5S	C20-C17-O19-C1
7	A	2030	Y01	CAC-CBB-CBE-CAP
7	A	2030	Y01	CAC-CBB-CBE-CBI
10	A	2018	PCW	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
7	A	2030	Y01	CAJ-CAO-CBB-CAC
7	A	2030	Y01	CAO-CBB-CBE-CBI
10	A	2027	PCW	O11-C11-O3-C3
10	A	2027	PCW	C12-C11-O3-C3
5	A	2001	NAG	O5-C5-C6-O6
7	A	2030	Y01	CAO-CBB-CBE-CAP
9	A	2025	LPE	O1-C1-C2-O2H
5	A	2001	NAG	C4-C5-C6-O6
10	A	2028	PCW	C12-C11-O3-C3
7	A	2005	Y01	CAR-CBC-OAW-CAY
9	A	2023	LPE	C31-C32-N-C2N
9	A	2023	LPE	C31-C32-N-C3N
10	A	2016	PCW	C4-C5-N-C8
10	A	2018	PCW	C4-C5-N-C7
7	A	2009	Y01	CAR-CBC-OAW-CAY
7	A	2030	Y01	CAJ-CAO-CBB-CBE
9	A	2014	LPE	O1-C1-C2-O2H
10	A	2013	PCW	C32-C31-O2-C2
9	A	2026	LPE	C31-C32-N-C3N
10	A	2016	PCW	C4-C5-N-C7
9	A	2014	LPE	O1-C11-C12-C13
10	A	2028	PCW	O11-C11-O3-C3
9	A	2020	LPE	O1-C1-C2-O2H
9	A	2011	LPE	C31-O33-P-O3
9	A	2014	LPE	C3-O3-P-O33
9	A	2015	LPE	C3-O3-P-O33
9	A	2019	LPE	C31-O33-P-O3
9	A	2022	LPE	C3-O3-P-O33
9	A	2023	LPE	C31-O33-P-O3
9	A	2025	LPE	C3-O3-P-O33
9	A	2026	LPE	C31-O33-P-O3
9	B	304	LPE	C31-O33-P-O3
10	A	2013	PCW	C4-O4P-P-O3P
10	A	2016	PCW	C4-O4P-P-O3P
10	A	2018	PCW	C4-O4P-P-O3P
10	A	2028	PCW	C1-O3P-P-O4P
10	A	2013	PCW	O31-C31-O2-C2
7	A	2005	Y01	CAV-CBC-OAW-CAY
7	A	2009	Y01	CAV-CBC-OAW-CAY
9	A	2010	LPE	O1-C11-C12-C13
9	A	2014	LPE	C31-C32-N-C1N
9	A	2014	LPE	C31-C32-N-C2N

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Mol	Chain	Res	Type	Atoms
9	A	2014	LPE	C31-C32-N-C3N
10	A	2018	PCW	C4-C5-N-C6
10	A	2028	PCW	C32-C31-O2-C2
9	A	2020	LPE	O1-C1-C2-C3
10	A	2028	PCW	O31-C31-O2-C2
6	A	2017	P5S	C25-C26-C27-C28
6	A	2029	P5S	C17-C20-C21-C22
6	A	2029	P5S	C42-C43-C44-C45
9	A	2011	LPE	O1-C11-C12-C13
9	A	2023	LPE	C31-C32-N-C1N
10	A	2028	PCW	C4-C5-N-C8
9	A	2020	LPE	C12-C13-C14-C15
6	A	2017	P5S	C27-C28-C29-C30
10	A	2027	PCW	C33-C34-C35-C36
9	A	2020	LPE	C14-C15-C16-C17
10	A	2016	PCW	C4-C5-N-C6
10	A	2018	PCW	C4-C5-N-C8
6	A	2029	P5S	C21-C22-C23-C24
10	A	2027	PCW	C31-C32-C33-C34
9	A	2024	LPE	C13-C14-C15-C16
9	A	2011	LPE	C13-C14-C15-C16
9	A	2026	LPE	C31-C32-N-C1N
9	A	2026	LPE	C31-C32-N-C2N
6	A	2029	P5S	C38-C39-C40-C41
6	A	2029	P5S	C3-O16-P12-OG
9	A	2011	LPE	C3-O3-P-O33
10	A	2016	PCW	C35-C36-C37-C38
6	A	2029	P5S	C40-C41-C42-C43
6	A	2029	P5S	C43-C44-C45-C46
9	A	2010	LPE	C2-C1-O1-C11
7	A	2030	Y01	CAN-CAJ-CAO-CBB
10	A	2016	PCW	C34-C35-C36-C37
9	B	304	LPE	C2-C3-O3-P
10	A	2013	PCW	C12-C11-O3-C3
9	A	2026	LPE	C2-C1-O1-C11
9	A	2015	LPE	O1-C1-C2-C3
9	A	2015	LPE	O1-C1-C2-O2H
9	A	2019	LPE	C2-C1-O1-C11
9	A	2012	LPE	C3-O3-P-O33
9	A	2020	LPE	C16-C17-C18-C19
9	A	2020	LPE	C11-C12-C13-C14
6	A	2029	P5S	C2-C3-O16-P12

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Mol	Chain	Res	Type	Atoms
10	A	2018	PCW	C2-C1-O3P-P
7	A	2009	Y01	CAO-CAJ-CAN-CBA
7	A	2005	Y01	CAO-CAJ-CAN-CBA
6	A	2002	P5S	C1-C2-O37-C38
10	A	2013	PCW	O11-C11-O3-C3
6	A	2029	P5S	C39-C38-O37-C2
9	A	2020	LPE	C12-C11-O1-C1
6	A	2029	P5S	CA-CB-OG-P12
6	A	2029	P5S	O47-C38-O37-C2
10	A	2027	PCW	O31-C31-O2-C2
9	B	304	LPE	C2-C1-O1-C11
9	A	2012	LPE	C12-C11-O1-C1
5	A	2008	NAG	C8-C7-N2-C2
9	A	2012	LPE	C31-O33-P-O3
9	A	2020	LPE	C31-O33-P-O3
9	A	2024	LPE	C31-O33-P-O3
10	A	2027	PCW	C1-O3P-P-O4P
9	A	2010	LPE	C2-C3-O3-P
9	A	2012	LPE	C2-C3-O3-P
6	A	2029	P5S	C3-O16-P12-O15
9	A	2011	LPE	C3-O3-P-O32
9	A	2011	LPE	C31-O33-P-O31
9	A	2012	LPE	C3-O3-P-O31
9	A	2020	LPE	C3-O3-P-O32
9	A	2022	LPE	C3-O3-P-O31
9	A	2023	LPE	C31-O33-P-O31
9	A	2025	LPE	C3-O3-P-O31
9	A	2026	LPE	C31-O33-P-O31
9	B	304	LPE	C31-O33-P-O31
10	A	2013	PCW	C4-O4P-P-O2P
10	A	2016	PCW	C4-O4P-P-O2P
10	A	2018	PCW	C4-O4P-P-O2P
10	A	2027	PCW	C4-O4P-P-O2P
10	A	2028	PCW	C1-O3P-P-O2P
9	A	2011	LPE	C32-C31-O33-P
9	B	304	LPE	C32-C31-O33-P
9	A	2014	LPE	C12-C11-O1-C1
9	A	2010	LPE	C11-C12-C13-C14
9	A	2024	LPE	C2-C1-O1-C11
9	A	2014	LPE	C13-C14-C15-C16
10	A	2027	PCW	C34-C35-C36-C37
9	A	2010	LPE	O33-C31-C32-N

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Mol	Chain	Res	Type	Atoms
9	A	2012	LPE	O33-C31-C32-N
9	A	2015	LPE	O33-C31-C32-N
9	A	2019	LPE	O33-C31-C32-N
9	A	2020	LPE	O33-C31-C32-N
9	A	2021	LPE	O33-C31-C32-N
9	A	2022	LPE	O33-C31-C32-N
9	A	2023	LPE	O33-C31-C32-N
9	A	2024	LPE	O33-C31-C32-N
9	A	2025	LPE	O33-C31-C32-N
9	B	304	LPE	O33-C31-C32-N
10	A	2028	PCW	O4P-C4-C5-N
9	A	2015	LPE	C12-C11-O1-C1
10	A	2027	PCW	C32-C31-O2-C2
6	A	2002	P5S	CB-OG-P12-O16
6	A	2017	P5S	CB-OG-P12-O16
9	A	2010	LPE	C3-O3-P-O33
9	A	2015	LPE	C31-O33-P-O3
9	A	2021	LPE	C31-O33-P-O3
9	A	2024	LPE	C3-O3-P-O33
9	A	2026	LPE	C3-O3-P-O33
10	A	2016	PCW	C1-O3P-P-O4P
10	A	2018	PCW	C1-O3P-P-O4P
10	A	2027	PCW	C4-O4P-P-O3P
10	A	2016	PCW	C17-C18-C19-C20
10	A	2016	PCW	C37-C38-C39-C40
10	A	2027	PCW	C11-C12-C13-C14
9	A	2025	LPE	C2-C1-O1-C11
9	A	2014	LPE	C11-C12-C13-C14
5	A	2008	NAG	O7-C7-N2-C2
6	A	2002	P5S	O-C-CA-N
10	A	2027	PCW	C21-C22-C23-C24
6	A	2029	P5S	C41-C42-C43-C44
9	A	2015	LPE	C2-C3-O3-P
10	A	2013	PCW	C19-C20-C21-C22
9	A	2010	LPE	C31-C32-N-C2N
6	A	2002	P5S	OXT-C-CA-CB
10	A	2016	PCW	C39-C40-C41-C42
10	A	2018	PCW	O3-C11-C12-C13
9	A	2020	LPE	C13-C14-C15-C16
9	A	2012	LPE	C1-C2-C3-O3
9	A	2010	LPE	C16-C17-C18-C19
6	A	2017	P5S	CB-OG-P12-O13

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Mol	Chain	Res	Type	Atoms
9	A	2015	LPE	C31-O33-P-O31
9	A	2021	LPE	C31-O33-P-O31
10	A	2016	PCW	C1-O3P-P-O2P
10	A	2018	PCW	C1-O3P-P-O2P
10	A	2027	PCW	C4-C5-N-C6
9	A	2010	LPE	C32-C31-O33-P
9	A	2015	LPE	C32-C31-O33-P
9	A	2023	LPE	C32-C31-O33-P
10	A	2018	PCW	C5-C4-O4P-P
9	A	2012	LPE	C31-C32-N-C2N
10	A	2027	PCW	O3-C11-C12-C13
7	A	2005	Y01	CAN-CAJ-CAO-CBB
7	A	2009	Y01	CAN-CAJ-CAO-CBB

There are no ring outliers.

29 monomers are involved in 247 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2006	9Z9	33	0
6	A	2017	P5S	17	0
6	A	2029	P5S	2	0
7	A	2007	Y01	19	0
9	A	2026	LPE	2	0
10	A	2018	PCW	22	0
7	A	2003	Y01	5	0
9	A	2015	LPE	5	0
9	A	2019	LPE	1	0
10	A	2013	PCW	7	0
9	A	2021	LPE	4	0
9	A	2011	LPE	1	0
7	A	2004	Y01	8	0
9	A	2012	LPE	4	0
10	A	2016	PCW	16	0
10	A	2028	PCW	1	0
9	A	2020	LPE	2	0
9	A	2025	LPE	1	0
9	A	2023	LPE	14	0
7	A	2005	Y01	27	0
9	A	2014	LPE	18	0
7	A	2030	Y01	9	0
9	A	2022	LPE	8	0
6	A	2002	P5S	5	0

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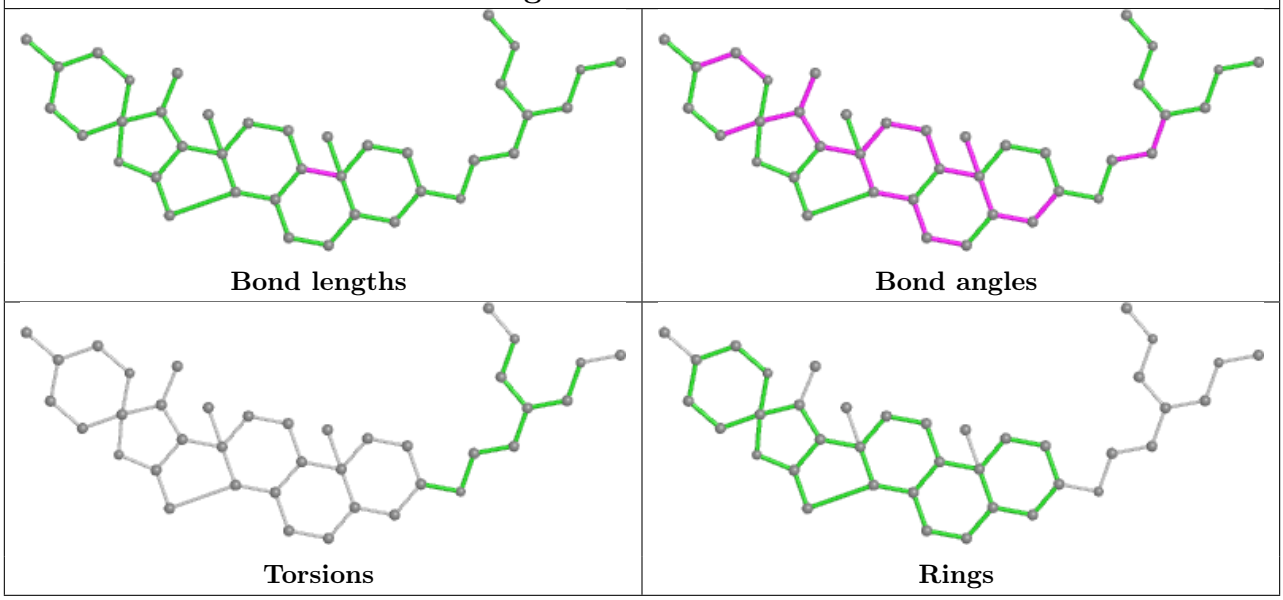
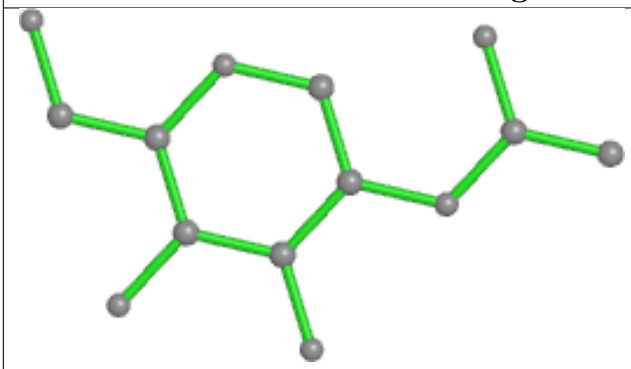
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2009	Y01	6	0
5	B	302	NAG	6	0
9	B	304	LPE	9	0
10	A	2027	PCW	5	0
9	A	2010	LPE	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

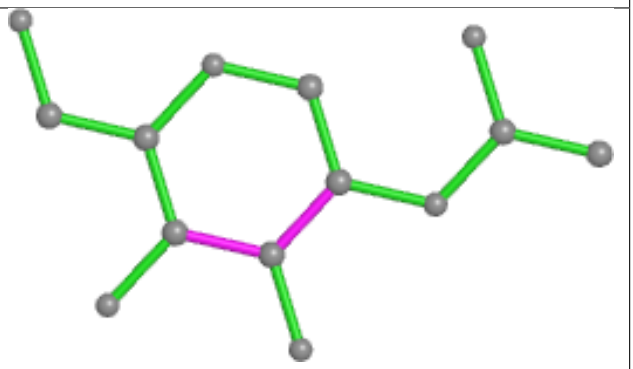
Ligand 9Z9 A 2006



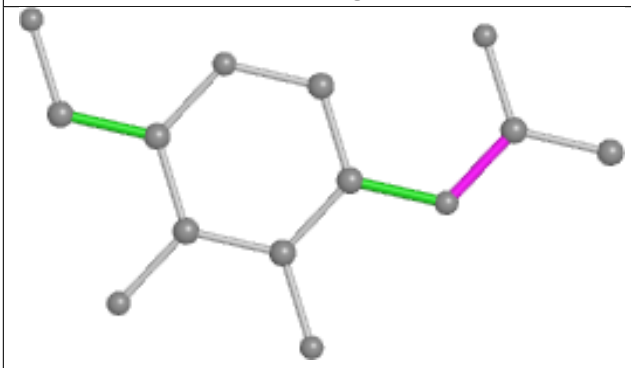
Ligand NAG A 2008



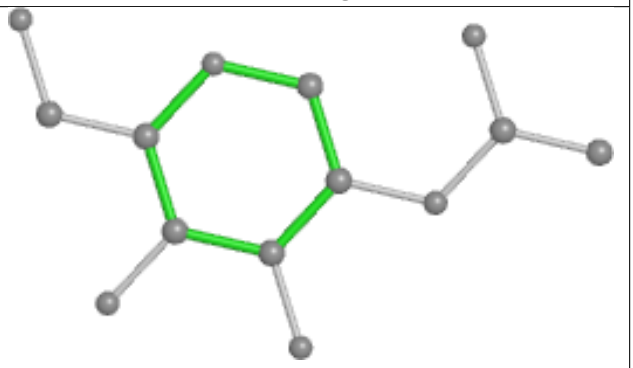
Bond lengths



Bond angles

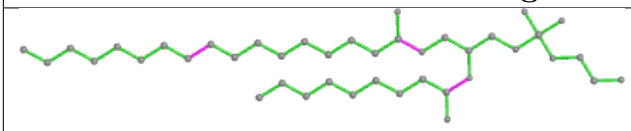


Torsions

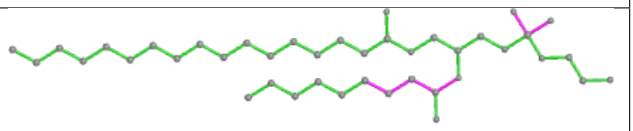


Rings

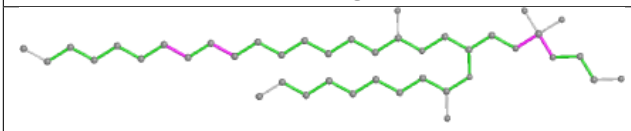
Ligand P5S A 2017



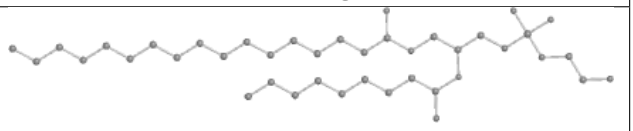
Bond lengths



Bond angles

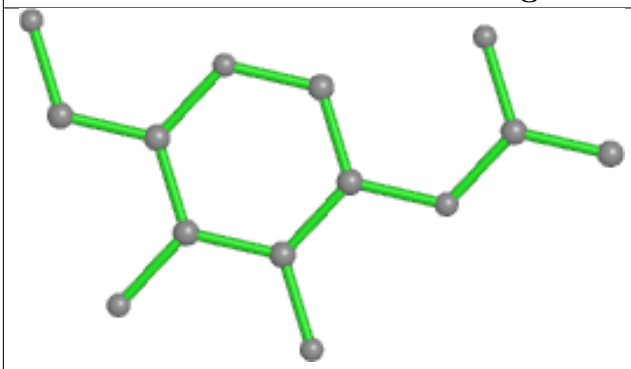


Torsions



Rings

Ligand NAG B 303



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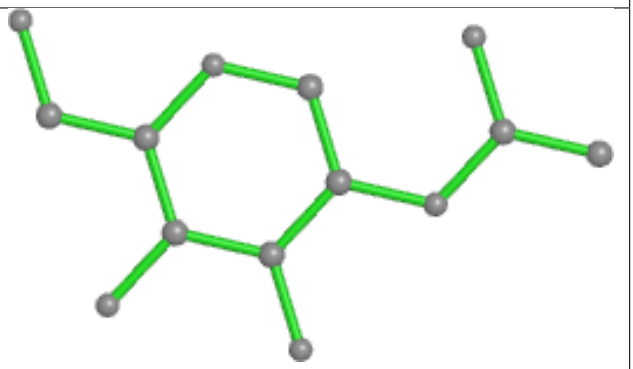
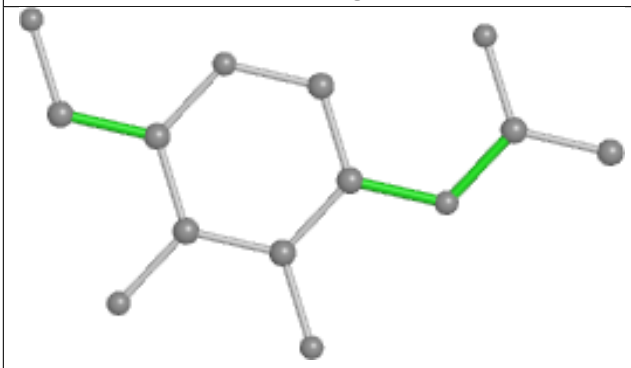
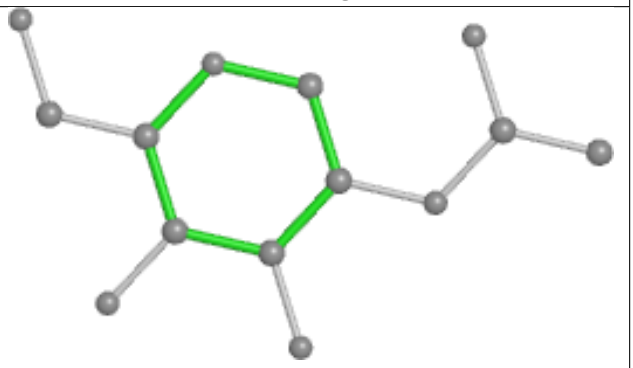


Bond angles

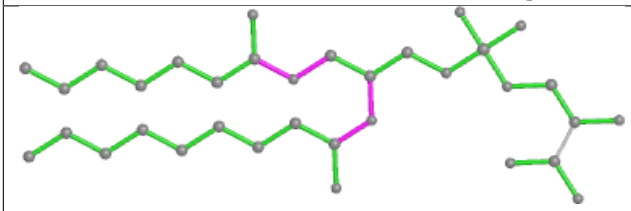


Torsions



Rings

Ligand P5S A 2029



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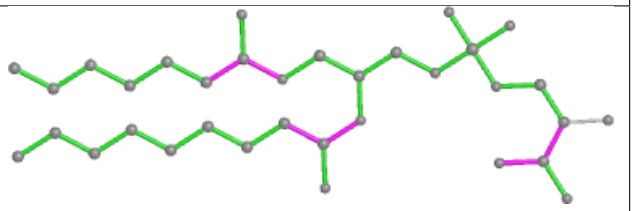
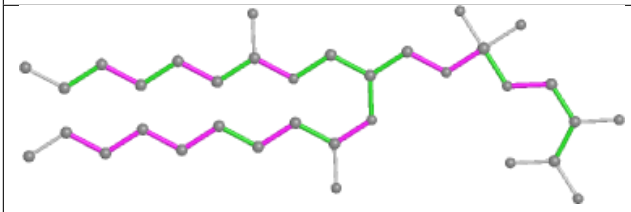


Bond angles



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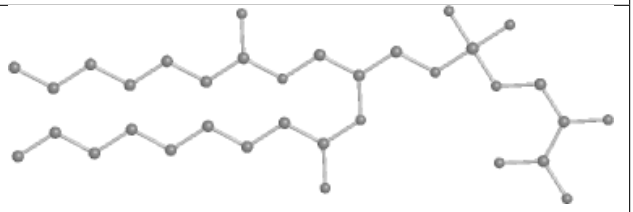
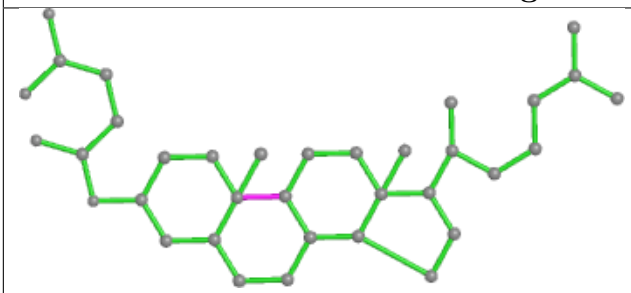


Rings

Ligand Y01 A 2007



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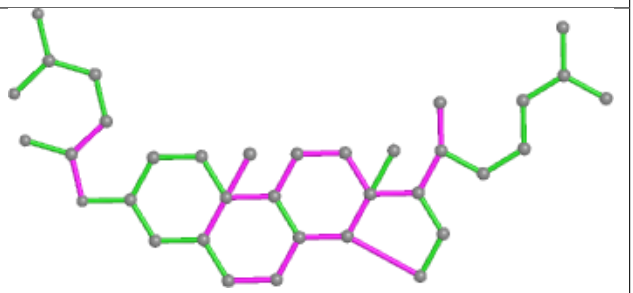

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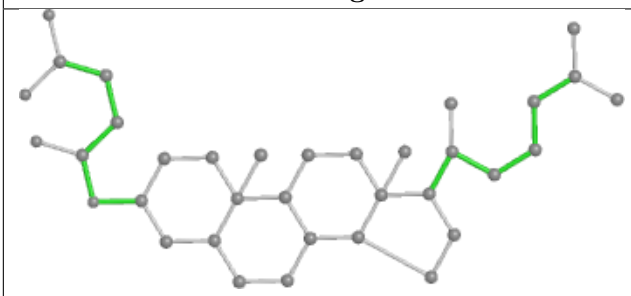

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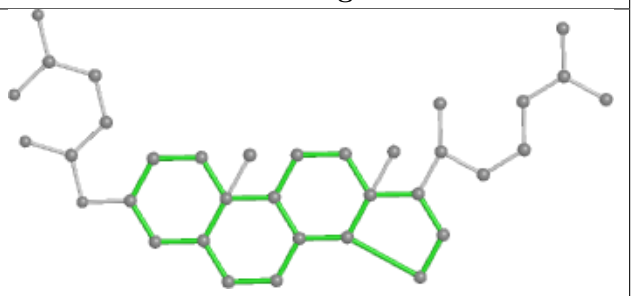
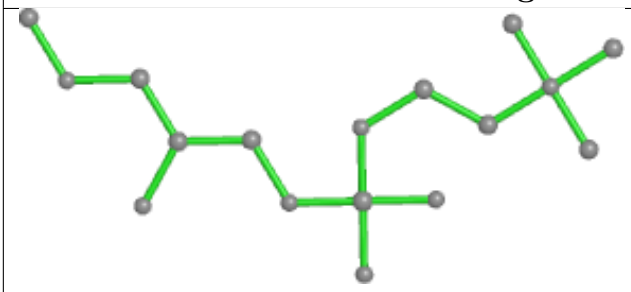


Rings

Ligand LPE A 2026



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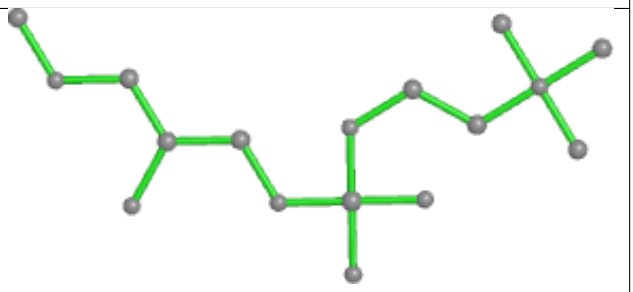
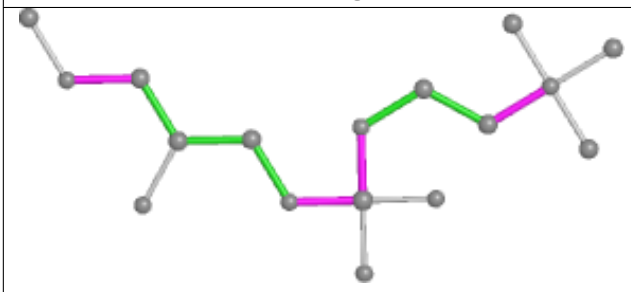


Bond angles



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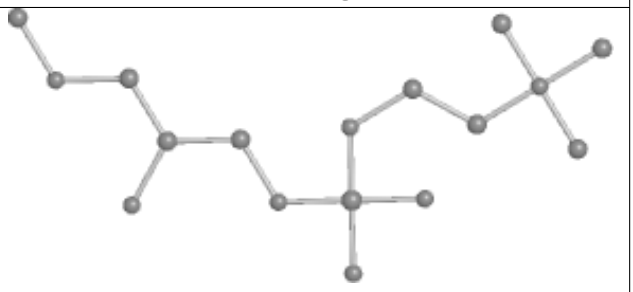
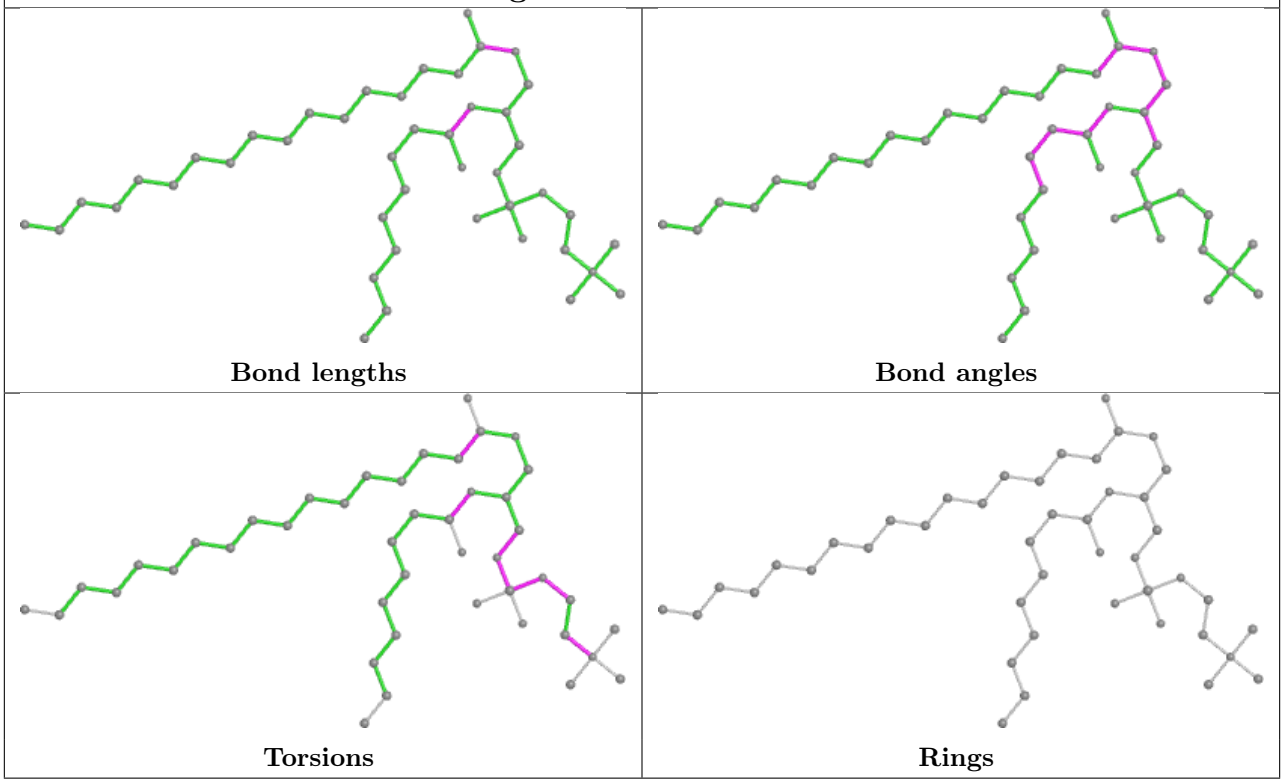
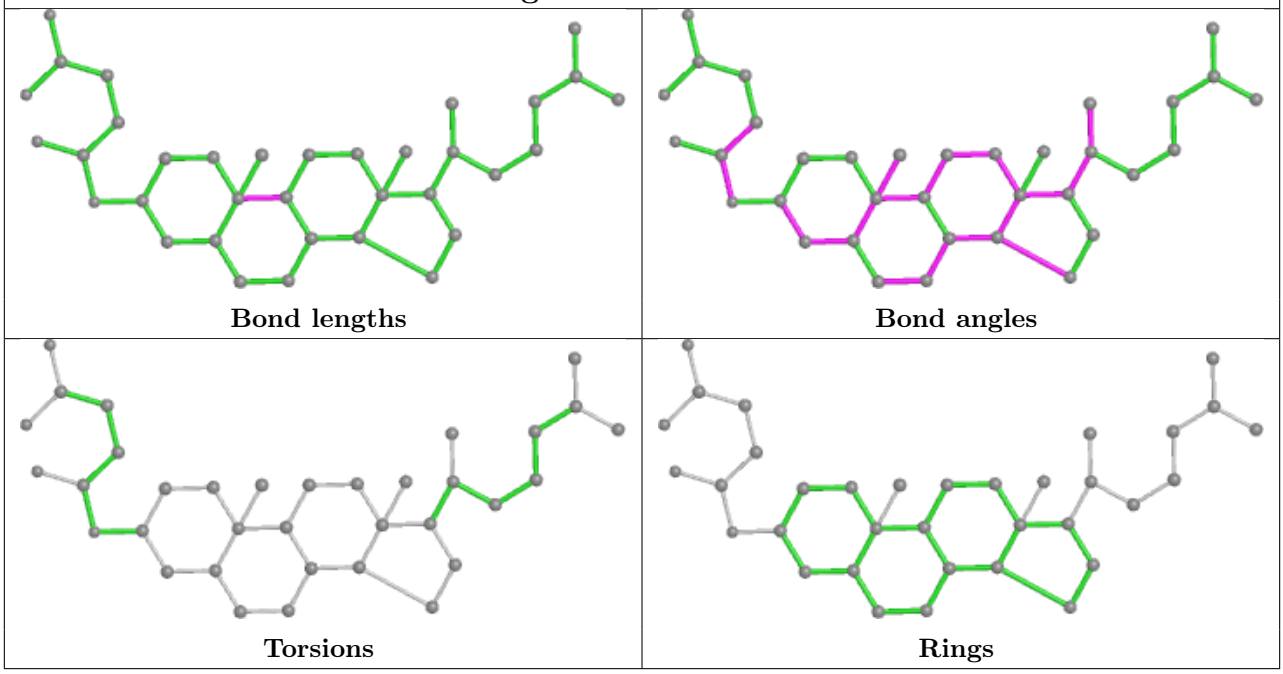


Rings

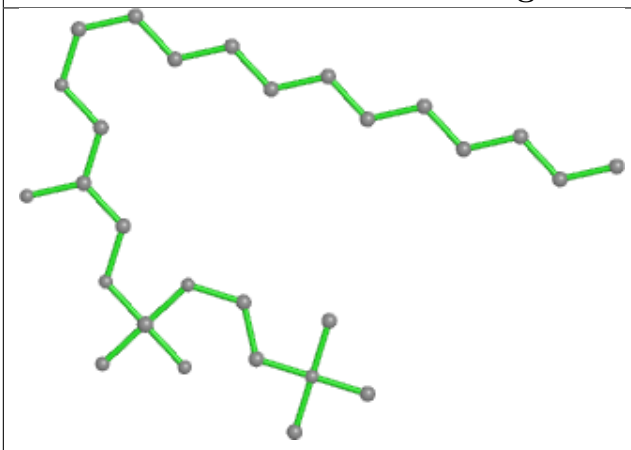
Ligand PCW A 2018



Ligand Y01 A 2003



Ligand LPE A 2015



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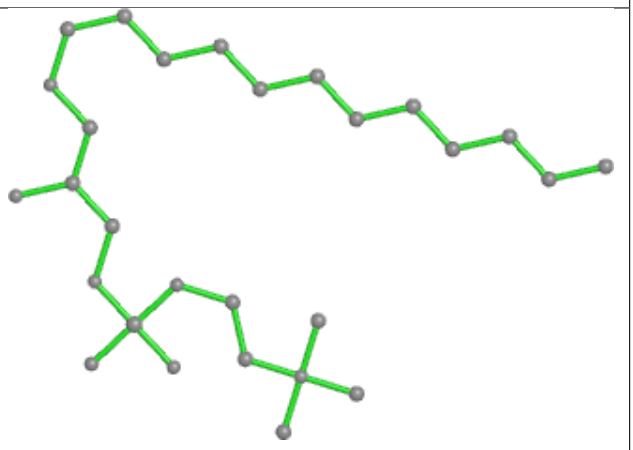
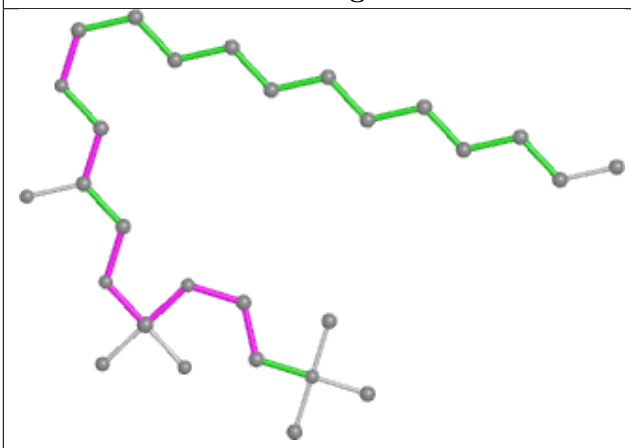
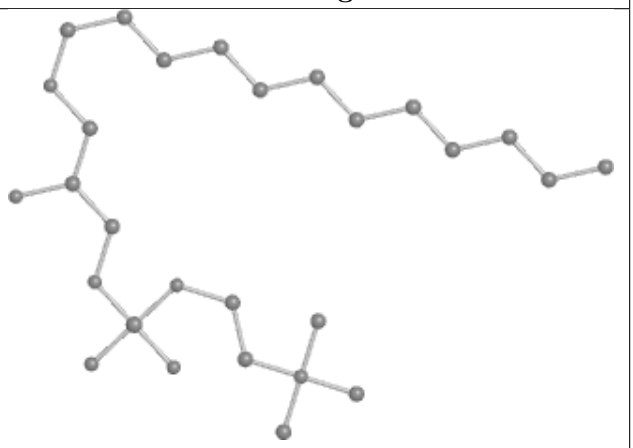


Bond angles

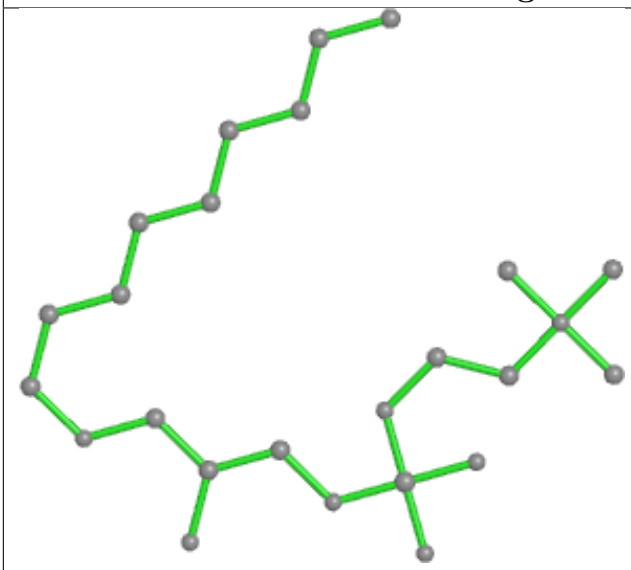


Torsions

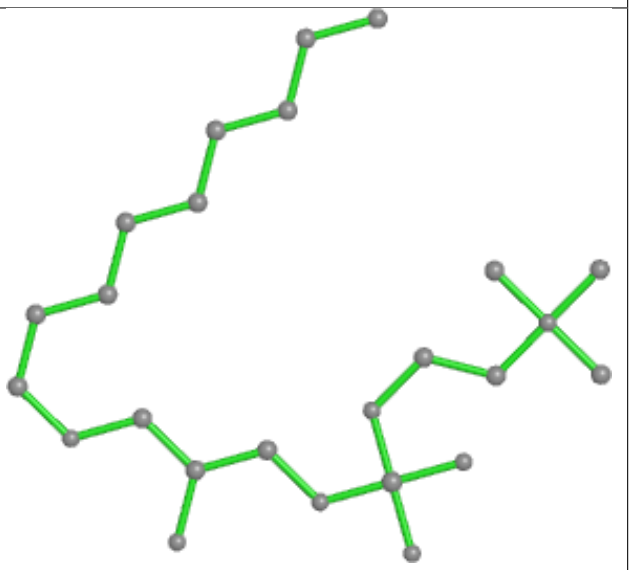


Rings

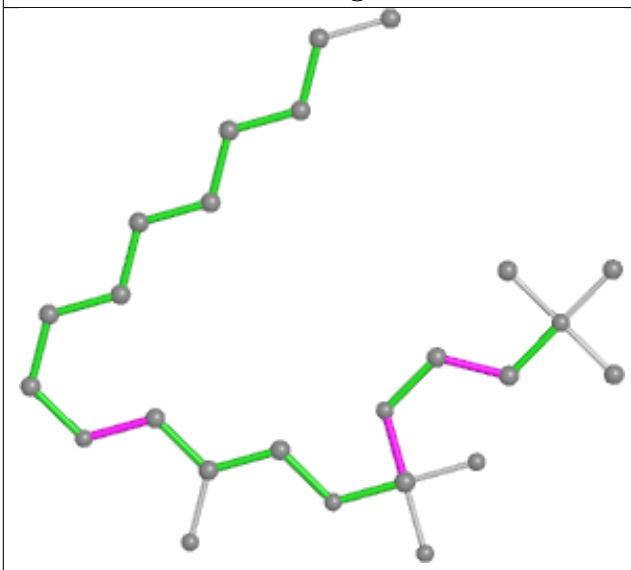
Ligand LPE A 2019



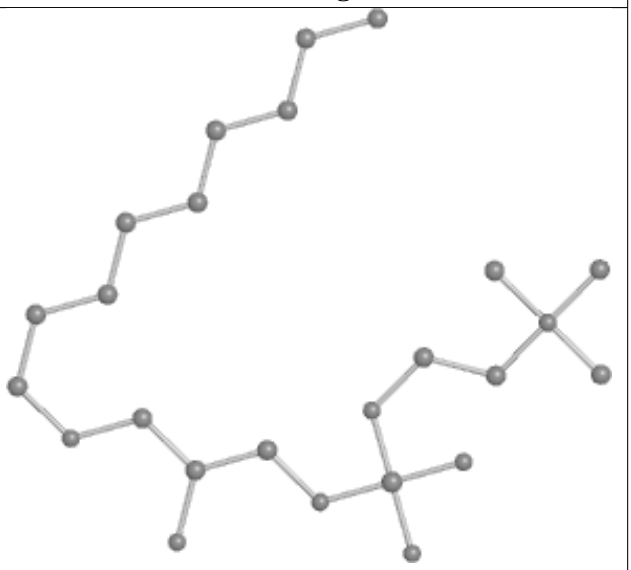
Bond lengths



Bond angles

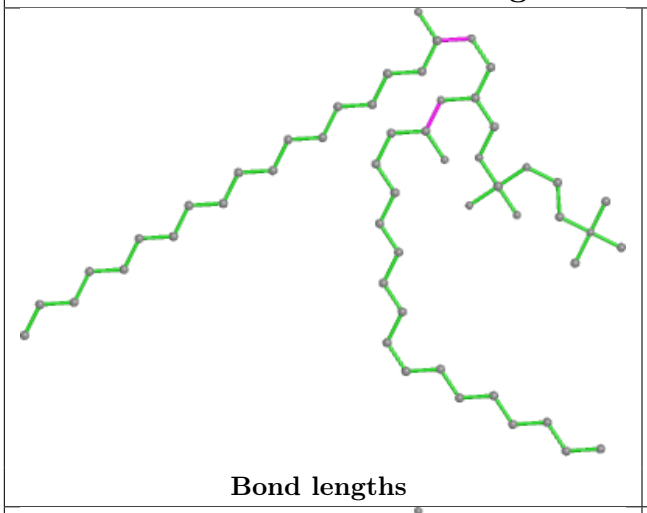


Torsions

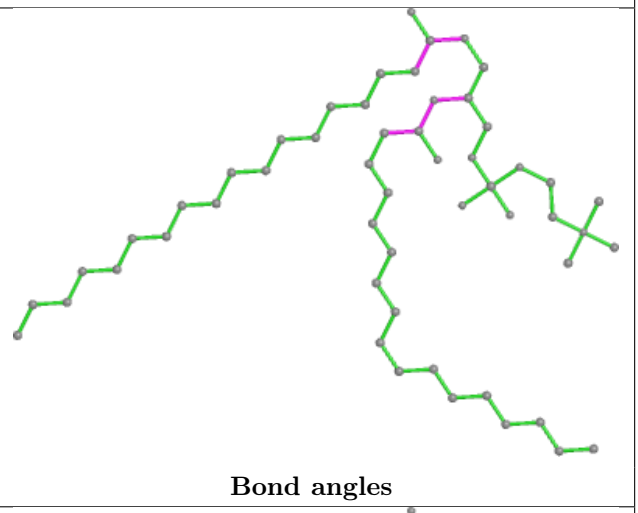


Rings

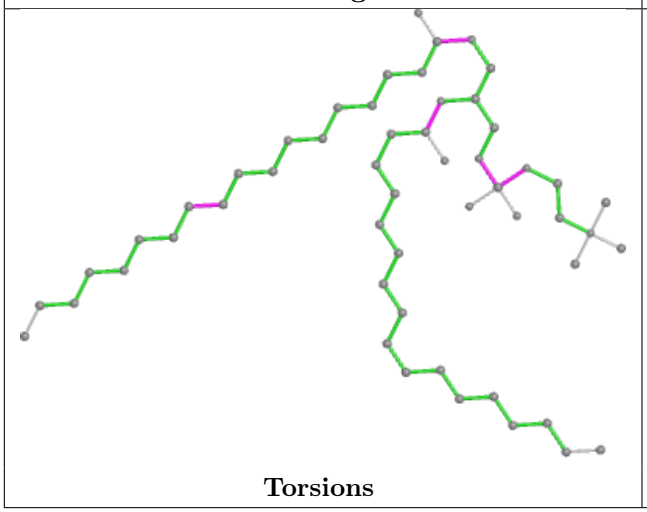
Ligand PCW A 2013



Bond lengths



Bond angles



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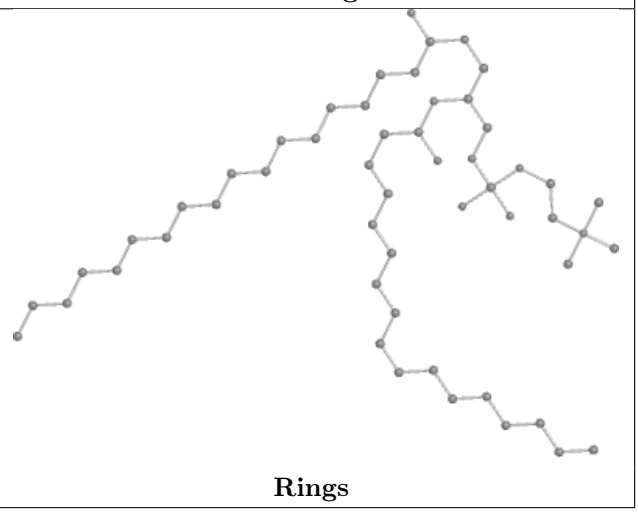
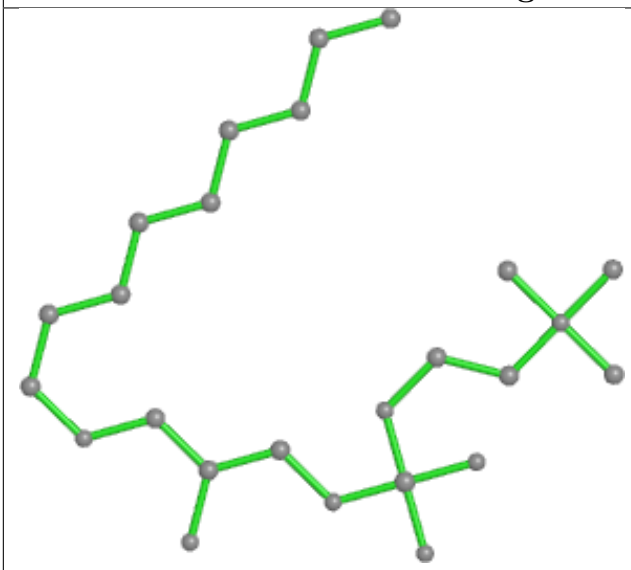


Rings

Ligand LPE A 2021



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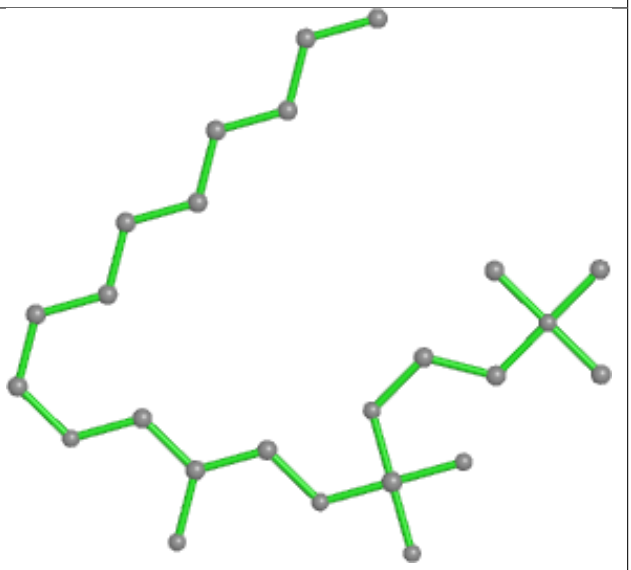
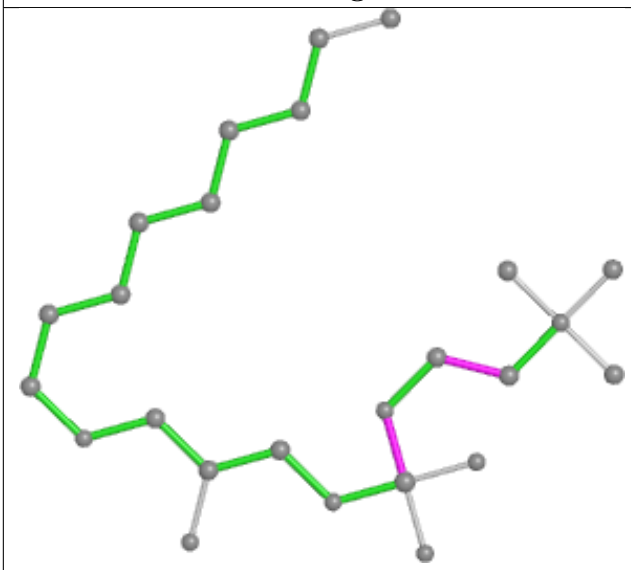


Bond angles



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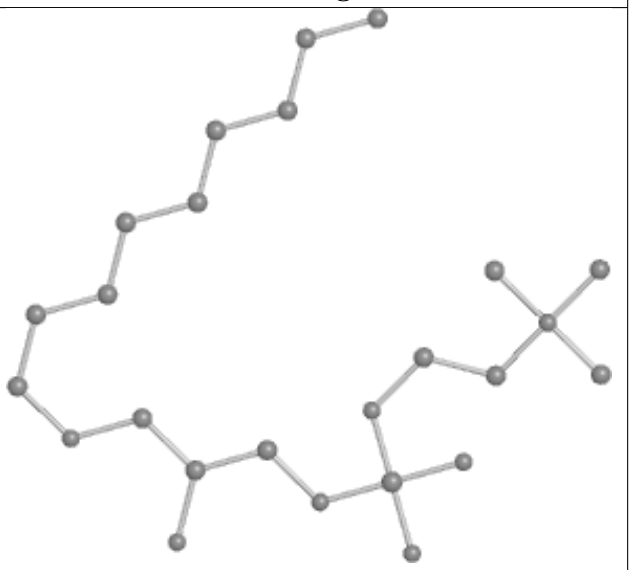
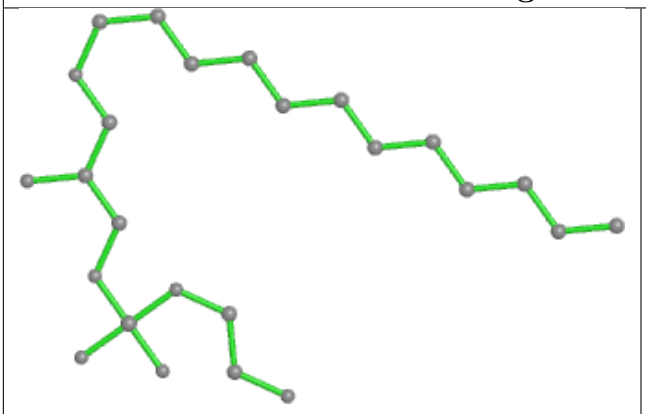


Rings

Ligand LPE A 2011



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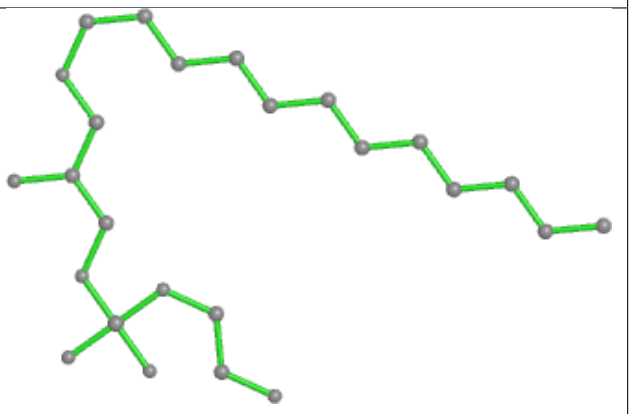
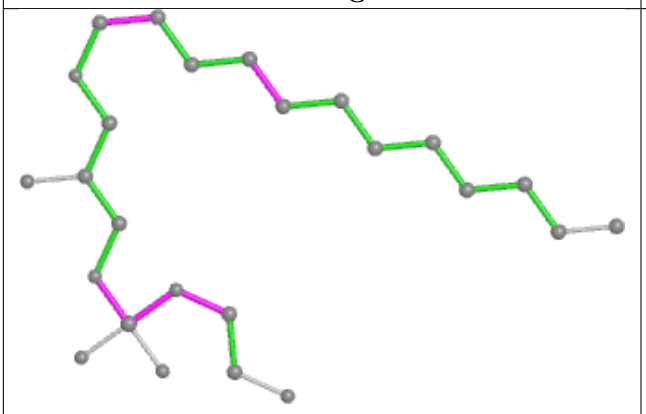


Bond angles



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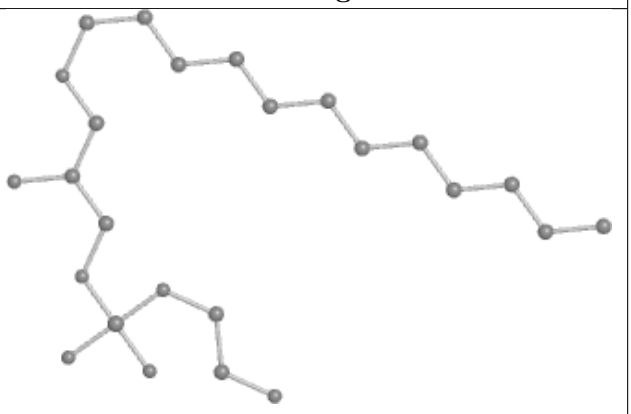
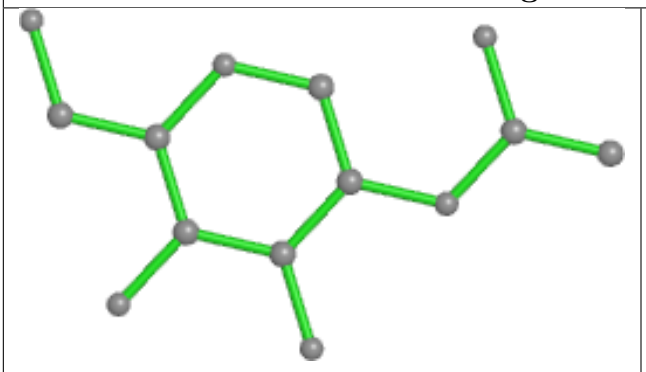
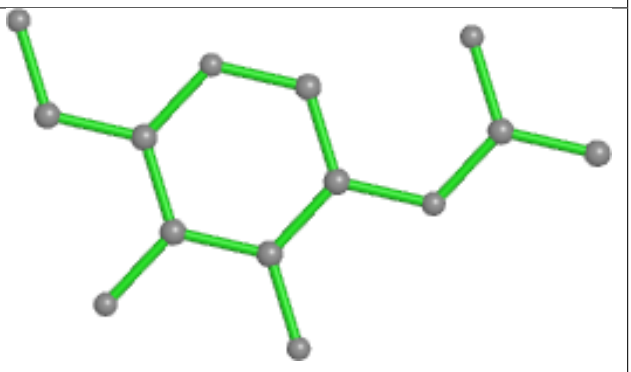


Rings

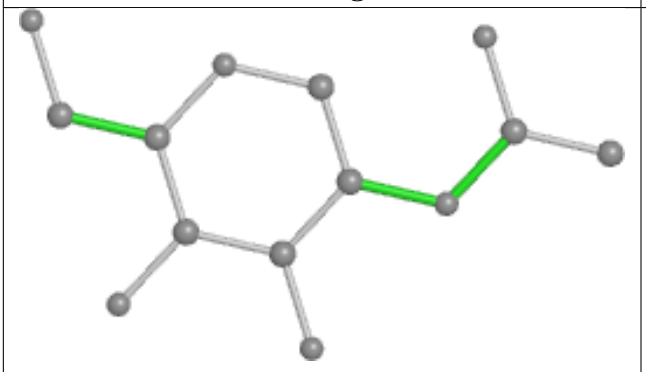
Ligand NAG B 301



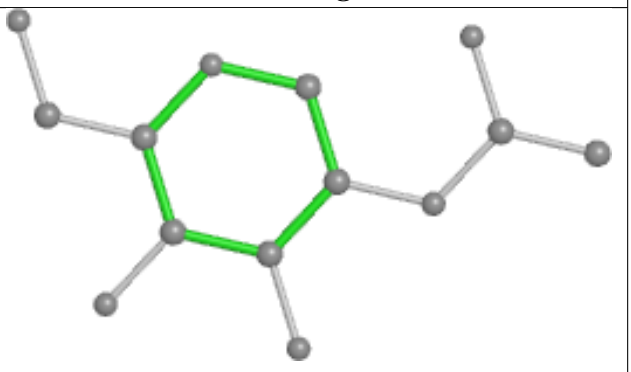
Bond lengths



Bond angles

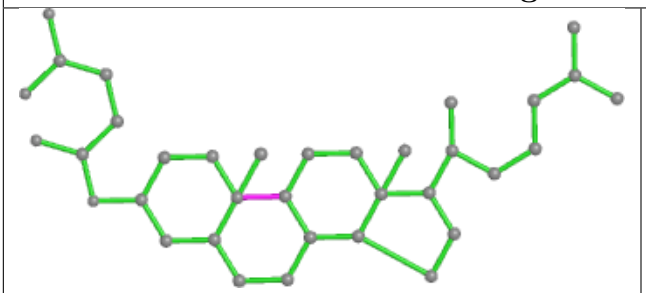


Torsions



Rings

Ligand Y01 A 2004



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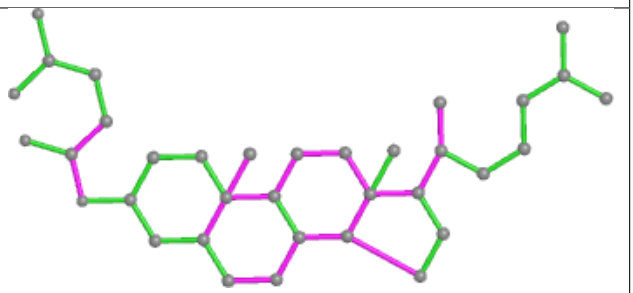

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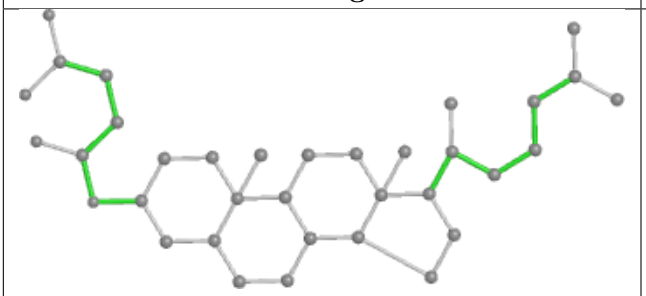
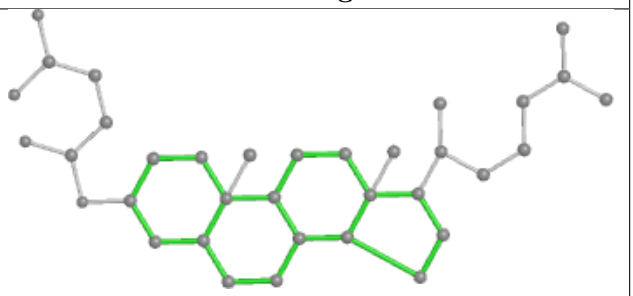
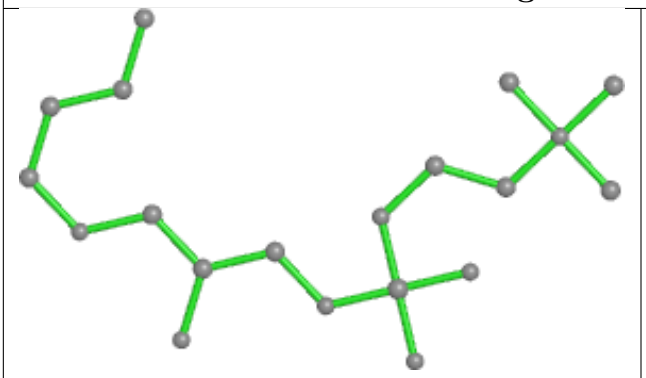


Torsions



Rings

Ligand LPE A 2012



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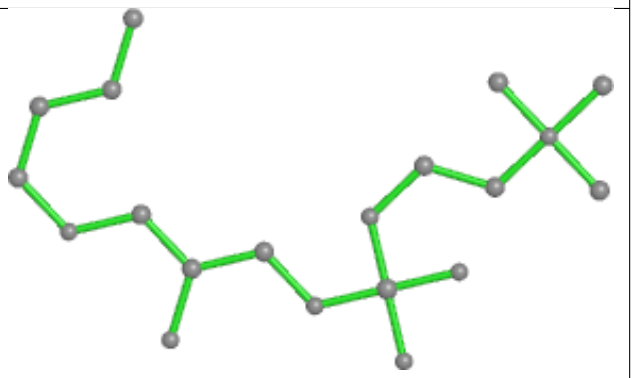
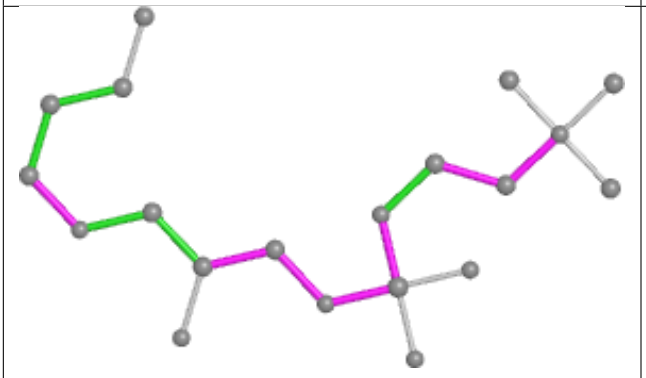


Bond angles



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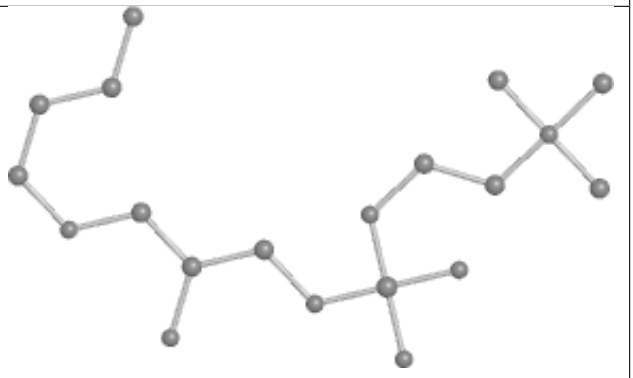
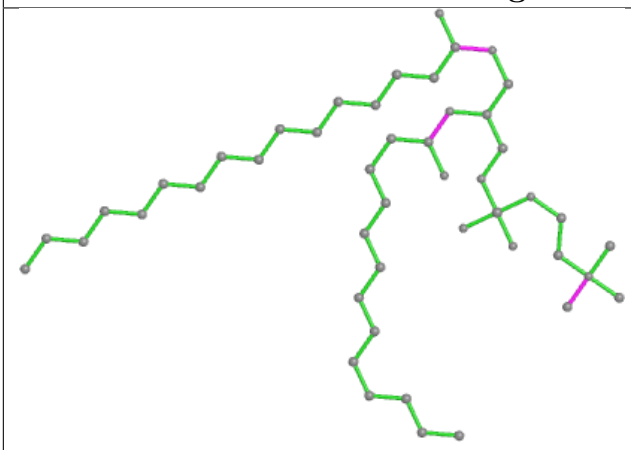


Rings

Ligand PCW A 2016



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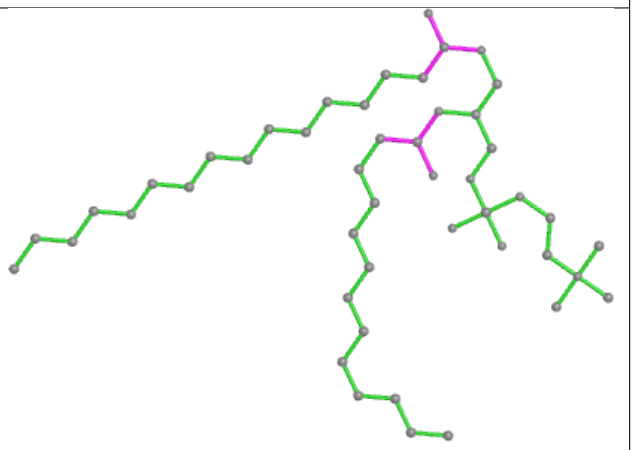
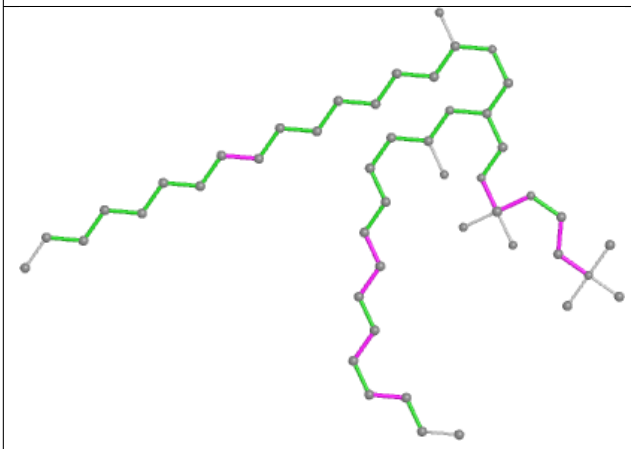


Bond angles



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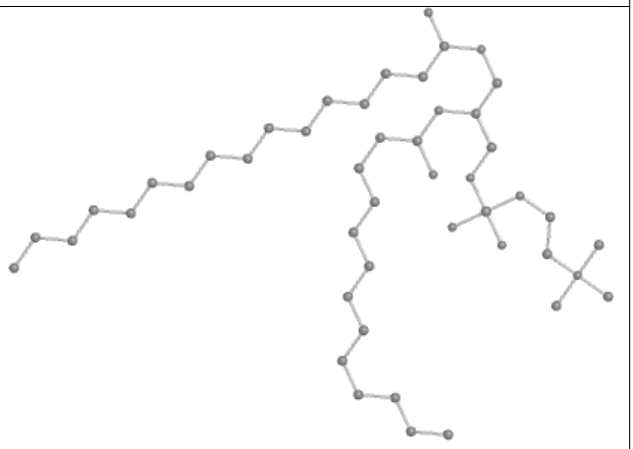
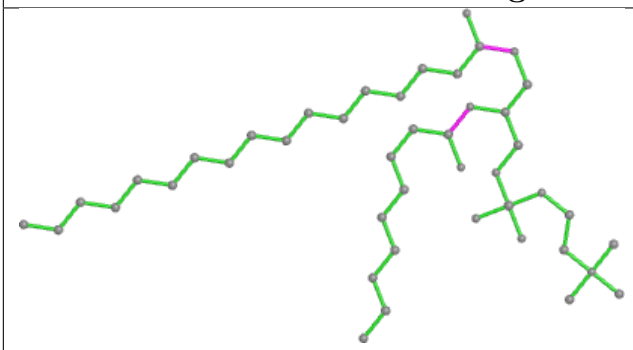


Rings

Ligand PCW A 2028



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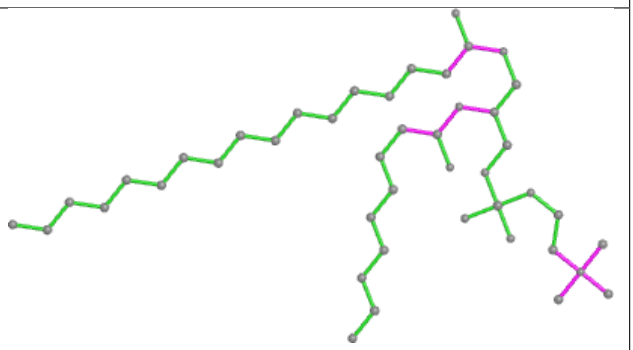

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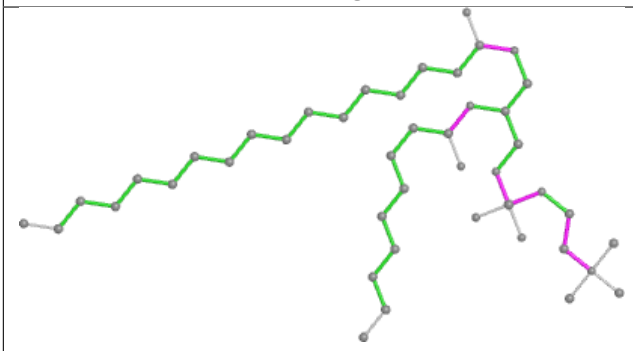

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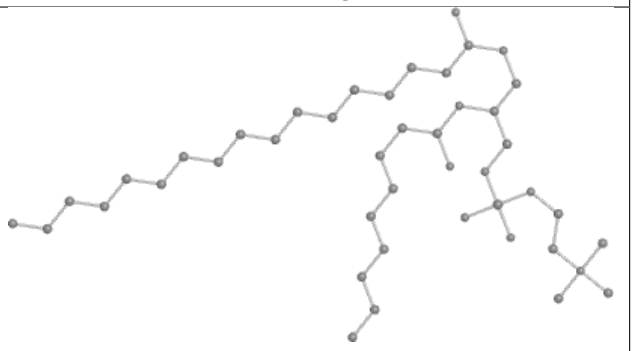
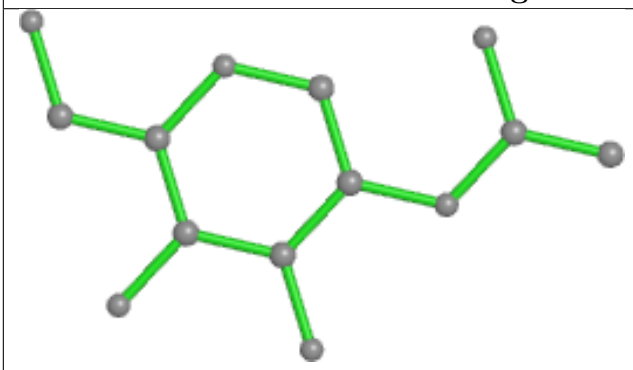


Rings

Ligand NAG A 2001



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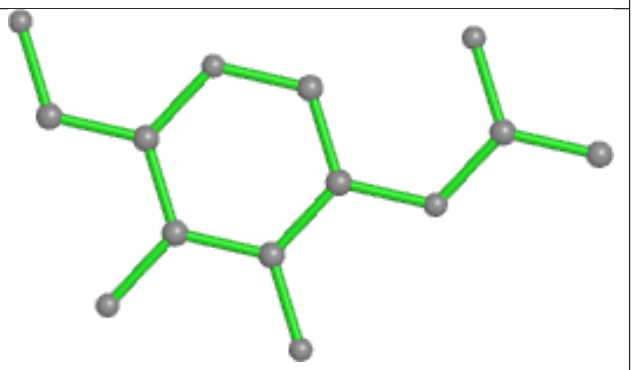

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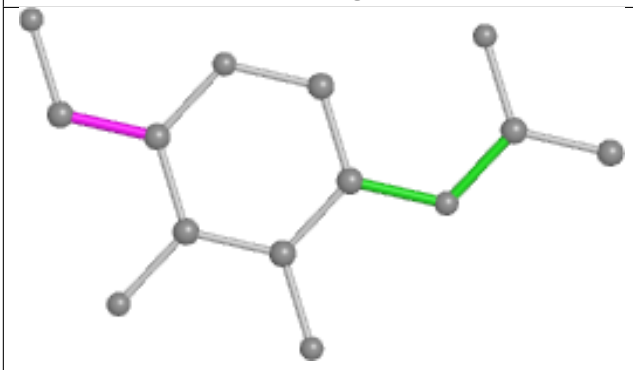

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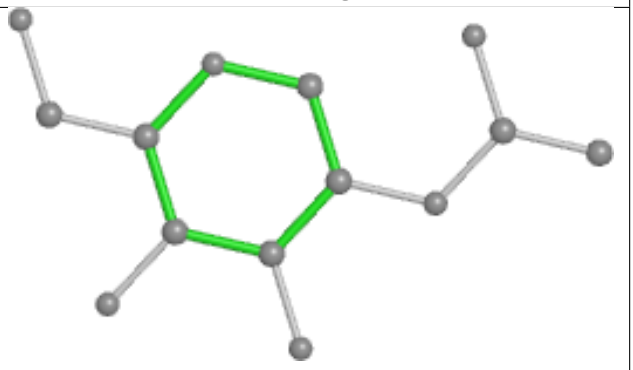
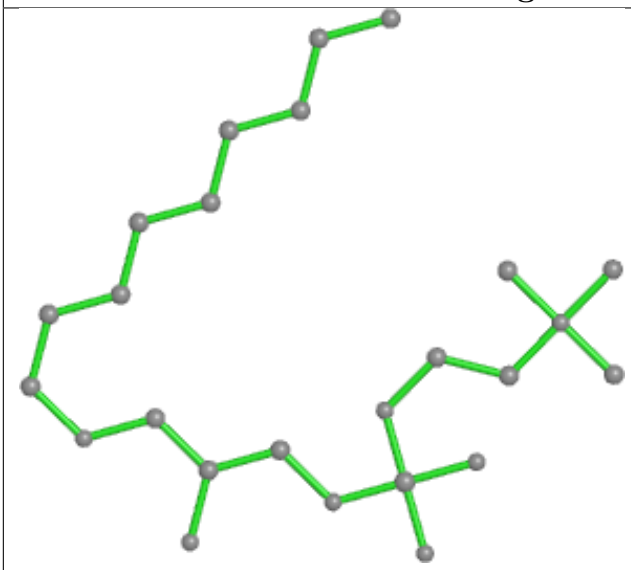


Rings

Ligand LPE A 2020



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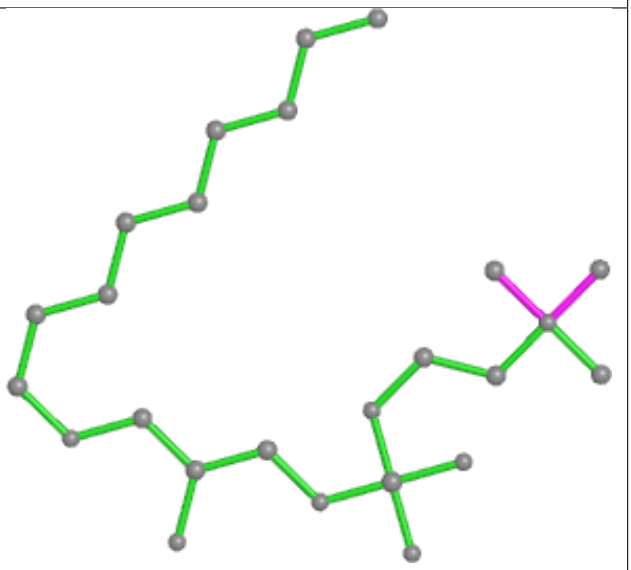

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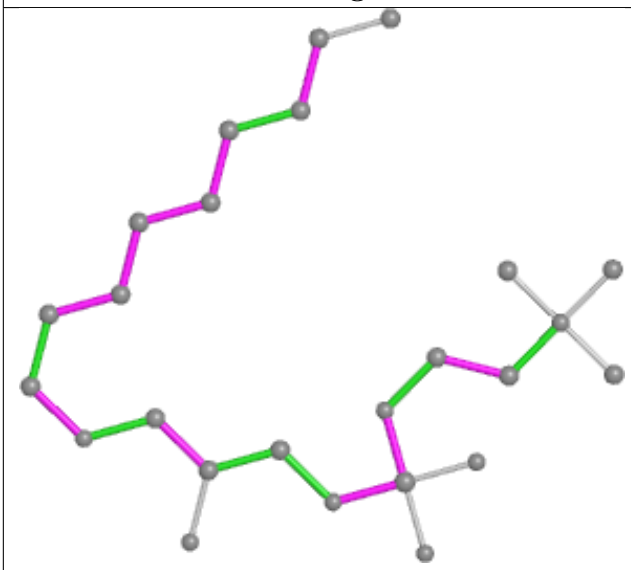

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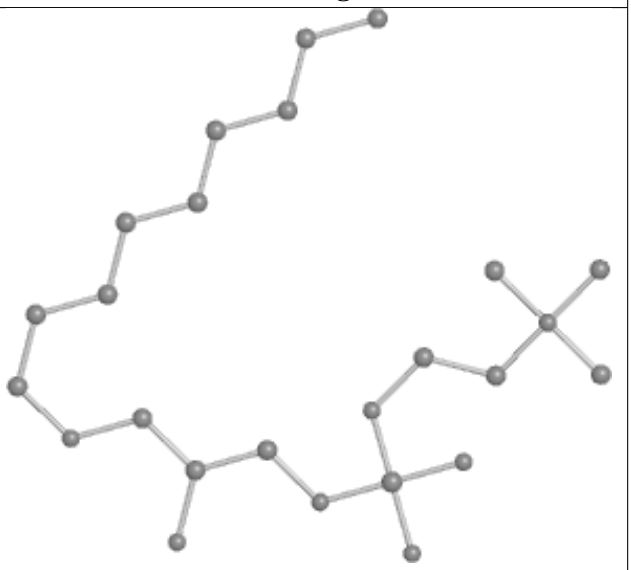
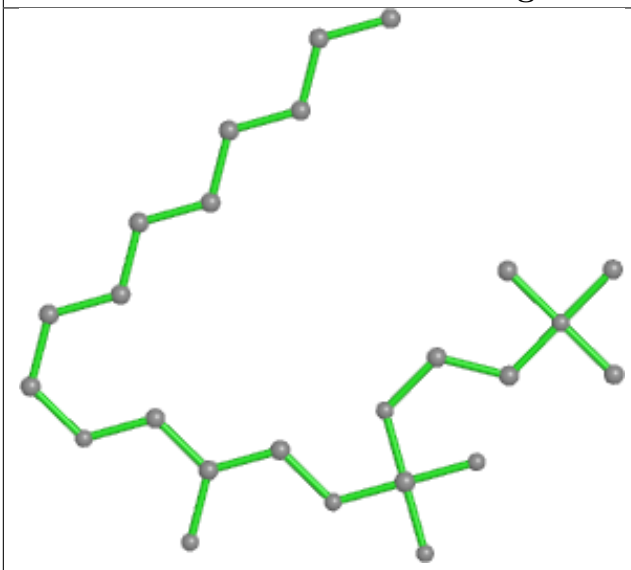


Rings

Ligand LPE A 2025



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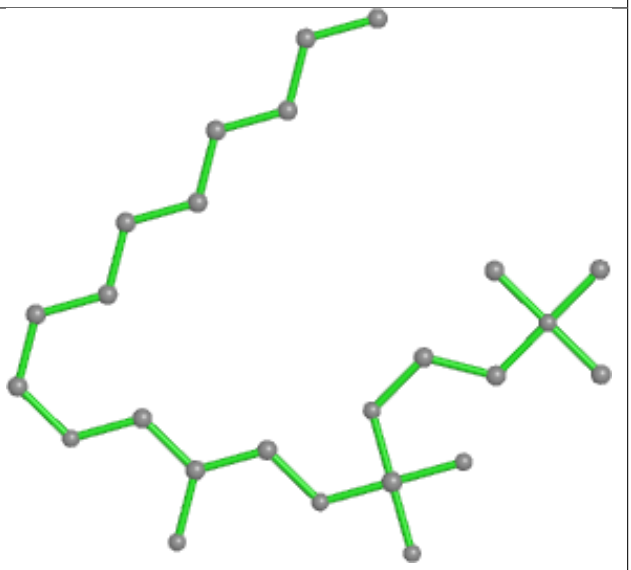

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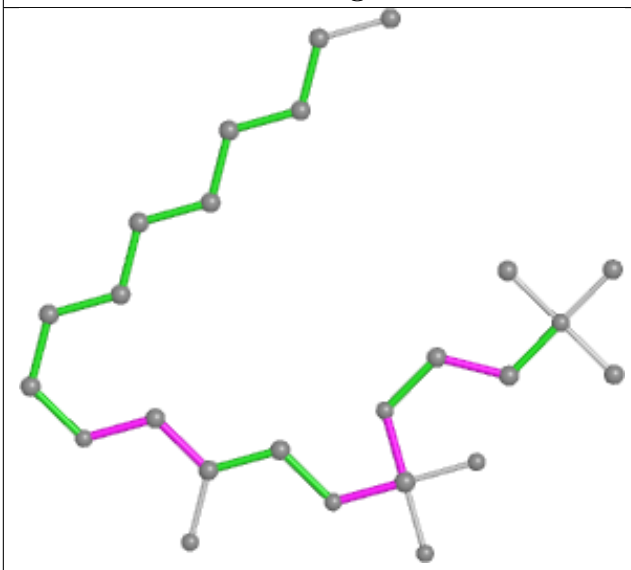

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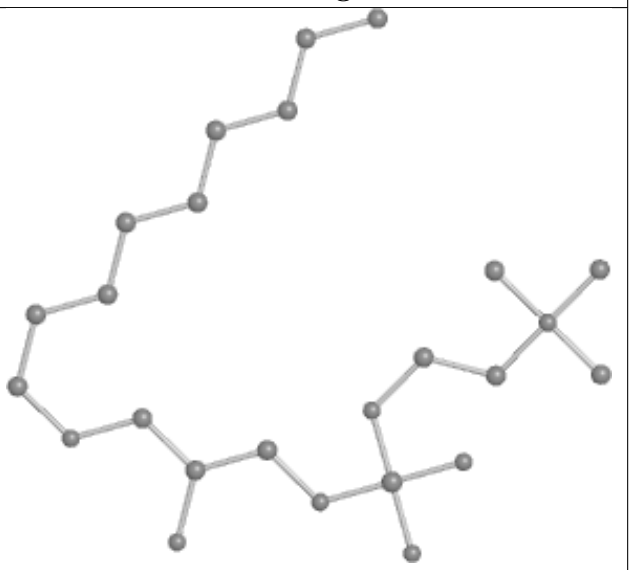
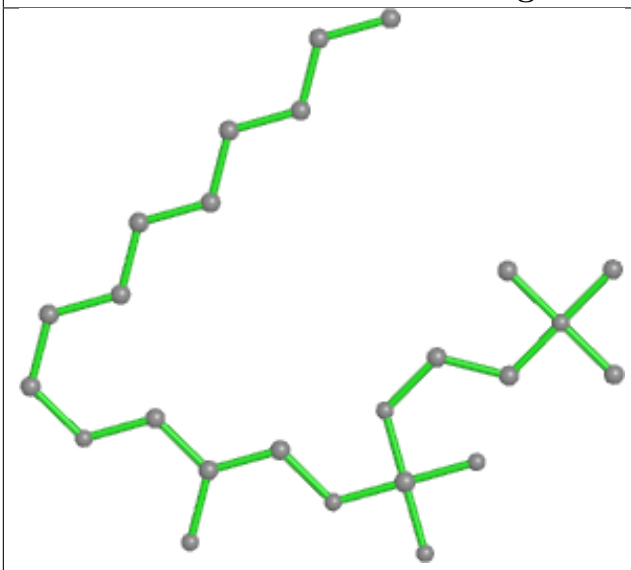


Rings

Ligand LPE A 2023



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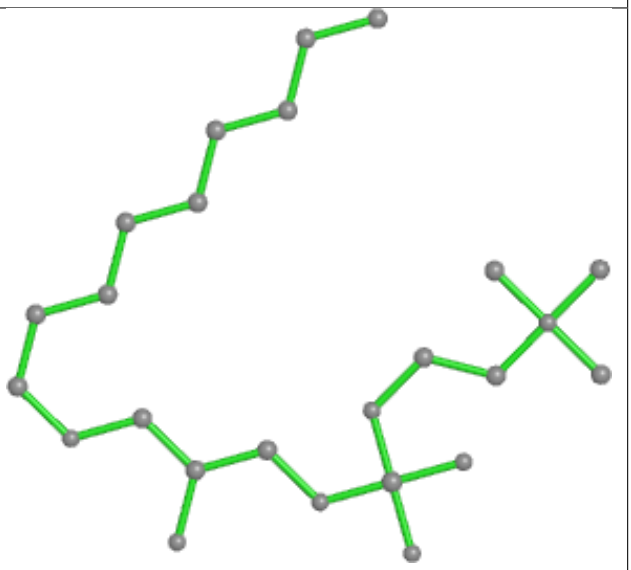

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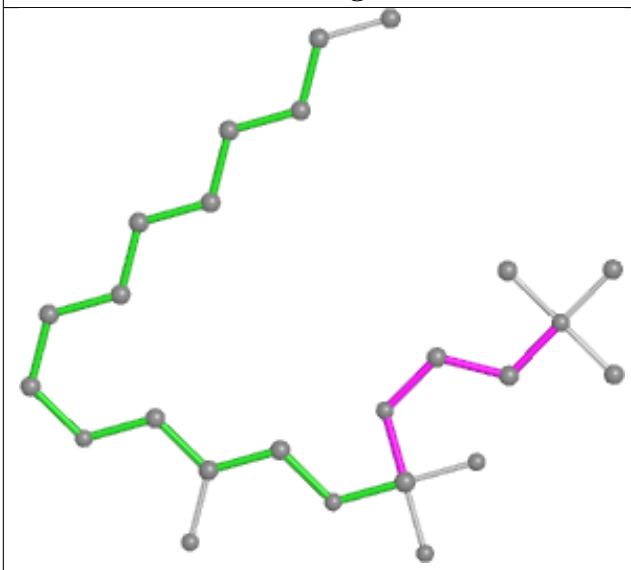

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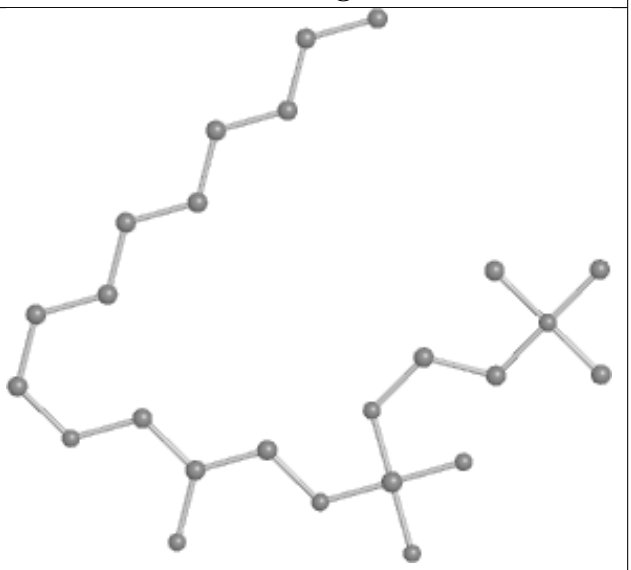
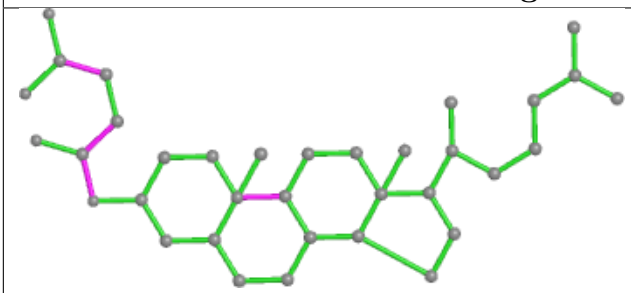


Rings

Ligand Y01 A 2005



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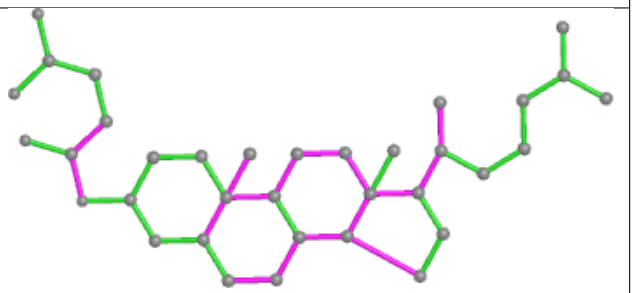

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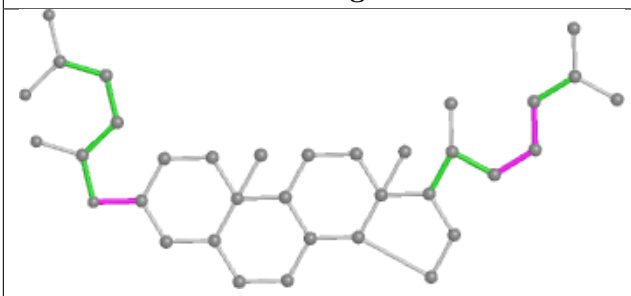

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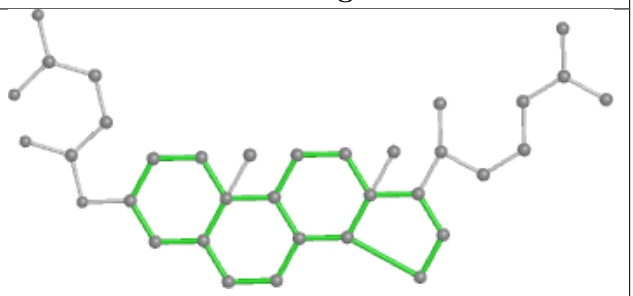
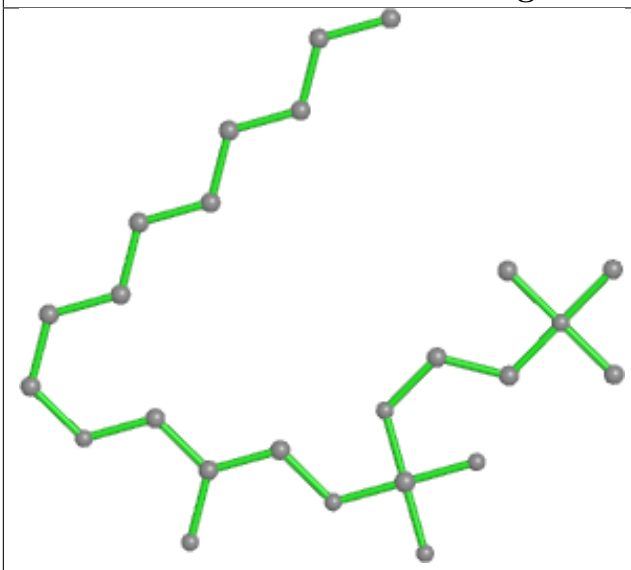


Rings

Ligand LPE A 2024



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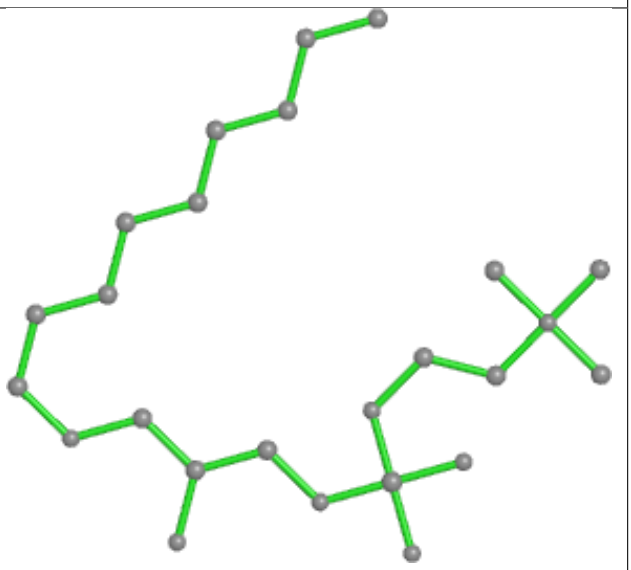
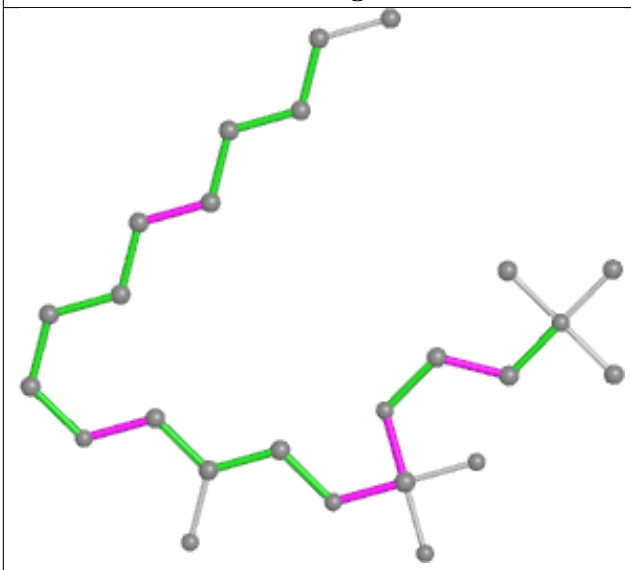


Bond angles



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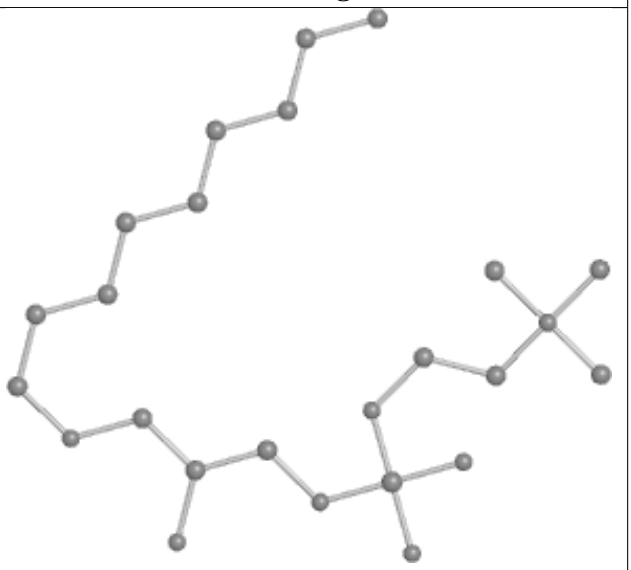
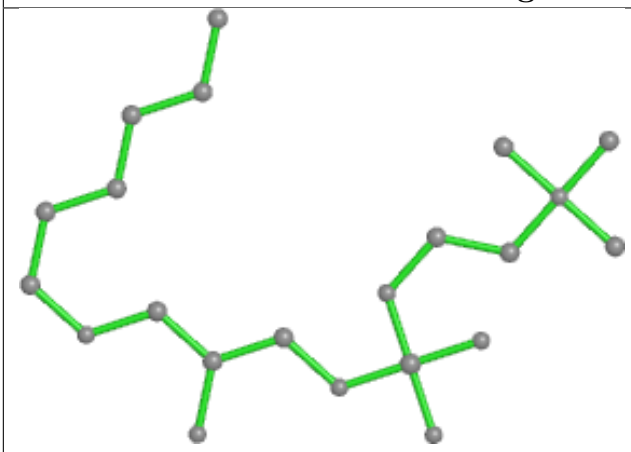


Rings

Ligand LPE A 2014



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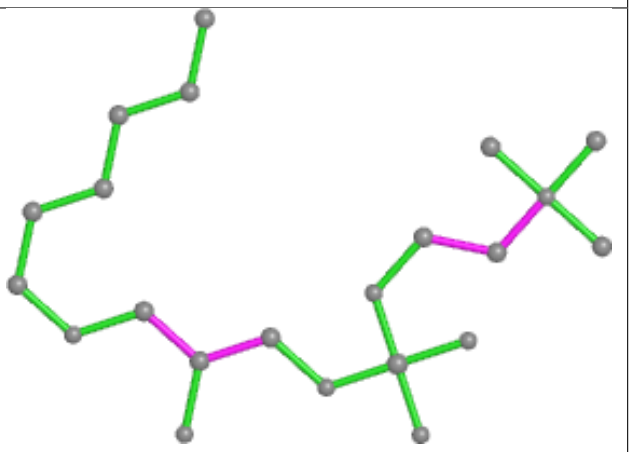
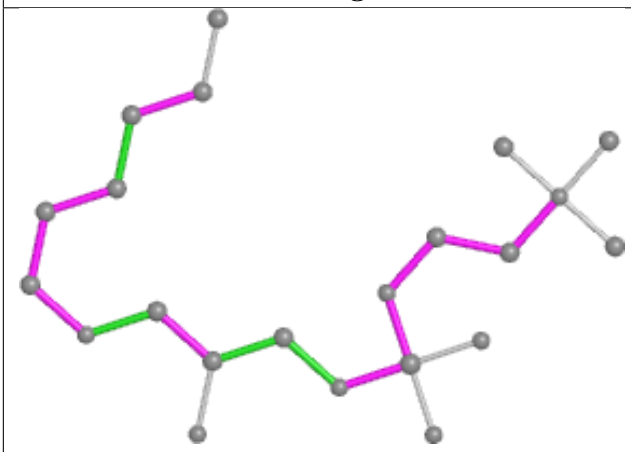


Bond angles



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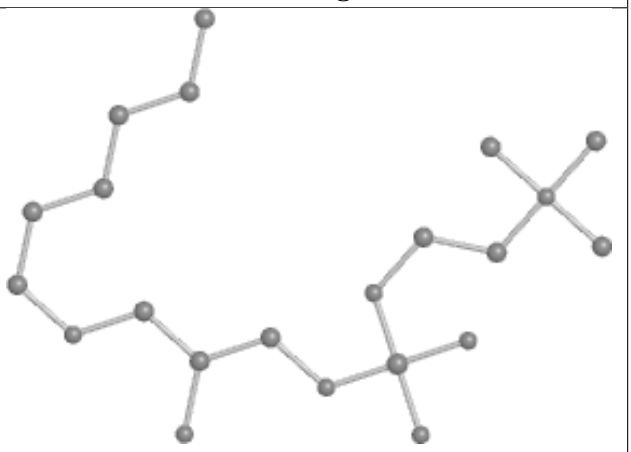
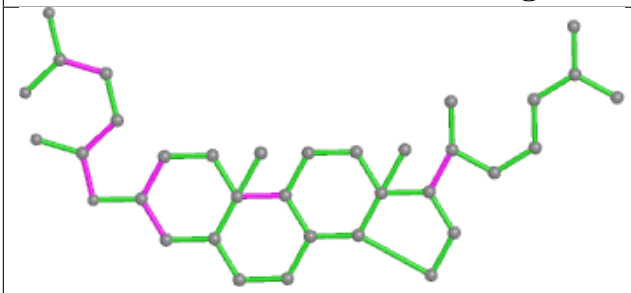


Rings

Ligand Y01 A 2030



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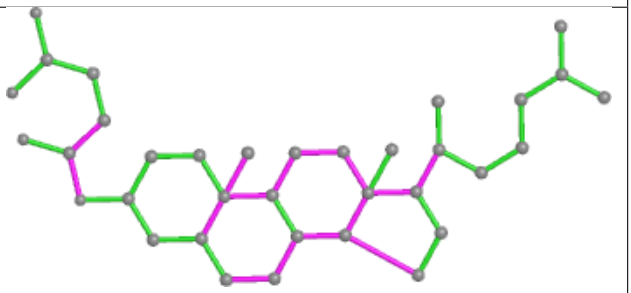

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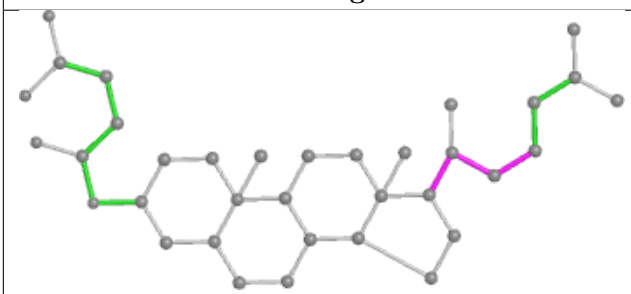

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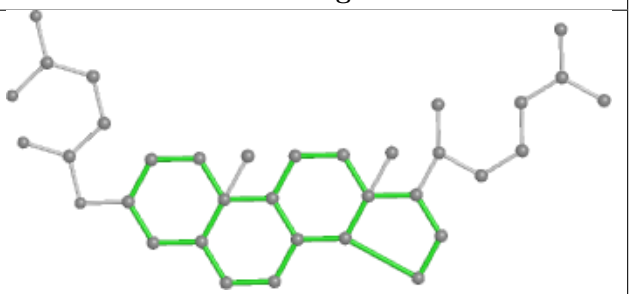
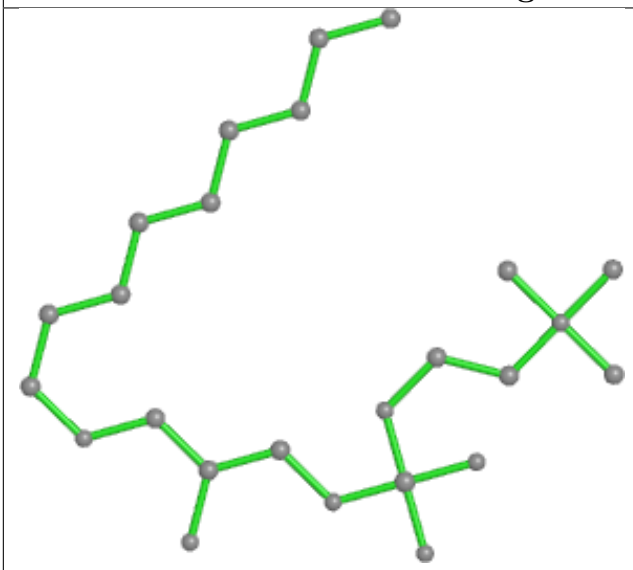


Rings

Ligand LPE A 2022



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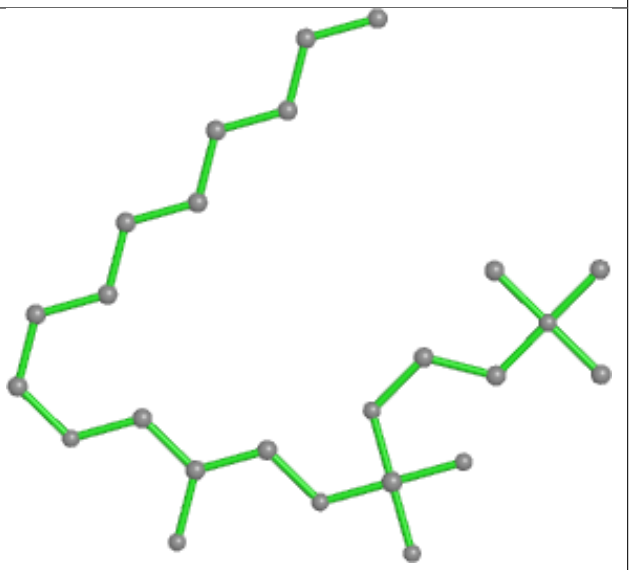
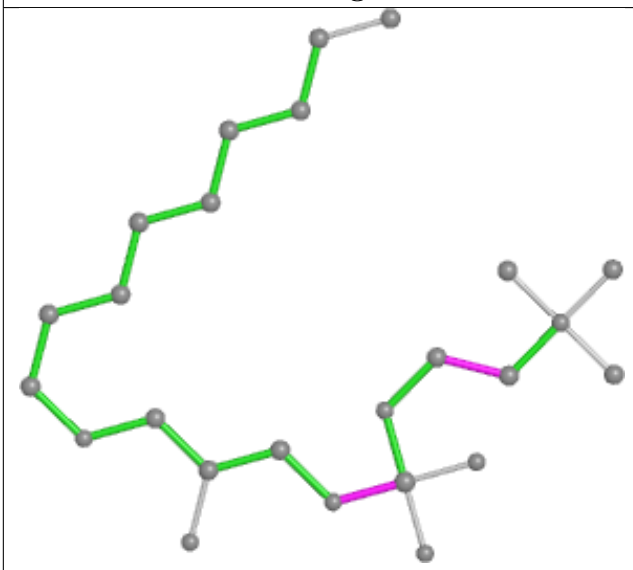


Bond angles



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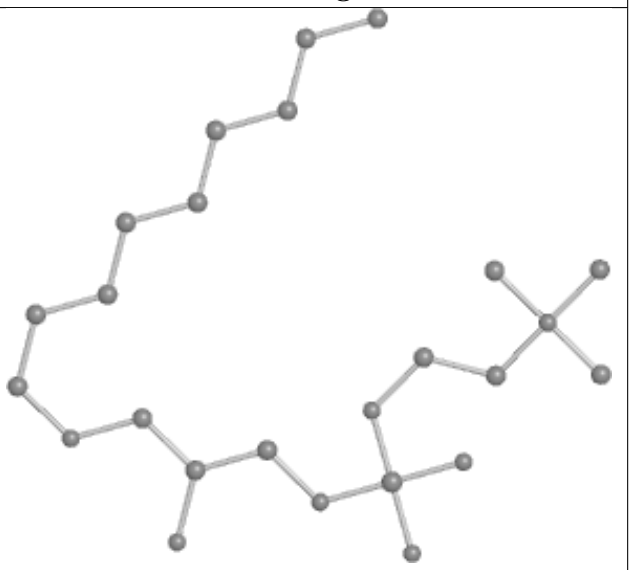
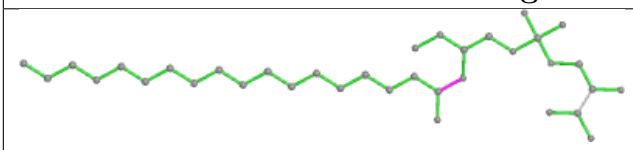


Rings

Ligand P5S A 2002



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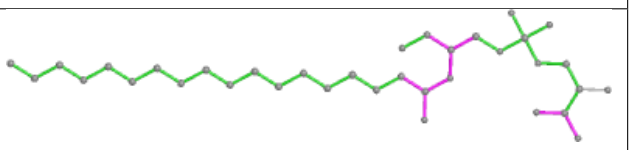
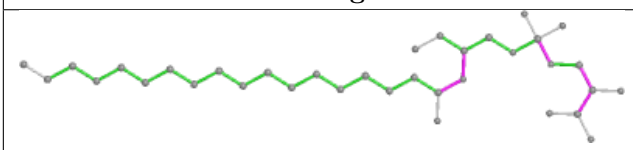


Bond angles



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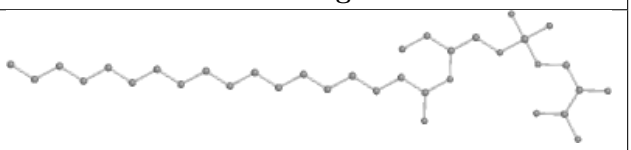
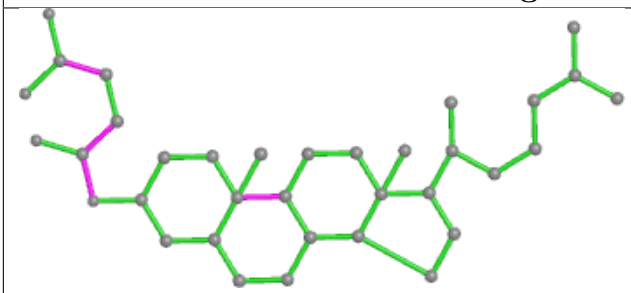


Rings

Ligand Y01 A 2009



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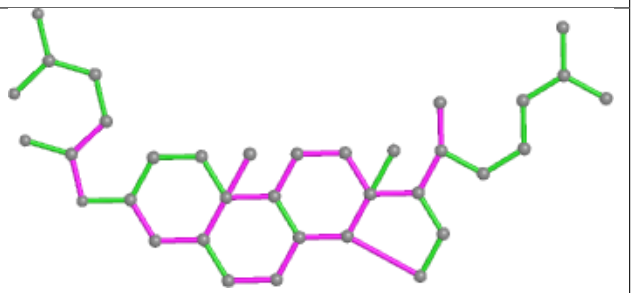
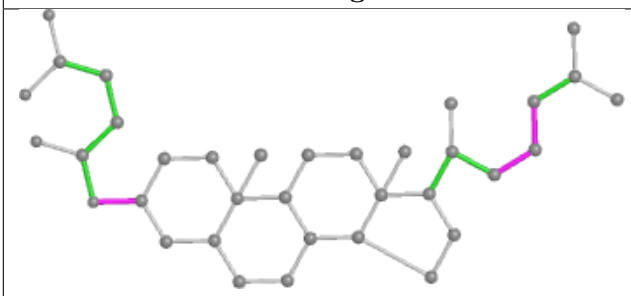


Bond angles



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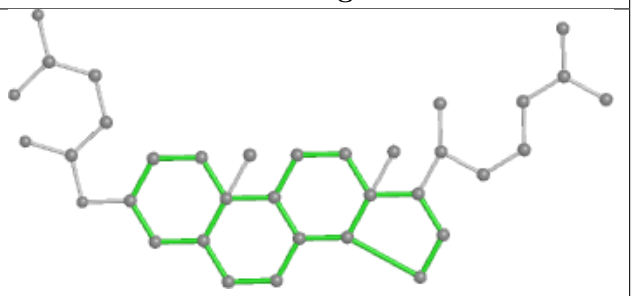
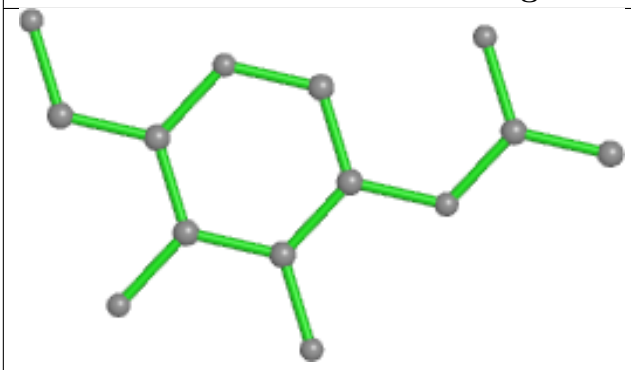
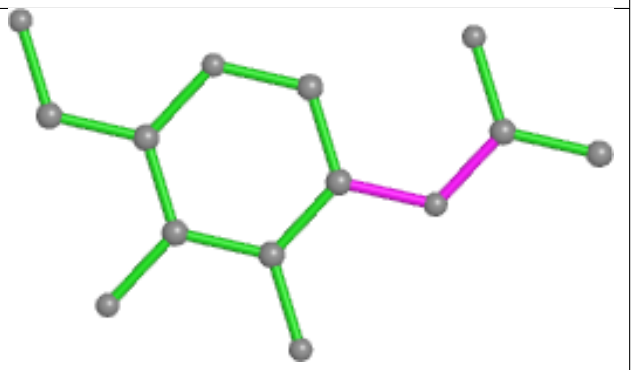


Rings

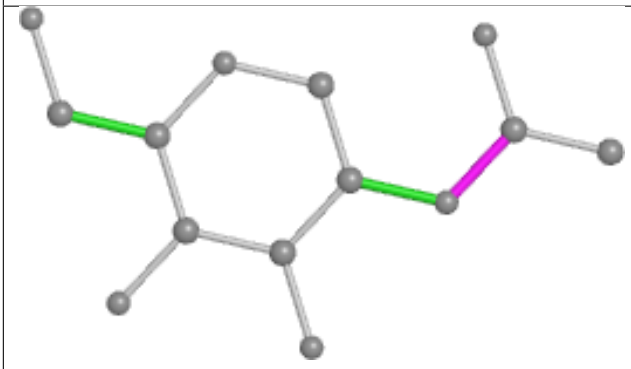
Ligand NAG B 302



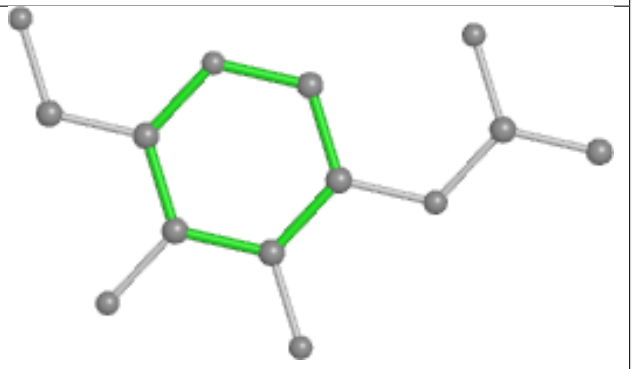
Bond lengths



Bond angles

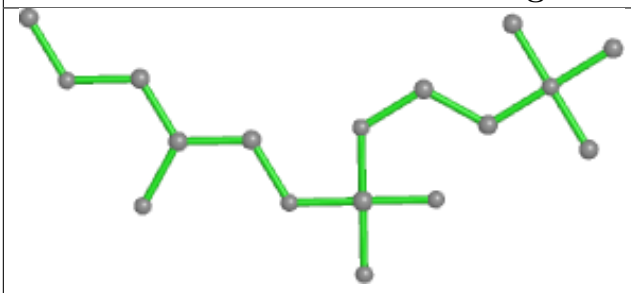


Torsions

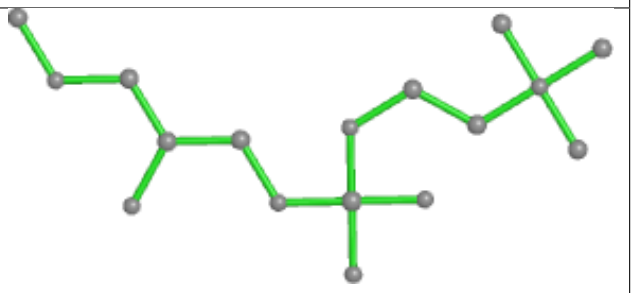


Rings

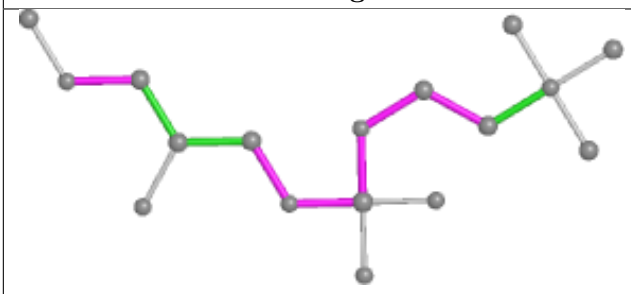
Ligand LPE B 304



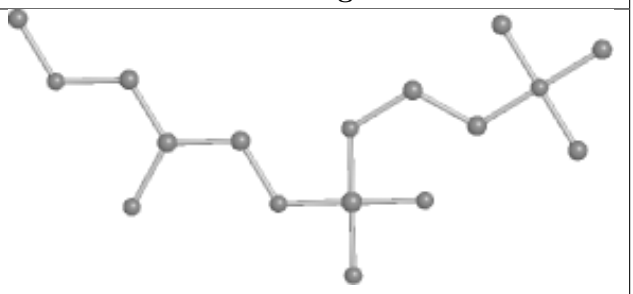
Bond lengths



Bond angles

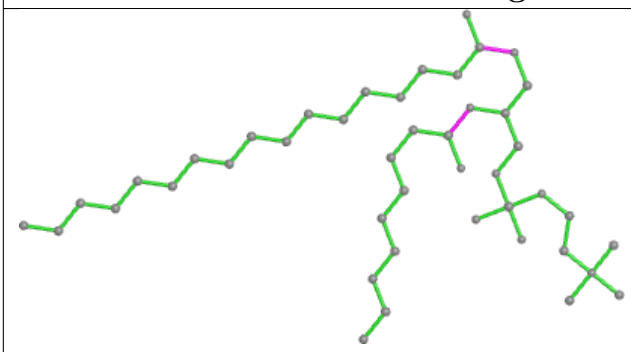


Torsions

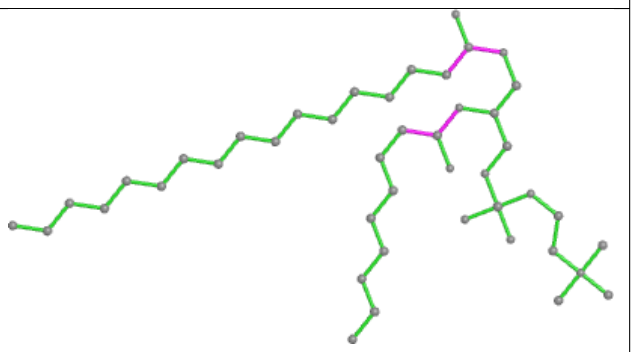


Rings

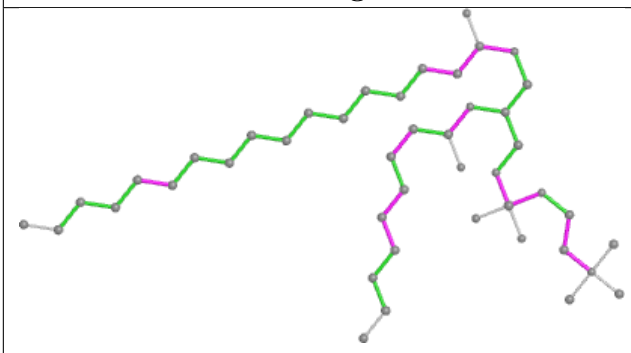
Ligand PCW A 2027



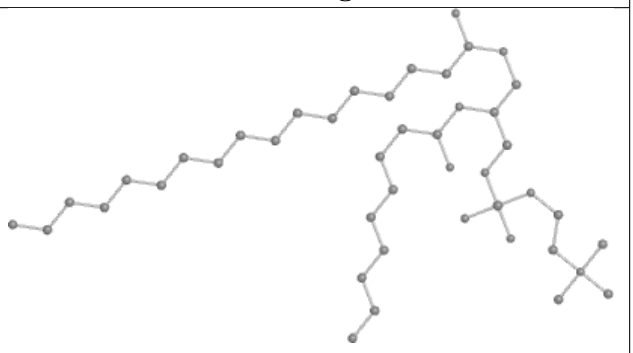
Bond lengths



Bond angles

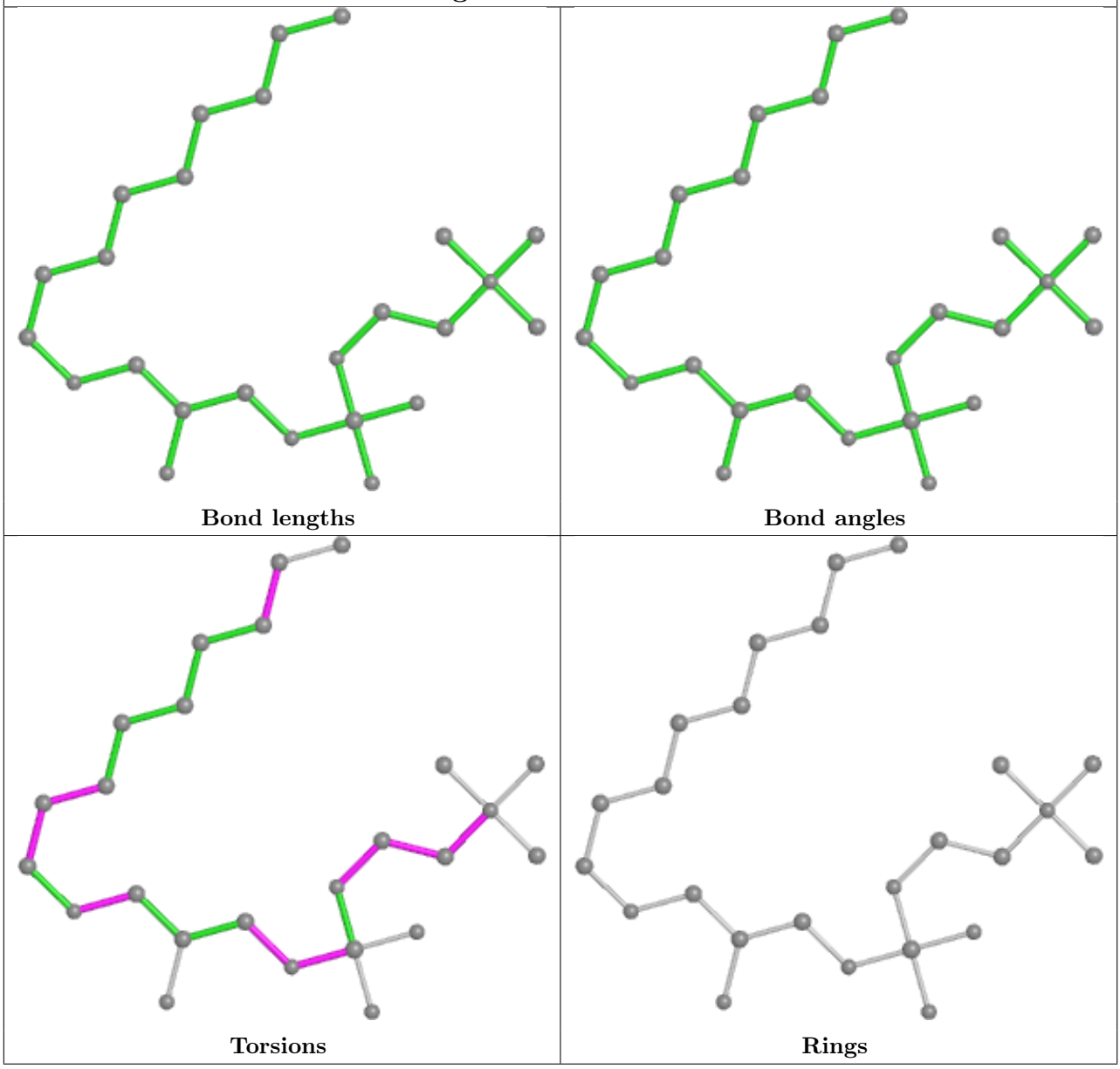


Torsions



Rings

Ligand LPE A 2010



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.

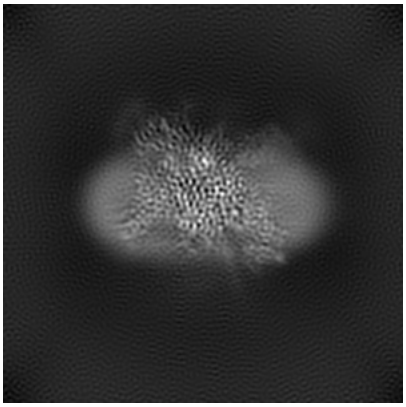
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32369. These allow visual inspection of the internal detail of the map and identification of artifacts.

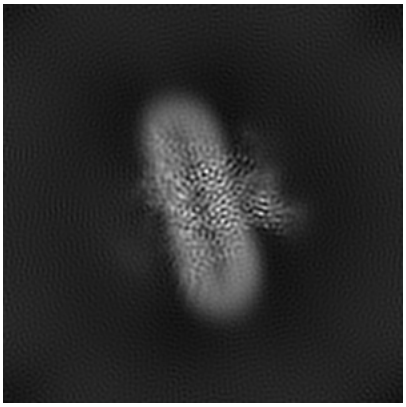
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

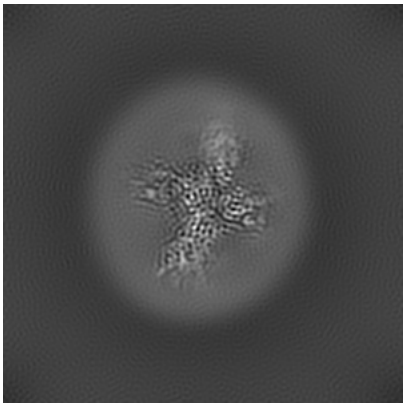
6.1.1 Primary map



X



Y

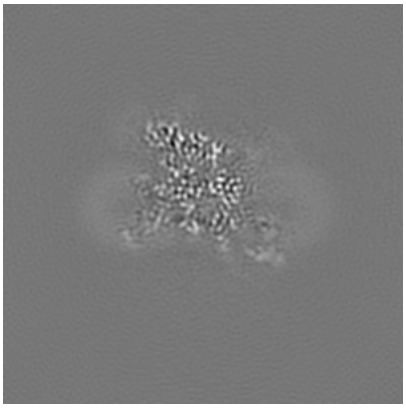


Z

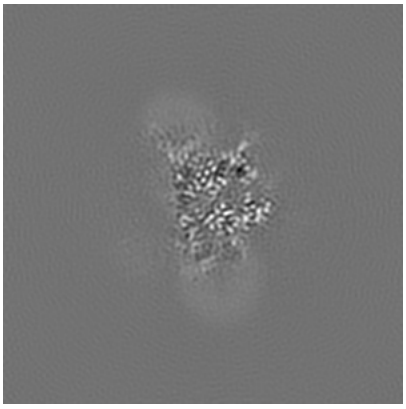
The images above show the map projected in three orthogonal directions.

6.2 Central slices

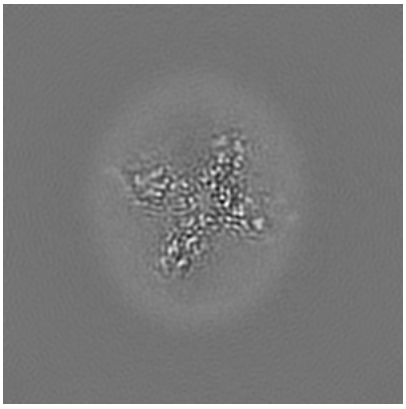
6.2.1 Primary map



X Index: 128



Y Index: 128

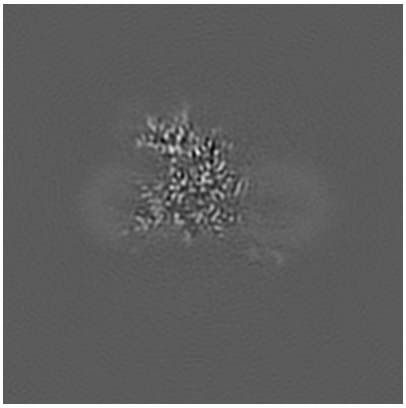


Z Index: 128

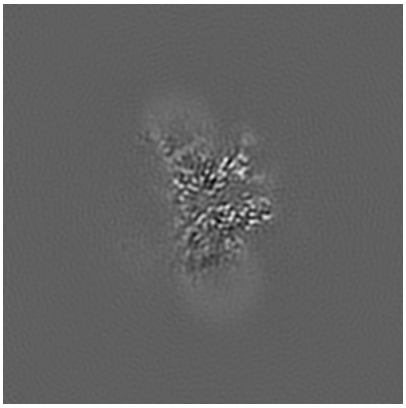
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

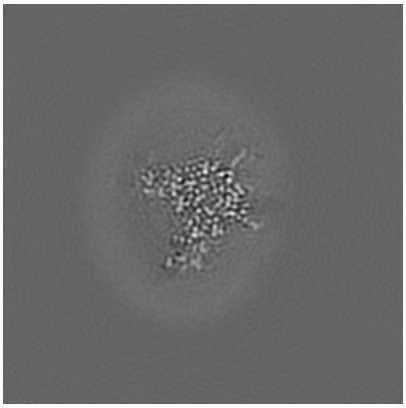
6.3.1 Primary map



X Index: 122



Y Index: 130



Z Index: 138

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.43. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

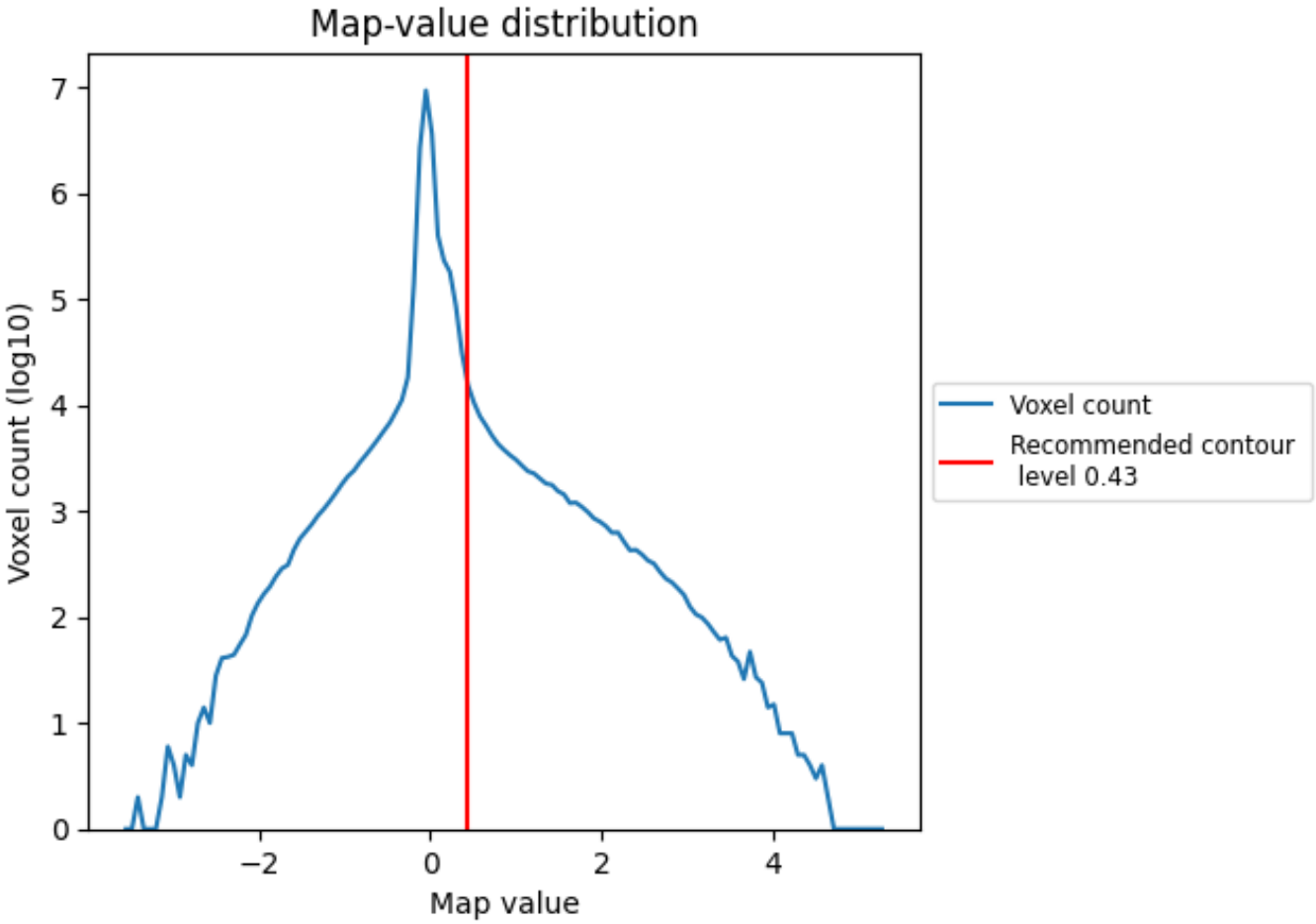
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

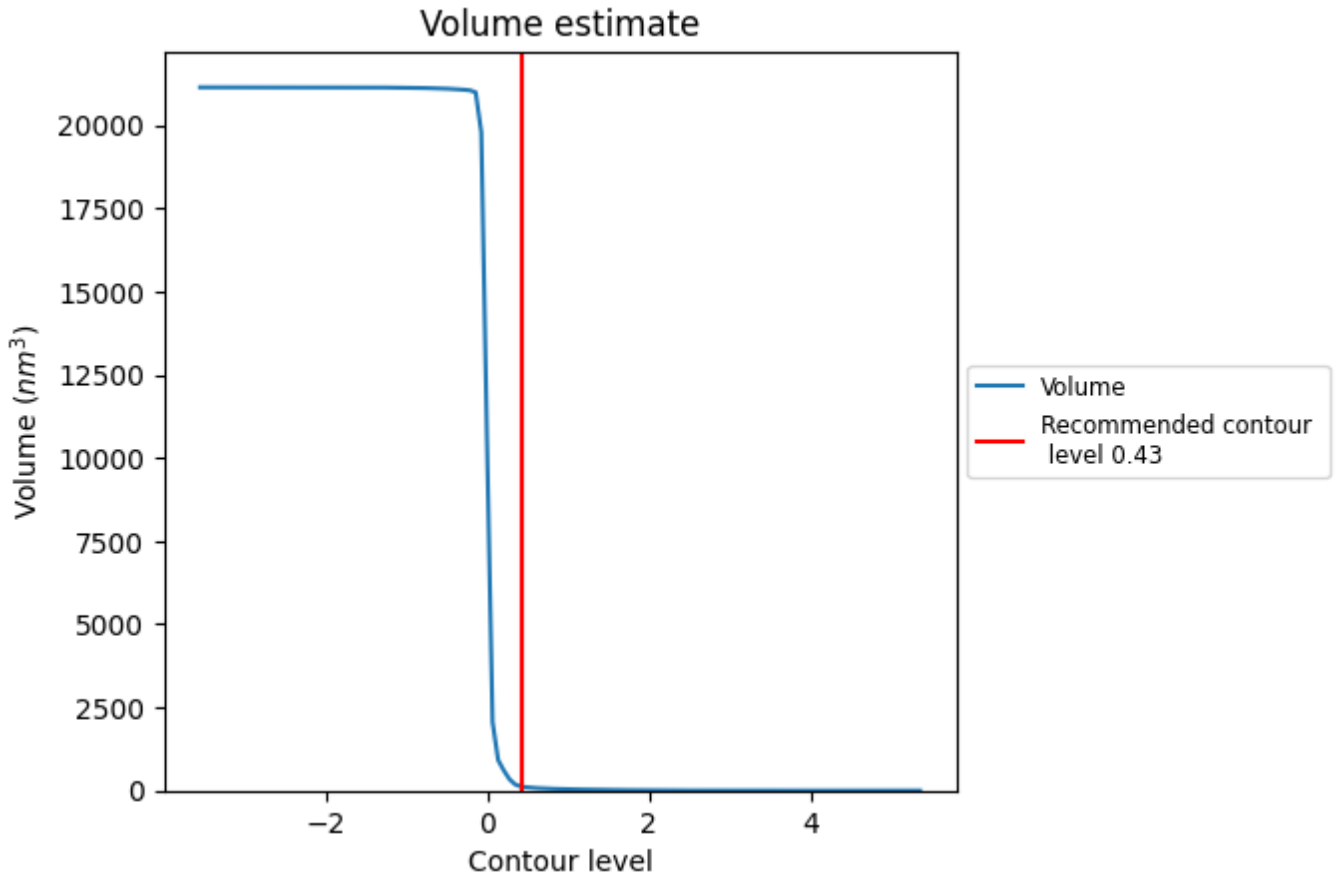
This section contains the results of statistical analysis of the map.

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.

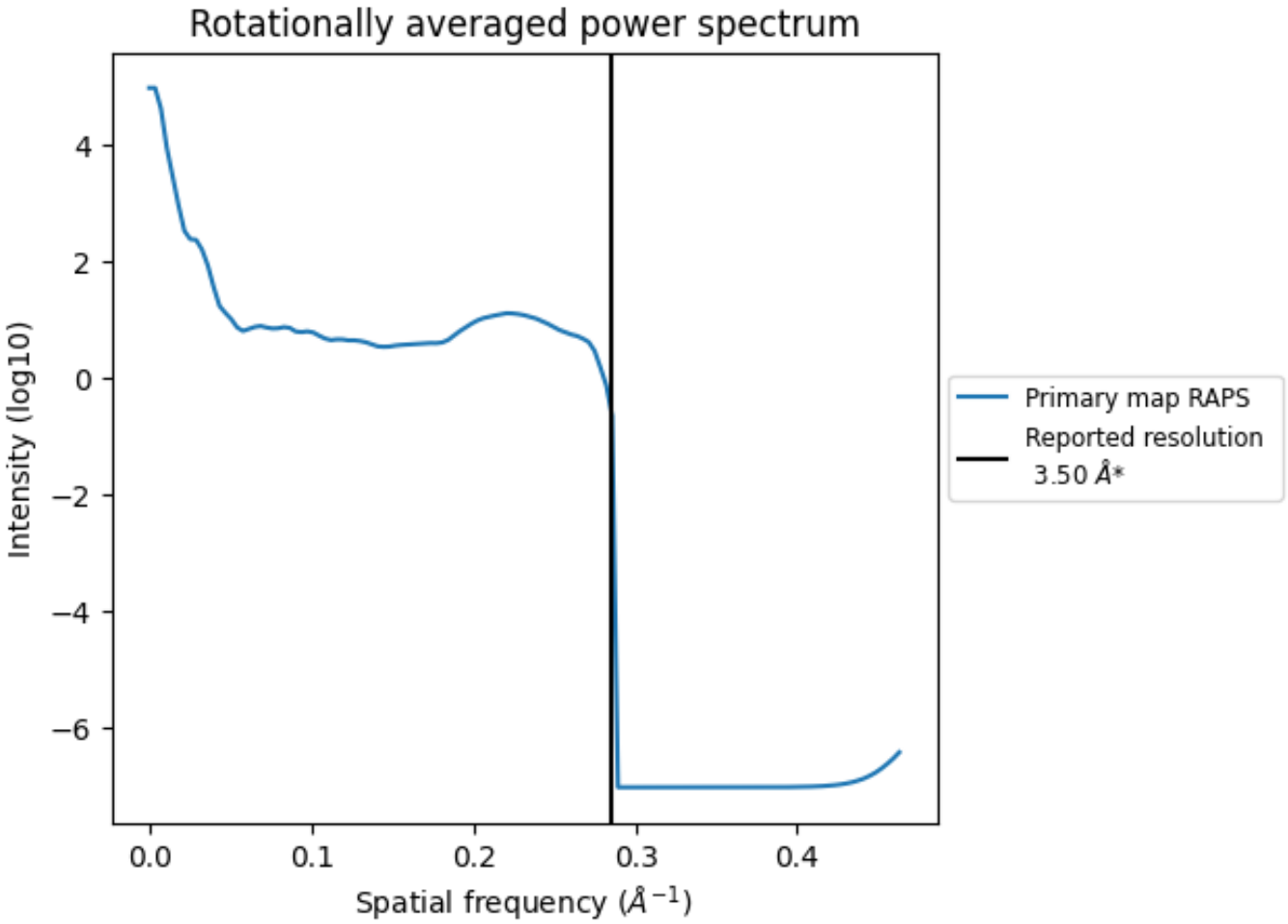
7.2 Volume estimate



The volume at the recommended contour level is 118 nm^3; this corresponds to an approximate mass of 106 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}

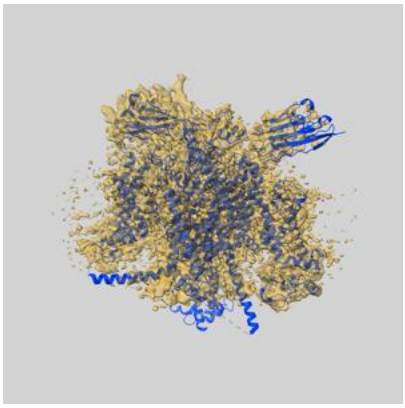
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

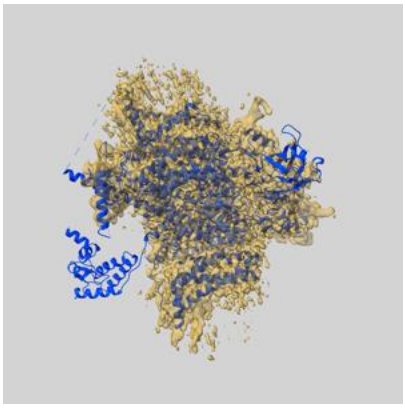
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32369 and PDB model 7W9L. Per-residue inclusion information can be found in section 3 on page 11.

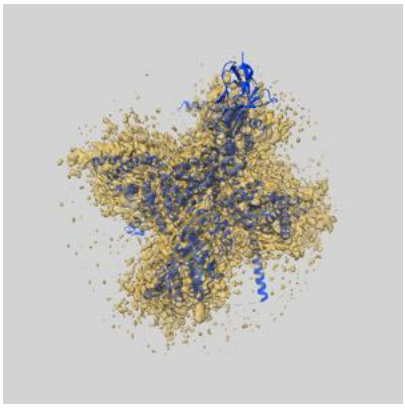
9.1 Map-model overlay



X



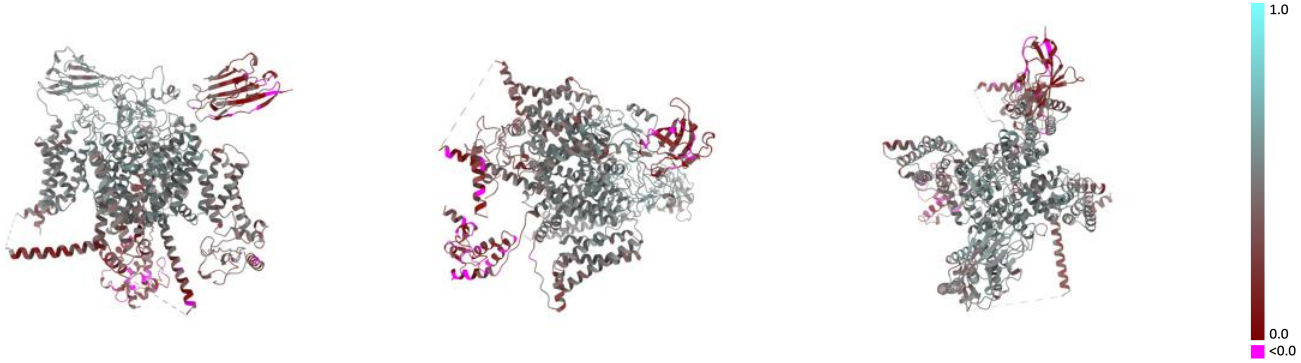
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.43 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.

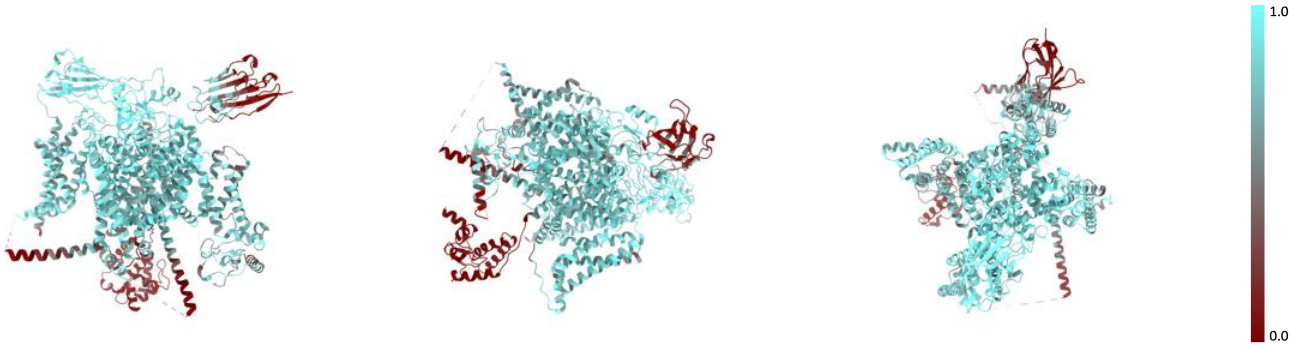
9.2 Q-score mapped to coordinate model (i)



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.

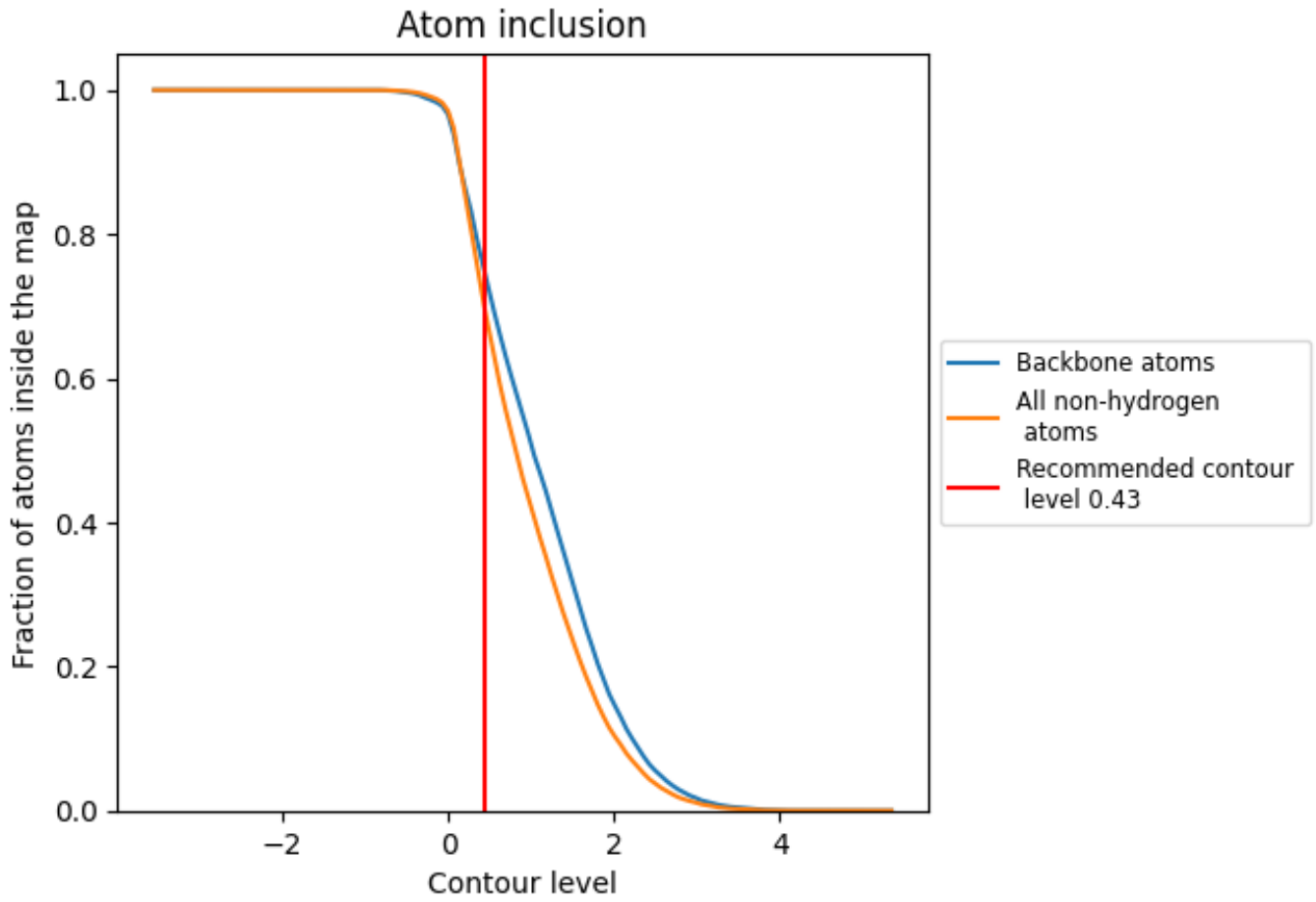
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.43).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 70% 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 (0.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7008	0.4140
A	0.7109	0.4230
B	0.8601	0.4750
C	0.3260	0.2170
D	0.7500	0.3970
E	0.6429	0.2600
F	0.8571	0.4420