Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 12:46 AM JST

PDB ID	:	7W9T
EMDB ID	:	EMD-32372
Title	:	Cryo-EM structure of human Nav1.7(E406K) in complex with auxiliary beta subunits, huwentoxin-IV and saxitoxin (S6IV alpha helix conformer)
Authors	:	Yan, N.; Huang, G.; Liu, D.; Wei, P.
Deposited on	:	2021-12-10
Resolution	:	3.00 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:

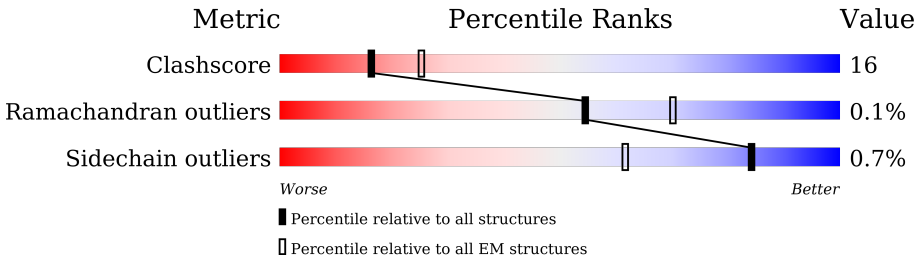
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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	25% 50% 20% 30%
2	B	218	8% 56% 22% • 21%
3	C	215	48% 51% 5% 45%
4	D	2	50% 100%
4	E	2	50% 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
11	PCW	A	2013	-	-	X	-
6	NAG	A	2008	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 14841 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	1417	11419	7539	1798	1997	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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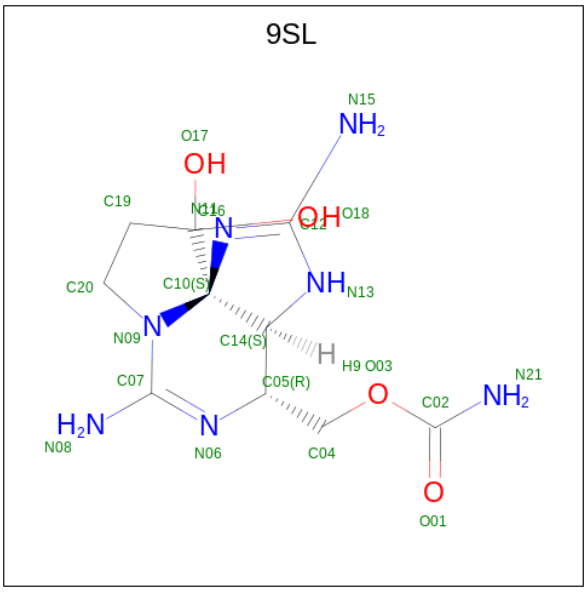
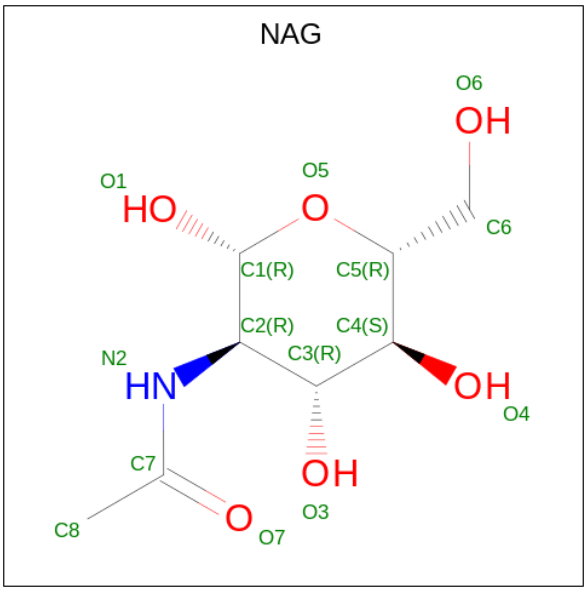
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is [(3aS,4R,10aS)-2,6-diamino-10,10-dihydroxy-3a,4,9,10-tetrahydro-3H,8H-pyrrolo[1,2-c]purin-4-yl]methyl carbamate (three-letter code: 9SL) (formula: $C_{10}H_{17}N_7O_4$) (labeled as "Ligand of Interest" by depositor).



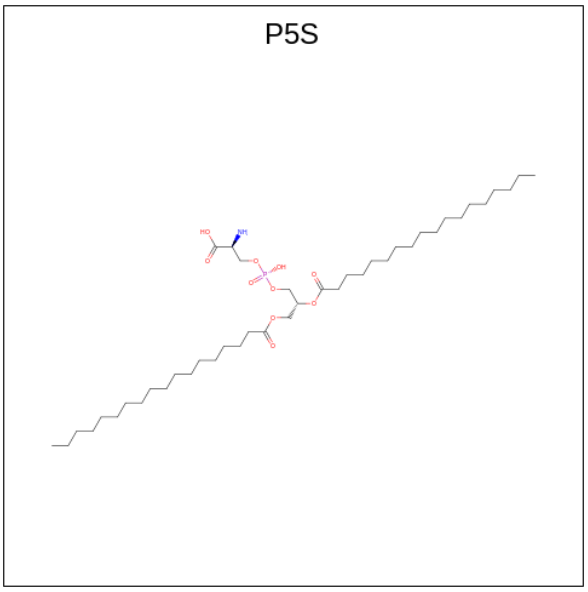
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			21	10	7	4	

- Molecule 6 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).



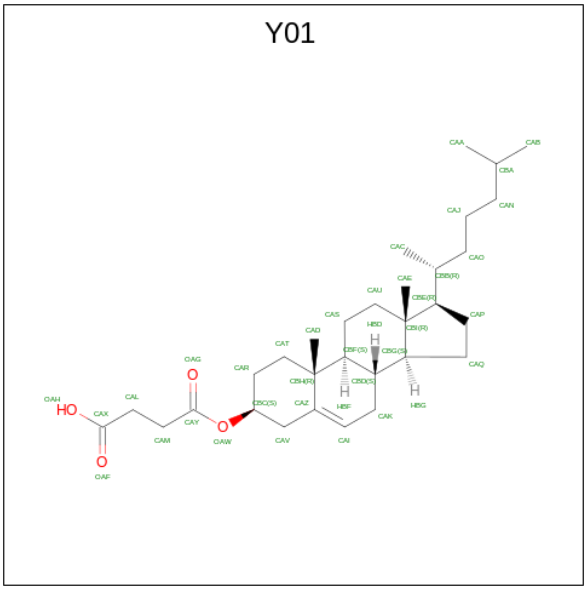
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			28	16	2	10	
6	A	1	Total	C	N	O	0
			28	16	2	10	
6	B	1	Total	C	N	O	0
			42	24	3	15	
6	B	1	Total	C	N	O	0
			42	24	3	15	
6	B	1	Total	C	N	O	0
			42	24	3	15	

- Molecule 7 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
7	A	1	Total	C	N	O	P	0
			76	55	2	17	2	
7	A	1	Total	C	N	O	P	0
			76	55	2	17	2	

- Molecule 8 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			175	155	20	
8	A	1	Total	C	O	0
			175	155	20	

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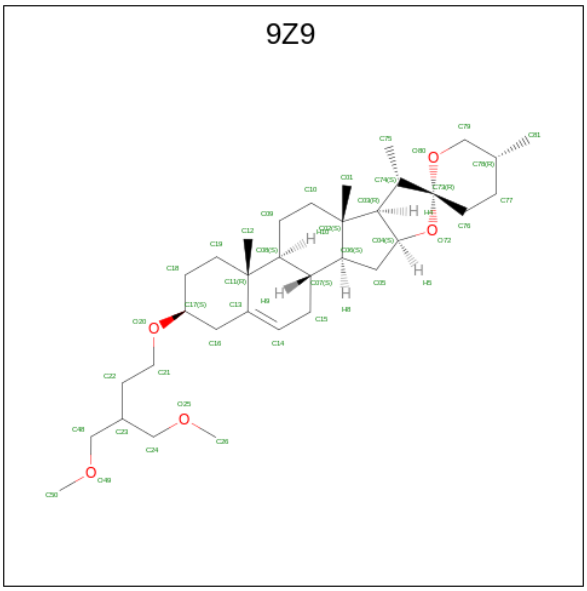
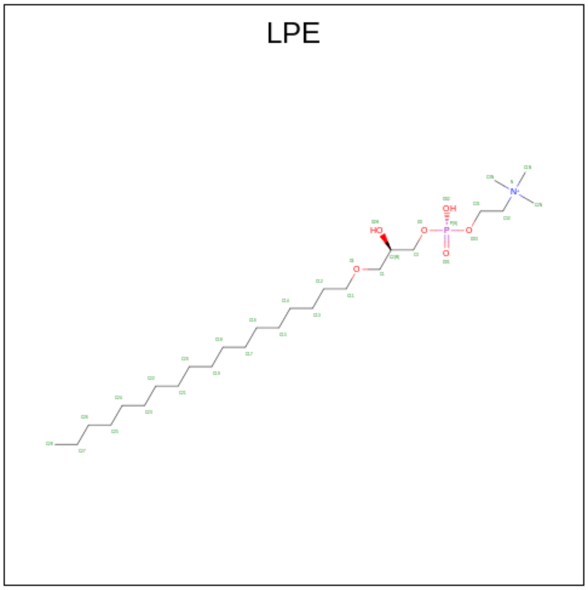
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total 175	C 155	O 20	0
8	A	1	Total 175	C 155	O 20	0
8	A	1	Total 175	C 155	O 20	0

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



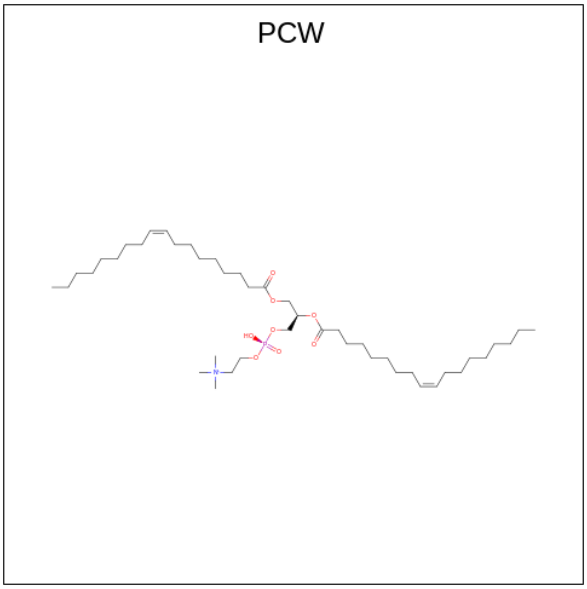
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total 39	C 34	O 5	0

- Molecule 10 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula: $C_{26}H_{57}NO_6P$).



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

- Molecule 11 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



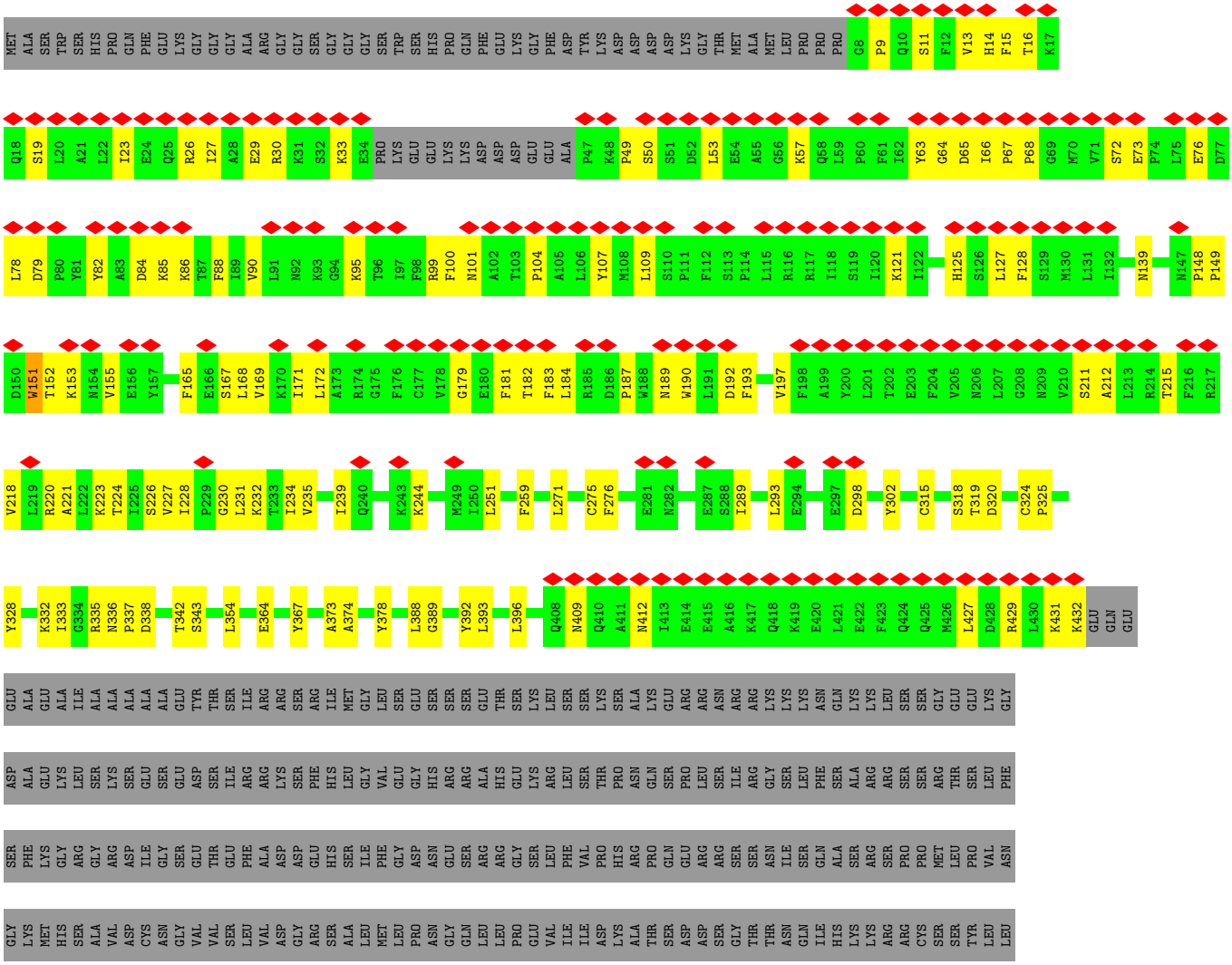
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
11	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
11	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
11	A	1	Total	C	N	O	P	0
			232	182	5	40	5	
11	A	1	Total	C	N	O	P	0
			232	182	5	40	5	

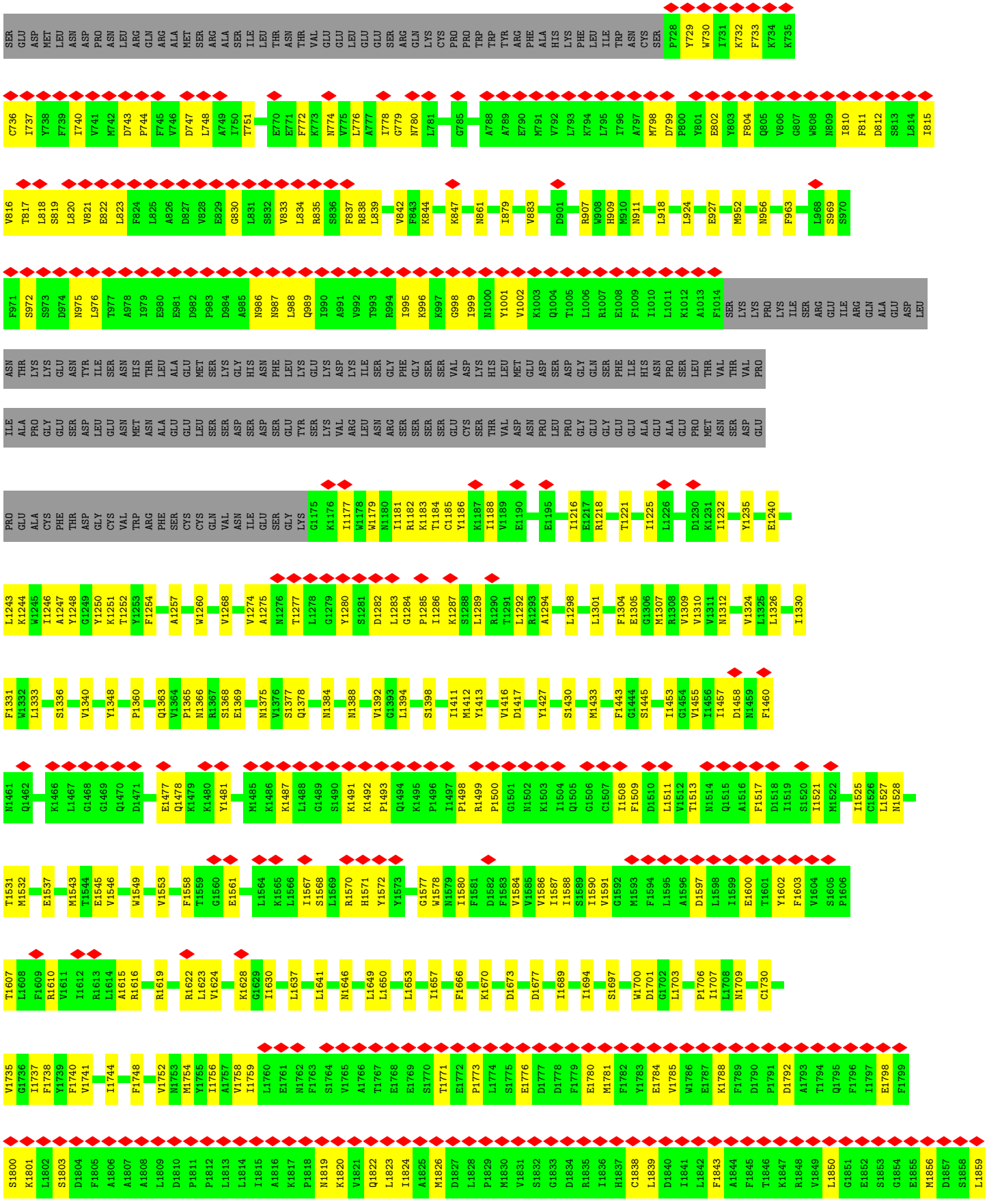
3 Residue-property plots (i)

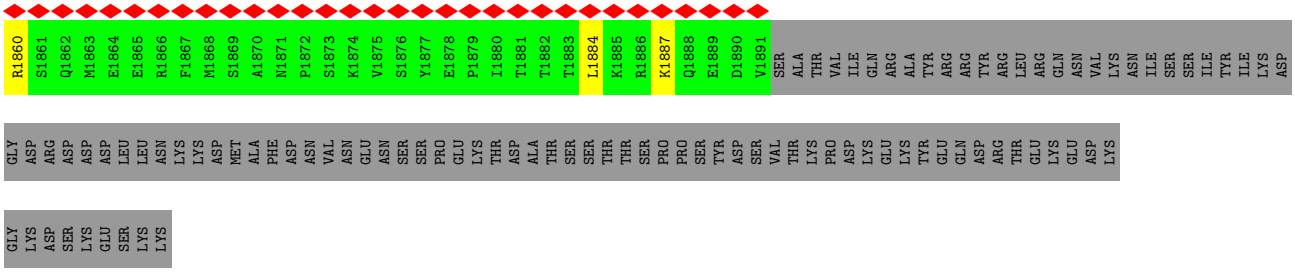
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

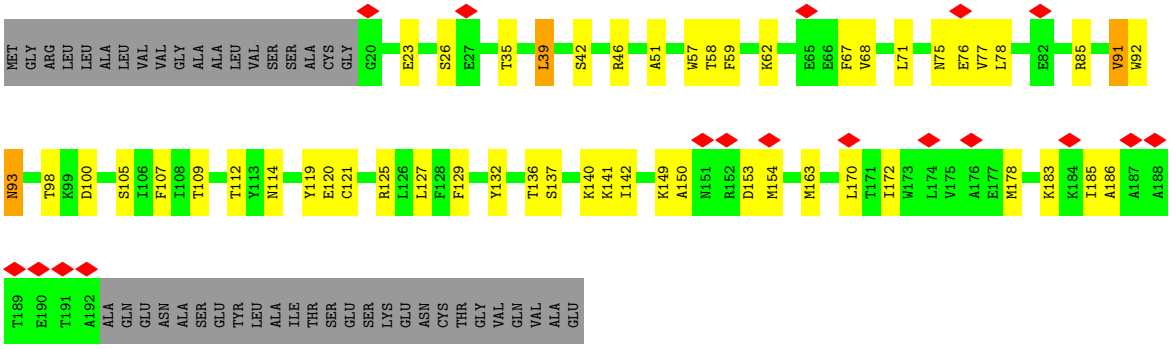



SER GLU ASP MET LEU ASN ASP PRO ASN LEU ARG GLN ARG ALA MET SER ARG ALA SER ILE LEU THR ASN THR VAL GLU GLU LEU GLU GLU SER ARG GLN LYS CYS PRO PRO TRP TRP TYR ARG PHE ALA HIS LYS PHE LEU ILE TRP ASN CYS SER P728 Y729 W730 I731 K732 F733 K734 K735
C736 I737 Y738 F739 I740 V741 M742 D743 P744 F745 V746 D747 L748 A749 T750 T751 E770 E771 F772 K773 N774 V775 L776 A777 L778 G779 N780 L781 G785 A788 A789 E790 M791 V792 L793 K794 L795 I796 A797 M798 D799 P800 Y801 E802 Y803 F804 Q805 V806 G807 W808 N809 I810 F811 D812 S813 L814 I815
V816 T817 L818 S819 L820 V821 E822 L823 F824 L825 A826 D827 V828 E829 G830 L831 S832 V833 L834 R835 S836 F837 R838 L839 V842 F843 K844 K847 N861 I879 V883 D901 R907 W908 H909 M910 N911 L918 L924 E927 M952 N956 F963 L968 S969 S970
P971 S972 S973 D974 N975 L976 T977 A978 I979 E980 E981 D982 P983 D984 A985 N986 N987 L988 Q989 T990 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 GLU LEU SER SER SER ASP ASP SER GLU TYR SER LYS VAL ARG LEU ASN ARG SER 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 K1176 I1177 W1178 W1179 N1180 I1181 R1182 K1183 T1184 C1185 Y1186 K1187 I1188 V1189 E1190 E1195 I1216 E1217 R1218 T1221 I1225 L1226 D1230 K1231 I1232 Y1235 E1240
L1243 K1244 W1245 I1246 A1247 Y1248 G1249 Y1250 K1251 T1252 Y1253 F1254 A1257 W1260 V1268 V1274 A1275 N1276 T1277 L1278 G1279 Y1280 S1281 D1282 L1283 G1284 P1285 I1286 K1287 S1288 L1289 R1290 T1291 L1292 R1293 A1294 L1298 L1301 F1304 E1305 G1306 M1307 R1308 V1309 V1310 V1311 N1312 V1324 L1325 L1326 I1330
F1331 W1332 L1333 S1336 V1340 Y1348 P1360 Q1363 V1364 P1365 N1366 R1367 S1368 E1369 N1375 V1376 S1377 Q1378 N1384 N1388 V1392 G1393 L1394 S1398 I1411 M1412 Y1413 V1416 D1417 Y1427 S1430 M1433 F1443 G1444 S1445 I1453 G1454 V1455 I1456 I1457 D1458 N1459 F1460
N1461 Q1462 K1466 L1467 G1468 G1469 Q1470 D1471 E1477 Q1478 K1479 K1480 Y1481 M1485 K1486 K1487 L1488 G1489 S1490 K1491 K1492 P1493 Q1494 K1495 P1496 I1497 P1498 R1499 P1500 G1501 N1502 K1503 I1504 Q1505 G1506 C1507 I1508 F1509 D1510 L1511 V1512 T1513 N1514 Q1515 A1516 F1517 D1518 I1519 S1520 I1521 M1522 I1525 C1526 L1527 N1528
T1531 M1532 E1537 M1543 T1544 E1545 V1546 W1549 V1553 F1558 T1559 G1560 E1561 L1564 K1565 L1566 I1567 S1568 L1569 R1570 H1571 Y1572 Y1573 G1577 W1578 N1579 I1580 F1581 D1582 F1583 V1584 V1585 V1586 I1587 I1588 S1589 I1590 V1591 G1592 M1593 F1594 L1595 A1596 D1597 L1598 I1599 E1600 T1601 Y1602 F1603 V1604 S1605 P1606
T1607 L1608 F1609 R1610 V1611 I1612 R1613 L1614 A1615 R1616 R1619 R1622 L1623 V1624 K1628 G1629 I1630 L1637 L1641 N1646 L1649 L1650 L1653 I1657 F1666 K1670 D1673 D1677 I1689 I1694 S1697 W1700 D1701 G1702 L1703 P1706 I1707 L1708 N1709 C1730
V1735 G1736 I1737 F1738 Y1739 F1740 V1741 I1744 F1748 V1752 N1753 M1754 Y1755 I1756 A1757 V1758 I1759 L1760 E1761 N1762 F1763 S1764 V1765 A1766 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



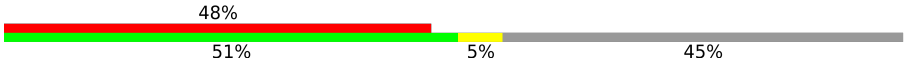
• Molecule 2: Sodium channel subunit beta-1

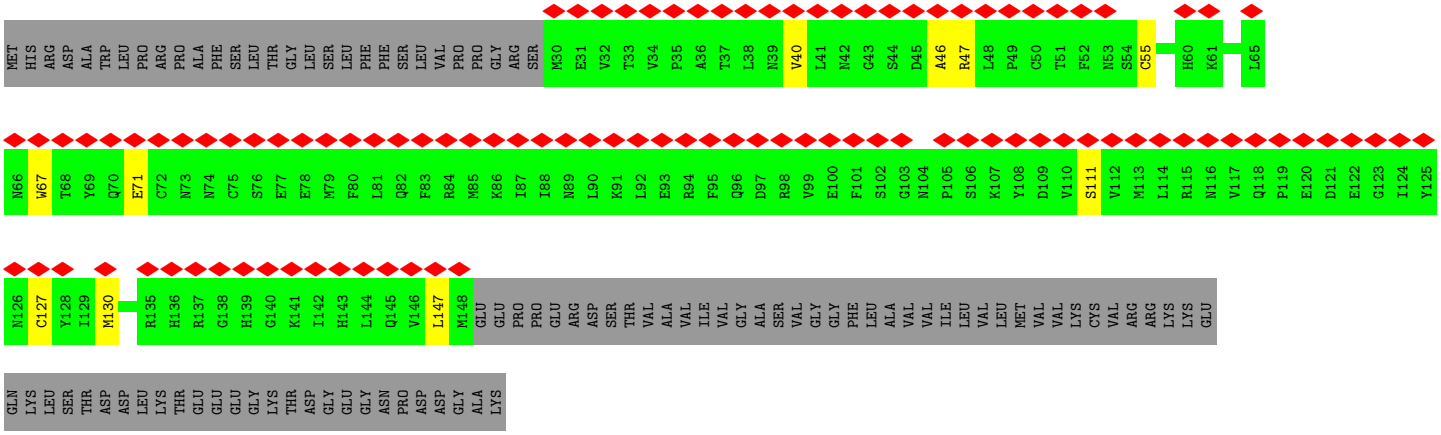
Chain B:



• Molecule 3: Sodium channel subunit beta-2

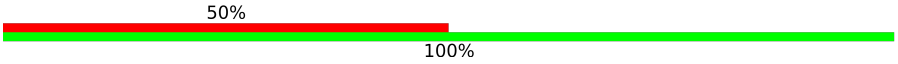
Chain C:





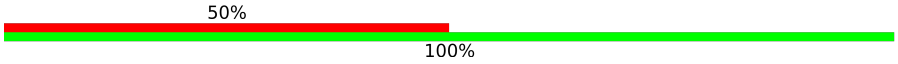
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



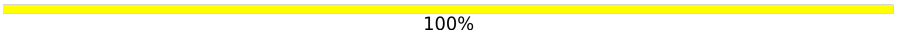
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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	165021	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	2.876	Depositor
Minimum map value	-1.308	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.098	Depositor
Recommended contour level	0.63	Depositor
Map size (Å)	261.84, 261.84, 261.84	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.41	0/11693	0.52	1/15834 (0.0%)
2	B	0.41	0/1442	0.50	0/1949
3	C	0.36	0/1011	0.58	0/1367
All	All	0.40	0/14146	0.53	1/19150 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	275	CYS	CA-CB-SG	5.84	124.52	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11419	0	11645	357	0
2	B	1416	0	1380	45	0
3	C	980	0	935	3	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
5	A	21	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	28	0	26	9	0
6	B	42	0	39	0	0
7	A	76	0	96	21	0
8	A	175	0	245	48	0
9	A	39	0	0	9	0
10	A	312	0	426	79	0
10	B	17	0	19	10	0
11	A	232	0	321	35	0
All	All	14841	0	15207	473	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 16.

All (473) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1602:TYR:CE2	1:A:1603:PHE:CE1	1.76	1.65
1:A:1602:TYR:CE2	1:A:1603:PHE:HE1	1.04	1.64
1:A:1602:TYR:CD2	1:A:1603:PHE:CE1	1.92	1.53
1:A:1602:TYR:CD2	1:A:1603:PHE:CD1	2.18	1.28
1:A:1602:TYR:HD2	1:A:1603:PHE:CD1	1.52	1.26
2:B:178:MET:CE	10:B:304:LPE:H12	1.70	1.21
1:A:1738:PHE:CD2	10:A:2014:LPE:H1N2	1.75	1.20
1:A:1330:ILE:CD1	8:A:2006:Y01:HAB2	1.71	1.18
1:A:1738:PHE:CE2	10:A:2014:LPE:H1N2	1.81	1.15
1:A:1330:ILE:HD12	8:A:2006:Y01:HAB2	1.34	1.09
1:A:963:PHE:CE1	9:A:2007:9Z9:C77	2.37	1.08
1:A:1257:ALA:CB	10:A:2015:LPE:H31	1.84	1.07
1:A:1330:ILE:HD12	8:A:2006:Y01:CAB	1.85	1.07
2:B:178:MET:HE3	10:B:304:LPE:C1	1.86	1.04
11:A:2013:PCW:C37	8:A:2029:Y01:HAQ1	1.89	1.02
1:A:1602:TYR:HE2	1:A:1603:PHE:CE1	1.30	1.02
2:B:178:MET:CE	10:B:304:LPE:C1	2.37	1.02
1:A:1375:ASN:ND2	6:A:2008:NAG:C2	2.23	1.00
11:A:2013:PCW:H371	8:A:2029:Y01:HAQ1	1.45	0.99
11:A:2013:PCW:C37	8:A:2029:Y01:CAQ	2.45	0.94
1:A:1307:MET:CE	10:A:2023:LPE:C19	2.46	0.93
2:B:178:MET:HE3	10:B:304:LPE:H12	0.95	0.93
1:A:1375:ASN:CG	6:A:2008:NAG:C1	2.36	0.92
10:A:2021:LPE:H1N3	10:A:2022:LPE:O32	1.70	0.92
1:A:1301:LEU:HD11	10:A:2014:LPE:H151	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2012:LPE:H1N1	11:A:2013:PCW:C8	2.04	0.88
1:A:1738:PHE:CE2	10:A:2014:LPE:C1N	2.56	0.88
1:A:1307:MET:HE1	10:A:2023:LPE:C19	2.04	0.88
1:A:1457:ILE:HD13	9:A:2007:9Z9:C12	2.04	0.87
1:A:364:GLU:OE2	5:A:2001:9SL:N11	2.07	0.86
1:A:1624:VAL:HG21	7:A:2017:P5S:H29A	1.57	0.85
1:A:1179:TRP:CZ3	10:A:2025:LPE:H321	2.13	0.84
1:A:1324:VAL:HG21	1:A:1455:VAL:HG21	1.57	0.84
1:A:1653:LEU:HD23	10:A:2014:LPE:C16	2.07	0.84
1:A:1257:ALA:HB1	10:A:2015:LPE:H31	1.60	0.83
1:A:1307:MET:HE3	10:A:2023:LPE:C19	2.08	0.83
10:A:2012:LPE:H1N1	11:A:2013:PCW:H83	1.59	0.82
1:A:1735:VAL:HG23	10:A:2014:LPE:H2N1	1.62	0.82
1:A:1301:LEU:HD11	10:A:2014:LPE:C15	2.10	0.81
1:A:1457:ILE:CD1	9:A:2007:9Z9:C12	2.59	0.80
1:A:1477:GLU:HG3	10:A:2019:LPE:H1N1	1.65	0.79
2:B:178:MET:HE1	10:B:304:LPE:C1	2.11	0.78
1:A:1578:TRP:CH2	7:A:2017:P5S:H26	2.19	0.77
1:A:1330:ILE:CD1	8:A:2006:Y01:CAB	2.52	0.77
1:A:963:PHE:HE1	9:A:2007:9Z9:C77	1.95	0.76
1:A:1375:ASN:O	6:A:2008:NAG:H82	1.85	0.76
1:A:1738:PHE:HD2	10:A:2014:LPE:H1N2	1.43	0.75
11:A:2013:PCW:H372	8:A:2029:Y01:CAQ	2.16	0.75
1:A:1508:ILE:HA	1:A:1511:LEU:HD12	1.69	0.74
2:B:178:MET:HE1	10:B:304:LPE:O2H	1.88	0.74
1:A:1735:VAL:CG2	10:A:2014:LPE:H2N1	2.18	0.74
11:A:2013:PCW:H381	8:A:2029:Y01:HAQ2	1.71	0.73
1:A:1384:ASN:OD1	1:A:1388:ASN:ND2	2.22	0.72
1:A:1781:MET:HA	1:A:1784:GLU:HG2	1.69	0.72
10:A:2021:LPE:C32	10:A:2022:LPE:H31	2.19	0.72
1:A:1477:GLU:HG3	10:A:2019:LPE:C1N	2.20	0.72
1:A:1785:VAL:HA	1:A:1788:LYS:HD2	1.72	0.72
1:A:1282:ASP:HA	1:A:1287:LYS:HG3	1.70	0.71
1:A:1738:PHE:HE2	10:A:2014:LPE:C1N	2.02	0.71
11:A:2013:PCW:H381	8:A:2029:Y01:CAQ	2.21	0.71
1:A:1477:GLU:CG	10:A:2019:LPE:H1N1	2.21	0.70
1:A:1257:ALA:HB3	10:A:2015:LPE:H31	1.71	0.69
1:A:1330:ILE:HD12	8:A:2006:Y01:CAA	2.22	0.69
1:A:1578:TRP:CH2	7:A:2017:P5S:C26	2.75	0.69
11:A:2013:PCW:H372	8:A:2029:Y01:HAQ1	1.71	0.68
11:A:2013:PCW:C38	8:A:2029:Y01:CAQ	2.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:HIS:HD2	1:A:911:ASN:H	1.43	0.67
7:A:2003:P5S:H54A	10:A:2025:LPE:H171	1.76	0.67
10:A:2021:LPE:H321	10:A:2022:LPE:H31	1.77	0.67
1:A:1677:ASP:OD2	2:B:46:ARG:NH2	2.27	0.67
1:A:1558:PHE:O	1:A:1561:GLU:HG2	1.95	0.66
1:A:1653:LEU:CD2	10:A:2014:LPE:C16	2.74	0.66
10:A:2012:LPE:H1N1	11:A:2013:PCW:H82	1.77	0.66
1:A:9:PRO:HA	1:A:63:TYR:HA	1.78	0.66
1:A:1251:LYS:CE	10:A:2026:LPE:H312	2.26	0.65
11:A:2013:PCW:C37	8:A:2029:Y01:HAQ2	2.27	0.65
1:A:293:LEU:HD22	1:A:298:ASP:HB3	1.79	0.65
1:A:1366:ASN:OD1	1:A:1368:SER:OG	2.11	0.64
1:A:1330:ILE:HD13	8:A:2006:Y01:HAB2	1.74	0.64
1:A:64:GLY:O	1:A:95:LYS:NZ	2.30	0.64
1:A:1602:TYR:CE2	1:A:1603:PHE:CZ	2.73	0.64
1:A:1375:ASN:OD1	6:A:2008:NAG:C1	2.46	0.64
1:A:1330:ILE:HD11	8:A:2006:Y01:HAJ1	1.80	0.63
1:A:1179:TRP:CZ3	10:A:2025:LPE:C32	2.81	0.63
1:A:324:CYS:SG	1:A:328:TYR:HB2	2.38	0.63
2:B:51:ALA:HB2	2:B:127:LEU:HD13	1.80	0.63
1:A:230:GLY:O	1:A:234:ILE:HG12	1.99	0.62
1:A:1759:ILE:CD1	9:A:2007:9Z9:C03	2.78	0.62
1:A:927:GLU:OE2	5:A:2001:9SL:C04	2.48	0.62
1:A:1298:LEU:CD2	10:A:2014:LPE:H151	2.30	0.62
1:A:1330:ILE:HD12	8:A:2006:Y01:HAA3	1.82	0.62
10:A:2021:LPE:H321	10:A:2022:LPE:O32	1.99	0.62
11:A:2013:PCW:C38	8:A:2029:Y01:HAQ2	2.30	0.61
1:A:1257:ALA:CB	10:A:2015:LPE:C3	2.72	0.61
2:B:178:MET:CE	10:B:304:LPE:O2H	2.48	0.61
1:A:816:VAL:O	1:A:820:LEU:HG	2.01	0.60
1:A:388:LEU:HD11	7:A:2017:P5S:H34	1.83	0.60
1:A:99:ARG:HG2	1:A:181:PHE:CE2	2.36	0.60
8:A:2009:Y01:HAC1	8:A:2009:Y01:HAE2	1.83	0.60
1:A:1218:ARG:NH2	2:B:23:GLU:O	2.28	0.60
1:A:1578:TRP:CZ3	7:A:2017:P5S:H26	2.36	0.60
8:A:2004:Y01:HAC1	8:A:2004:Y01:HAE2	1.84	0.60
8:A:2005:Y01:HAE2	8:A:2005:Y01:HAC1	1.83	0.60
1:A:1375:ASN:ND2	6:A:2008:NAG:H2	2.16	0.60
1:A:1375:ASN:HD22	6:A:2008:NAG:C7	2.15	0.60
1:A:730:TRP:HA	1:A:733:PHE:CZ	2.36	0.59
1:A:65:ASP:OD1	1:A:66:ILE:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PRO:HB2	1:A:151:TRP:HD1	1.67	0.59
1:A:1250:TYR:H	7:A:2003:P5S:H45	1.67	0.59
8:A:2006:Y01:HAC1	8:A:2006:Y01:HAE2	1.83	0.59
1:A:27:ILE:HA	1:A:30:ARG:HD2	1.84	0.59
2:B:129:PHE:HB2	2:B:132:TYR:HB3	1.84	0.59
1:A:183:PHE:HD2	1:A:184:LEU:HD22	1.68	0.59
1:A:1257:ALA:HB3	10:A:2015:LPE:C3	2.32	0.59
1:A:1577:GLY:H	11:A:2018:PCW:H51	1.68	0.58
1:A:1673:ASP:OD1	1:A:1673:ASP:O	2.21	0.58
11:A:2013:PCW:H381	8:A:2029:Y01:CAP	2.33	0.58
11:A:2018:PCW:H19	11:A:2027:PCW:H261	1.85	0.58
2:B:136:THR:HG22	2:B:137:SER:H	1.68	0.58
2:B:91:VAL:HG23	2:B:107:PHE:HB3	1.85	0.58
1:A:1304:PHE:CE2	10:A:2023:LPE:C19	2.87	0.58
11:A:2013:PCW:H371	8:A:2029:Y01:CAQ	2.21	0.58
1:A:1513:THR:HG22	1:A:1513:THR:O	2.02	0.58
11:A:2013:PCW:H372	8:A:2029:Y01:HAQ2	1.83	0.58
1:A:1641:LEU:HB3	10:A:2019:LPE:H11	1.85	0.57
1:A:1771:THR:HG23	1:A:1773:PRO:HD3	1.85	0.57
1:A:1850:LEU:HD23	1:A:1856:MET:HG2	1.86	0.57
1:A:86:LYS:NZ	1:A:86:LYS:H	2.01	0.57
1:A:1430:SER:HB3	1:A:1433:MET:HG2	1.86	0.57
7:A:2003:P5S:H42	10:A:2026:LPE:O32	2.05	0.57
2:B:23:GLU:OE1	2:B:140:LYS:NZ	2.37	0.57
1:A:388:LEU:O	1:A:392:TYR:HB3	2.04	0.57
7:A:2017:P5S:C35	7:A:2017:P5S:C46	2.83	0.57
1:A:179:GLY:H	1:A:182:THR:HG21	1.69	0.57
1:A:834:LEU:HD21	1:A:835:ARG:HH11	1.69	0.57
10:A:2010:LPE:O32	10:A:2012:LPE:H3N1	2.05	0.56
1:A:1331:PHE:CZ	1:A:1443:PHE:HB3	2.40	0.56
1:A:1375:ASN:ND2	6:A:2008:NAG:C7	2.68	0.56
1:A:318:SER:OG	1:A:319:THR:N	2.39	0.56
1:A:1607:THR:HA	1:A:1610:ARG:HH11	1.71	0.56
1:A:1348:TYR:CE2	1:A:1384:ASN:HB2	2.41	0.56
7:A:2003:P5S:H46	10:A:2025:LPE:H11	1.88	0.56
10:A:2011:LPE:H21	11:A:2013:PCW:H131	1.88	0.56
1:A:1628:LYS:NZ	7:A:2017:P5S:O13	2.33	0.56
2:B:153:ASP:OD1	2:B:154:MET:N	2.40	0.55
1:A:1521:ILE:HD12	1:A:1561:GLU:OE2	2.05	0.55
1:A:1251:LYS:HE2	10:A:2026:LPE:C31	2.36	0.55
1:A:1304:PHE:HE2	10:A:2023:LPE:C19	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1602:TYR:CE2	1:A:1603:PHE:CD1	2.62	0.55
1:A:223:LYS:O	1:A:227:VAL:HG22	2.06	0.54
2:B:57:TRP:HB2	2:B:71:LEU:HG	1.89	0.54
2:B:93:ASN:HB3	2:B:105:SER:OG	2.07	0.54
2:B:98:THR:C	2:B:100:ASP:H	2.09	0.54
1:A:226:SER:HA	1:A:232:LYS:HE2	1.90	0.54
1:A:1307:MET:HE1	10:A:2023:LPE:C18	2.37	0.54
1:A:1824:ILE:HG21	1:A:1887:LYS:HD3	1.89	0.54
1:A:1457:ILE:HD12	9:A:2007:9Z9:C12	2.36	0.54
1:A:1184:THR:O	1:A:1188:ILE:HG12	2.08	0.53
1:A:737:ILE:HA	1:A:740:ILE:HB	1.89	0.53
1:A:1375:ASN:OD1	6:A:2008:NAG:O5	2.27	0.53
2:B:178:MET:CE	10:B:304:LPE:C2	2.87	0.53
1:A:812:ASP:OD1	1:A:844:LYS:NZ	2.31	0.53
1:A:998:GLY:O	1:A:1002:VAL:HG23	2.08	0.53
1:A:1491:LYS:NZ	11:A:2027:PCW:H72	2.22	0.53
1:A:1737:ILE:O	1:A:1741:VAL:HG12	2.07	0.53
1:A:1580:ILE:O	1:A:1584:VAL:HG23	2.09	0.53
1:A:335:ARG:NH1	1:A:336:ASN:O	2.40	0.53
1:A:1250:TYR:OH	10:A:2025:LPE:H172	2.09	0.53
1:A:1478:GLN:HG2	10:A:2019:LPE:H311	1.90	0.53
1:A:1602:TYR:HD2	1:A:1603:PHE:CE1	1.63	0.53
10:A:2021:LPE:C3N	10:A:2022:LPE:H31	2.39	0.52
1:A:1331:PHE:HZ	1:A:1443:PHE:HB3	1.72	0.52
10:A:2012:LPE:C1N	11:A:2013:PCW:H82	2.39	0.52
7:A:2003:P5S:H42	10:A:2026:LPE:P	2.49	0.52
1:A:778:ILE:HG13	1:A:779:GLY:N	2.24	0.52
1:A:861:ASN:ND2	1:A:969:SER:OG	2.43	0.52
1:A:1567:ILE:HD12	1:A:1568:SER:N	2.25	0.52
1:A:1588:ILE:HG22	1:A:1615:ALA:HB1	1.91	0.52
1:A:1179:TRP:HZ3	10:A:2025:LPE:H321	1.68	0.52
1:A:1298:LEU:HD23	10:A:2014:LPE:C16	2.40	0.52
1:A:1251:LYS:HZ1	10:A:2026:LPE:H3N2	1.75	0.52
1:A:1577:GLY:HA2	1:A:1580:ILE:HD12	1.91	0.52
10:A:2010:LPE:O32	10:A:2012:LPE:C3N	2.58	0.52
1:A:149:PRO:HB2	1:A:151:TRP:CD1	2.44	0.52
1:A:1499:ARG:HD2	1:A:1500:PRO:HD2	1.92	0.52
1:A:804:PHE:O	1:A:810:ILE:HD11	2.10	0.51
1:A:1294:ALA:O	1:A:1657:ILE:HG23	2.10	0.51
8:A:2004:Y01:HAE2	8:A:2004:Y01:CAC	2.41	0.51
1:A:101:ASN:OD1	1:A:101:ASN:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:ARG:NH2	3:C:111[B]:SER:OG	2.43	0.51
1:A:729:TYR:HA	1:A:732:LYS:HD2	1.93	0.51
1:A:1838:CYS:SG	1:A:1839:LEU:N	2.84	0.51
1:A:151:TRP:O	1:A:155:VAL:HG23	2.11	0.51
1:A:1377:SER:OG	1:A:1378:GLN:N	2.44	0.51
1:A:165:PHE:O	1:A:169:VAL:HG23	2.11	0.51
1:A:1365:PRO:HD2	1:A:1369:GLU:HG3	1.92	0.51
1:A:324:CYS:SG	1:A:325:PRO:HD2	2.51	0.51
1:A:1330:ILE:CD1	8:A:2006:Y01:HAA3	2.41	0.50
1:A:86:LYS:H	1:A:86:LYS:HZ2	1.59	0.50
1:A:1250:TYR:HD2	7:A:2003:P5S:H45A	1.77	0.50
1:A:1624:VAL:HG21	7:A:2017:P5S:C29	2.33	0.50
1:A:1570:ARG:HG3	1:A:1571:HIS:H	1.75	0.50
1:A:72:SER:OG	1:A:121:LYS:HE3	2.10	0.50
1:A:834:LEU:O	1:A:838:ARG:HG2	2.12	0.50
1:A:1301:LEU:HD11	10:A:2014:LPE:H152	1.92	0.50
1:A:1417:ASP:OD1	1:A:1427:TYR:HA	2.12	0.50
1:A:211:SER:O	1:A:215:THR:HG23	2.12	0.50
1:A:1251:LYS:HZ3	10:A:2026:LPE:H1N3	1.76	0.50
7:A:2003:P5S:H50	10:A:2025:LPE:H122	1.94	0.50
8:A:2006:Y01:HAE2	8:A:2006:Y01:CAC	2.41	0.50
10:A:2012:LPE:C1N	11:A:2013:PCW:C8	2.86	0.50
1:A:167:SER:O	1:A:171:ILE:HG13	2.12	0.49
1:A:811:PHE:CZ	1:A:815:ILE:HD11	2.47	0.49
1:A:995:ILE:O	1:A:999:ILE:HG12	2.12	0.49
2:B:178:MET:HE1	10:B:304:LPE:C2	2.42	0.49
1:A:1235:TYR:HE2	2:B:170:LEU:HD11	1.77	0.49
1:A:1250:TYR:CE2	7:A:2003:P5S:H49	2.47	0.49
1:A:1307:MET:HE1	10:A:2023:LPE:H182	1.93	0.49
1:A:50:SER:N	1:A:79:ASP:OD2	2.43	0.49
2:B:78:LEU:HD12	2:B:92:TRP:HB2	1.94	0.49
10:A:2021:LPE:H3N2	10:A:2022:LPE:H31	1.94	0.49
1:A:1738:PHE:HE2	10:A:2014:LPE:H1N3	1.78	0.49
1:A:221:ALA:O	1:A:224:THR:OG1	2.28	0.49
7:A:2003:P5S:H46	10:A:2025:LPE:C1	2.42	0.48
1:A:1453:ILE:HG21	9:A:2007:9Z9:C76	2.43	0.48
2:B:185:ILE:HG13	2:B:186:ALA:N	2.28	0.48
1:A:1330:ILE:HD12	8:A:2006:Y01:CBA	2.41	0.48
1:A:1179:TRP:CD1	1:A:1183:LYS:HE2	2.48	0.48
8:A:2029:Y01:HAE2	8:A:2029:Y01:HBB	1.60	0.48
1:A:1584:VAL:O	1:A:1588:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1491:LYS:C	1:A:1493:PRO:HD3	2.34	0.48
1:A:1549:TRP:O	1:A:1553:VAL:HG23	2.12	0.48
1:A:73:GLU:H	1:A:90:VAL:HG23	1.77	0.48
1:A:812:ASP:O	1:A:816:VAL:HG23	2.13	0.48
1:A:1310:VAL:HG23	1:A:1650:LEU:HD22	1.95	0.48
1:A:1653:LEU:HD13	10:A:2023:LPE:H182	1.95	0.48
8:A:2005:Y01:HAC1	8:A:2005:Y01:HAU2	1.96	0.48
1:A:1185:CYS:SG	1:A:1246:ILE:HG21	2.54	0.48
1:A:1333:LEU:HD22	8:A:2029:Y01:HAA1	1.95	0.48
11:A:2018:PCW:C19	11:A:2027:PCW:H261	2.44	0.48
1:A:1525:ILE:HD13	1:A:1622:ARG:HB2	1.95	0.48
1:A:1752:VAL:O	1:A:1756:ILE:HG12	2.13	0.48
8:A:2004:Y01:HAC1	8:A:2004:Y01:HAU2	1.96	0.48
1:A:276:PHE:CE1	1:A:302:TYR:HB3	2.49	0.48
8:A:2009:Y01:OAG	8:A:2009:Y01:HAV2	2.14	0.48
1:A:364:GLU:OE2	5:A:2001:9SL:C12	2.61	0.47
1:A:1251:LYS:CE	10:A:2026:LPE:C31	2.92	0.47
1:A:392:TYR:CZ	1:A:1637:LEU:HB2	2.50	0.47
2:B:178:MET:HE1	10:B:304:LPE:O1	2.12	0.47
8:A:2006:Y01:HAC1	8:A:2006:Y01:HAU2	1.96	0.47
11:A:2018:PCW:H31	11:A:2027:PCW:H31	1.95	0.47
1:A:228:ILE:HD12	1:A:231:LEU:HD22	1.95	0.47
1:A:90:VAL:HG12	1:A:100:PHE:HE2	1.79	0.47
1:A:1289:LEU:HD13	1:A:1292:LEU:HD12	1.96	0.47
8:A:2006:Y01:HAV2	8:A:2006:Y01:OAG	2.14	0.47
8:A:2009:Y01:HAC1	8:A:2009:Y01:HAU2	1.96	0.47
11:A:2018:PCW:H31	11:A:2027:PCW:C3	2.45	0.47
1:A:324:CYS:SG	1:A:328:TYR:CB	3.03	0.47
1:A:1478:GLN:HG2	10:A:2019:LPE:C31	2.45	0.47
1:A:1260:TRP:CE3	8:A:2004:Y01:CAE	2.98	0.47
1:A:320:ASP:HB3	10:A:2021:LPE:H1N2	1.97	0.47
7:A:2003:P5S:H43A	10:A:2026:LPE:H12	1.96	0.47
1:A:1392:VAL:HB	8:A:2029:Y01:HBG	1.97	0.46
1:A:747:ASP:OD1	1:A:987:ASN:HB2	2.14	0.46
1:A:1186:TYR:HA	1:A:1247:ALA:HB1	1.97	0.46
1:A:1260:TRP:CE3	8:A:2004:Y01:HAE3	2.50	0.46
1:A:1586:VAL:O	1:A:1590:ILE:HG22	2.15	0.46
1:A:817:THR:O	1:A:821:VAL:HG23	2.15	0.46
1:A:822:GLU:HG2	1:A:834:LEU:HD22	1.95	0.46
1:A:1260:TRP:CZ3	8:A:2004:Y01:HAE3	2.49	0.46
1:A:53:LEU:HD13	1:A:78:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ASP:OD1	1:A:85:LYS:N	2.48	0.46
1:A:271:LEU:HD12	1:A:343:SER:HA	1.97	0.46
1:A:13:VAL:HG23	1:A:76:GLU:HB2	1.97	0.46
1:A:907:ARG:HD2	1:A:1413:TYR:CD1	2.50	0.46
1:A:972:SER:O	1:A:976:LEU:HG	2.16	0.46
1:A:1251:LYS:NZ	10:A:2026:LPE:H1N3	2.31	0.46
1:A:139:ASN:HD21	1:A:220:ARG:HD2	1.81	0.46
1:A:972:SER:HB2	1:A:975:ASN:ND2	2.31	0.46
1:A:1280:TYR:HB3	1:A:1283:LEU:CD1	2.46	0.46
1:A:125:HIS:CE1	1:A:127:LEU:HD23	2.51	0.46
1:A:128:PHE:CG	1:A:128:PHE:O	2.69	0.46
1:A:148:PRO:HB3	1:A:152:THR:HG21	1.97	0.46
1:A:839:LEU:O	1:A:842:VAL:HG23	2.16	0.46
1:A:1677:ASP:OD1	1:A:1677:ASP:N	2.48	0.46
1:A:332:LYS:NZ	1:A:1537:GLU:OE2	2.41	0.46
1:A:798:MET:HG2	1:A:802:GLU:HB2	1.97	0.46
1:A:1243:LEU:HA	1:A:1243:LEU:HD23	1.77	0.46
1:A:1822:GLN:O	1:A:1826:MET:HG3	2.16	0.46
1:A:259:PHE:HZ	1:A:388:LEU:HD13	1.81	0.45
1:A:820:LEU:HA	1:A:823:LEU:HG	1.98	0.45
1:A:1275:ALA:HB1	1:A:1286:ILE:HD13	1.98	0.45
1:A:1491:LYS:HZ1	11:A:2027:PCW:H72	1.81	0.45
1:A:1709:ASN:O	1:A:1730:CYS:HB2	2.17	0.45
2:B:26:SER:HB2	2:B:39:LEU:H	1.80	0.45
1:A:212:ALA:O	1:A:215:THR:OG1	2.29	0.45
1:A:1179:TRP:CH2	10:A:2025:LPE:H321	2.52	0.45
1:A:1232:ILE:HG13	2:B:163:MET:HG3	1.98	0.45
1:A:1298:LEU:CD2	10:A:2014:LPE:C15	2.93	0.45
8:A:2009:Y01:HAE2	8:A:2009:Y01:CAC	2.41	0.45
1:A:811:PHE:O	1:A:815:ILE:HG13	2.16	0.45
1:A:1748:PHE:O	1:A:1752:VAL:HG23	2.16	0.45
1:A:88:PHE:CE1	1:A:100:PHE:HB2	2.52	0.45
1:A:1754:MET:O	1:A:1758:VAL:HG23	2.17	0.45
1:A:374:ALA:HB1	1:A:378:TYR:CD2	2.51	0.45
1:A:963:PHE:CD1	9:A:2007:9Z9:C77	2.97	0.45
1:A:1330:ILE:HD13	8:A:2029:Y01:HAA3	1.97	0.45
1:A:1177:ILE:O	1:A:1181:ILE:HG12	2.17	0.45
2:B:42:SER:O	2:B:42:SER:OG	2.33	0.45
1:A:367:TYR:OH	1:A:1689:ILE:HG23	2.17	0.45
1:A:15:PHE:HA	1:A:76:GLU:HG3	1.99	0.44
1:A:1457:ILE:HG13	1:A:1458:ASP:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1509:PHE:CD2	1:A:1509:PHE:C	2.90	0.44
10:A:2014:LPE:O32	10:A:2015:LPE:H201	2.16	0.44
1:A:168:LEU:O	1:A:172:LEU:HB2	2.17	0.44
1:A:189:ASN:HA	1:A:192:ASP:OD1	2.17	0.44
1:A:1326:LEU:HD23	1:A:1326:LEU:HA	1.79	0.44
2:B:42:SER:OG	2:B:125:ARG:NH2	2.49	0.44
1:A:14:HIS:O	1:A:16:THR:HG23	2.16	0.44
1:A:1375:ASN:O	6:A:2008:NAG:C8	2.59	0.44
2:B:121:CYS:HB3	2:B:140:LYS:HB2	1.99	0.44
1:A:1623:LEU:HD23	1:A:1623:LEU:HA	1.82	0.44
1:A:1697:SER:O	1:A:1700:TRP:HD1	2.00	0.44
1:A:289:ILE:HD13	1:A:289:ILE:HA	1.81	0.44
1:A:338:ASP:HB2	1:A:342:THR:HG22	1.99	0.44
1:A:847:LYS:HD3	1:A:847:LYS:HA	1.72	0.44
11:A:2028:PCW:H322	11:A:2028:PCW:H351	1.81	0.44
8:A:2009:Y01:HAN2	8:A:2009:Y01:HAC3	2.00	0.44
1:A:774:ASN:O	1:A:778:ILE:HG23	2.18	0.44
1:A:1333:LEU:HA	1:A:1336:SER:OG	2.18	0.44
1:A:193:PHE:O	1:A:197:VAL:HG23	2.18	0.44
1:A:1268:VAL:HG13	1:A:1289:LEU:HD12	2.00	0.44
1:A:1792:ASP:N	1:A:1792:ASP:OD2	2.44	0.44
2:B:35:THR:HG22	2:B:109:THR:HA	1.99	0.44
1:A:772:PHE:O	1:A:776:LEU:HG	2.18	0.44
1:A:776:LEU:O	1:A:780:ASN:ND2	2.51	0.44
1:A:988:LEU:C	1:A:988:LEU:HD23	2.38	0.44
1:A:816:VAL:O	1:A:819:SER:OG	2.28	0.43
1:A:986:ASN:O	1:A:989:GLN:N	2.50	0.43
1:A:1216:ILE:HD12	1:A:1216:ILE:HA	1.89	0.43
1:A:1666:PHE:CD1	1:A:1707:ILE:HD13	2.53	0.43
11:A:2013:PCW:H63	11:A:2013:PCW:H41	1.69	0.43
2:B:119:TYR:HB2	2:B:142:ILE:HB	2.00	0.43
1:A:1282:ASP:HA	1:A:1287:LYS:CG	2.43	0.43
1:A:1412:MET:O	1:A:1416:VAL:HG13	2.19	0.43
10:A:2026:LPE:H312	10:A:2026:LPE:H3N2	1.72	0.43
1:A:251:LEU:HB2	1:A:1630:ILE:HD12	1.99	0.43
1:A:1481:TYR:CD2	10:A:2019:LPE:H321	2.53	0.43
1:A:1528:ASN:HD21	1:A:1619:ARG:HH11	1.67	0.43
1:A:1694:ILE:HG21	1:A:1703:LEU:HD12	1.99	0.43
1:A:427:LEU:O	1:A:431:LYS:HG2	2.17	0.43
1:A:830:GLY:O	1:A:833:VAL:HG22	2.18	0.43
1:A:1670:LYS:HB3	1:A:1670:LYS:HE2	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1759:ILE:HD13	9:A:2007:9Z9:C03	2.48	0.43
1:A:19:SER:O	1:A:23:ILE:HG13	2.17	0.43
1:A:23:ILE:HG12	1:A:26:ARG:NH2	2.33	0.43
1:A:139:ASN:ND2	1:A:220:ARG:HD2	2.33	0.43
1:A:244:LYS:HE3	1:A:244:LYS:HB3	1.84	0.43
1:A:1248:TYR:O	1:A:1252:THR:OG1	2.36	0.43
10:A:2019:LPE:H311	10:A:2019:LPE:H2N3	1.61	0.43
1:A:333:ILE:HD12	1:A:333:ILE:HA	1.78	0.43
1:A:1179:TRP:HZ3	10:A:2025:LPE:O31	2.01	0.43
1:A:1517:PHE:O	1:A:1521:ILE:HG12	2.17	0.43
1:A:1707:ILE:HD12	1:A:1740:PHE:HE2	1.84	0.43
1:A:215:THR:O	1:A:218:VAL:HG12	2.19	0.43
10:A:2021:LPE:C1N	10:A:2022:LPE:O32	2.55	0.43
1:A:736:CYS:O	1:A:740:ILE:HG13	2.19	0.43
1:A:1798:GLU:HB3	1:A:1801:LYS:HE2	2.00	0.43
1:A:1824:ILE:HG22	1:A:1884:LEU:HD12	2.01	0.43
8:A:2005:Y01:HAE2	8:A:2005:Y01:CAC	2.41	0.43
1:A:23:ILE:HG21	1:A:86:LYS:HA	2.01	0.42
1:A:918:LEU:HD23	1:A:918:LEU:HA	1.85	0.42
2:B:58:THR:O	2:B:120:GLU:N	2.46	0.42
2:B:178:MET:HE2	2:B:178:MET:HB3	1.83	0.42
1:A:1250:TYR:CE2	7:A:2003:P5S:C49	3.02	0.42
1:A:1250:TYR:HD1	1:A:1254:PHE:HE2	1.67	0.42
2:B:58:THR:CG2	2:B:67:PHE:HB3	2.49	0.42
1:A:153:LYS:HE2	1:A:153:LYS:HB3	1.86	0.42
1:A:389:GLY:O	1:A:393:LEU:HB2	2.19	0.42
1:A:1250:TYR:HE2	10:A:2025:LPE:H152	1.84	0.42
2:B:172:ILE:HD13	2:B:172:ILE:HA	1.86	0.42
1:A:1602:TYR:CD2	1:A:1603:PHE:CZ	2.86	0.42
1:A:57:LYS:HE3	1:A:57:LYS:HB3	1.83	0.42
1:A:396:LEU:HD23	1:A:396:LEU:HA	1.75	0.42
8:A:2006:Y01:HAC3	8:A:2006:Y01:HAN2	2.00	0.42
1:A:14:HIS:HD1	1:A:73:GLU:CD	2.22	0.42
1:A:952:MET:O	1:A:956:ASN:ND2	2.31	0.42
1:A:1221:THR:O	1:A:1225:ILE:HG12	2.19	0.42
1:A:1498:PRO:HG2	1:A:1572:TYR:CZ	2.55	0.42
2:B:59:PHE:HE2	2:B:85:ARG:HH21	1.68	0.42
2:B:119:TYR:O	2:B:141:LYS:HA	2.20	0.42
1:A:743:ASP:N	1:A:744:PRO:HD2	2.35	0.42
1:A:819:SER:O	1:A:823:LEU:HG	2.17	0.42
1:A:1798:GLU:HG2	1:A:1800:SER:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2012:LPE:H1N3	11:A:2013:PCW:O4P	2.20	0.42
1:A:1284:GLY:HA3	1:A:1285:PRO:HD3	1.92	0.41
1:A:1843:PHE:CZ	1:A:1860:ARG:HB2	2.55	0.41
1:A:1856:MET:SD	1:A:1859:LEU:HD21	2.60	0.41
7:A:2003:P5S:H56A	7:A:2003:P5S:H53	1.86	0.41
8:A:2029:Y01:HAP1	8:A:2029:Y01:HAO2	1.36	0.41
1:A:11:SER:OG	1:A:78:LEU:HD11	2.20	0.41
1:A:1336:SER:O	1:A:1340:VAL:HG23	2.20	0.41
1:A:1388:ASN:OD1	1:A:1394:LEU:HD13	2.20	0.41
1:A:1741:VAL:HG13	10:A:2011:LPE:H171	2.02	0.41
2:B:149:LYS:HD2	2:B:149:LYS:HA	1.76	0.41
1:A:171:ILE:HG12	1:A:183:PHE:CD1	2.55	0.41
1:A:799:ASP:HB3	1:A:802:GLU:HG2	2.02	0.41
1:A:1274:VAL:HA	1:A:1277:THR:HG22	2.03	0.41
1:A:1706:PRO:HA	1:A:1709:ASN:HD21	1.85	0.41
3:C:40:VAL:HG11	3:C:46:ALA:HB2	2.03	0.41
1:A:996:LYS:HA	1:A:999:ILE:HG12	2.02	0.41
1:A:1280:TYR:HB3	1:A:1283:LEU:HD12	2.02	0.41
1:A:1543:MET:HA	1:A:1546:VAL:HG22	2.02	0.41
2:B:183:LYS:HD2	2:B:183:LYS:HA	1.87	0.41
1:A:1587:ILE:O	1:A:1591:VAL:HG12	2.21	0.41
1:A:1597:ASP:HA	1:A:1600:GLU:OE1	2.20	0.41
11:A:2027:PCW:H42	11:A:2027:PCW:H63	1.59	0.41
2:B:112:THR:HG23	2:B:114:ASN:H	1.83	0.41
1:A:29:GLU:HB3	1:A:33:LYS:NZ	2.35	0.41
1:A:1301:LEU:HD23	1:A:1301:LEU:HA	1.89	0.41
1:A:49:PRO:HB3	1:A:82:TYR:CE2	2.55	0.41
1:A:1186:TYR:CA	1:A:1247:ALA:HB1	2.51	0.41
1:A:1532:MET:HE2	1:A:1616:ARG:HG3	2.03	0.41
1:A:1740:PHE:O	1:A:1744:ILE:HG23	2.20	0.41
8:A:2006:Y01:HAS2	8:A:2006:Y01:HAE1	1.81	0.41
2:B:58:THR:HG23	2:B:68:VAL:C	2.41	0.41
1:A:67:PRO:HA	1:A:68:PRO:HD3	1.92	0.41
1:A:748:LEU:HA	1:A:751:THR:HG22	2.02	0.41
1:A:1398:SER:HB3	1:A:1411:ILE:HD13	2.02	0.41
1:A:1460:PHE:HD2	1:A:1756:ILE:HG21	1.84	0.41
1:A:1820:LYS:O	1:A:1824:ILE:HG12	2.20	0.41
3:C:67:TRP:CZ2	3:C:127:CYS:HB3	2.55	0.41
1:A:104:PRO:HA	1:A:109:LEU:O	2.20	0.41
1:A:224:THR:HA	1:A:227:VAL:CG2	2.51	0.41
1:A:354:LEU:HD12	1:A:354:LEU:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:998:GLY:O	1:A:1001:TYR:HB3	2.21	0.41
1:A:1360:PRO:HD2	1:A:1363:GLN:HE21	1.86	0.41
1:A:1487:LYS:HE3	1:A:1487:LYS:HB2	1.82	0.41
1:A:1491:LYS:O	1:A:1493:PRO:HD3	2.20	0.41
7:A:2017:P5S:O18	11:A:2018:PCW:O2P	2.39	0.41
1:A:879:ILE:O	1:A:883:VAL:HG12	2.20	0.41
1:A:1527:LEU:O	1:A:1531:THR:HG23	2.21	0.41
1:A:1588:ILE:HG12	11:A:2028:PCW:H252	2.01	0.41
11:A:2027:PCW:H341	11:A:2027:PCW:H371	1.56	0.41
2:B:59:PHE:HB2	2:B:119:TYR:CD1	2.56	0.41
1:A:315:CYS:O	1:A:373:ALA:HA	2.21	0.40
1:A:429:ARG:HA	1:A:432:LYS:HE2	2.02	0.40
1:A:730:TRP:HA	1:A:733:PHE:CE2	2.56	0.40
1:A:924:LEU:HA	1:A:924:LEU:HD23	1.76	0.40
1:A:1182:ARG:HG2	1:A:1246:ILE:O	2.21	0.40
1:A:1478:GLN:HE22	1:A:1646:ASN:HD21	1.68	0.40
1:A:818:LEU:HG	1:A:837:PHE:CD2	2.55	0.40
1:A:1309:VAL:HA	1:A:1312:ASN:ND2	2.37	0.40
1:A:1701:ASP:N	1:A:1701:ASP:OD1	2.54	0.40
1:A:1776:GLU:O	1:A:1780:GLU:HG2	2.21	0.40
1:A:1819:ASN:O	1:A:1823:LEU:HG	2.21	0.40
10:A:2012:LPE:C1N	11:A:2013:PCW:O4P	2.69	0.40
2:B:75:ASN:O	2:B:77:VAL:N	2.54	0.40
1:A:29:GLU:O	1:A:33:LYS:HG3	2.22	0.40
1:A:171:ILE:HG12	1:A:183:PHE:CG	2.56	0.40
1:A:1545:GLU:HG2	1:A:1549:TRP:CD1	2.57	0.40
10:A:2021:LPE:H2N3	10:A:2021:LPE:H311	1.78	0.40
1:A:187:PRO:O	1:A:190:TRP:HB2	2.21	0.40
1:A:235:VAL:O	1:A:239:ILE:HG12	2.21	0.40
1:A:337:PRO:HG2	1:A:342:THR:HG23	2.04	0.40
1:A:1240:GLU:O	1:A:1244:LYS:HG3	2.22	0.40
11:A:2016:PCW:H42	11:A:2016:PCW:H83	1.62	0.40
2:B:62:LYS:HE2	2:B:62:LYS:HB3	1.89	0.40
2:B:149:LYS:HZ3	2:B:150:ALA:HB3	1.87	0.40
1:A:104:PRO:HB2	1:A:107:TYR:HA	2.03	0.40
1:A:1305:GLU:H	1:A:1305:GLU:CD	2.23	0.40
1:A:1649:LEU:HA	1:A:1649:LEU:HD23	1.79	0.40
1:A:1803:SER:O	1:A:1819:ASN:ND2	2.53	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	1409/2031 (69%)	1337 (95%)	71 (5%)	1 (0%)	51 85
2	B	171/218 (78%)	156 (91%)	14 (8%)	1 (1%)	25 64
3	C	120/215 (56%)	116 (97%)	4 (3%)	0	100 100
All	All	1700/2464 (69%)	1609 (95%)	89 (5%)	2 (0%)	54 85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1492	LYS
2	B	76	GLU

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	1266/1809 (70%)	1262 (100%)	4 (0%)	92 97
2	B	157/190 (83%)	154 (98%)	3 (2%)	57 84
3	C	114/193 (59%)	110 (96%)	4 (4%)	36 71
All	All	1537/2192 (70%)	1526 (99%)	11 (1%)	84 94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	TRP

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Mol	Chain	Res	Type
1	A	409	ASN
1	A	412	ASN
1	A	1445	SER
2	B	39	LEU
2	B	91	VAL
2	B	93	ASN
3	C	55	CYS
3	C	71	GLU
3	C	130	MET
3	C	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	278	ASN
1	A	323	GLN
1	A	365	ASN
1	A	408	GLN
1	A	409	ASN
1	A	412	ASN
1	A	425	GLN
1	A	757	ASN
1	A	780	ASN
1	A	809	ASN
1	A	861	ASN
1	A	909	HIS
1	A	911	ASN
1	A	941	GLN
1	A	961	ASN
1	A	975	ASN
1	A	987	ASN
1	A	1363	GLN
1	A	1378	GLN
1	A	1478	GLN
1	A	1494	GLN
1	A	1502	ASN
1	A	1528	ASN
1	A	1721	HIS
1	A	1871	ASN
2	B	102	GLN
2	B	115	HIS

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Mol	Chain	Res	Type
3	C	53	ASN
3	C	82	GLN
3	C	118	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	0.25	0	17,19,21	0.46	0
4	NAG	D	2	4	14,14,15	0.24	0	17,19,21	0.38	0
4	NAG	E	1	1,4	14,14,15	0.18	0	17,19,21	0.46	0
4	NAG	E	2	4	14,14,15	0.45	0	17,19,21	0.66	0
4	NAG	F	1	4,2	14,14,15	0.57	0	17,19,21	1.19	2 (11%)
4	NAG	F	2	4	14,14,15	0.65	0	17,19,21	1.20	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,2	-	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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	1	NAG	C1-O5-C5	2.72	115.87	112.19
4	F	1	NAG	C3-C4-C5	-2.65	105.52	110.24
4	F	2	NAG	C4-C3-C2	-2.42	107.47	111.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

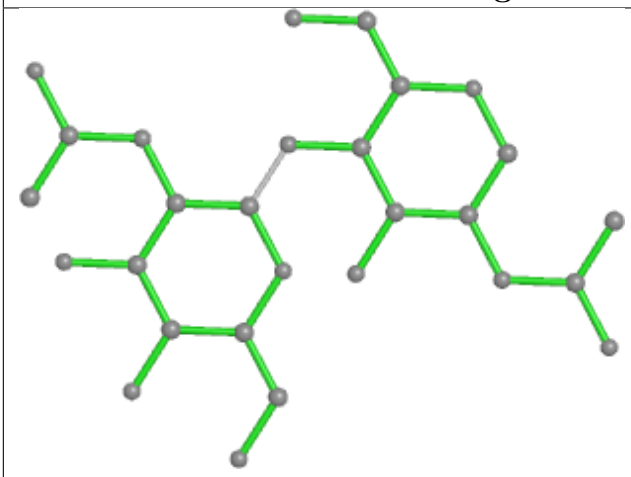
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6

There are no ring outliers.

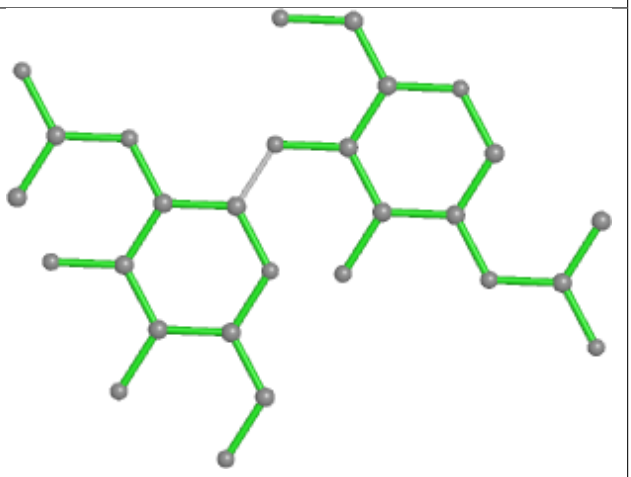
No monomer is involved in short contacts.

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

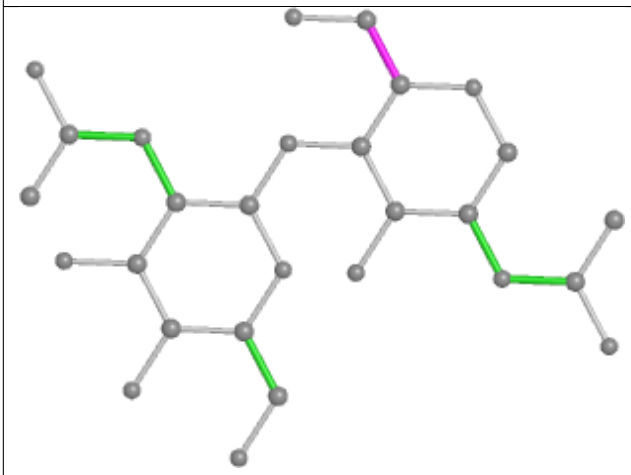
Oligosaccharide Chain D



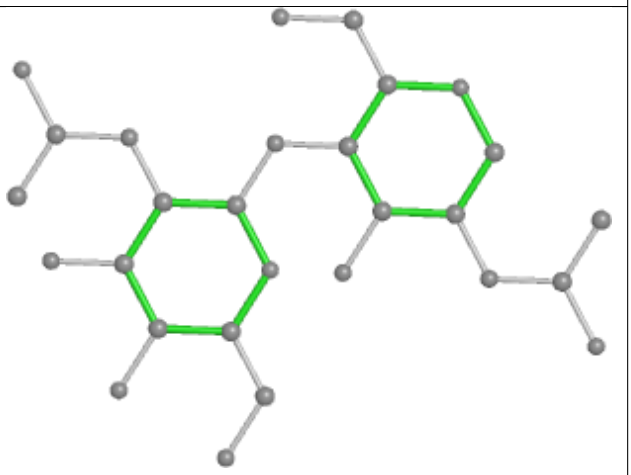
Bond lengths



Bond angles

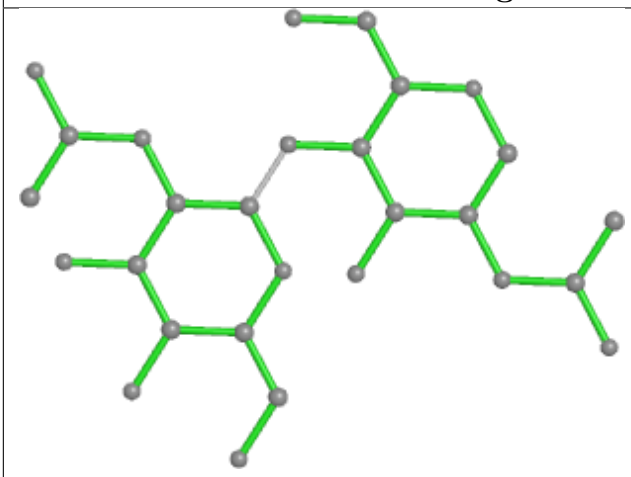


Torsions

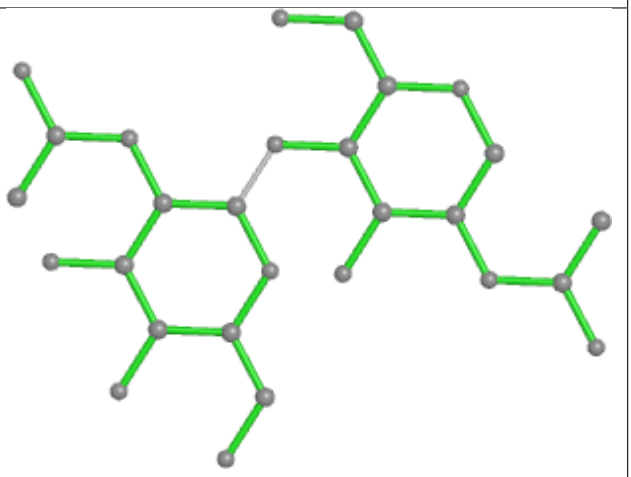


Rings

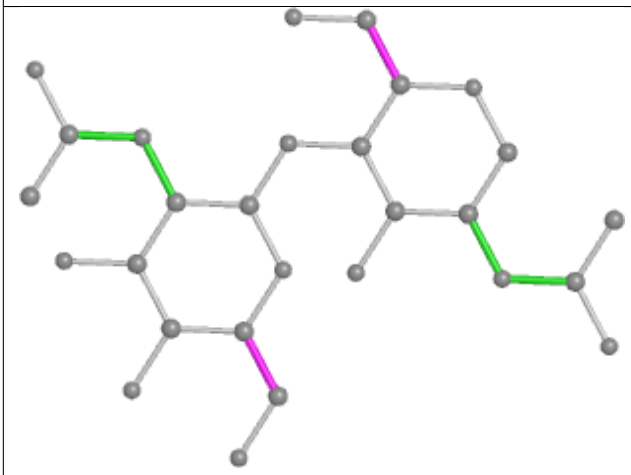
Oligosaccharide Chain E



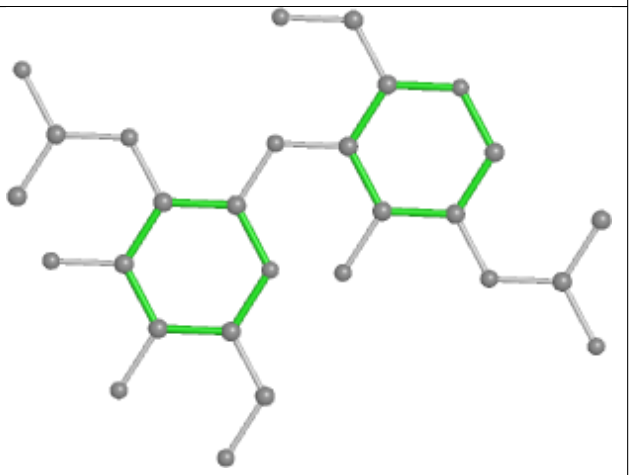
Bond lengths



Bond angles

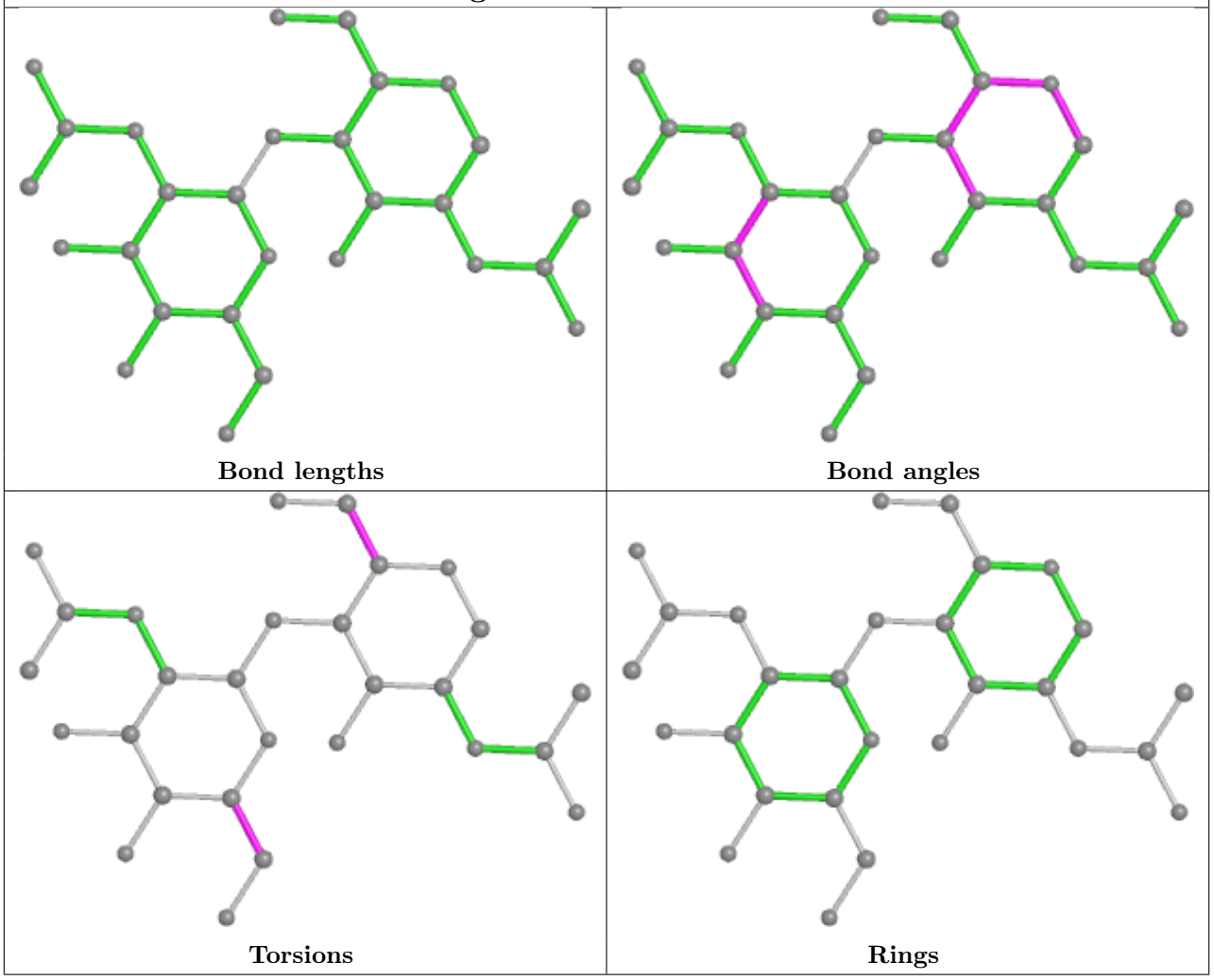


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

33 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	$\#\|Z\| > 2$
10	LPE	A	2026	-	16,16,33	0.68	0	20,22,39	0.67	0
5	9SL	A	2001	-	17,23,23	3.61	8 (47%)	13,37,37	3.02	6 (46%)
10	LPE	A	2010	-	24,24,33	0.52	0	28,30,39	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	LPE	A	2012	-	19,19,33	0.62	0	23,25,39	0.51	0
6	NAG	B	301	2	14,14,15	0.64	0	17,19,21	0.98	0
10	LPE	A	2022	-	24,24,33	0.53	0	28,30,39	0.63	0
11	PCW	A	2027	-	43,43,53	1.03	2 (4%)	49,51,61	0.94	2 (4%)
6	NAG	A	2008	1	14,14,15	0.30	0	17,19,21	1.00	1 (5%)
8	Y01	A	2005	-	38,38,38	0.66	1 (2%)	57,57,57	1.79	11 (19%)
6	NAG	A	2002	1	14,14,15	0.34	0	17,19,21	0.44	0
10	LPE	A	2024	-	24,24,33	0.52	0	28,30,39	0.62	0
6	NAG	B	302	2	14,14,15	0.18	0	17,19,21	0.41	0
8	Y01	A	2006	-	38,38,38	1.15	4 (10%)	57,57,57	1.74	12 (21%)
9	9Z9	A	2007	-	44,44,44	0.70	1 (2%)	66,68,68	1.45	12 (18%)
10	LPE	A	2021	-	24,24,33	0.54	0	28,30,39	0.68	1 (3%)
10	LPE	A	2020	-	24,24,33	0.85	0	28,30,39	0.92	1 (3%)
6	NAG	B	303	2	14,14,15	0.25	0	17,19,21	0.42	0
10	LPE	A	2015	-	27,27,33	0.54	0	31,33,39	0.61	0
10	LPE	A	2023	-	24,24,33	0.53	0	28,30,39	0.54	0
10	LPE	A	2025	-	24,24,33	0.54	0	28,30,39	0.50	0
11	PCW	A	2013	-	52,52,53	0.93	2 (3%)	58,60,61	0.97	2 (3%)
10	LPE	A	2011	-	24,24,33	0.33	0	25,27,39	0.60	0
10	LPE	B	304	-	16,16,33	0.67	0	20,22,39	0.60	0
8	Y01	A	2004	-	38,38,38	0.66	1 (2%)	57,57,57	1.79	11 (19%)
11	PCW	A	2018	-	43,43,53	1.01	2 (4%)	49,51,61	1.12	5 (10%)
8	Y01	A	2009	-	38,38,38	1.15	4 (10%)	57,57,57	1.74	10 (17%)
10	LPE	A	2019	-	24,24,33	0.60	0	28,30,39	0.89	1 (3%)
7	P5S	A	2003	-	33,34,53	0.76	1 (3%)	36,40,60	1.80	5 (13%)
8	Y01	A	2029	-	38,38,38	1.62	7 (18%)	57,57,57	1.63	10 (17%)
11	PCW	A	2016	-	46,46,53	0.99	3 (6%)	52,54,61	1.18	4 (7%)
11	PCW	A	2028	-	43,43,53	0.99	2 (4%)	49,51,61	2.90	6 (12%)
7	P5S	A	2017	-	40,40,53	1.14	3 (7%)	43,45,60	1.37	3 (6%)
10	LPE	A	2014	-	21,21,33	0.68	0	25,27,39	1.03	2 (8%)

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
10	LPE	A	2026	-	-	7/17/17/34	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	9SL	A	2001	-	-	4/5/53/53	0/3/3/3
10	LPE	A	2010	-	-	10/25/25/34	-
10	LPE	A	2012	-	-	10/20/20/34	-
6	NAG	B	301	2	-	0/6/23/26	0/1/1/1
10	LPE	A	2022	-	-	3/25/25/34	-
11	PCW	A	2027	-	-	16/47/47/57	-
6	NAG	A	2008	1	-	2/6/23/26	0/1/1/1
8	Y01	A	2005	-	-	0/19/77/77	0/4/4/4
6	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
10	LPE	A	2024	-	-	6/25/25/34	-
6	NAG	B	302	2	-	0/6/23/26	0/1/1/1
8	Y01	A	2006	-	-	4/19/77/77	0/4/4/4
9	9Z9	A	2007	-	-	0/12/100/100	0/6/6/6
10	LPE	A	2021	-	-	3/25/25/34	-
10	LPE	A	2020	-	-	12/25/25/34	-
6	NAG	B	303	2	-	0/6/23/26	0/1/1/1
10	LPE	A	2015	-	-	10/28/28/34	-
10	LPE	A	2023	-	-	8/25/25/34	-
10	LPE	A	2025	-	-	10/25/25/34	-
11	PCW	A	2013	-	-	16/56/56/57	-
10	LPE	A	2011	-	-	8/25/25/34	-
10	LPE	B	304	-	-	9/17/17/34	-
8	Y01	A	2004	-	-	0/19/77/77	0/4/4/4
11	PCW	A	2018	-	-	12/47/47/57	-
8	Y01	A	2009	-	-	4/19/77/77	0/4/4/4
10	LPE	A	2019	-	-	7/25/25/34	-
7	P5S	A	2003	-	-	28/39/39/59	-
8	Y01	A	2029	-	-	7/19/77/77	0/4/4/4
11	PCW	A	2016	-	-	13/50/50/57	-
11	PCW	A	2028	-	-	12/47/47/57	-
7	P5S	A	2017	-	-	8/44/44/59	-
10	LPE	A	2014	-	-	15/22/22/34	-

All (41) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2001	9SL	C12-N13	8.85	1.49	1.35
5	A	2001	9SL	C07-N08	6.10	1.45	1.34
5	A	2001	9SL	C02-N21	5.95	1.44	1.33
5	A	2001	9SL	C12-N15	4.57	1.45	1.34
7	A	2017	P5S	O37-C38	4.42	1.46	1.34
11	A	2027	PCW	O3-C11	4.41	1.46	1.33
8	A	2029	Y01	CBB-CBE	-4.36	1.46	1.54
11	A	2028	PCW	O3-C11	4.28	1.45	1.33
11	A	2013	PCW	O2-C31	4.17	1.46	1.34
11	A	2013	PCW	O3-C11	4.15	1.45	1.33
8	A	2029	Y01	CAR-CBC	-4.15	1.40	1.51
11	A	2028	PCW	O2-C31	4.10	1.45	1.34
11	A	2018	PCW	O2-C31	3.96	1.45	1.34
7	A	2017	P5S	O19-C17	3.94	1.44	1.33
11	A	2027	PCW	O2-C31	3.88	1.45	1.34
11	A	2018	PCW	O3-C11	3.87	1.44	1.33
11	A	2016	PCW	O3-C11	3.85	1.44	1.33
8	A	2029	Y01	OAW-CAY	3.70	1.44	1.34
11	A	2016	PCW	O2-C31	3.67	1.44	1.34
5	A	2001	9SL	C05-C14	3.64	1.60	1.52
8	A	2006	Y01	OAW-CAY	3.62	1.44	1.34
8	A	2009	Y01	OAW-CAY	3.59	1.44	1.34
5	A	2001	9SL	O01-C02	-3.45	1.17	1.21
7	A	2003	P5S	O37-C38	3.41	1.43	1.34
7	A	2017	P5S	C28-C27	-3.35	1.32	1.51
5	A	2001	9SL	O03-C02	2.94	1.39	1.35
8	A	2029	Y01	CAV-CBC	2.91	1.59	1.52
5	A	2001	9SL	C05-N06	-2.44	1.43	1.47
8	A	2009	Y01	CAM-CAY	2.39	1.57	1.50
8	A	2006	Y01	CAM-CAY	2.39	1.57	1.50
8	A	2029	Y01	CAM-CAY	2.38	1.57	1.50
8	A	2006	Y01	CAL-CAX	2.23	1.55	1.50
8	A	2009	Y01	CAL-CAX	2.22	1.55	1.50
8	A	2004	Y01	CBH-CBF	-2.22	1.52	1.56
8	A	2029	Y01	CBH-CBF	-2.21	1.52	1.56
8	A	2009	Y01	CBH-CBF	-2.19	1.52	1.56
9	A	2007	9Z9	C11-C08	-2.17	1.52	1.56
8	A	2029	Y01	CAL-CAX	2.16	1.55	1.50
11	A	2016	PCW	C6-N	-2.15	1.43	1.50
8	A	2006	Y01	CBH-CBF	-2.12	1.52	1.56
8	A	2005	Y01	CBH-CBF	-2.12	1.52	1.56

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	2028	PCW	C8-N-C6	-12.10	77.88	108.97
11	A	2028	PCW	C8-N-C7	-12.03	78.04	108.97
5	A	2001	9SL	O03-C02-N21	7.82	120.78	111.08
11	A	2028	PCW	C8-N-C5	-7.81	77.97	109.92
7	A	2003	P5S	OG-CB-CA	7.06	114.22	108.06
8	A	2006	Y01	CBI-CBE-CBB	-5.93	110.19	119.49
8	A	2004	Y01	CBI-CBE-CBB	-5.92	110.22	119.49
8	A	2009	Y01	CBI-CBE-CBB	-5.92	110.22	119.49
8	A	2005	Y01	CBI-CBE-CBB	-5.90	110.24	119.49
7	A	2017	P5S	O37-C38-C39	5.47	123.29	111.50
11	A	2016	PCW	O2-C31-C32	4.84	121.93	111.50
8	A	2005	Y01	CBI-CBG-CBD	-4.83	107.22	114.38
8	A	2004	Y01	CBI-CBG-CBD	-4.78	107.30	114.38
8	A	2029	Y01	CBI-CBG-CBD	-4.75	107.35	114.38
8	A	2009	Y01	CBI-CBG-CBD	-4.73	107.38	114.38
8	A	2006	Y01	CBI-CBG-CBD	-4.73	107.38	114.38
9	A	2007	9Z9	C02-C06-C07	-4.38	107.90	114.38
5	A	2001	9SL	O01-C02-N21	-4.26	118.48	125.51
8	A	2029	Y01	CBI-CBE-CBB	-4.18	112.94	119.49
7	A	2003	P5S	OXT-C-O	-4.09	114.81	124.09
8	A	2005	Y01	OAW-CAY-CAM	3.98	120.08	111.50
8	A	2004	Y01	OAW-CAY-CAM	3.98	120.08	111.50
10	A	2020	LPE	C3N-N-C2N	3.93	119.07	108.97
11	A	2013	PCW	O2-C31-C32	3.88	119.86	111.50
8	A	2009	Y01	OAW-CAY-CAM	3.74	119.56	111.50
8	A	2006	Y01	OAW-CAY-CAM	3.74	119.55	111.50
11	A	2028	PCW	O2-C31-C32	3.70	119.47	111.50
7	A	2003	P5S	O37-C38-C39	3.67	119.41	111.50
8	A	2029	Y01	OAW-CAY-CAM	3.59	119.24	111.50
9	A	2007	9Z9	C21-C22-C23	-3.50	109.45	113.88
8	A	2009	Y01	CAS-CAU-CBI	-3.35	107.04	112.78
8	A	2006	Y01	CAS-CAU-CBI	-3.32	107.08	112.78
8	A	2005	Y01	CAS-CAU-CBI	-3.32	107.08	112.78
8	A	2004	Y01	CAS-CAU-CBI	-3.32	107.09	112.78
8	A	2029	Y01	CAS-CAU-CBI	-3.32	107.09	112.78
9	A	2007	9Z9	C09-C10-C02	-3.30	107.12	112.78
5	A	2001	9SL	N09-C07-N06	-3.29	120.83	125.42
11	A	2027	PCW	O2-C31-C32	3.26	118.52	111.50
9	A	2007	9Z9	C02-C03-C74	-3.25	109.52	120.56
5	A	2001	9SL	N13-C12-N11	-3.08	107.66	115.45
11	A	2016	PCW	O3-C11-C12	3.05	121.49	111.91
8	A	2004	Y01	CAD-CBH-CBF	-2.99	108.12	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	2005	Y01	CAD-CBH-CBF	-2.95	108.17	111.68
8	A	2009	Y01	CAD-CBH-CBF	-2.94	108.18	111.68
8	A	2006	Y01	CAD-CBH-CBF	-2.94	108.18	111.68
7	A	2003	P5S	OXT-C-CA	2.91	123.31	113.38
11	A	2018	PCW	C3-C2-C1	-2.90	104.92	111.79
6	A	2008	NAG	C4-C3-C2	-2.90	106.77	111.02
8	A	2029	Y01	CAD-CBH-CBF	-2.89	108.23	111.68
10	A	2014	LPE	C3-C2-C1	-2.85	104.41	112.79
9	A	2007	9Z9	C12-C11-C08	-2.84	108.29	111.68
9	A	2007	9Z9	C76-C73-C74	-2.81	109.92	115.69
11	A	2018	PCW	O2-C31-C32	2.78	117.50	111.50
11	A	2028	PCW	O3-C11-C12	2.76	120.57	111.91
8	A	2029	Y01	CBG-CBI-CBE	2.71	103.28	100.07
8	A	2005	Y01	CBG-CBI-CBE	2.70	103.27	100.07
8	A	2009	Y01	CBG-CBI-CBE	2.69	103.26	100.07
8	A	2004	Y01	CBG-CBI-CBE	2.69	103.26	100.07
8	A	2006	Y01	CBG-CBI-CBE	2.68	103.25	100.07
11	A	2028	PCW	C7-N-C6	2.67	115.83	108.97
10	A	2014	LPE	C31-C32-N	-2.56	107.24	115.78
8	A	2005	Y01	CAS-CBF-CBH	-2.53	109.75	113.08
11	A	2018	PCW	O3-C11-C12	2.52	119.81	111.91
9	A	2007	9Z9	C75-C74-C73	-2.51	110.33	114.92
9	A	2007	9Z9	C09-C08-C11	-2.50	109.78	113.08
8	A	2029	Y01	CAS-CBF-CBH	-2.49	109.80	113.08
8	A	2006	Y01	CAS-CBF-CBH	-2.47	109.82	113.08
5	A	2001	9SL	O03-C02-O01	-2.46	120.74	123.07
8	A	2009	Y01	CBD-CAK-CAI	-2.46	109.19	112.73
8	A	2004	Y01	CAS-CBF-CBH	-2.46	109.84	113.08
8	A	2004	Y01	CBD-CAK-CAI	-2.46	109.20	112.73
8	A	2009	Y01	CAS-CBF-CBH	-2.46	109.84	113.08
11	A	2013	PCW	O3-C11-C12	2.43	119.54	111.91
8	A	2005	Y01	CBD-CAK-CAI	-2.43	109.24	112.73
9	A	2007	9Z9	C07-C15-C14	-2.42	109.25	112.73
8	A	2006	Y01	CBD-CAK-CAI	-2.42	109.26	112.73
8	A	2029	Y01	CBD-CAK-CAI	-2.41	109.26	112.73
7	A	2017	P5S	C41-C40-C39	-2.36	104.70	113.19
8	A	2004	Y01	CBF-CBH-CAZ	2.35	113.33	109.65
8	A	2029	Y01	CBF-CBH-CAZ	2.35	113.33	109.65
8	A	2009	Y01	CBF-CBH-CAZ	2.34	113.31	109.65
8	A	2006	Y01	CBF-CBH-CAZ	2.32	113.29	109.65
5	A	2001	9SL	O03-C04-C05	2.31	112.95	108.40
11	A	2027	PCW	O3-C11-C12	2.31	119.14	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	2003	P5S	C2-O37-C38	-2.30	112.14	117.79
8	A	2005	Y01	CAC-CBB-CBE	-2.27	109.45	112.92
8	A	2005	Y01	CBF-CBH-CAZ	2.27	113.20	109.65
9	A	2007	9Z9	C08-C11-C13	2.25	113.18	109.65
8	A	2006	Y01	CAC-CBB-CBE	-2.23	109.51	112.92
8	A	2009	Y01	CAC-CBB-CBE	-2.22	109.53	112.92
8	A	2004	Y01	CAC-CBB-CBE	-2.21	109.54	112.92
10	A	2021	LPE	C31-C32-N	-2.17	108.53	115.78
11	A	2018	PCW	C34-C33-C32	-2.16	105.44	113.19
10	A	2019	LPE	C31-C32-N	-2.13	108.68	115.78
11	A	2016	PCW	O2-C31-O31	-2.12	118.58	123.70
7	A	2017	P5S	O15-P12-O13	2.11	122.65	112.24
9	A	2007	9Z9	O80-C79-C78	-2.07	109.20	112.18
11	A	2018	PCW	O3-C3-C2	2.06	114.44	108.43
8	A	2004	Y01	CAQ-CBG-CBD	-2.04	115.72	119.08
8	A	2005	Y01	CAQ-CBG-CBD	-2.04	115.73	119.08
11	A	2016	PCW	O3-C11-O11	-2.04	118.45	123.59
8	A	2006	Y01	CAQ-CBG-CBD	-2.03	115.73	119.08
9	A	2007	9Z9	C17-C16-C13	-2.03	108.37	111.52
8	A	2006	Y01	CBC-CAV-CAZ	-2.02	108.37	111.52
8	A	2029	Y01	CAQ-CBG-CBD	-2.02	115.76	119.08

There are no chirality outliers.

All (246) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2001	9SL	O01-C02-O03-C04
5	A	2001	9SL	N21-C02-O03-C04
5	A	2001	9SL	O03-C04-C05-N06
5	A	2001	9SL	O03-C04-C05-C14
7	A	2003	P5S	C-CA-CB-OG
7	A	2003	P5S	N-CA-CB-OG
7	A	2003	P5S	CB-OG-P12-O13
7	A	2003	P5S	C3-O16-P12-OG
7	A	2003	P5S	C3-O16-P12-O13
7	A	2003	P5S	C3-O16-P12-O15
7	A	2017	P5S	CB-OG-P12-O15
7	A	2017	P5S	C3-O16-P12-OG
7	A	2017	P5S	C3-O16-P12-O13
7	A	2017	P5S	C3-O16-P12-O15
10	A	2010	LPE	C3-O3-P-O31
10	A	2011	LPE	C3-O3-P-O31

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Mol	Chain	Res	Type	Atoms
10	A	2012	LPE	C3-O3-P-O32
10	A	2012	LPE	C31-O33-P-O31
10	A	2014	LPE	O1-C1-C2-C3
10	A	2014	LPE	C3-O3-P-O32
10	A	2014	LPE	C31-O33-P-O3
10	A	2014	LPE	C31-O33-P-O31
10	A	2014	LPE	C32-C31-O33-P
10	A	2014	LPE	O33-C31-C32-N
10	A	2015	LPE	C3-O3-P-O32
10	A	2019	LPE	C31-O33-P-O31
10	A	2019	LPE	O33-C31-C32-N
10	A	2020	LPE	C31-O33-P-O31
10	A	2021	LPE	C31-O33-P-O31
10	A	2023	LPE	C31-O33-P-O32
10	A	2024	LPE	C31-O33-P-O31
10	A	2025	LPE	O1-C1-C2-C3
10	A	2025	LPE	C3-O3-P-O32
10	A	2025	LPE	C31-O33-P-O3
10	A	2025	LPE	C31-O33-P-O31
10	A	2025	LPE	C31-O33-P-O32
10	B	304	LPE	C3-O3-P-O31
10	B	304	LPE	C3-O3-P-O32
10	B	304	LPE	C3-O3-P-O33
11	A	2016	PCW	O4P-C4-C5-N
11	A	2018	PCW	C32-C31-O2-C2
11	A	2027	PCW	O4P-C4-C5-N
11	A	2027	PCW	C1-O3P-P-O2P
8	A	2029	Y01	CAC-CBB-CBE-CAP
8	A	2029	Y01	CAC-CBB-CBE-CBI
11	A	2018	PCW	O31-C31-O2-C2
8	A	2029	Y01	CAJ-CAO-CBB-CAC
8	A	2029	Y01	CAO-CBB-CBE-CBI
11	A	2027	PCW	O11-C11-O3-C3
11	A	2027	PCW	C12-C11-O3-C3
6	A	2002	NAG	O5-C5-C6-O6
8	A	2029	Y01	CAO-CBB-CBE-CAP
10	A	2025	LPE	O1-C1-C2-O2H
6	A	2002	NAG	C4-C5-C6-O6
6	A	2008	NAG	C8-C7-N2-C2
8	A	2006	Y01	CAR-CBC-OAW-CAY
10	A	2023	LPE	C31-C32-N-C2N
10	A	2023	LPE	C31-C32-N-C3N

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Mol	Chain	Res	Type	Atoms
11	A	2016	PCW	C4-C5-N-C8
11	A	2018	PCW	C4-C5-N-C7
11	A	2028	PCW	C12-C11-O3-C3
8	A	2009	Y01	CAR-CBC-OAW-CAY
8	A	2029	Y01	CAJ-CAO-CBB-CBE
6	A	2008	NAG	O7-C7-N2-C2
11	A	2028	PCW	O11-C11-O3-C3
10	A	2014	LPE	O1-C1-C2-O2H
10	A	2026	LPE	C31-C32-N-C3N
11	A	2016	PCW	C4-C5-N-C7
7	A	2003	P5S	C38-C39-C40-C41
10	A	2014	LPE	O1-C11-C12-C13
10	A	2020	LPE	O1-C1-C2-O2H
7	A	2003	P5S	CB-OG-P12-O16
10	A	2011	LPE	C3-O3-P-O33
10	A	2011	LPE	C31-O33-P-O3
10	A	2014	LPE	C3-O3-P-O33
10	A	2015	LPE	C3-O3-P-O33
10	A	2022	LPE	C3-O3-P-O33
10	A	2023	LPE	C31-O33-P-O3
10	A	2025	LPE	C3-O3-P-O33
10	A	2026	LPE	C31-O33-P-O3
10	B	304	LPE	C31-O33-P-O3
11	A	2013	PCW	C4-O4P-P-O3P
11	A	2016	PCW	C4-O4P-P-O3P
11	A	2018	PCW	C4-O4P-P-O3P
8	A	2006	Y01	CAV-CBC-OAW-CAY
8	A	2009	Y01	CAV-CBC-OAW-CAY
10	A	2010	LPE	O1-C11-C12-C13
10	A	2014	LPE	C31-C32-N-C1N
10	A	2014	LPE	C31-C32-N-C2N
10	A	2014	LPE	C31-C32-N-C3N
11	A	2018	PCW	C4-C5-N-C6
11	A	2028	PCW	C4-C5-N-C8
10	A	2020	LPE	O1-C1-C2-C3
7	A	2003	P5S	C46-C48-C49-C50
7	A	2017	P5S	C25-C26-C27-C28
10	A	2011	LPE	O1-C11-C12-C13
10	A	2023	LPE	C31-C32-N-C1N
10	A	2020	LPE	C12-C13-C14-C15
7	A	2003	P5S	C51-C52-C53-C54
7	A	2017	P5S	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
7	A	2003	P5S	C41-C42-C43-C44
11	A	2027	PCW	C33-C34-C35-C36
7	A	2003	P5S	C52-C53-C54-C55
10	A	2020	LPE	C14-C15-C16-C17
11	A	2016	PCW	C4-C5-N-C6
11	A	2013	PCW	C24-C25-C26-C27
11	A	2013	PCW	C32-C31-O2-C2
11	A	2013	PCW	C32-C33-C34-C35
7	A	2003	P5S	C48-C49-C50-C51
11	A	2027	PCW	C31-C32-C33-C34
10	A	2024	LPE	C13-C14-C15-C16
10	A	2011	LPE	C13-C14-C15-C16
10	A	2026	LPE	C31-C32-N-C1N
10	A	2026	LPE	C31-C32-N-C2N
11	A	2018	PCW	C4-C5-N-C8
11	A	2013	PCW	O31-C31-O2-C2
7	A	2003	P5S	C39-C38-O37-C2
11	A	2028	PCW	C32-C31-O2-C2
11	A	2016	PCW	C35-C36-C37-C38
10	A	2010	LPE	C2-C1-O1-C11
8	A	2029	Y01	CAN-CAJ-CAO-CBB
11	A	2013	PCW	C41-C42-C43-C44
11	A	2016	PCW	C34-C35-C36-C37
7	A	2003	P5S	O47-C38-O37-C2
7	A	2003	P5S	C1-C2-C3-O16
11	A	2028	PCW	O31-C31-O2-C2
10	B	304	LPE	C2-C3-O3-P
10	A	2026	LPE	C2-C1-O1-C11
10	A	2015	LPE	O1-C1-C2-C3
10	A	2015	LPE	O1-C1-C2-O2H
10	A	2012	LPE	C3-O3-P-O33
10	A	2020	LPE	C16-C17-C18-C19
10	A	2020	LPE	C11-C12-C13-C14
7	A	2003	P5S	C2-C3-O16-P12
11	A	2018	PCW	C2-C1-O3P-P
10	A	2019	LPE	C2-C1-O1-C11
8	A	2006	Y01	CAO-CAJ-CAN-CBA
8	A	2009	Y01	CAO-CAJ-CAN-CBA
7	A	2003	P5S	O37-C2-C3-O16
10	A	2020	LPE	C12-C11-O1-C1
7	A	2003	P5S	C40-C41-C42-C43
11	A	2027	PCW	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
10	B	304	LPE	C2-C1-O1-C11
10	A	2012	LPE	C12-C11-O1-C1
10	A	2012	LPE	C31-O33-P-O3
10	A	2020	LPE	C31-O33-P-O3
10	A	2021	LPE	C31-O33-P-O3
10	A	2024	LPE	C31-O33-P-O3
11	A	2027	PCW	C1-O3P-P-O4P
10	A	2010	LPE	C2-C3-O3-P
10	A	2012	LPE	C2-C3-O3-P
7	A	2003	P5S	CB-OG-P12-O15
10	A	2011	LPE	C3-O3-P-O32
10	A	2011	LPE	C31-O33-P-O31
10	A	2012	LPE	C3-O3-P-O31
10	A	2020	LPE	C3-O3-P-O32
10	A	2022	LPE	C3-O3-P-O31
10	A	2023	LPE	C31-O33-P-O31
10	A	2025	LPE	C3-O3-P-O31
10	A	2026	LPE	C31-O33-P-O31
10	B	304	LPE	C31-O33-P-O31
11	A	2013	PCW	C4-C5-N-C6
11	A	2013	PCW	C4-C5-N-C7
11	A	2013	PCW	C4-O4P-P-O2P
11	A	2016	PCW	C4-O4P-P-O2P
11	A	2018	PCW	C4-O4P-P-O2P
11	A	2027	PCW	C4-O4P-P-O2P
10	A	2011	LPE	C32-C31-O33-P
10	B	304	LPE	C32-C31-O33-P
10	A	2019	LPE	C12-C11-O1-C1
10	A	2010	LPE	C11-C12-C13-C14
10	A	2024	LPE	C2-C1-O1-C11
10	A	2014	LPE	C13-C14-C15-C16
11	A	2027	PCW	C34-C35-C36-C37
10	A	2010	LPE	O33-C31-C32-N
10	A	2012	LPE	O33-C31-C32-N
10	A	2015	LPE	O33-C31-C32-N
10	A	2020	LPE	O33-C31-C32-N
10	A	2021	LPE	O33-C31-C32-N
10	A	2022	LPE	O33-C31-C32-N
10	A	2023	LPE	O33-C31-C32-N
10	A	2024	LPE	O33-C31-C32-N
10	A	2025	LPE	O33-C31-C32-N
10	B	304	LPE	O33-C31-C32-N

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Mol	Chain	Res	Type	Atoms
11	A	2028	PCW	O4P-C4-C5-N
10	A	2014	LPE	C12-C11-O1-C1
7	A	2003	P5S	C50-C51-C52-C53
10	A	2015	LPE	C12-C11-O1-C1
11	A	2013	PCW	C4-C5-N-C8
11	A	2027	PCW	C32-C31-O2-C2
11	A	2028	PCW	C19-C20-C21-C22
7	A	2017	P5S	CB-OG-P12-O16
10	A	2010	LPE	C3-O3-P-O33
10	A	2015	LPE	C31-O33-P-O3
10	A	2019	LPE	C31-O33-P-O3
10	A	2024	LPE	C3-O3-P-O33
10	A	2026	LPE	C3-O3-P-O33
11	A	2016	PCW	C1-O3P-P-O4P
11	A	2018	PCW	C1-O3P-P-O4P
11	A	2027	PCW	C4-O4P-P-O3P
11	A	2028	PCW	C1-O3P-P-O4P
11	A	2028	PCW	C4-O4P-P-O3P
11	A	2016	PCW	C17-C18-C19-C20
11	A	2016	PCW	C37-C38-C39-C40
11	A	2013	PCW	C23-C24-C25-C26
11	A	2027	PCW	C11-C12-C13-C14
10	A	2025	LPE	C2-C1-O1-C11
10	A	2014	LPE	C11-C12-C13-C14
7	A	2003	P5S	C43-C44-C45-C46
11	A	2013	PCW	C44-C45-C46-C47
7	A	2003	P5S	C39-C40-C41-C42
11	A	2027	PCW	C21-C22-C23-C24
7	A	2003	P5S	O19-C1-C2-O37
7	A	2003	P5S	C53-C54-C55-C56
10	A	2015	LPE	C2-C3-O3-P
11	A	2013	PCW	C13-C14-C15-C16
11	A	2013	PCW	C17-C18-C19-C20
11	A	2013	PCW	C39-C40-C41-C42
11	A	2028	PCW	C17-C18-C19-C20
10	A	2010	LPE	C31-C32-N-C2N
11	A	2016	PCW	C39-C40-C41-C42
11	A	2018	PCW	O3-C11-C12-C13
10	A	2012	LPE	C1-C2-C3-O3
10	A	2020	LPE	C13-C14-C15-C16
10	A	2010	LPE	C16-C17-C18-C19
11	A	2013	PCW	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
7	A	2017	P5S	CB-OG-P12-O13
10	A	2015	LPE	C31-O33-P-O31
10	A	2019	LPE	C3-O3-P-O31
11	A	2016	PCW	C1-O3P-P-O2P
11	A	2018	PCW	C1-O3P-P-O2P
11	A	2027	PCW	C4-C5-N-C6
11	A	2028	PCW	C1-O3P-P-O2P
11	A	2028	PCW	C4-O4P-P-O2P
10	A	2010	LPE	C32-C31-O33-P
10	A	2015	LPE	C32-C31-O33-P
10	A	2019	LPE	C32-C31-O33-P
10	A	2023	LPE	C32-C31-O33-P
11	A	2018	PCW	C5-C4-O4P-P
7	A	2003	P5S	C49-C50-C51-C52
10	A	2012	LPE	C31-C32-N-C2N
11	A	2027	PCW	O3-C11-C12-C13
7	A	2003	P5S	O37-C38-C39-C40
8	A	2006	Y01	CAN-CAJ-CAO-CBB
8	A	2009	Y01	CAN-CAJ-CAO-CBB
7	A	2003	P5S	O47-C38-C39-C40

There are no ring outliers.

27 monomers are involved in 185 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	2026	LPE	10	0
5	A	2001	9SL	3	0
10	A	2010	LPE	2	0
10	A	2012	LPE	9	0
10	A	2022	LPE	7	0
11	A	2027	PCW	8	0
6	A	2008	NAG	9	0
8	A	2005	Y01	3	0
8	A	2006	Y01	16	0
9	A	2007	9Z9	9	0
10	A	2021	LPE	9	0
10	A	2015	LPE	6	0
10	A	2023	LPE	8	0
10	A	2025	LPE	11	0
11	A	2013	PCW	22	0
10	A	2011	LPE	2	0
10	B	304	LPE	10	0

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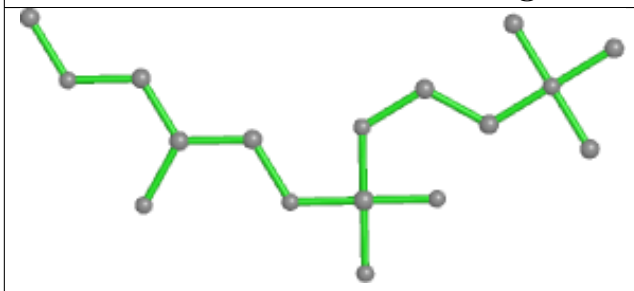
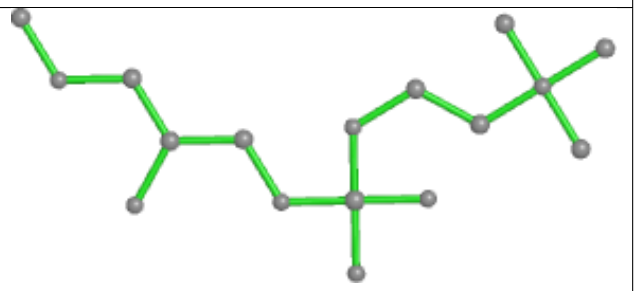
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2004	Y01	6	0
11	A	2018	PCW	6	0
8	A	2009	Y01	5	0
10	A	2019	LPE	8	0
7	A	2003	P5S	12	0
8	A	2029	Y01	18	0
11	A	2016	PCW	1	0
11	A	2028	PCW	2	0
7	A	2017	P5S	9	0
10	A	2014	LPE	17	0

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.

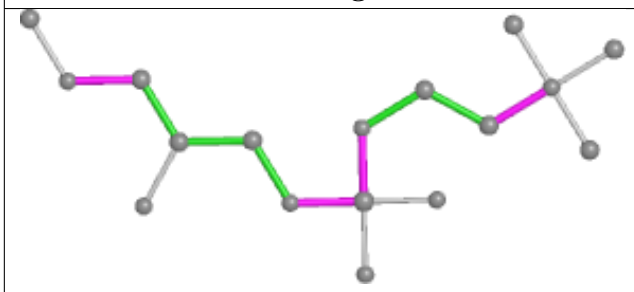
Ligand LPE A 2026



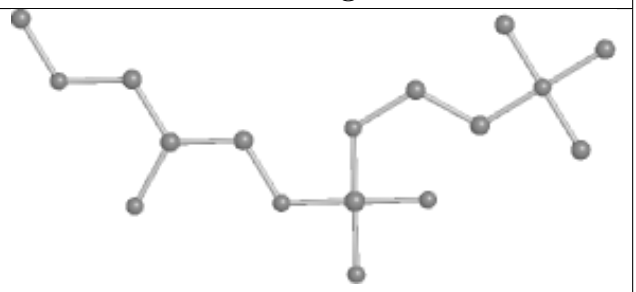
Bond lengths



Bond angles

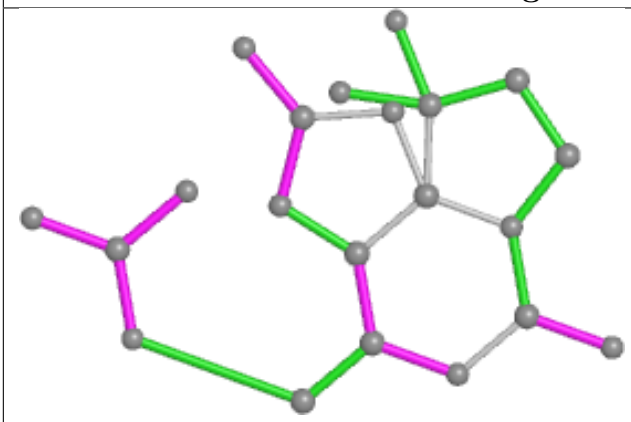


Torsions

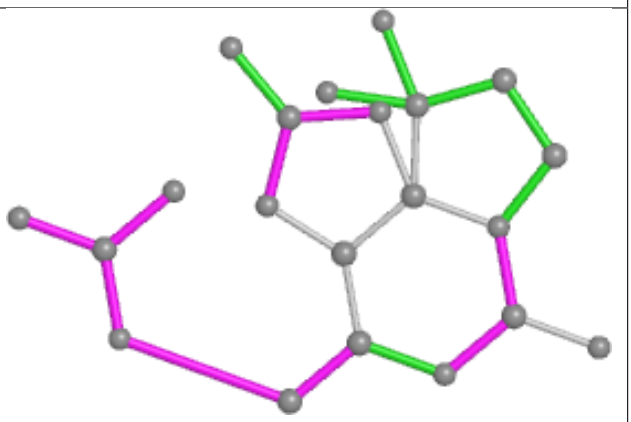


Rings

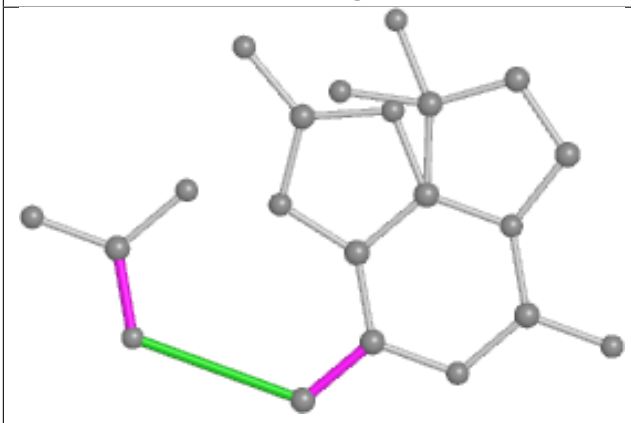
Ligand 9SL A 2001



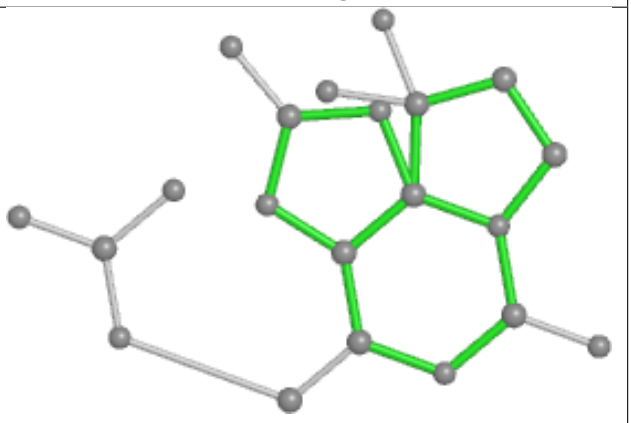
Bond lengths



Bond angles

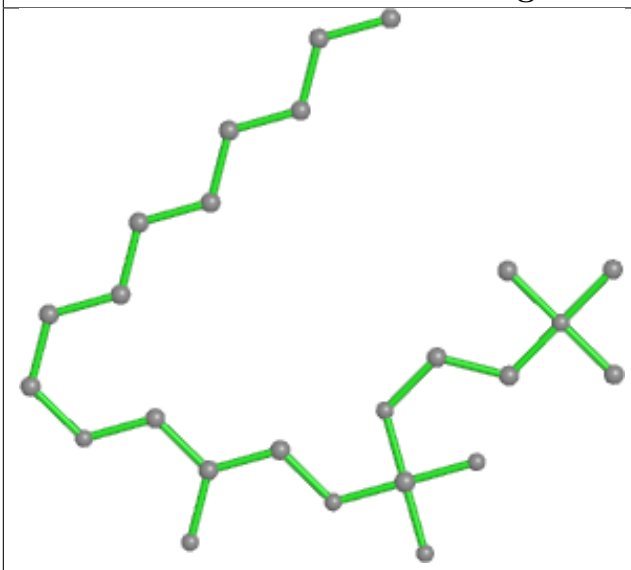


Torsions

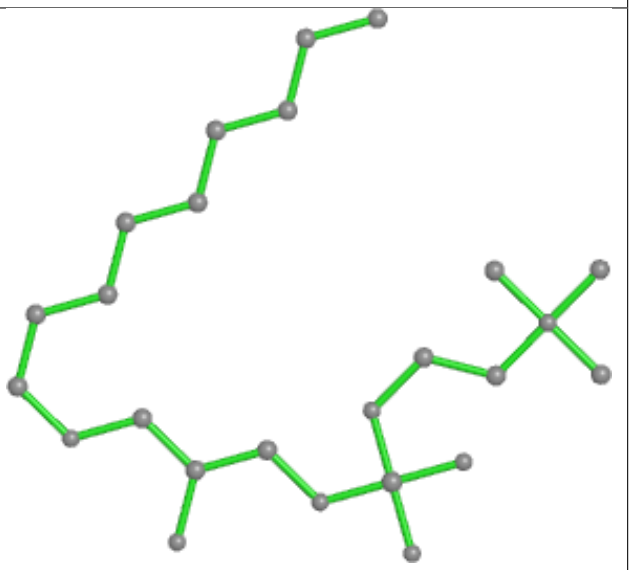


Rings

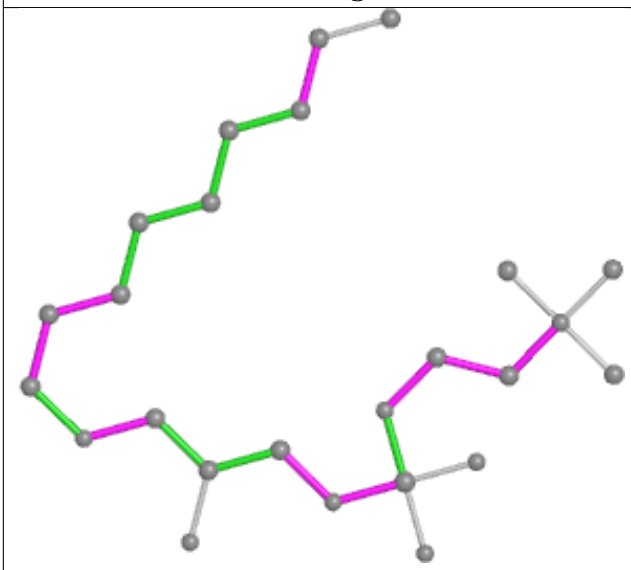
Ligand LPE A 2010



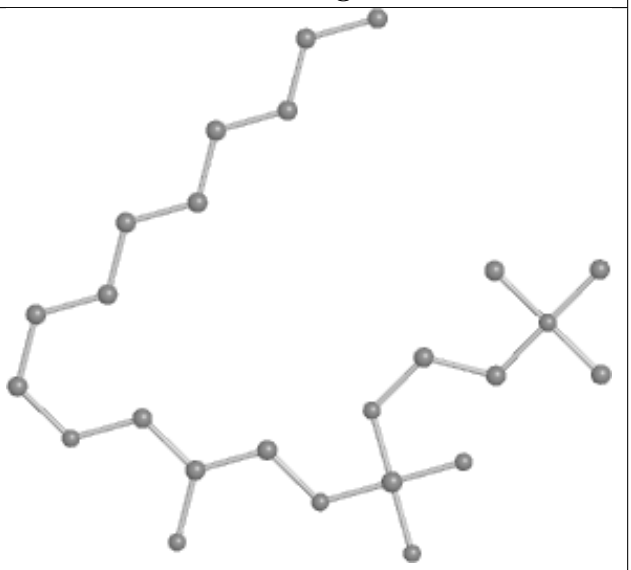
Bond lengths



Bond angles

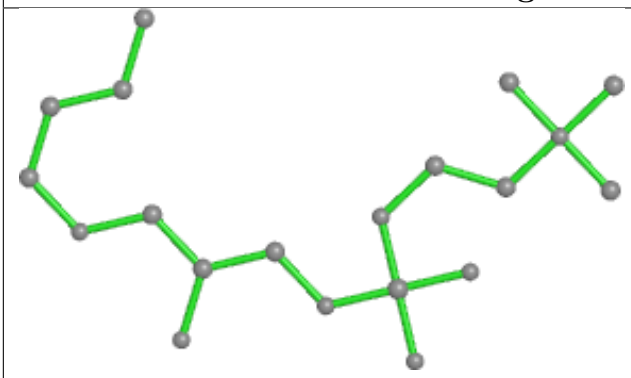


Torsions

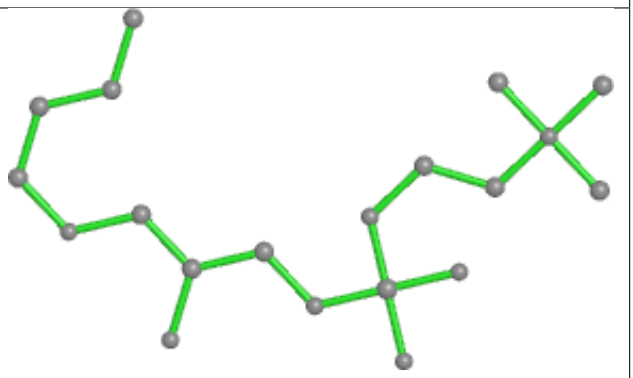


Rings

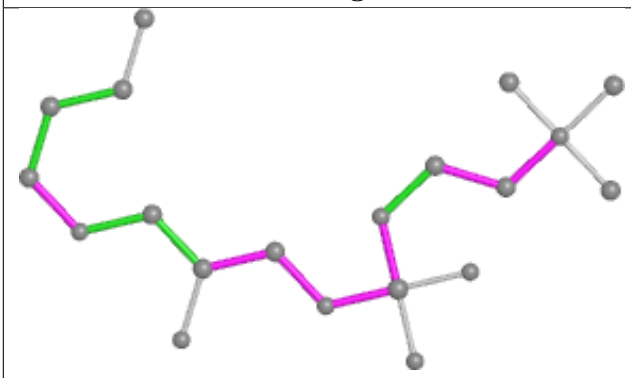
Ligand LPE A 2012



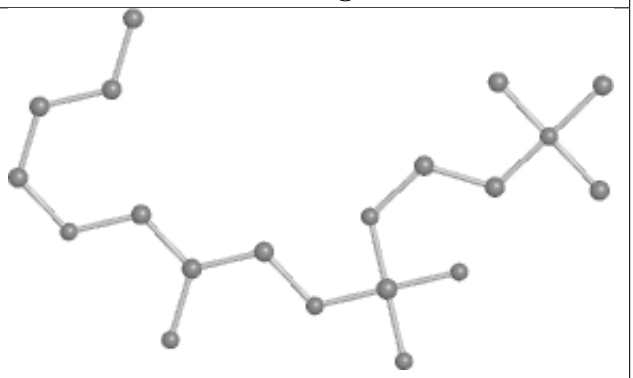
Bond lengths



Bond angles

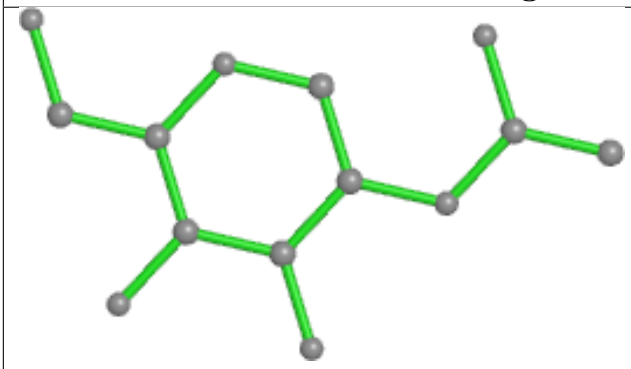


Torsions

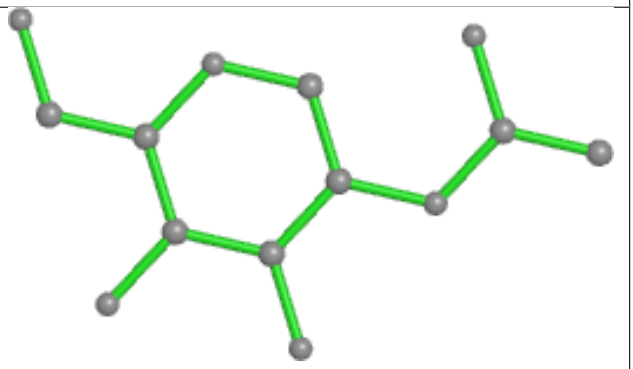


Rings

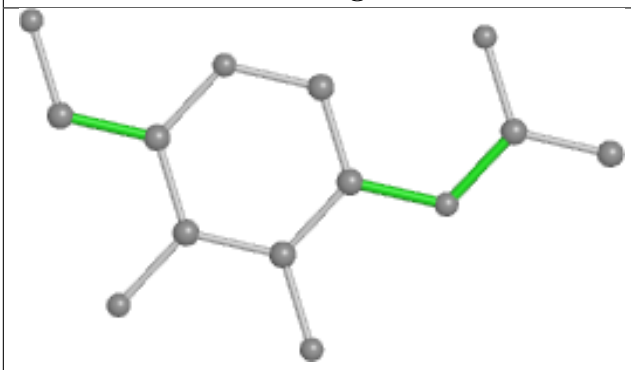
Ligand NAG B 301



Bond lengths



Bond angles



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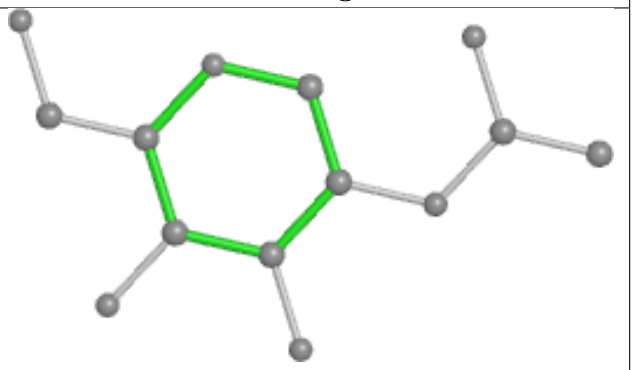
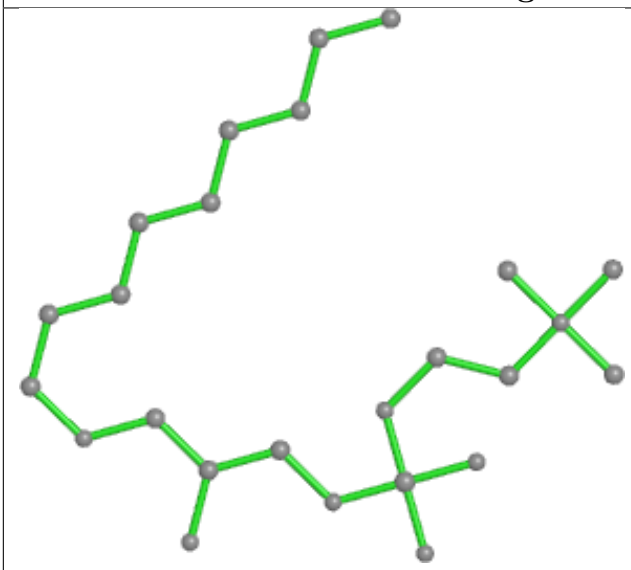


Rings

Ligand LPE A 2022



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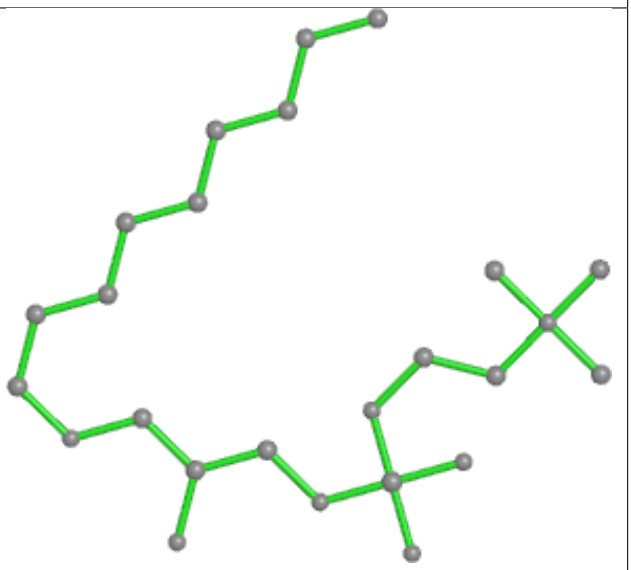
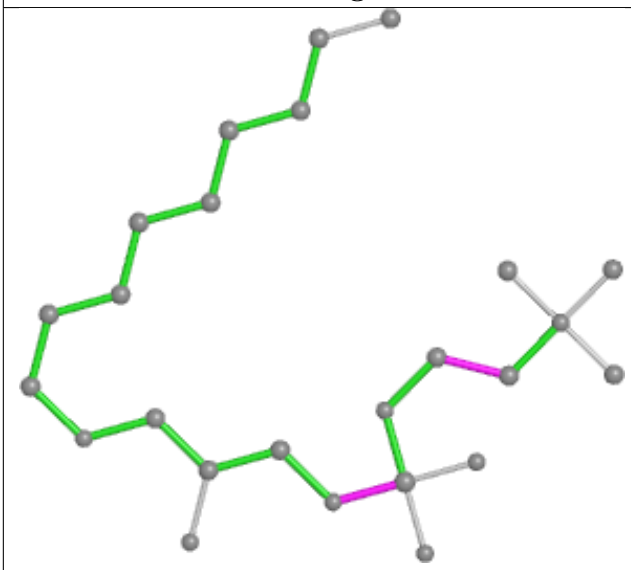


Bond angles



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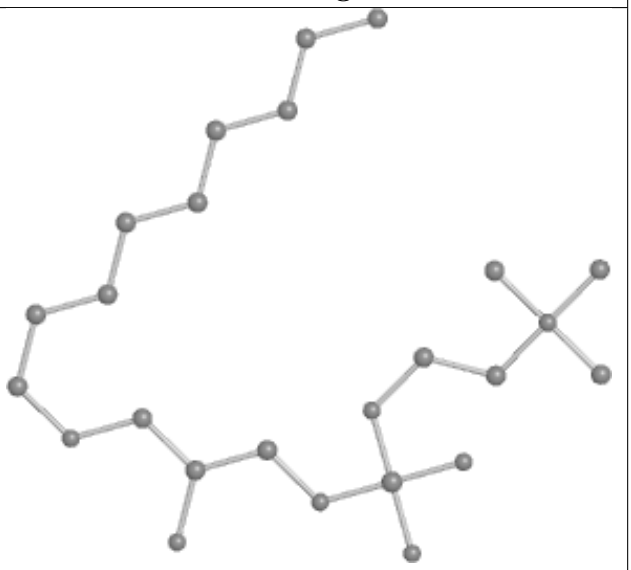
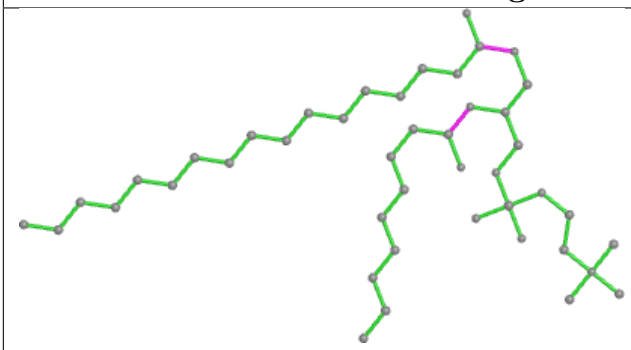
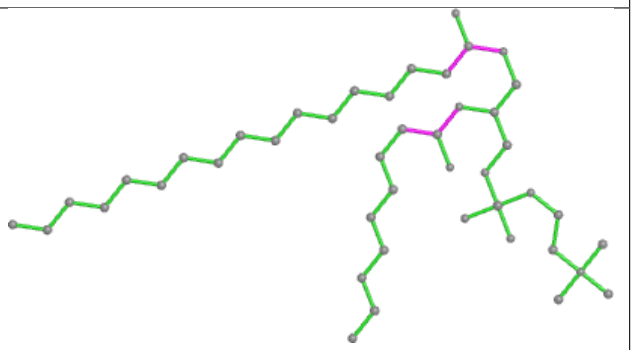


Rings

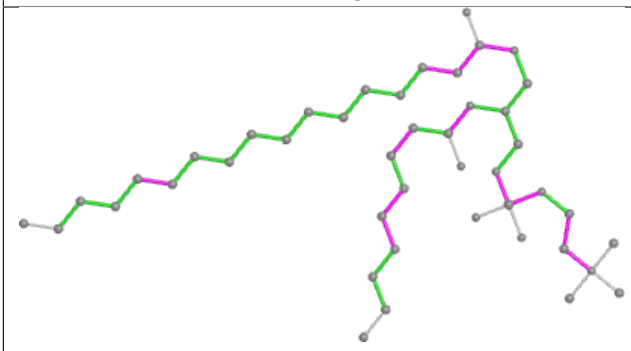
Ligand PCW A 2027



Bond lengths



Bond angles



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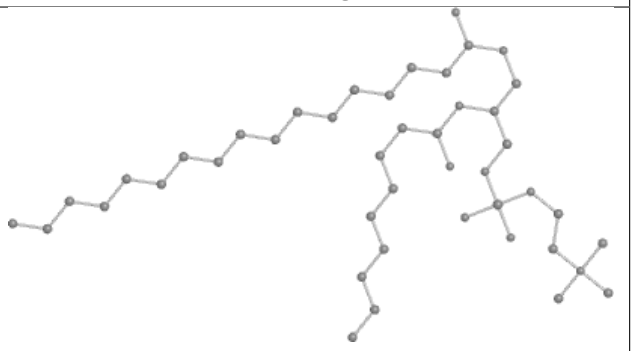
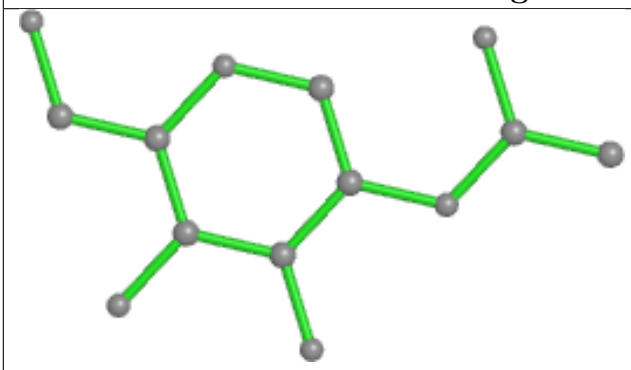


Rings

Ligand NAG A 2008



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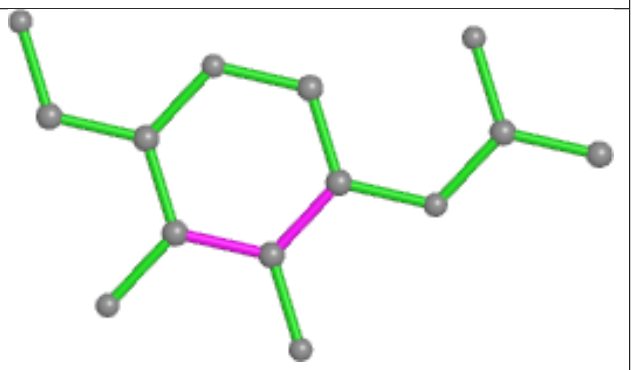
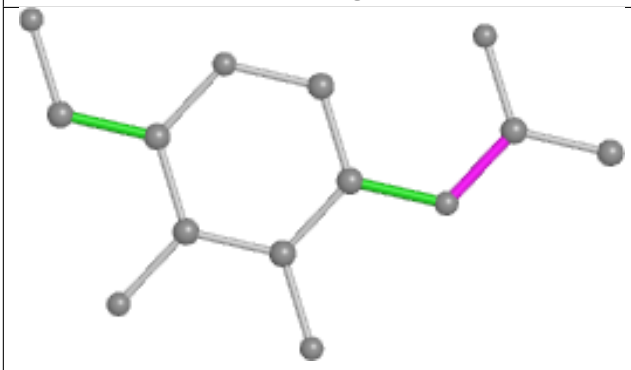
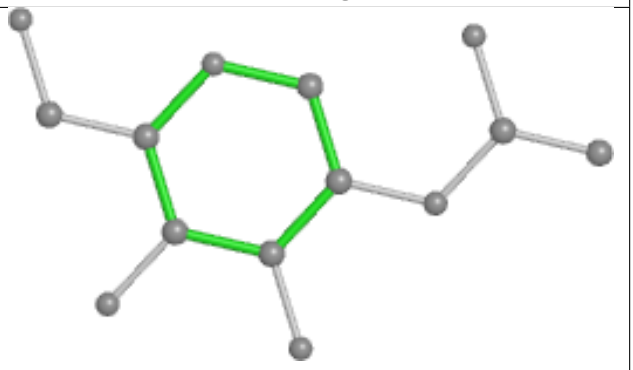


Bond angles

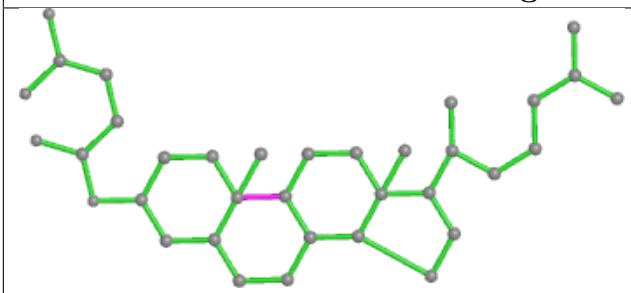


Torsions

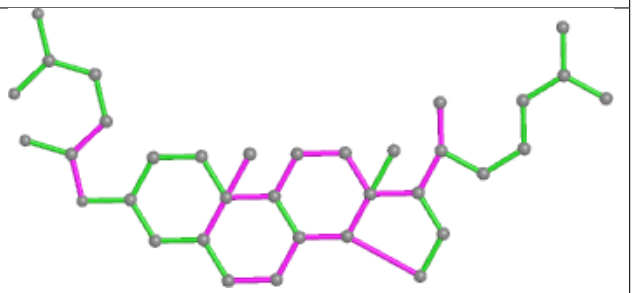


Rings

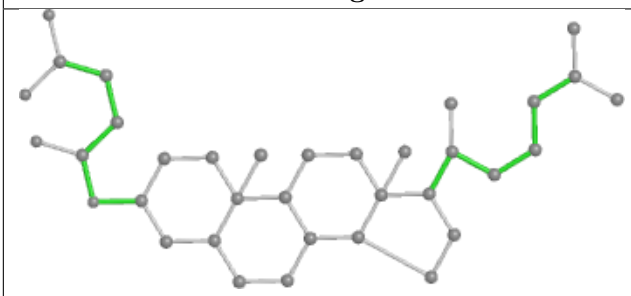
Ligand Y01 A 2005



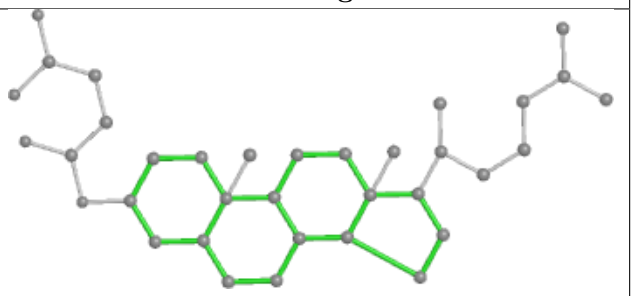
Bond lengths



Bond angles

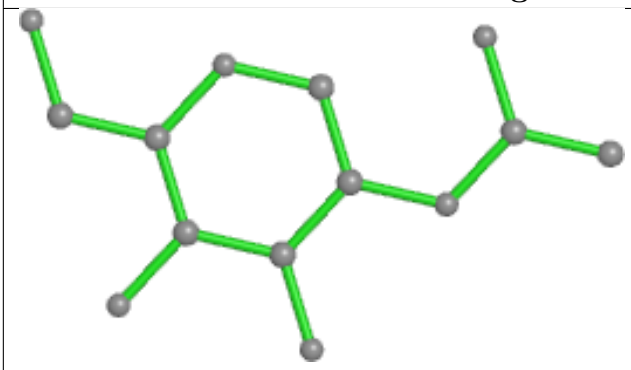


Torsions

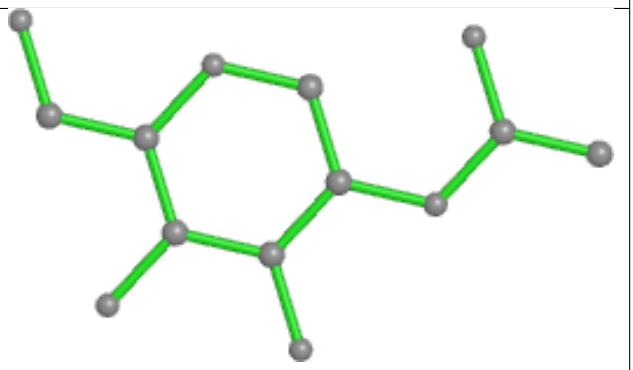


Rings

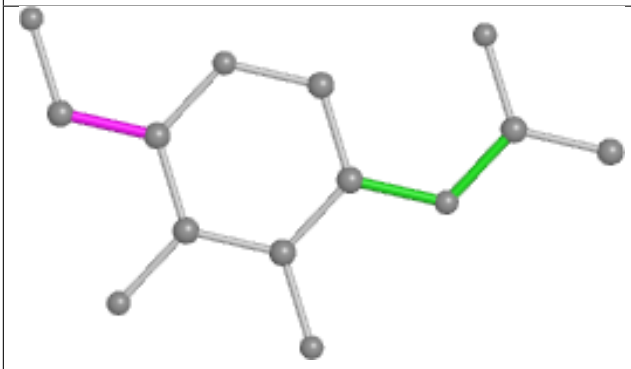
Ligand NAG A 2002



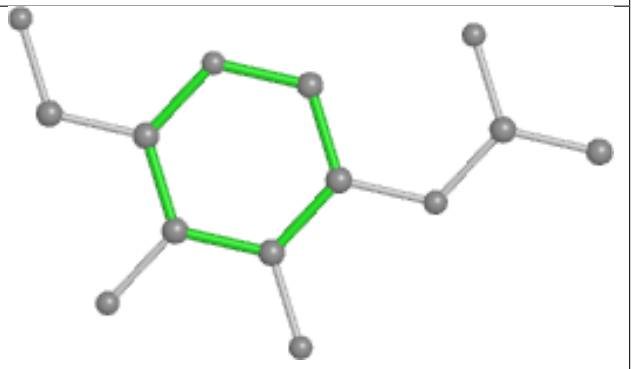
Bond lengths



Bond angles

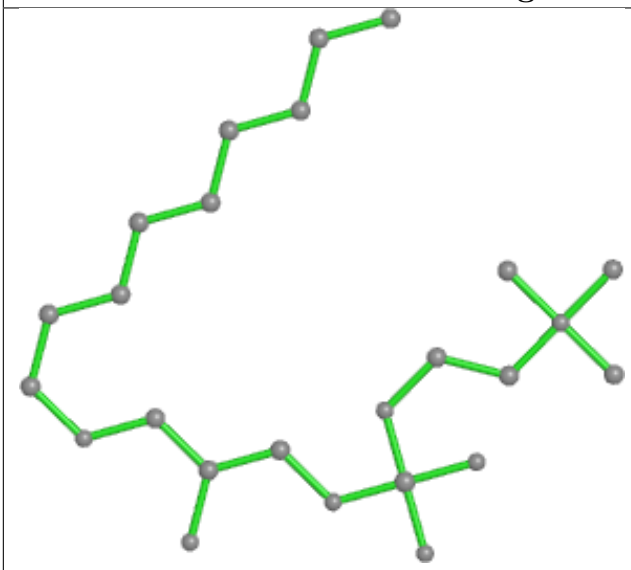


Torsions

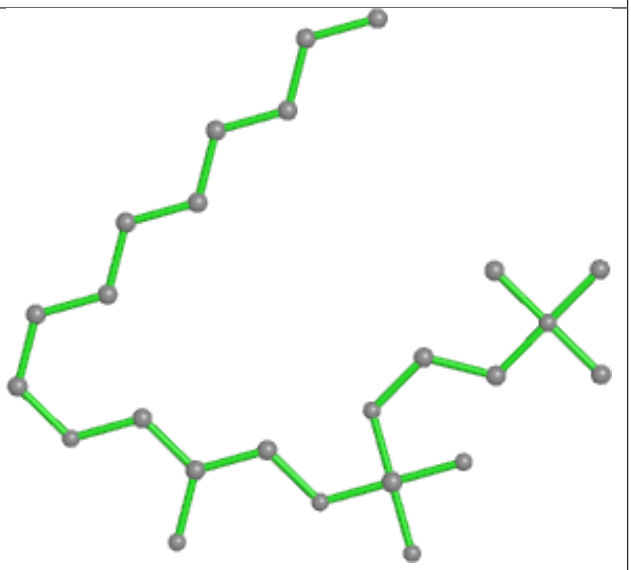


Rings

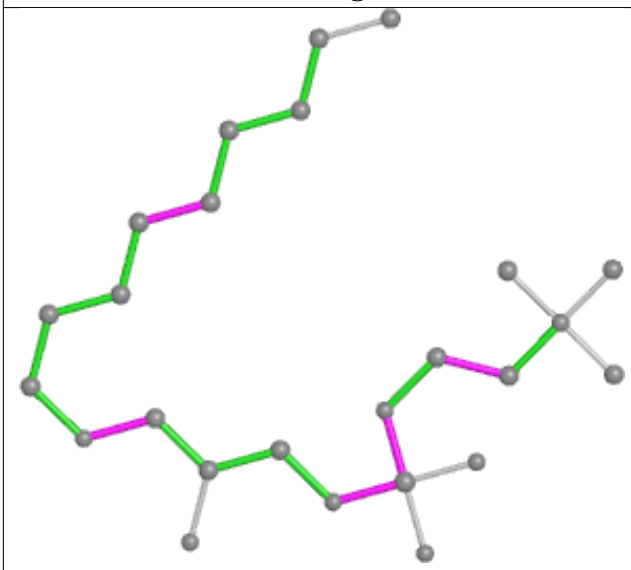
Ligand LPE A 2024



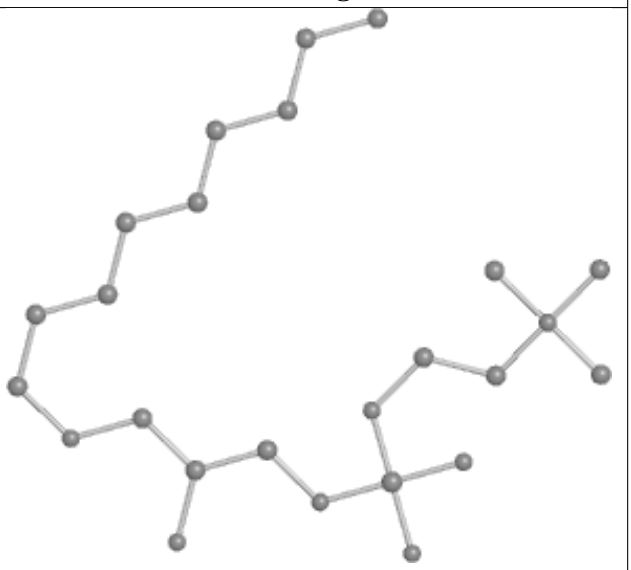
Bond lengths



Bond angles

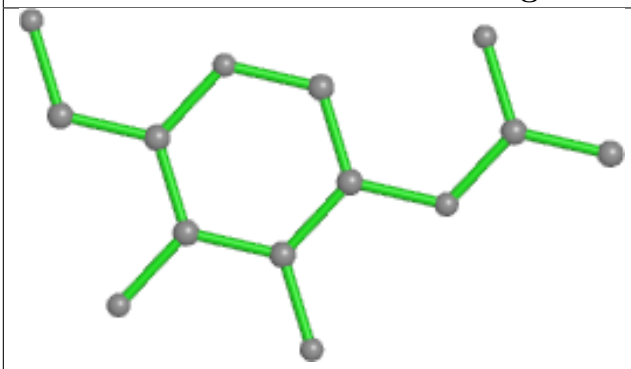


Torsions



Rings

Ligand NAG B 302



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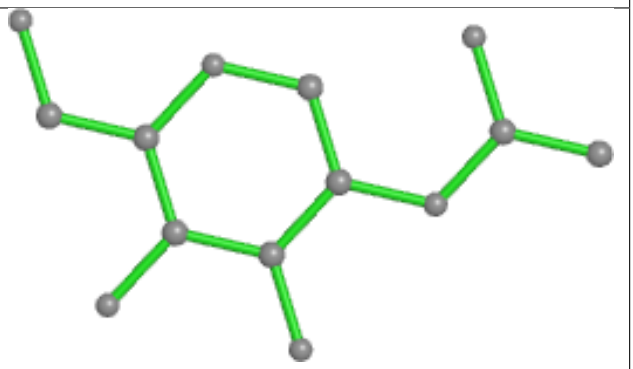
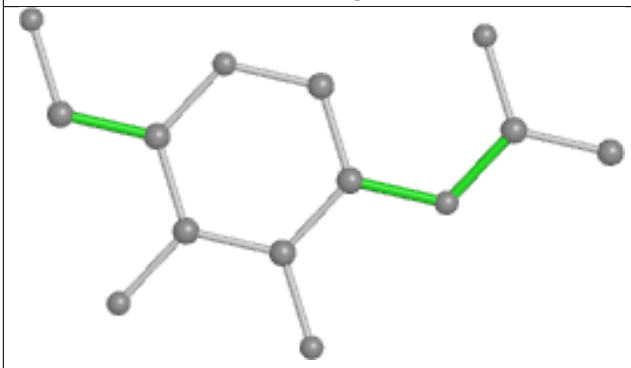


Bond angles



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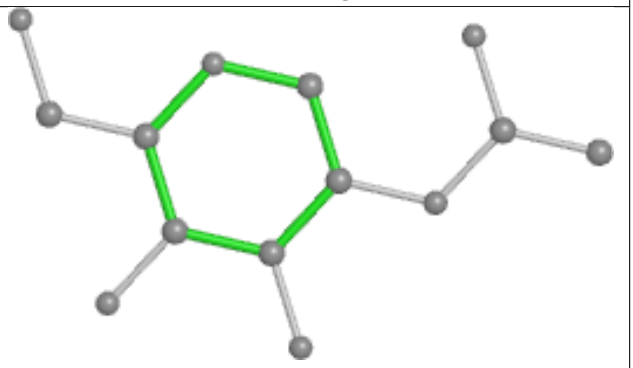
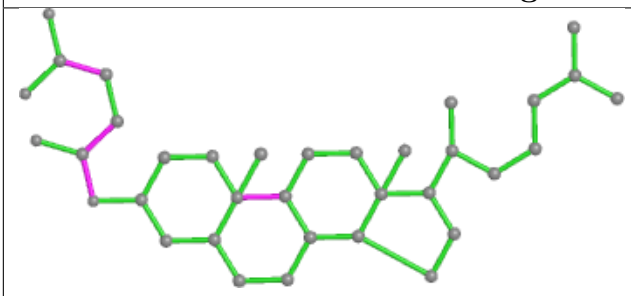


Rings

Ligand Y01 A 2006



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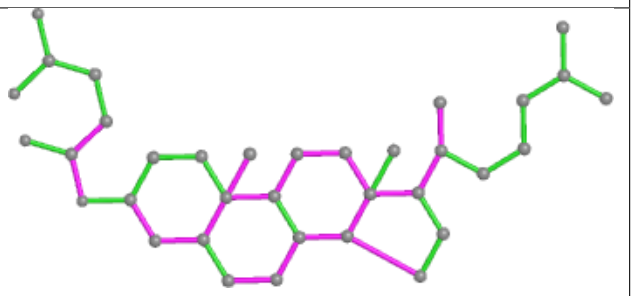
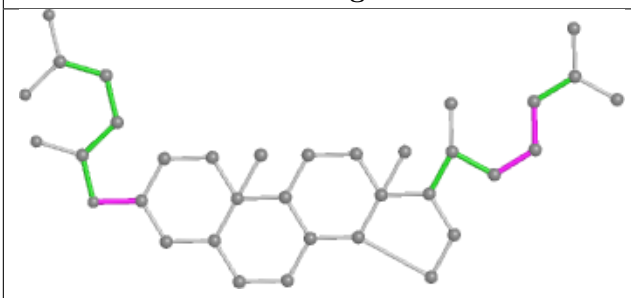


Bond angles



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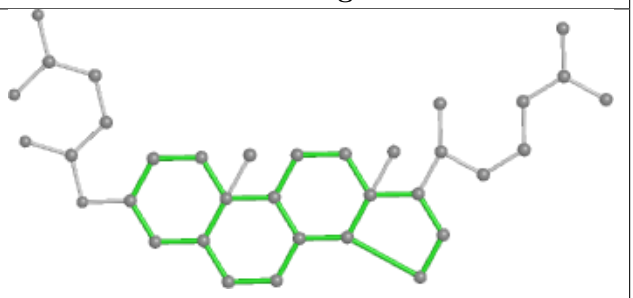
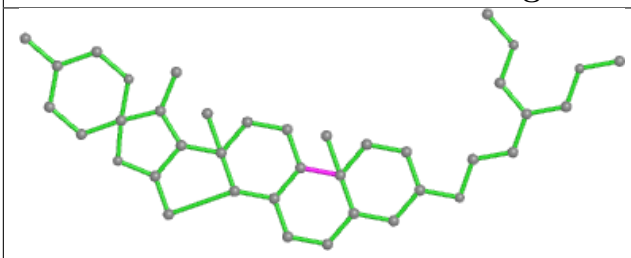


Rings

Ligand 9Z9 A 2007



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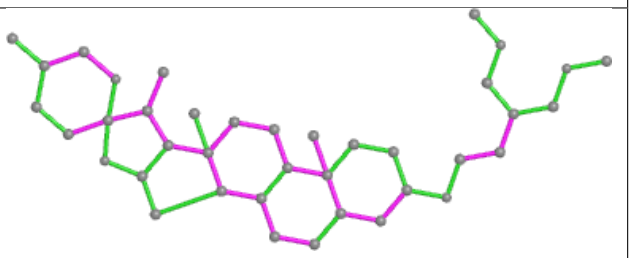
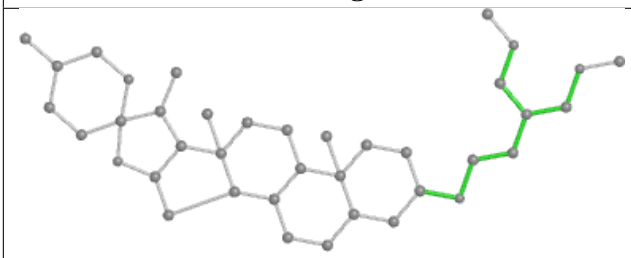


Bond angles



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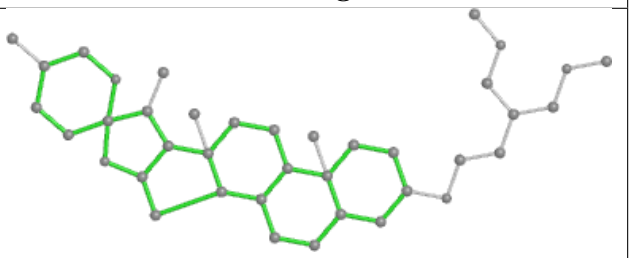
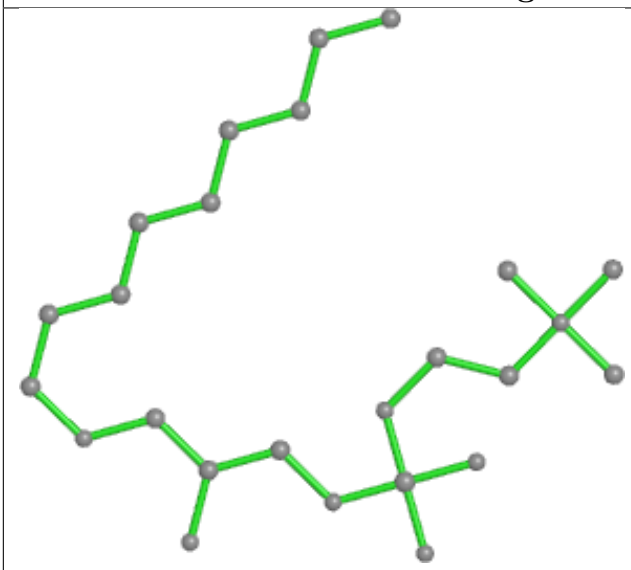


Rings

Ligand LPE A 2021



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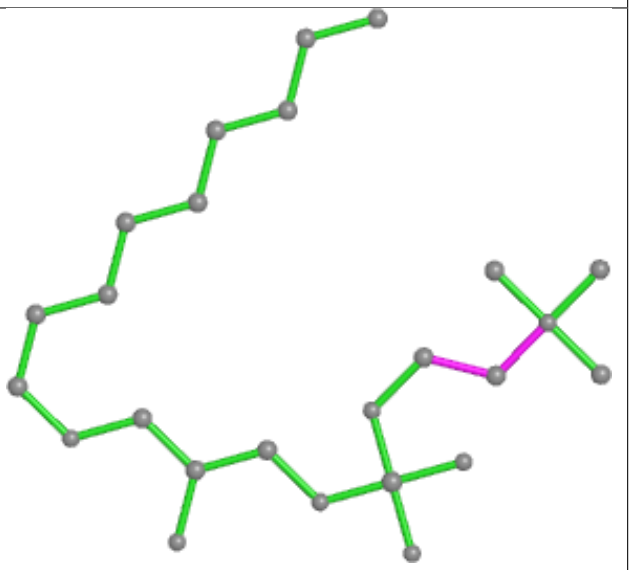

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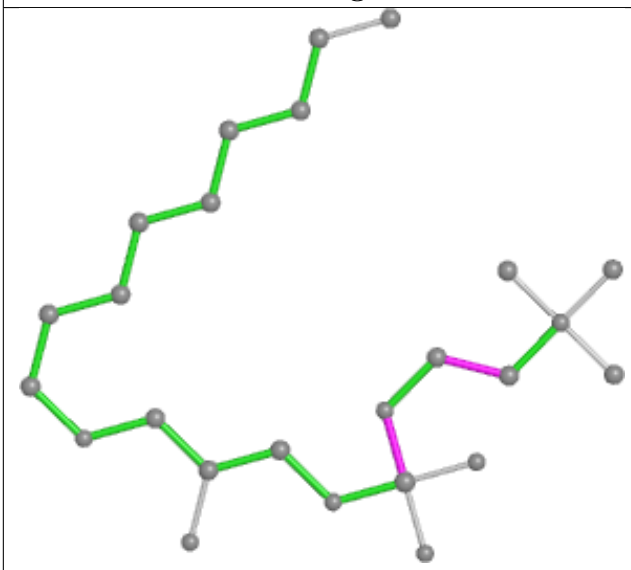

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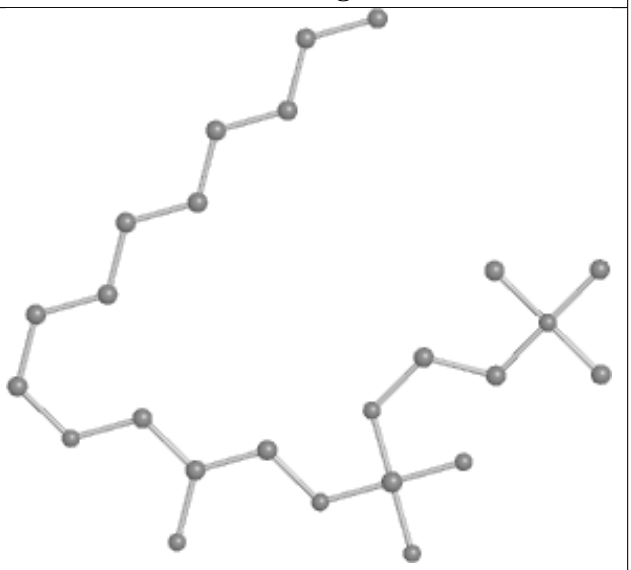
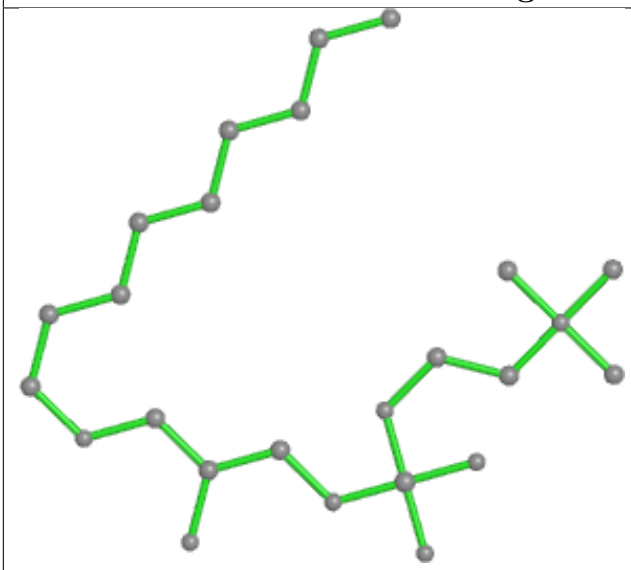


Rings

Ligand LPE A 2020



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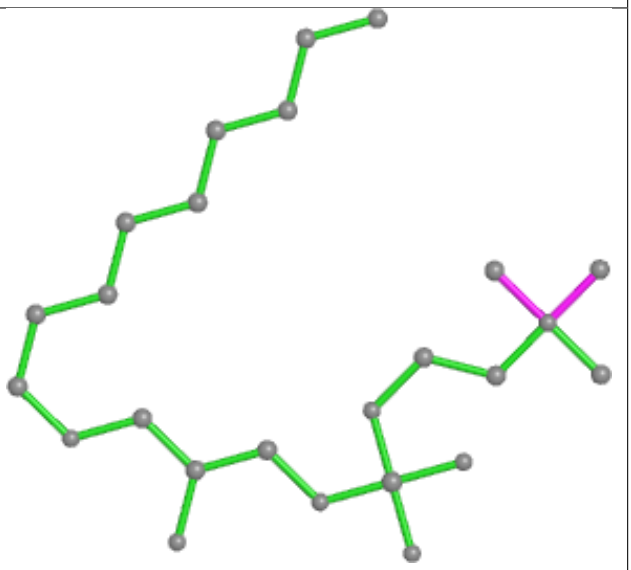
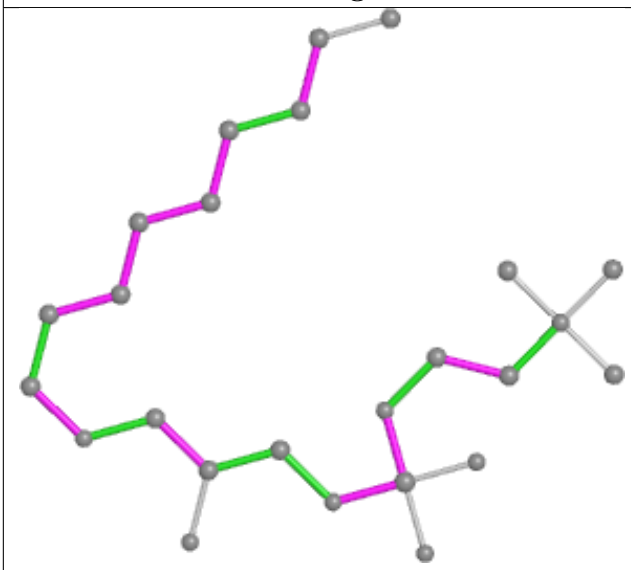


Bond angles



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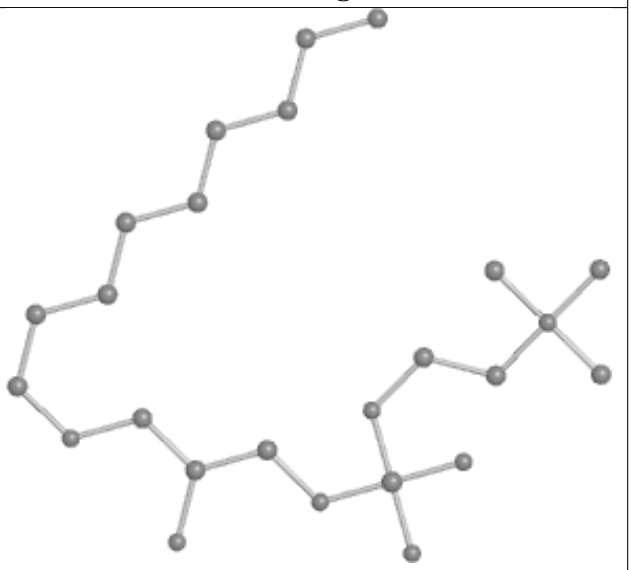
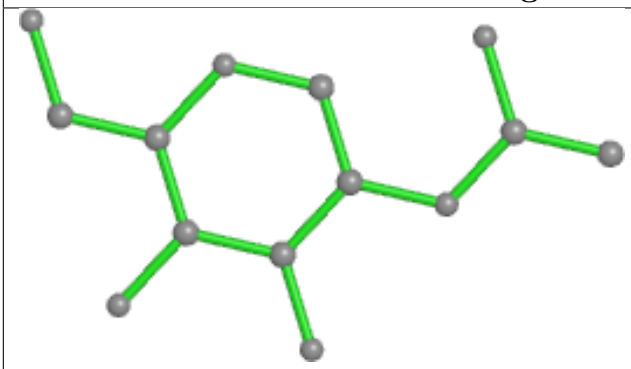


Rings

Ligand NAG B 303



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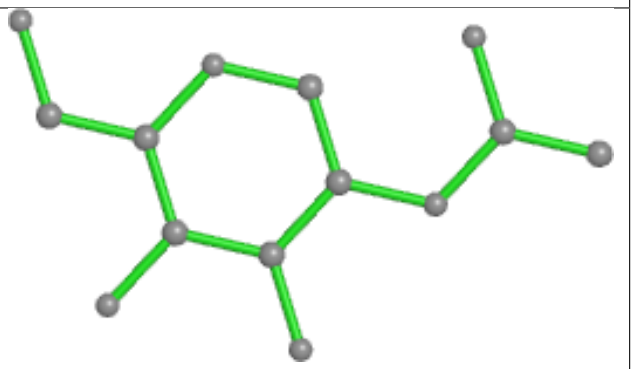
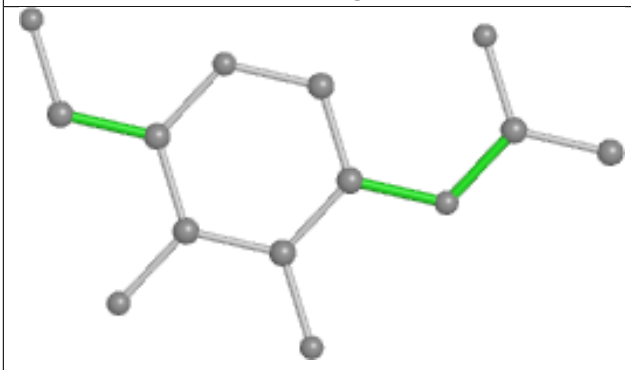


Bond angles



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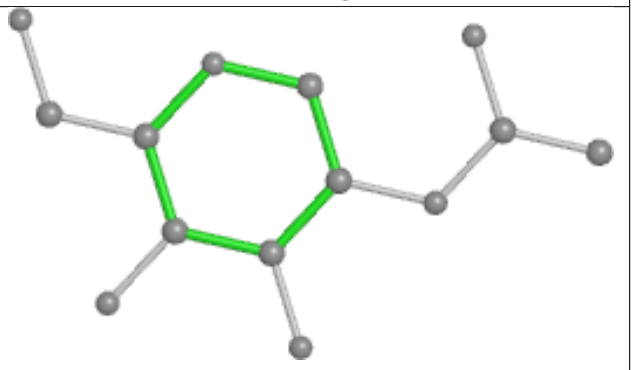
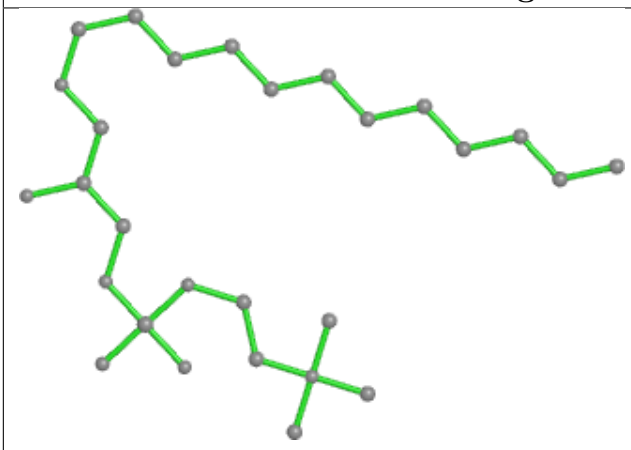


Rings

Ligand LPE A 2015



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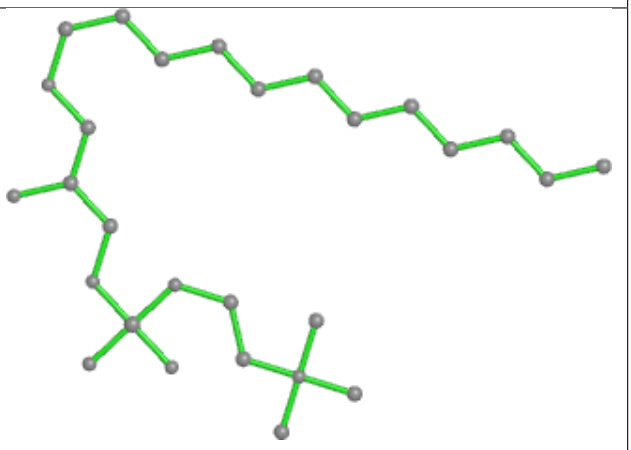
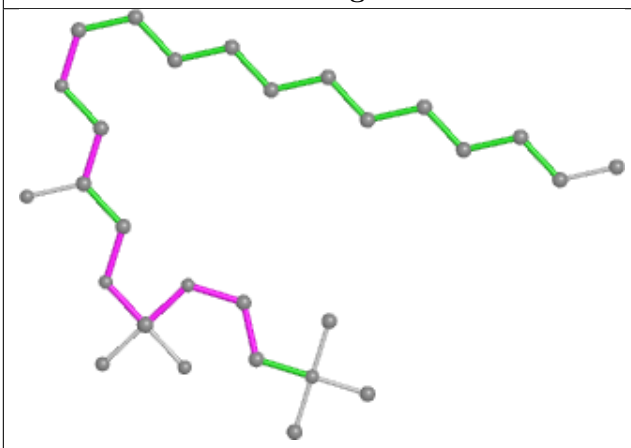


Bond angles



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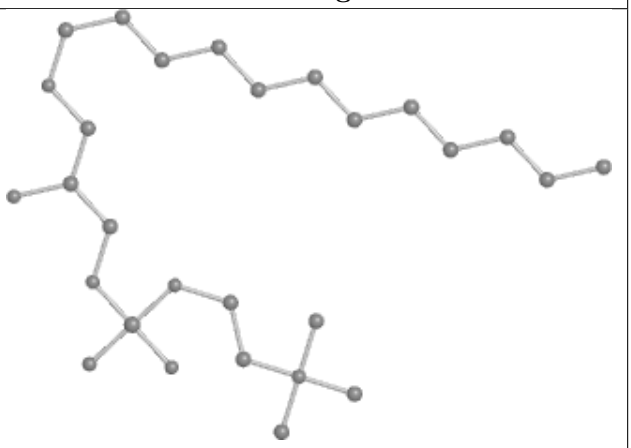
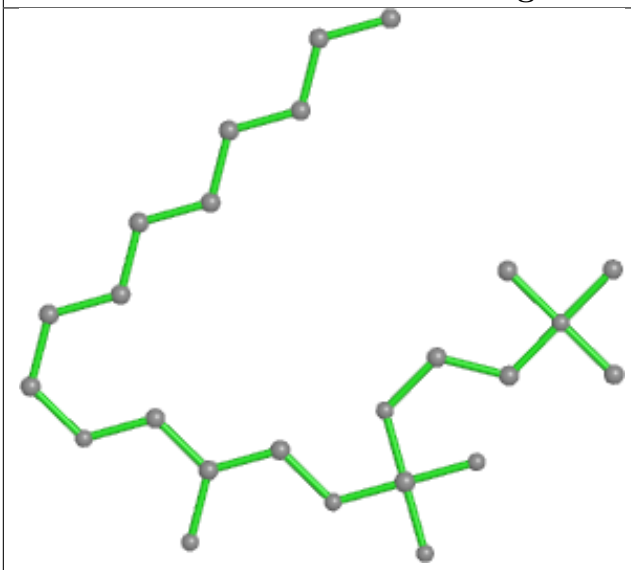


Rings

Ligand LPE A 2023



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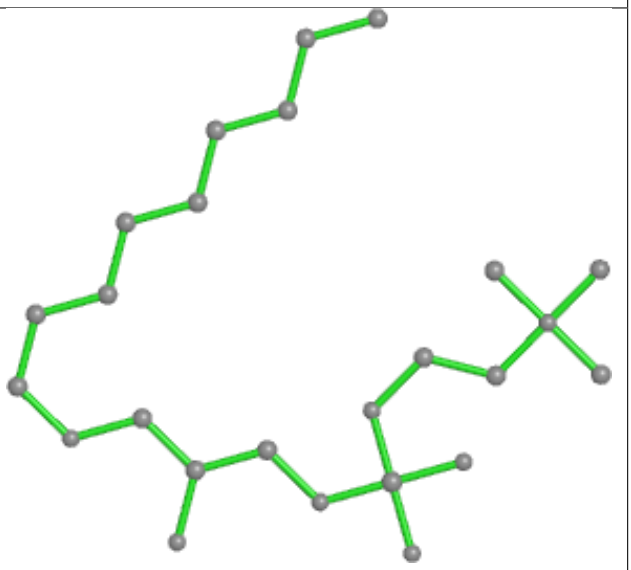
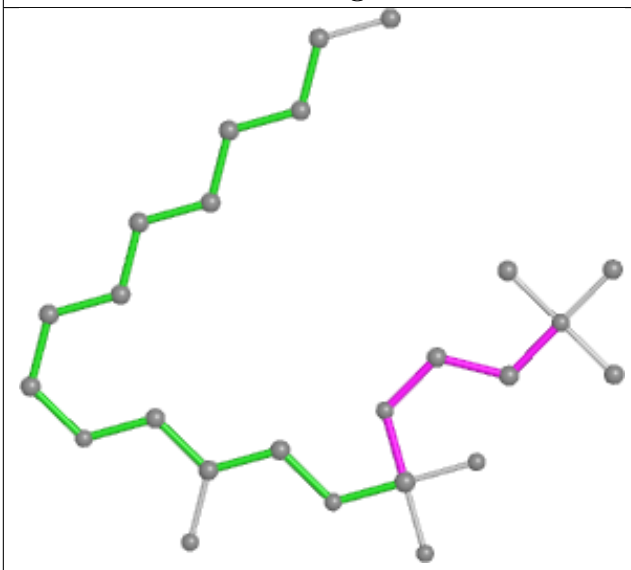


Bond angles



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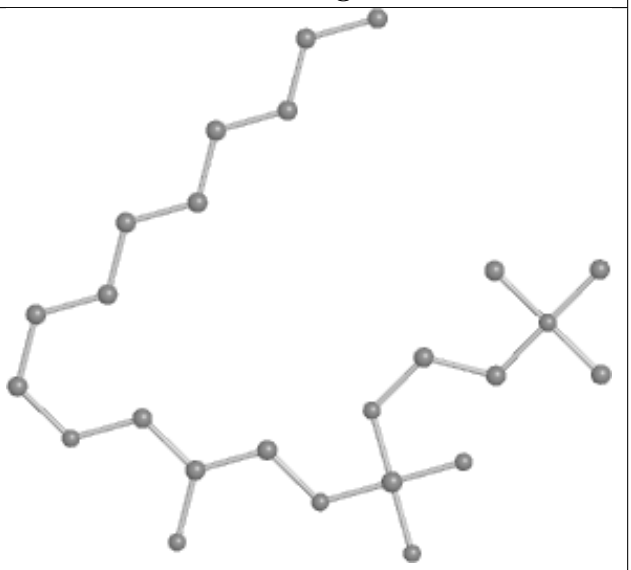
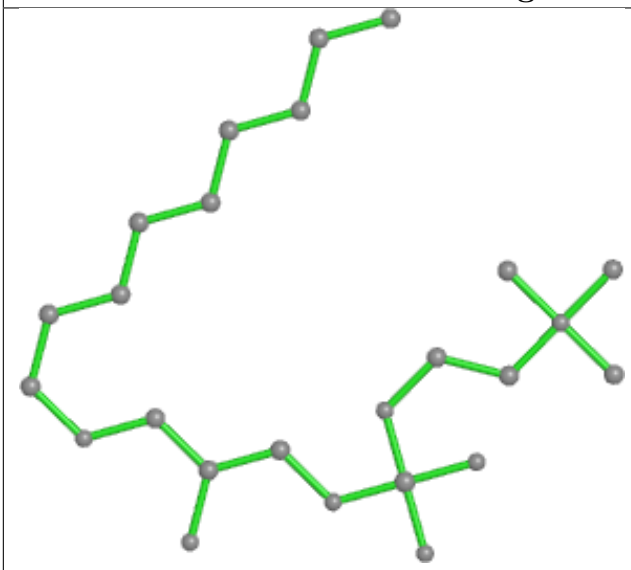


Rings

Ligand LPE A 2025



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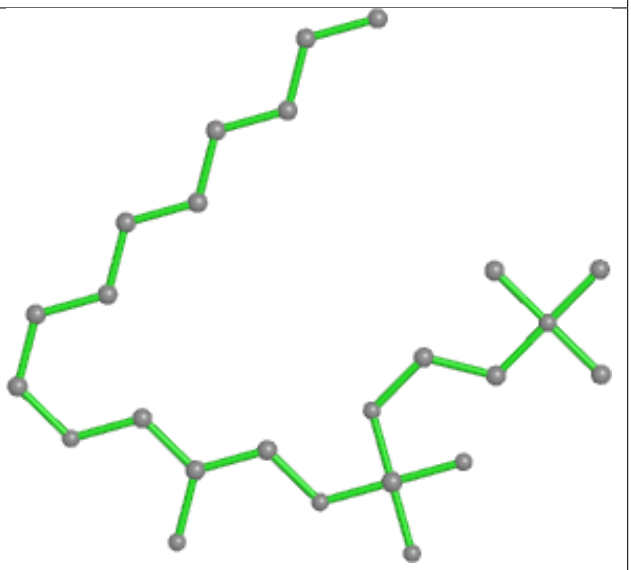
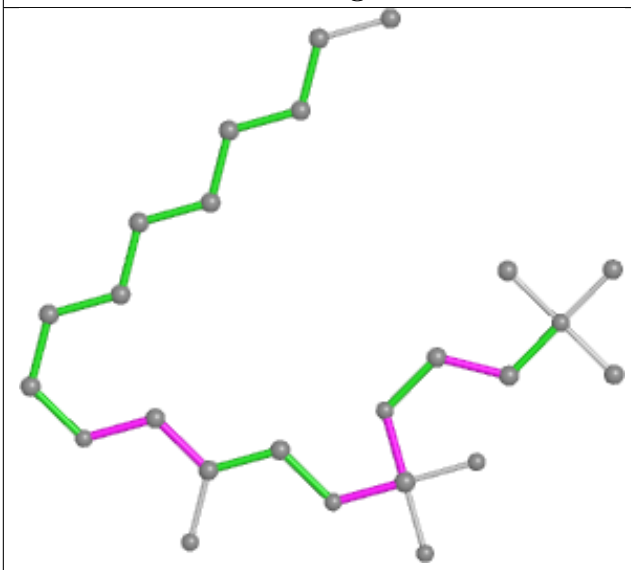


Bond angles



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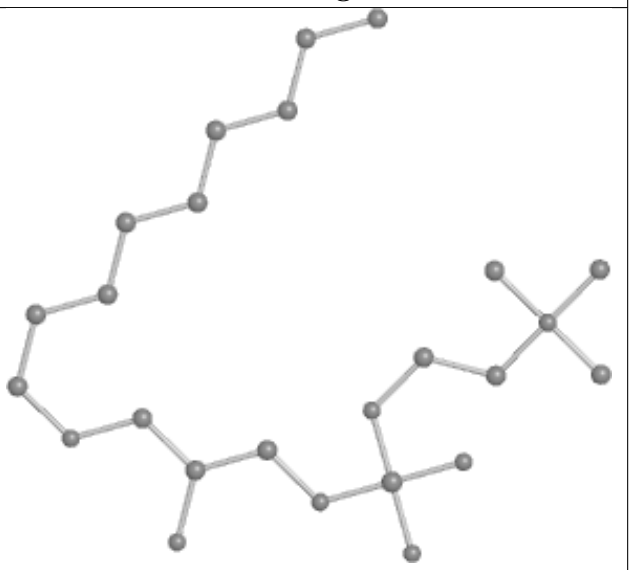
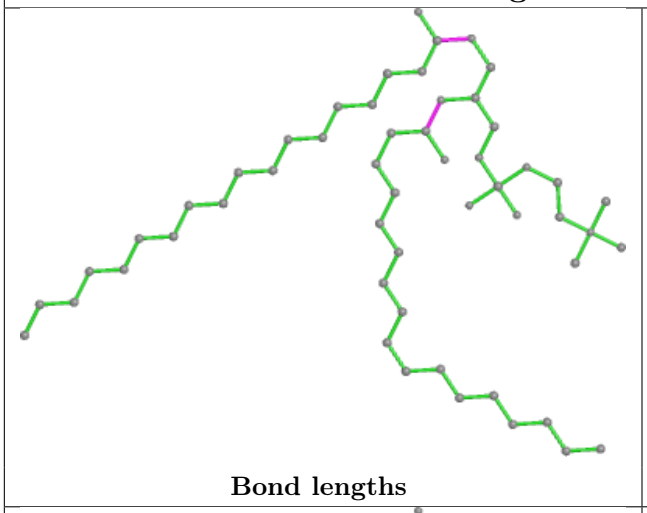


Rings

Ligand PCW A 2013



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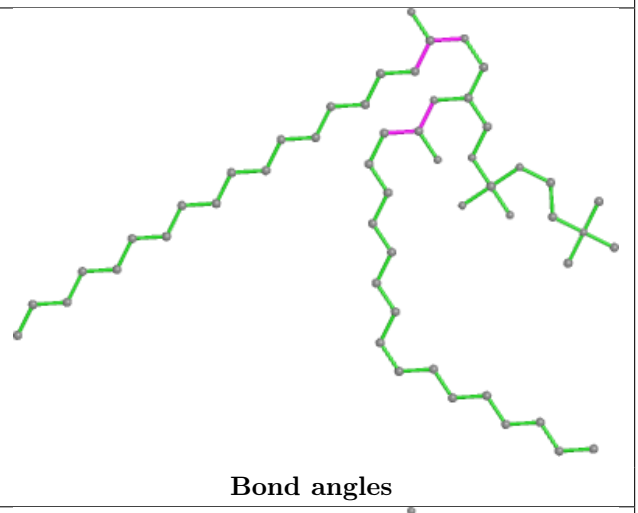
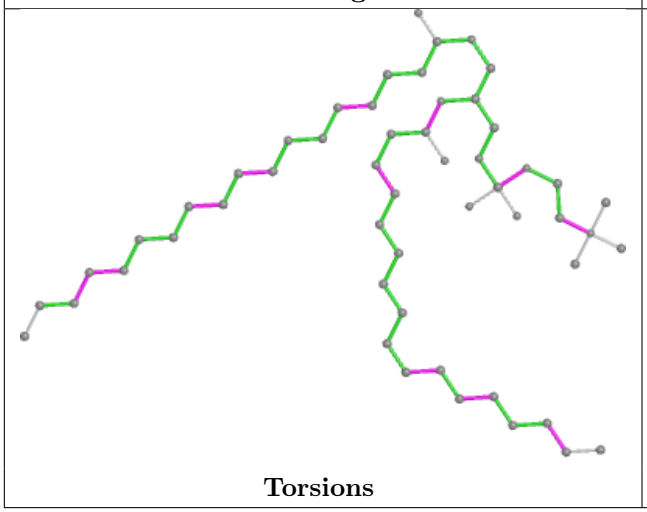


Bond angles



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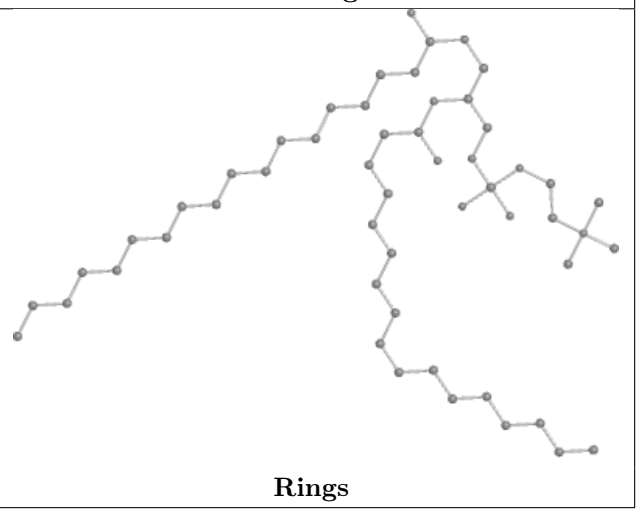
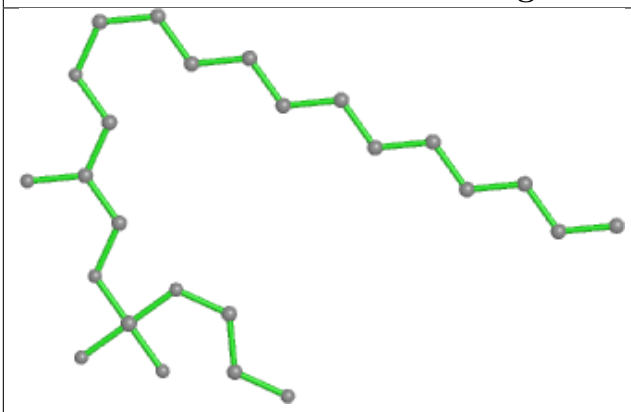


Rings

Ligand LPE A 2011



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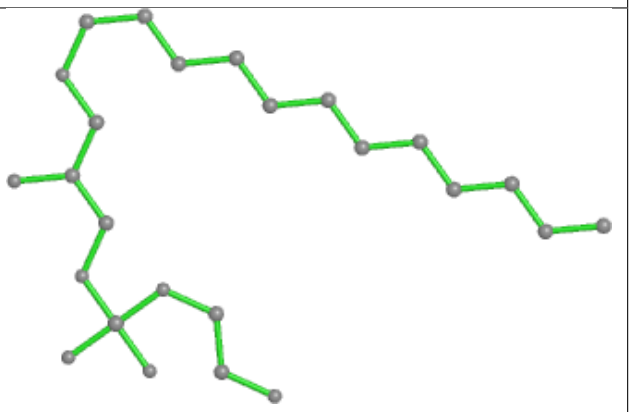
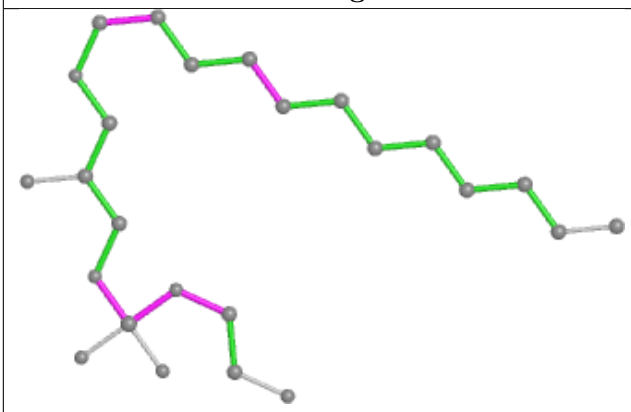


Bond angles



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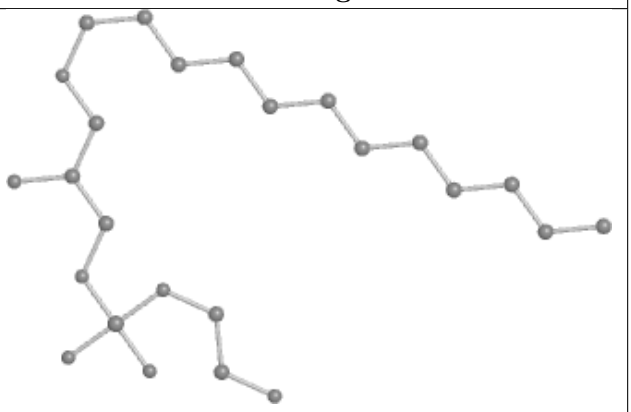
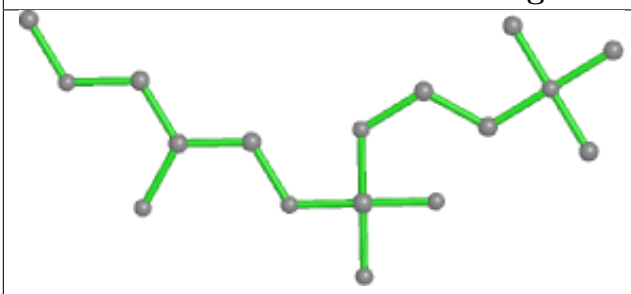


Rings

Ligand LPE B 304



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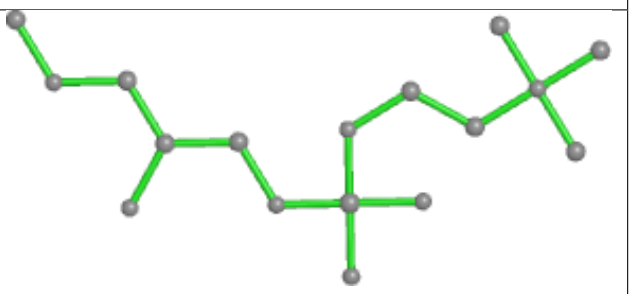
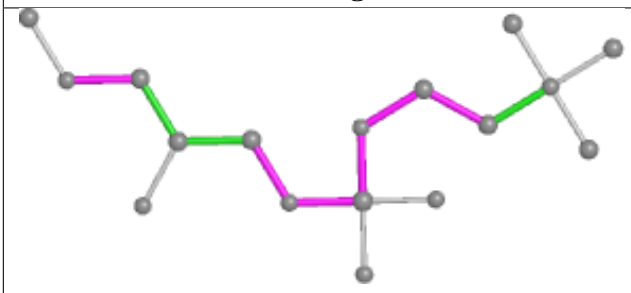


Bond angles



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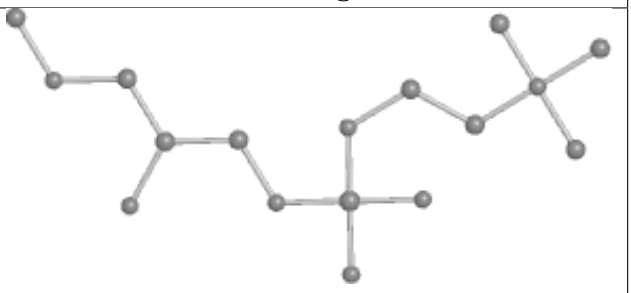
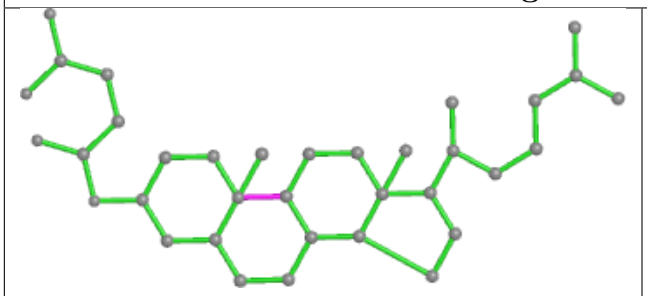


Rings

Ligand Y01 A 2004



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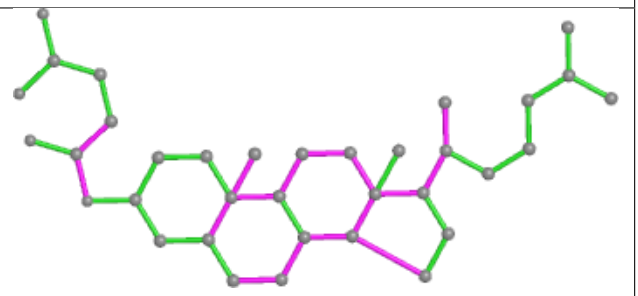
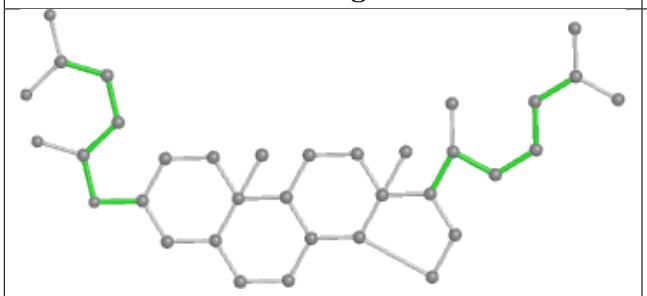
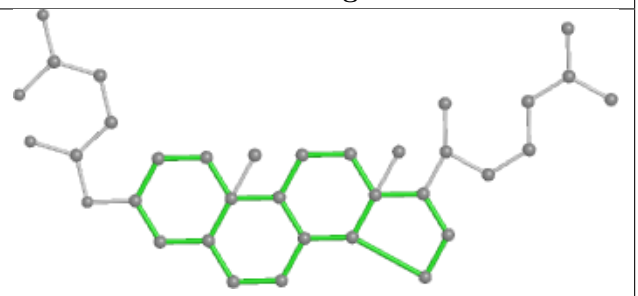


Bond angles

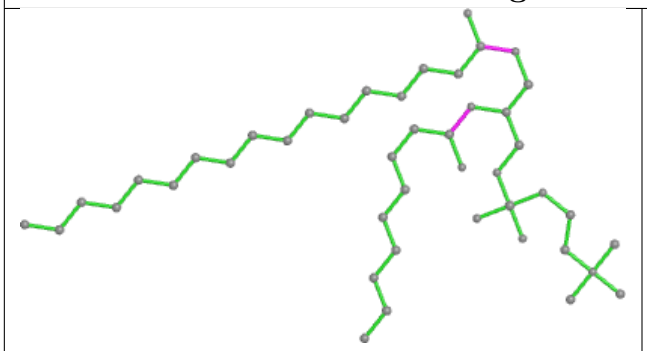


Torsions



Rings

Ligand PCW A 2018



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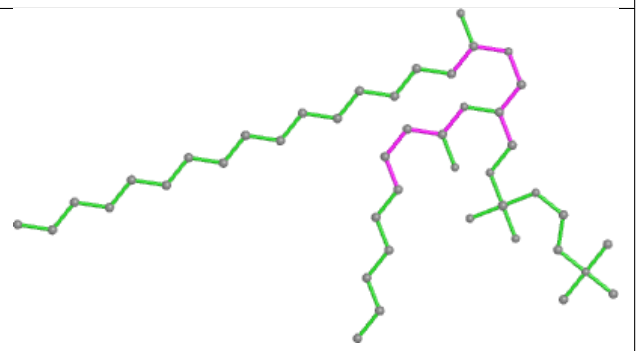
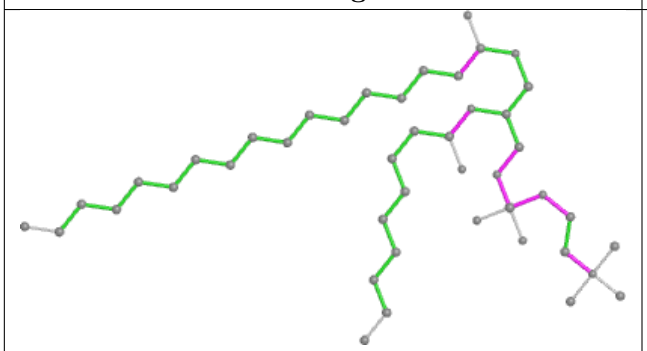
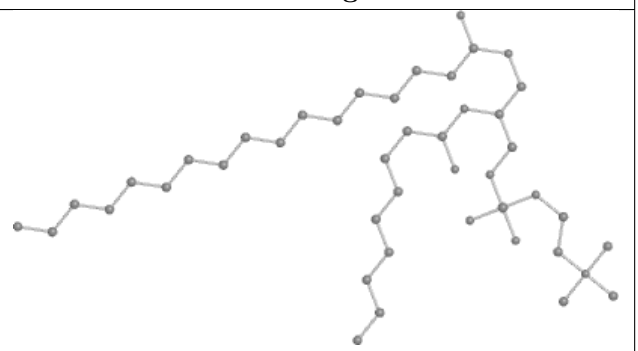


Bond angles

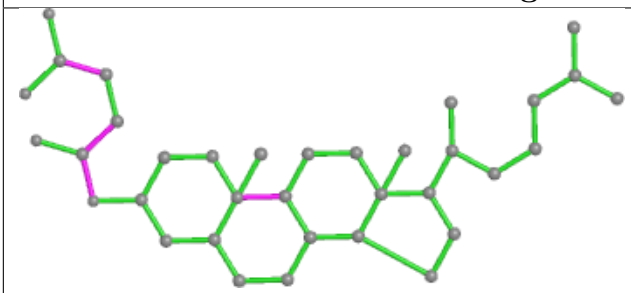


Torsions

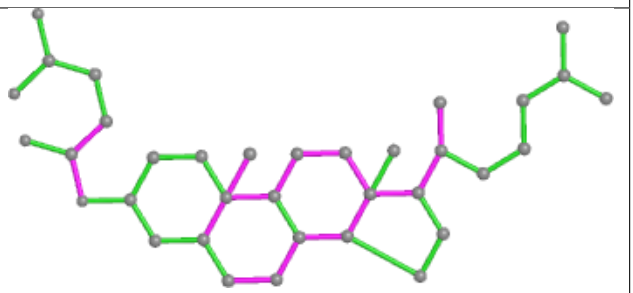


Rings

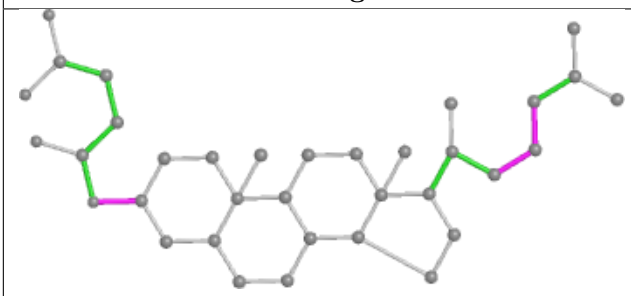
Ligand Y01 A 2009



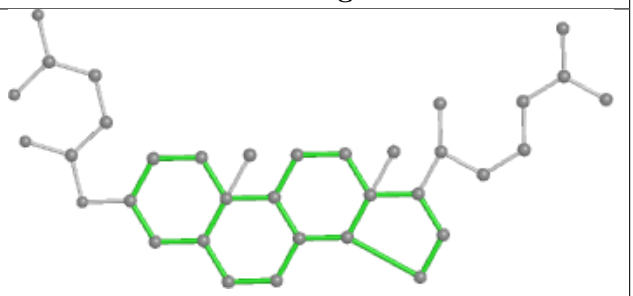
Bond lengths



Bond angles

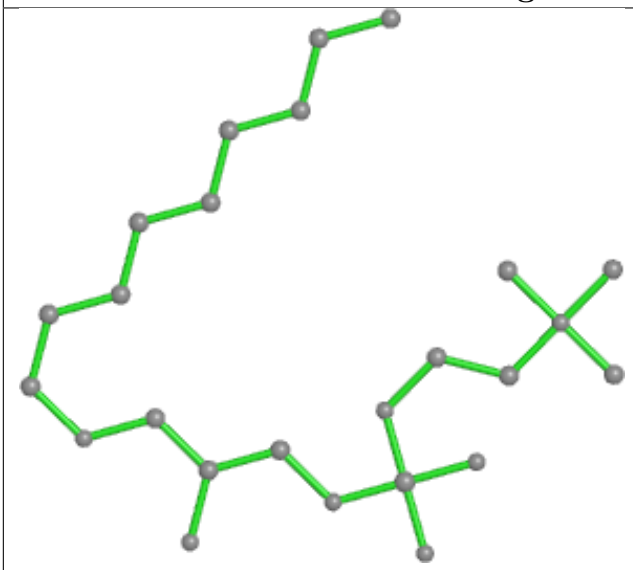


Torsions

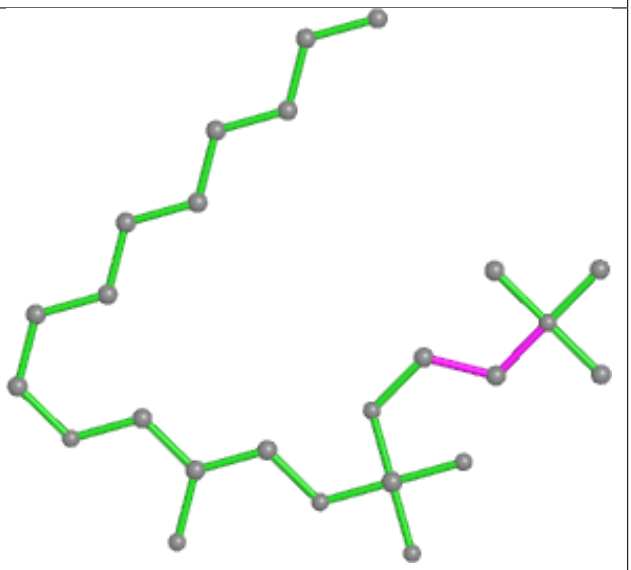


Rings

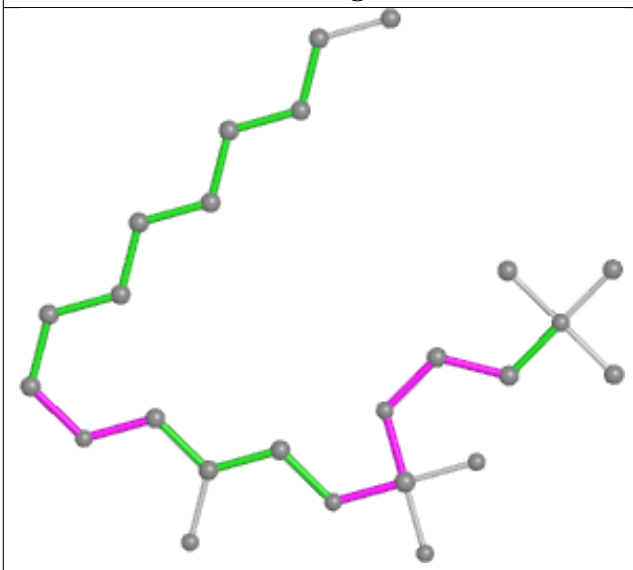
Ligand LPE A 2019



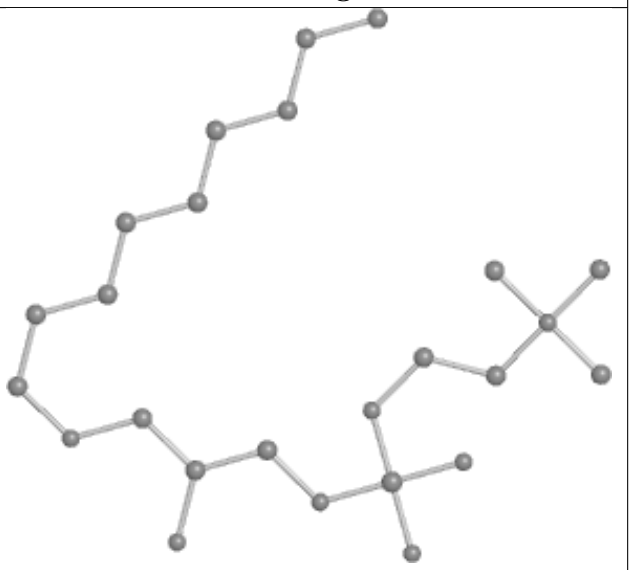
Bond lengths



Bond angles

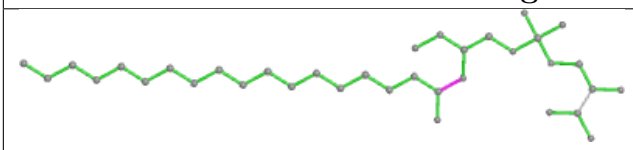


Torsions

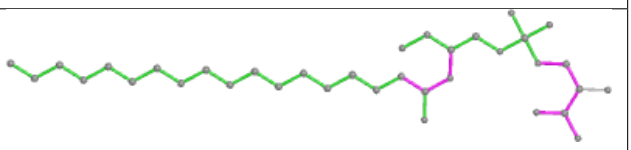


Rings

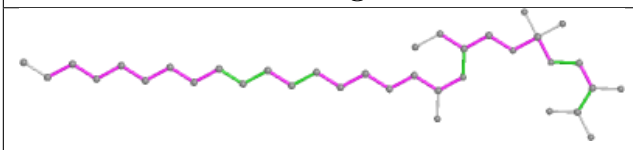
Ligand P5S A 2003



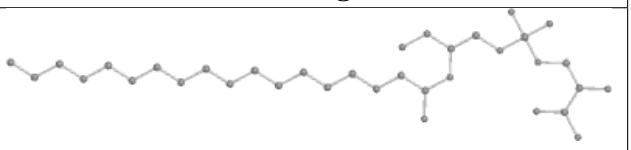
Bond lengths



Bond angles

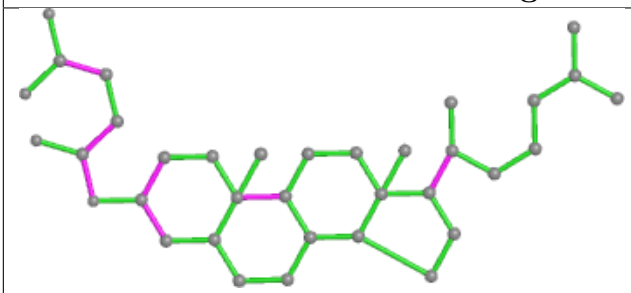


Torsions

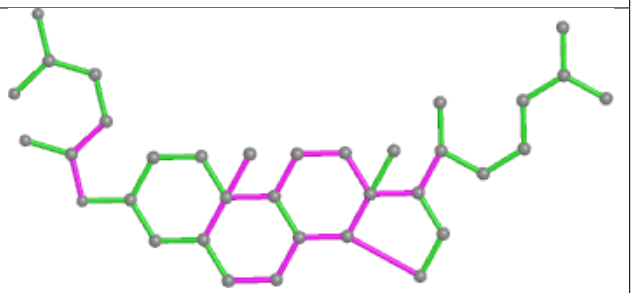


Rings

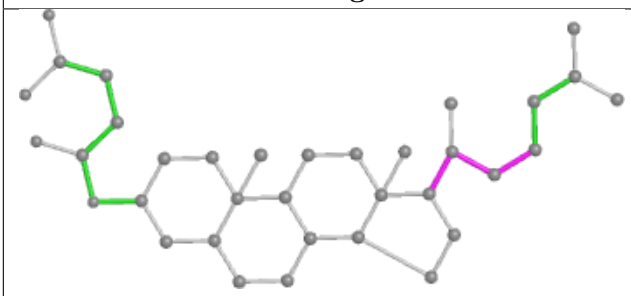
Ligand Y01 A 2029



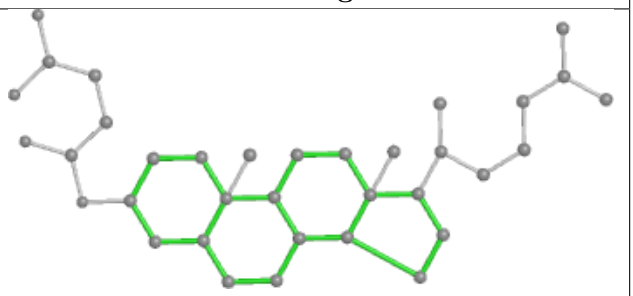
Bond lengths



Bond angles

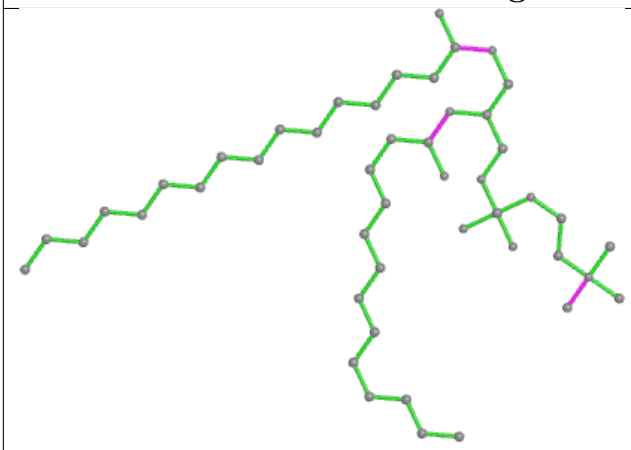


Torsions

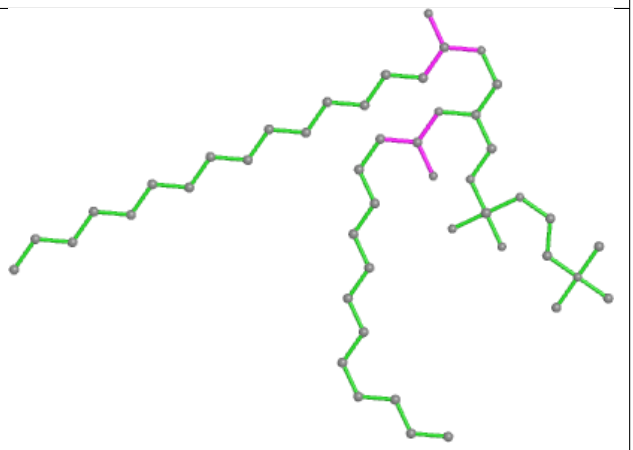


Rings

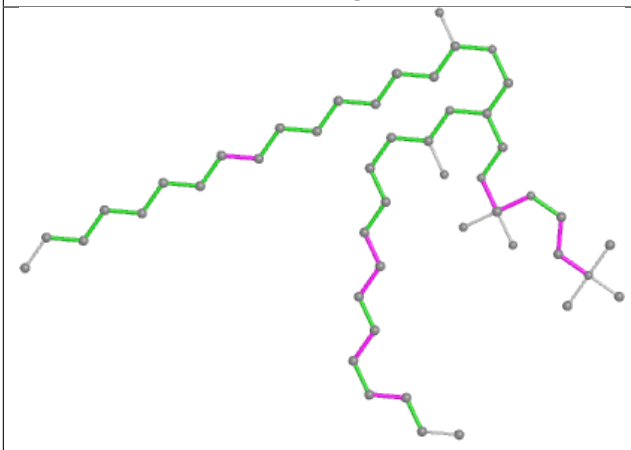
Ligand PCW A 2016



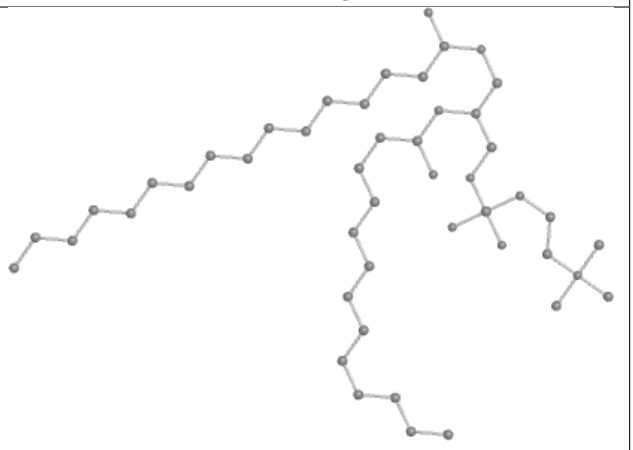
Bond lengths



Bond angles

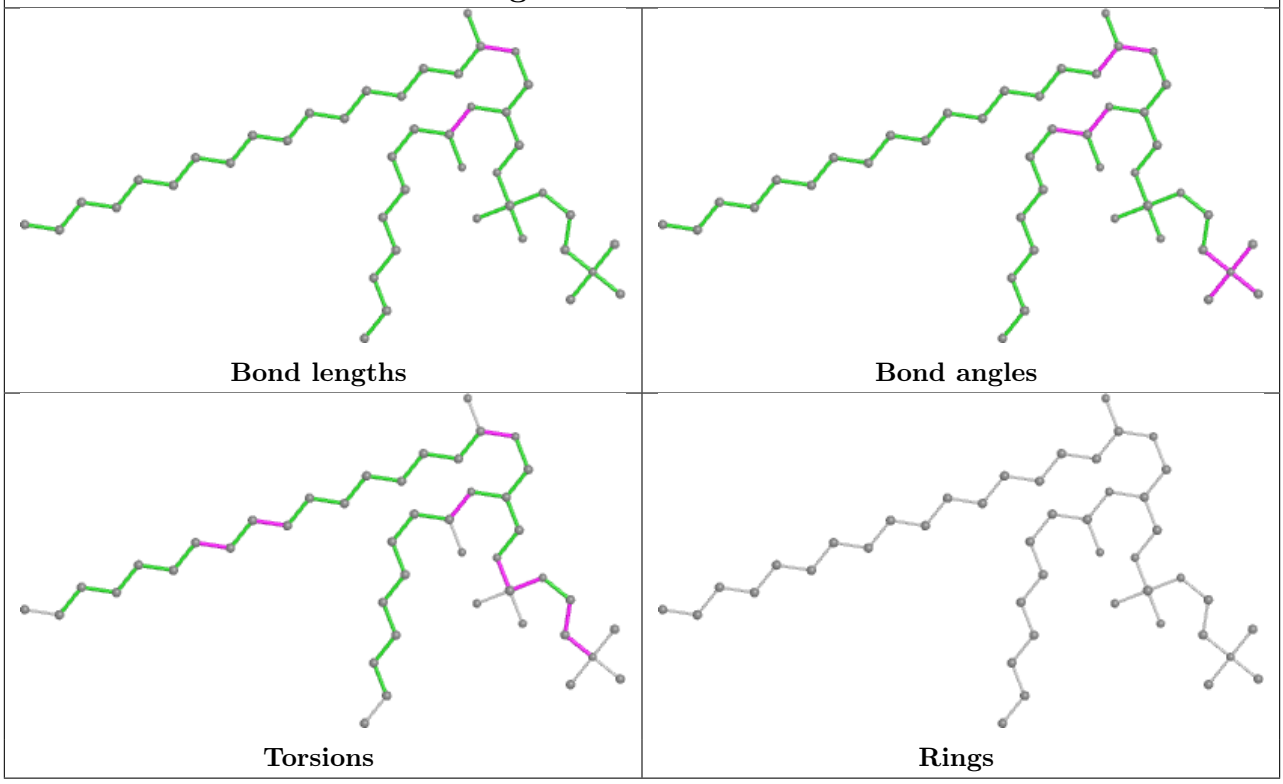


Torsions

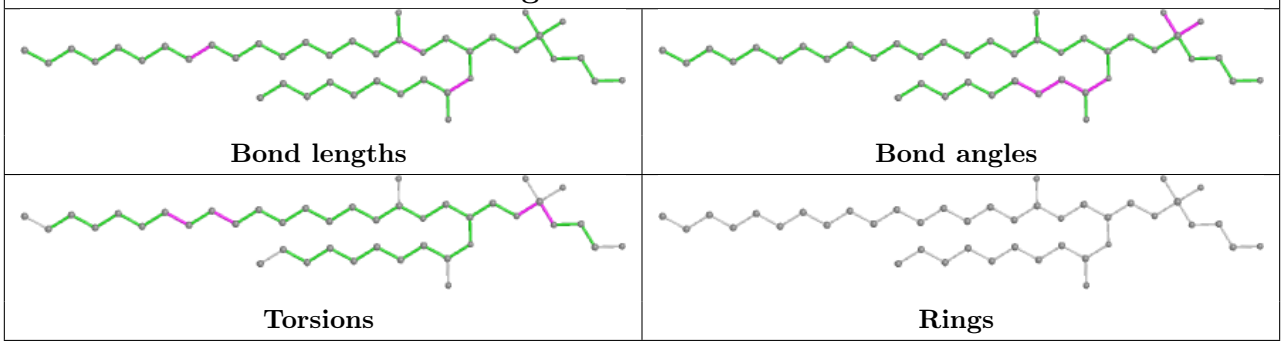


Rings

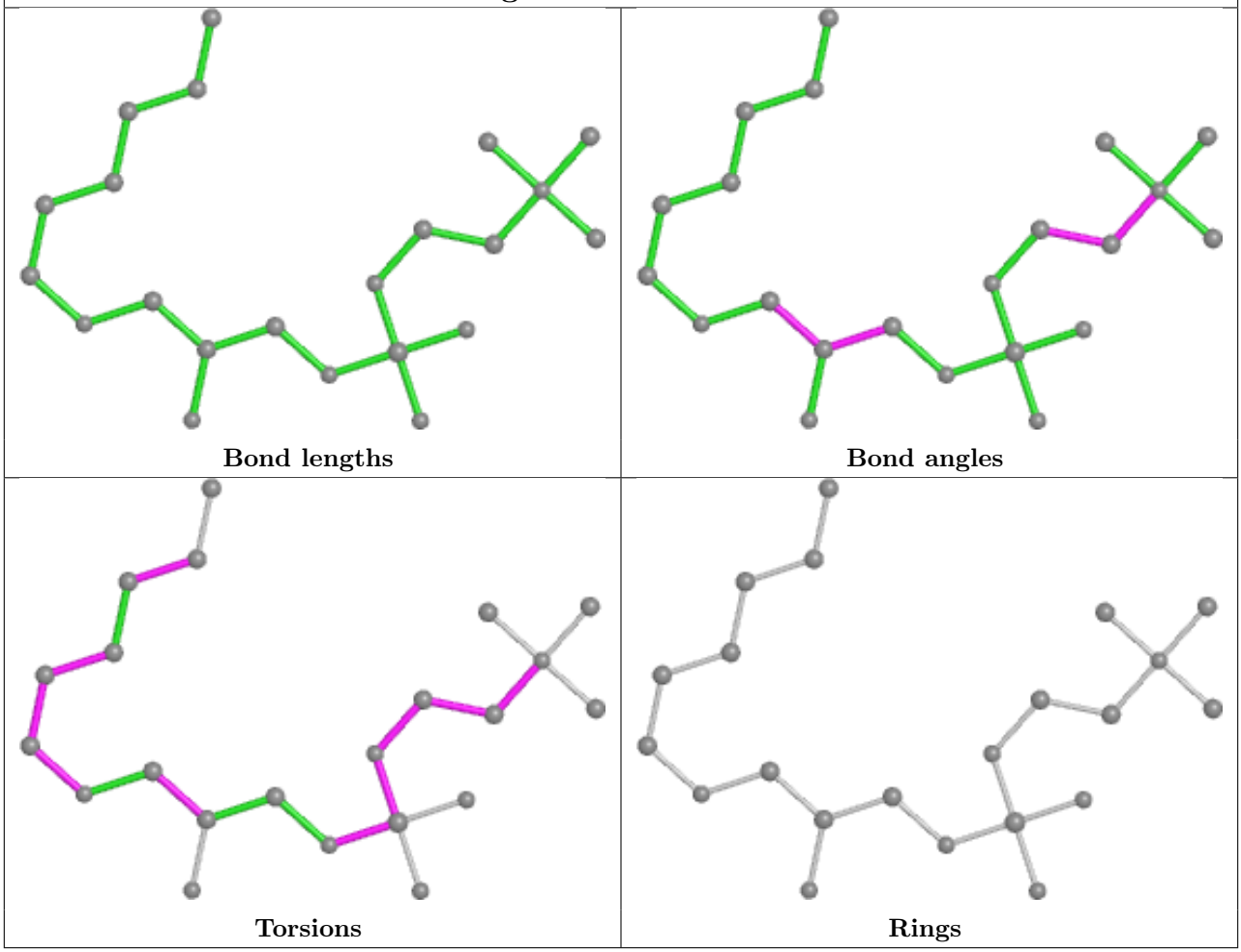
Ligand PCW A 2028



Ligand P5S A 2017



Ligand LPE A 2014



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.

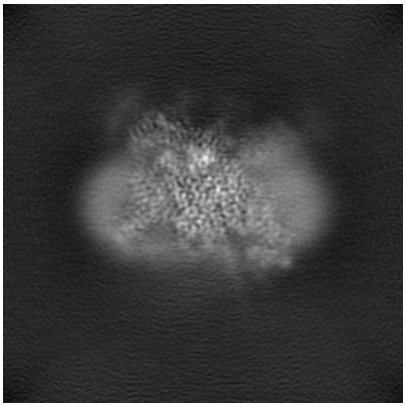
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32372. These allow visual inspection of the internal detail of the map and identification of artifacts.

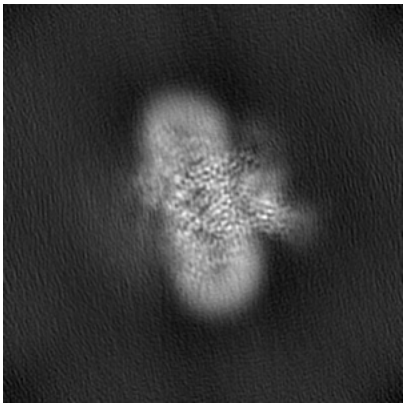
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

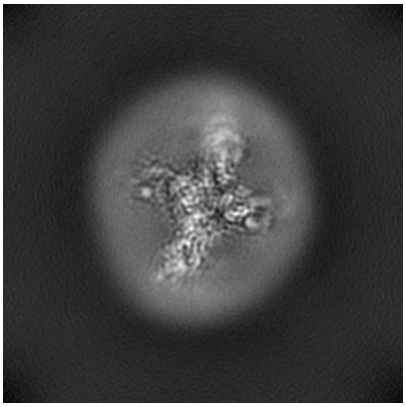
6.1.1 Primary map



X



Y

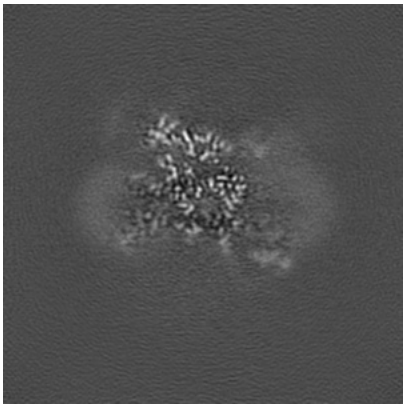


Z

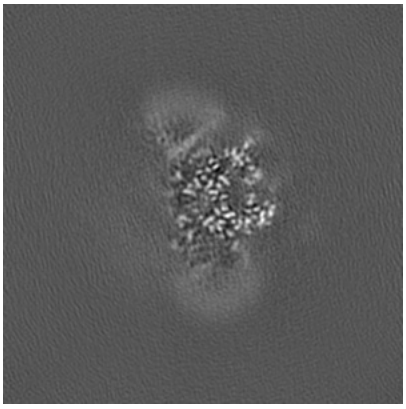
The images above show the map projected in three orthogonal directions.

6.2 Central slices

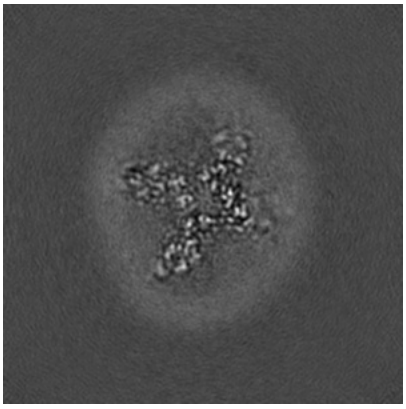
6.2.1 Primary map



X Index: 120



Y Index: 120

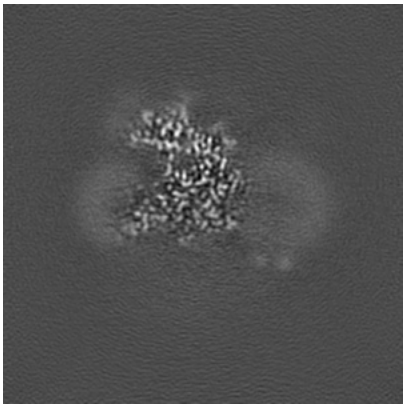


Z Index: 120

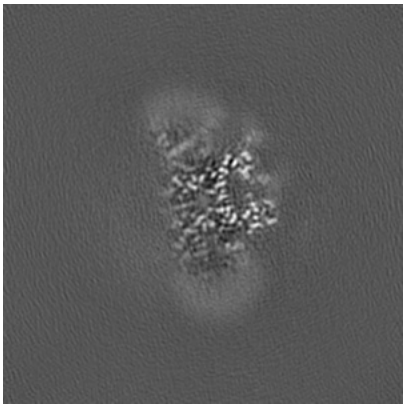
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

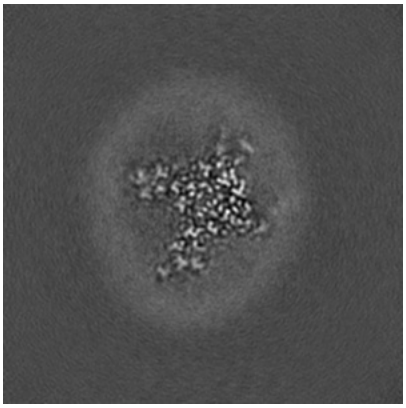
6.3.1 Primary map



X Index: 112



Y Index: 122

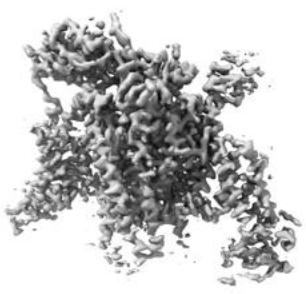


Z Index: 126

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 0.63. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

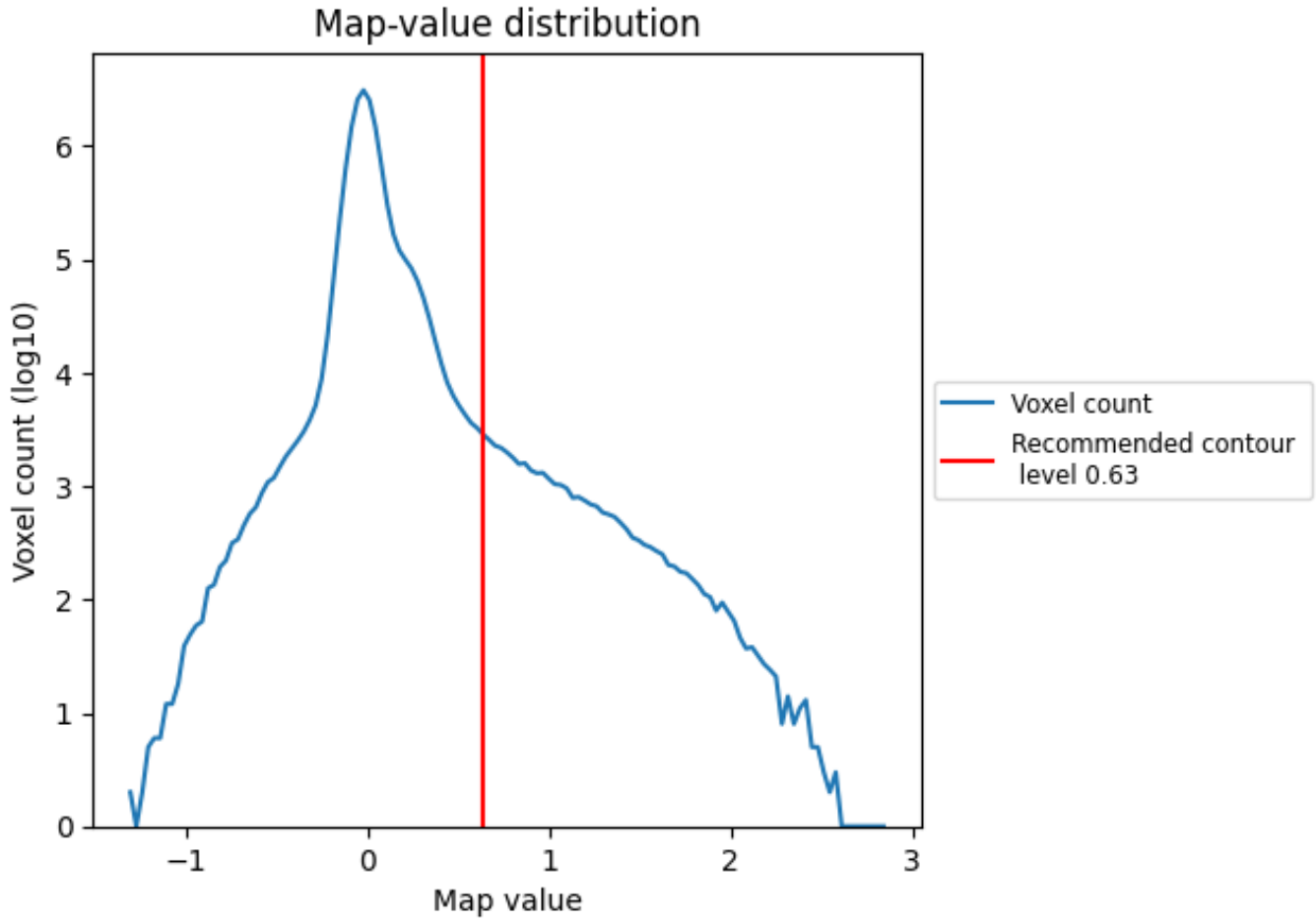
6.5 Mask visualisation (i)

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

7 Map analysis

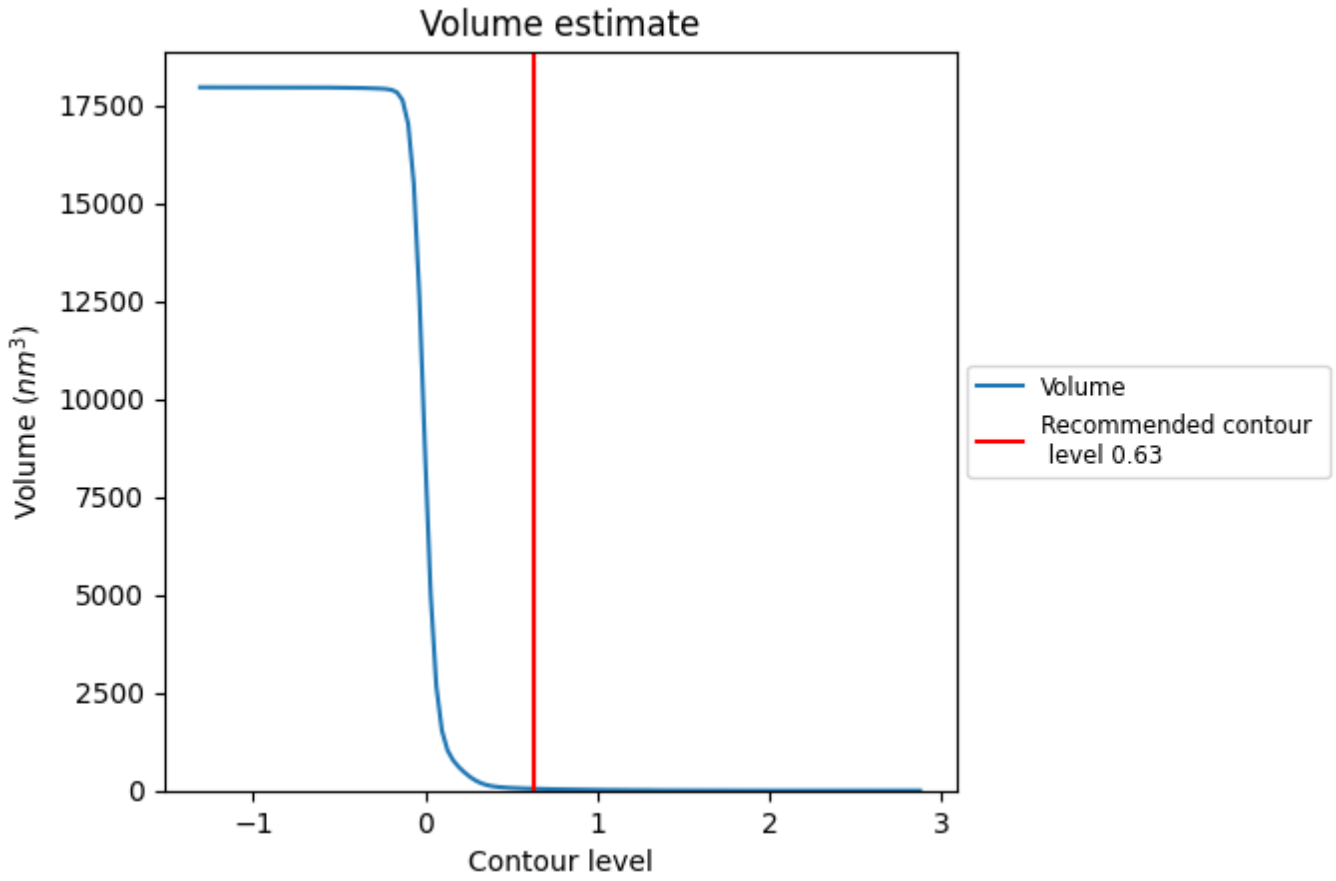
This section contains the results of statistical analysis of the map.

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.

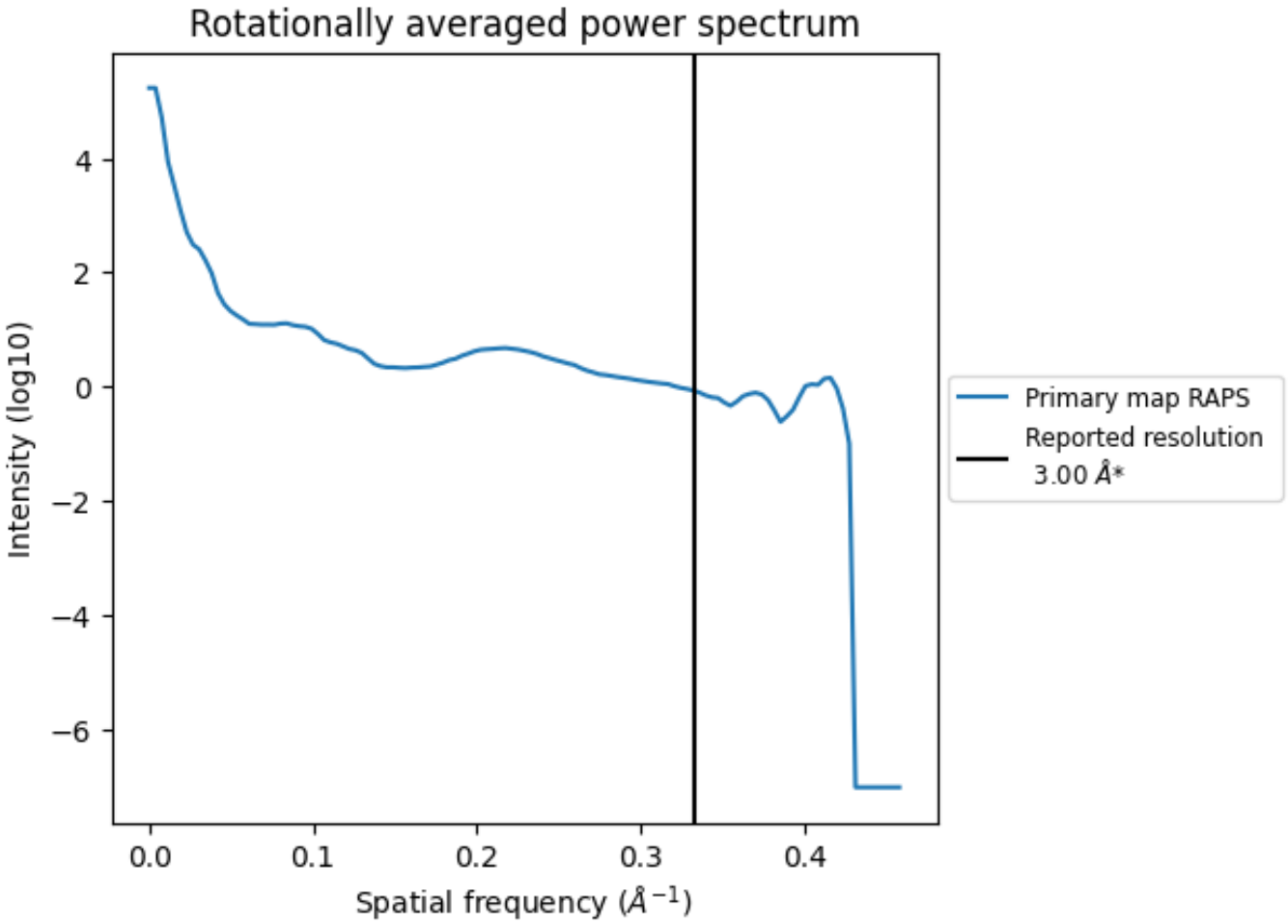
7.2 Volume estimate



The volume at the recommended contour level is 46 nm^3; this corresponds to an approximate mass of 42 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 0.333 Å^{-1}

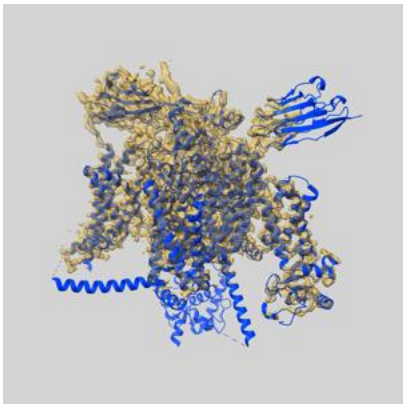
8 Fourier-Shell correlation (i)

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

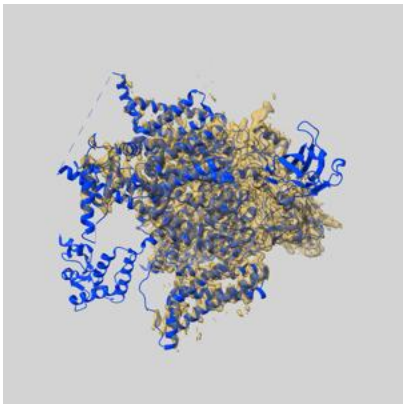
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32372 and PDB model 7W9T. Per-residue inclusion information can be found in section 3 on page 12.

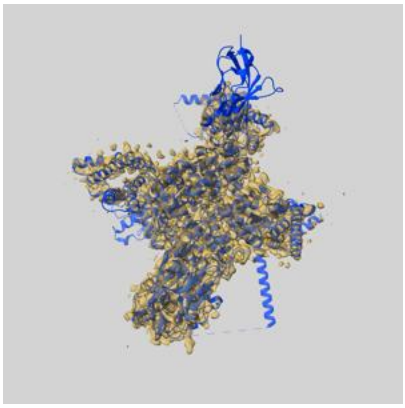
9.1 Map-model overlay



X



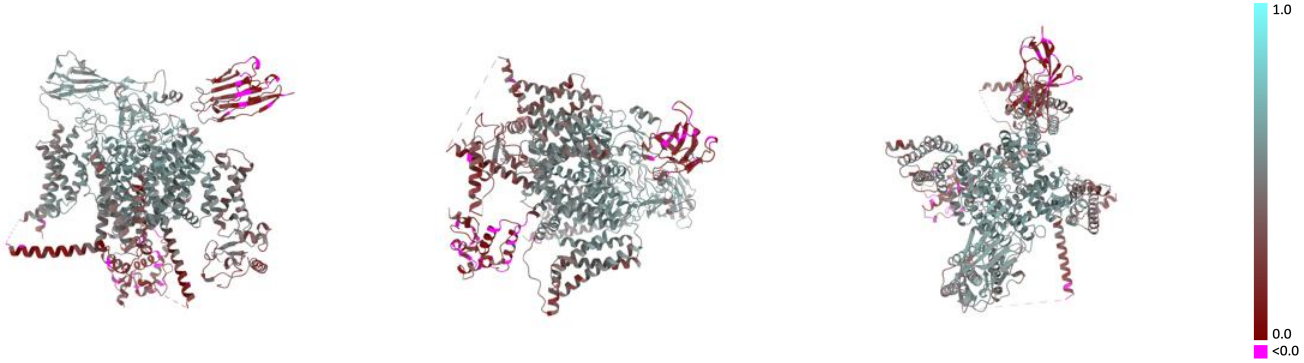
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.63 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.

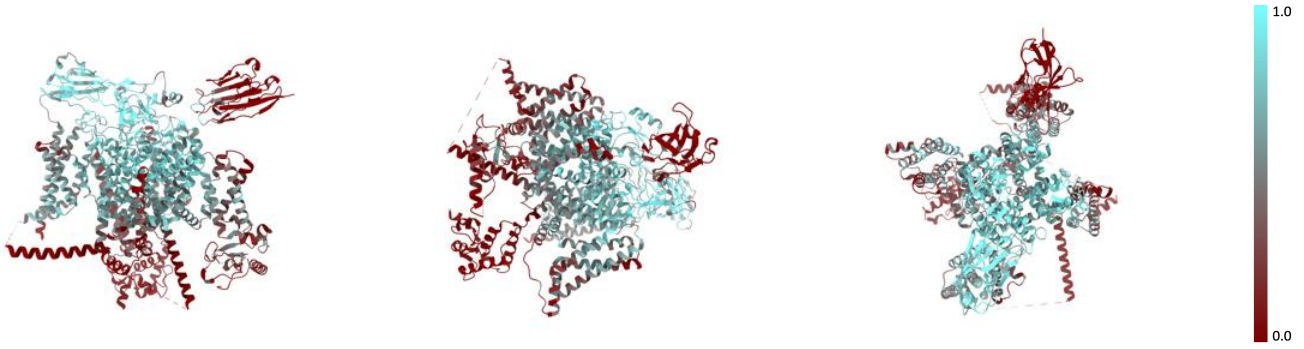
9.2 Q-score mapped to coordinate model (i)



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.

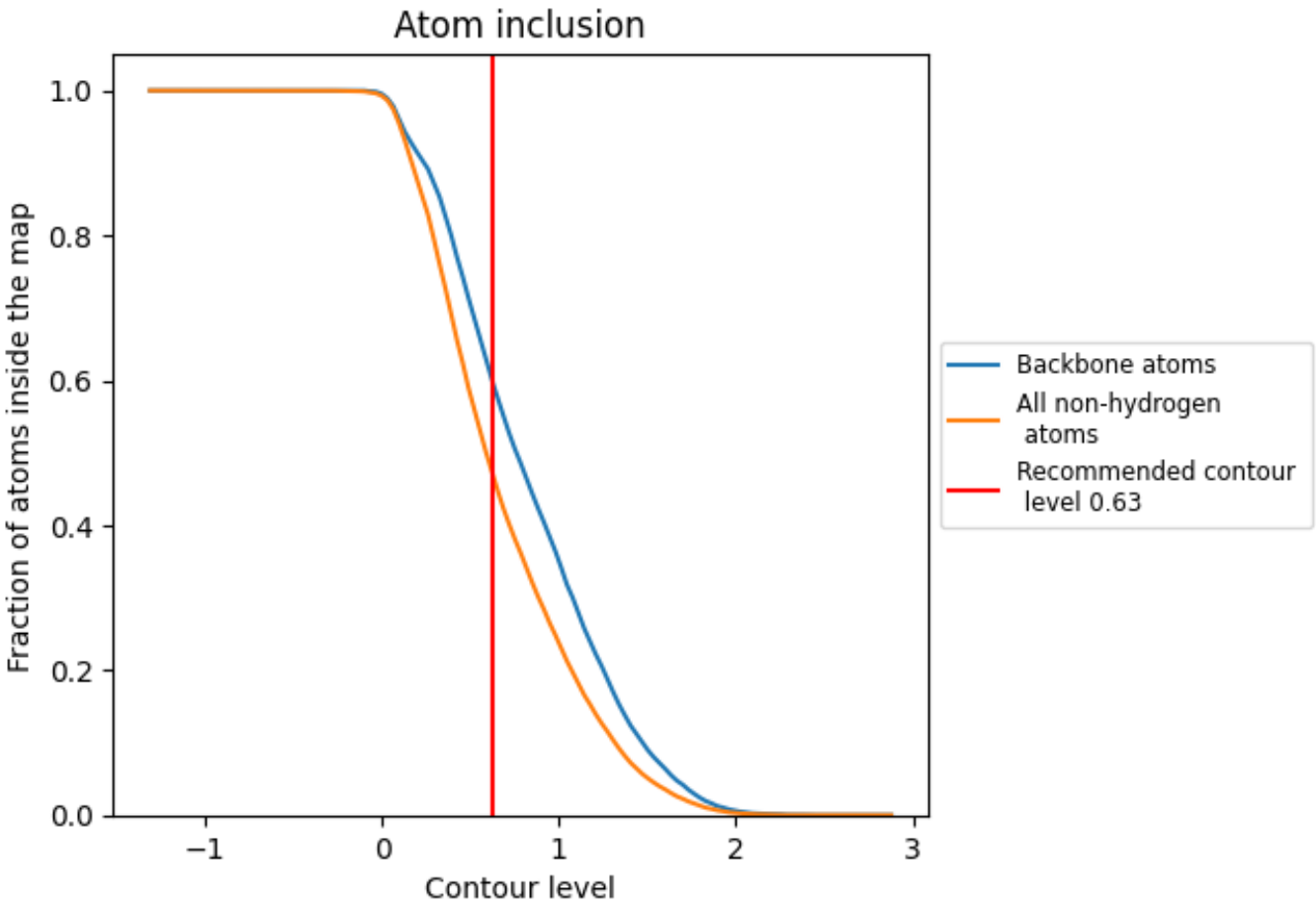
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.63).

9.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 47% 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 (0.63) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4676	0.4310
A	0.4677	0.4410
B	0.6939	0.5070
C	0.1125	0.1840
D	0.4643	0.4680
E	0.5714	0.4350
F	0.6786	0.4410