Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 04:02 PM JST

PDB ID	:	6JB1
EMDB ID	:	EMD-9787
Title	:	Structure of pancreatic ATP-sensitive potassium channel bound with repaglinide and ATPgammaS at 3.3A resolution
Authors	:	Chen, L.; Ding, D.; Wang, M.; Wu, J.-X.; Kang, Y.
Deposited on	:	2019-01-25
Resolution	:	3.30 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:

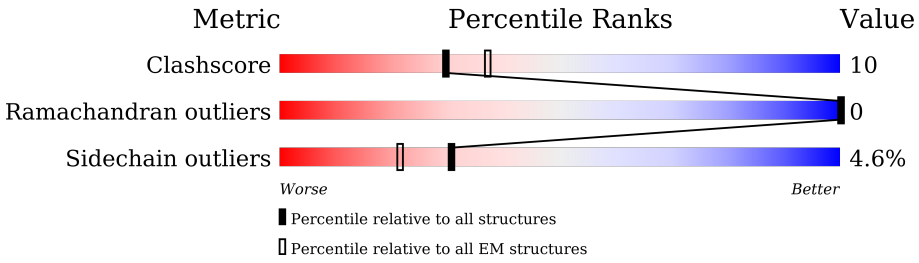
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	390	55% 27% • 16%
1	C	390	55% 28% • 16%
1	E	390	54% 28% • 16%
1	G	390	54% 28% • 16%
2	B	1582	16% 69% 16% • 14%
2	D	1582	16% 69% 16% • 14%
2	F	1582	16% 70% 16% • 14%
2	H	1582	16% 70% 15% • 14%

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
5	AJP	B	1601	X	-	-	-
5	AJP	D	1601	X	-	-	-
5	AJP	F	1601	X	-	-	-
5	AJP	H	1601	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 52028 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.

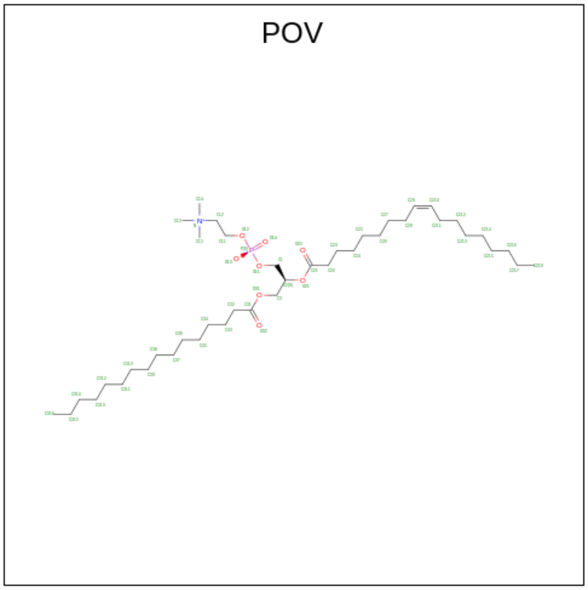
- Molecule 1 is a protein called ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	327	Total	C	N	O	S	0	0
			2543	1641	440	446	16		
1	C	327	Total	C	N	O	S	0	0
			2543	1641	440	446	16		
1	E	327	Total	C	N	O	S	0	0
			2543	1641	440	446	16		
1	G	327	Total	C	N	O	S	0	0
			2543	1641	440	446	16		

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8 isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1366	Total	C	N	O	S	0	0
			9890	6419	1693	1735	43		
2	D	1366	Total	C	N	O	S	0	0
			9890	6419	1693	1735	43		
2	F	1366	Total	C	N	O	S	0	0
			9890	6419	1693	1735	43		
2	H	1366	Total	C	N	O	S	0	0
			9890	6419	1693	1735	43		

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O P 31 22 1 7 1	0
3	B	1	Total C N O P 272 199 7 59 7	0
3	B	1	Total C N O P 272 199 7 59 7	0
3	B	1	Total C N O P 272 199 7 59 7	0
3	B	1	Total C N O P 272 199 7 59 7	0
3	B	1	Total C N O P 272 199 7 59 7	0
3	B	1	Total C N O P 272 199 7 59 7	0
3	B	1	Total C N O P 272 199 7 59 7	0
3	B	1	Total C N O P 272 199 7 59 7	0
3	C	1	Total C N O P 31 22 1 7 1	0
3	D	1	Total C N O P 272 199 7 59 7	0
3	D	1	Total C N O P 272 199 7 59 7	0
3	D	1	Total C N O P 272 199 7 59 7	0
3	D	1	Total C N O P 272 199 7 59 7	0

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Mol	Chain	Residues	Atoms	AltConf
3	D	1	Total C N O P 272 199 7 59 7	0
3	D	1	Total C N O P 272 199 7 59 7	0
3	D	1	Total C N O P 272 199 7 59 7	0
3	D	1	Total C N O P 272 199 7 59 7	0
3	E	1	Total C N O P 31 22 1 7 1	0
3	F	1	Total C N O P 272 199 7 59 7	0
3	F	1	Total C N O P 272 199 7 59 7	0
3	F	1	Total C N O P 272 199 7 59 7	0
3	F	1	Total C N O P 272 199 7 59 7	0
3	F	1	Total C N O P 272 199 7 59 7	0
3	F	1	Total C N O P 272 199 7 59 7	0
3	F	1	Total C N O P 272 199 7 59 7	0
3	F	1	Total C N O P 272 199 7 59 7	0
3	G	1	Total C N O P 31 22 1 7 1	0
3	H	1	Total C N O P 272 199 7 59 7	0
3	H	1	Total C N O P 272 199 7 59 7	0
3	H	1	Total C N O P 272 199 7 59 7	0
3	H	1	Total C N O P 272 199 7 59 7	0
3	H	1	Total C N O P 272 199 7 59 7	0
3	H	1	Total C N O P 272 199 7 59 7	0
3	H	1	Total C N O P 272 199 7 59 7	0

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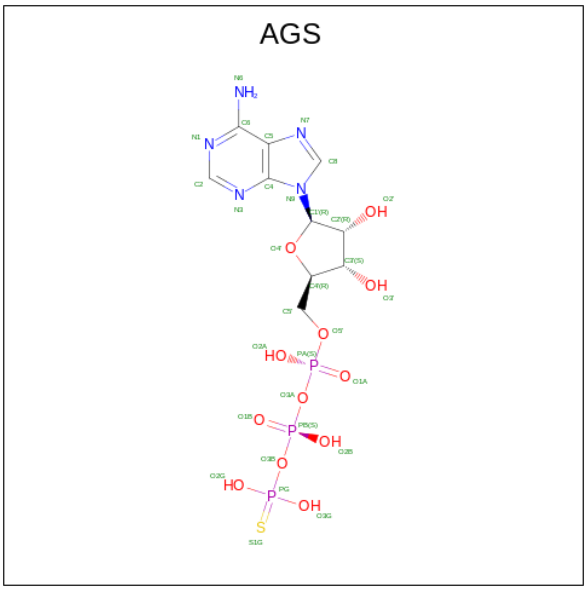
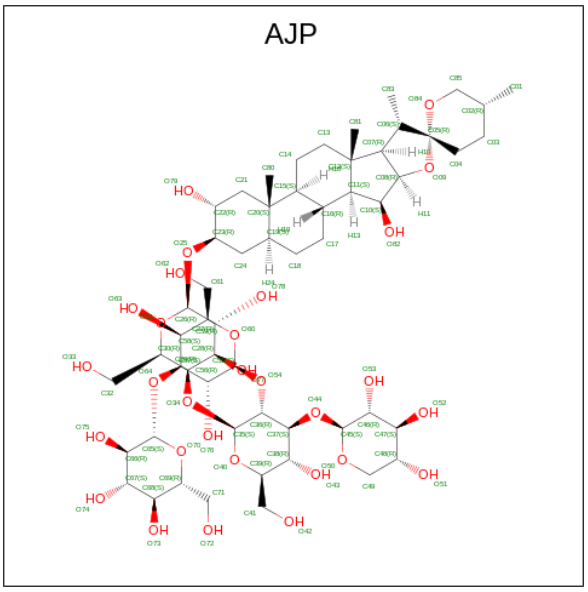
Mol	Chain	Residues	Atoms					AltConf
3	H	1	Total	C	N	O	P	0
			272	199	7	59	7	

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



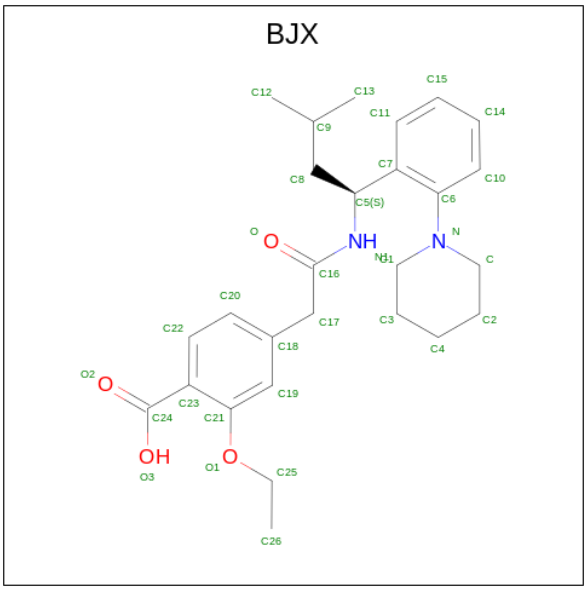
Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	G	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	H	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 5 is Digitonin (three-letter code: AJP) (formula: $C_{56}H_{92}O_{29}$).



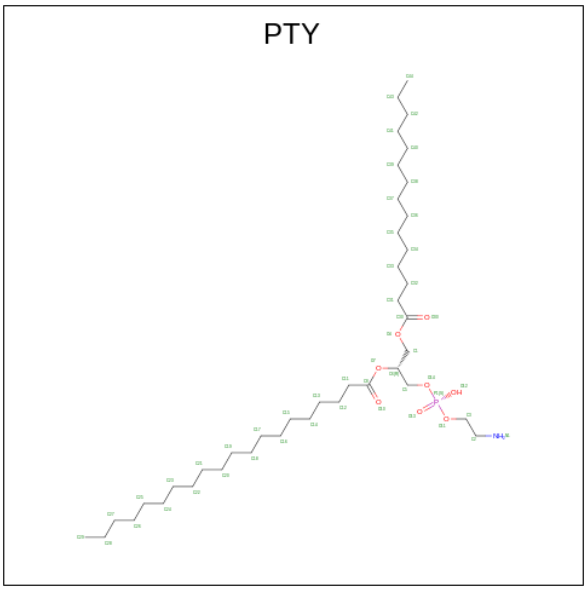
Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	C	O	0
			74	50	24	
5	D	1	Total	C	O	0
			74	50	24	
5	F	1	Total	C	O	0
			74	50	24	
5	H	1	Total	C	O	0
			74	50	24	

- Molecule 6 is Repaglinide (three-letter code: BJX) (formula: $C_{27}H_{36}N_2O_4$).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			33	27	2	4	
6	D	1	Total	C	N	O	0
			33	27	2	4	
6	F	1	Total	C	N	O	0
			33	27	2	4	
6	H	1	Total	C	N	O	0
			33	27	2	4	

- Molecule 7 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	B	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	B	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	B	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	D	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	D	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	D	1	Total	C	N	O	P	0
			102	65	4	29	4	

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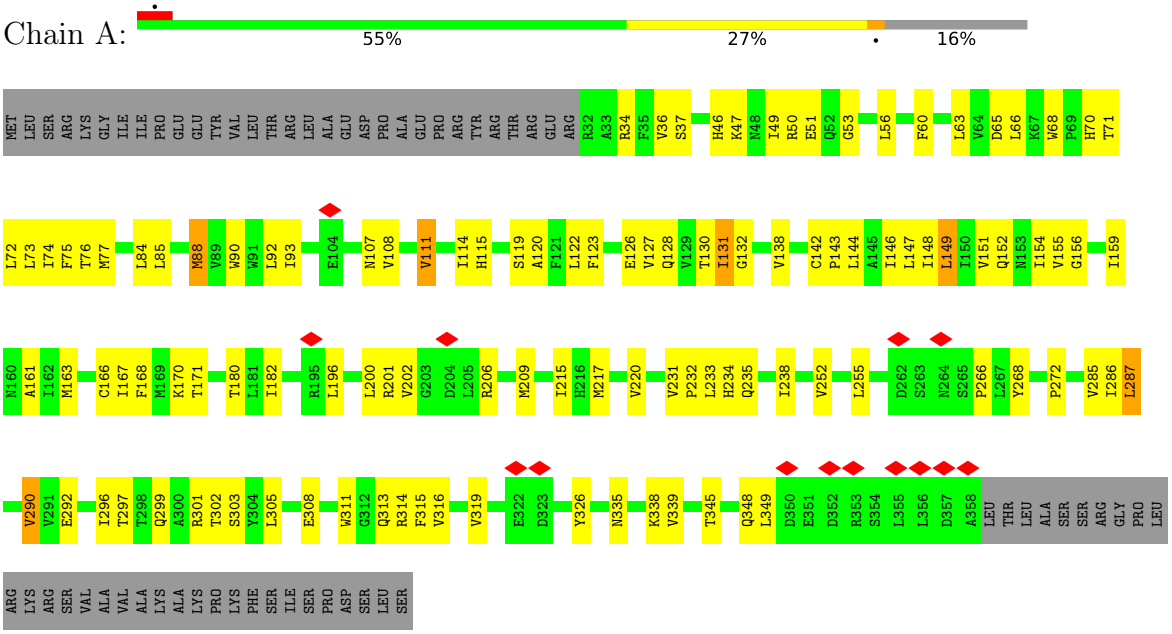
Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	F	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	F	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	F	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	F	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	H	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	H	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	H	1	Total	C	N	O	P	0
			102	65	4	29	4	
7	H	1	Total	C	N	O	P	0
			102	65	4	29	4	

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.

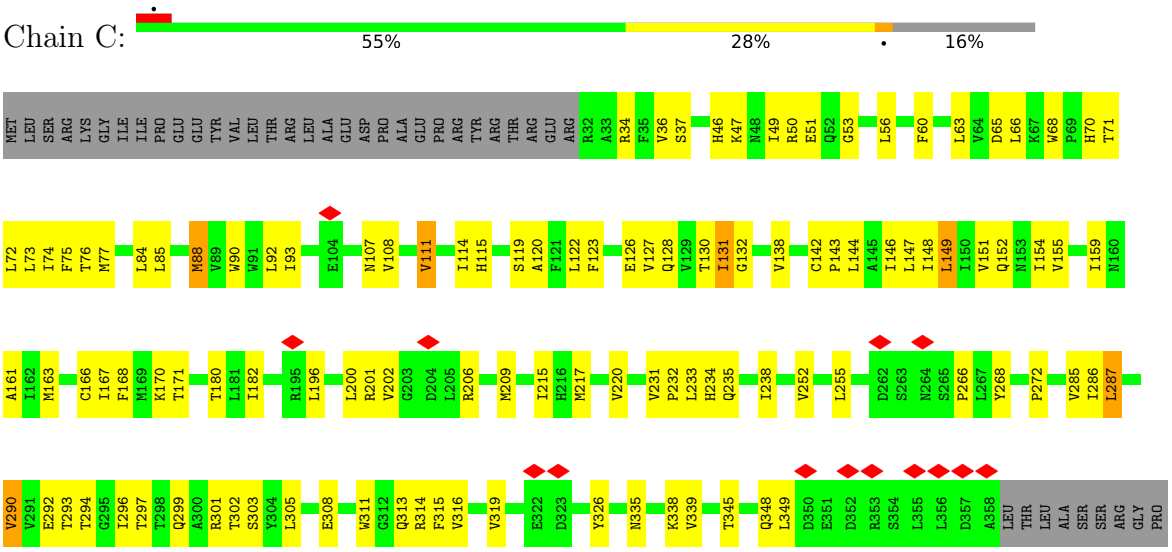
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain A:



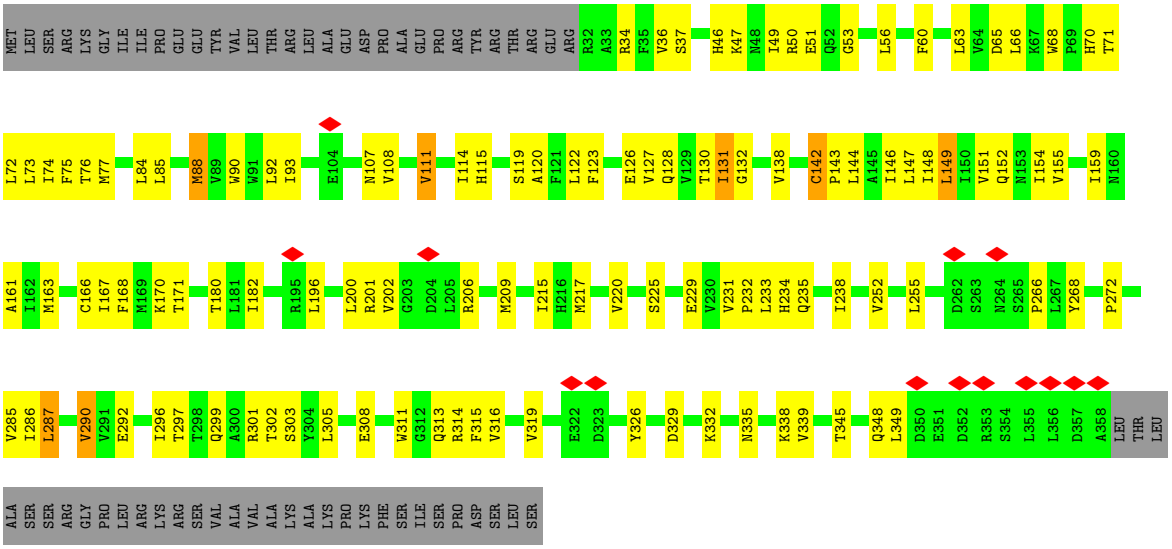
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain C:



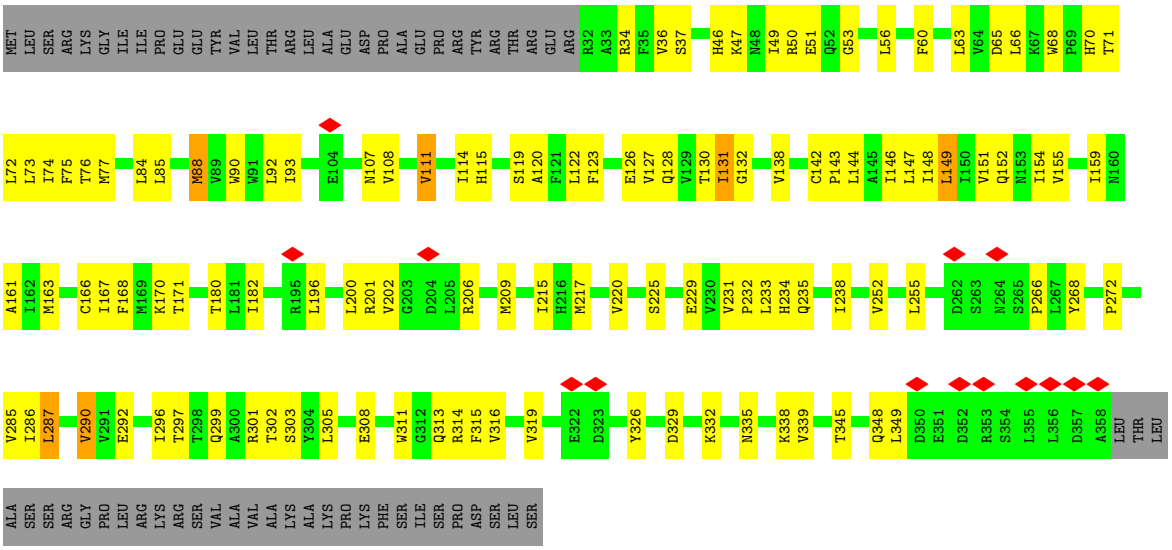
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain E:



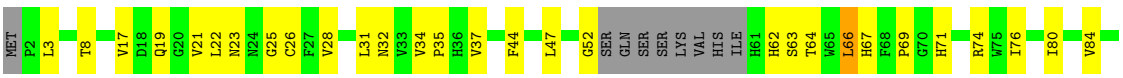
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

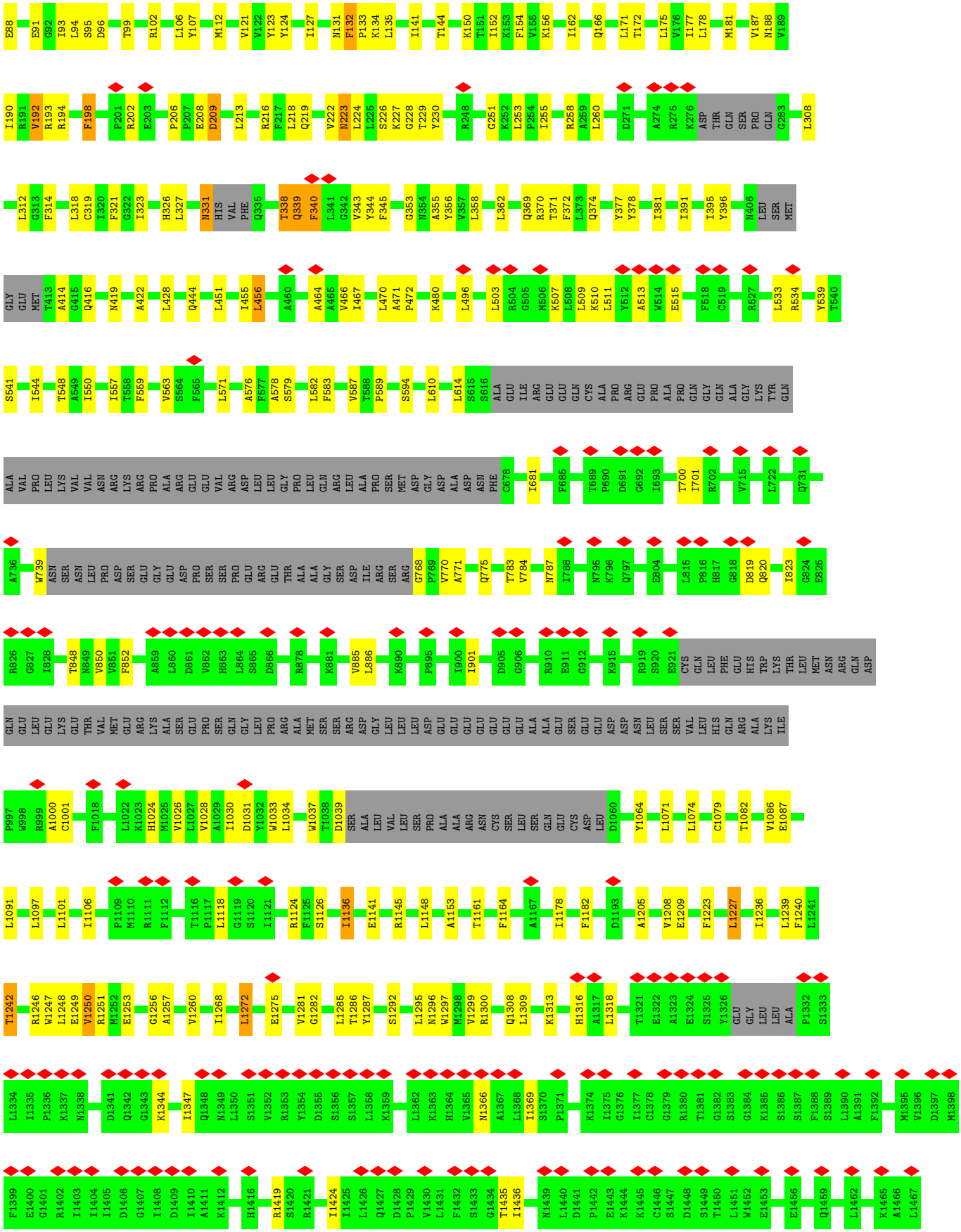
Chain G:

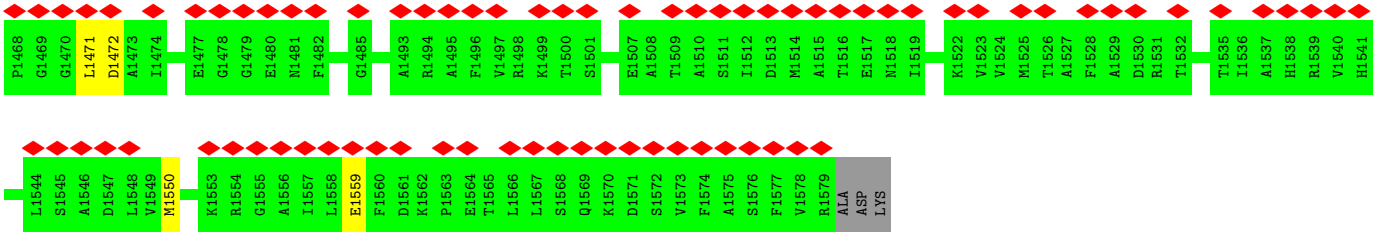


• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

Chain B:

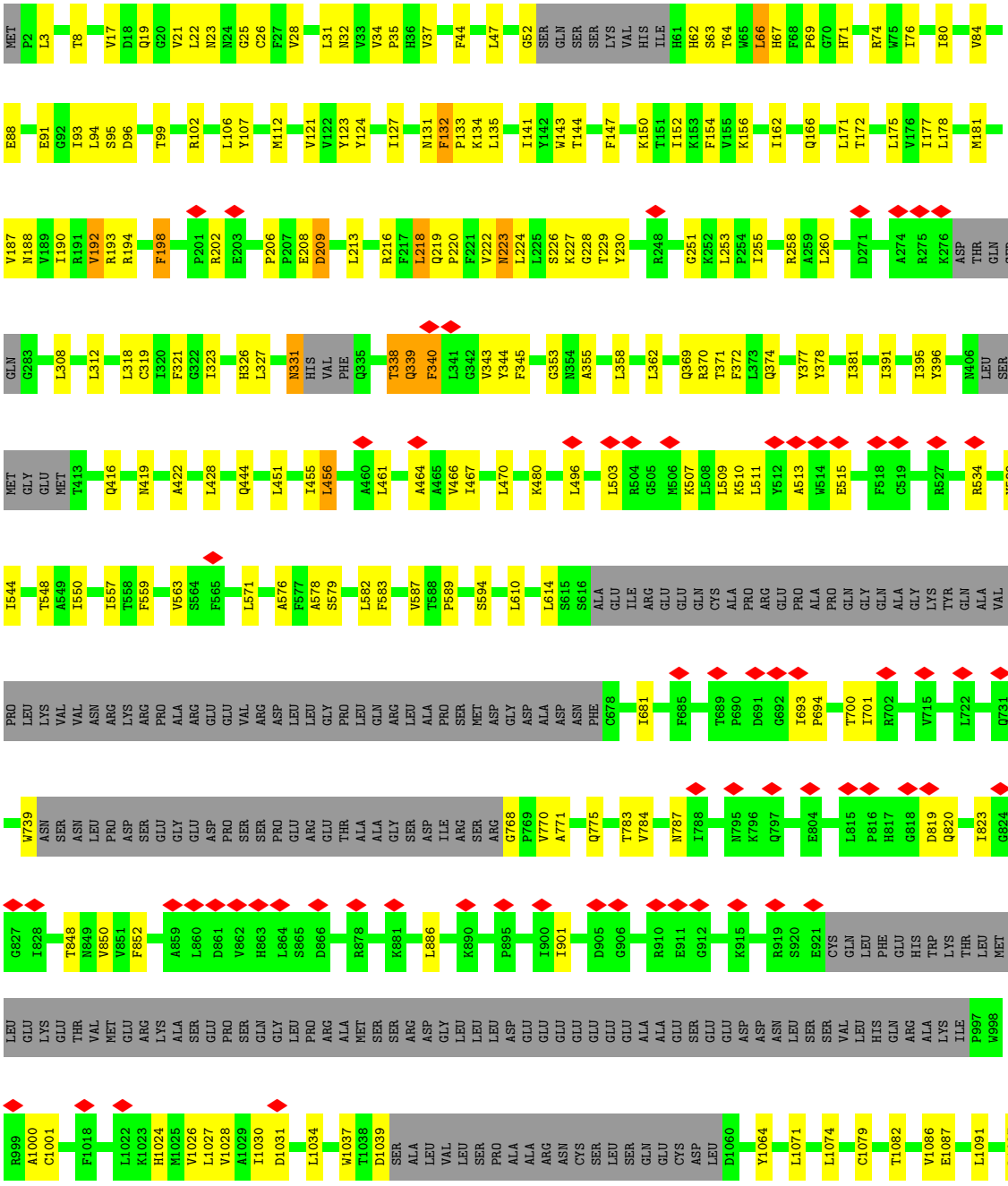


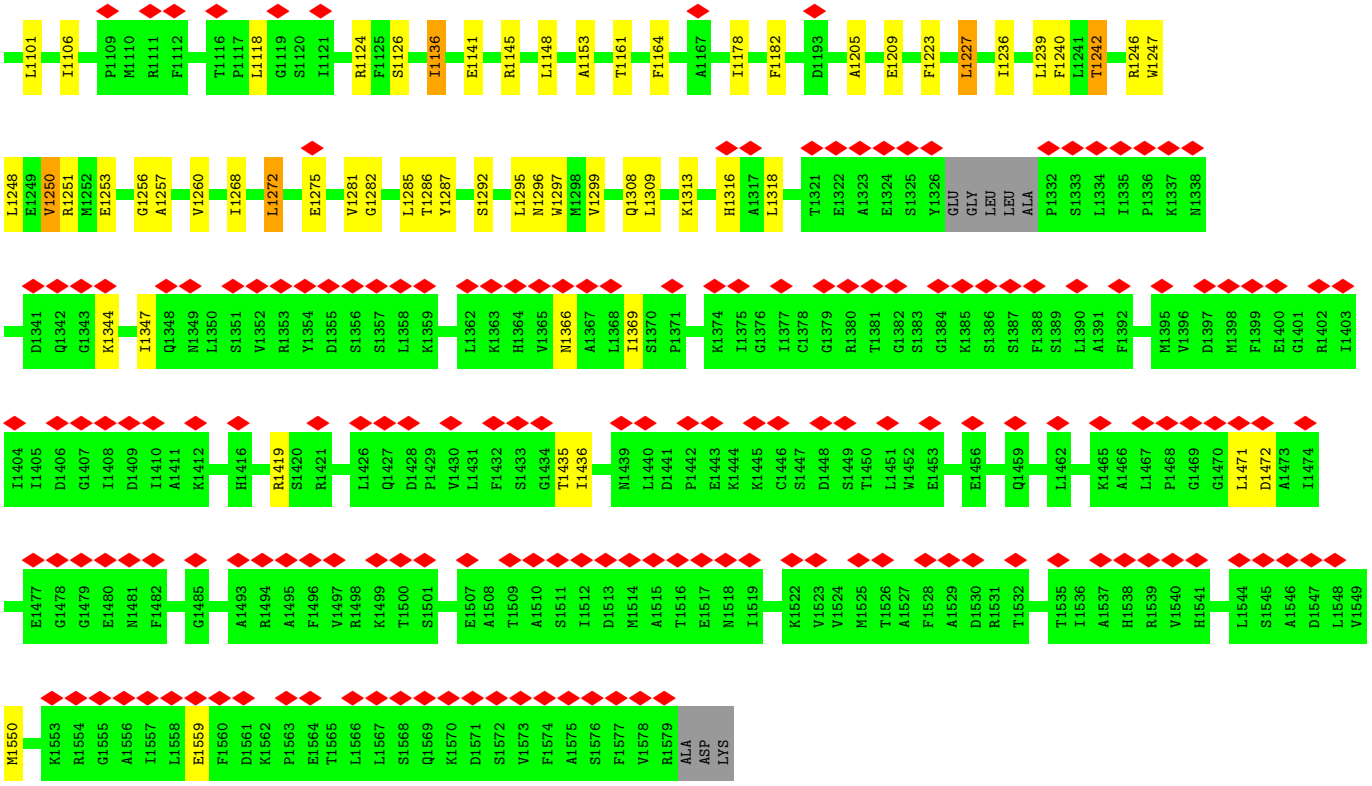




• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

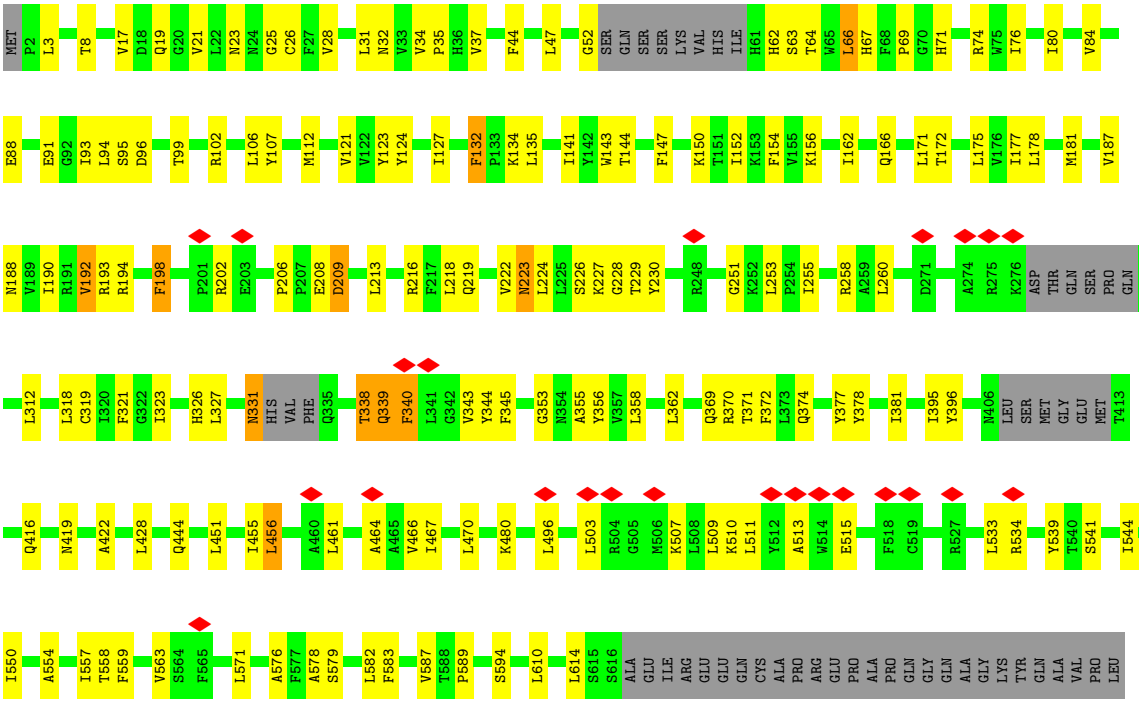
Chain D:

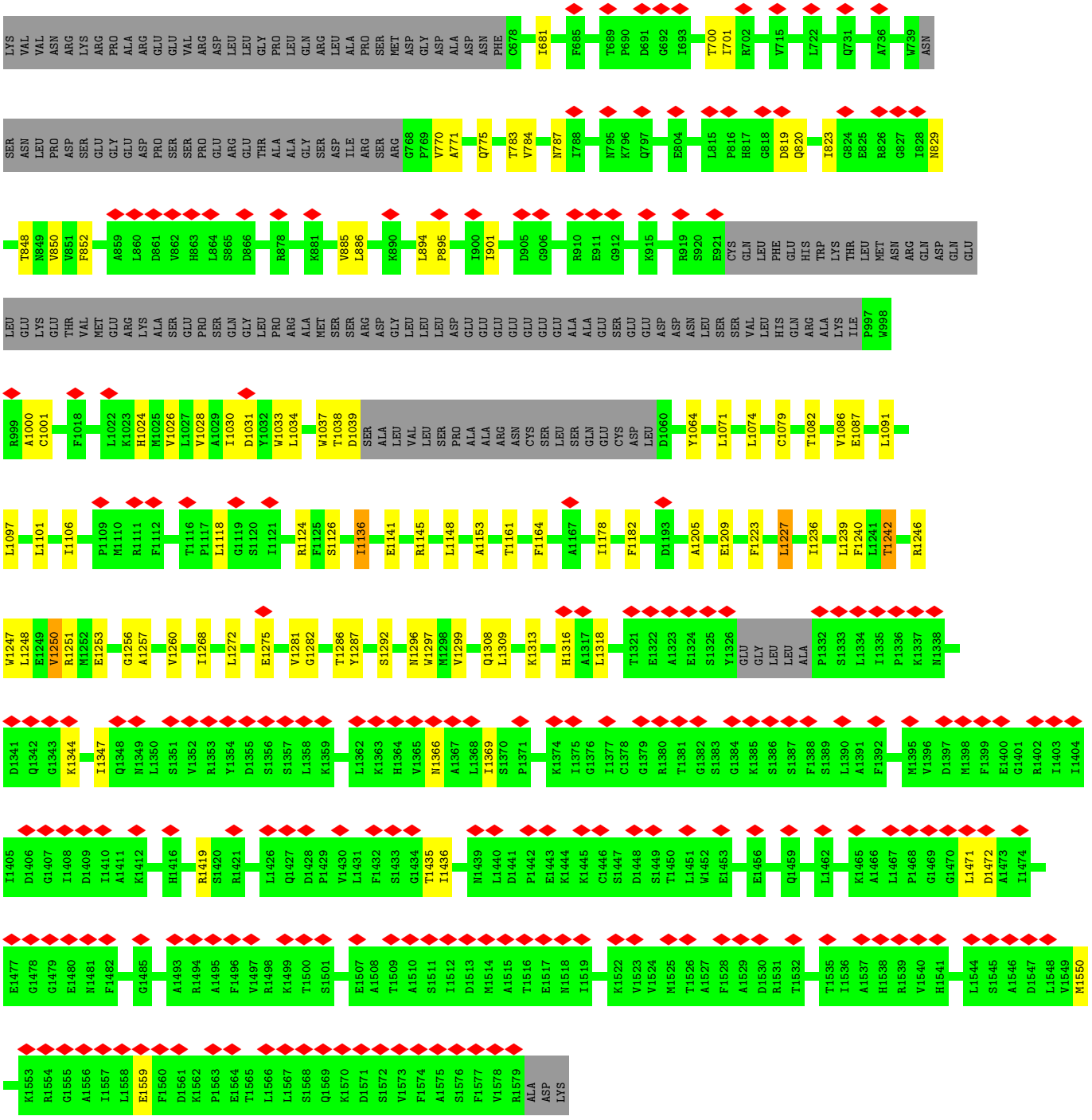




• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

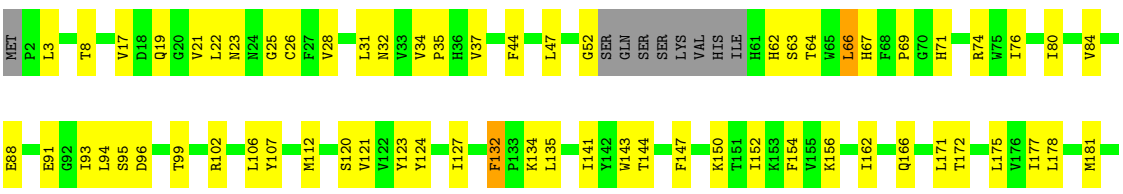
Chain F:

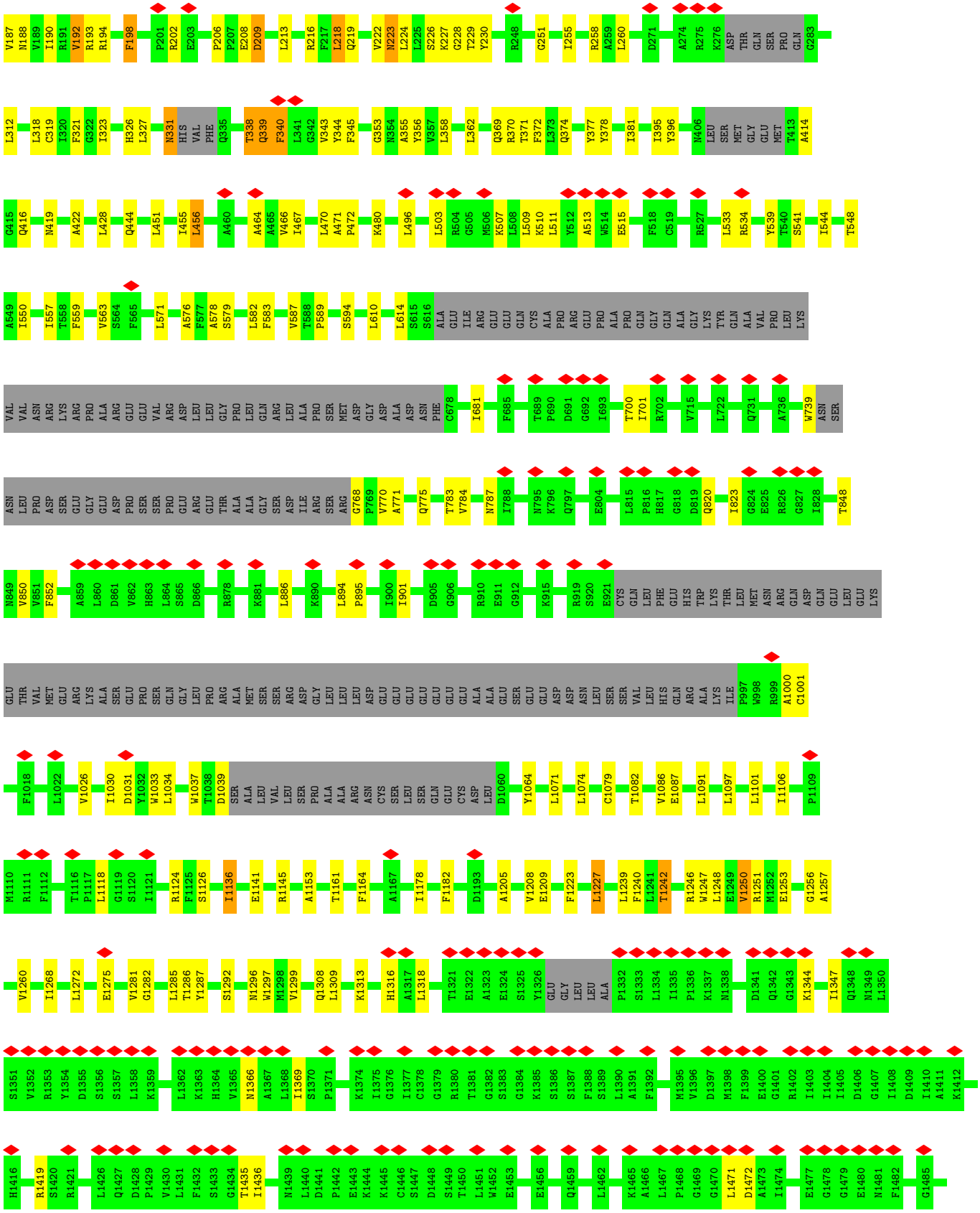




• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

Chain H:




V187 N188 V189 I190 R191 V192 R193 R194 F198 P201 R202 E203 P206 P207 E208 D209 L213 R216 F217 L218 Q219 V222 N223 L224 L225 S226 K227 G228 T229 Y230 R248 G251 I255 R258 A259 L260 D271 A274 R275 K276 ASP THR GLN SER PRO GLN G283
L312 L318 C319 I320 F321 G322 I323 H326 L327 N331 HIS VAL PHE Q335 T338 Q339 F340 L341 G342 V343 Y344 F345 G353 N354 A355 Y356 V357 L358 L362 Q369 R370 T371 F372 L373 Q374 Y377 Y378 I381 I395 Y396 N406 LEU SER MET GLY GLU MET T413 A414
G415 Q416 N419 A422 L428 Q444 L451 I455 L456 A460 A464 A465 V466 I467 L470 A471 P472 K480 L496 L503 R504 G505 M506 K507 L508 L509 K510 L511 Y512 A513 W514 E515 F518 C519 R527 L533 R534 Y539 T540 S541 I544 T548
A549 I550 I557 T558 F559 V563 S564 F565 L571 A576 F577 A578 S579 L582 F583 V587 T588 P589 S594 L610 L614 S615 S616 ALA GLU ILE ARG GLU GLU GLN CYS ALA PRO ARG GLU PRO ALA PRO GLN GLY GLN ALA GLY LYS TYR GLN ALA VAL PRO LEU LYS
VAL VAL ASN ARG LYS ARG PRO ALA ARG GLU GLU VAL ARG ASP LEU LEU GLY PRO LEU GLN ARG LEU ALA PRO SER MET ASP GLY ASP ALA ASP ASN PHE C678 I681 F685 T689 P690 D691 G692 I693 T700 I701 R702 V715 L722 Q731 A736 W739 ASN SER
ASN LEU PRO ASP SER GLU GLY GLU ASP PRO SER SER PRO GLU ARG GLU THR ALA ALA GLY SER ASP ILE ARG SER ARG G768 P769 V770 A771 Q775 T783 V784 N787 I788 N795 K796 Q797 E804 L815 P816 H817 G818 D819 Q820 I823 G824 E825 R826 G827 I828 T848
N849 V850 Y851 F852 A859 L860 D861 V862 H863 L864 S865 D866 R878 K881 L886 K890 L894 P895 I900 I901 D905 G906 R910 E911 G912 K915 R919 S920 E921 CYS GLN LEU PHE GLU HIS TRP LYS THR LEU MET ASN ARG GLN ASP GLN GLU LEU GLU LYS
GLU THR VAL MET GLU ARG LYS ALA SER GLU PRO SER GLN GLY LEU PRO ARG ALA MET SER SER ARG ASP GLY LEU LEU LEU ASP GLU GLU GLU GLU GLU GLU GLU GLU ALA ALA GLU GLU SER GLU GLU ASP ASP ASN LEU SER SER VAL LEU HIS GLN ARG ALA LYS ILE P997 W998 R999 A1000 C1001
F1018 L1022 V1026 I1030 D1031 Y1032 W1033 L1034 W1037 T1038 D1039 SER ALA LEU VAL LEU SER PRO ALA ALA ARG ASN CYS SER LEU SER GLN GLU CYS ASP LEU D1060 Y1064 L1071 L1074 C1079 T1082 V1086 E1087 L1091 L1097 L1101 I1106 P1109
M1110 R1111 F1112 T1116 P1117 L1118 G1119 S1120 I1121 R1124 F1125 S1126 I1136 E1141 R1145 A1153 T1161 F1164 A1167 I1178 F1182 D1193 A1205 V1208 E1209 F1223 L1227 L1239 F1240 L1241 T1242 R1246 W1247 L1248 E1249 V1250 R1251 M1252 E1253 G1256 A1257
V1260 I1268 L1272 E1275 V1281 G1282 L1285 T1286 Y1287 S1292 N1296 W1297 M1298 V1299 Q1308 L1309 K1313 H1316 A1317 L1318 T1321 E1322 A1323 E1324 S1325 Y1326 GLU GLY LEU LEU ALA P1332 S1333 L1334 I1335 P1336 K1337 N1338 D1341 Q1342 G1343 K1344 I1347 Q1348 N1349 L1350
S1351 V1352 R1353 Y1354 D1355 S1356 S1357 L1358 K1359 L1362 K1363 H1364 V1365 N1366 A1367 L1368 I1369 S1370 P1371 K1374 I1375 G1376 I1377 C1378 G1379 R1380 T1381 G1382 S1383 G1384 K1385 S1386 S1387 F1388 S1389 L1390 A1391 F1392 M1395 V1396 D1397 M1398 F1399 E1400 G1401 R1402 I1403 I1404 I1405 D1406 G1407 I1408 D1409 I1410 A1411 K1412
H1416 R1419 S1420 R1421 L1426 Q1427 D1428 P1429 V1430 L1431 F1432 S1433 G1434 T1435 I1436 N1439 L1440 D1441 P1442 E1443 K1444 K1445 C1446 S1447 D1448 S1449 T1450 L1451 W1452 E1453 E1456 Q1459 L1462 K1465 A1466 L1467 P1468 G1469 G1470 L1471 D1472 A1473 I1474 E1477 G1478 G1479 E1480 N1481 F1482 G1485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L1544
S1545
A1546
D1547
L1548
V1549
M1550
K1553
R1554
G1555
A1556
I1557
L1558
E1559
F1560

D1561
K1562
P1563
E1564
T1565
L1566
L1567
S1568
Q1569
K1570
D1571
S1572
V1573
F1574
A1575
S1576
F1577
V1578
R1579
ALA
ASP
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	277548	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	27.764	Depositor
Minimum map value	-15.475	Depositor
Average map value	0.095	Depositor
Map value standard deviation	0.834	Depositor
Recommended contour level	3.8	Depositor
Map size (Å)	338.944, 338.944, 338.944	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.324, 1.324, 1.324	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BJX, AGS, AJP, POV, PTY

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	0.36	0/2600	0.54	0/3535
1	C	0.36	0/2600	0.54	0/3535
1	E	0.36	0/2600	0.54	0/3535
1	G	0.36	0/2600	0.54	0/3535
2	B	0.28	0/10097	0.43	0/13798
2	D	0.28	0/10097	0.43	0/13798
2	F	0.28	0/10097	0.43	0/13798
2	H	0.28	0/10097	0.43	0/13798
All	All	0.30	0/50788	0.45	0/69332

There are no bond length outliers.

There are no bond angle outliers.

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	2543	0	2571	79	0
1	C	2543	0	2571	80	0
1	E	2543	0	2571	78	0
1	G	2543	0	2571	79	0
2	B	9890	0	9397	178	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	9890	0	9397	180	0
2	F	9890	0	9397	172	0
2	H	9890	0	9397	170	0
3	A	31	0	40	4	0
3	B	272	0	346	21	0
3	C	31	0	40	3	0
3	D	272	0	346	19	0
3	E	31	0	40	4	0
3	F	272	0	346	18	0
3	G	31	0	40	4	0
3	H	272	0	346	19	0
4	A	31	0	12	2	0
4	B	31	0	12	1	0
4	C	31	0	12	2	0
4	D	31	0	12	1	0
4	E	31	0	12	2	0
4	F	31	0	12	1	0
4	G	31	0	12	2	0
4	H	31	0	12	1	0
5	B	74	0	0	1	0
5	D	74	0	0	1	0
5	F	74	0	0	1	0
5	H	74	0	0	1	0
6	B	33	0	0	2	0
6	D	33	0	0	2	0
6	F	33	0	0	2	0
6	H	33	0	0	2	0
7	B	102	0	108	7	0
7	D	102	0	108	7	0
7	F	102	0	108	7	0
7	H	102	0	108	7	0
All	All	52028	0	49944	1026	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 10.

All (1026) 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:130:THR:HA	1:G:131:ILE:HG22	1.59	0.85
1:E:131:ILE:HG22	1:G:130:THR:HA	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ILE:HG22	1:C:130:THR:HA	1.59	0.84
1:C:131:ILE:HG22	1:E:130:THR:HA	1.59	0.84
2:F:371:THR:HG21	7:F:1615:PTY:H141	1.63	0.80
2:D:371:THR:HG21	7:D:1615:PTY:H141	1.63	0.80
2:H:371:THR:HG21	7:H:1615:PTY:H141	1.63	0.79
2:B:371:THR:HG21	7:B:1615:PTY:H141	1.63	0.79
2:B:1030:ILE:HG22	2:B:1071:LEU:HB3	1.67	0.77
2:H:1030:ILE:HG22	2:H:1071:LEU:HB3	1.67	0.77
2:D:1030:ILE:HG22	2:D:1071:LEU:HB3	1.67	0.76
2:F:1030:ILE:HG22	2:F:1071:LEU:HB3	1.67	0.75
1:A:47:LYS:HA	2:B:62:HIS:HB3	1.72	0.72
1:C:47:LYS:HA	2:D:62:HIS:HB3	1.72	0.71
2:B:470:LEU:HB2	2:B:550:ILE:HG21	1.72	0.71
1:G:47:LYS:HA	2:H:62:HIS:HB3	1.72	0.71
2:H:470:LEU:HB2	2:H:550:ILE:HG21	1.72	0.71
2:H:1344:LYS:HA	2:H:1369:ILE:O	1.91	0.71
2:B:1344:LYS:HA	2:B:1369:ILE:O	1.91	0.70
2:D:470:LEU:HB2	2:D:550:ILE:HG21	1.72	0.70
2:F:1344:LYS:HA	2:F:1369:ILE:O	1.91	0.70
1:E:47:LYS:HA	2:F:62:HIS:HB3	1.72	0.70
2:F:470:LEU:HB2	2:F:550:ILE:HG21	1.72	0.70
2:D:1344:LYS:HA	2:D:1369:ILE:O	1.91	0.70
2:B:548:THR:OG1	2:B:1145:ARG:NH2	2.27	0.68
2:H:548:THR:OG1	2:H:1145:ARG:NH2	2.27	0.68
2:D:548:THR:OG1	2:D:1145:ARG:NH2	2.27	0.68
2:F:548:THR:OG1	2:F:1145:ARG:NH2	2.27	0.68
2:F:31:LEU:HD21	3:F:1609:POV:H25	1.76	0.68
2:D:31:LEU:HD21	3:D:1609:POV:H25	1.76	0.67
2:F:166:GLN:HG2	2:F:345:PHE:HB3	1.77	0.67
2:H:166:GLN:HG2	2:H:345:PHE:HB3	1.77	0.67
2:B:166:GLN:HG2	2:B:345:PHE:HB3	1.77	0.67
2:H:31:LEU:HD21	3:H:1609:POV:H25	1.76	0.66
1:G:84:LEU:HD22	3:H:1608:POV:H29	1.78	0.66
2:B:31:LEU:HD21	3:B:1609:POV:H25	1.76	0.66
1:A:84:LEU:HD22	3:B:1608:POV:H29	1.78	0.65
1:C:84:LEU:HD22	3:D:1608:POV:H29	1.78	0.65
2:D:166:GLN:HG2	2:D:345:PHE:HB3	1.77	0.65
1:E:84:LEU:HD22	3:F:1608:POV:H29	1.78	0.65
2:B:456:LEU:HD13	2:B:579:SER:HB3	1.79	0.65
2:D:456:LEU:HD13	2:D:579:SER:HB3	1.79	0.65
4:G:401:AGS:H5'2	4:G:401:AGS:O1B	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:401:AGS:H5'2	4:C:401:AGS:O1B	1.96	0.64
4:A:402:AGS:H5'2	4:A:402:AGS:O1B	1.96	0.64
4:E:401:AGS:H5'2	4:E:401:AGS:O1B	1.96	0.64
3:F:1604:POV:H27	3:F:1605:POV:H22	1.79	0.64
2:F:456:LEU:HD13	2:F:579:SER:HB3	1.79	0.64
3:B:1604:POV:H27	3:B:1605:POV:H22	1.79	0.64
2:D:444:GLN:HG2	2:D:589:PRO:HG2	1.80	0.64
2:D:510:LYS:O	2:D:1419:ARG:NH1	2.31	0.64
2:F:444:GLN:HG2	2:F:589:PRO:HG2	1.80	0.63
2:D:312:LEU:HB3	2:D:369:GLN:HB2	1.80	0.63
2:F:510:LYS:O	2:F:1419:ARG:NH1	2.31	0.63
3:D:1604:POV:H27	3:D:1605:POV:H22	1.79	0.63
2:H:456:LEU:HD13	2:H:579:SER:HB3	1.79	0.63
2:F:312:LEU:HB3	2:F:369:GLN:HB2	1.80	0.63
2:D:69:PRO:HG2	2:D:192:VAL:HG11	1.80	0.63
3:D:1604:POV:H28A	3:D:1606:POV:H35	1.81	0.63
2:H:312:LEU:HB3	2:H:369:GLN:HB2	1.80	0.63
3:H:1604:POV:H28A	3:H:1606:POV:H35	1.81	0.63
2:B:510:LYS:O	2:B:1419:ARG:NH1	2.31	0.63
2:H:69:PRO:HG2	2:H:192:VAL:HG11	1.80	0.62
1:A:51:GLU:HG2	1:A:53:GLY:H	1.64	0.62
2:D:370:ARG:HD3	2:D:1253:GLU:HB3	1.81	0.62
1:G:126:GLU:HB3	1:G:132:GLY:HA2	1.81	0.62
2:F:370:ARG:HD3	2:F:1253:GLU:HB3	1.81	0.62
2:F:69:PRO:HG2	2:F:192:VAL:HG11	1.80	0.62
2:F:541:SER:HB2	2:F:1087:GLU:HG3	1.82	0.62
2:B:312:LEU:HB3	2:B:369:GLN:HB2	1.80	0.62
2:D:1124:ARG:HG3	2:D:1318:LEU:HD13	1.82	0.62
2:H:510:LYS:O	2:H:1419:ARG:NH1	2.31	0.62
2:H:1153:ALA:HA	2:H:1287:TYR:HD2	1.65	0.62
2:B:69:PRO:HG2	2:B:192:VAL:HG11	1.80	0.62
2:B:444:GLN:HG2	2:B:589:PRO:HG2	1.80	0.62
1:A:126:GLU:HB3	1:A:132:GLY:HA2	1.81	0.62
2:B:701:ILE:HD13	2:B:901:ILE:HD13	1.82	0.62
1:E:51:GLU:HG2	1:E:53:GLY:H	1.64	0.62
1:G:51:GLU:HG2	1:G:53:GLY:H	1.64	0.62
2:H:541:SER:HB2	2:H:1087:GLU:HG3	1.82	0.62
2:F:701:ILE:HD13	2:F:901:ILE:HD13	1.82	0.62
2:F:1153:ALA:HA	2:F:1287:TYR:HD2	1.65	0.62
2:H:444:GLN:HG2	2:H:589:PRO:HG2	1.80	0.62
1:A:115:HIS:O	3:B:1608:POV:H12A	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:HIS:O	3:F:1608:POV:H12A	2.00	0.62
1:E:126:GLU:HB3	1:E:132:GLY:HA2	1.81	0.62
2:H:319:CYS:HB3	2:H:362:LEU:HD12	1.82	0.62
3:H:1604:POV:H27	3:H:1605:POV:H22	1.79	0.62
2:B:319:CYS:HB3	2:B:362:LEU:HD12	1.82	0.61
1:C:126:GLU:HB3	1:C:132:GLY:HA2	1.81	0.61
1:E:123:PHE:O	1:E:127:VAL:HG12	2.00	0.61
2:F:319:CYS:HB3	2:F:362:LEU:HD12	1.82	0.61
1:A:123:PHE:O	1:A:127:VAL:HG12	2.00	0.61
1:C:51:GLU:HG2	1:C:53:GLY:H	1.64	0.61
2:D:1153:ALA:HA	2:D:1287:TYR:HD2	1.65	0.61
2:B:370:ARG:HD3	2:B:1253:GLU:HB3	1.81	0.61
3:B:1604:POV:H28A	3:B:1606:POV:H35	1.81	0.61
3:B:1611:POV:H24	3:B:1611:POV:H34A	1.82	0.61
1:G:115:HIS:O	3:H:1608:POV:H12A	2.00	0.61
2:H:370:ARG:HD3	2:H:1253:GLU:HB3	1.81	0.61
2:H:701:ILE:HD13	2:H:901:ILE:HD13	1.82	0.61
2:B:1153:ALA:HA	2:B:1287:TYR:HD2	1.65	0.61
2:D:222:VAL:HG23	2:D:227:LYS:HG3	1.81	0.61
2:D:701:ILE:HD13	2:D:901:ILE:HD13	1.82	0.61
1:G:123:PHE:O	1:G:127:VAL:HG12	2.00	0.61
2:H:76:ILE:HG12	7:H:1613:PTY:HC51	1.83	0.61
2:B:76:ILE:HG12	7:B:1613:PTY:HC51	1.83	0.61
3:D:1611:POV:H34A	3:D:1611:POV:H24	1.82	0.61
2:D:76:ILE:HG12	7:D:1613:PTY:HC51	1.83	0.61
2:D:319:CYS:HB3	2:D:362:LEU:HD12	1.82	0.61
2:B:222:VAL:HG23	2:B:227:LYS:HG3	1.81	0.61
2:F:76:ILE:HG12	7:F:1613:PTY:HC51	1.83	0.61
1:C:115:HIS:O	3:D:1608:POV:H12A	2.00	0.60
3:F:1604:POV:H28A	3:F:1606:POV:H35	1.81	0.60
3:F:1611:POV:H34A	3:F:1611:POV:H24	1.82	0.60
1:A:345:THR:HG23	1:A:348:GLN:H	1.66	0.60
2:B:66:LEU:HD22	2:B:67:HIS:H	1.66	0.60
2:B:541:SER:HB2	2:B:1087:GLU:HG3	1.82	0.60
1:E:345:THR:HG23	1:E:348:GLN:H	1.66	0.60
2:H:222:VAL:HG23	2:H:227:LYS:HG3	1.81	0.60
3:H:1611:POV:H34A	3:H:1611:POV:H24	1.82	0.60
2:D:66:LEU:HD22	2:D:67:HIS:H	1.66	0.60
2:D:515:GLU:HB2	2:D:1106:ILE:HD12	1.84	0.60
2:F:1124:ARG:HG3	2:F:1318:LEU:HD13	1.82	0.60
2:H:1124:ARG:HG3	2:H:1318:LEU:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:515:GLU:HB2	2:F:1106:ILE:HD12	1.84	0.60
2:B:1124:ARG:HG3	2:B:1318:LEU:HD13	1.82	0.60
1:C:123:PHE:O	1:C:127:VAL:HG12	2.00	0.60
2:F:222:VAL:HG23	2:F:227:LYS:HG3	1.81	0.60
2:H:515:GLU:HB2	2:H:1106:ILE:HD12	1.84	0.60
2:B:515:GLU:HB2	2:B:1106:ILE:HD12	1.84	0.60
2:D:74:ARG:HD3	2:D:124:TYR:CE2	2.37	0.60
2:D:541:SER:HB2	2:D:1087:GLU:HG3	1.82	0.60
2:B:74:ARG:HD3	2:B:124:TYR:CE2	2.37	0.60
2:B:321:PHE:HB2	2:B:578:ALA:HB2	1.84	0.60
2:D:91:GLU:O	2:D:95:SER:HB2	2.01	0.60
2:D:1037:TRP:CD1	2:D:1064:TYR:HB3	2.37	0.60
1:C:345:THR:HG23	1:C:348:GLN:H	1.66	0.60
2:H:321:PHE:HB2	2:H:578:ALA:HB2	1.84	0.59
2:D:177:ILE:O	2:D:181:MET:HG2	2.03	0.59
2:F:91:GLU:O	2:F:95:SER:HB2	2.01	0.59
2:B:177:ILE:O	2:B:181:MET:HG2	2.03	0.59
1:E:111:VAL:HB	1:E:138:VAL:HA	1.85	0.59
2:F:1037:TRP:CD1	2:F:1064:TYR:HB3	2.37	0.59
2:F:66:LEU:HD22	2:F:67:HIS:H	1.66	0.59
2:H:66:LEU:HD22	2:H:67:HIS:H	1.66	0.59
1:G:111:VAL:HB	1:G:138:VAL:HA	1.85	0.59
1:C:111:VAL:HB	1:C:138:VAL:HA	1.85	0.59
2:H:74:ARG:HD3	2:H:124:TYR:CE2	2.37	0.59
1:A:111:VAL:HB	1:A:138:VAL:HA	1.85	0.59
2:F:219:GLN:HE22	2:F:230:TYR:HD1	1.50	0.59
2:F:544:ILE:HD13	2:F:1141:GLU:HG2	1.85	0.59
2:H:91:GLU:O	2:H:95:SER:HB2	2.01	0.59
2:H:177:ILE:O	2:H:181:MET:HG2	2.03	0.59
2:B:91:GLU:O	2:B:95:SER:HB2	2.01	0.59
2:H:1037:TRP:CD1	2:H:1064:TYR:HB3	2.37	0.58
2:B:1037:TRP:CD1	2:B:1064:TYR:HB3	2.37	0.58
2:D:219:GLN:HE22	2:D:230:TYR:HD1	1.50	0.58
1:G:345:THR:HG23	1:G:348:GLN:H	1.66	0.58
2:H:544:ILE:HD13	2:H:1141:GLU:HG2	1.85	0.58
2:F:74:ARG:HD3	2:F:124:TYR:CE2	2.37	0.58
2:F:321:PHE:HB2	2:F:578:ALA:HB2	1.84	0.58
2:D:321:PHE:HB2	2:D:578:ALA:HB2	1.84	0.58
2:F:1347:ILE:O	2:F:1366:ASN:HA	2.04	0.58
2:H:1347:ILE:O	2:H:1366:ASN:HA	2.04	0.58
2:B:1347:ILE:O	2:B:1366:ASN:HA	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:177:ILE:O	2:F:181:MET:HG2	2.03	0.57
2:H:99:THR:O	2:H:102:ARG:NH2	2.37	0.57
2:B:219:GLN:HE22	2:B:230:TYR:HD1	1.50	0.57
2:B:544:ILE:HD13	2:B:1141:GLU:HG2	1.85	0.57
2:B:1246:ARG:HA	2:B:1246:ARG:HH11	1.69	0.57
2:D:80:ILE:HG12	7:D:1613:PTY:H132	1.87	0.57
2:D:1246:ARG:HA	2:D:1246:ARG:HH11	1.69	0.57
2:H:219:GLN:HE22	2:H:230:TYR:HD1	1.50	0.57
2:F:1246:ARG:HA	2:F:1246:ARG:HH11	1.69	0.57
2:H:1246:ARG:HH11	2:H:1246:ARG:HA	1.69	0.57
2:D:99:THR:O	2:D:102:ARG:NH2	2.37	0.57
2:D:338:THR:HA	2:D:344:TYR:HA	1.86	0.57
2:D:544:ILE:HD13	2:D:1141:GLU:HG2	1.85	0.57
2:D:1347:ILE:O	2:D:1366:ASN:HA	2.04	0.57
2:F:80:ILE:HG12	7:F:1613:PTY:H132	1.87	0.57
2:B:3:LEU:O	3:B:1608:POV:H1A	2.05	0.57
2:H:3:LEU:O	3:H:1608:POV:H1A	2.05	0.57
2:B:66:LEU:HB2	2:B:206:PRO:HG3	1.87	0.57
2:B:99:THR:O	2:B:102:ARG:NH2	2.37	0.56
2:B:80:ILE:HG12	7:B:1613:PTY:H132	1.87	0.56
1:E:329:ASP:OD2	1:E:332:LYS:NZ	2.31	0.56
2:H:80:ILE:HG12	7:H:1613:PTY:H132	1.87	0.56
1:C:314:ARG:HH21	1:C:339:VAL:HG21	1.70	0.56
1:E:314:ARG:HH21	1:E:339:VAL:HG21	1.70	0.56
2:F:99:THR:O	2:F:102:ARG:NH2	2.37	0.56
2:B:338:THR:HA	2:B:344:TYR:HA	1.86	0.56
2:F:3:LEU:O	3:F:1608:POV:H1A	2.05	0.56
2:F:338:THR:HA	2:F:344:TYR:HA	1.86	0.56
1:G:231:VAL:HG23	1:G:234:HIS:HB2	1.87	0.56
1:G:314:ARG:HH21	1:G:339:VAL:HG21	1.70	0.56
2:B:1000:ALA:HB2	2:B:1313:LYS:HB2	1.88	0.56
1:C:70:HIS:O	1:C:74:ILE:HG12	2.05	0.56
1:C:231:VAL:HG23	1:C:234:HIS:HB2	1.87	0.56
2:F:455:ILE:HG22	2:F:456:LEU:HD12	1.88	0.56
2:D:3:LEU:O	3:D:1608:POV:H1A	2.05	0.56
1:G:70:HIS:O	1:G:74:ILE:HG12	2.05	0.56
2:D:66:LEU:HB2	2:D:206:PRO:HG3	1.87	0.56
2:D:455:ILE:HG22	2:D:456:LEU:HD12	1.88	0.56
2:F:102:ARG:HD3	3:F:1604:POV:H23	1.88	0.56
2:F:1000:ALA:HB2	2:F:1313:LYS:HB2	1.88	0.56
2:H:102:ARG:HD3	3:H:1604:POV:H23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:338:THR:HA	2:H:344:TYR:HA	1.86	0.56
1:A:231:VAL:HG23	1:A:234:HIS:HB2	1.87	0.56
1:A:314:ARG:HH21	1:A:339:VAL:HG21	1.70	0.56
2:D:1000:ALA:HB2	2:D:1313:LYS:HB2	1.88	0.56
1:E:231:VAL:HG23	1:E:234:HIS:HB2	1.87	0.56
2:H:1000:ALA:HB2	2:H:1313:LYS:HB2	1.88	0.56
1:E:70:HIS:O	1:E:74:ILE:HG12	2.05	0.55
2:H:66:LEU:HB2	2:H:206:PRO:HG3	1.87	0.55
2:D:102:ARG:HD3	3:D:1604:POV:H23	1.88	0.55
2:F:216:ARG:H	2:F:251:GLY:HA3	1.71	0.55
2:H:188:ASN:O	2:H:192:VAL:HG12	2.06	0.55
1:A:70:HIS:O	1:A:74:ILE:HG12	2.05	0.55
2:B:216:ARG:H	2:B:251:GLY:HA3	1.71	0.55
2:F:66:LEU:HB2	2:F:206:PRO:HG3	1.87	0.55
2:H:455:ILE:HG22	2:H:456:LEU:HD12	1.88	0.55
2:H:216:ARG:H	2:H:251:GLY:HA3	1.71	0.55
2:B:455:ILE:HG22	2:B:456:LEU:HD12	1.88	0.55
2:D:188:ASN:O	2:D:192:VAL:HG12	2.06	0.55
2:F:681:ILE:O	2:F:700:THR:HA	2.07	0.55
2:B:102:ARG:HD3	3:B:1604:POV:H23	1.88	0.55
2:B:188:ASN:O	2:B:192:VAL:HG12	2.06	0.55
2:B:681:ILE:O	2:B:700:THR:HA	2.07	0.55
1:C:128:GLN:OE1	1:C:152:GLN:NE2	2.30	0.55
2:D:681:ILE:O	2:D:700:THR:HA	2.07	0.55
2:F:188:ASN:O	2:F:192:VAL:HG12	2.06	0.55
1:E:128:GLN:OE1	1:E:152:GLN:NE2	2.30	0.54
2:D:216:ARG:H	2:D:251:GLY:HA3	1.71	0.54
2:D:372:PHE:HZ	7:D:1613:PTY:HC6	1.73	0.54
1:G:196:LEU:HD13	1:G:349:LEU:HD22	1.90	0.54
2:H:372:PHE:HZ	7:H:1613:PTY:HC6	1.73	0.54
1:G:286:ILE:HG13	1:G:301:ARG:HB3	1.89	0.54
1:A:286:ILE:HG13	1:A:301:ARG:HB3	1.89	0.54
2:B:355:ALA:O	2:B:1268:ILE:HD13	2.08	0.54
2:B:372:PHE:HZ	7:B:1613:PTY:HC6	1.73	0.54
1:C:93:ILE:HG23	3:C:402:POV:H3A	1.90	0.54
2:H:355:ALA:O	2:H:1268:ILE:HD13	2.08	0.54
2:H:681:ILE:O	2:H:700:THR:HA	2.07	0.54
2:H:187:VAL:O	2:H:190:ILE:HG22	2.08	0.54
1:C:286:ILE:HG13	1:C:301:ARG:HB3	1.89	0.54
2:D:466:VAL:HG21	2:D:557:ILE:HG21	1.90	0.54
2:F:187:VAL:O	2:F:190:ILE:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LEU:HD13	1:A:349:LEU:HD22	1.90	0.53
2:B:187:VAL:O	2:B:190:ILE:HG22	2.08	0.53
2:F:355:ALA:O	2:F:1268:ILE:HD13	2.08	0.53
1:A:285:VAL:HG22	1:A:302:THR:HG22	1.90	0.53
2:B:466:VAL:HG21	2:B:557:ILE:HG21	1.90	0.53
2:D:355:ALA:O	2:D:1268:ILE:HD13	2.08	0.53
1:G:285:VAL:HG22	1:G:302:THR:HG22	1.90	0.53
1:A:93:ILE:HG23	3:A:401:POV:H3A	1.90	0.53
1:G:93:ILE:HG23	3:G:402:POV:H3A	1.90	0.53
2:H:1178:ILE:HD13	2:H:1251:ARG:HB3	1.90	0.53
2:H:466:VAL:HG21	2:H:557:ILE:HG21	1.90	0.53
2:D:187:VAL:O	2:D:190:ILE:HG22	2.08	0.53
2:D:467:ILE:HD12	2:D:550:ILE:HG22	1.91	0.53
2:F:372:PHE:HZ	7:F:1613:PTY:HC6	1.73	0.53
2:F:467:ILE:HD12	2:F:550:ILE:HG22	1.91	0.53
1:G:329:ASP:OD2	1:G:332:LYS:NZ	2.31	0.53
2:H:32:ASN:O	2:H:35:PRO:HD2	2.09	0.53
2:B:32:ASN:O	2:B:35:PRO:HD2	2.09	0.53
1:C:196:LEU:HD13	1:C:349:LEU:HD22	1.90	0.53
1:E:93:ILE:HG23	3:E:402:POV:H3A	1.90	0.53
1:E:201:ARG:NH2	1:E:315:PHE:HB3	2.24	0.53
2:F:32:ASN:O	2:F:35:PRO:HD2	2.09	0.53
2:D:228:GLY:HA3	7:D:1615:PTY:H112	1.91	0.53
1:A:201:ARG:NH2	1:A:315:PHE:HB3	2.24	0.53
2:F:228:GLY:HA3	7:F:1615:PTY:H112	1.91	0.53
2:F:1178:ILE:HD13	2:F:1251:ARG:HB3	1.90	0.53
2:H:209:ASP:OD1	2:H:209:ASP:N	2.42	0.53
1:C:285:VAL:HG22	1:C:302:THR:HG22	1.90	0.53
2:H:467:ILE:HD12	2:H:550:ILE:HG22	1.91	0.53
1:E:285:VAL:HG22	1:E:302:THR:HG22	1.90	0.52
1:E:286:ILE:HG13	1:E:301:ARG:HB3	1.89	0.52
1:G:201:ARG:NH2	1:G:315:PHE:HB3	2.24	0.52
2:B:1178:ILE:HD13	2:B:1251:ARG:HB3	1.90	0.52
2:F:209:ASP:N	2:F:209:ASP:OD1	2.42	0.52
2:F:466:VAL:HG21	2:F:557:ILE:HG21	1.90	0.52
2:B:467:ILE:HD12	2:B:550:ILE:HG22	1.91	0.52
2:D:93:ILE:HG23	3:D:1604:POV:H24A	1.91	0.52
1:E:122:LEU:O	1:E:126:GLU:HG3	2.09	0.52
1:G:122:LEU:O	1:G:126:GLU:HG3	2.09	0.52
1:A:122:LEU:O	1:A:126:GLU:HG3	2.09	0.52
1:C:201:ARG:NH2	1:C:315:PHE:HB3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:228:GLY:HA3	7:H:1615:PTY:H112	1.91	0.52
2:D:32:ASN:O	2:D:35:PRO:HD2	2.09	0.52
1:G:107:ASN:OD1	1:G:108:VAL:N	2.43	0.52
2:B:208:GLU:H	2:B:208:GLU:CD	2.13	0.52
2:B:228:GLY:HA3	7:B:1615:PTY:H112	1.91	0.52
1:E:196:LEU:HD13	1:E:349:LEU:HD22	1.90	0.52
2:F:93:ILE:HG23	3:F:1604:POV:H24A	1.91	0.52
2:B:93:ILE:HG23	3:B:1604:POV:H24A	1.91	0.52
2:H:17:VAL:HB	2:H:21:VAL:HG22	1.92	0.52
1:C:122:LEU:O	1:C:126:GLU:HG3	2.09	0.51
2:D:503:LEU:HB3	2:D:1118:LEU:HD11	1.92	0.51
2:F:503:LEU:HB3	2:F:1118:LEU:HD11	1.92	0.51
2:B:209:ASP:OD1	2:B:209:ASP:N	2.42	0.51
2:D:1178:ILE:HD13	2:D:1251:ARG:HB3	1.90	0.51
1:C:147:LEU:O	1:C:151:VAL:HG23	2.11	0.51
2:D:208:GLU:H	2:D:208:GLU:CD	2.13	0.51
2:D:775:GLN:OE1	4:D:1602:AGS:S1G	2.69	0.51
1:E:107:ASN:OD1	1:E:108:VAL:N	2.43	0.51
2:H:93:ILE:HG23	3:H:1604:POV:H24A	1.91	0.51
2:F:17:VAL:HB	2:F:21:VAL:HG22	1.92	0.51
2:H:25:GLY:HA2	2:H:28:VAL:HG12	1.93	0.51
2:H:208:GLU:H	2:H:208:GLU:CD	2.13	0.51
2:H:503:LEU:HB3	2:H:1118:LEU:HD11	1.92	0.51
1:A:180:THR:HG21	1:A:206:ARG:HD2	1.93	0.51
2:B:503:LEU:HB3	2:B:1118:LEU:HD11	1.92	0.51
1:C:217:MET:HG2	1:C:285:VAL:HG12	1.92	0.51
1:G:126:GLU:HA	1:G:131:ILE:HG12	1.93	0.51
1:A:107:ASN:OD1	1:A:108:VAL:N	2.43	0.51
1:C:36:VAL:HB	1:C:303:SER:OG	2.11	0.51
1:C:313:GLN:HA	1:C:338:LYS:HA	1.93	0.51
2:D:377:TYR:O	2:D:381:ILE:HG12	2.11	0.51
1:E:126:GLU:HA	1:E:131:ILE:HG12	1.93	0.51
2:F:377:TYR:O	2:F:381:ILE:HG12	2.11	0.51
1:E:217:MET:HG2	1:E:285:VAL:HG12	1.92	0.51
2:H:47:LEU:HD21	2:H:123:TYR:HA	1.93	0.51
1:A:147:LEU:O	1:A:151:VAL:HG23	2.11	0.50
2:D:17:VAL:HB	2:D:21:VAL:HG22	1.92	0.50
2:D:47:LEU:HD21	2:D:123:TYR:HA	1.93	0.50
2:H:775:GLN:OE1	4:H:1602:AGS:S1G	2.69	0.50
1:A:126:GLU:HA	1:A:131:ILE:HG12	1.93	0.50
2:B:17:VAL:HB	2:B:21:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:377:TYR:O	2:B:381:ILE:HG12	2.11	0.50
1:E:313:GLN:HA	1:E:338:LYS:HA	1.93	0.50
1:G:180:THR:HG21	1:G:206:ARG:HD2	1.93	0.50
1:A:217:MET:HG2	1:A:285:VAL:HG12	1.92	0.50
2:B:25:GLY:HA2	2:B:28:VAL:HG12	1.93	0.50
2:B:563:VAL:HG21	2:B:1037:TRP:CH2	2.47	0.50
2:D:563:VAL:HG21	2:D:1037:TRP:CH2	2.47	0.50
2:F:208:GLU:H	2:F:208:GLU:CD	2.13	0.50
2:F:775:GLN:OE1	4:F:1602:AGS:S1G	2.69	0.50
2:F:25:GLY:HA2	2:F:28:VAL:HG12	1.93	0.50
2:F:563:VAL:HG21	2:F:1037:TRP:CH2	2.47	0.50
2:H:377:TYR:O	2:H:381:ILE:HG12	2.11	0.50
2:D:783:THR:HB	2:D:820:GLN:HA	1.94	0.50
2:D:1039:ASP:OD1	2:D:1039:ASP:N	2.40	0.50
1:E:36:VAL:HB	1:E:303:SER:OG	2.11	0.50
1:E:147:LEU:O	1:E:151:VAL:HG23	2.11	0.50
1:G:217:MET:HG2	1:G:285:VAL:HG12	1.92	0.50
2:B:84:VAL:HG13	2:B:171:LEU:HD22	1.94	0.50
1:C:126:GLU:HA	1:C:131:ILE:HG12	1.93	0.50
1:C:180:THR:HG21	1:C:206:ARG:HD2	1.93	0.50
2:F:47:LEU:HD21	2:F:123:TYR:HA	1.93	0.50
2:H:71:HIS:NE2	2:H:223:ASN:HA	2.26	0.50
1:A:36:VAL:HB	1:A:303:SER:OG	2.11	0.50
2:B:47:LEU:HD21	2:B:123:TYR:HA	1.93	0.50
1:C:46:HIS:HB3	1:C:49:ILE:HD11	1.94	0.50
2:B:123:TYR:CZ	2:B:127:ILE:HD11	2.47	0.50
2:D:84:VAL:HG13	2:D:171:LEU:HD22	1.94	0.50
2:F:71:HIS:NE2	2:F:223:ASN:HA	2.26	0.50
1:A:313:GLN:HA	1:A:338:LYS:HA	1.93	0.50
2:B:187:VAL:HA	2:B:190:ILE:HG22	1.94	0.50
2:B:775:GLN:OE1	4:B:1602:AGS:S1G	2.69	0.50
1:C:107:ASN:OD1	1:C:108:VAL:N	2.43	0.50
2:F:783:THR:HB	2:F:820:GLN:HA	1.94	0.50
1:G:313:GLN:HA	1:G:338:LYS:HA	1.93	0.50
2:B:71:HIS:NE2	2:B:223:ASN:HA	2.26	0.49
2:B:783:THR:HB	2:B:820:GLN:HA	1.94	0.49
2:D:96:ASP:HB3	2:D:106:LEU:HD12	1.94	0.49
2:D:123:TYR:CZ	2:D:127:ILE:HD11	2.47	0.49
1:E:290:VAL:HA	1:E:297:THR:HA	1.94	0.49
1:G:290:VAL:HA	1:G:297:THR:HA	1.94	0.49
2:H:96:ASP:HB3	2:H:106:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:PRO:HB2	1:G:319:VAL:HB	1.94	0.49
2:D:25:GLY:HA2	2:D:28:VAL:HG12	1.93	0.49
1:E:319:VAL:HB	1:G:232:PRO:HB2	1.94	0.49
3:B:1607:POV:H23	3:B:1607:POV:H33A	1.95	0.49
2:F:123:TYR:CZ	2:F:127:ILE:HD11	2.47	0.49
1:G:147:LEU:O	1:G:151:VAL:HG23	2.11	0.49
2:H:123:TYR:CZ	2:H:127:ILE:HD11	2.47	0.49
1:C:290:VAL:HA	1:C:297:THR:HA	1.94	0.49
1:G:36:VAL:HB	1:G:303:SER:OG	2.11	0.49
2:H:84:VAL:HG13	2:H:171:LEU:HD22	1.94	0.49
2:H:783:THR:HB	2:H:820:GLN:HA	1.94	0.49
1:A:290:VAL:HA	1:A:297:THR:HA	1.94	0.49
2:D:71:HIS:NE2	2:D:223:ASN:HA	2.26	0.49
3:D:1607:POV:H33A	3:D:1607:POV:H23	1.95	0.49
1:E:180:THR:HG21	1:E:206:ARG:HD2	1.93	0.49
2:B:96:ASP:HB3	2:B:106:LEU:HD12	1.94	0.49
1:C:209:MET:O	1:C:292:GLU:HB2	2.13	0.49
1:E:138:VAL:HG11	1:E:149:LEU:HD22	1.95	0.49
1:A:46:HIS:HB3	1:A:49:ILE:HD11	1.94	0.49
2:D:1296:ASN:HA	2:D:1299:VAL:HG12	1.95	0.49
1:E:46:HIS:HB3	1:E:49:ILE:HD11	1.94	0.49
1:E:85:LEU:O	1:E:88:MET:HB3	2.13	0.49
1:E:272:PRO:HG3	1:E:311:TRP:CZ2	2.48	0.49
2:F:84:VAL:HG13	2:F:171:LEU:HD22	1.94	0.49
2:H:28:VAL:HG23	2:H:152:ILE:HG22	1.95	0.49
1:A:85:LEU:O	1:A:88:MET:HB3	2.13	0.49
2:B:1097:LEU:HD11	2:B:1316:HIS:NE2	2.28	0.49
1:C:85:LEU:O	1:C:88:MET:HB3	2.13	0.49
2:D:1097:LEU:HD11	2:D:1316:HIS:NE2	2.28	0.49
2:F:187:VAL:HA	2:F:190:ILE:HG22	1.94	0.49
2:B:783:THR:O	2:B:787:ASN:ND2	2.37	0.49
1:C:290:VAL:HG21	1:E:297:THR:HB	1.95	0.49
1:E:290:VAL:HG21	1:G:297:THR:HB	1.95	0.49
2:H:563:VAL:HG21	2:H:1037:TRP:CH2	2.47	0.49
2:H:1039:ASP:OD1	2:H:1039:ASP:N	2.40	0.49
1:E:209:MET:O	1:E:292:GLU:HB2	2.13	0.49
1:G:46:HIS:HB3	1:G:49:ILE:HD11	1.94	0.49
1:G:85:LEU:O	1:G:88:MET:HB3	2.13	0.49
1:A:114:ILE:HD12	1:A:120:ALA:HA	1.95	0.48
2:B:150:LYS:HE3	2:B:175:LEU:HD12	1.95	0.48
1:C:272:PRO:HG3	1:C:311:TRP:CZ2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1607:POV:H23	3:H:1607:POV:H33A	1.95	0.48
1:A:138:VAL:HG11	1:A:149:LEU:HD22	1.95	0.48
1:A:272:PRO:HG3	1:A:311:TRP:CZ2	2.48	0.48
2:B:162:ILE:HD13	2:B:339:GLN:HG2	1.96	0.48
2:D:74:ARG:HD3	2:D:124:TYR:CZ	2.48	0.48
2:D:187:VAL:HA	2:D:190:ILE:HG22	1.94	0.48
2:D:783:THR:O	2:D:787:ASN:ND2	2.37	0.48
1:G:272:PRO:HG3	1:G:311:TRP:CZ2	2.48	0.48
2:H:166:GLN:N	2:H:166:GLN:OE1	2.47	0.48
2:H:1097:LEU:HD11	2:H:1316:HIS:NE2	2.28	0.48
1:G:114:ILE:HD12	1:G:120:ALA:HA	1.95	0.48
1:A:128:GLN:OE1	1:A:152:GLN:NE2	2.30	0.48
1:A:209:MET:O	1:A:292:GLU:HB2	2.13	0.48
1:A:319:VAL:HB	1:C:232:PRO:HB2	1.94	0.48
2:B:74:ARG:HD3	2:B:124:TYR:CZ	2.48	0.48
1:C:319:VAL:HB	1:E:232:PRO:HB2	1.94	0.48
2:D:166:GLN:N	2:D:166:GLN:OE1	2.47	0.48
2:F:150:LYS:HE3	2:F:175:LEU:HD12	1.95	0.48
2:H:162:ILE:HD13	2:H:339:GLN:HG2	1.96	0.48
2:F:28:VAL:HG23	2:F:152:ILE:HG22	1.95	0.48
2:F:96:ASP:HB3	2:F:106:LEU:HD12	1.94	0.48
5:F:1601:AJP:O76	5:F:1601:AJP:O77	2.32	0.48
2:H:74:ARG:HD3	2:H:124:TYR:CZ	2.48	0.48
2:B:1026:VAL:HG21	2:B:1074:LEU:HD22	1.96	0.48
2:D:381:ILE:HD11	6:D:1603:BJX:C20	2.44	0.48
2:F:166:GLN:N	2:F:166:GLN:OE1	2.47	0.48
2:F:323:ILE:HD13	2:F:1268:ILE:HD11	1.96	0.48
1:G:138:VAL:HG11	1:G:149:LEU:HD22	1.95	0.48
2:H:187:VAL:HA	2:H:190:ILE:HG22	1.94	0.48
2:H:323:ILE:HD13	2:H:1268:ILE:HD11	1.96	0.48
2:B:28:VAL:HG23	2:B:152:ILE:HG22	1.95	0.48
2:F:480:LYS:HB3	2:F:539:TYR:CE2	2.49	0.48
3:F:1607:POV:H23	3:F:1607:POV:H33A	1.95	0.48
1:G:209:MET:O	1:G:292:GLU:HB2	2.13	0.48
1:A:151:VAL:O	1:A:155:VAL:HG13	2.14	0.48
5:B:1601:AJP:O76	5:B:1601:AJP:O77	2.32	0.48
1:C:114:ILE:HD12	1:C:120:ALA:HA	1.95	0.48
2:D:162:ILE:HD13	2:D:339:GLN:HG2	1.96	0.48
5:D:1601:AJP:O76	5:D:1601:AJP:O77	2.32	0.48
2:F:74:ARG:HD3	2:F:124:TYR:CZ	2.48	0.48
2:F:381:ILE:HD11	6:F:1603:BJX:C20	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:VAL:HG21	1:C:297:THR:HB	1.95	0.48
2:B:419:ASN:HA	2:B:422:ALA:HB3	1.95	0.48
1:C:138:VAL:HG11	1:C:149:LEU:HD22	1.95	0.48
1:C:151:VAL:O	1:C:155:VAL:HG13	2.14	0.48
2:F:162:ILE:HD13	2:F:339:GLN:HG2	1.96	0.48
2:F:1296:ASN:HA	2:F:1299:VAL:HG12	1.95	0.48
2:H:419:ASN:HA	2:H:422:ALA:HB3	1.95	0.48
1:A:297:THR:HB	1:G:290:VAL:HG21	1.95	0.48
2:B:166:GLN:OE1	2:B:166:GLN:N	2.47	0.48
2:D:419:ASN:HA	2:D:422:ALA:HB3	1.95	0.48
2:D:1026:VAL:HG21	2:D:1074:LEU:HD22	1.96	0.48
2:F:194:ARG:HH12	2:F:202:ARG:HE	1.61	0.48
2:H:194:ARG:HH12	2:H:202:ARG:HE	1.61	0.48
2:H:1296:ASN:HA	2:H:1299:VAL:HG12	1.95	0.48
1:C:220:VAL:HG22	1:C:235:GLN:HG2	1.96	0.47
2:H:1026:VAL:HG21	2:H:1074:LEU:HD22	1.96	0.47
5:H:1601:AJP:O76	5:H:1601:AJP:O77	2.32	0.47
2:B:326:HIS:ND1	2:B:353:GLY:O	2.47	0.47
2:B:1296:ASN:HA	2:B:1299:VAL:HG12	1.95	0.47
2:H:784:VAL:HG22	2:H:823:ILE:HD11	1.97	0.47
2:B:194:ARG:HH12	2:B:202:ARG:HE	1.61	0.47
2:B:323:ILE:HD13	2:B:1268:ILE:HD11	1.96	0.47
2:B:381:ILE:HD11	6:B:1603:BJX:C20	2.44	0.47
2:D:1246:ARG:NH2	6:D:1603:BJX:O2	2.47	0.47
1:E:155:VAL:O	1:E:159:ILE:HG23	2.14	0.47
2:F:1030:ILE:HG13	2:F:1031:ASP:N	2.29	0.47
1:G:155:VAL:O	1:G:159:ILE:HG23	2.14	0.47
2:H:141:ILE:O	2:H:144:THR:HB	2.15	0.47
2:H:381:ILE:HD11	6:H:1603:BJX:C20	2.44	0.47
1:A:220:VAL:HG22	1:A:235:GLN:HG2	1.96	0.47
2:B:318:LEU:HD23	2:B:455:ILE:HD11	1.96	0.47
1:C:319:VAL:HG11	1:E:233:LEU:HG	1.96	0.47
2:D:150:LYS:HE3	2:D:175:LEU:HD12	1.95	0.47
2:D:194:ARG:HH12	2:D:202:ARG:HE	1.61	0.47
2:D:1030:ILE:HG13	2:D:1031:ASP:N	2.29	0.47
1:E:319:VAL:HG11	1:G:233:LEU:HG	1.96	0.47
2:F:1097:LEU:HD11	2:F:1316:HIS:NE2	2.28	0.47
2:F:1246:ARG:NH2	6:F:1603:BJX:O2	2.47	0.47
2:H:150:LYS:HE3	2:H:175:LEU:HD12	1.95	0.47
1:C:63:LEU:HD11	1:C:74:ILE:HG21	1.97	0.47
1:C:155:VAL:O	1:C:159:ILE:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:TYR:CE2	1:E:233:LEU:HD21	2.49	0.47
2:D:28:VAL:HG23	2:D:152:ILE:HG22	1.95	0.47
1:E:114:ILE:HD12	1:E:120:ALA:HA	1.95	0.47
1:E:220:VAL:HG22	1:E:235:GLN:HG2	1.96	0.47
1:E:326:TYR:CE2	1:G:233:LEU:HD21	2.49	0.47
2:F:318:LEU:HD23	2:F:455:ILE:HD11	1.96	0.47
2:F:496:LEU:HD23	2:F:496:LEU:HA	1.78	0.47
2:F:784:VAL:HG22	2:F:823:ILE:HD11	1.97	0.47
1:G:151:VAL:O	1:G:155:VAL:HG13	2.14	0.47
1:G:220:VAL:HG22	1:G:235:GLN:HG2	1.96	0.47
2:D:480:LYS:HB3	2:D:539:TYR:CE2	2.49	0.47
1:G:63:LEU:HD11	1:G:74:ILE:HG21	1.97	0.47
1:A:63:LEU:HD11	1:A:74:ILE:HG21	1.97	0.47
2:B:141:ILE:O	2:B:144:THR:HB	2.15	0.47
2:B:1030:ILE:HG13	2:B:1031:ASP:N	2.29	0.47
2:B:1148:LEU:HD23	2:B:1148:LEU:HA	1.78	0.47
2:D:318:LEU:HD23	2:D:455:ILE:HD11	1.96	0.47
3:D:1605:POV:H211	3:D:1605:POV:H28	1.68	0.47
1:E:63:LEU:HD11	1:E:74:ILE:HG21	1.97	0.47
1:E:75:PHE:CE1	1:E:163:MET:HB3	2.50	0.47
1:E:151:VAL:O	1:E:155:VAL:HG13	2.14	0.47
2:F:1026:VAL:HG21	2:F:1074:LEU:HD22	1.96	0.47
2:H:1030:ILE:HG13	2:H:1031:ASP:N	2.29	0.47
3:H:1608:POV:H34	3:H:1608:POV:H25	1.97	0.47
1:A:326:TYR:CE2	1:C:233:LEU:HD21	2.49	0.47
2:F:416:GLN:HA	2:F:419:ASN:ND2	2.30	0.47
2:F:419:ASN:HA	2:F:422:ALA:HB3	1.95	0.47
2:H:326:HIS:ND1	2:H:353:GLY:O	2.47	0.47
2:B:416:GLN:HA	2:B:419:ASN:ND2	2.30	0.47
2:B:480:LYS:HB3	2:B:539:TYR:CE2	2.49	0.47
2:B:784:VAL:HG22	2:B:823:ILE:HD11	1.97	0.47
1:C:75:PHE:CE1	1:C:163:MET:HB3	2.50	0.47
2:D:1282:GLY:O	2:D:1286:THR:HG23	2.15	0.47
3:H:1608:POV:H33A	3:H:1608:POV:H22A	1.96	0.47
1:A:233:LEU:HD21	1:G:326:TYR:CE2	2.49	0.47
2:D:141:ILE:O	2:D:144:THR:HB	2.15	0.47
2:H:480:LYS:HB3	2:H:539:TYR:CE2	2.49	0.47
1:A:299:GLN:HE21	1:A:301:ARG:HD3	1.81	0.46
2:B:1282:GLY:O	2:B:1286:THR:HG23	2.15	0.46
3:B:1608:POV:H25	3:B:1608:POV:H34	1.97	0.46
2:H:318:LEU:HD23	2:H:455:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1001:CYS:HB2	2:H:1309:LEU:HD21	1.97	0.46
2:H:1246:ARG:NH2	6:H:1603:BJX:O2	2.47	0.46
1:A:75:PHE:CE1	1:A:163:MET:HB3	2.50	0.46
2:B:374:GLN:HG3	2:B:1250:VAL:HG23	1.97	0.46
2:D:323:ILE:HD13	2:D:1268:ILE:HD11	1.96	0.46
2:D:496:LEU:HD23	2:D:496:LEU:HA	1.78	0.46
1:G:299:GLN:HE21	1:G:301:ARG:HD3	1.81	0.46
2:H:416:GLN:HA	2:H:419:ASN:ND2	2.30	0.46
2:B:1272:LEU:HD12	2:B:1272:LEU:HA	1.81	0.46
2:F:1247:TRP:O	2:F:1251:ARG:HG2	2.16	0.46
2:F:1282:GLY:O	2:F:1286:THR:HG23	2.15	0.46
2:H:1247:TRP:O	2:H:1251:ARG:HG2	2.16	0.46
1:C:305:LEU:H	1:C:308:GLU:HG3	1.80	0.46
2:F:141:ILE:O	2:F:144:THR:HB	2.15	0.46
2:F:1246:ARG:HA	2:F:1246:ARG:HD3	1.77	0.46
1:A:233:LEU:HG	1:G:319:VAL:HG11	1.96	0.46
3:B:1604:POV:H13B	3:B:1604:POV:H11	1.65	0.46
3:B:1608:POV:H33A	3:B:1608:POV:H22A	1.96	0.46
2:D:374:GLN:HG3	2:D:1250:VAL:HG23	1.97	0.46
2:D:784:VAL:HG22	2:D:823:ILE:HD11	1.97	0.46
2:F:507:LYS:O	2:F:511:LEU:HG	2.16	0.46
2:H:534:ARG:HA	2:H:1091:LEU:HD11	1.98	0.46
2:F:1001:CYS:HB2	2:F:1309:LEU:HD21	1.97	0.46
2:H:135:LEU:HA	2:H:135:LEU:HD23	1.72	0.46
2:H:396:TYR:CD1	2:H:1227:LEU:HD13	2.51	0.46
2:D:416:GLN:HA	2:D:419:ASN:ND2	2.30	0.46
2:D:507:LYS:O	2:D:511:LEU:HG	2.16	0.46
3:D:1608:POV:H25	3:D:1608:POV:H34	1.97	0.46
2:F:396:TYR:OH	2:F:1223:PHE:HB3	2.16	0.46
2:F:533:LEU:HD23	2:F:533:LEU:HA	1.82	0.46
2:F:534:ARG:HA	2:F:1091:LEU:HD11	1.98	0.46
3:F:1608:POV:H25	3:F:1608:POV:H34	1.97	0.46
1:A:305:LEU:H	1:A:308:GLU:HG3	1.80	0.46
2:B:213:LEU:HD23	2:B:213:LEU:HA	1.83	0.46
3:B:1605:POV:H13B	3:B:1605:POV:H11	1.66	0.46
2:D:326:HIS:ND1	2:D:353:GLY:O	2.47	0.46
3:D:1604:POV:H13B	3:D:1604:POV:H11	1.65	0.46
1:E:75:PHE:HE1	1:E:163:MET:HB3	1.80	0.46
2:F:1161:THR:HG22	2:F:1164:PHE:H	1.81	0.46
3:F:1608:POV:H22A	3:F:1608:POV:H33A	1.96	0.46
1:G:75:PHE:CE1	1:G:163:MET:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1256:GLY:HA3	2:H:1292:SER:HB2	1.98	0.46
2:H:1282:GLY:O	2:H:1286:THR:HG23	2.15	0.46
1:C:299:GLN:HE21	1:C:301:ARG:HD3	1.81	0.46
3:D:1608:POV:H22A	3:D:1608:POV:H33A	1.96	0.46
1:E:305:LEU:H	1:E:308:GLU:HG3	1.80	0.46
2:H:1296:ASN:OD1	2:H:1297:TRP:N	2.49	0.46
1:A:60:PHE:CD1	1:G:171:THR:HG23	2.52	0.46
1:A:155:VAL:O	1:A:159:ILE:HG23	2.14	0.46
2:B:396:TYR:OH	2:B:1223:PHE:HB3	2.16	0.46
2:B:1246:ARG:HA	2:B:1246:ARG:HD3	1.77	0.46
3:D:1605:POV:H13B	3:D:1605:POV:H11	1.66	0.46
2:F:1256:GLY:HA3	2:F:1292:SER:HB2	1.98	0.46
2:H:374:GLN:HG3	2:H:1250:VAL:HG23	1.97	0.46
2:H:507:LYS:O	2:H:511:LEU:HG	2.16	0.46
1:A:319:VAL:HG11	1:C:233:LEU:HG	1.96	0.45
2:F:226:SER:HB2	7:F:1614:PTY:HC51	1.99	0.45
1:A:68:TRP:CZ2	1:A:170:LYS:HG2	2.51	0.45
1:A:171:THR:HG23	1:C:60:PHE:CD1	2.52	0.45
2:B:327:LEU:HD21	2:B:1281:VAL:HG11	1.98	0.45
2:B:507:LYS:O	2:B:511:LEU:HG	2.16	0.45
2:B:1001:CYS:HB2	2:B:1309:LEU:HD21	1.97	0.45
1:C:68:TRP:CZ2	1:C:170:LYS:HG2	2.51	0.45
2:D:209:ASP:N	2:D:209:ASP:OD1	2.42	0.45
2:F:327:LEU:HD21	2:F:1281:VAL:HG11	1.98	0.45
1:G:75:PHE:HE1	1:G:163:MET:HB3	1.80	0.45
1:G:305:LEU:H	1:G:308:GLU:HG3	1.80	0.45
2:B:1296:ASN:OD1	2:B:1297:TRP:N	2.49	0.45
2:D:1161:THR:HG22	2:D:1164:PHE:H	1.81	0.45
2:D:1256:GLY:HA3	2:D:1292:SER:HB2	1.98	0.45
2:F:396:TYR:CD1	2:F:1227:LEU:HD13	2.51	0.45
1:G:68:TRP:CZ2	1:G:170:LYS:HG2	2.51	0.45
2:H:226:SER:HB2	7:H:1614:PTY:HC51	1.99	0.45
3:H:1605:POV:H211	3:H:1605:POV:H28	1.68	0.45
2:D:1247:TRP:O	2:D:1251:ARG:HG2	2.16	0.45
1:E:171:THR:HG23	1:G:60:PHE:CD1	2.52	0.45
1:E:299:GLN:HE21	1:E:301:ARG:HD3	1.81	0.45
2:F:374:GLN:HG3	2:F:1250:VAL:HG23	1.97	0.45
2:B:69:PRO:CG	2:B:192:VAL:HG11	2.47	0.45
2:D:226:SER:HB2	7:D:1614:PTY:HC51	1.99	0.45
2:D:396:TYR:CD1	2:D:1227:LEU:HD13	2.51	0.45
1:E:68:TRP:CZ2	1:E:170:LYS:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1296:ASN:OD1	2:F:1297:TRP:N	2.49	0.45
1:G:128:GLN:OE1	1:G:152:GLN:NE2	2.30	0.45
1:A:75:PHE:HE1	1:A:163:MET:HB3	1.80	0.45
2:B:1161:THR:HG22	2:B:1164:PHE:H	1.81	0.45
2:D:396:TYR:OH	2:D:1223:PHE:HB3	2.16	0.45
2:D:1031:ASP:OD2	2:D:1287:TYR:OH	2.26	0.45
2:B:226:SER:HB2	7:B:1614:PTY:HC51	1.99	0.45
2:B:534:ARG:HA	2:B:1091:LEU:HD11	1.98	0.45
2:D:230:TYR:CE2	2:D:1246:ARG:HB3	2.52	0.45
2:D:534:ARG:HA	2:D:1091:LEU:HD11	1.98	0.45
2:F:194:ARG:HH22	2:F:202:ARG:HH11	1.64	0.45
2:F:326:HIS:ND1	2:F:353:GLY:O	2.47	0.45
1:G:151:VAL:HA	1:G:154:ILE:HG12	1.99	0.45
2:H:69:PRO:CG	2:H:192:VAL:HG11	2.47	0.45
2:H:230:TYR:CE2	2:H:1246:ARG:HB3	2.52	0.45
2:H:583:PHE:O	2:H:587:VAL:HG23	2.17	0.45
2:B:1247:TRP:O	2:B:1251:ARG:HG2	2.16	0.45
2:B:1256:GLY:HA3	2:B:1292:SER:HB2	1.98	0.45
1:C:75:PHE:HE1	1:C:163:MET:HB3	1.80	0.45
2:D:1296:ASN:OD1	2:D:1297:TRP:N	2.49	0.45
2:B:193:ARG:HE	2:B:193:ARG:HB3	1.53	0.45
2:B:230:TYR:CE2	2:B:1246:ARG:HB3	2.52	0.45
1:C:151:VAL:HA	1:C:154:ILE:HG12	1.99	0.45
2:D:1148:LEU:HD23	2:D:1148:LEU:HA	1.78	0.45
2:F:194:ARG:HD3	2:F:198:PHE:CE1	2.52	0.45
2:H:194:ARG:HD3	2:H:198:PHE:CE1	2.52	0.45
2:H:1161:THR:HG22	2:H:1164:PHE:H	1.81	0.45
2:B:396:TYR:CD1	2:B:1227:LEU:HD13	2.51	0.45
2:D:194:ARG:HH22	2:D:202:ARG:HH11	1.64	0.45
2:D:1001:CYS:HB2	2:D:1309:LEU:HD21	1.97	0.45
3:D:1608:POV:H13B	3:D:1608:POV:H11	1.80	0.45
2:H:327:LEU:HD21	2:H:1281:VAL:HG11	1.98	0.45
2:H:783:THR:O	2:H:787:ASN:ND2	2.37	0.45
2:D:583:PHE:O	2:D:587:VAL:HG23	2.17	0.44
1:E:215:ILE:HG12	1:E:287:LEU:HB2	1.99	0.44
2:H:396:TYR:OH	2:H:1223:PHE:HB3	2.16	0.44
2:B:194:ARG:HD3	2:B:198:PHE:CE1	2.52	0.44
2:B:466:VAL:HG21	2:B:557:ILE:HD13	1.99	0.44
2:B:571:LEU:HG	2:B:576:ALA:HB2	1.99	0.44
2:B:1205:ALA:O	2:B:1209:GLU:HG2	2.17	0.44
2:D:194:ARG:HD3	2:D:198:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:571:LEU:HG	2:D:576:ALA:HB2	1.99	0.44
2:H:466:VAL:HG21	2:H:557:ILE:HD13	1.99	0.44
2:H:1205:ALA:O	2:H:1209:GLU:HG2	2.17	0.44
1:A:88:MET:SD	3:B:1608:POV:H26A	2.58	0.44
1:C:171:THR:HG23	1:E:60:PHE:CD1	2.52	0.44
2:F:783:THR:O	2:F:787:ASN:ND2	2.37	0.44
2:B:219:GLN:HG2	2:B:378:TYR:CZ	2.53	0.44
2:B:583:PHE:O	2:B:587:VAL:HG23	2.17	0.44
2:B:1039:ASP:OD1	2:B:1039:ASP:N	2.40	0.44
2:B:1106:ILE:HD13	2:B:1106:ILE:HA	1.81	0.44
2:D:327:LEU:HD21	2:D:1281:VAL:HG11	1.98	0.44
2:D:1205:ALA:O	2:D:1209:GLU:HG2	2.17	0.44
1:E:144:LEU:HD22	3:E:402:POV:O31	2.17	0.44
2:H:156:LYS:HD3	2:H:156:LYS:HA	1.81	0.44
2:H:513:ALA:HB2	2:H:1419:ARG:HG3	2.00	0.44
2:H:571:LEU:HG	2:H:576:ALA:HB2	1.99	0.44
1:A:161:ALA:CB	1:G:167:ILE:HD11	2.48	0.44
1:A:215:ILE:HG12	1:A:287:LEU:HB2	1.99	0.44
2:B:135:LEU:HD23	2:B:135:LEU:HA	1.72	0.44
1:C:88:MET:SD	3:D:1608:POV:H26A	2.58	0.44
2:F:496:LEU:HD21	2:F:1126:SER:HA	2.00	0.44
1:G:143:PRO:O	1:G:146:ILE:N	2.51	0.44
2:H:194:ARG:HH22	2:H:202:ARG:HH11	1.64	0.44
2:H:533:LEU:HD23	2:H:533:LEU:HA	1.82	0.44
2:H:1026:VAL:O	2:H:1030:ILE:HG23	2.18	0.44
1:A:167:ILE:HD11	1:C:161:ALA:CB	2.48	0.44
2:B:22:LEU:HD12	2:B:22:LEU:HA	1.82	0.44
2:B:132:PHE:CE1	2:B:134:LYS:HB2	2.53	0.44
2:B:509:LEU:O	2:B:513:ALA:N	2.51	0.44
2:B:770:VAL:HG11	2:B:852:PHE:CE2	2.53	0.44
1:C:167:ILE:HD11	1:E:161:ALA:CB	2.48	0.44
2:D:63:SER:O	2:D:64:THR:OG1	2.33	0.44
2:H:132:PHE:CE1	2:H:134:LYS:HB2	2.53	0.44
1:C:154:ILE:HG13	1:C:155:VAL:N	2.33	0.44
1:C:168:PHE:CE2	1:E:168:PHE:HE2	2.36	0.44
2:D:770:VAL:HG11	2:D:852:PHE:CE2	2.53	0.44
2:D:1026:VAL:O	2:D:1030:ILE:HG23	2.18	0.44
2:F:1205:ALA:O	2:F:1209:GLU:HG2	2.17	0.44
1:G:215:ILE:HG12	1:G:287:LEU:HB2	1.99	0.44
2:H:381:ILE:HG21	2:H:1242:THR:OG1	2.18	0.44
1:A:34:ARG:HD3	1:A:37:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ARG:HD3	1:C:37:SER:HA	2.00	0.44
1:C:144:LEU:HD22	3:C:402:POV:O31	2.17	0.44
1:E:151:VAL:HA	1:E:154:ILE:HG12	1.99	0.44
1:E:167:ILE:HD11	1:G:161:ALA:CB	2.48	0.44
2:F:132:PHE:CE1	2:F:134:LYS:HB2	2.53	0.44
2:F:513:ALA:HB2	2:F:1419:ARG:HG3	2.00	0.44
1:A:168:PHE:CE2	1:C:168:PHE:HE2	2.36	0.44
2:B:88:GLU:O	2:B:91:GLU:HG3	2.18	0.44
2:B:194:ARG:HH22	2:B:202:ARG:HH11	1.64	0.44
2:B:1026:VAL:O	2:B:1030:ILE:HG23	2.18	0.44
2:D:1272:LEU:HD12	2:D:1272:LEU:HA	1.81	0.44
2:D:1295:LEU:HD23	2:D:1295:LEU:HA	1.89	0.44
1:E:143:PRO:O	1:E:146:ILE:N	2.51	0.44
2:F:230:TYR:CE2	2:F:1246:ARG:HB3	2.52	0.44
1:G:88:MET:SD	3:H:1608:POV:H26A	2.58	0.44
1:G:154:ILE:HG13	1:G:155:VAL:N	2.33	0.44
2:H:96:ASP:OD2	2:H:107:TYR:HE2	2.01	0.44
2:H:464:ALA:HA	2:H:467:ILE:HG22	2.00	0.44
2:D:1106:ILE:HD13	2:D:1106:ILE:HA	1.81	0.43
2:F:63:SER:O	2:F:64:THR:OG1	2.33	0.43
2:H:1246:ARG:HA	2:H:1246:ARG:HD3	1.77	0.43
1:A:144:LEU:HD22	3:A:401:POV:O31	2.17	0.43
1:C:50:ARG:N	4:C:401:AGS:N1	2.67	0.43
1:C:238:ILE:HG22	1:C:266:PRO:HD2	2.00	0.43
1:C:314:ARG:NH2	1:C:339:VAL:HG21	2.34	0.43
2:D:132:PHE:CE1	2:D:134:LYS:HB2	2.53	0.43
2:D:219:GLN:HG2	2:D:378:TYR:CZ	2.53	0.43
1:E:314:ARG:NH2	1:E:339:VAL:HG21	2.34	0.43
2:F:381:ILE:HG21	2:F:1242:THR:OG1	2.18	0.43
2:F:583:PHE:O	2:F:587:VAL:HG23	2.17	0.43
3:F:1605:POV:H211	3:F:1605:POV:H28	1.68	0.43
1:G:34:ARG:HD3	1:G:37:SER:HA	2.00	0.43
1:G:238:ILE:HG22	1:G:266:PRO:HD2	2.00	0.43
2:H:559:PHE:HE2	2:H:1034:LEU:HD11	1.83	0.43
2:H:770:VAL:HG11	2:H:852:PHE:CE2	2.53	0.43
2:H:1082:THR:O	2:H:1086:VAL:HG13	2.18	0.43
1:A:151:VAL:HA	1:A:154:ILE:HG12	1.99	0.43
1:A:154:ILE:HG13	1:A:155:VAL:N	2.33	0.43
2:B:533:LEU:HD23	2:B:533:LEU:HA	1.82	0.43
2:B:559:PHE:HE2	2:B:1034:LEU:HD11	1.83	0.43
2:B:1101:LEU:HD11	2:B:1318:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1246:ARG:NH2	6:B:1603:BJX:O2	2.47	0.43
2:B:1436:ILE:HB	2:B:1471:LEU:HA	2.00	0.43
2:D:1091:LEU:HD23	2:D:1091:LEU:HA	1.89	0.43
2:D:1436:ILE:HB	2:D:1471:LEU:HA	2.00	0.43
1:E:88:MET:SD	3:F:1608:POV:H26A	2.58	0.43
1:E:154:ILE:HG13	1:E:155:VAL:N	2.33	0.43
1:G:50:ARG:N	4:G:401:AGS:N1	2.67	0.43
2:H:509:LEU:O	2:H:513:ALA:N	2.51	0.43
1:A:238:ILE:HG22	1:A:266:PRO:HD2	2.00	0.43
2:B:496:LEU:HD21	2:B:1126:SER:HA	2.00	0.43
1:C:215:ILE:HG12	1:C:287:LEU:HB2	1.99	0.43
2:D:22:LEU:HD12	2:D:22:LEU:HA	1.82	0.43
2:D:213:LEU:HD23	2:D:213:LEU:HA	1.83	0.43
2:H:22:LEU:HD12	2:H:22:LEU:HA	1.82	0.43
2:B:1082:THR:O	2:B:1086:VAL:HG13	2.18	0.43
2:D:466:VAL:HG21	2:D:557:ILE:HD13	1.99	0.43
2:F:88:GLU:O	2:F:91:GLU:HG3	2.18	0.43
2:F:466:VAL:HG21	2:F:557:ILE:HD13	1.99	0.43
2:F:509:LEU:O	2:F:513:ALA:N	2.51	0.43
2:H:88:GLU:O	2:H:91:GLU:HG3	2.18	0.43
1:C:143:PRO:O	1:C:146:ILE:N	2.51	0.43
2:D:88:GLU:O	2:D:91:GLU:HG3	2.18	0.43
2:D:255:ILE:HG12	2:D:258:ARG:HE	1.84	0.43
2:D:496:LEU:HD21	2:D:1126:SER:HA	2.00	0.43
2:D:1082:THR:O	2:D:1086:VAL:HG13	2.18	0.43
2:F:219:GLN:HG2	2:F:378:TYR:CZ	2.53	0.43
2:F:255:ILE:HG12	2:F:258:ARG:HE	1.84	0.43
2:F:559:PHE:HE2	2:F:1034:LEU:HD11	1.83	0.43
2:F:571:LEU:HG	2:F:576:ALA:HB2	1.99	0.43
2:F:1082:THR:O	2:F:1086:VAL:HG13	2.18	0.43
2:H:63:SER:O	2:H:64:THR:OG1	2.33	0.43
1:A:168:PHE:HE2	1:G:168:PHE:CE2	2.36	0.43
2:B:464:ALA:HA	2:B:467:ILE:HG22	2.00	0.43
1:E:168:PHE:CE2	1:G:168:PHE:HE2	2.36	0.43
2:F:1026:VAL:O	2:F:1030:ILE:HG23	2.18	0.43
2:F:1136:ILE:HD12	2:F:1308:GLN:HB3	2.00	0.43
2:F:1148:LEU:HD23	2:F:1148:LEU:HA	1.78	0.43
1:G:314:ARG:NH2	1:G:339:VAL:HG21	2.34	0.43
2:H:218:LEU:H	2:H:218:LEU:HG	1.73	0.43
1:A:66:LEU:HD23	1:A:66:LEU:HA	1.84	0.43
2:D:156:LYS:HA	2:D:156:LYS:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:513:ALA:HB2	2:D:1419:ARG:HG3	2.00	0.43
1:G:34:ARG:HB2	1:G:305:LEU:HD21	2.01	0.43
1:G:144:LEU:HD22	3:G:402:POV:O31	2.17	0.43
2:B:340:PHE:HB2	2:B:343:VAL:HB	2.01	0.43
3:B:1608:POV:H13B	3:B:1608:POV:H11	1.80	0.43
1:E:90:TRP:CZ2	1:E:148:ILE:HG22	2.54	0.43
2:F:1182:PHE:CE2	2:F:1248:LEU:HD22	2.54	0.43
1:G:316:VAL:HG11	1:G:335:ASN:HB2	2.01	0.43
2:H:106:LEU:HD23	2:H:106:LEU:HA	1.84	0.43
2:H:219:GLN:HG2	2:H:378:TYR:CZ	2.53	0.43
2:H:255:ILE:HG12	2:H:258:ARG:HE	1.84	0.43
2:B:381:ILE:HG21	2:B:1242:THR:OG1	2.18	0.43
2:D:154:PHE:HD1	2:D:172:THR:HG23	1.84	0.43
2:D:509:LEU:O	2:D:513:ALA:N	2.51	0.43
2:D:1124:ARG:HA	2:D:1124:ARG:HD3	1.85	0.43
2:D:1182:PHE:CE2	2:D:1248:LEU:HD22	2.54	0.43
1:E:34:ARG:HD3	1:E:37:SER:HA	2.00	0.43
2:F:143:TRP:O	2:F:147:PHE:N	2.40	0.43
2:H:193:ARG:HE	2:H:193:ARG:HB3	1.53	0.43
1:A:143:PRO:O	1:A:146:ILE:N	2.51	0.42
1:C:66:LEU:HD23	1:C:66:LEU:HA	1.84	0.42
2:D:143:TRP:O	2:D:147:PHE:N	2.40	0.42
2:D:340:PHE:HB2	2:D:343:VAL:HB	2.01	0.42
2:D:381:ILE:HG21	2:D:1242:THR:OG1	2.18	0.42
1:E:316:VAL:HG11	1:E:335:ASN:HB2	2.01	0.42
2:F:340:PHE:HB2	2:F:343:VAL:HB	2.01	0.42
2:F:770:VAL:HG11	2:F:852:PHE:CE2	2.53	0.42
2:F:1436:ILE:HB	2:F:1471:LEU:HA	2.00	0.42
2:H:496:LEU:HD21	2:H:1126:SER:HA	2.00	0.42
2:H:1101:LEU:HD11	2:H:1318:LEU:HD22	2.00	0.42
2:H:1182:PHE:CE2	2:H:1248:LEU:HD22	2.54	0.42
2:H:1436:ILE:HB	2:H:1471:LEU:HA	2.00	0.42
2:B:63:SER:O	2:B:64:THR:OG1	2.33	0.42
2:B:1182:PHE:CE2	2:B:1248:LEU:HD22	2.54	0.42
1:C:90:TRP:CZ2	1:C:148:ILE:HG22	2.54	0.42
1:C:316:VAL:HG11	1:C:335:ASN:HB2	2.01	0.42
2:D:96:ASP:OD2	2:D:107:TYR:HE2	2.01	0.42
2:D:1101:LEU:HD11	2:D:1318:LEU:HD22	2.00	0.42
1:E:34:ARG:HB2	1:E:305:LEU:HD21	2.01	0.42
2:F:154:PHE:HD1	2:F:172:THR:HG23	1.84	0.42
1:G:90:TRP:CZ2	1:G:148:ILE:HG22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:340:PHE:HB2	2:H:343:VAL:HB	2.01	0.42
1:A:66:LEU:HD21	2:B:52:GLY:HA3	2.02	0.42
2:B:255:ILE:HG12	2:B:258:ARG:HE	1.84	0.42
2:B:1136:ILE:HD12	2:B:1308:GLN:HB3	2.00	0.42
1:C:73:LEU:HA	1:C:76:THR:HG22	2.02	0.42
2:D:1136:ILE:HD12	2:D:1308:GLN:HB3	2.00	0.42
1:E:50:ARG:N	4:E:401:AGS:N1	2.67	0.42
1:E:73:LEU:HA	1:E:76:THR:HG22	2.02	0.42
2:B:154:PHE:HD1	2:B:172:THR:HG23	1.84	0.42
2:B:156:LYS:HA	2:B:156:LYS:HD3	1.81	0.42
2:B:1239:LEU:O	2:B:1242:THR:HG22	2.20	0.42
1:C:231:VAL:HA	1:C:232:PRO:HD3	1.90	0.42
2:D:76:ILE:HD11	7:D:1613:PTY:O13	2.20	0.42
2:D:464:ALA:HA	2:D:467:ILE:HG22	2.00	0.42
1:E:238:ILE:HG22	1:E:266:PRO:HD2	2.00	0.42
2:F:1101:LEU:HD11	2:F:1318:LEU:HD22	2.00	0.42
2:H:76:ILE:HD11	7:H:1613:PTY:O13	2.20	0.42
2:H:319:CYS:SG	2:H:362:LEU:HB2	2.60	0.42
1:A:34:ARG:HB2	1:A:305:LEU:HD21	2.01	0.42
2:B:1295:LEU:HD23	2:B:1295:LEU:HA	1.89	0.42
2:D:771:ALA:HB2	2:D:848:THR:HG21	2.02	0.42
2:D:1239:LEU:O	2:D:1242:THR:HG22	2.20	0.42
2:F:80:ILE:HG22	2:F:178:LEU:HD11	2.01	0.42
2:F:464:ALA:HA	2:F:467:ILE:HG22	2.00	0.42
2:H:1550:MET:HA	2:H:1559:GLU:HA	2.02	0.42
2:B:80:ILE:HG22	2:B:178:LEU:HD11	2.01	0.42
2:B:395:ILE:HG21	2:B:610:LEU:HD11	2.02	0.42
2:D:819:ASP:OD1	2:D:820:GLN:N	2.46	0.42
2:H:213:LEU:HD23	2:H:213:LEU:HA	1.83	0.42
2:H:395:ILE:HG21	2:H:610:LEU:HD11	2.02	0.42
1:A:90:TRP:CZ2	1:A:148:ILE:HG22	2.54	0.42
2:B:513:ALA:HB2	2:B:1419:ARG:HG3	2.00	0.42
2:B:771:ALA:HB2	2:B:848:THR:HG21	2.02	0.42
2:D:319:CYS:SG	2:D:362:LEU:HB2	2.60	0.42
2:D:559:PHE:HE2	2:D:1034:LEU:HD11	1.83	0.42
1:E:92:LEU:HD22	2:F:34:VAL:HG21	2.02	0.42
2:F:96:ASP:OD2	2:F:107:TYR:HE2	2.01	0.42
2:F:771:ALA:HB2	2:F:848:THR:HG21	2.02	0.42
1:G:66:LEU:HD21	2:H:52:GLY:HA3	2.02	0.42
2:H:80:ILE:HG22	2:H:178:LEU:HD11	2.01	0.42
2:H:1239:LEU:O	2:H:1242:THR:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1435:THR:HB	2:H:1472:ASP:HA	2.01	0.42
1:A:50:ARG:N	4:A:402:AGS:N1	2.67	0.42
2:D:193:ARG:HE	2:D:193:ARG:HB3	1.53	0.42
2:D:395:ILE:HG21	2:D:610:LEU:HD11	2.02	0.42
2:D:1027:LEU:HD12	2:D:1027:LEU:HA	1.91	0.42
2:H:771:ALA:HB2	2:H:848:THR:HG21	2.02	0.42
2:B:96:ASP:OD2	2:B:107:TYR:HE2	2.01	0.42
3:B:1605:POV:H28	3:B:1605:POV:H211	1.68	0.42
1:C:66:LEU:HD21	2:D:52:GLY:HA3	2.02	0.42
2:F:76:ILE:HD11	7:F:1613:PTY:O13	2.20	0.42
2:H:496:LEU:HD23	2:H:496:LEU:HA	1.78	0.42
1:A:316:VAL:HG11	1:A:335:ASN:HB2	2.01	0.42
2:B:582:LEU:HD23	2:B:582:LEU:HA	1.94	0.42
2:D:1239:LEU:HD12	2:D:1239:LEU:HA	1.87	0.42
2:F:213:LEU:HD23	2:F:213:LEU:HA	1.83	0.42
2:F:829:ASN:OD1	2:F:829:ASN:N	2.45	0.42
2:F:1039:ASP:OD1	2:F:1039:ASP:N	2.40	0.42
1:G:233:LEU:HD23	1:G:233:LEU:HA	1.85	0.42
2:B:319:CYS:SG	2:B:362:LEU:HB2	2.60	0.41
2:B:1550:MET:HA	2:B:1559:GLU:HA	2.02	0.41
2:D:69:PRO:CG	2:D:192:VAL:HG11	2.47	0.41
2:D:80:ILE:HG22	2:D:178:LEU:HD11	2.01	0.41
2:F:319:CYS:SG	2:F:362:LEU:HB2	2.60	0.41
2:F:770:VAL:HG22	2:F:850:VAL:HB	2.02	0.41
2:F:1239:LEU:HD12	2:F:1239:LEU:HA	1.87	0.41
1:G:73:LEU:HA	1:G:76:THR:HG22	2.02	0.41
2:H:1136:ILE:HD12	2:H:1308:GLN:HB3	2.00	0.41
3:H:1607:POV:H36A	3:H:1608:POV:H37A	2.01	0.41
3:A:401:POV:O13	3:B:1609:POV:H12A	2.20	0.41
1:C:51:GLU:HG2	1:C:53:GLY:N	2.33	0.41
1:C:92:LEU:HD22	2:D:34:VAL:HG21	2.02	0.41
3:C:402:POV:O13	3:D:1609:POV:H12A	2.20	0.41
2:D:135:LEU:HD23	2:D:135:LEU:HA	1.72	0.41
2:D:770:VAL:HG22	2:D:850:VAL:HB	2.02	0.41
2:F:1435:THR:HB	2:F:1472:ASP:HA	2.01	0.41
1:G:114:ILE:HA	1:G:119:SER:HB3	2.03	0.41
1:A:73:LEU:HA	1:A:76:THR:HG22	2.02	0.41
2:B:76:ILE:HD11	7:B:1613:PTY:O13	2.20	0.41
2:D:461:LEU:HD23	2:D:461:LEU:HA	1.92	0.41
2:D:1285:LEU:HD23	2:D:1285:LEU:HA	1.86	0.41
2:F:219:GLN:HG2	2:F:378:TYR:OH	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:461:LEU:HD23	2:F:461:LEU:HA	1.92	0.41
2:F:1239:LEU:O	2:F:1242:THR:HG22	2.20	0.41
2:H:1285:LEU:HA	2:H:1285:LEU:HD23	1.86	0.41
2:B:219:GLN:HG2	2:B:378:TYR:OH	2.21	0.41
1:C:34:ARG:HB2	1:C:305:LEU:HD21	2.01	0.41
2:D:253:LEU:HD23	2:D:1236:ILE:HD13	2.02	0.41
2:H:23:ASN:HB3	2:H:156:LYS:NZ	2.35	0.41
1:A:114:ILE:HA	1:A:119:SER:HB3	2.03	0.41
2:B:253:LEU:HD23	2:B:1236:ILE:HD13	2.02	0.41
2:B:739:TRP:HE1	2:B:768:GLY:N	2.19	0.41
2:B:819:ASP:OD1	2:B:820:GLN:N	2.46	0.41
2:D:1550:MET:HA	2:D:1559:GLU:HA	2.02	0.41
2:F:219:GLN:NE2	2:F:230:TYR:HD1	2.18	0.41
3:B:1607:POV:H36A	3:B:1608:POV:H37A	2.01	0.41
2:D:391:ILE:HD13	2:D:391:ILE:HA	1.93	0.41
3:D:1607:POV:H36A	3:D:1608:POV:H37A	2.01	0.41
2:F:576:ALA:HB1	2:F:1034:LEU:HD21	2.02	0.41
2:H:451:LEU:HB3	2:H:582:LEU:HD11	2.03	0.41
2:H:1079:CYS:O	2:H:1082:THR:HG22	2.21	0.41
2:B:770:VAL:HG22	2:B:850:VAL:HB	2.02	0.41
2:B:1079:CYS:O	2:B:1082:THR:HG22	2.21	0.41
2:B:1257:ALA:O	2:B:1260:VAL:HG12	2.20	0.41
2:D:1257:ALA:O	2:D:1260:VAL:HG12	2.20	0.41
2:D:1435:THR:HB	2:D:1472:ASP:HA	2.01	0.41
2:F:395:ILE:HG21	2:F:610:LEU:HD11	2.02	0.41
2:F:554:ALA:O	2:F:558:THR:OG1	2.33	0.41
2:F:1079:CYS:O	2:F:1082:THR:HG22	2.21	0.41
2:F:1550:MET:HA	2:F:1559:GLU:HA	2.02	0.41
1:G:66:LEU:HD23	1:G:66:LEU:HA	1.84	0.41
3:G:402:POV:O13	3:H:1609:POV:H12A	2.20	0.41
2:H:143:TRP:O	2:H:147:PHE:N	2.40	0.41
2:H:154:PHE:HD1	2:H:172:THR:HG23	1.84	0.41
2:H:770:VAL:HG22	2:H:850:VAL:HB	2.02	0.41
1:C:201:ARG:HH11	1:C:201:ARG:HG3	1.86	0.41
3:E:402:POV:O13	3:F:1609:POV:H12A	2.20	0.41
2:F:23:ASN:HB3	2:F:156:LYS:NZ	2.35	0.41
2:F:253:LEU:HD23	2:F:1236:ILE:HD13	2.02	0.41
2:H:894:LEU:HB2	2:H:895:PRO:HD3	2.03	0.41
2:H:1033:TRP:O	2:H:1037:TRP:HB2	2.21	0.41
1:A:63:LEU:HD12	1:A:63:LEU:HA	1.89	0.41
1:A:92:LEU:HD22	2:B:34:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:LEU:HA	1:A:233:LEU:HD23	1.85	0.41
3:A:401:POV:H11A	3:B:1609:POV:H15A	2.03	0.41
2:B:451:LEU:HB3	2:B:582:LEU:HD11	2.03	0.41
2:B:1435:THR:HB	2:B:1472:ASP:HA	2.01	0.41
1:C:126:GLU:HB3	1:C:132:GLY:CA	2.51	0.41
2:D:219:GLN:NE2	2:D:230:TYR:HD1	2.18	0.41
2:D:331:ASN:OD1	2:D:331:ASN:N	2.54	0.41
1:E:66:LEU:HD21	2:F:52:GLY:HA3	2.02	0.41
1:E:114:ILE:HA	1:E:119:SER:HB3	2.03	0.41
1:E:201:ARG:HG3	1:E:201:ARG:HH11	1.86	0.41
1:E:225:SER:HB3	1:E:229:GLU:H	1.86	0.41
2:F:356:TYR:CE1	3:F:1611:POV:H1A	2.56	0.41
2:F:451:LEU:HB3	2:F:582:LEU:HD11	2.03	0.41
2:F:852:PHE:CD1	2:F:885:VAL:HB	2.56	0.41
2:F:894:LEU:HB2	2:F:895:PRO:HD3	2.03	0.41
2:F:1257:ALA:O	2:F:1260:VAL:HG12	2.20	0.41
3:F:1607:POV:H36A	3:F:1608:POV:H37A	2.01	0.41
1:G:92:LEU:HD22	2:H:34:VAL:HG21	2.02	0.41
1:G:225:SER:HB3	1:G:229:GLU:H	1.86	0.41
2:H:219:GLN:HG2	2:H:378:TYR:OH	2.21	0.41
2:H:1257:ALA:O	2:H:1260:VAL:HG12	2.20	0.41
2:B:511:LEU:HB3	2:B:1424:ILE:HG21	2.03	0.41
2:B:576:ALA:HB1	2:B:1034:LEU:HD21	2.02	0.41
2:D:23:ASN:HB3	2:D:156:LYS:NZ	2.35	0.41
2:D:219:GLN:HG2	2:D:378:TYR:OH	2.21	0.41
2:D:739:TRP:HE1	2:D:768:GLY:N	2.19	0.41
2:F:69:PRO:CG	2:F:192:VAL:HG11	2.47	0.41
2:F:819:ASP:OD1	2:F:820:GLN:N	2.46	0.41
2:H:576:ALA:HB1	2:H:1034:LEU:HD21	2.02	0.41
2:H:739:TRP:HE1	2:H:768:GLY:N	2.19	0.41
2:H:1124:ARG:HD3	2:H:1124:ARG:HA	1.85	0.41
2:B:331:ASN:OD1	2:B:331:ASN:N	2.54	0.40
2:B:471:ALA:HB3	2:B:472:PRO:HD3	2.02	0.40
2:B:496:LEU:HA	2:B:496:LEU:HD23	1.78	0.40
2:B:1024:HIS:O	2:B:1028:VAL:HG12	2.21	0.40
2:D:378:TYR:HB2	2:D:1246:ARG:HG3	2.03	0.40
2:D:1079:CYS:O	2:D:1082:THR:HG22	2.21	0.40
2:F:378:TYR:HB2	2:F:1246:ARG:HG3	2.03	0.40
2:F:1033:TRP:O	2:F:1037:TRP:HB2	2.21	0.40
1:G:201:ARG:HG3	1:G:201:ARG:HH11	1.86	0.40
3:G:402:POV:H11A	3:H:1609:POV:H15A	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:331:ASN:OD1	2:H:331:ASN:N	2.54	0.40
2:H:356:TYR:CE1	3:H:1611:POV:H1A	2.56	0.40
1:A:201:ARG:HG3	1:A:201:ARG:HH11	1.86	0.40
2:B:356:TYR:CE1	3:B:1611:POV:H1A	2.56	0.40
2:B:1249:GLU:OE2	2:B:1300:ARG:NH2	2.53	0.40
1:C:114:ILE:HA	1:C:119:SER:HB3	2.03	0.40
2:D:576:ALA:HB1	2:D:1034:LEU:HD21	2.02	0.40
2:D:1024:HIS:O	2:D:1028:VAL:HG12	2.21	0.40
1:E:142:CYS:HA	1:E:143:PRO:HD3	1.93	0.40
2:F:331:ASN:OD1	2:F:331:ASN:N	2.54	0.40
2:H:120:SER:HG	2:H:143:TRP:HZ2	1.69	0.40
2:H:1106:ILE:HA	2:H:1106:ILE:HD13	1.81	0.40
3:H:1608:POV:H13B	3:H:1608:POV:H11	1.80	0.40
1:A:314:ARG:NH2	1:A:339:VAL:HG21	2.34	0.40
2:B:131:ASN:O	2:B:133:PRO:HD3	2.21	0.40
2:B:391:ILE:HD13	2:B:391:ILE:HA	1.93	0.40
2:B:414:ALA:HA	2:B:1208:VAL:HG11	2.03	0.40
2:B:852:PHE:CD1	2:B:885:VAL:HB	2.56	0.40
2:B:1033:TRP:O	2:B:1037:TRP:HB2	2.21	0.40
2:D:131:ASN:O	2:D:133:PRO:HD3	2.21	0.40
2:F:1024:HIS:O	2:F:1028:VAL:HG12	2.21	0.40
2:F:1034:LEU:O	2:F:1038:THR:HG23	2.22	0.40
2:B:314:PHE:HD1	2:B:314:PHE:HA	1.76	0.40
2:B:1285:LEU:HA	2:B:1285:LEU:HD23	1.86	0.40
1:C:293:THR:OG1	1:C:294:THR:N	2.55	0.40
2:D:218:LEU:H	2:D:218:LEU:HG	1.73	0.40
2:D:219:GLN:HB3	2:D:220:PRO:HD3	2.04	0.40
2:D:308:LEU:HD23	2:D:372:PHE:HE2	1.87	0.40
2:D:451:LEU:HB3	2:D:582:LEU:HD11	2.03	0.40
3:E:402:POV:H11A	3:F:1609:POV:H15A	2.03	0.40
2:F:135:LEU:HD23	2:F:135:LEU:HA	1.72	0.40
2:H:471:ALA:HB3	2:H:472:PRO:HD3	2.02	0.40
1:A:128:GLN:HE21	1:A:156:GLY:HA2	1.87	0.40
2:B:23:ASN:HB3	2:B:156:LYS:NZ	2.35	0.40
2:B:308:LEU:HD23	2:B:372:PHE:HE2	1.87	0.40
2:D:222:VAL:HB	2:D:226:SER:HB3	2.04	0.40
2:D:693:ILE:HA	2:D:694:PRO:HD3	1.93	0.40
2:F:193:ARG:HE	2:F:193:ARG:HB3	1.53	0.40
2:F:222:VAL:HB	2:F:226:SER:HB3	2.04	0.40
2:H:414:ALA:HA	2:H:1208:VAL:HG11	2.03	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	325/390 (83%)	305 (94%)	20 (6%)	0	100	100
1	C	325/390 (83%)	305 (94%)	20 (6%)	0	100	100
1	E	325/390 (83%)	305 (94%)	20 (6%)	0	100	100
1	G	325/390 (83%)	305 (94%)	20 (6%)	0	100	100
2	B	1346/1582 (85%)	1284 (95%)	62 (5%)	0	100	100
2	D	1346/1582 (85%)	1284 (95%)	62 (5%)	0	100	100
2	F	1346/1582 (85%)	1284 (95%)	62 (5%)	0	100	100
2	H	1346/1582 (85%)	1284 (95%)	62 (5%)	0	100	100
All	All	6684/7888 (85%)	6356 (95%)	328 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/339 (81%)	256 (93%)	20 (7%)	14	41
1	C	276/339 (81%)	256 (93%)	20 (7%)	14	41
1	E	276/339 (81%)	256 (93%)	20 (7%)	14	41
1	G	276/339 (81%)	256 (93%)	20 (7%)	14	41
2	B	931/1371 (68%)	896 (96%)	35 (4%)	33	62
2	D	931/1371 (68%)	896 (96%)	35 (4%)	33	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	931/1371 (68%)	896 (96%)	35 (4%)	33 62
2	H	931/1371 (68%)	896 (96%)	35 (4%)	33 62
All	All	4828/6840 (71%)	4608 (95%)	220 (5%)	31 58

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	65	ASP
1	A	71	THR
1	A	72	LEU
1	A	77	MET
1	A	88	MET
1	A	111	VAL
1	A	131	ILE
1	A	142	CYS
1	A	149	LEU
1	A	166	CYS
1	A	182	ILE
1	A	200	LEU
1	A	202	VAL
1	A	252	VAL
1	A	255	LEU
1	A	268	TYR
1	A	287	LEU
1	A	290	VAL
1	A	296	ILE
2	B	8	THR
2	B	19	GLN
2	B	26	CYS
2	B	37	VAL
2	B	44	PHE
2	B	66	LEU
2	B	94	LEU
2	B	112	MET
2	B	121	VAL
2	B	132	PHE
2	B	192	VAL
2	B	198	PHE
2	B	209	ASP
2	B	218	LEU

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Mol	Chain	Res	Type
2	B	223	ASN
2	B	224	LEU
2	B	229	THR
2	B	260	LEU
2	B	331	ASN
2	B	338	THR
2	B	339	GLN
2	B	340	PHE
2	B	358	LEU
2	B	428	LEU
2	B	456	LEU
2	B	594	SER
2	B	614	LEU
2	B	886	LEU
2	B	1136	ILE
2	B	1227	LEU
2	B	1240	PHE
2	B	1242	THR
2	B	1250	VAL
2	B	1272	LEU
2	B	1275	GLU
1	C	56	LEU
1	C	65	ASP
1	C	71	THR
1	C	72	LEU
1	C	77	MET
1	C	88	MET
1	C	111	VAL
1	C	131	ILE
1	C	142	CYS
1	C	149	LEU
1	C	166	CYS
1	C	182	ILE
1	C	200	LEU
1	C	202	VAL
1	C	252	VAL
1	C	255	LEU
1	C	268	TYR
1	C	287	LEU
1	C	290	VAL
1	C	296	ILE
2	D	8	THR

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Mol	Chain	Res	Type
2	D	19	GLN
2	D	26	CYS
2	D	37	VAL
2	D	44	PHE
2	D	66	LEU
2	D	94	LEU
2	D	112	MET
2	D	121	VAL
2	D	132	PHE
2	D	192	VAL
2	D	198	PHE
2	D	209	ASP
2	D	218	LEU
2	D	223	ASN
2	D	224	LEU
2	D	229	THR
2	D	260	LEU
2	D	331	ASN
2	D	338	THR
2	D	339	GLN
2	D	340	PHE
2	D	358	LEU
2	D	428	LEU
2	D	456	LEU
2	D	594	SER
2	D	614	LEU
2	D	886	LEU
2	D	1136	ILE
2	D	1227	LEU
2	D	1240	PHE
2	D	1242	THR
2	D	1250	VAL
2	D	1272	LEU
2	D	1275	GLU
1	E	56	LEU
1	E	65	ASP
1	E	71	THR
1	E	72	LEU
1	E	77	MET
1	E	88	MET
1	E	111	VAL
1	E	131	ILE

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Mol	Chain	Res	Type
1	E	142	CYS
1	E	149	LEU
1	E	166	CYS
1	E	182	ILE
1	E	200	LEU
1	E	202	VAL
1	E	252	VAL
1	E	255	LEU
1	E	268	TYR
1	E	287	LEU
1	E	290	VAL
1	E	296	ILE
2	F	8	THR
2	F	19	GLN
2	F	26	CYS
2	F	37	VAL
2	F	44	PHE
2	F	66	LEU
2	F	94	LEU
2	F	112	MET
2	F	121	VAL
2	F	132	PHE
2	F	192	VAL
2	F	198	PHE
2	F	209	ASP
2	F	218	LEU
2	F	223	ASN
2	F	224	LEU
2	F	229	THR
2	F	260	LEU
2	F	331	ASN
2	F	338	THR
2	F	339	GLN
2	F	340	PHE
2	F	358	LEU
2	F	428	LEU
2	F	456	LEU
2	F	594	SER
2	F	614	LEU
2	F	886	LEU
2	F	1136	ILE
2	F	1227	LEU

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Mol	Chain	Res	Type
2	F	1240	PHE
2	F	1242	THR
2	F	1250	VAL
2	F	1272	LEU
2	F	1275	GLU
1	G	56	LEU
1	G	65	ASP
1	G	71	THR
1	G	72	LEU
1	G	77	MET
1	G	88	MET
1	G	111	VAL
1	G	131	ILE
1	G	142	CYS
1	G	149	LEU
1	G	166	CYS
1	G	182	ILE
1	G	200	LEU
1	G	202	VAL
1	G	252	VAL
1	G	255	LEU
1	G	268	TYR
1	G	287	LEU
1	G	290	VAL
1	G	296	ILE
2	H	8	THR
2	H	19	GLN
2	H	26	CYS
2	H	37	VAL
2	H	44	PHE
2	H	66	LEU
2	H	94	LEU
2	H	112	MET
2	H	121	VAL
2	H	132	PHE
2	H	192	VAL
2	H	198	PHE
2	H	209	ASP
2	H	218	LEU
2	H	223	ASN
2	H	224	LEU
2	H	229	THR

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Mol	Chain	Res	Type
2	H	260	LEU
2	H	331	ASN
2	H	338	THR
2	H	339	GLN
2	H	340	PHE
2	H	358	LEU
2	H	428	LEU
2	H	456	LEU
2	H	594	SER
2	H	614	LEU
2	H	886	LEU
2	H	1136	ILE
2	H	1227	LEU
2	H	1240	PHE
2	H	1242	THR
2	H	1250	VAL
2	H	1272	LEU
2	H	1275	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	299	GLN
2	B	219	GLN
2	B	437	ASN
1	C	46	HIS
1	C	299	GLN
2	D	219	GLN
2	D	437	ASN
1	E	46	HIS
1	E	299	GLN
2	F	219	GLN
2	F	437	ASN
1	G	46	HIS
1	G	299	GLN
2	H	219	GLN
2	H	437	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

68 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	$\#\|Z\| > 2$
7	PTY	F	1612	-	31,31,49	1.25	2 (6%)	34,36,54	1.27	2 (5%)
3	POV	F	1609	-	24,24,51	1.08	1 (4%)	29,31,59	1.05	1 (3%)
3	POV	B	1607	-	40,40,51	1.10	2 (5%)	46,48,59	1.12	4 (8%)
3	POV	B	1606	-	39,39,51	1.13	2 (5%)	45,47,59	1.06	2 (4%)
3	POV	D	1608	-	35,35,51	1.19	2 (5%)	41,43,59	1.27	4 (9%)
4	AGS	F	1602	-	26,33,33	1.88	3 (11%)	26,52,52	1.46	4 (15%)
7	PTY	B	1613	-	26,26,49	1.36	2 (7%)	29,31,54	1.16	2 (6%)
7	PTY	B	1614	-	21,21,49	1.12	1 (4%)	23,25,54	0.93	1 (4%)
3	POV	A	401	-	30,30,51	0.98	1 (3%)	35,37,59	1.04	3 (8%)
6	BJX	D	1603	-	35,35,35	1.87	5 (14%)	47,47,47	1.43	7 (14%)
7	PTY	H	1612	-	31,31,49	1.25	2 (6%)	34,36,54	1.27	2 (5%)
5	AJP	H	1601	-	83,83,95	0.64	0	125,131,149	1.31	13 (10%)
3	POV	B	1604	-	35,35,51	1.18	2 (5%)	41,43,59	1.09	2 (4%)
6	BJX	B	1603	-	35,35,35	1.87	5 (14%)	47,47,47	1.43	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	POV	H	1611	-	27,27,51	1.27	2 (7%)	29,29,59	1.23	2 (6%)
3	POV	B	1608	-	35,35,51	1.19	2 (5%)	41,43,59	1.27	4 (9%)
3	POV	B	1611	-	27,27,51	1.27	2 (7%)	29,29,59	1.23	2 (6%)
7	PTY	B	1615	-	20,20,49	1.22	2 (10%)	22,24,54	1.30	3 (13%)
3	POV	H	1605	-	40,40,51	1.11	2 (5%)	46,48,59	1.02	2 (4%)
6	BJX	F	1603	-	35,35,35	1.87	5 (14%)	47,47,47	1.43	7 (14%)
3	POV	D	1609	-	24,24,51	1.08	1 (4%)	29,31,59	1.05	1 (3%)
4	AGS	D	1602	-	26,33,33	1.88	3 (11%)	26,52,52	1.46	4 (15%)
3	POV	F	1608	-	35,35,51	1.19	2 (5%)	41,43,59	1.27	4 (9%)
7	PTY	D	1613	-	26,26,49	1.36	2 (7%)	29,31,54	1.16	2 (6%)
3	POV	D	1607	-	40,40,51	1.10	2 (5%)	46,48,59	1.12	4 (8%)
3	POV	D	1604	-	35,35,51	1.18	2 (5%)	41,43,59	1.09	2 (4%)
3	POV	D	1606	-	39,39,51	1.13	2 (5%)	45,47,59	1.06	2 (4%)
4	AGS	E	401	-	26,33,33	1.87	3 (11%)	26,52,52	1.45	5 (19%)
3	POV	D	1610	-	24,24,51	1.03	1 (4%)	29,31,59	1.16	2 (6%)
7	PTY	B	1612	-	31,31,49	1.25	2 (6%)	34,36,54	1.27	2 (5%)
3	POV	F	1607	-	40,40,51	1.10	2 (5%)	46,48,59	1.12	4 (8%)
6	BJX	H	1603	-	35,35,35	1.87	5 (14%)	47,47,47	1.43	7 (14%)
3	POV	B	1610	-	24,24,51	1.03	1 (4%)	29,31,59	1.16	2 (6%)
3	POV	H	1608	-	35,35,51	1.19	2 (5%)	41,43,59	1.27	4 (9%)
3	POV	D	1605	-	40,40,51	1.11	2 (5%)	46,48,59	1.02	2 (4%)
5	AJP	B	1601	-	83,83,95	0.64	0	125,131,149	1.31	13 (10%)
7	PTY	D	1612	-	31,31,49	1.25	2 (6%)	34,36,54	1.27	2 (5%)
3	POV	F	1604	-	35,35,51	1.18	2 (5%)	41,43,59	1.09	2 (4%)
7	PTY	D	1615	-	20,20,49	1.22	2 (10%)	22,24,54	1.30	3 (13%)
3	POV	B	1609	-	24,24,51	1.08	1 (4%)	29,31,59	1.05	1 (3%)
4	AGS	B	1602	-	26,33,33	1.88	3 (11%)	26,52,52	1.46	4 (15%)
3	POV	F	1611	-	27,27,51	1.27	2 (7%)	29,29,59	1.23	2 (6%)
3	POV	G	402	-	30,30,51	0.98	1 (3%)	35,37,59	1.04	3 (8%)
3	POV	C	402	-	30,30,51	0.98	1 (3%)	35,37,59	1.04	3 (8%)
3	POV	H	1610	-	24,24,51	1.03	1 (4%)	29,31,59	1.16	2 (6%)
3	POV	F	1605	-	40,40,51	1.11	2 (5%)	46,48,59	1.02	2 (4%)
7	PTY	H	1614	-	21,21,49	1.12	1 (4%)	23,25,54	0.93	1 (4%)
3	POV	H	1609	-	24,24,51	1.08	1 (4%)	29,31,59	1.05	1 (3%)
3	POV	B	1605	-	40,40,51	1.11	2 (5%)	46,48,59	1.02	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	AGS	A	402	-	26,33,33	1.87	3 (11%)	26,52,52	1.45	5 (19%)
3	POV	E	402	-	30,30,51	0.98	1 (3%)	35,37,59	1.04	3 (8%)
4	AGS	G	401	-	26,33,33	1.87	3 (11%)	26,52,52	1.45	5 (19%)
4	AGS	H	1602	-	26,33,33	1.88	3 (11%)	26,52,52	1.46	4 (15%)
7	PTY	D	1614	-	21,21,49	1.12	1 (4%)	23,25,54	0.93	1 (4%)
7	PTY	F	1615	-	20,20,49	1.22	2 (10%)	22,24,54	1.30	3 (13%)
3	POV	H	1607	-	40,40,51	1.10	2 (5%)	46,48,59	1.12	4 (8%)
3	POV	H	1604	-	35,35,51	1.18	2 (5%)	41,43,59	1.09	2 (4%)
7	PTY	H	1613	-	26,26,49	1.36	2 (7%)	29,31,54	1.16	2 (6%)
3	POV	H	1606	-	39,39,51	1.13	2 (5%)	45,47,59	1.06	2 (4%)
7	PTY	F	1614	-	21,21,49	1.12	1 (4%)	23,25,54	0.93	1 (4%)
3	POV	F	1606	-	39,39,51	1.13	2 (5%)	45,47,59	1.06	2 (4%)
7	PTY	H	1615	-	20,20,49	1.22	2 (10%)	22,24,54	1.30	3 (13%)
5	AJP	D	1601	-	83,83,95	0.64	0	125,131,149	1.31	13 (10%)
4	AGS	C	401	-	26,33,33	1.87	3 (11%)	26,52,52	1.45	5 (19%)
3	POV	D	1611	-	27,27,51	1.27	2 (7%)	29,29,59	1.23	2 (6%)
3	POV	F	1610	-	24,24,51	1.03	1 (4%)	29,31,59	1.16	2 (6%)
7	PTY	F	1613	-	26,26,49	1.36	2 (7%)	29,31,54	1.16	2 (6%)
5	AJP	F	1601	-	83,83,95	0.64	0	125,131,149	1.31	13 (10%)

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
7	PTY	F	1612	-	-	14/35/35/53	-
3	POV	F	1609	-	-	10/27/27/55	-
3	POV	B	1607	-	-	14/44/44/55	-
3	POV	B	1606	-	-	17/43/43/55	-
3	POV	D	1608	-	-	12/39/39/55	-
4	AGS	F	1602	-	-	2/17/38/38	0/3/3/3
7	PTY	B	1613	-	-	15/30/30/53	-
7	PTY	B	1614	-	-	13/23/23/53	-
3	POV	A	401	-	-	5/33/33/55	-
6	BJX	D	1603	-	-	13/27/35/35	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PTY	H	1612	-	-	14/35/35/53	-
5	AJP	H	1601	-	29/29/33/38	11/22/194/220	0/10/10/11
3	POV	B	1604	-	-	13/39/39/55	-
6	BJX	B	1603	-	-	13/27/35/35	0/3/3/3
3	POV	H	1611	-	-	11/29/29/55	-
3	POV	B	1608	-	-	12/39/39/55	-
3	POV	B	1611	-	-	11/29/29/55	-
7	PTY	B	1615	-	-	14/22/22/53	-
3	POV	H	1605	-	-	14/44/44/55	-
6	BJX	F	1603	-	-	13/27/35/35	0/3/3/3
3	POV	D	1609	-	-	10/27/27/55	-
4	AGS	D	1602	-	-	2/17/38/38	0/3/3/3
3	POV	F	1608	-	-	12/39/39/55	-
7	PTY	D	1613	-	-	15/30/30/53	-
3	POV	D	1607	-	-	14/44/44/55	-
3	POV	D	1604	-	-	13/39/39/55	-
3	POV	D	1606	-	-	17/43/43/55	-
4	AGS	E	401	-	-	2/17/38/38	0/3/3/3
3	POV	D	1610	-	-	6/27/27/55	-
7	PTY	B	1612	-	-	14/35/35/53	-
3	POV	F	1607	-	-	14/44/44/55	-
6	BJX	H	1603	-	-	13/27/35/35	0/3/3/3
3	POV	B	1610	-	-	6/27/27/55	-
3	POV	H	1608	-	-	12/39/39/55	-
3	POV	D	1605	-	-	14/44/44/55	-
5	AJP	B	1601	-	29/29/33/38	11/22/194/220	0/10/10/11
7	PTY	D	1612	-	-	14/35/35/53	-
3	POV	F	1604	-	-	13/39/39/55	-
7	PTY	D	1615	-	-	14/22/22/53	-
3	POV	B	1609	-	-	10/27/27/55	-
4	AGS	B	1602	-	-	2/17/38/38	0/3/3/3
3	POV	F	1611	-	-	11/29/29/55	-
3	POV	G	402	-	-	5/33/33/55	-
3	POV	C	402	-	-	5/33/33/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	H	1610	-	-	6/27/27/55	-
3	POV	F	1605	-	-	14/44/44/55	-
7	PTY	H	1614	-	-	13/23/23/53	-
3	POV	H	1609	-	-	10/27/27/55	-
3	POV	B	1605	-	-	14/44/44/55	-
4	AGS	A	402	-	-	2/17/38/38	0/3/3/3
3	POV	E	402	-	-	5/33/33/55	-
4	AGS	G	401	-	-	2/17/38/38	0/3/3/3
4	AGS	H	1602	-	-	2/17/38/38	0/3/3/3
7	PTY	D	1614	-	-	13/23/23/53	-
7	PTY	F	1615	-	-	14/22/22/53	-
3	POV	H	1607	-	-	14/44/44/55	-
3	POV	H	1604	-	-	13/39/39/55	-
7	PTY	H	1613	-	-	15/30/30/53	-
3	POV	H	1606	-	-	17/43/43/55	-
7	PTY	F	1614	-	-	13/23/23/53	-
3	POV	F	1606	-	-	17/43/43/55	-
7	PTY	H	1615	-	-	14/22/22/53	-
5	AJP	D	1601	-	29/29/33/38	11/22/194/220	0/10/10/11
4	AGS	C	401	-	-	2/17/38/38	0/3/3/3
3	POV	D	1611	-	-	11/29/29/55	-
3	POV	F	1610	-	-	6/27/27/55	-
7	PTY	F	1613	-	-	15/30/30/53	-
5	AJP	F	1601	-	29/29/33/38	11/22/194/220	0/10/10/11

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1603	BJX	C6-C7	8.50	1.49	1.40
6	D	1603	BJX	C6-C7	8.50	1.49	1.40
6	F	1603	BJX	C6-C7	8.50	1.49	1.40
6	H	1603	BJX	C6-C7	8.50	1.49	1.40
4	A	402	AGS	PG-S1G	8.02	2.08	1.90
4	C	401	AGS	PG-S1G	8.02	2.08	1.90
4	E	401	AGS	PG-S1G	8.02	2.08	1.90
4	G	401	AGS	PG-S1G	8.02	2.08	1.90
4	B	1602	AGS	PG-S1G	8.01	2.08	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1602	AGS	PG-S1G	8.01	2.08	1.90
4	F	1602	AGS	PG-S1G	8.01	2.08	1.90
4	H	1602	AGS	PG-S1G	8.01	2.08	1.90
7	B	1612	PTY	O7-C8	4.68	1.47	1.34
7	D	1612	PTY	O7-C8	4.68	1.47	1.34
7	F	1612	PTY	O7-C8	4.68	1.47	1.34
7	H	1612	PTY	O7-C8	4.68	1.47	1.34
7	B	1614	PTY	O4-C30	4.63	1.46	1.33
7	D	1614	PTY	O4-C30	4.63	1.46	1.33
7	F	1614	PTY	O4-C30	4.63	1.46	1.33
7	H	1614	PTY	O4-C30	4.63	1.46	1.33
7	B	1613	PTY	O4-C30	4.62	1.46	1.33
7	D	1613	PTY	O4-C30	4.62	1.46	1.33
7	F	1613	PTY	O4-C30	4.62	1.46	1.33
7	H	1613	PTY	O4-C30	4.62	1.46	1.33
3	B	1605	POV	O31-C31	4.59	1.46	1.33
3	D	1605	POV	O31-C31	4.59	1.46	1.33
3	F	1605	POV	O31-C31	4.59	1.46	1.33
3	H	1605	POV	O31-C31	4.59	1.46	1.33
3	B	1608	POV	O31-C31	4.57	1.46	1.33
3	D	1608	POV	O31-C31	4.57	1.46	1.33
3	F	1608	POV	O31-C31	4.57	1.46	1.33
3	H	1608	POV	O31-C31	4.57	1.46	1.33
3	B	1604	POV	O31-C31	4.53	1.46	1.33
3	D	1604	POV	O31-C31	4.53	1.46	1.33
3	F	1604	POV	O31-C31	4.53	1.46	1.33
3	H	1604	POV	O31-C31	4.53	1.46	1.33
3	B	1606	POV	O31-C31	4.53	1.46	1.33
3	D	1606	POV	O31-C31	4.53	1.46	1.33
3	F	1606	POV	O31-C31	4.53	1.46	1.33
3	H	1606	POV	O31-C31	4.53	1.46	1.33
3	B	1607	POV	O21-C21	4.52	1.47	1.34
3	D	1607	POV	O21-C21	4.52	1.47	1.34
3	F	1607	POV	O21-C21	4.52	1.47	1.34
3	H	1607	POV	O21-C21	4.52	1.47	1.34
7	B	1615	PTY	O7-C8	4.48	1.46	1.34
7	D	1615	PTY	O7-C8	4.48	1.46	1.34
7	F	1615	PTY	O7-C8	4.48	1.46	1.34
7	H	1615	PTY	O7-C8	4.48	1.46	1.34
3	B	1611	POV	O31-C31	4.48	1.46	1.33
3	D	1611	POV	O31-C31	4.48	1.46	1.33
3	F	1611	POV	O31-C31	4.48	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1611	POV	O31-C31	4.48	1.46	1.33
7	B	1613	PTY	O7-C8	4.42	1.46	1.34
7	D	1613	PTY	O7-C8	4.42	1.46	1.34
7	F	1613	PTY	O7-C8	4.42	1.46	1.34
7	H	1613	PTY	O7-C8	4.42	1.46	1.34
3	A	401	POV	O21-C21	4.42	1.46	1.34
3	C	402	POV	O21-C21	4.42	1.46	1.34
3	E	402	POV	O21-C21	4.42	1.46	1.34
3	G	402	POV	O21-C21	4.42	1.46	1.34
7	B	1612	PTY	O4-C30	4.40	1.46	1.33
7	D	1612	PTY	O4-C30	4.40	1.46	1.33
7	F	1612	PTY	O4-C30	4.40	1.46	1.33
7	H	1612	PTY	O4-C30	4.40	1.46	1.33
3	B	1606	POV	O21-C21	4.39	1.46	1.34
3	D	1606	POV	O21-C21	4.39	1.46	1.34
3	F	1606	POV	O21-C21	4.39	1.46	1.34
3	H	1606	POV	O21-C21	4.39	1.46	1.34
3	B	1609	POV	O21-C21	4.34	1.46	1.34
3	D	1609	POV	O21-C21	4.34	1.46	1.34
3	F	1609	POV	O21-C21	4.34	1.46	1.34
3	H	1609	POV	O21-C21	4.34	1.46	1.34
3	B	1605	POV	O21-C21	4.27	1.46	1.34
3	D	1605	POV	O21-C21	4.27	1.46	1.34
3	F	1605	POV	O21-C21	4.27	1.46	1.34
3	H	1605	POV	O21-C21	4.27	1.46	1.34
3	B	1604	POV	O21-C21	4.25	1.46	1.34
3	D	1604	POV	O21-C21	4.25	1.46	1.34
3	F	1604	POV	O21-C21	4.25	1.46	1.34
3	H	1604	POV	O21-C21	4.25	1.46	1.34
3	B	1611	POV	O21-C21	4.23	1.46	1.34
3	D	1611	POV	O21-C21	4.23	1.46	1.34
3	F	1611	POV	O21-C21	4.23	1.46	1.34
3	H	1611	POV	O21-C21	4.23	1.46	1.34
3	B	1607	POV	O31-C31	4.23	1.45	1.33
3	D	1607	POV	O31-C31	4.23	1.45	1.33
3	F	1607	POV	O31-C31	4.23	1.45	1.33
3	H	1607	POV	O31-C31	4.23	1.45	1.33
3	B	1608	POV	O21-C21	4.10	1.45	1.34
3	D	1608	POV	O21-C21	4.10	1.45	1.34
3	F	1608	POV	O21-C21	4.10	1.45	1.34
3	H	1608	POV	O21-C21	4.10	1.45	1.34
3	B	1610	POV	O21-C21	4.00	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1610	POV	O21-C21	4.00	1.45	1.34
3	F	1610	POV	O21-C21	4.00	1.45	1.34
3	H	1610	POV	O21-C21	4.00	1.45	1.34
6	B	1603	BJX	C23-C21	3.86	1.47	1.40
6	D	1603	BJX	C23-C21	3.86	1.47	1.40
6	F	1603	BJX	C23-C21	3.86	1.47	1.40
6	H	1603	BJX	C23-C21	3.86	1.47	1.40
6	B	1603	BJX	O2-C24	3.66	1.33	1.22
6	D	1603	BJX	O2-C24	3.66	1.33	1.22
6	F	1603	BJX	O2-C24	3.66	1.33	1.22
6	H	1603	BJX	O2-C24	3.66	1.33	1.22
6	B	1603	BJX	O3-C24	-2.70	1.22	1.30
6	D	1603	BJX	O3-C24	-2.70	1.22	1.30
6	F	1603	BJX	O3-C24	-2.70	1.22	1.30
6	H	1603	BJX	O3-C24	-2.70	1.22	1.30
6	B	1603	BJX	C7-C5	-2.56	1.48	1.52
6	D	1603	BJX	C7-C5	-2.56	1.48	1.52
6	F	1603	BJX	C7-C5	-2.56	1.48	1.52
6	H	1603	BJX	C7-C5	-2.56	1.48	1.52
4	A	402	AGS	C5-C4	2.45	1.47	1.40
4	C	401	AGS	C5-C4	2.45	1.47	1.40
4	E	401	AGS	C5-C4	2.45	1.47	1.40
4	G	401	AGS	C5-C4	2.45	1.47	1.40
4	B	1602	AGS	C5-C4	2.43	1.47	1.40
4	D	1602	AGS	C5-C4	2.43	1.47	1.40
4	F	1602	AGS	C5-C4	2.43	1.47	1.40
4	H	1602	AGS	C5-C4	2.43	1.47	1.40
7	B	1615	PTY	O7-C6	-2.17	1.43	1.47
7	D	1615	PTY	O7-C6	-2.17	1.43	1.47
7	F	1615	PTY	O7-C6	-2.17	1.43	1.47
7	H	1615	PTY	O7-C6	-2.17	1.43	1.47
4	A	402	AGS	PG-O2G	2.04	1.61	1.54
4	C	401	AGS	PG-O2G	2.04	1.61	1.54
4	E	401	AGS	PG-O2G	2.04	1.61	1.54
4	G	401	AGS	PG-O2G	2.04	1.61	1.54
4	B	1602	AGS	PG-O2G	2.04	1.61	1.54
4	D	1602	AGS	PG-O2G	2.04	1.61	1.54
4	F	1602	AGS	PG-O2G	2.04	1.61	1.54
4	H	1602	AGS	PG-O2G	2.04	1.61	1.54

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1608	POV	O21-C21-C22	5.06	122.41	111.50
3	D	1608	POV	O21-C21-C22	5.06	122.41	111.50
3	F	1608	POV	O21-C21-C22	5.06	122.41	111.50
3	H	1608	POV	O21-C21-C22	5.06	122.41	111.50
5	B	1601	AJP	C12-C07-C08	-5.04	99.43	104.88
5	D	1601	AJP	C12-C07-C08	-5.04	99.43	104.88
5	F	1601	AJP	C12-C07-C08	-5.04	99.43	104.88
5	H	1601	AJP	C12-C07-C08	-5.04	99.43	104.88
7	B	1612	PTY	O7-C8-C11	5.03	122.34	111.50
7	D	1612	PTY	O7-C8-C11	5.03	122.34	111.50
7	F	1612	PTY	O7-C8-C11	5.03	122.34	111.50
7	H	1612	PTY	O7-C8-C11	5.03	122.34	111.50
5	B	1601	AJP	O09-C08-C10	5.00	120.47	110.17
5	D	1601	AJP	O09-C08-C10	5.00	120.47	110.17
5	F	1601	AJP	O09-C08-C10	5.00	120.47	110.17
5	H	1601	AJP	O09-C08-C10	5.00	120.47	110.17
3	B	1607	POV	O21-C21-C22	4.80	121.84	111.50
3	D	1607	POV	O21-C21-C22	4.80	121.84	111.50
3	F	1607	POV	O21-C21-C22	4.80	121.84	111.50
3	H	1607	POV	O21-C21-C22	4.80	121.84	111.50
3	A	401	POV	O21-C21-C22	4.56	121.34	111.50
3	C	402	POV	O21-C21-C22	4.56	121.34	111.50
3	E	402	POV	O21-C21-C22	4.56	121.34	111.50
3	G	402	POV	O21-C21-C22	4.56	121.34	111.50
3	B	1606	POV	O21-C21-C22	4.50	121.20	111.50
3	D	1606	POV	O21-C21-C22	4.50	121.20	111.50
3	F	1606	POV	O21-C21-C22	4.50	121.20	111.50
3	H	1606	POV	O21-C21-C22	4.50	121.20	111.50
3	B	1611	POV	O21-C21-C22	4.30	120.76	111.50
3	D	1611	POV	O21-C21-C22	4.30	120.76	111.50
3	F	1611	POV	O21-C21-C22	4.30	120.76	111.50
3	H	1611	POV	O21-C21-C22	4.30	120.76	111.50
3	B	1605	POV	O21-C21-C22	4.23	120.61	111.50
3	D	1605	POV	O21-C21-C22	4.23	120.61	111.50
3	F	1605	POV	O21-C21-C22	4.23	120.61	111.50
3	H	1605	POV	O21-C21-C22	4.23	120.61	111.50
6	B	1603	BJX	C-N-C1	4.20	120.79	111.52
6	D	1603	BJX	C-N-C1	4.20	120.79	111.52
6	F	1603	BJX	C-N-C1	4.20	120.79	111.52
6	H	1603	BJX	C-N-C1	4.20	120.79	111.52
3	B	1604	POV	O21-C21-C22	4.20	120.54	111.50
3	D	1604	POV	O21-C21-C22	4.20	120.54	111.50
3	F	1604	POV	O21-C21-C22	4.20	120.54	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1604	POV	O21-C21-C22	4.20	120.54	111.50
3	B	1609	POV	O21-C21-C22	4.15	120.45	111.50
3	D	1609	POV	O21-C21-C22	4.15	120.45	111.50
3	F	1609	POV	O21-C21-C22	4.15	120.45	111.50
3	H	1609	POV	O21-C21-C22	4.15	120.45	111.50
5	B	1601	AJP	C20-C15-C16	-4.09	108.12	112.42
5	D	1601	AJP	C20-C15-C16	-4.09	108.12	112.42
5	F	1601	AJP	C20-C15-C16	-4.09	108.12	112.42
5	H	1601	AJP	C20-C15-C16	-4.09	108.12	112.42
3	B	1610	POV	O21-C21-C22	4.01	120.15	111.50
3	D	1610	POV	O21-C21-C22	4.01	120.15	111.50
3	F	1610	POV	O21-C21-C22	4.01	120.15	111.50
3	H	1610	POV	O21-C21-C22	4.01	120.15	111.50
7	B	1613	PTY	O7-C8-C11	4.01	120.14	111.50
7	D	1613	PTY	O7-C8-C11	4.01	120.14	111.50
7	F	1613	PTY	O7-C8-C11	4.01	120.14	111.50
7	H	1613	PTY	O7-C8-C11	4.01	120.14	111.50
7	B	1615	PTY	O7-C8-C11	3.95	120.00	111.50
7	D	1615	PTY	O7-C8-C11	3.95	120.00	111.50
7	F	1615	PTY	O7-C8-C11	3.95	120.00	111.50
7	H	1615	PTY	O7-C8-C11	3.95	120.00	111.50
4	B	1602	AGS	C3'-C2'-C1'	3.39	106.08	100.98
4	D	1602	AGS	C3'-C2'-C1'	3.39	106.08	100.98
4	F	1602	AGS	C3'-C2'-C1'	3.39	106.08	100.98
4	H	1602	AGS	C3'-C2'-C1'	3.39	106.08	100.98
5	B	1601	AJP	C12-C07-C06	3.38	132.05	120.56
5	D	1601	AJP	C12-C07-C06	3.38	132.05	120.56
5	F	1601	AJP	C12-C07-C06	3.38	132.05	120.56
5	H	1601	AJP	C12-C07-C06	3.38	132.05	120.56
6	B	1603	BJX	C7-C6-N	3.31	124.51	119.32
6	D	1603	BJX	C7-C6-N	3.31	124.51	119.32
6	F	1603	BJX	C7-C6-N	3.31	124.51	119.32
6	H	1603	BJX	C7-C6-N	3.31	124.51	119.32
4	A	402	AGS	N3-C2-N1	-3.30	123.52	128.68
4	C	401	AGS	N3-C2-N1	-3.30	123.52	128.68
4	E	401	AGS	N3-C2-N1	-3.30	123.52	128.68
4	G	401	AGS	N3-C2-N1	-3.30	123.52	128.68
4	B	1602	AGS	N3-C2-N1	-3.29	123.53	128.68
4	D	1602	AGS	N3-C2-N1	-3.29	123.53	128.68
4	F	1602	AGS	N3-C2-N1	-3.29	123.53	128.68
4	H	1602	AGS	N3-C2-N1	-3.29	123.53	128.68
3	B	1610	POV	C2-O21-C21	-3.15	110.03	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1610	POV	C2-O21-C21	-3.15	110.03	117.79
3	F	1610	POV	C2-O21-C21	-3.15	110.03	117.79
3	H	1610	POV	C2-O21-C21	-3.15	110.03	117.79
4	A	402	AGS	PA-O3A-PB	-3.04	122.41	132.83
4	C	401	AGS	PA-O3A-PB	-3.04	122.41	132.83
4	E	401	AGS	PA-O3A-PB	-3.04	122.41	132.83
4	G	401	AGS	PA-O3A-PB	-3.04	122.41	132.83
6	B	1603	BJX	C10-C6-N	-3.00	117.51	122.30
6	D	1603	BJX	C10-C6-N	-3.00	117.51	122.30
6	F	1603	BJX	C10-C6-N	-3.00	117.51	122.30
6	H	1603	BJX	C10-C6-N	-3.00	117.51	122.30
4	A	402	AGS	C3'-C2'-C1'	3.00	105.50	100.98
4	C	401	AGS	C3'-C2'-C1'	3.00	105.50	100.98
4	E	401	AGS	C3'-C2'-C1'	3.00	105.50	100.98
4	G	401	AGS	C3'-C2'-C1'	3.00	105.50	100.98
4	B	1602	AGS	PA-O3A-PB	-2.97	122.62	132.83
4	D	1602	AGS	PA-O3A-PB	-2.97	122.62	132.83
4	F	1602	AGS	PA-O3A-PB	-2.97	122.62	132.83
4	H	1602	AGS	PA-O3A-PB	-2.97	122.62	132.83
3	B	1607	POV	O31-C31-C32	2.95	121.17	111.91
3	D	1607	POV	O31-C31-C32	2.95	121.17	111.91
3	F	1607	POV	O31-C31-C32	2.95	121.17	111.91
3	H	1607	POV	O31-C31-C32	2.95	121.17	111.91
7	B	1615	PTY	C6-O7-C8	-2.90	114.15	117.88
7	D	1615	PTY	C6-O7-C8	-2.90	114.15	117.88
7	F	1615	PTY	C6-O7-C8	-2.90	114.15	117.88
7	H	1615	PTY	C6-O7-C8	-2.90	114.15	117.88
7	B	1613	PTY	O4-C30-C31	2.88	120.94	111.91
7	D	1613	PTY	O4-C30-C31	2.88	120.94	111.91
7	F	1613	PTY	O4-C30-C31	2.88	120.94	111.91
7	H	1613	PTY	O4-C30-C31	2.88	120.94	111.91
7	B	1614	PTY	O4-C30-C31	2.87	120.92	111.91
7	D	1614	PTY	O4-C30-C31	2.87	120.92	111.91
7	F	1614	PTY	O4-C30-C31	2.87	120.92	111.91
7	H	1614	PTY	O4-C30-C31	2.87	120.92	111.91
7	B	1612	PTY	O4-C30-C31	2.80	120.69	111.91
7	D	1612	PTY	O4-C30-C31	2.80	120.69	111.91
7	F	1612	PTY	O4-C30-C31	2.80	120.69	111.91
7	H	1612	PTY	O4-C30-C31	2.80	120.69	111.91
3	B	1605	POV	O31-C31-C32	2.75	120.55	111.91
3	D	1605	POV	O31-C31-C32	2.75	120.55	111.91
3	F	1605	POV	O31-C31-C32	2.75	120.55	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1605	POV	O31-C31-C32	2.75	120.55	111.91
3	B	1608	POV	C2-O21-C21	-2.72	111.11	117.79
3	D	1608	POV	C2-O21-C21	-2.72	111.11	117.79
3	F	1608	POV	C2-O21-C21	-2.72	111.11	117.79
3	H	1608	POV	C2-O21-C21	-2.72	111.11	117.79
3	B	1611	POV	O31-C31-C32	2.70	120.38	111.91
3	D	1611	POV	O31-C31-C32	2.70	120.38	111.91
3	F	1611	POV	O31-C31-C32	2.70	120.38	111.91
3	H	1611	POV	O31-C31-C32	2.70	120.38	111.91
5	B	1601	AJP	C11-C12-C07	-2.64	95.69	100.19
5	D	1601	AJP	C11-C12-C07	-2.64	95.69	100.19
5	F	1601	AJP	C11-C12-C07	-2.64	95.69	100.19
5	H	1601	AJP	C11-C12-C07	-2.64	95.69	100.19
4	B	1602	AGS	C4-C5-N7	-2.62	106.67	109.40
4	D	1602	AGS	C4-C5-N7	-2.62	106.67	109.40
4	F	1602	AGS	C4-C5-N7	-2.62	106.67	109.40
4	H	1602	AGS	C4-C5-N7	-2.62	106.67	109.40
6	B	1603	BJX	C2-C-N	-2.60	105.98	111.05
6	D	1603	BJX	C2-C-N	-2.60	105.98	111.05
6	F	1603	BJX	C2-C-N	-2.60	105.98	111.05
6	H	1603	BJX	C2-C-N	-2.60	105.98	111.05
3	B	1606	POV	O31-C31-C32	2.56	119.93	111.91
3	D	1606	POV	O31-C31-C32	2.56	119.93	111.91
3	F	1606	POV	O31-C31-C32	2.56	119.93	111.91
3	H	1606	POV	O31-C31-C32	2.56	119.93	111.91
3	B	1607	POV	O31-C31-O32	-2.48	117.34	123.59
3	D	1607	POV	O31-C31-O32	-2.48	117.34	123.59
3	F	1607	POV	O31-C31-O32	-2.48	117.34	123.59
3	H	1607	POV	O31-C31-O32	-2.48	117.34	123.59
6	B	1603	BJX	C21-C23-C24	-2.46	119.29	123.74
6	D	1603	BJX	C21-C23-C24	-2.46	119.29	123.74
6	F	1603	BJX	C21-C23-C24	-2.46	119.29	123.74
6	H	1603	BJX	C21-C23-C24	-2.46	119.29	123.74
3	B	1608	POV	C23-C22-C21	-2.44	104.74	113.62
3	D	1608	POV	C23-C22-C21	-2.44	104.74	113.62
3	F	1608	POV	C23-C22-C21	-2.44	104.74	113.62
3	H	1608	POV	C23-C22-C21	-2.44	104.74	113.62
5	B	1601	AJP	C45-O44-C37	-2.43	111.94	117.96
5	D	1601	AJP	C45-O44-C37	-2.43	111.94	117.96
5	F	1601	AJP	C45-O44-C37	-2.43	111.94	117.96
5	H	1601	AJP	C45-O44-C37	-2.43	111.94	117.96
3	B	1604	POV	O31-C31-C32	2.41	119.49	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1604	POV	O31-C31-C32	2.41	119.49	111.91
3	F	1604	POV	O31-C31-C32	2.41	119.49	111.91
3	H	1604	POV	O31-C31-C32	2.41	119.49	111.91
5	B	1601	AJP	O34-C29-C28	2.35	113.53	107.28
5	D	1601	AJP	O34-C29-C28	2.35	113.53	107.28
5	F	1601	AJP	O34-C29-C28	2.35	113.53	107.28
5	H	1601	AJP	O34-C29-C28	2.35	113.53	107.28
5	B	1601	AJP	C24-C19-C20	-2.35	110.16	112.66
5	D	1601	AJP	C24-C19-C20	-2.35	110.16	112.66
5	F	1601	AJP	C24-C19-C20	-2.35	110.16	112.66
5	H	1601	AJP	C24-C19-C20	-2.35	110.16	112.66
4	A	402	AGS	C4-C5-N7	-2.31	106.99	109.40
4	C	401	AGS	C4-C5-N7	-2.31	106.99	109.40
4	E	401	AGS	C4-C5-N7	-2.31	106.99	109.40
4	G	401	AGS	C4-C5-N7	-2.31	106.99	109.40
5	B	1601	AJP	C12-C11-C16	-2.31	110.51	113.82
5	D	1601	AJP	C12-C11-C16	-2.31	110.51	113.82
5	F	1601	AJP	C12-C11-C16	-2.31	110.51	113.82
5	H	1601	AJP	C12-C11-C16	-2.31	110.51	113.82
6	B	1603	BJX	C3-C1-N	-2.30	106.56	111.05
6	D	1603	BJX	C3-C1-N	-2.30	106.56	111.05
6	F	1603	BJX	C3-C1-N	-2.30	106.56	111.05
6	H	1603	BJX	C3-C1-N	-2.30	106.56	111.05
5	B	1601	AJP	O40-C39-C38	2.24	113.77	109.69
5	D	1601	AJP	O40-C39-C38	2.24	113.77	109.69
5	F	1601	AJP	O40-C39-C38	2.24	113.77	109.69
5	H	1601	AJP	O40-C39-C38	2.24	113.77	109.69
6	B	1603	BJX	C5-N1-C16	-2.22	119.79	123.33
6	D	1603	BJX	C5-N1-C16	-2.22	119.79	123.33
6	F	1603	BJX	C5-N1-C16	-2.22	119.79	123.33
6	H	1603	BJX	C5-N1-C16	-2.22	119.79	123.33
7	B	1615	PTY	O7-C6-C5	2.20	111.23	106.13
7	D	1615	PTY	O7-C6-C5	2.20	111.23	106.13
7	F	1615	PTY	O7-C6-C5	2.20	111.23	106.13
7	H	1615	PTY	O7-C6-C5	2.20	111.23	106.13
5	B	1601	AJP	C18-C17-C16	-2.20	108.52	112.14
5	D	1601	AJP	C18-C17-C16	-2.20	108.52	112.14
5	F	1601	AJP	C18-C17-C16	-2.20	108.52	112.14
5	H	1601	AJP	C18-C17-C16	-2.20	108.52	112.14
3	B	1608	POV	O21-C21-O22	-2.07	118.69	123.70
3	D	1608	POV	O21-C21-O22	-2.07	118.69	123.70
3	F	1608	POV	O21-C21-O22	-2.07	118.69	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1608	POV	O21-C21-O22	-2.07	118.69	123.70
4	A	402	AGS	C2-N1-C6	2.07	122.30	118.75
4	C	401	AGS	C2-N1-C6	2.07	122.30	118.75
4	E	401	AGS	C2-N1-C6	2.07	122.30	118.75
4	G	401	AGS	C2-N1-C6	2.07	122.30	118.75
3	B	1607	POV	O21-C21-O22	-2.06	118.71	123.70
3	D	1607	POV	O21-C21-O22	-2.06	118.71	123.70
3	F	1607	POV	O21-C21-O22	-2.06	118.71	123.70
3	H	1607	POV	O21-C21-O22	-2.06	118.71	123.70
3	A	401	POV	C1-C2-C3	-2.06	106.99	111.80
3	C	402	POV	C1-C2-C3	-2.06	106.99	111.80
3	E	402	POV	C1-C2-C3	-2.06	106.99	111.80
3	G	402	POV	C1-C2-C3	-2.06	106.99	111.80
5	B	1601	AJP	C06-C07-C08	-2.04	100.63	104.34
5	D	1601	AJP	C06-C07-C08	-2.04	100.63	104.34
5	F	1601	AJP	C06-C07-C08	-2.04	100.63	104.34
5	H	1601	AJP	C06-C07-C08	-2.04	100.63	104.34
3	A	401	POV	O21-C21-O22	-2.01	118.85	123.70
3	C	402	POV	O21-C21-O22	-2.01	118.85	123.70
3	E	402	POV	O21-C21-O22	-2.01	118.85	123.70
3	G	402	POV	O21-C21-O22	-2.01	118.85	123.70
5	B	1601	AJP	C35-O40-C39	2.01	117.63	113.69
5	D	1601	AJP	C35-O40-C39	2.01	117.63	113.69
5	F	1601	AJP	C35-O40-C39	2.01	117.63	113.69
5	H	1601	AJP	C35-O40-C39	2.01	117.63	113.69

All (116) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1601	AJP	C12
5	B	1601	AJP	C59
5	B	1601	AJP	C05
5	B	1601	AJP	C45
5	B	1601	AJP	C36
5	B	1601	AJP	C10
5	B	1601	AJP	C15
5	B	1601	AJP	C47
5	B	1601	AJP	C57
5	B	1601	AJP	C19
5	B	1601	AJP	C26
5	B	1601	AJP	C39
5	B	1601	AJP	C38

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Mol	Chain	Res	Type	Atom
5	B	1601	AJP	C23
5	B	1601	AJP	C27
5	B	1601	AJP	C22
5	B	1601	AJP	C11
5	B	1601	AJP	C02
5	B	1601	AJP	C28
5	B	1601	AJP	C48
5	B	1601	AJP	C30
5	B	1601	AJP	C07
5	B	1601	AJP	C35
5	B	1601	AJP	C16
5	B	1601	AJP	C20
5	B	1601	AJP	C55
5	B	1601	AJP	C37
5	B	1601	AJP	C56
5	B	1601	AJP	C46
5	D	1601	AJP	C12
5	D	1601	AJP	C59
5	D	1601	AJP	C05
5	D	1601	AJP	C45
5	D	1601	AJP	C36
5	D	1601	AJP	C10
5	D	1601	AJP	C15
5	D	1601	AJP	C47
5	D	1601	AJP	C57
5	D	1601	AJP	C19
5	D	1601	AJP	C26
5	D	1601	AJP	C39
5	D	1601	AJP	C38
5	D	1601	AJP	C23
5	D	1601	AJP	C27
5	D	1601	AJP	C22
5	D	1601	AJP	C11
5	D	1601	AJP	C02
5	D	1601	AJP	C28
5	D	1601	AJP	C48
5	D	1601	AJP	C30
5	D	1601	AJP	C07
5	D	1601	AJP	C35
5	D	1601	AJP	C16
5	D	1601	AJP	C20
5	D	1601	AJP	C55

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Mol	Chain	Res	Type	Atom
5	D	1601	AJP	C37
5	D	1601	AJP	C56
5	D	1601	AJP	C46
5	F	1601	AJP	C12
5	F	1601	AJP	C59
5	F	1601	AJP	C05
5	F	1601	AJP	C45
5	F	1601	AJP	C36
5	F	1601	AJP	C10
5	F	1601	AJP	C15
5	F	1601	AJP	C47
5	F	1601	AJP	C57
5	F	1601	AJP	C19
5	F	1601	AJP	C26
5	F	1601	AJP	C39
5	F	1601	AJP	C38
5	F	1601	AJP	C23
5	F	1601	AJP	C27
5	F	1601	AJP	C22
5	F	1601	AJP	C11
5	F	1601	AJP	C02
5	F	1601	AJP	C28
5	F	1601	AJP	C48
5	F	1601	AJP	C30
5	F	1601	AJP	C07
5	F	1601	AJP	C35
5	F	1601	AJP	C16
5	F	1601	AJP	C20
5	F	1601	AJP	C55
5	F	1601	AJP	C37
5	F	1601	AJP	C56
5	F	1601	AJP	C46
5	H	1601	AJP	C12
5	H	1601	AJP	C59
5	H	1601	AJP	C05
5	H	1601	AJP	C45
5	H	1601	AJP	C36
5	H	1601	AJP	C10
5	H	1601	AJP	C15
5	H	1601	AJP	C47
5	H	1601	AJP	C57
5	H	1601	AJP	C19

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Mol	Chain	Res	Type	Atom
5	H	1601	AJP	C26
5	H	1601	AJP	C39
5	H	1601	AJP	C38
5	H	1601	AJP	C23
5	H	1601	AJP	C27
5	H	1601	AJP	C22
5	H	1601	AJP	C11
5	H	1601	AJP	C02
5	H	1601	AJP	C28
5	H	1601	AJP	C48
5	H	1601	AJP	C30
5	H	1601	AJP	C07
5	H	1601	AJP	C35
5	H	1601	AJP	C16
5	H	1601	AJP	C20
5	H	1601	AJP	C55
5	H	1601	AJP	C37
5	H	1601	AJP	C56
5	H	1601	AJP	C46

All (744) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	POV	C22-C21-O21-C2
3	B	1604	POV	C11-O12-P-O14
3	B	1604	POV	C22-C21-O21-C2
3	B	1605	POV	C11-O12-P-O11
3	B	1605	POV	C11-O12-P-O13
3	B	1605	POV	C11-O12-P-O14
3	B	1606	POV	C1-O11-P-O14
3	B	1606	POV	C11-O12-P-O14
3	B	1606	POV	C22-C21-O21-C2
3	B	1607	POV	C11-O12-P-O14
3	B	1607	POV	O12-C11-C12-N
3	B	1607	POV	C12-C11-O12-P
3	B	1607	POV	C22-C21-O21-C2
3	B	1607	POV	O22-C21-O21-C2
3	B	1608	POV	C1-O11-P-O14
3	B	1608	POV	C11-O12-P-O11
3	B	1608	POV	C11-O12-P-O14
3	B	1608	POV	C22-C21-O21-C2
3	B	1609	POV	C11-O12-P-O13

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Mol	Chain	Res	Type	Atoms
3	B	1609	POV	C22-C21-O21-C2
3	B	1610	POV	O22-C21-O21-C2
3	B	1611	POV	C22-C21-O21-C2
3	C	402	POV	C22-C21-O21-C2
3	D	1604	POV	C11-O12-P-O14
3	D	1604	POV	C22-C21-O21-C2
3	D	1605	POV	C11-O12-P-O11
3	D	1605	POV	C11-O12-P-O13
3	D	1605	POV	C11-O12-P-O14
3	D	1606	POV	C1-O11-P-O14
3	D	1606	POV	C11-O12-P-O14
3	D	1606	POV	C22-C21-O21-C2
3	D	1607	POV	C11-O12-P-O14
3	D	1607	POV	O12-C11-C12-N
3	D	1607	POV	C12-C11-O12-P
3	D	1607	POV	C22-C21-O21-C2
3	D	1607	POV	O22-C21-O21-C2
3	D	1608	POV	C1-O11-P-O14
3	D	1608	POV	C11-O12-P-O11
3	D	1608	POV	C11-O12-P-O14
3	D	1608	POV	C22-C21-O21-C2
3	D	1609	POV	C11-O12-P-O13
3	D	1609	POV	C22-C21-O21-C2
3	D	1610	POV	O22-C21-O21-C2
3	D	1611	POV	C22-C21-O21-C2
3	E	402	POV	C22-C21-O21-C2
3	F	1604	POV	C11-O12-P-O14
3	F	1604	POV	C22-C21-O21-C2
3	F	1605	POV	C11-O12-P-O11
3	F	1605	POV	C11-O12-P-O13
3	F	1605	POV	C11-O12-P-O14
3	F	1606	POV	C1-O11-P-O14
3	F	1606	POV	C11-O12-P-O14
3	F	1606	POV	C22-C21-O21-C2
3	F	1607	POV	C11-O12-P-O14
3	F	1607	POV	O12-C11-C12-N
3	F	1607	POV	C12-C11-O12-P
3	F	1607	POV	C22-C21-O21-C2
3	F	1607	POV	O22-C21-O21-C2
3	F	1608	POV	C1-O11-P-O14
3	F	1608	POV	C11-O12-P-O11
3	F	1608	POV	C11-O12-P-O14

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Mol	Chain	Res	Type	Atoms
3	F	1608	POV	C22-C21-O21-C2
3	F	1609	POV	C11-O12-P-O13
3	F	1609	POV	C22-C21-O21-C2
3	F	1610	POV	O22-C21-O21-C2
3	F	1611	POV	C22-C21-O21-C2
3	G	402	POV	C22-C21-O21-C2
3	H	1604	POV	C11-O12-P-O14
3	H	1604	POV	C22-C21-O21-C2
3	H	1605	POV	C11-O12-P-O11
3	H	1605	POV	C11-O12-P-O13
3	H	1605	POV	C11-O12-P-O14
3	H	1606	POV	C1-O11-P-O14
3	H	1606	POV	C11-O12-P-O14
3	H	1606	POV	C22-C21-O21-C2
3	H	1607	POV	C11-O12-P-O14
3	H	1607	POV	O12-C11-C12-N
3	H	1607	POV	C12-C11-O12-P
3	H	1607	POV	C22-C21-O21-C2
3	H	1607	POV	O22-C21-O21-C2
3	H	1608	POV	C1-O11-P-O14
3	H	1608	POV	C11-O12-P-O11
3	H	1608	POV	C11-O12-P-O14
3	H	1608	POV	C22-C21-O21-C2
3	H	1609	POV	C11-O12-P-O13
3	H	1609	POV	C22-C21-O21-C2
3	H	1610	POV	O22-C21-O21-C2
3	H	1611	POV	C22-C21-O21-C2
4	A	402	AGS	O4'-C4'-C5'-O5'
4	B	1602	AGS	PB-O3B-PG-O2G
4	B	1602	AGS	PB-O3B-PG-O3G
4	C	401	AGS	O4'-C4'-C5'-O5'
4	D	1602	AGS	PB-O3B-PG-O2G
4	D	1602	AGS	PB-O3B-PG-O3G
4	E	401	AGS	O4'-C4'-C5'-O5'
4	F	1602	AGS	PB-O3B-PG-O2G
4	F	1602	AGS	PB-O3B-PG-O3G
4	G	401	AGS	O4'-C4'-C5'-O5'
4	H	1602	AGS	PB-O3B-PG-O2G
4	H	1602	AGS	PB-O3B-PG-O3G
5	B	1601	AJP	C35-C36-O54-C55
5	D	1601	AJP	C35-C36-O54-C55
5	F	1601	AJP	C35-C36-O54-C55

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Mol	Chain	Res	Type	Atoms
5	H	1601	AJP	C35-C36-O54-C55
7	B	1612	PTY	N1-C2-C3-O11
7	B	1612	PTY	C2-C3-O11-P1
7	B	1612	PTY	C11-C8-O7-C6
7	B	1613	PTY	C11-C8-O7-C6
7	B	1613	PTY	C5-O14-P1-O11
7	B	1613	PTY	C5-O14-P1-O12
7	B	1613	PTY	C5-O14-P1-O13
7	B	1614	PTY	O4-C1-C6-C5
7	B	1615	PTY	O14-C5-C6-O7
7	B	1615	PTY	C11-C8-O7-C6
7	B	1615	PTY	C5-O14-P1-O12
7	D	1612	PTY	N1-C2-C3-O11
7	D	1612	PTY	C2-C3-O11-P1
7	D	1612	PTY	C11-C8-O7-C6
7	D	1613	PTY	C11-C8-O7-C6
7	D	1613	PTY	C5-O14-P1-O11
7	D	1613	PTY	C5-O14-P1-O12
7	D	1613	PTY	C5-O14-P1-O13
7	D	1614	PTY	O4-C1-C6-C5
7	D	1615	PTY	O14-C5-C6-O7
7	D	1615	PTY	C11-C8-O7-C6
7	D	1615	PTY	C5-O14-P1-O12
7	F	1612	PTY	N1-C2-C3-O11
7	F	1612	PTY	C2-C3-O11-P1
7	F	1612	PTY	C11-C8-O7-C6
7	F	1613	PTY	C11-C8-O7-C6
7	F	1613	PTY	C5-O14-P1-O11
7	F	1613	PTY	C5-O14-P1-O12
7	F	1613	PTY	C5-O14-P1-O13
7	F	1614	PTY	O4-C1-C6-C5
7	F	1615	PTY	O14-C5-C6-O7
7	F	1615	PTY	C11-C8-O7-C6
7	F	1615	PTY	C5-O14-P1-O12
7	H	1612	PTY	N1-C2-C3-O11
7	H	1612	PTY	C2-C3-O11-P1
7	H	1612	PTY	C11-C8-O7-C6
7	H	1613	PTY	C11-C8-O7-C6
7	H	1613	PTY	C5-O14-P1-O11
7	H	1613	PTY	C5-O14-P1-O12
7	H	1613	PTY	C5-O14-P1-O13
7	H	1614	PTY	O4-C1-C6-C5

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Mol	Chain	Res	Type	Atoms
7	H	1615	PTY	O14-C5-C6-O7
7	H	1615	PTY	C11-C8-O7-C6
7	H	1615	PTY	C5-O14-P1-O12
7	B	1612	PTY	O30-C30-O4-C1
7	B	1613	PTY	O30-C30-O4-C1
7	D	1612	PTY	O30-C30-O4-C1
7	D	1613	PTY	O30-C30-O4-C1
7	F	1612	PTY	O30-C30-O4-C1
7	F	1613	PTY	O30-C30-O4-C1
7	H	1612	PTY	O30-C30-O4-C1
7	H	1613	PTY	O30-C30-O4-C1
3	B	1604	POV	O22-C21-O21-C2
3	B	1608	POV	O22-C21-O21-C2
3	B	1609	POV	O22-C21-O21-C2
3	B	1611	POV	O22-C21-O21-C2
3	D	1604	POV	O22-C21-O21-C2
3	D	1608	POV	O22-C21-O21-C2
3	D	1609	POV	O22-C21-O21-C2
3	D	1611	POV	O22-C21-O21-C2
3	F	1604	POV	O22-C21-O21-C2
3	F	1608	POV	O22-C21-O21-C2
3	F	1609	POV	O22-C21-O21-C2
3	F	1611	POV	O22-C21-O21-C2
3	H	1604	POV	O22-C21-O21-C2
3	H	1608	POV	O22-C21-O21-C2
3	H	1609	POV	O22-C21-O21-C2
3	H	1611	POV	O22-C21-O21-C2
7	B	1613	PTY	O10-C8-O7-C6
7	B	1615	PTY	O10-C8-O7-C6
7	D	1613	PTY	O10-C8-O7-C6
7	D	1615	PTY	O10-C8-O7-C6
7	F	1613	PTY	O10-C8-O7-C6
7	F	1615	PTY	O10-C8-O7-C6
7	H	1613	PTY	O10-C8-O7-C6
7	H	1615	PTY	O10-C8-O7-C6
7	B	1612	PTY	C31-C30-O4-C1
7	D	1612	PTY	C31-C30-O4-C1
7	F	1612	PTY	C31-C30-O4-C1
7	H	1612	PTY	C31-C30-O4-C1
3	B	1610	POV	C22-C21-O21-C2
3	D	1610	POV	C22-C21-O21-C2
3	F	1610	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
3	H	1610	POV	C22-C21-O21-C2
7	B	1613	PTY	C31-C30-O4-C1
7	D	1613	PTY	C31-C30-O4-C1
7	F	1613	PTY	C31-C30-O4-C1
7	H	1613	PTY	C31-C30-O4-C1
3	A	401	POV	O22-C21-O21-C2
3	B	1606	POV	O22-C21-O21-C2
3	C	402	POV	O22-C21-O21-C2
3	D	1606	POV	O22-C21-O21-C2
3	E	402	POV	O22-C21-O21-C2
3	F	1606	POV	O22-C21-O21-C2
3	G	402	POV	O22-C21-O21-C2
3	H	1606	POV	O22-C21-O21-C2
7	B	1612	PTY	O10-C8-O7-C6
7	D	1612	PTY	O10-C8-O7-C6
7	F	1612	PTY	O10-C8-O7-C6
7	H	1612	PTY	O10-C8-O7-C6
3	B	1607	POV	C32-C31-O31-C3
3	D	1607	POV	C32-C31-O31-C3
3	F	1607	POV	C32-C31-O31-C3
3	H	1607	POV	C32-C31-O31-C3
7	B	1614	PTY	C31-C30-O4-C1
7	D	1614	PTY	C31-C30-O4-C1
7	F	1614	PTY	C31-C30-O4-C1
7	H	1614	PTY	C31-C30-O4-C1
3	B	1607	POV	O32-C31-O31-C3
3	D	1607	POV	O32-C31-O31-C3
3	F	1607	POV	O32-C31-O31-C3
3	H	1607	POV	O32-C31-O31-C3
7	B	1614	PTY	O4-C1-C6-O7
7	D	1614	PTY	O4-C1-C6-O7
7	F	1614	PTY	O4-C1-C6-O7
7	H	1614	PTY	O4-C1-C6-O7
3	B	1611	POV	C33-C34-C35-C36
3	D	1611	POV	C33-C34-C35-C36
3	F	1611	POV	C33-C34-C35-C36
3	H	1611	POV	C33-C34-C35-C36
5	B	1601	AJP	O50-C45-O44-C37
5	D	1601	AJP	O50-C45-O44-C37
5	F	1601	AJP	O50-C45-O44-C37
5	H	1601	AJP	O50-C45-O44-C37
4	A	402	AGS	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	C	401	AGS	C3'-C4'-C5'-O5'
4	E	401	AGS	C3'-C4'-C5'-O5'
4	G	401	AGS	C3'-C4'-C5'-O5'
7	B	1614	PTY	O30-C30-O4-C1
7	D	1614	PTY	O30-C30-O4-C1
7	F	1614	PTY	O30-C30-O4-C1
7	H	1614	PTY	O30-C30-O4-C1
7	B	1615	PTY	C1-C6-O7-C8
7	B	1615	PTY	C5-C6-O7-C8
7	D	1615	PTY	C1-C6-O7-C8
7	D	1615	PTY	C5-C6-O7-C8
7	F	1615	PTY	C1-C6-O7-C8
7	F	1615	PTY	C5-C6-O7-C8
7	H	1615	PTY	C1-C6-O7-C8
7	H	1615	PTY	C5-C6-O7-C8
5	B	1601	AJP	O40-C39-C41-O42
5	D	1601	AJP	O40-C39-C41-O42
5	F	1601	AJP	O40-C39-C41-O42
5	H	1601	AJP	O40-C39-C41-O42
3	B	1604	POV	C21-C22-C23-C24
3	D	1604	POV	C21-C22-C23-C24
3	F	1604	POV	C21-C22-C23-C24
3	H	1604	POV	C21-C22-C23-C24
3	B	1608	POV	C32-C31-O31-C3
3	D	1608	POV	C32-C31-O31-C3
3	F	1608	POV	C32-C31-O31-C3
3	H	1608	POV	C32-C31-O31-C3
3	B	1606	POV	C1-O11-P-O12
3	B	1608	POV	C1-O11-P-O12
3	B	1609	POV	C11-O12-P-O11
3	D	1606	POV	C1-O11-P-O12
3	D	1608	POV	C1-O11-P-O12
3	D	1609	POV	C11-O12-P-O11
3	F	1606	POV	C1-O11-P-O12
3	F	1608	POV	C1-O11-P-O12
3	F	1609	POV	C11-O12-P-O11
3	H	1606	POV	C1-O11-P-O12
3	H	1608	POV	C1-O11-P-O12
3	H	1609	POV	C11-O12-P-O11
7	B	1612	PTY	C3-O11-P1-O14
7	B	1614	PTY	C3-O11-P1-O14
7	D	1612	PTY	C3-O11-P1-O14

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Mol	Chain	Res	Type	Atoms
7	D	1614	PTY	C3-O11-P1-O14
7	F	1612	PTY	C3-O11-P1-O14
7	F	1614	PTY	C3-O11-P1-O14
7	H	1612	PTY	C3-O11-P1-O14
7	H	1614	PTY	C3-O11-P1-O14
3	B	1610	POV	C21-C22-C23-C24
3	D	1610	POV	C21-C22-C23-C24
3	F	1610	POV	C21-C22-C23-C24
3	H	1610	POV	C21-C22-C23-C24
7	B	1614	PTY	C31-C32-C33-C34
7	D	1614	PTY	C31-C32-C33-C34
7	F	1614	PTY	C31-C32-C33-C34
7	H	1614	PTY	C31-C32-C33-C34
7	B	1612	PTY	C1-C6-O7-C8
7	D	1612	PTY	C1-C6-O7-C8
7	F	1612	PTY	C1-C6-O7-C8
7	H	1612	PTY	C1-C6-O7-C8
3	B	1608	POV	C32-C33-C34-C35
3	D	1608	POV	C32-C33-C34-C35
3	F	1608	POV	C32-C33-C34-C35
3	H	1608	POV	C32-C33-C34-C35
3	B	1606	POV	C22-C23-C24-C25
3	D	1606	POV	C22-C23-C24-C25
3	F	1606	POV	C22-C23-C24-C25
3	H	1606	POV	C22-C23-C24-C25
7	B	1614	PTY	C32-C33-C34-C35
7	B	1615	PTY	C12-C13-C14-C15
7	D	1614	PTY	C32-C33-C34-C35
7	D	1615	PTY	C12-C13-C14-C15
7	F	1614	PTY	C32-C33-C34-C35
7	F	1615	PTY	C12-C13-C14-C15
7	H	1614	PTY	C32-C33-C34-C35
7	H	1615	PTY	C12-C13-C14-C15
5	B	1601	AJP	C28-C29-O34-C35
5	D	1601	AJP	C28-C29-O34-C35
5	F	1601	AJP	C28-C29-O34-C35
5	H	1601	AJP	C28-C29-O34-C35
6	B	1603	BJX	C21-C23-C24-O3
6	D	1603	BJX	C21-C23-C24-O3
6	F	1603	BJX	C21-C23-C24-O3
6	H	1603	BJX	C21-C23-C24-O3
5	B	1601	AJP	O31-C30-C32-O33

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Mol	Chain	Res	Type	Atoms
5	D	1601	AJP	O31-C30-C32-O33
5	F	1601	AJP	O31-C30-C32-O33
5	H	1601	AJP	O31-C30-C32-O33
7	B	1614	PTY	C33-C34-C35-C36
7	D	1614	PTY	C33-C34-C35-C36
7	F	1614	PTY	C33-C34-C35-C36
7	H	1614	PTY	C33-C34-C35-C36
3	B	1608	POV	O32-C31-O31-C3
3	D	1608	POV	O32-C31-O31-C3
3	F	1608	POV	O32-C31-O31-C3
3	H	1608	POV	O32-C31-O31-C3
7	B	1615	PTY	C11-C12-C13-C14
7	D	1615	PTY	C11-C12-C13-C14
7	F	1615	PTY	C11-C12-C13-C14
7	H	1615	PTY	C11-C12-C13-C14
5	B	1601	AJP	C30-C29-O34-C35
5	D	1601	AJP	C30-C29-O34-C35
5	F	1601	AJP	C30-C29-O34-C35
5	H	1601	AJP	C30-C29-O34-C35
3	B	1604	POV	C32-C31-O31-C3
3	D	1604	POV	C32-C31-O31-C3
3	F	1604	POV	C32-C31-O31-C3
3	H	1604	POV	C32-C31-O31-C3
3	B	1606	POV	O11-C1-C2-O21
3	D	1606	POV	O11-C1-C2-O21
3	F	1606	POV	O11-C1-C2-O21
3	H	1606	POV	O11-C1-C2-O21
6	B	1603	BJX	N1-C5-C8-C9
6	D	1603	BJX	N1-C5-C8-C9
6	F	1603	BJX	N1-C5-C8-C9
6	H	1603	BJX	N1-C5-C8-C9
6	B	1603	BJX	C21-C23-C24-O2
6	D	1603	BJX	C21-C23-C24-O2
6	F	1603	BJX	C21-C23-C24-O2
6	H	1603	BJX	C21-C23-C24-O2
3	B	1604	POV	O32-C31-O31-C3
3	D	1604	POV	O32-C31-O31-C3
3	F	1604	POV	O32-C31-O31-C3
3	H	1604	POV	O32-C31-O31-C3
3	B	1604	POV	C11-O12-P-O11
3	D	1604	POV	C11-O12-P-O11
3	F	1604	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
3	H	1604	POV	C11-O12-P-O11
7	B	1615	PTY	C5-O14-P1-O11
7	D	1615	PTY	C5-O14-P1-O11
7	F	1615	PTY	C5-O14-P1-O11
7	H	1615	PTY	C5-O14-P1-O11
3	B	1611	POV	C32-C31-O31-C3
3	D	1611	POV	C32-C31-O31-C3
3	F	1611	POV	C32-C31-O31-C3
3	H	1611	POV	C32-C31-O31-C3
5	B	1601	AJP	O60-C59-C61-O62
5	D	1601	AJP	O60-C59-C61-O62
5	F	1601	AJP	O60-C59-C61-O62
5	H	1601	AJP	O60-C59-C61-O62
3	B	1605	POV	C22-C21-O21-C2
3	D	1605	POV	C22-C21-O21-C2
3	F	1605	POV	C22-C21-O21-C2
3	H	1605	POV	C22-C21-O21-C2
3	B	1611	POV	O32-C31-O31-C3
3	D	1611	POV	O32-C31-O31-C3
3	F	1611	POV	O32-C31-O31-C3
3	H	1611	POV	O32-C31-O31-C3
3	B	1606	POV	O11-C1-C2-C3
3	D	1606	POV	O11-C1-C2-C3
3	F	1606	POV	O11-C1-C2-C3
3	H	1606	POV	O11-C1-C2-C3
7	B	1612	PTY	O14-C5-C6-C1
7	D	1612	PTY	O14-C5-C6-C1
7	F	1612	PTY	O14-C5-C6-C1
7	H	1612	PTY	O14-C5-C6-C1
5	B	1601	AJP	C37-C36-O54-C55
5	D	1601	AJP	C37-C36-O54-C55
5	F	1601	AJP	C37-C36-O54-C55
5	H	1601	AJP	C37-C36-O54-C55
6	B	1603	BJX	C26-C25-O1-C21
6	D	1603	BJX	C26-C25-O1-C21
6	F	1603	BJX	C26-C25-O1-C21
6	H	1603	BJX	C26-C25-O1-C21
3	B	1608	POV	C33-C34-C35-C36
3	D	1608	POV	C33-C34-C35-C36
3	F	1608	POV	C33-C34-C35-C36
3	H	1608	POV	C33-C34-C35-C36
3	B	1611	POV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
3	D	1611	POV	C25-C26-C27-C28
3	F	1611	POV	C25-C26-C27-C28
3	H	1611	POV	C25-C26-C27-C28
3	B	1608	POV	C34-C35-C36-C37
3	D	1608	POV	C34-C35-C36-C37
3	F	1608	POV	C34-C35-C36-C37
3	H	1608	POV	C34-C35-C36-C37
7	B	1615	PTY	O14-C5-C6-C1
7	D	1615	PTY	O14-C5-C6-C1
7	F	1615	PTY	O14-C5-C6-C1
7	H	1615	PTY	O14-C5-C6-C1
3	B	1608	POV	C24-C25-C26-C27
3	D	1608	POV	C24-C25-C26-C27
3	F	1608	POV	C24-C25-C26-C27
3	H	1608	POV	C24-C25-C26-C27
3	B	1607	POV	C11-O12-P-O11
3	D	1607	POV	C11-O12-P-O11
3	F	1607	POV	C11-O12-P-O11
3	H	1607	POV	C11-O12-P-O11
6	B	1603	BJX	C19-C21-O1-C25
6	D	1603	BJX	C19-C21-O1-C25
6	F	1603	BJX	C19-C21-O1-C25
6	H	1603	BJX	C19-C21-O1-C25
3	B	1605	POV	O22-C21-O21-C2
3	D	1605	POV	O22-C21-O21-C2
3	F	1605	POV	O22-C21-O21-C2
3	H	1605	POV	O22-C21-O21-C2
3	B	1605	POV	C36-C37-C38-C39
3	D	1605	POV	C36-C37-C38-C39
3	F	1605	POV	C36-C37-C38-C39
3	H	1605	POV	C36-C37-C38-C39
3	B	1605	POV	C33-C34-C35-C36
3	D	1605	POV	C33-C34-C35-C36
3	F	1605	POV	C33-C34-C35-C36
3	H	1605	POV	C33-C34-C35-C36
3	B	1605	POV	C2-C1-O11-P
3	D	1605	POV	C2-C1-O11-P
3	F	1605	POV	C2-C1-O11-P
3	H	1605	POV	C2-C1-O11-P
6	B	1603	BJX	C10-C6-N-C
6	D	1603	BJX	C10-C6-N-C
6	F	1603	BJX	C10-C6-N-C

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Mol	Chain	Res	Type	Atoms
6	H	1603	BJX	C10-C6-N-C
3	B	1605	POV	C32-C33-C34-C35
3	D	1605	POV	C32-C33-C34-C35
3	F	1605	POV	C32-C33-C34-C35
3	H	1605	POV	C32-C33-C34-C35
3	B	1604	POV	C2-C1-O11-P
3	D	1604	POV	C2-C1-O11-P
3	F	1604	POV	C2-C1-O11-P
3	H	1604	POV	C2-C1-O11-P
7	B	1612	PTY	O4-C1-C6-C5
7	B	1613	PTY	O4-C1-C6-C5
7	D	1612	PTY	O4-C1-C6-C5
7	D	1613	PTY	O4-C1-C6-C5
7	F	1612	PTY	O4-C1-C6-C5
7	F	1613	PTY	O4-C1-C6-C5
7	H	1612	PTY	O4-C1-C6-C5
7	H	1613	PTY	O4-C1-C6-C5
3	B	1606	POV	C35-C36-C37-C38
3	D	1606	POV	C35-C36-C37-C38
3	F	1606	POV	C35-C36-C37-C38
3	H	1606	POV	C35-C36-C37-C38
7	B	1613	PTY	O4-C1-C6-O7
7	D	1613	PTY	O4-C1-C6-O7
7	F	1613	PTY	O4-C1-C6-O7
7	H	1613	PTY	O4-C1-C6-O7
3	B	1604	POV	O21-C21-C22-C23
3	D	1604	POV	O21-C21-C22-C23
3	F	1604	POV	O21-C21-C22-C23
3	H	1604	POV	O21-C21-C22-C23
3	B	1605	POV	C1-O11-P-O12
3	B	1606	POV	C11-O12-P-O11
3	B	1610	POV	C1-O11-P-O12
3	D	1605	POV	C1-O11-P-O12
3	D	1606	POV	C11-O12-P-O11
3	D	1610	POV	C1-O11-P-O12
3	F	1605	POV	C1-O11-P-O12
3	F	1606	POV	C11-O12-P-O11
3	F	1610	POV	C1-O11-P-O12
3	H	1605	POV	C1-O11-P-O12
3	H	1606	POV	C11-O12-P-O11
3	H	1610	POV	C1-O11-P-O12
7	B	1614	PTY	C5-O14-P1-O11

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Mol	Chain	Res	Type	Atoms
7	B	1615	PTY	C3-O11-P1-O14
7	D	1614	PTY	C5-O14-P1-O11
7	D	1615	PTY	C3-O11-P1-O14
7	F	1614	PTY	C5-O14-P1-O11
7	F	1615	PTY	C3-O11-P1-O14
7	H	1614	PTY	C5-O14-P1-O11
7	H	1615	PTY	C3-O11-P1-O14
3	B	1609	POV	C11-C12-N-C13
3	D	1609	POV	C11-C12-N-C13
3	F	1609	POV	C11-C12-N-C13
3	H	1609	POV	C11-C12-N-C13
6	B	1603	BJX	C7-C5-C8-C9
6	D	1603	BJX	C7-C5-C8-C9
6	F	1603	BJX	C7-C5-C8-C9
6	H	1603	BJX	C7-C5-C8-C9
7	B	1612	PTY	C3-O11-P1-O12
7	B	1614	PTY	C3-O11-P1-O13
7	B	1615	PTY	C5-O14-P1-O13
7	D	1612	PTY	C3-O11-P1-O12
7	D	1614	PTY	C3-O11-P1-O13
7	D	1615	PTY	C5-O14-P1-O13
7	F	1612	PTY	C3-O11-P1-O12
7	F	1614	PTY	C3-O11-P1-O13
7	F	1615	PTY	C5-O14-P1-O13
7	H	1612	PTY	C3-O11-P1-O12
7	H	1614	PTY	C3-O11-P1-O13
7	H	1615	PTY	C5-O14-P1-O13
7	B	1613	PTY	C11-C12-C13-C14
7	D	1613	PTY	C11-C12-C13-C14
7	F	1613	PTY	C11-C12-C13-C14
7	H	1613	PTY	C11-C12-C13-C14
3	B	1605	POV	C22-C23-C24-C25
3	D	1605	POV	C22-C23-C24-C25
3	F	1605	POV	C22-C23-C24-C25
3	H	1605	POV	C22-C23-C24-C25
3	B	1605	POV	C34-C35-C36-C37
3	D	1605	POV	C34-C35-C36-C37
3	F	1605	POV	C34-C35-C36-C37
3	H	1605	POV	C34-C35-C36-C37
3	B	1604	POV	C12-C11-O12-P
3	D	1604	POV	C12-C11-O12-P
3	F	1604	POV	C12-C11-O12-P

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Mol	Chain	Res	Type	Atoms
3	H	1604	POV	C12-C11-O12-P
6	B	1603	BJX	N1-C5-C7-C6
6	D	1603	BJX	N1-C5-C7-C6
6	F	1603	BJX	N1-C5-C7-C6
6	H	1603	BJX	N1-C5-C7-C6
3	B	1605	POV	C25-C26-C27-C28
3	D	1605	POV	C25-C26-C27-C28
3	F	1605	POV	C25-C26-C27-C28
3	H	1605	POV	C25-C26-C27-C28
3	B	1606	POV	C21-C22-C23-C24
3	D	1606	POV	C21-C22-C23-C24
3	F	1606	POV	C21-C22-C23-C24
3	H	1606	POV	C21-C22-C23-C24
7	B	1612	PTY	O14-C5-C6-O7
7	D	1612	PTY	O14-C5-C6-O7
7	F	1612	PTY	O14-C5-C6-O7
7	H	1612	PTY	O14-C5-C6-O7
3	B	1607	POV	C31-C32-C33-C34
3	D	1607	POV	C31-C32-C33-C34
3	F	1607	POV	C31-C32-C33-C34
3	H	1607	POV	C31-C32-C33-C34
3	A	401	POV	O12-C11-C12-N
3	B	1606	POV	O12-C11-C12-N
3	B	1607	POV	C1-C2-C3-O31
3	B	1609	POV	O12-C11-C12-N
3	C	402	POV	O12-C11-C12-N
3	D	1606	POV	O12-C11-C12-N
3	D	1607	POV	C1-C2-C3-O31
3	D	1609	POV	O12-C11-C12-N
3	E	402	POV	O12-C11-C12-N
3	F	1606	POV	O12-C11-C12-N
3	F	1607	POV	C1-C2-C3-O31
3	F	1609	POV	O12-C11-C12-N
3	G	402	POV	O12-C11-C12-N
3	H	1606	POV	O12-C11-C12-N
3	H	1607	POV	C1-C2-C3-O31
3	H	1609	POV	O12-C11-C12-N
3	B	1607	POV	O21-C2-C3-O31
3	D	1607	POV	O21-C2-C3-O31
3	F	1607	POV	O21-C2-C3-O31
3	H	1607	POV	O21-C2-C3-O31
3	B	1604	POV	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
3	D	1604	POV	C33-C34-C35-C36
3	F	1604	POV	C33-C34-C35-C36
3	H	1604	POV	C33-C34-C35-C36
6	B	1603	BJX	O-C16-C17-C18
6	D	1603	BJX	O-C16-C17-C18
6	F	1603	BJX	O-C16-C17-C18
6	H	1603	BJX	O-C16-C17-C18
6	B	1603	BJX	C23-C21-O1-C25
6	D	1603	BJX	C23-C21-O1-C25
6	F	1603	BJX	C23-C21-O1-C25
6	H	1603	BJX	C23-C21-O1-C25
3	B	1606	POV	C31-C32-C33-C34
3	D	1606	POV	C31-C32-C33-C34
3	F	1606	POV	C31-C32-C33-C34
3	H	1606	POV	C31-C32-C33-C34
7	B	1615	PTY	C14-C15-C16-C17
7	D	1615	PTY	C14-C15-C16-C17
7	F	1615	PTY	C14-C15-C16-C17
7	H	1615	PTY	C14-C15-C16-C17
3	B	1609	POV	C11-C12-N-C15
3	D	1609	POV	C11-C12-N-C15
3	F	1609	POV	C11-C12-N-C15
3	H	1609	POV	C11-C12-N-C15
7	B	1612	PTY	O4-C1-C6-O7
7	D	1612	PTY	O4-C1-C6-O7
7	F	1612	PTY	O4-C1-C6-O7
7	H	1612	PTY	O4-C1-C6-O7
3	A	401	POV	C11-O12-P-O11
3	B	1607	POV	C1-O11-P-O12
3	B	1609	POV	C1-O11-P-O12
3	B	1610	POV	C11-O12-P-O11
3	C	402	POV	C11-O12-P-O11
3	D	1607	POV	C1-O11-P-O12
3	D	1609	POV	C1-O11-P-O12
3	D	1610	POV	C11-O12-P-O11
3	E	402	POV	C11-O12-P-O11
3	F	1607	POV	C1-O11-P-O12
3	F	1609	POV	C1-O11-P-O12
3	F	1610	POV	C11-O12-P-O11
3	G	402	POV	C11-O12-P-O11
3	H	1607	POV	C1-O11-P-O12
3	H	1609	POV	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
3	H	1610	POV	C11-O12-P-O11
7	B	1612	PTY	C5-O14-P1-O11
7	B	1613	PTY	C3-O11-P1-O14
7	D	1612	PTY	C5-O14-P1-O11
7	D	1613	PTY	C3-O11-P1-O14
7	F	1612	PTY	C5-O14-P1-O11
7	F	1613	PTY	C3-O11-P1-O14
7	H	1612	PTY	C5-O14-P1-O11
7	H	1613	PTY	C3-O11-P1-O14
5	B	1601	AJP	C38-C39-C41-O42
5	D	1601	AJP	C38-C39-C41-O42
5	F	1601	AJP	C38-C39-C41-O42
5	H	1601	AJP	C38-C39-C41-O42
7	B	1613	PTY	C6-C5-O14-P1
7	D	1613	PTY	C6-C5-O14-P1
7	F	1613	PTY	C6-C5-O14-P1
7	H	1613	PTY	C6-C5-O14-P1
3	B	1607	POV	O11-C1-C2-O21
3	D	1607	POV	O11-C1-C2-O21
3	F	1607	POV	O11-C1-C2-O21
3	H	1607	POV	O11-C1-C2-O21
6	B	1603	BJX	N1-C16-C17-C18
6	D	1603	BJX	N1-C16-C17-C18
6	F	1603	BJX	N1-C16-C17-C18
6	H	1603	BJX	N1-C16-C17-C18
3	B	1606	POV	C1-C2-C3-O31
3	D	1606	POV	C1-C2-C3-O31
3	F	1606	POV	C1-C2-C3-O31
3	H	1606	POV	C1-C2-C3-O31
7	B	1615	PTY	C8-C11-C12-C13
7	D	1615	PTY	C8-C11-C12-C13
7	F	1615	PTY	C8-C11-C12-C13
7	H	1615	PTY	C8-C11-C12-C13
3	B	1609	POV	C11-C12-N-C14
3	D	1609	POV	C11-C12-N-C14
3	F	1609	POV	C11-C12-N-C14
3	H	1609	POV	C11-C12-N-C14
3	B	1607	POV	O11-C1-C2-C3
3	D	1607	POV	O11-C1-C2-C3
3	F	1607	POV	O11-C1-C2-C3
3	H	1607	POV	O11-C1-C2-C3
3	B	1606	POV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
3	D	1606	POV	C24-C25-C26-C27
3	F	1606	POV	C24-C25-C26-C27
3	H	1606	POV	C24-C25-C26-C27
3	B	1609	POV	C22-C23-C24-C25
3	D	1609	POV	C22-C23-C24-C25
3	F	1609	POV	C22-C23-C24-C25
3	H	1609	POV	C22-C23-C24-C25
3	B	1611	POV	C32-C33-C34-C35
3	D	1611	POV	C32-C33-C34-C35
3	F	1611	POV	C32-C33-C34-C35
3	H	1611	POV	C32-C33-C34-C35
3	B	1611	POV	O11-C1-C2-O21
3	D	1611	POV	O11-C1-C2-O21
3	F	1611	POV	O11-C1-C2-O21
3	H	1611	POV	O11-C1-C2-O21
3	B	1605	POV	O21-C21-C22-C23
3	D	1605	POV	O21-C21-C22-C23
3	F	1605	POV	O21-C21-C22-C23
3	H	1605	POV	O21-C21-C22-C23
5	B	1601	AJP	C22-C23-O25-C26
5	D	1601	AJP	C22-C23-O25-C26
5	F	1601	AJP	C22-C23-O25-C26
5	H	1601	AJP	C22-C23-O25-C26
6	B	1603	BJX	C7-C6-N-C
6	D	1603	BJX	C7-C6-N-C
6	F	1603	BJX	C7-C6-N-C
6	H	1603	BJX	C7-C6-N-C
3	B	1611	POV	C34-C35-C36-C37
3	D	1611	POV	C34-C35-C36-C37
3	F	1611	POV	C34-C35-C36-C37
3	H	1611	POV	C34-C35-C36-C37
6	B	1603	BJX	N1-C5-C7-C11
6	D	1603	BJX	N1-C5-C7-C11
6	F	1603	BJX	N1-C5-C7-C11
6	H	1603	BJX	N1-C5-C7-C11
3	B	1604	POV	C32-C33-C34-C35
3	D	1604	POV	C32-C33-C34-C35
3	F	1604	POV	C32-C33-C34-C35
3	H	1604	POV	C32-C33-C34-C35
7	B	1614	PTY	O4-C30-C31-C32
7	D	1614	PTY	O4-C30-C31-C32
7	F	1614	PTY	O4-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
7	H	1614	PTY	O4-C30-C31-C32
7	B	1613	PTY	O4-C30-C31-C32
7	D	1613	PTY	O4-C30-C31-C32
7	F	1613	PTY	O4-C30-C31-C32
7	H	1613	PTY	O4-C30-C31-C32
3	B	1611	POV	O21-C21-C22-C23
3	D	1611	POV	O21-C21-C22-C23
3	F	1611	POV	O21-C21-C22-C23
3	H	1611	POV	O21-C21-C22-C23
3	B	1606	POV	C27-C28-C29-C210
3	D	1606	POV	C27-C28-C29-C210
3	F	1606	POV	C27-C28-C29-C210
3	H	1606	POV	C27-C28-C29-C210
5	B	1601	AJP	C36-C37-O44-C45
5	D	1601	AJP	C36-C37-O44-C45
5	F	1601	AJP	C36-C37-O44-C45
5	H	1601	AJP	C36-C37-O44-C45
3	B	1606	POV	C1-O11-P-O13
3	B	1610	POV	C11-O12-P-O14
3	D	1606	POV	C1-O11-P-O13
3	D	1610	POV	C11-O12-P-O14
3	F	1606	POV	C1-O11-P-O13
3	F	1610	POV	C11-O12-P-O14
3	H	1606	POV	C1-O11-P-O13
3	H	1610	POV	C11-O12-P-O14
7	B	1614	PTY	O30-C30-C31-C32
7	D	1614	PTY	O30-C30-C31-C32
7	F	1614	PTY	O30-C30-C31-C32
7	H	1614	PTY	O30-C30-C31-C32
3	A	401	POV	C12-C11-O12-P
3	C	402	POV	C12-C11-O12-P
3	E	402	POV	C12-C11-O12-P
3	G	402	POV	C12-C11-O12-P
7	B	1613	PTY	C2-C3-O11-P1
7	B	1614	PTY	C2-C3-O11-P1
7	D	1613	PTY	C2-C3-O11-P1
7	D	1614	PTY	C2-C3-O11-P1
7	F	1613	PTY	C2-C3-O11-P1
7	F	1614	PTY	C2-C3-O11-P1
7	H	1613	PTY	C2-C3-O11-P1
7	H	1614	PTY	C2-C3-O11-P1
3	B	1611	POV	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
3	D	1611	POV	O22-C21-C22-C23
3	F	1611	POV	O22-C21-C22-C23
3	H	1611	POV	O22-C21-C22-C23
3	B	1604	POV	O22-C21-C22-C23
3	D	1604	POV	O22-C21-C22-C23
3	F	1604	POV	O22-C21-C22-C23
3	H	1604	POV	O22-C21-C22-C23
7	B	1613	PTY	O30-C30-C31-C32
7	D	1613	PTY	O30-C30-C31-C32
7	F	1613	PTY	O30-C30-C31-C32
7	H	1613	PTY	O30-C30-C31-C32

There are no ring outliers.

60 monomers are involved in 137 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1609	POV	3	0
3	B	1607	POV	2	0
3	B	1606	POV	1	0
3	D	1608	POV	8	0
4	F	1602	AGS	1	0
7	B	1613	PTY	4	0
7	B	1614	PTY	1	0
3	A	401	POV	4	0
6	D	1603	BJX	2	0
5	H	1601	AJP	1	0
3	B	1604	POV	5	0
6	B	1603	BJX	2	0
3	H	1611	POV	2	0
3	B	1608	POV	8	0
3	B	1611	POV	2	0
7	B	1615	PTY	2	0
3	H	1605	POV	2	0
6	F	1603	BJX	2	0
3	D	1609	POV	2	0
4	D	1602	AGS	1	0
3	F	1608	POV	7	0
7	D	1613	PTY	4	0
3	D	1607	POV	2	0
3	D	1604	POV	5	0
3	D	1606	POV	1	0
4	E	401	AGS	2	0

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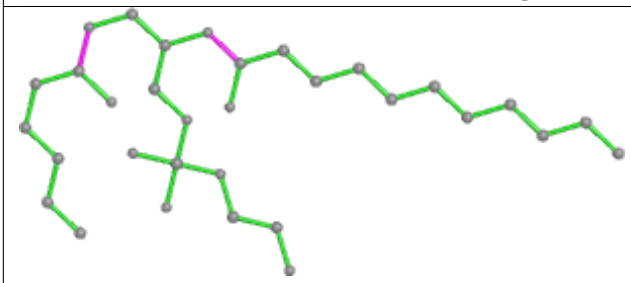
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1607	POV	2	0
6	H	1603	BJX	2	0
3	H	1608	POV	8	0
3	D	1605	POV	3	0
5	B	1601	AJP	1	0
3	F	1604	POV	4	0
7	D	1615	PTY	2	0
3	B	1609	POV	3	0
4	B	1602	AGS	1	0
3	F	1611	POV	2	0
3	G	402	POV	4	0
3	C	402	POV	3	0
3	F	1605	POV	2	0
7	H	1614	PTY	1	0
3	H	1609	POV	3	0
3	B	1605	POV	3	0
4	A	402	AGS	2	0
3	E	402	POV	4	0
4	G	401	AGS	2	0
4	H	1602	AGS	1	0
7	D	1614	PTY	1	0
7	F	1615	PTY	2	0
3	H	1607	POV	2	0
3	H	1604	POV	4	0
7	H	1613	PTY	4	0
3	H	1606	POV	1	0
7	F	1614	PTY	1	0
3	F	1606	POV	1	0
7	H	1615	PTY	2	0
5	D	1601	AJP	1	0
4	C	401	AGS	2	0
3	D	1611	POV	1	0
7	F	1613	PTY	4	0
5	F	1601	AJP	1	0

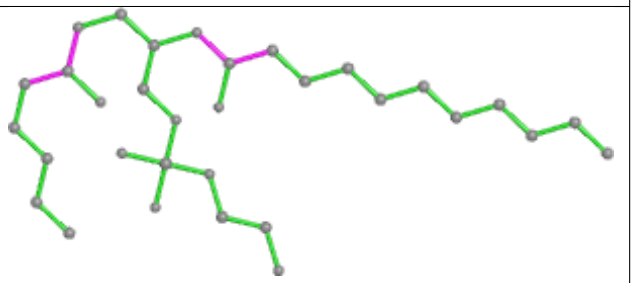
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

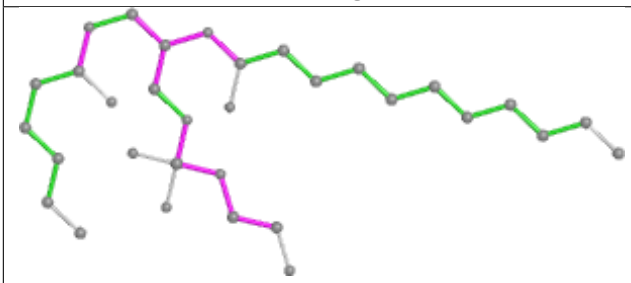
Ligand PTY F 1612



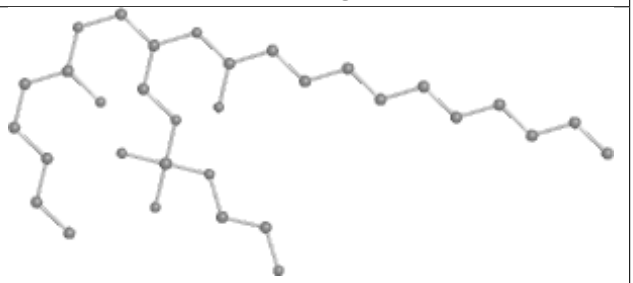
Bond lengths



Bond angles

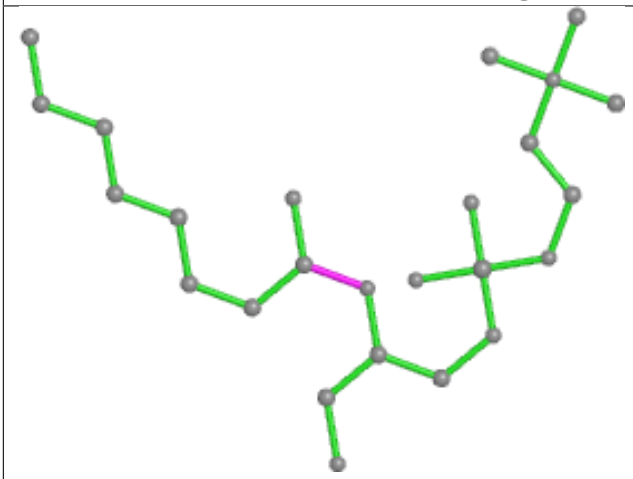


Torsions

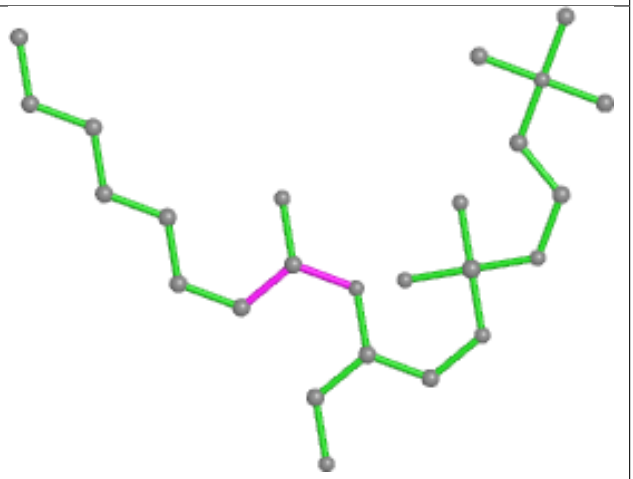


Rings

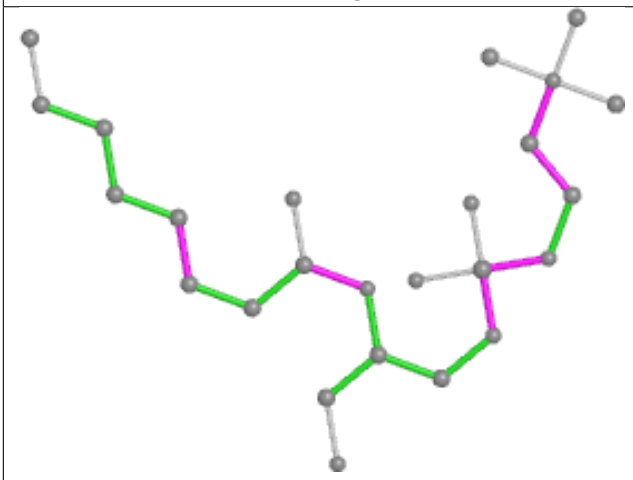
Ligand POV F 1609



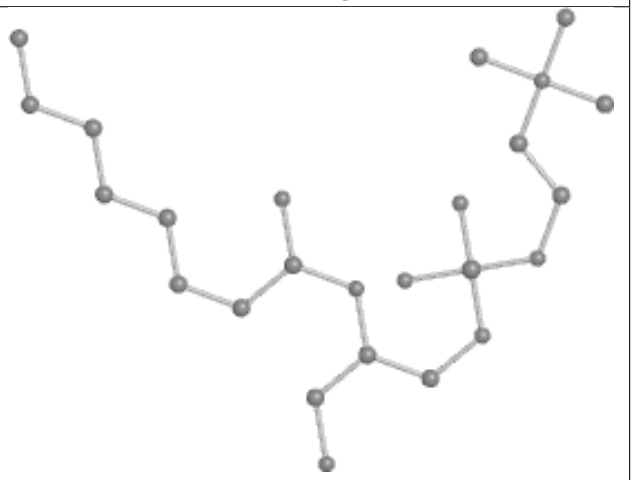
Bond lengths



Bond angles

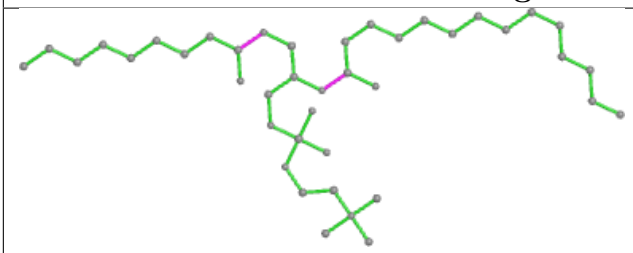


Torsions

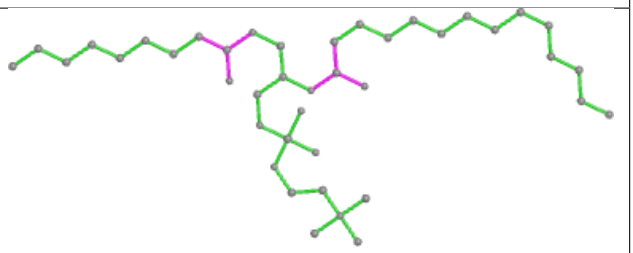


Rings

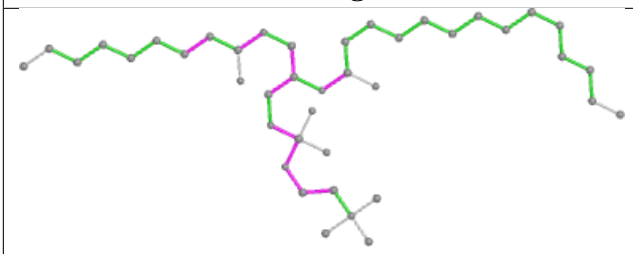
Ligand POV B 1607



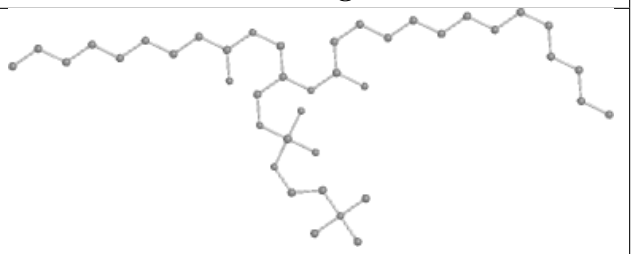
Bond lengths



Bond angles

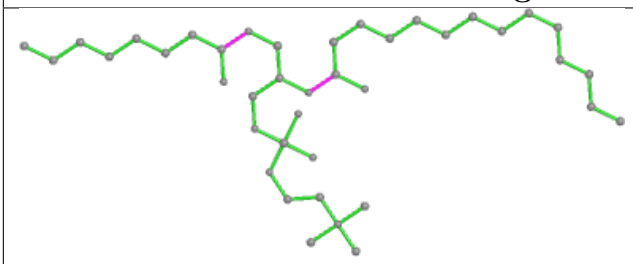


Torsions

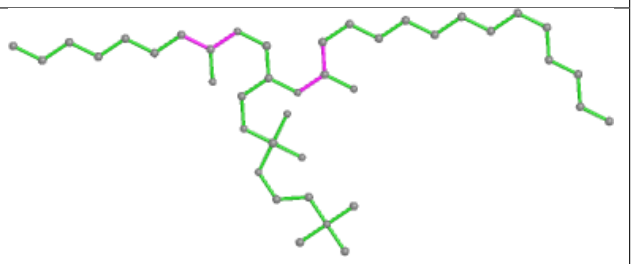


Rings

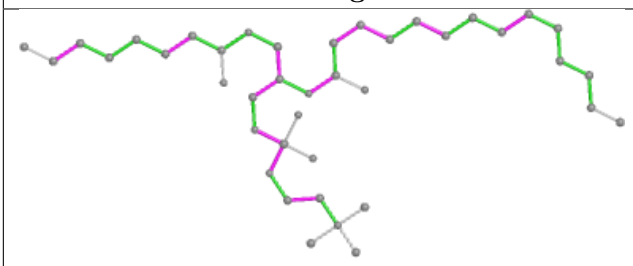
Ligand POV B 1606



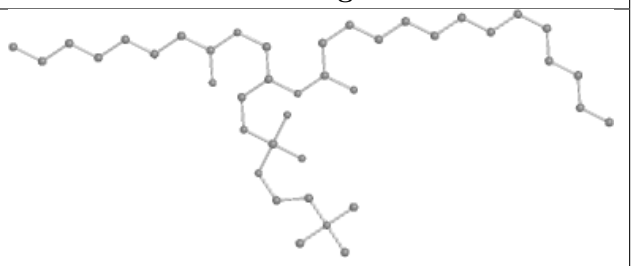
Bond lengths



Bond angles

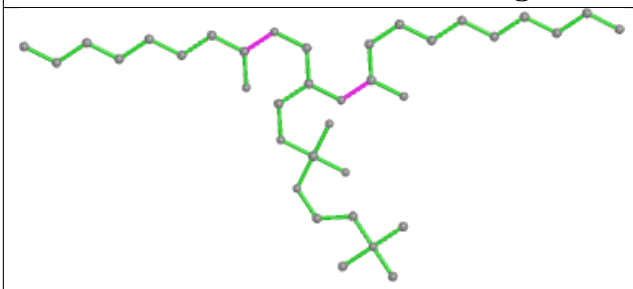


Torsions

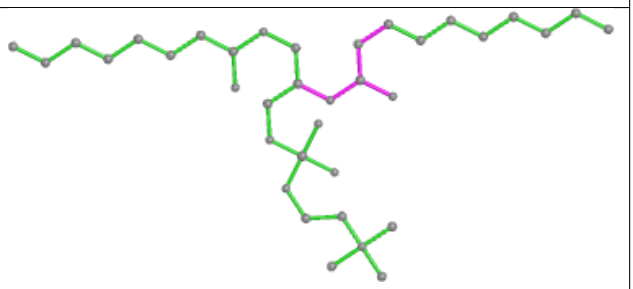


Rings

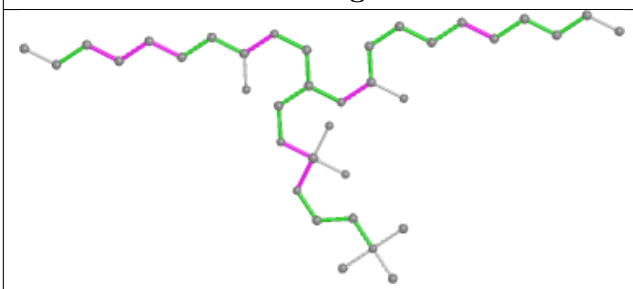
Ligand POV D 1608



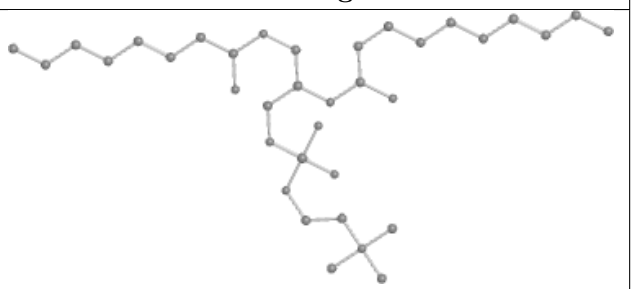
Bond lengths



Bond angles

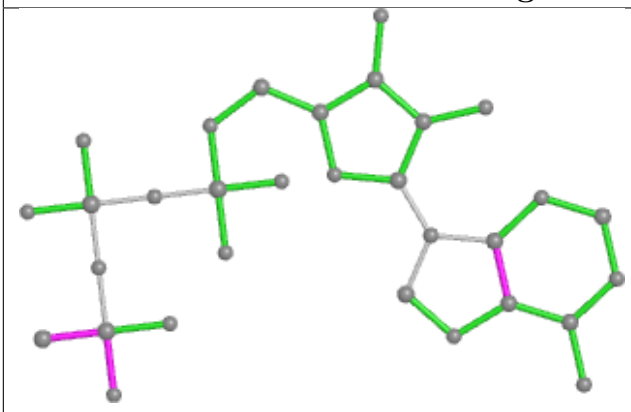


Torsions

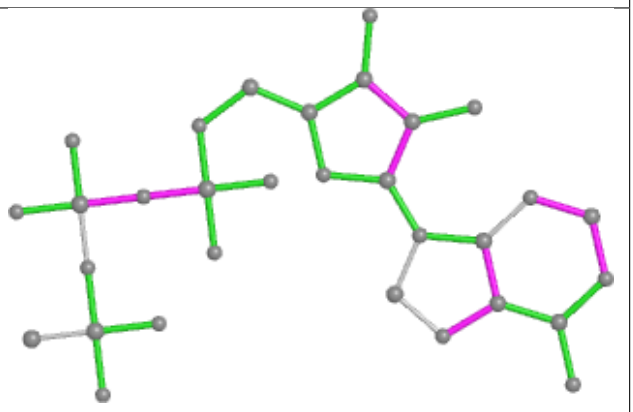


Rings

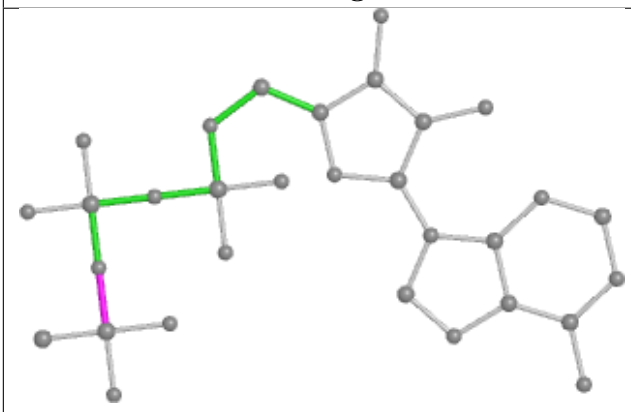
Ligand AGS F 1602



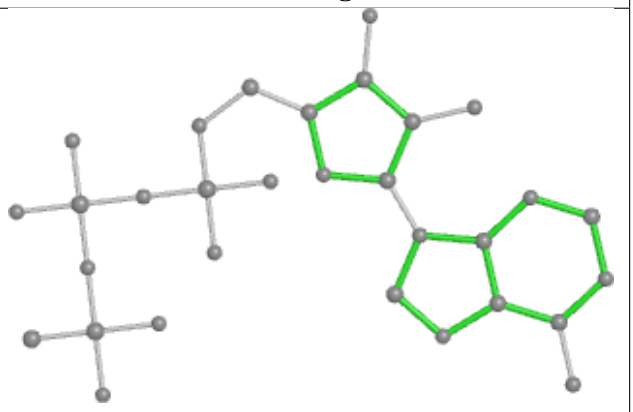
Bond lengths



Bond angles

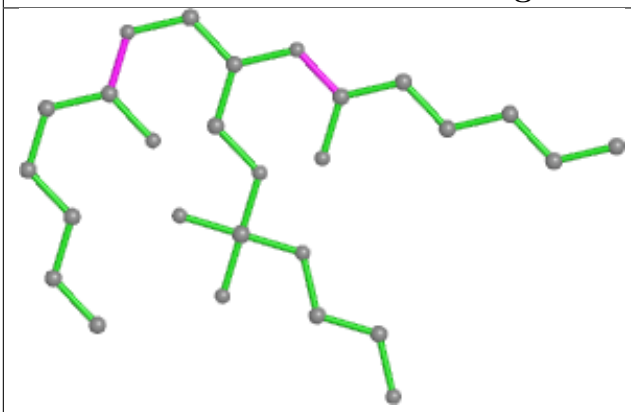


Torsions

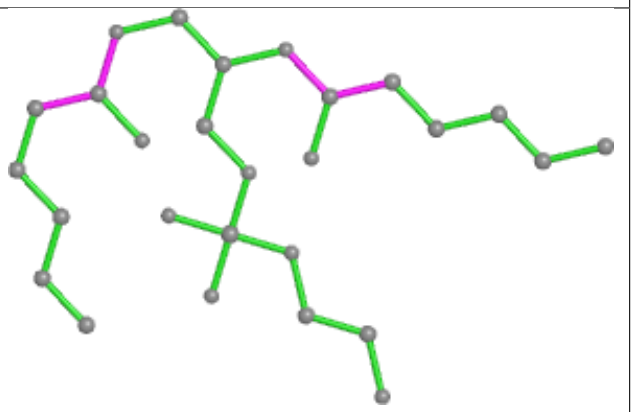


Rings

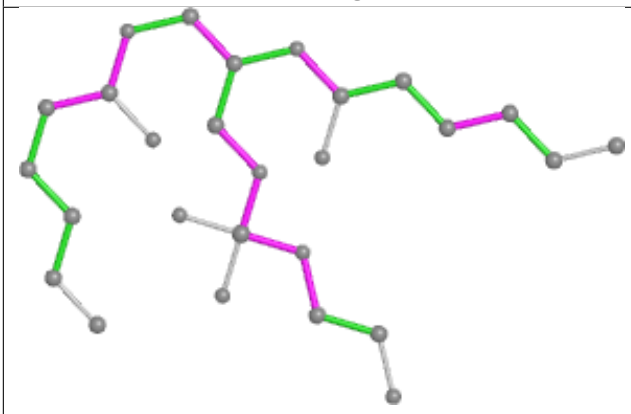
Ligand PTY B 1613



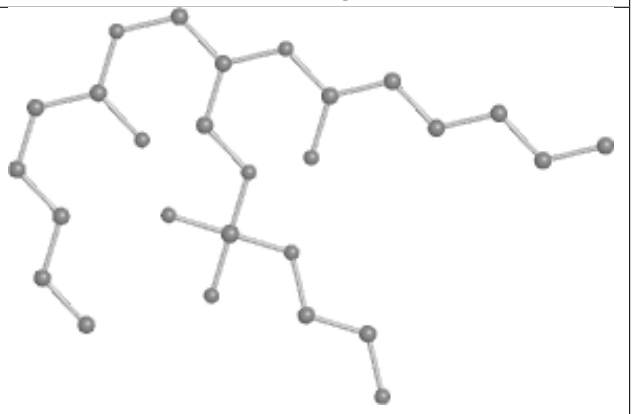
Bond lengths



Bond angles

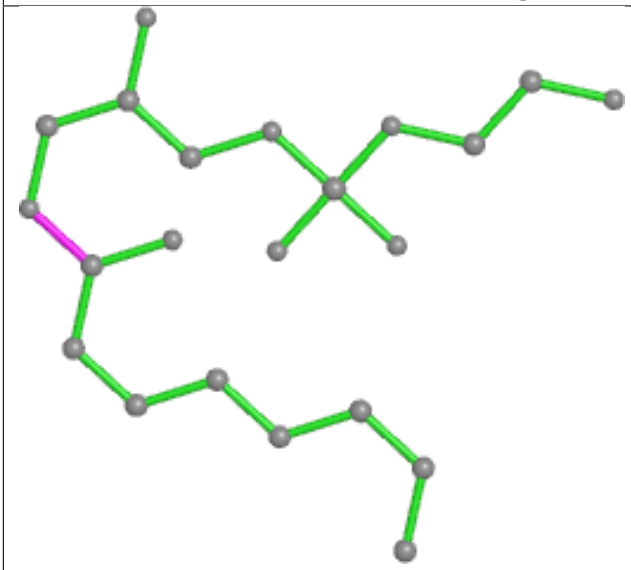


Torsions

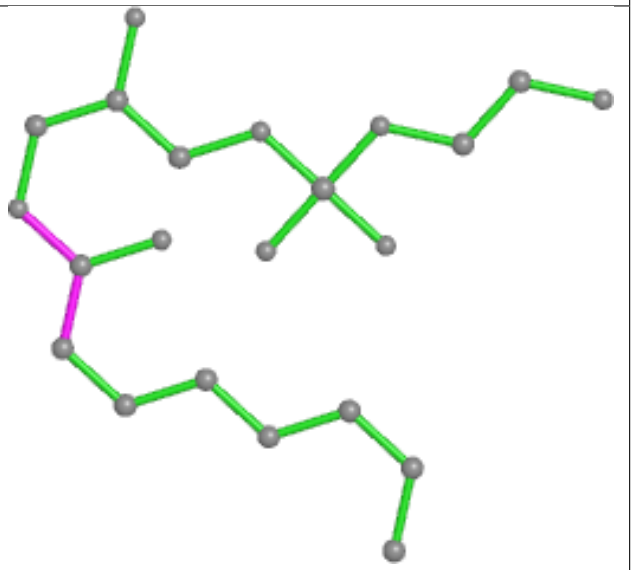


Rings

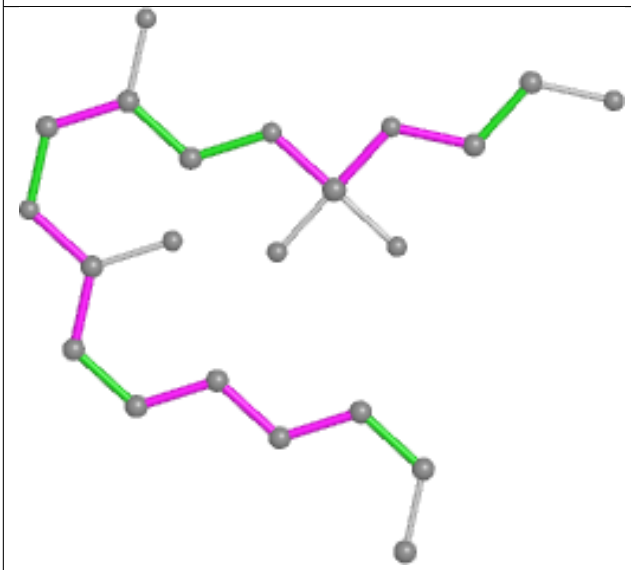
Ligand PTY B 1614



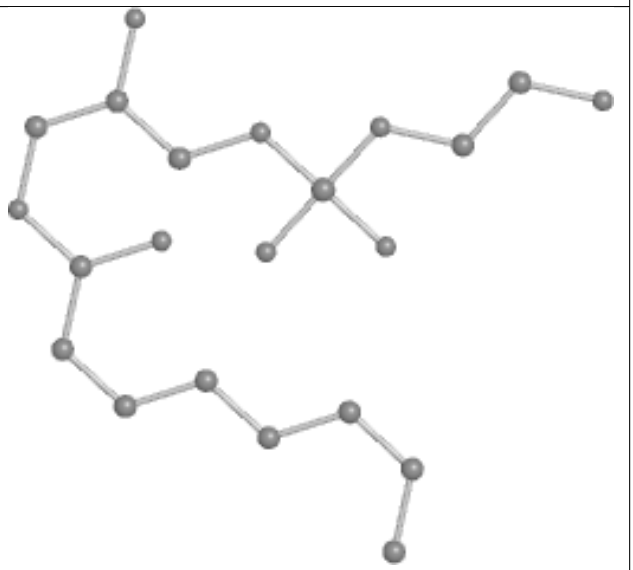
Bond lengths



Bond angles

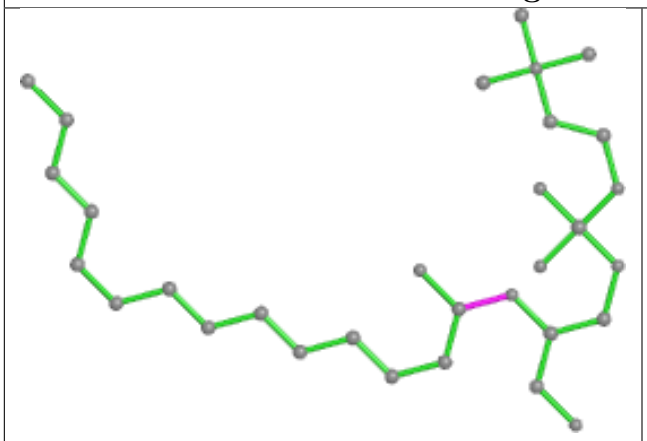


Torsions

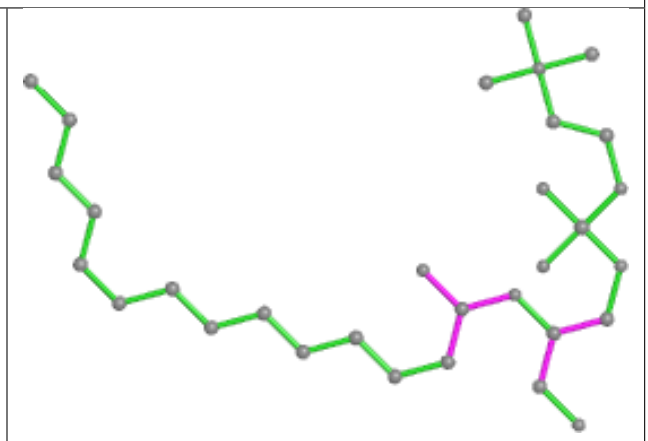


Rings

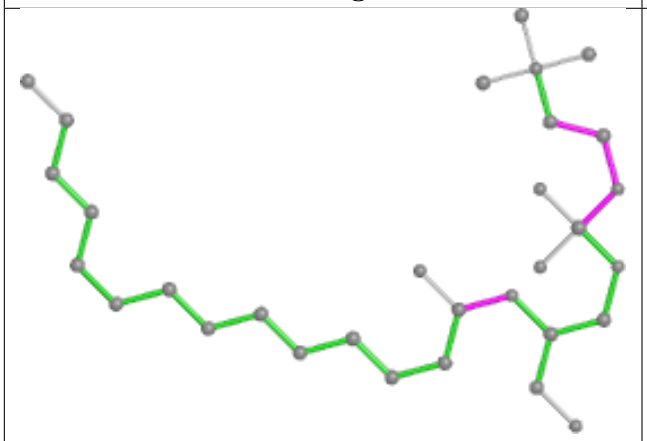
Ligand POV A 401



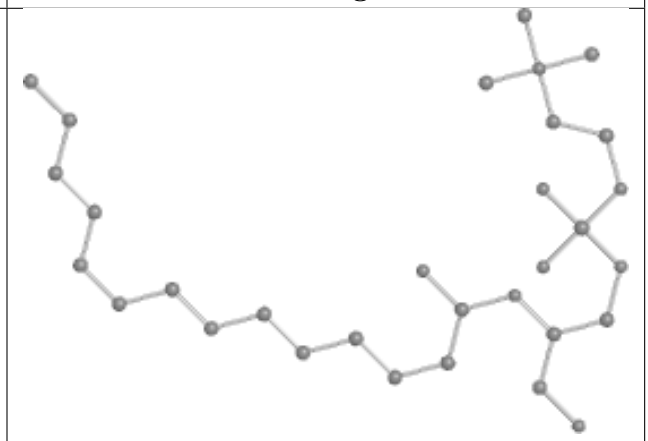
Bond lengths



Bond angles

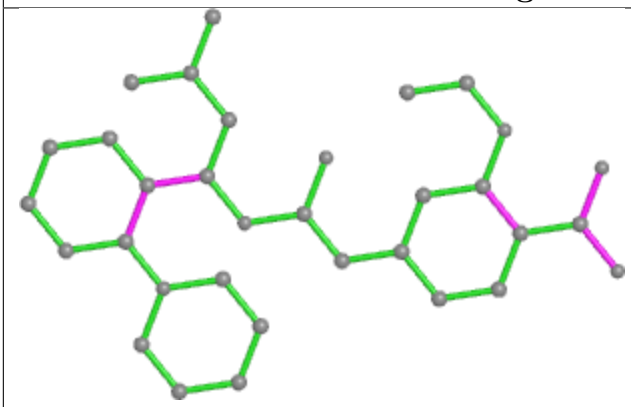


Torsions

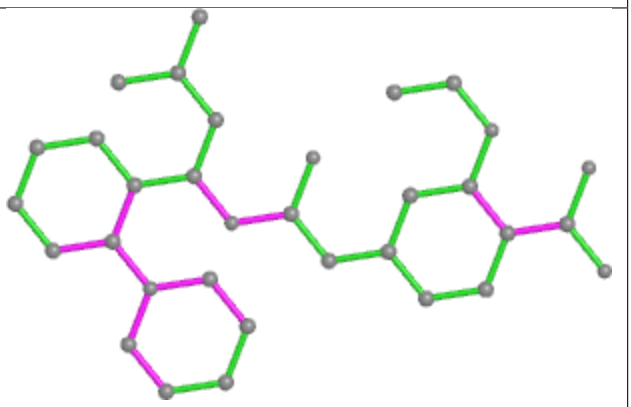


Rings

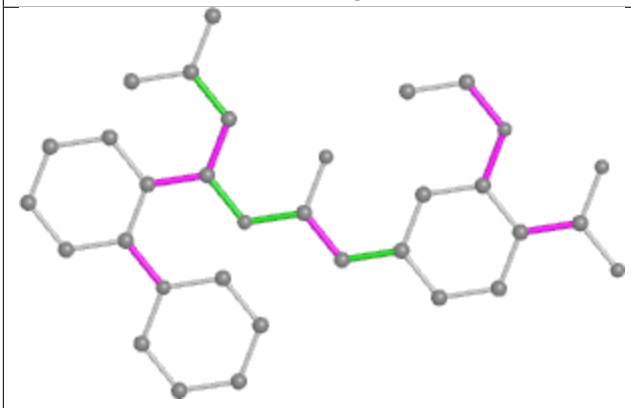
Ligand BJX D 1603



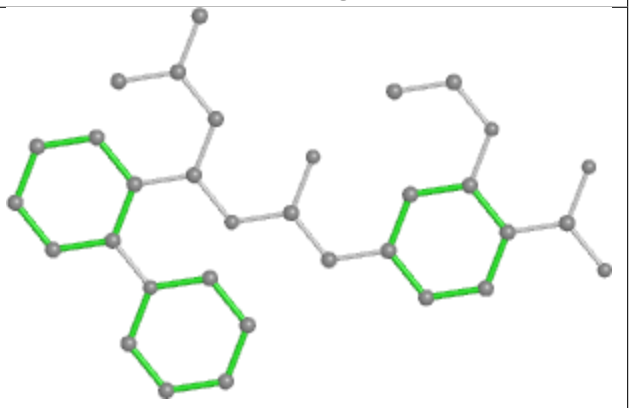
Bond lengths



Bond angles

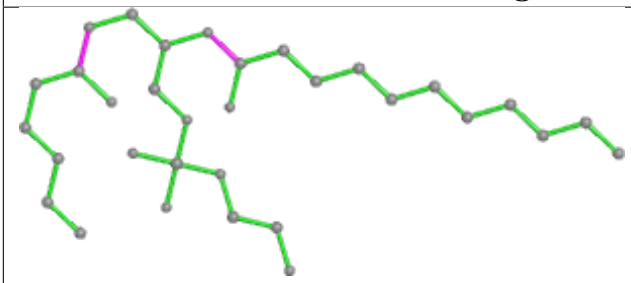


Torsions

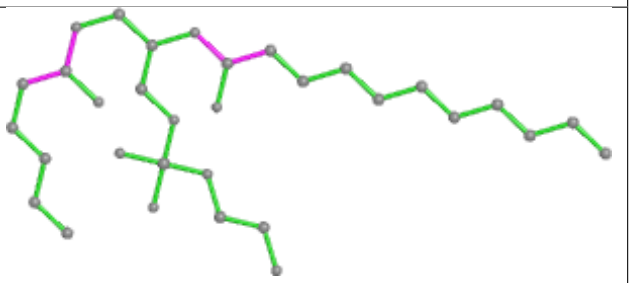


Rings

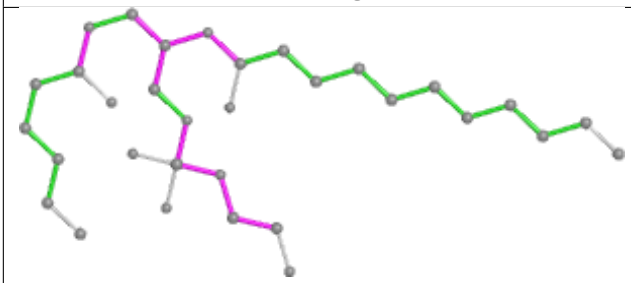
Ligand PTY H 1612



Bond lengths



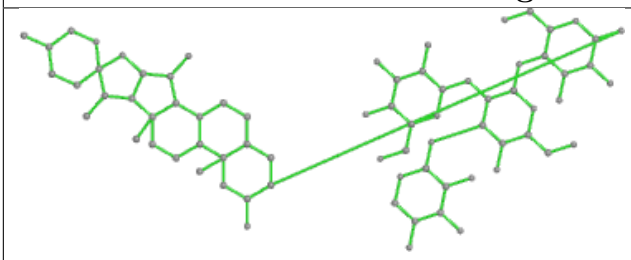
Bond angles



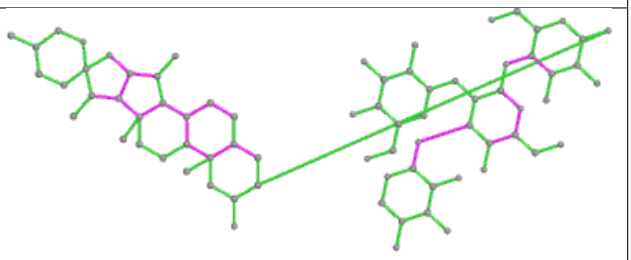
Torsions

Rings

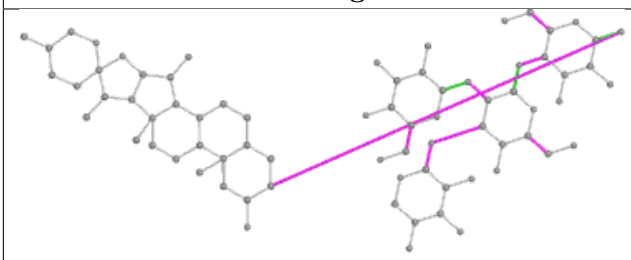
Ligand AJP H 1601



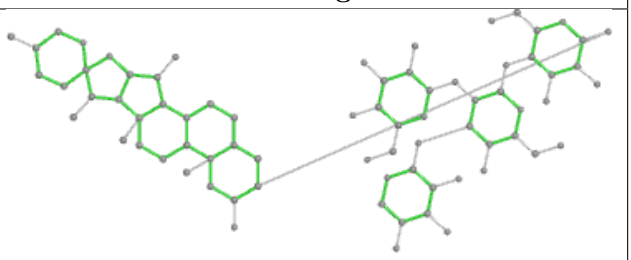
Bond lengths



Bond angles

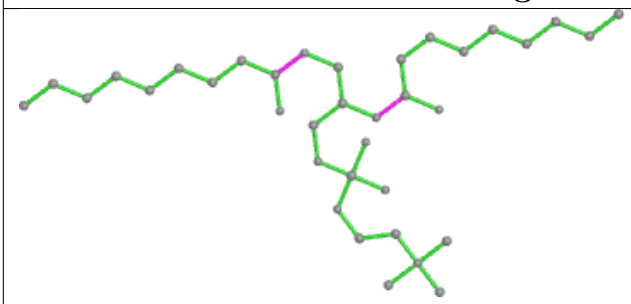


Torsions

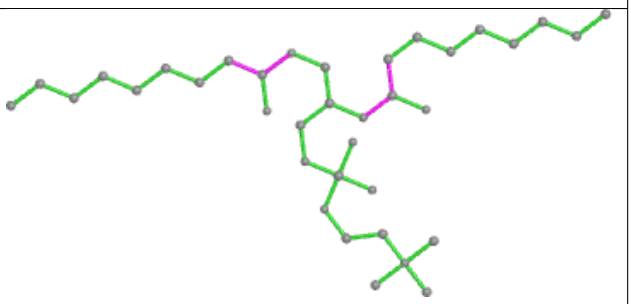


Rings

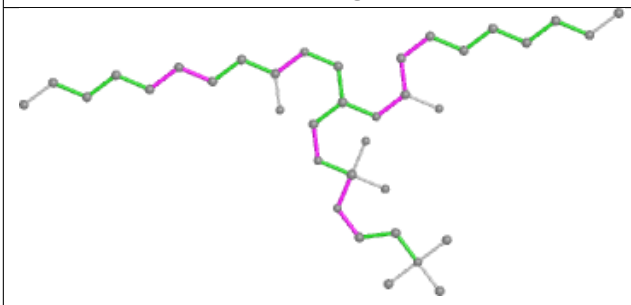
Ligand POV B 1604



Bond lengths



Bond angles



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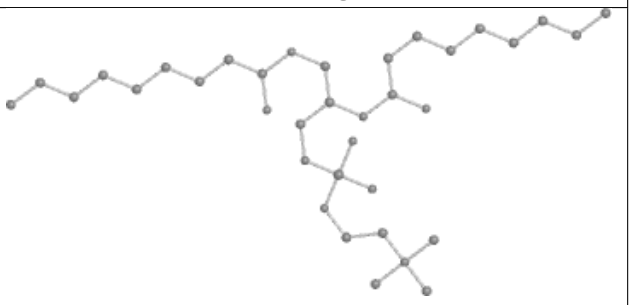
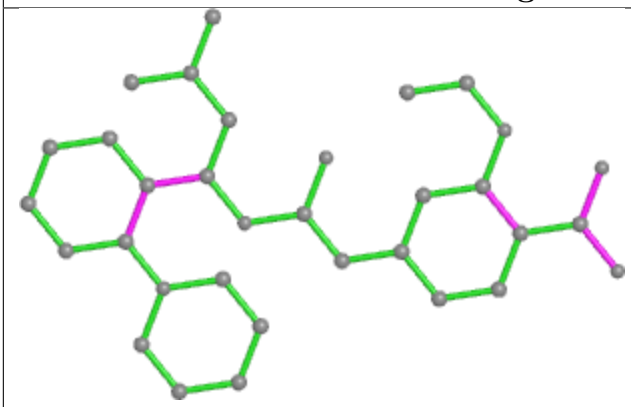
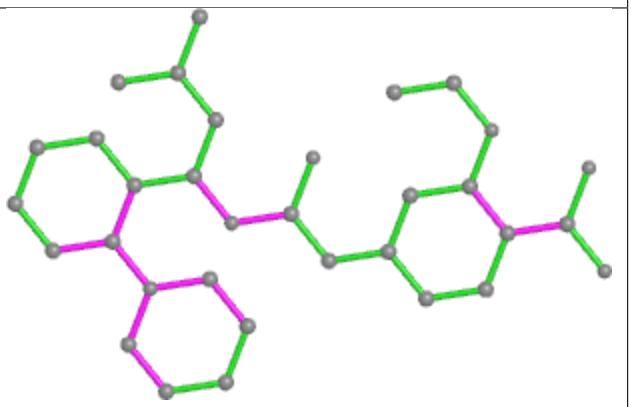


Rings

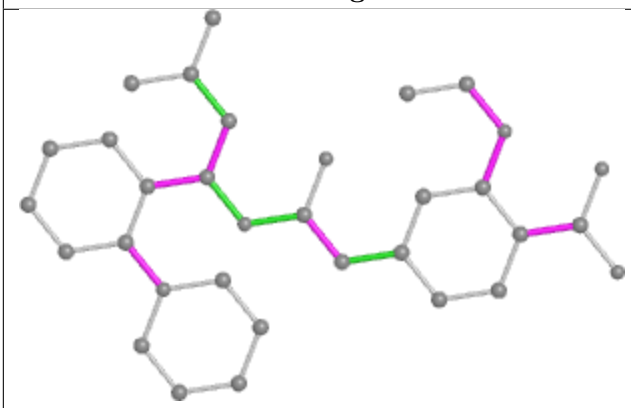
Ligand BJX B 1603



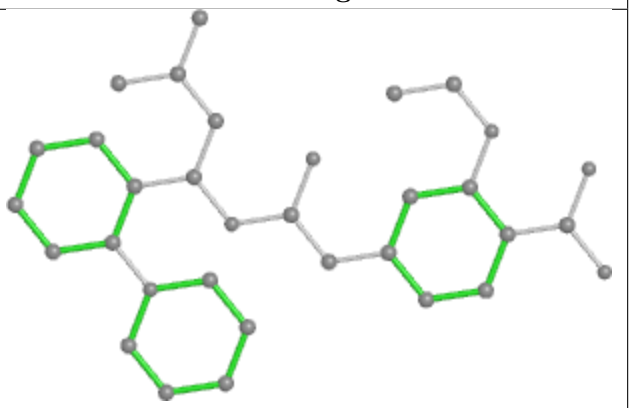
Bond lengths



Bond angles

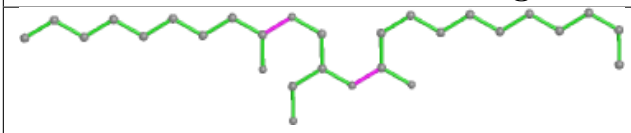


Torsions



Rings

Ligand POV H 1611



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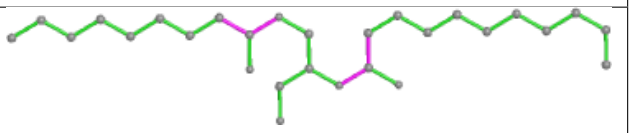
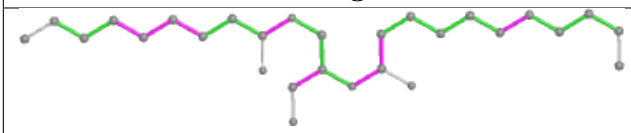
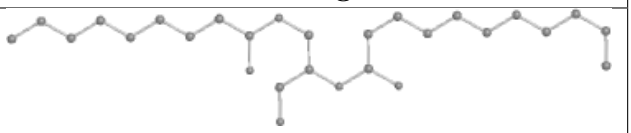


Bond angles

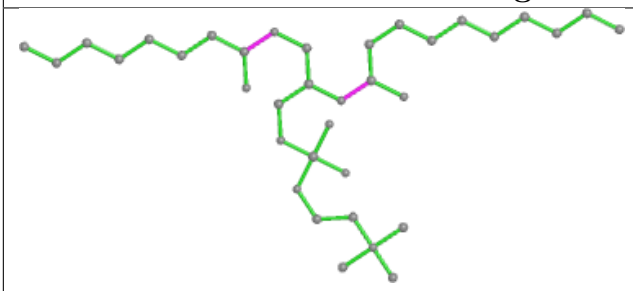


Torsions



Rings

Ligand POV B 1608



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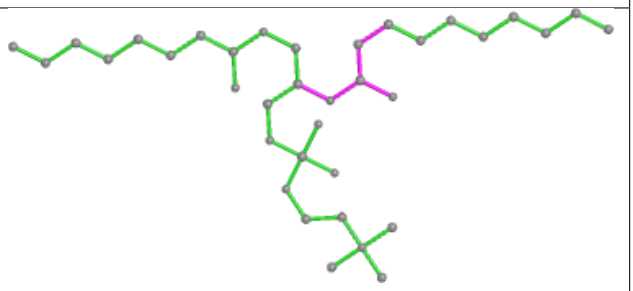
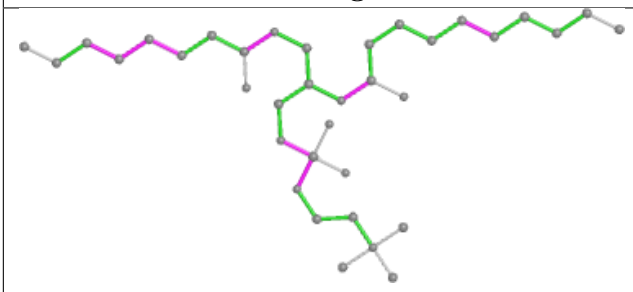
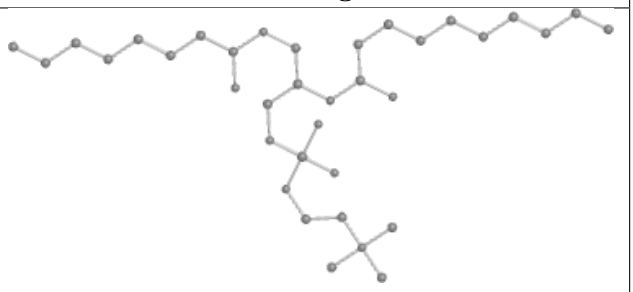


Bond angles

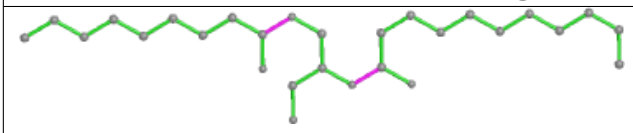


Torsions

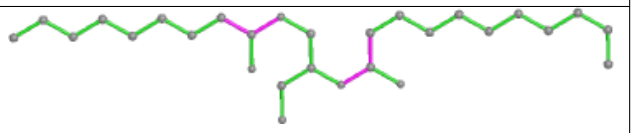


Rings

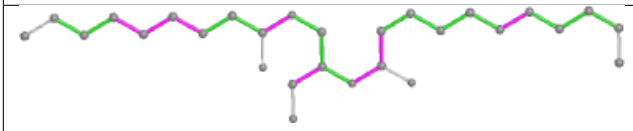
Ligand POV B 1611



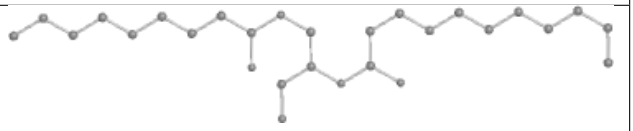
Bond lengths



Bond angles

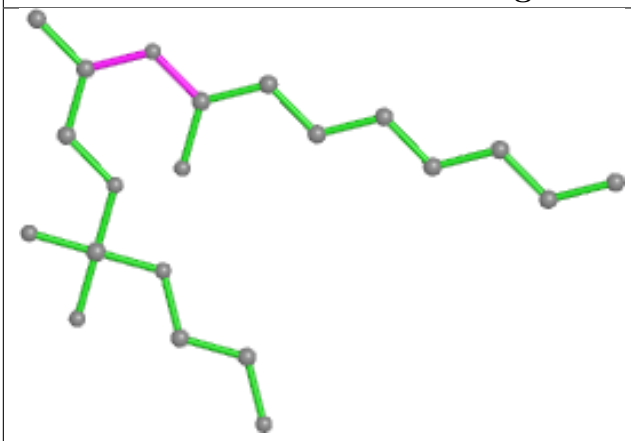


Torsions

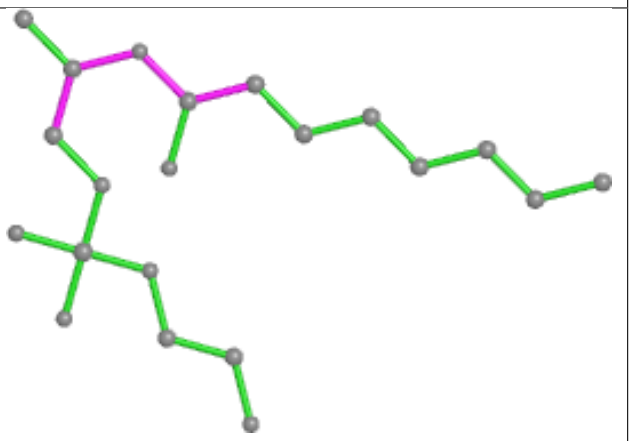


Rings

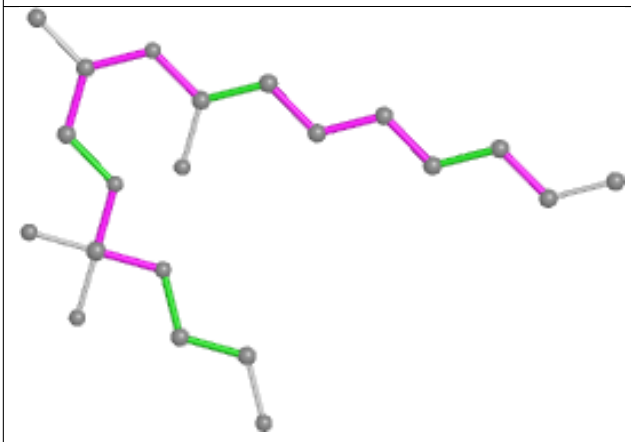
Ligand PTY B 1615



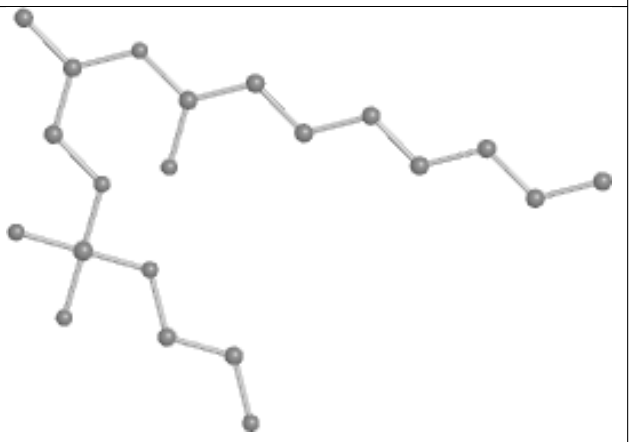
Bond lengths



Bond angles

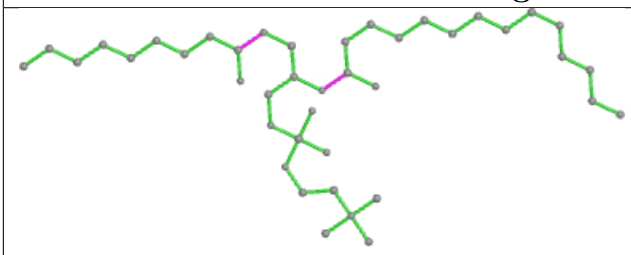


Torsions

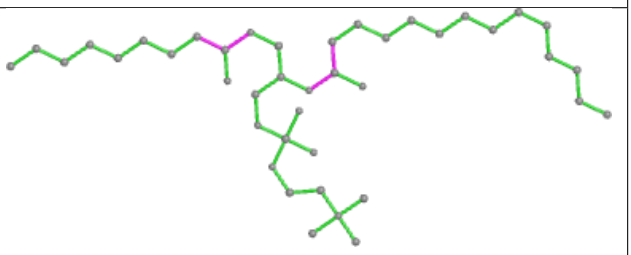


Rings

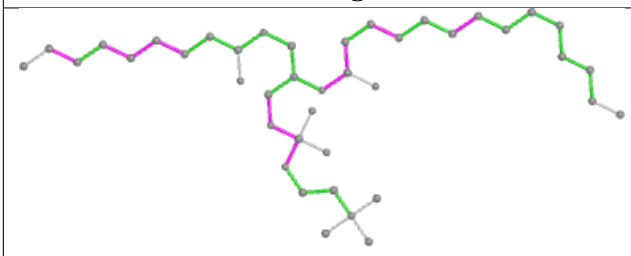
Ligand POV H 1605



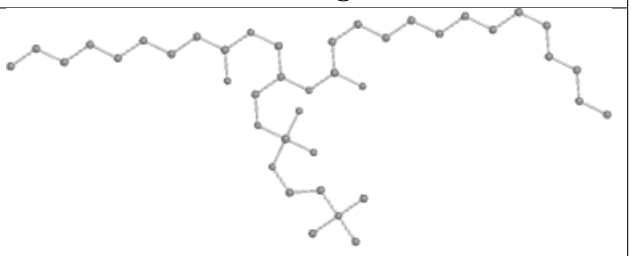
Bond lengths



Bond angles

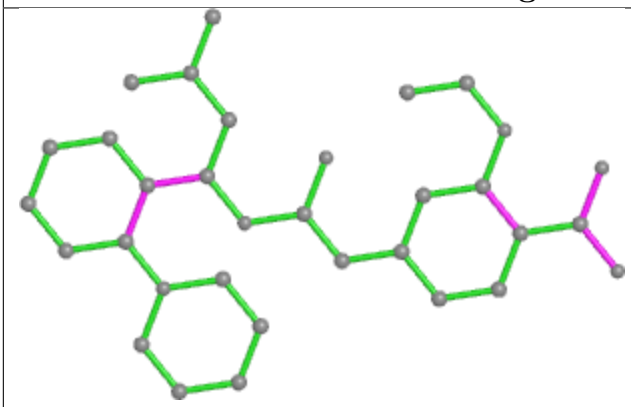


Torsions

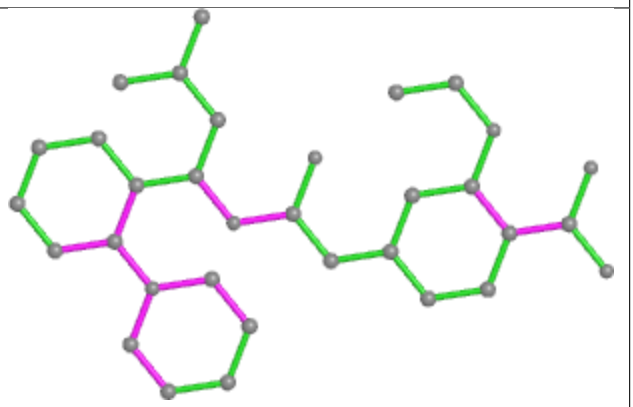


Rings

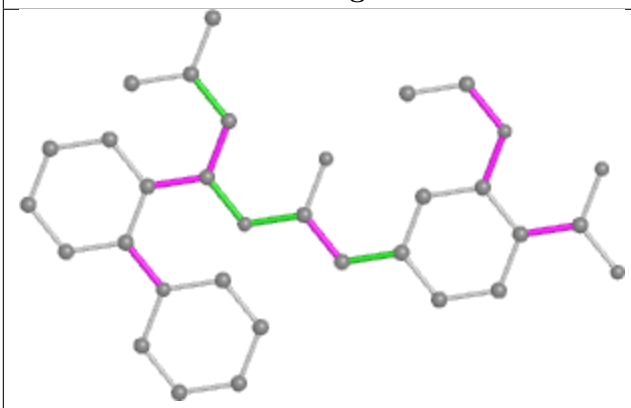
Ligand BJX F 1603



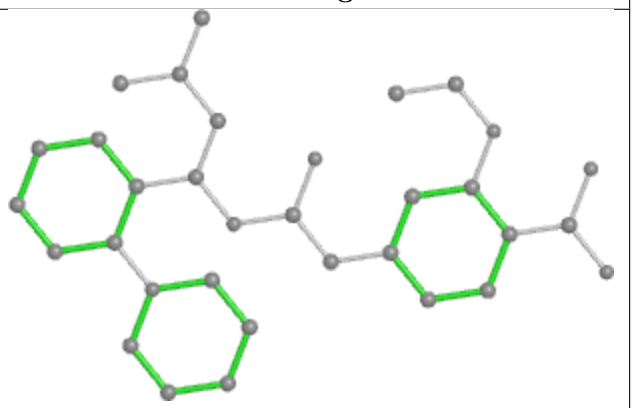
Bond lengths



Bond angles

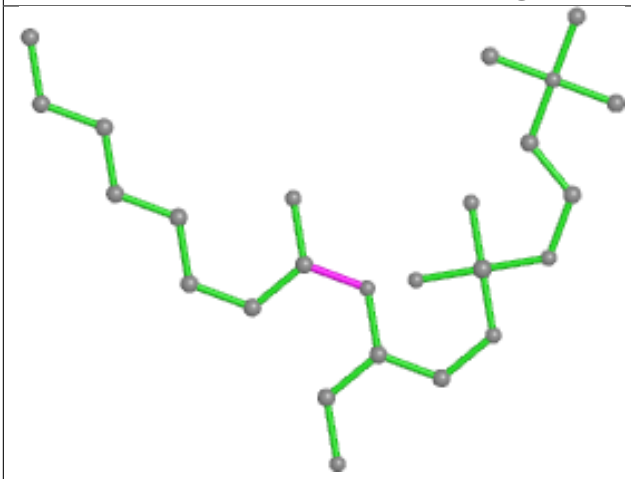


Torsions

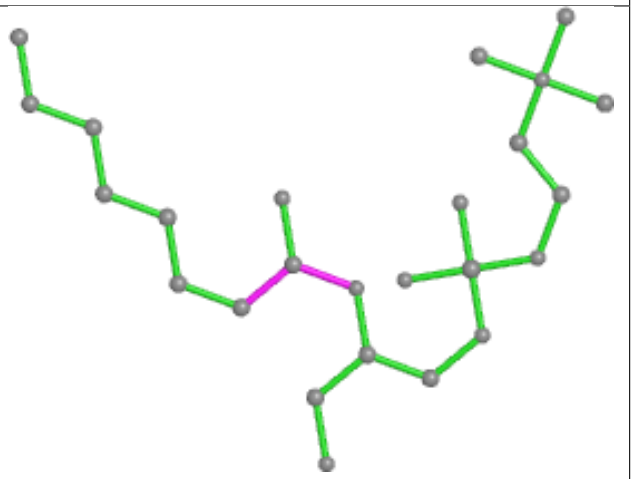


Rings

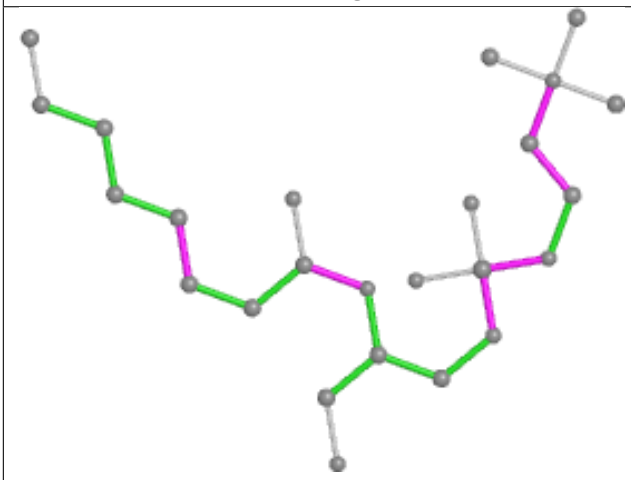
Ligand POV D 1609



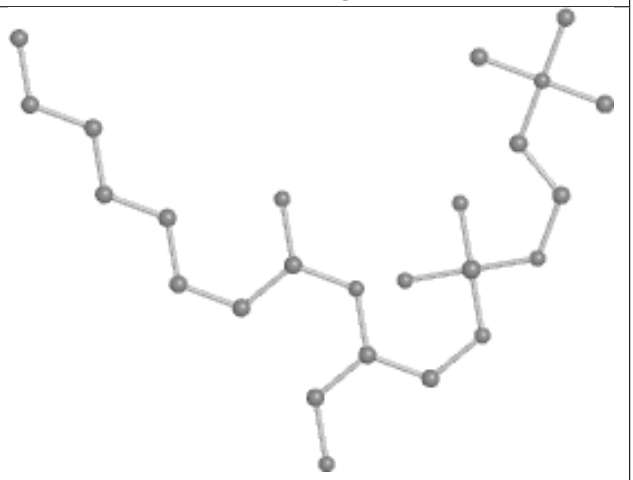
Bond lengths



Bond angles

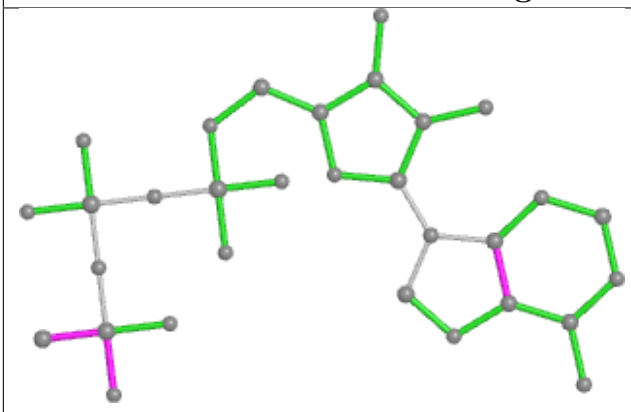


Torsions

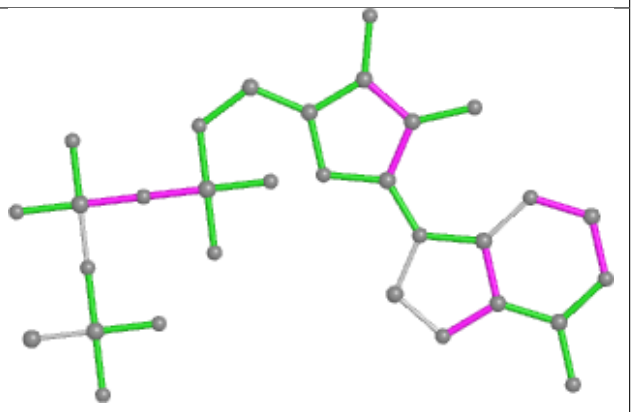


Rings

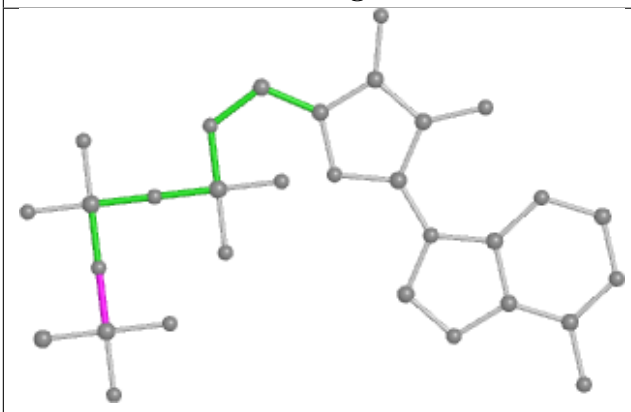
Ligand AGS D 1602



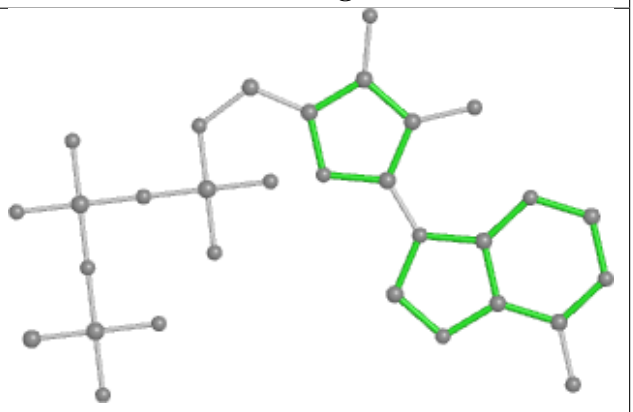
Bond lengths



Bond angles

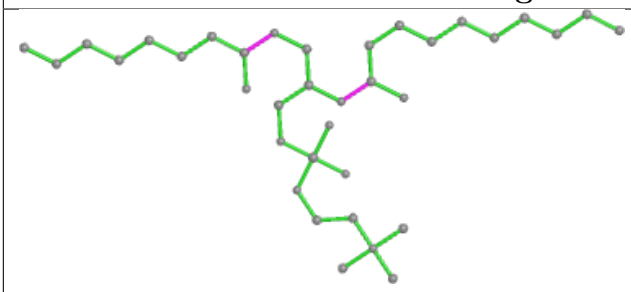


Torsions

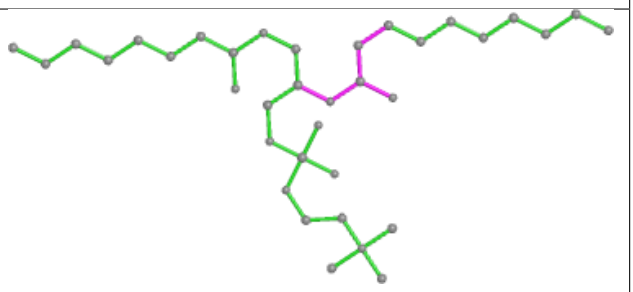


Rings

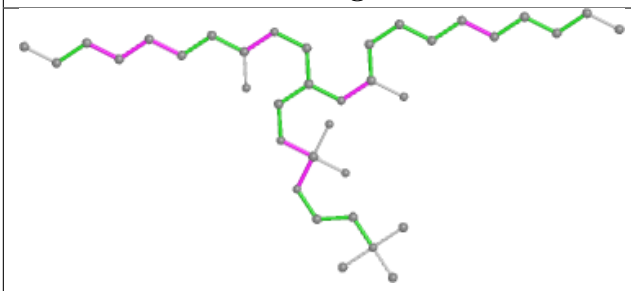
Ligand POV F 1608



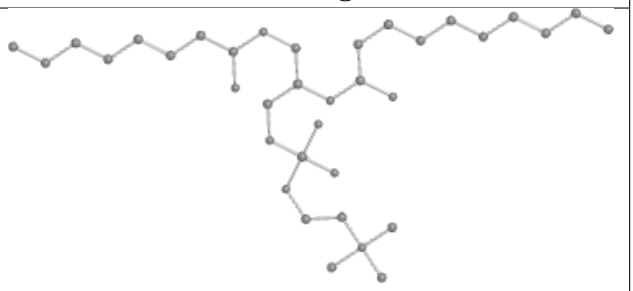
Bond lengths



Bond angles

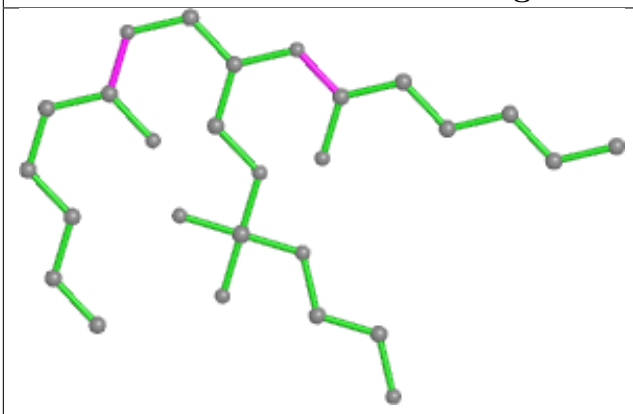


Torsions

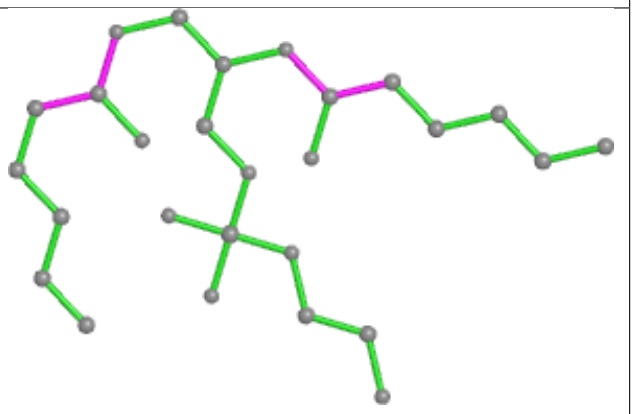


Rings

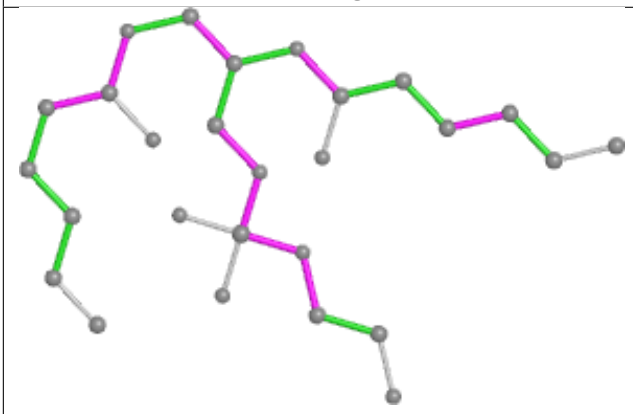
Ligand PTY D 1613



Bond lengths



Bond angles



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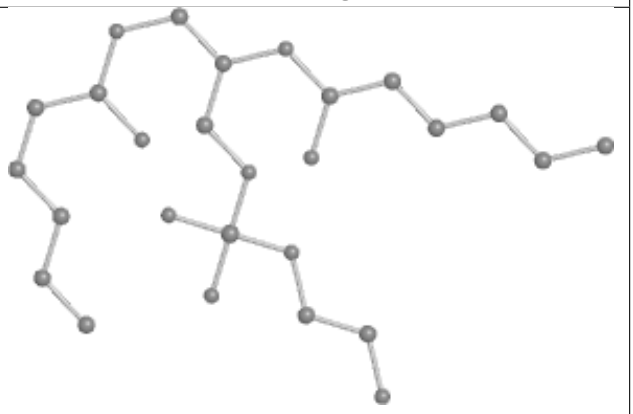
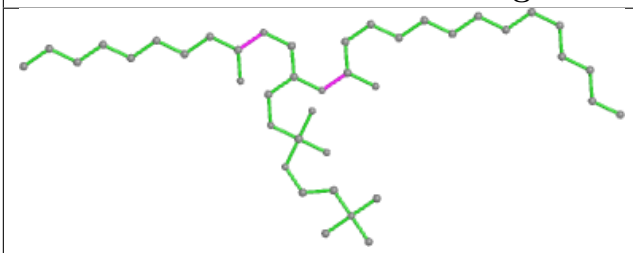
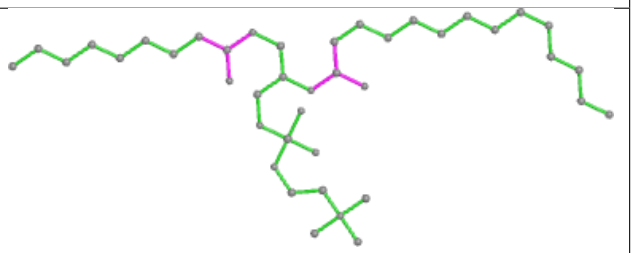


Rings

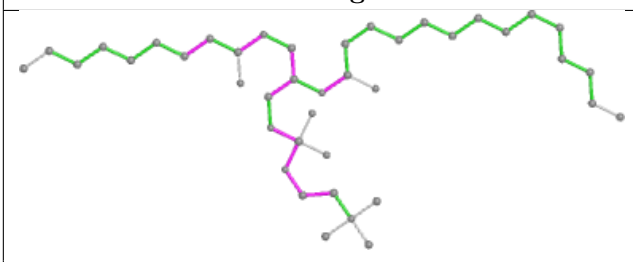
Ligand POV D 1607



Bond lengths



Bond angles



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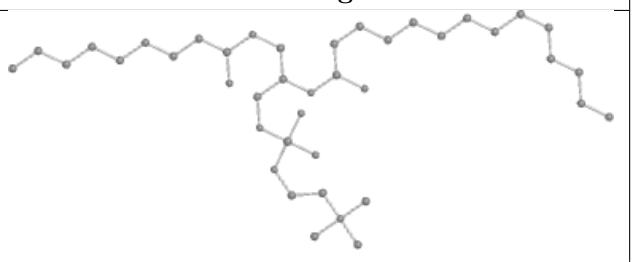
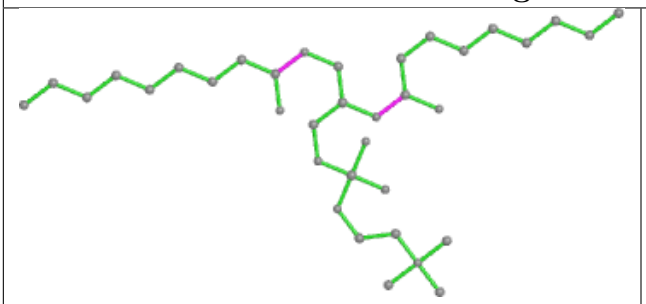


Rings

Ligand POV D 1604



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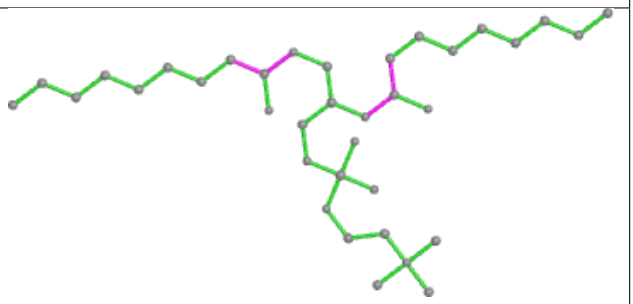
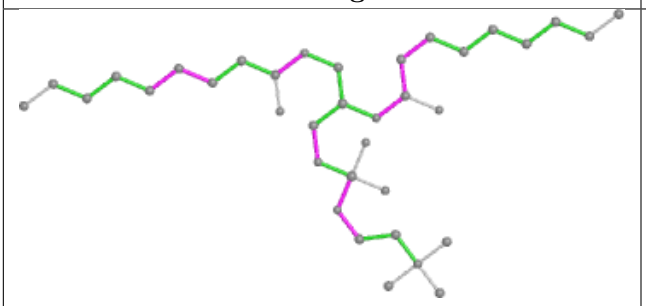


Bond angles



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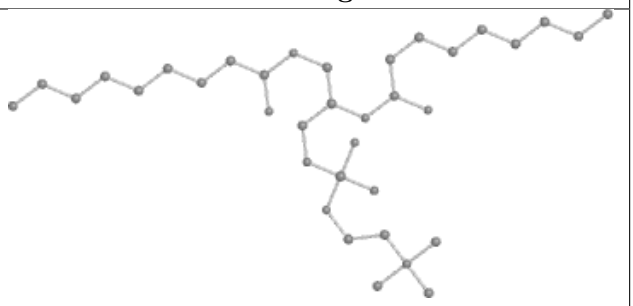
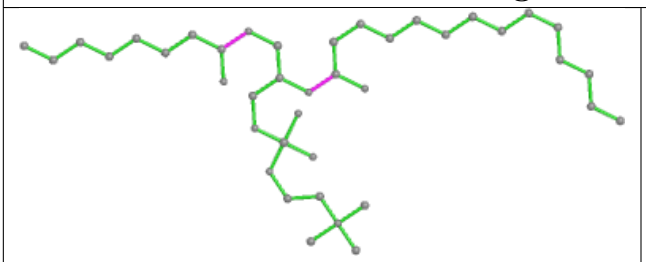


Rings

Ligand POV D 1606



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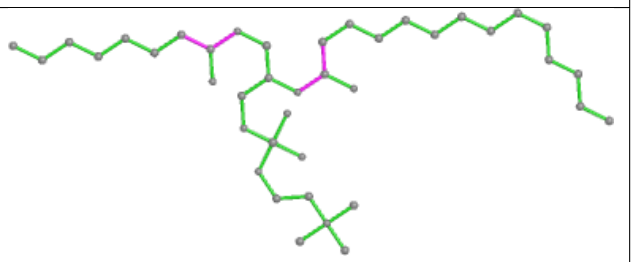
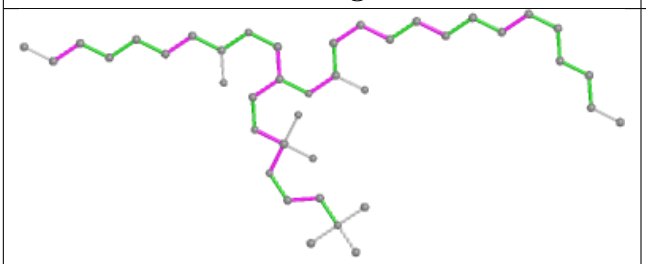


Bond angles



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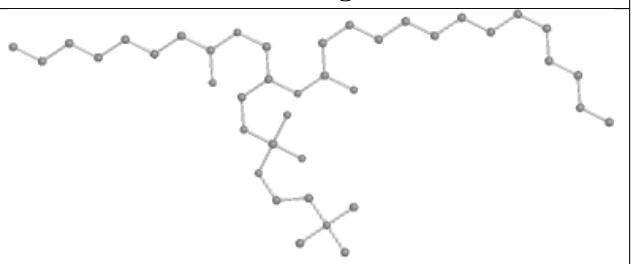
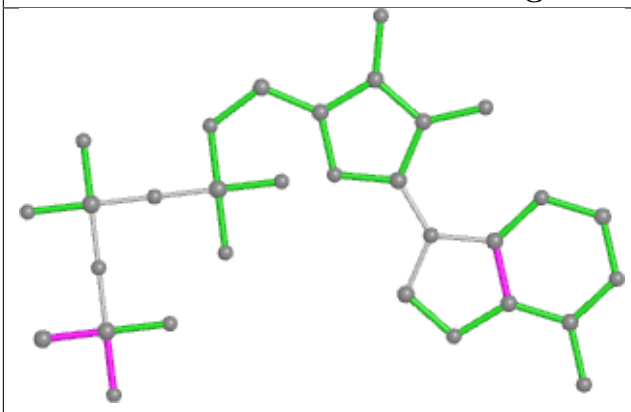


Rings

Ligand AGS E 401



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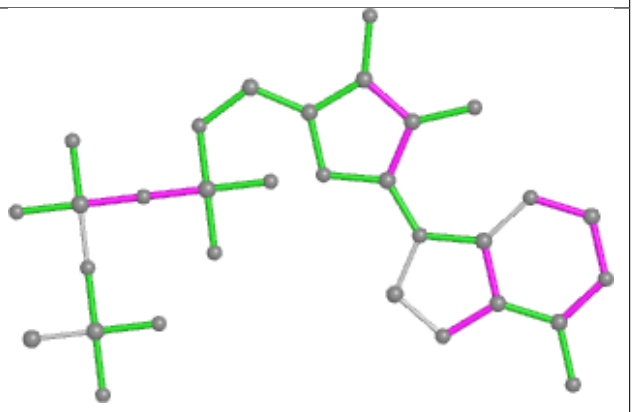
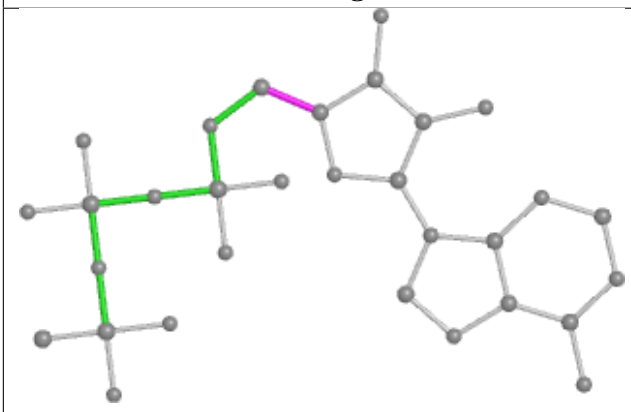


Bond angles



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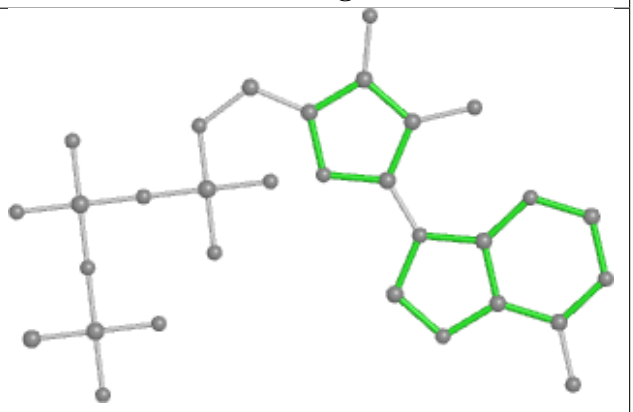
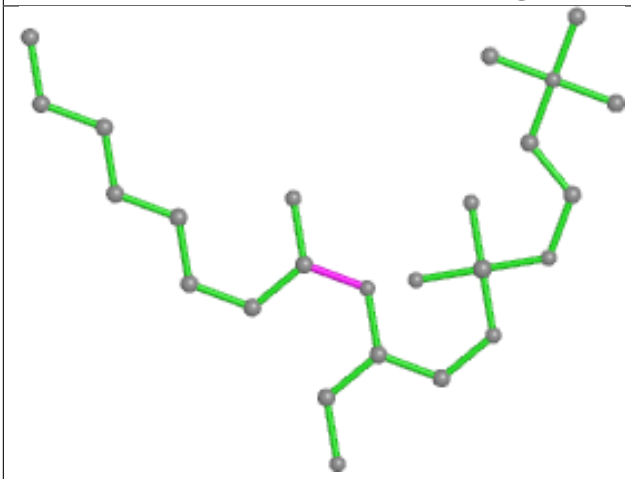


Rings

Ligand POV D 1610



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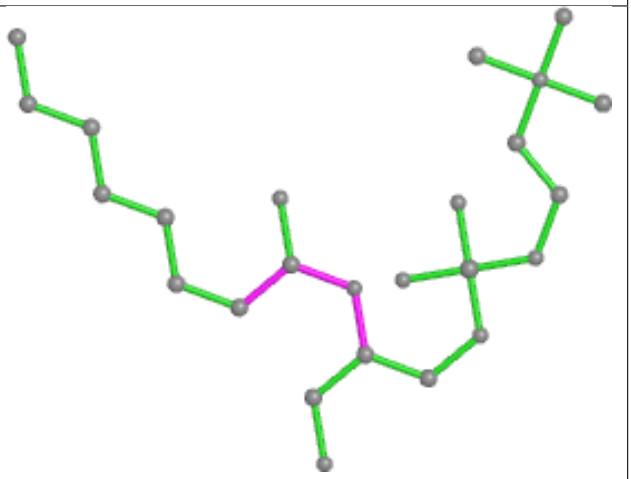
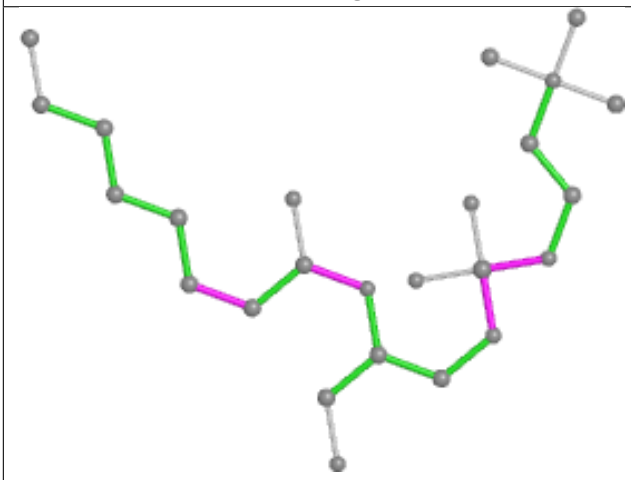


Bond angles



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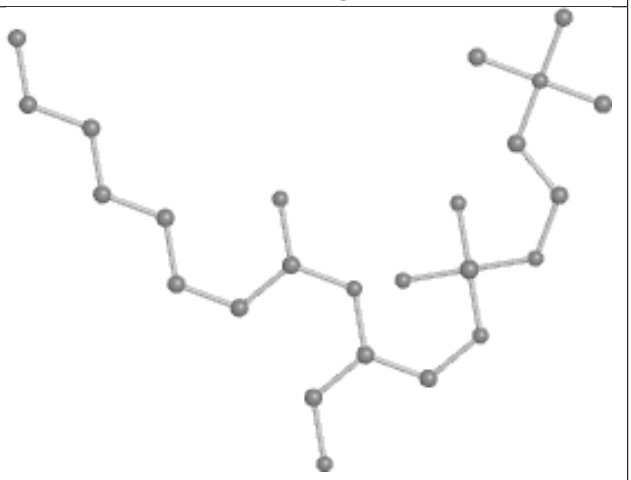
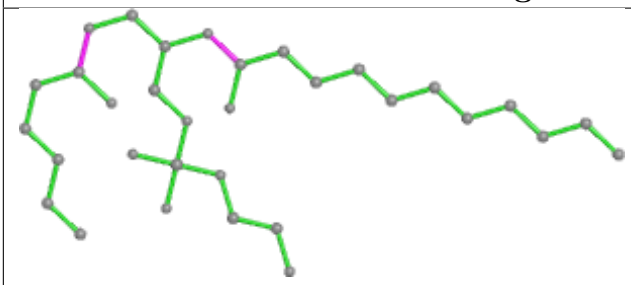


Rings

Ligand PTY B 1612



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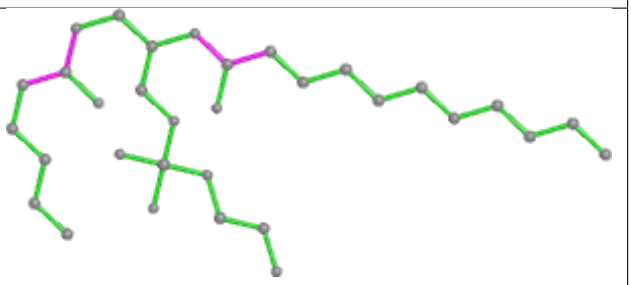
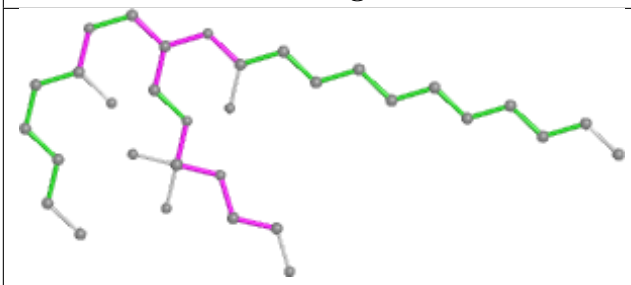


Bond angles



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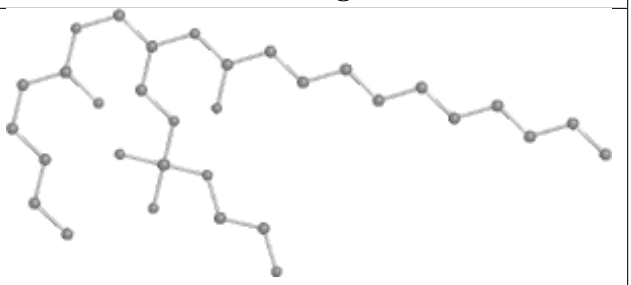
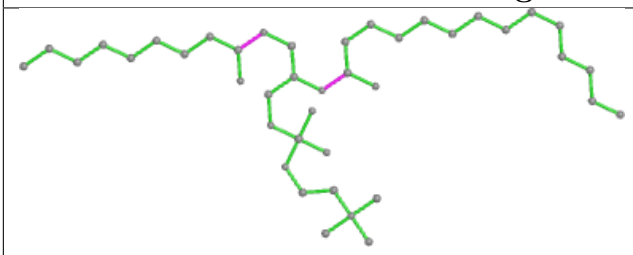


Rings

Ligand POV F 1607



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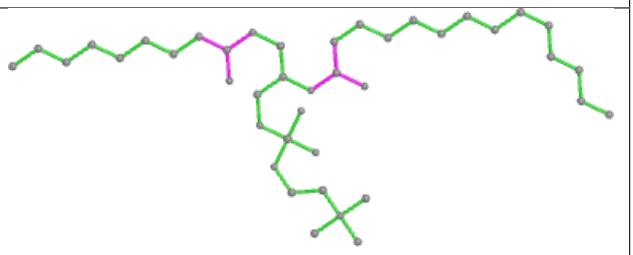
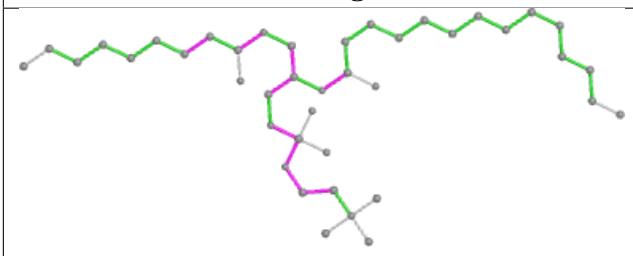
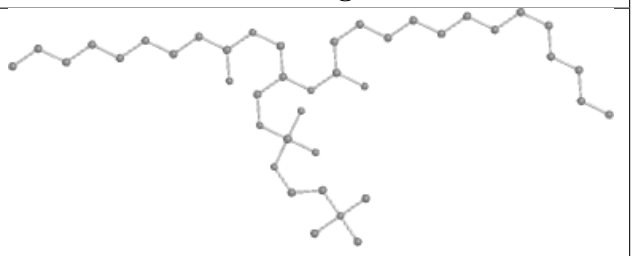


Bond angles

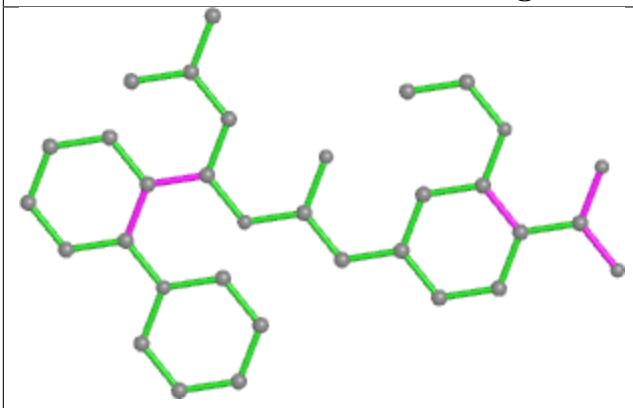


Torsions



Rings

Ligand BJX H 1603



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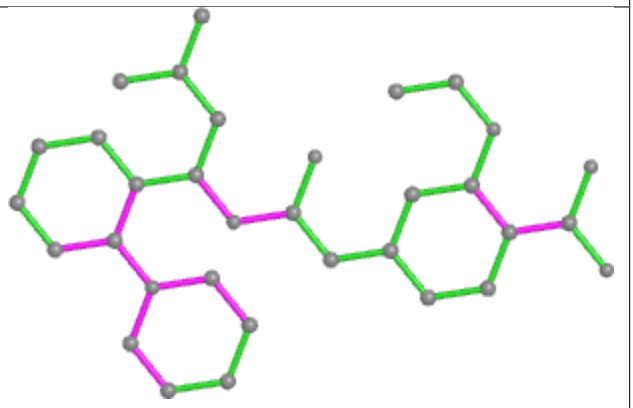
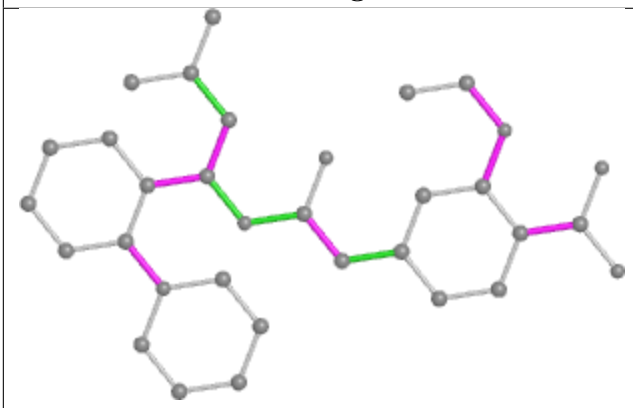
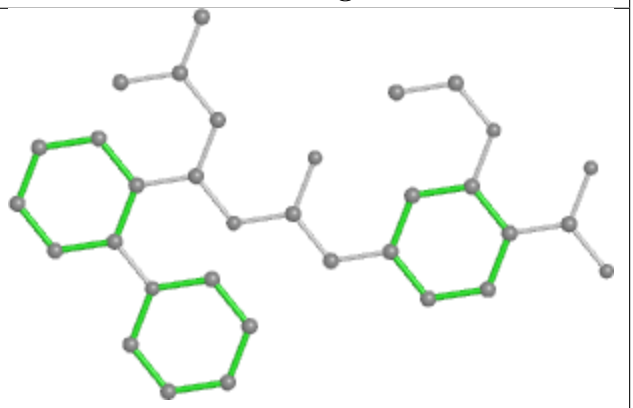


Bond angles

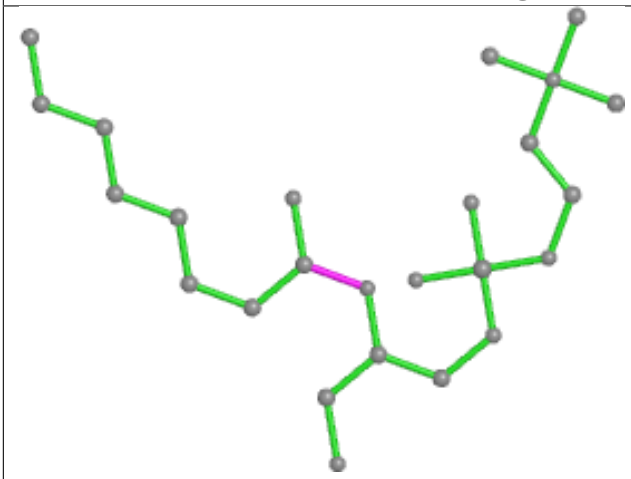


Torsions



Rings

Ligand POV B 1610



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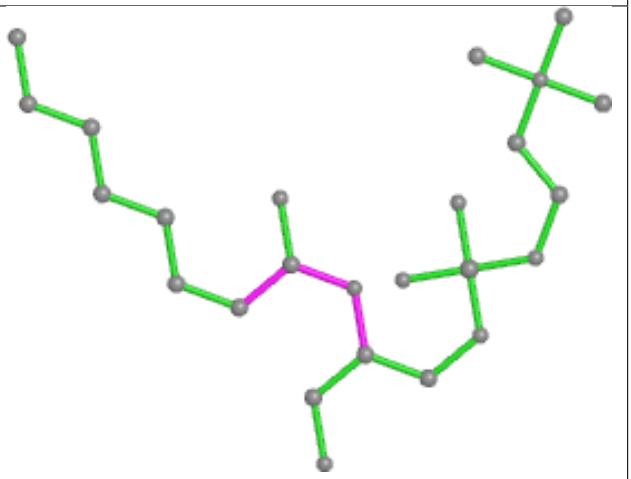
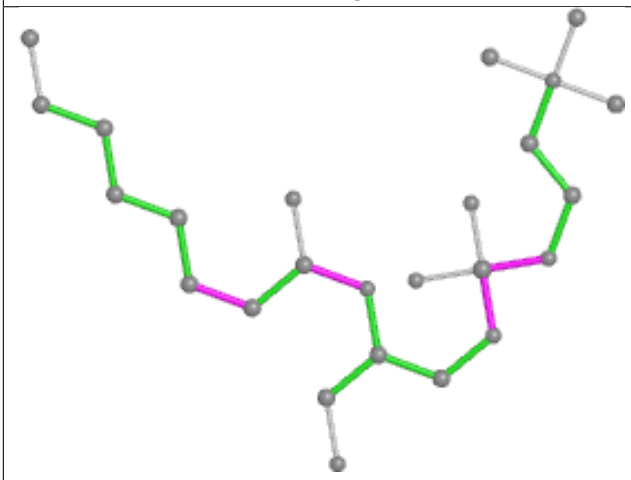


Bond angles



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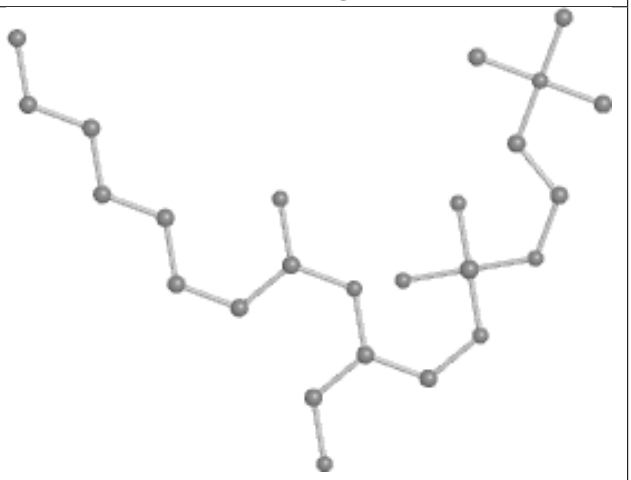
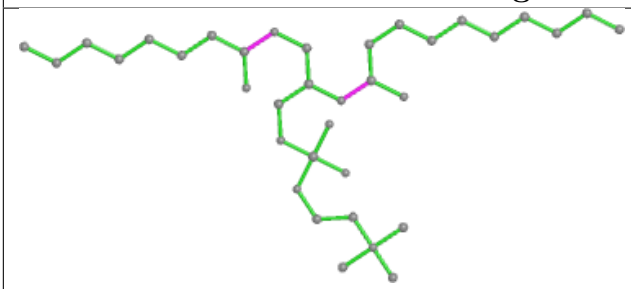


Rings

Ligand POV H 1608



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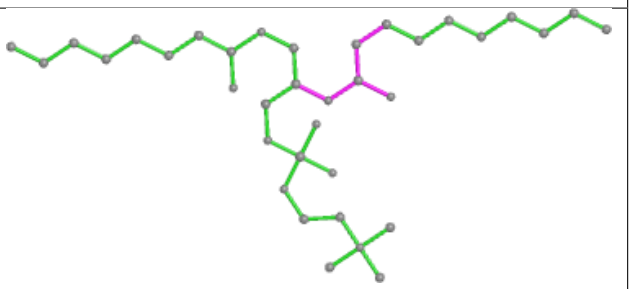
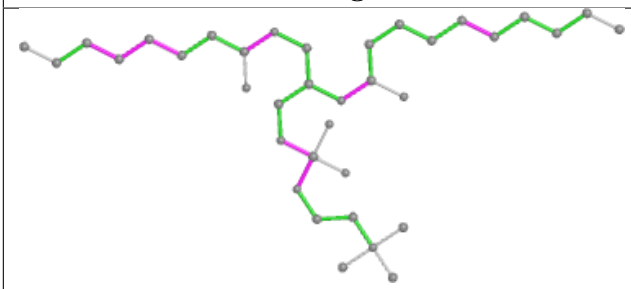
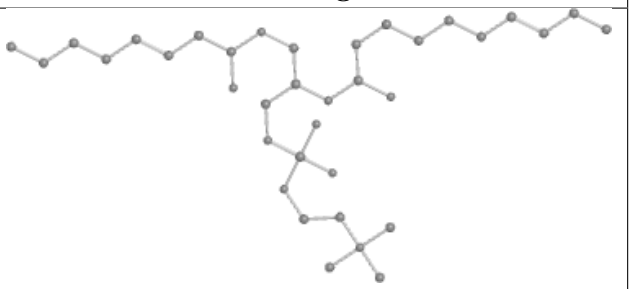


Bond angles

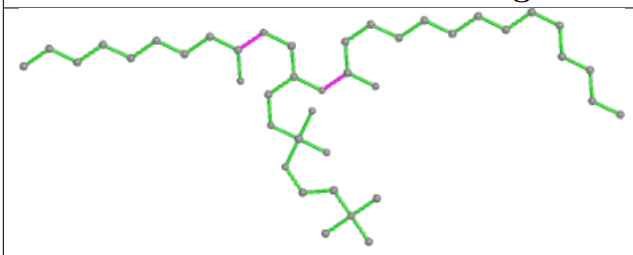


Torsions

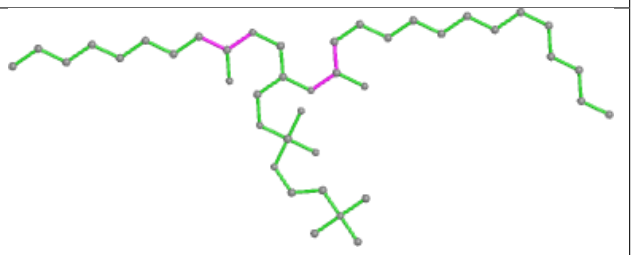


Rings

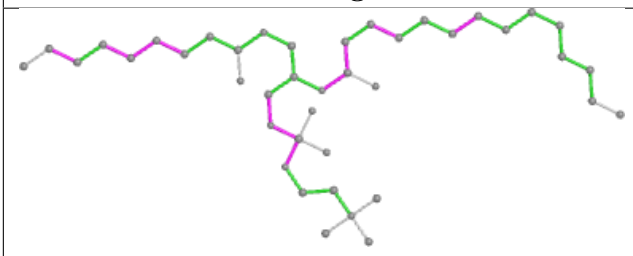
Ligand POV D 1605



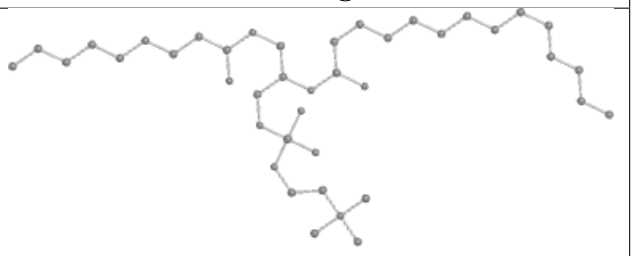
Bond lengths



Bond angles

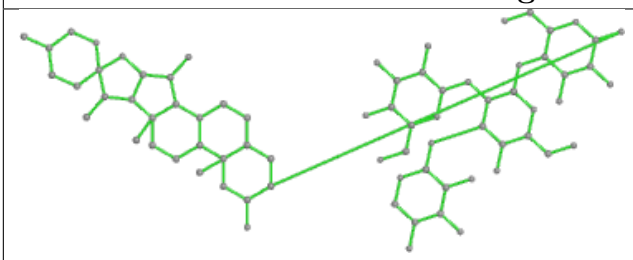


Torsions

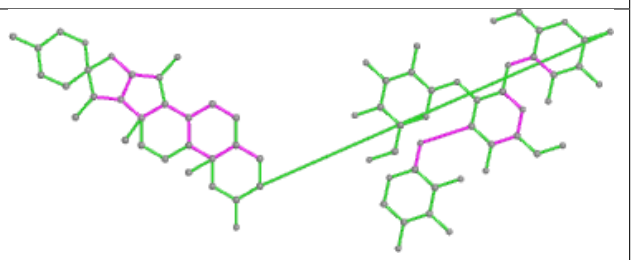


Rings

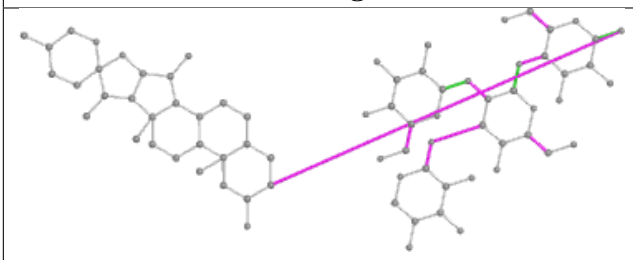
Ligand AJP B 1601



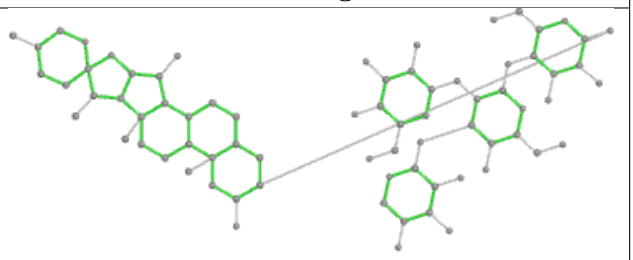
Bond lengths



Bond angles

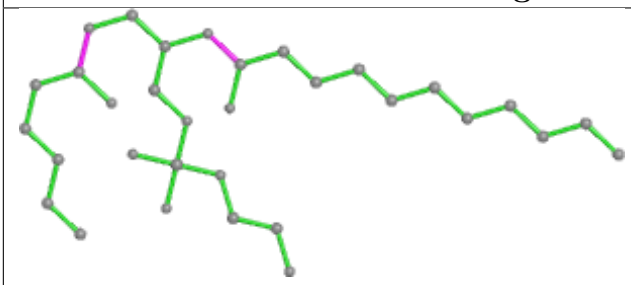


Torsions

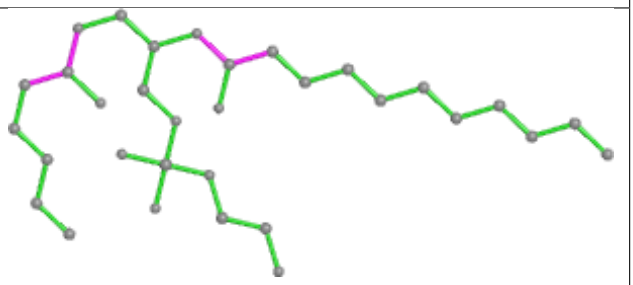


Rings

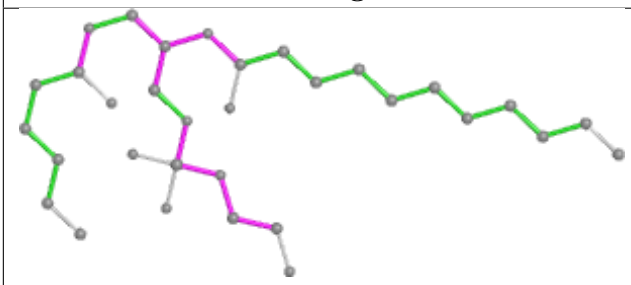
Ligand PTY D 1612



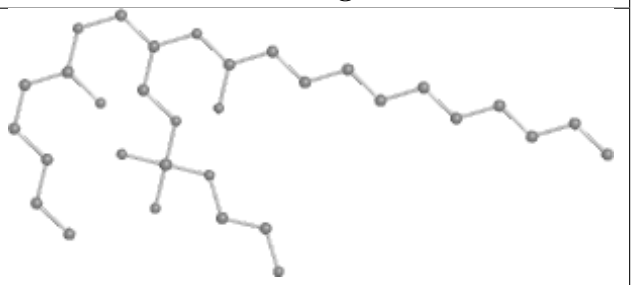
Bond lengths



Bond angles

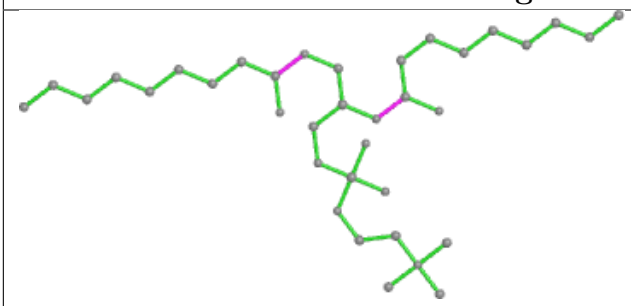


Torsions

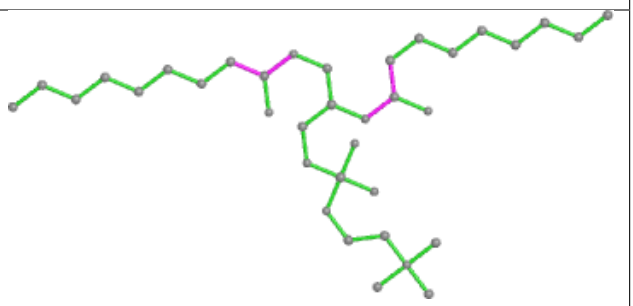


Rings

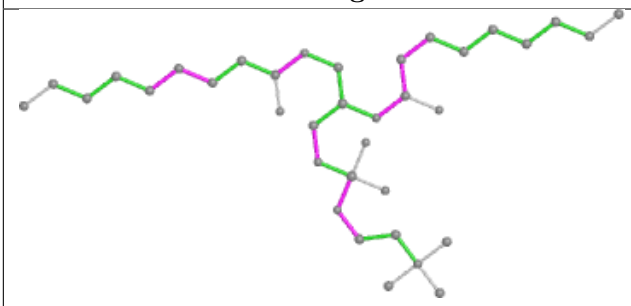
Ligand POV F 1604



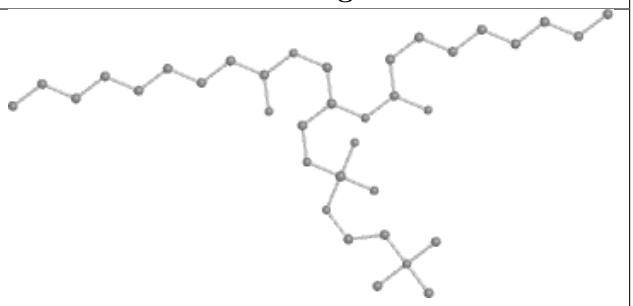
Bond lengths



Bond angles

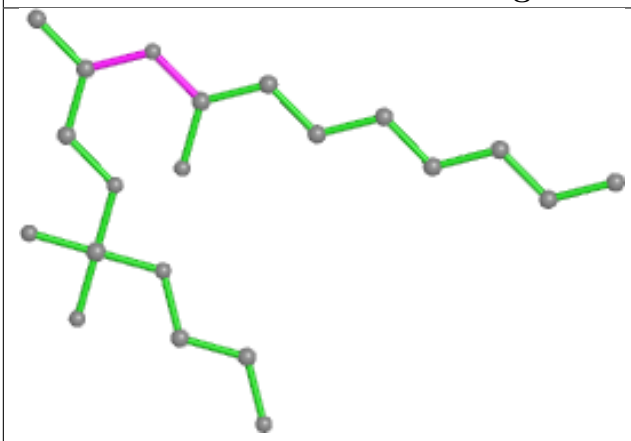


Torsions

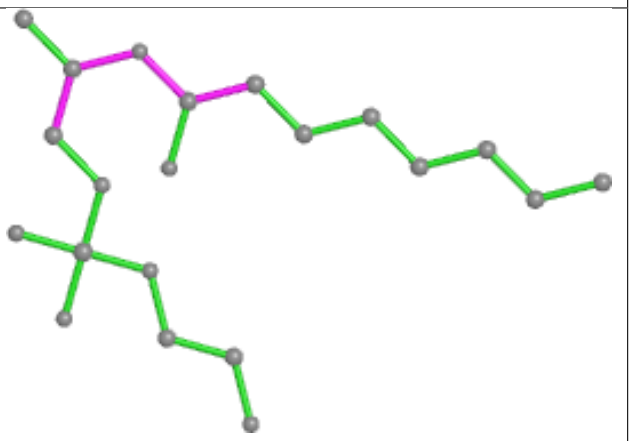


Rings

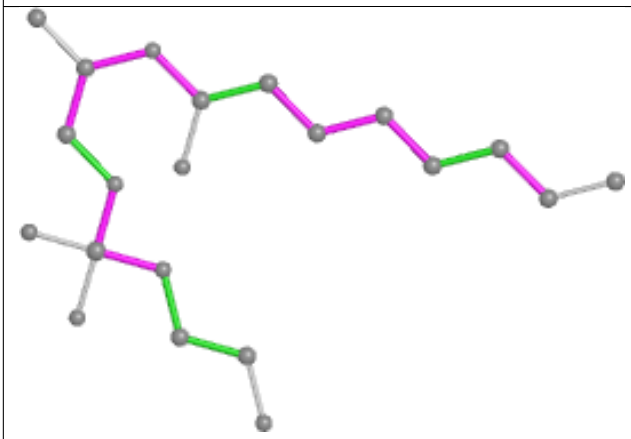
Ligand PTY D 1615



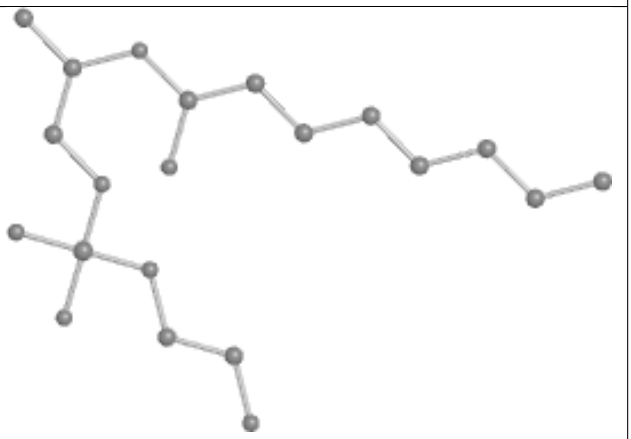
Bond lengths



Bond angles

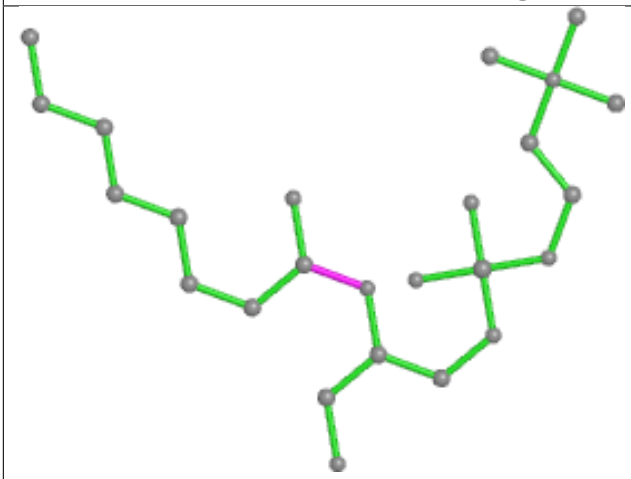


Torsions



Rings

Ligand POV B 1609



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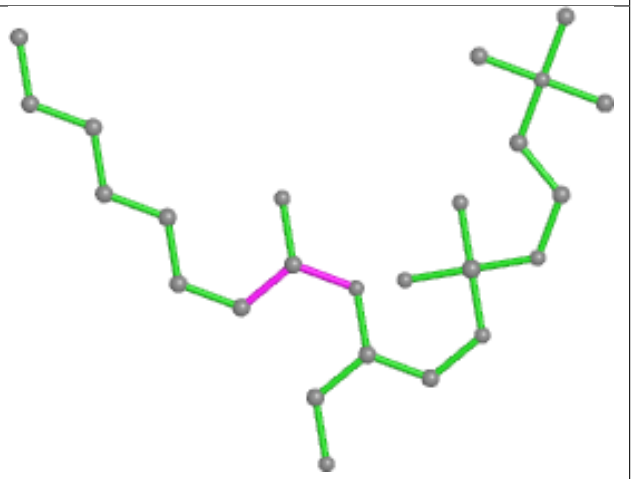
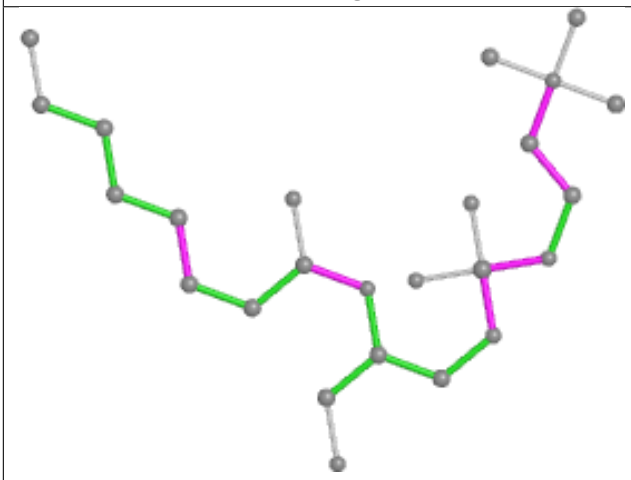
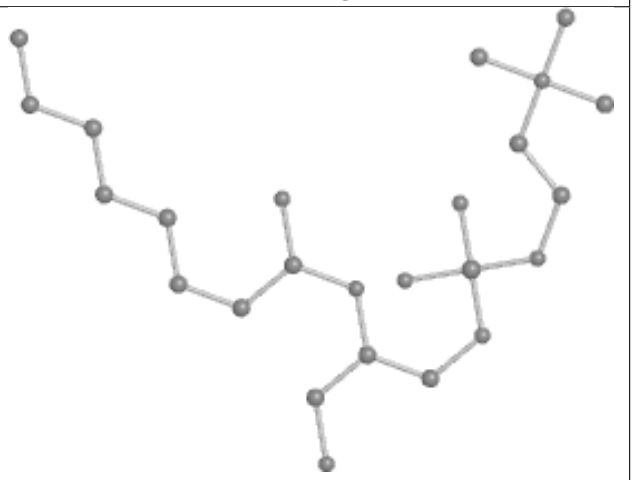


Bond angles

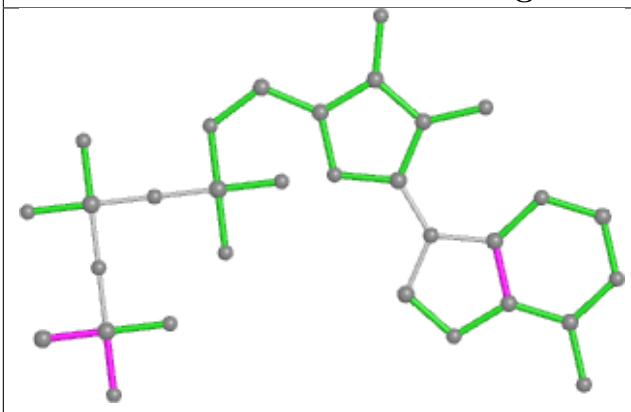


Torsions

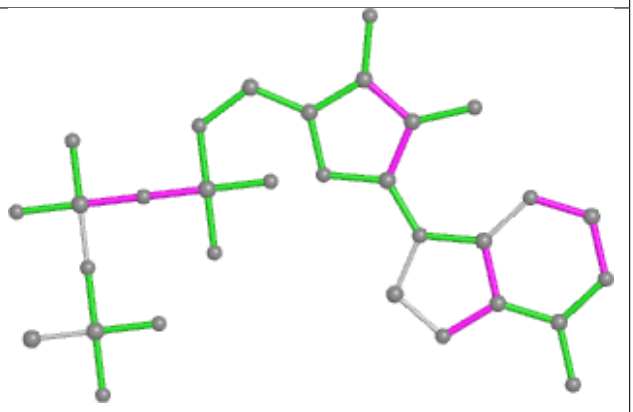


Rings

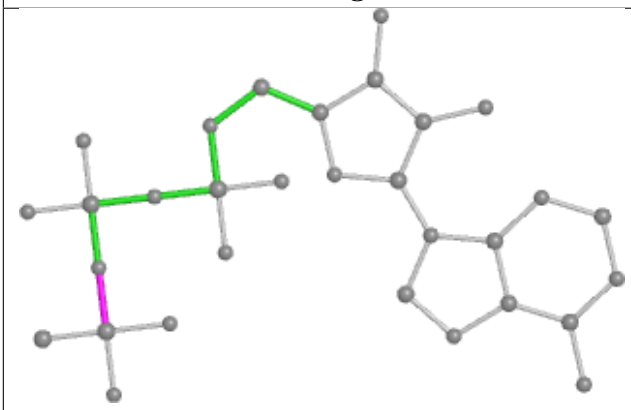
Ligand AGS B 1602



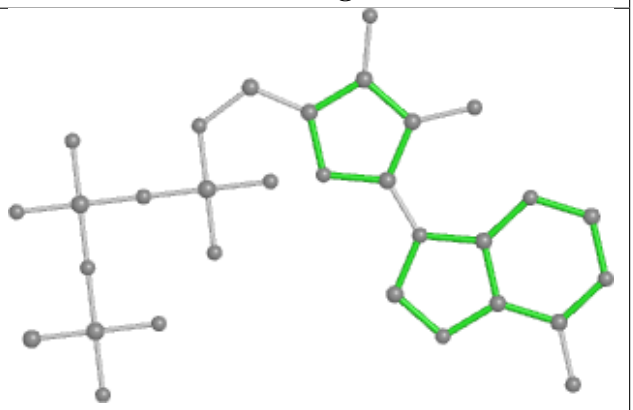
Bond lengths



Bond angles

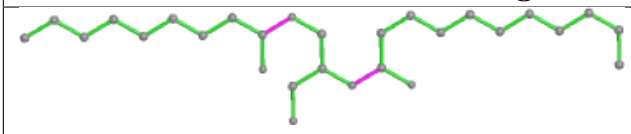


Torsions

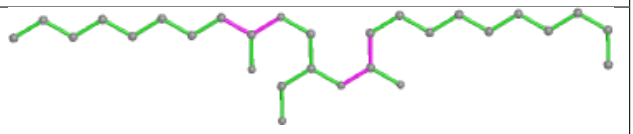


Rings

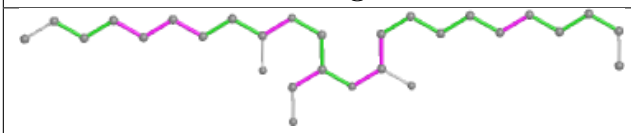
Ligand POV F 1611



Bond lengths



Bond angles



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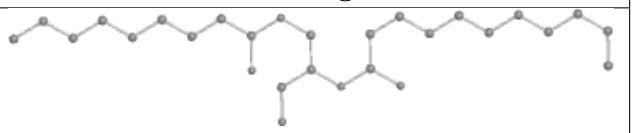
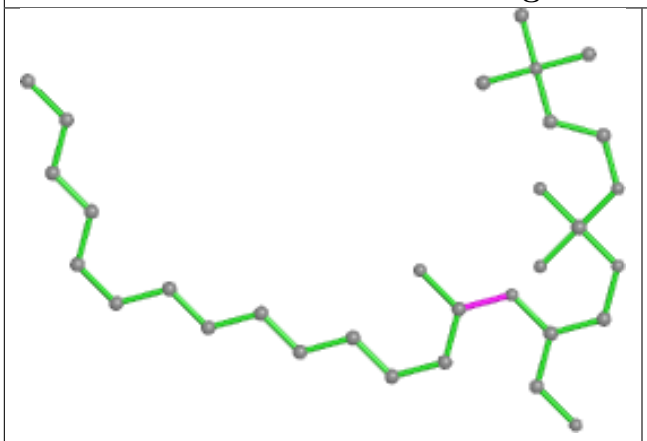


Rings

Ligand POV G 402



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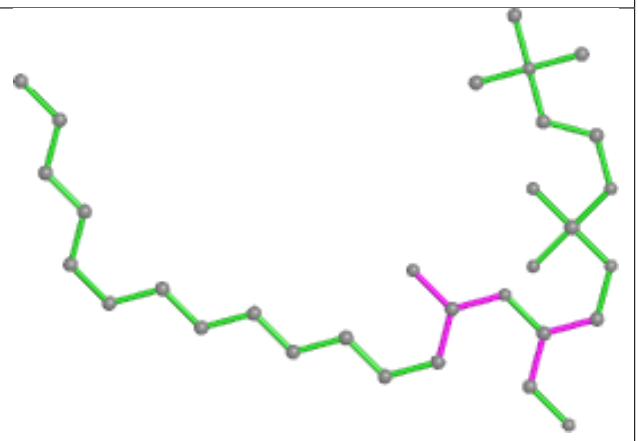
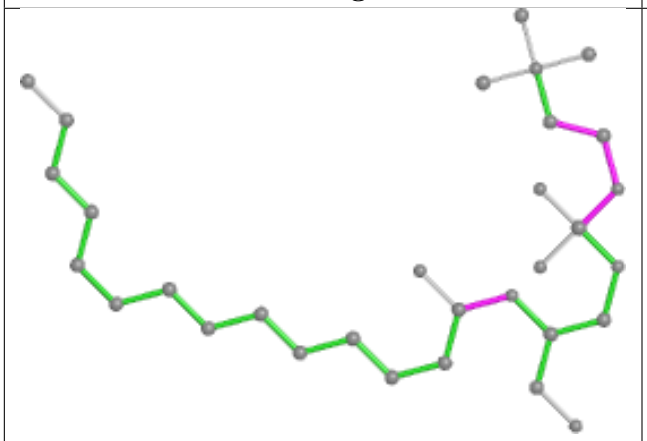
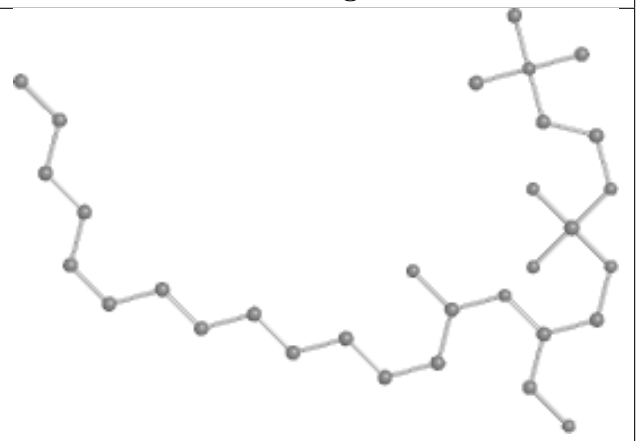


Bond angles

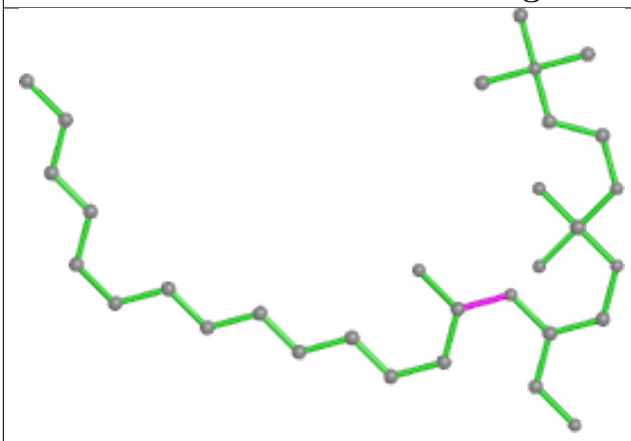


Torsions



Rings

Ligand POV C 402



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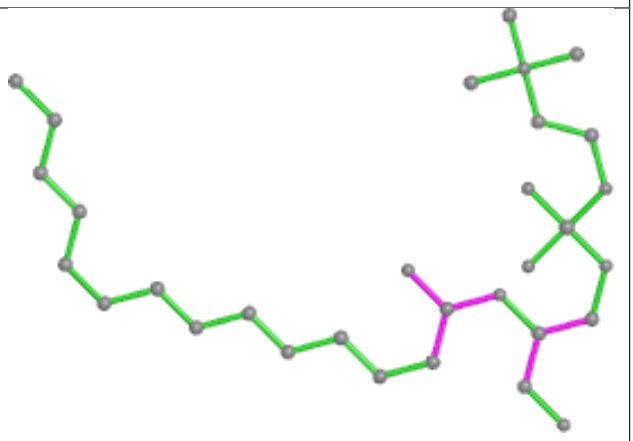
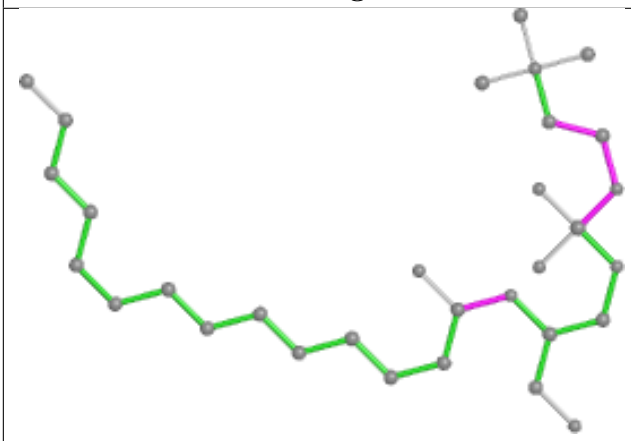
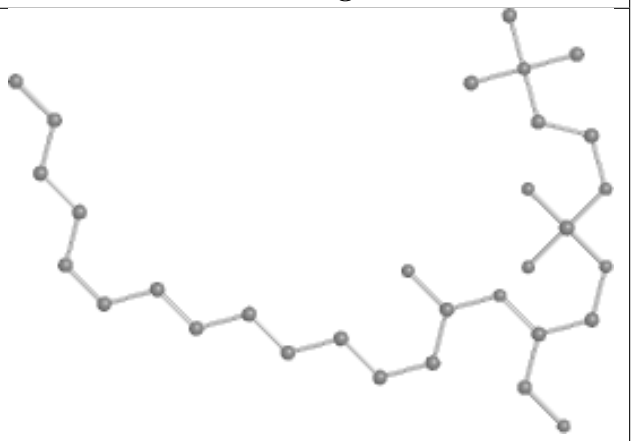


Bond angles

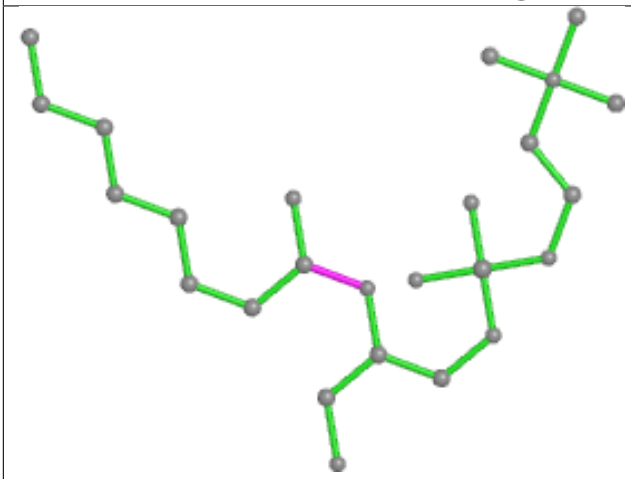


Torsions

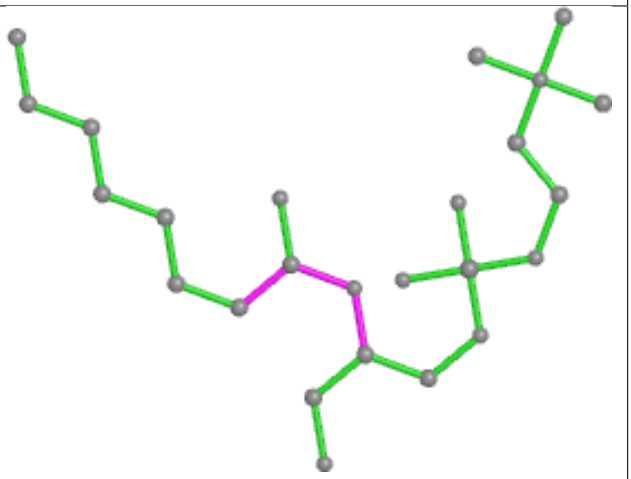


Rings

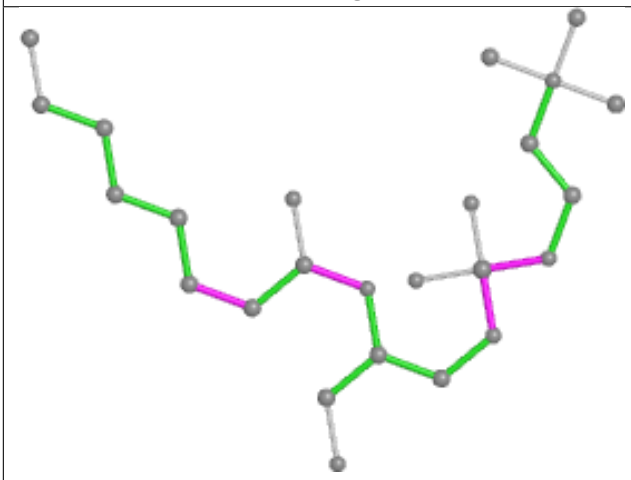
Ligand POV H 1610



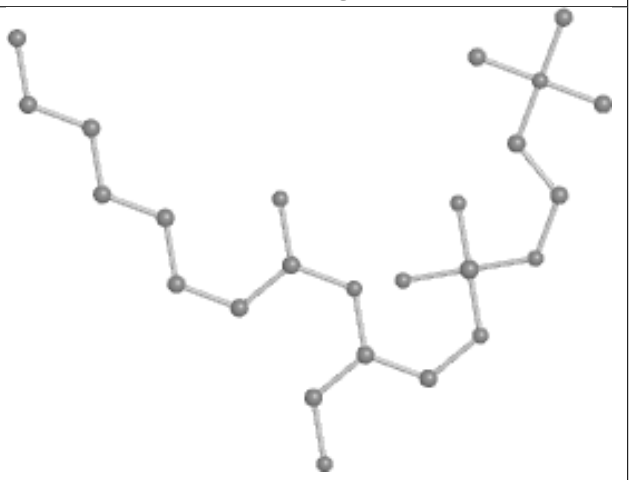
Bond lengths



Bond angles

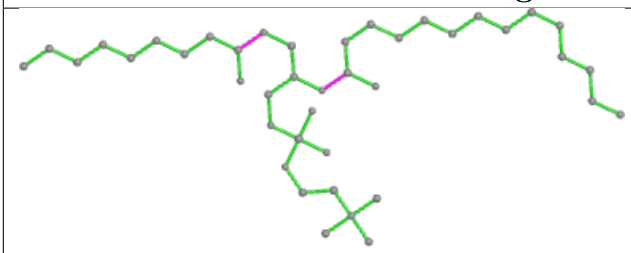


Torsions

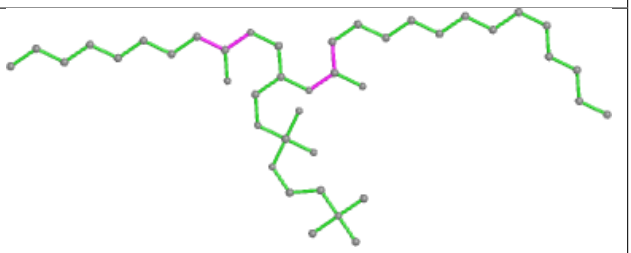


Rings

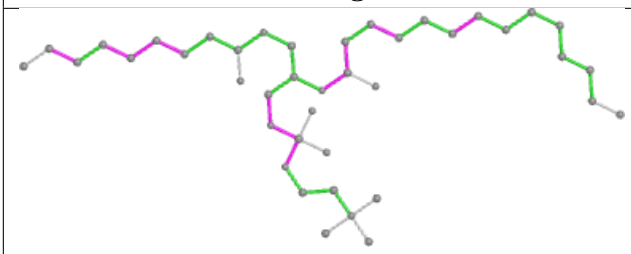
Ligand POV F 1605



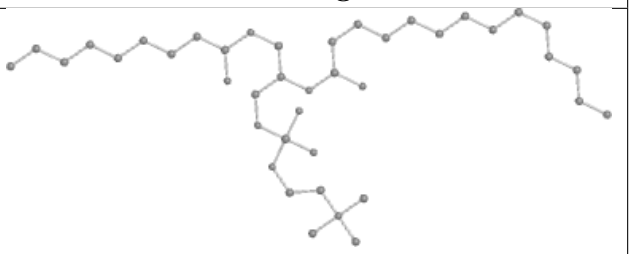
Bond lengths



Bond angles

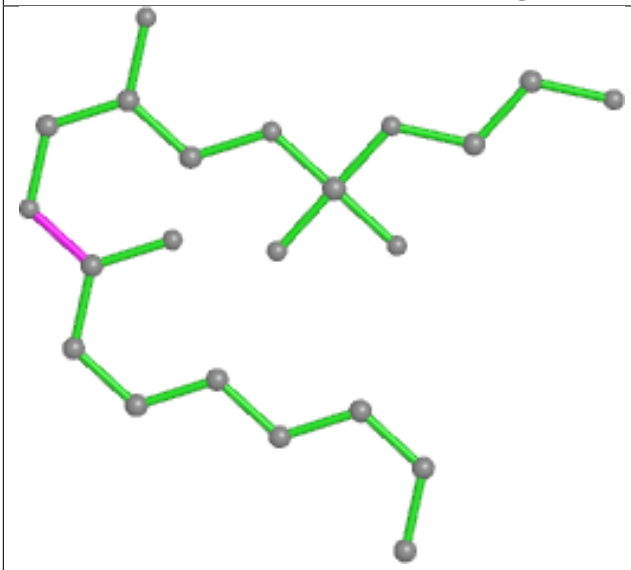


Torsions

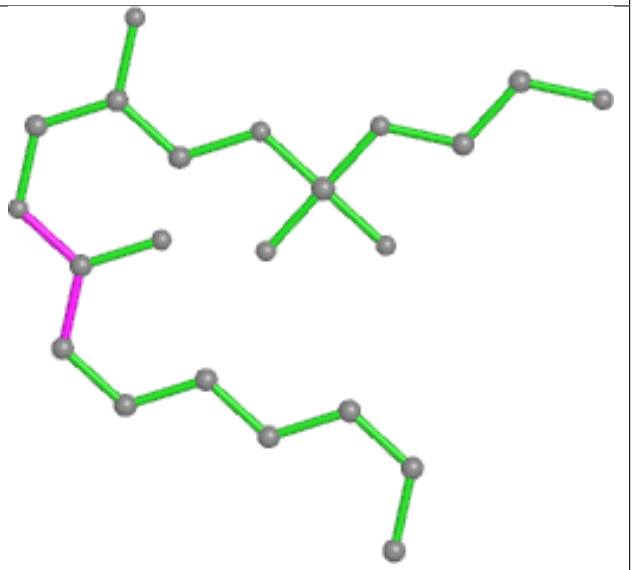


Rings

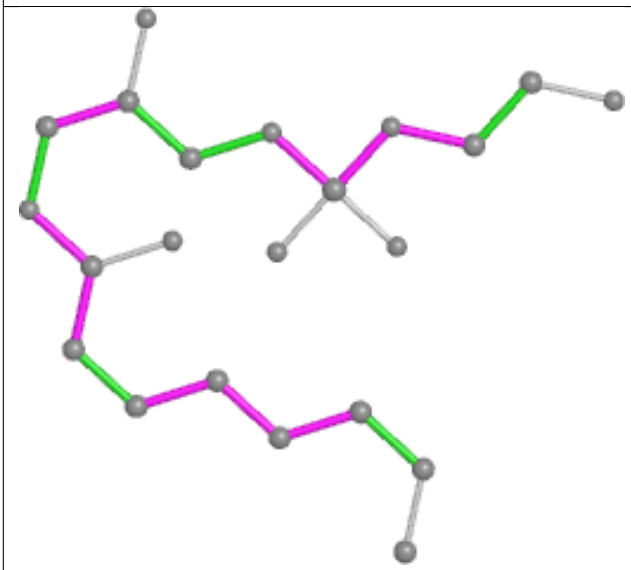
Ligand PTY H 1614



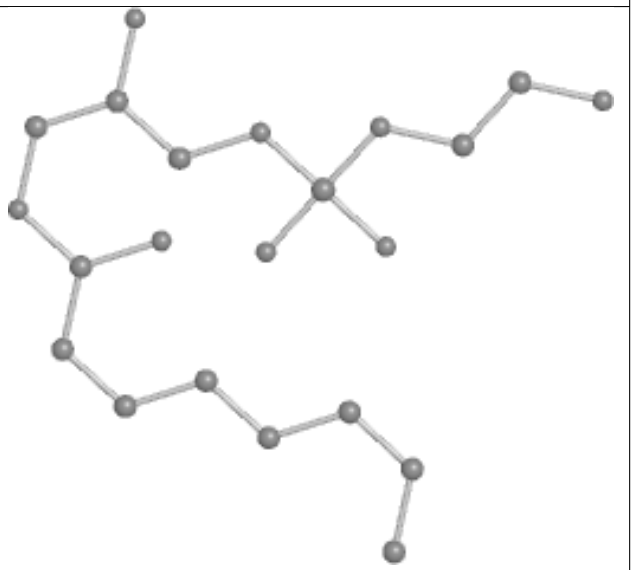
Bond lengths



Bond angles

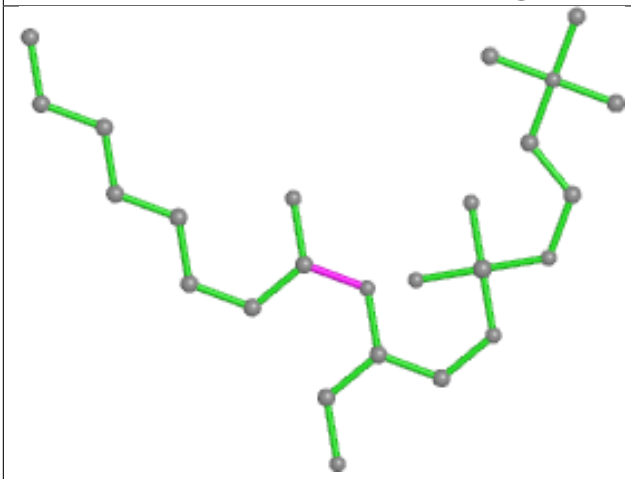


Torsions

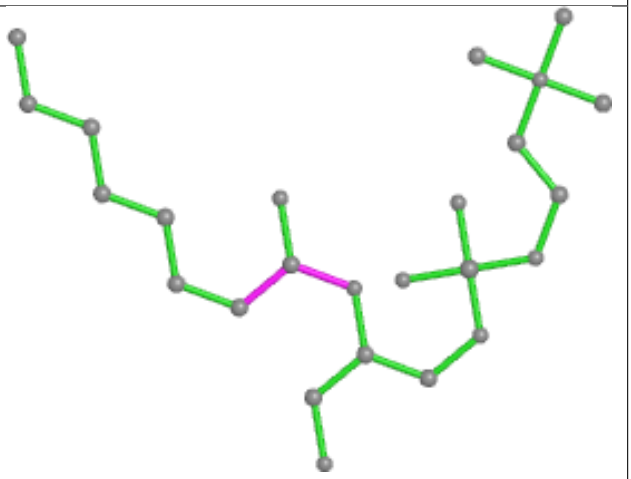


Rings

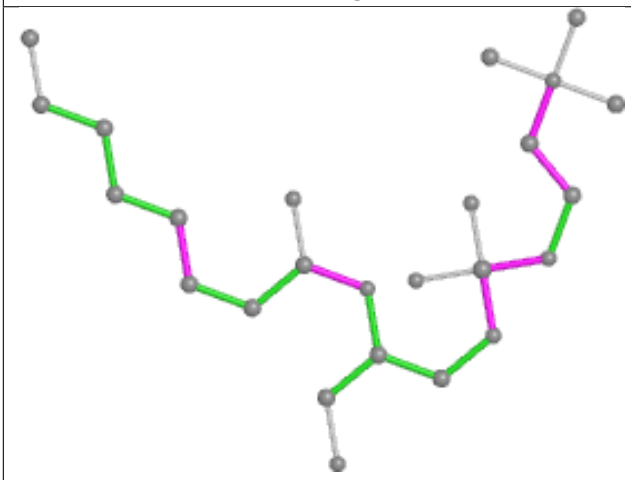
Ligand POV H 1609



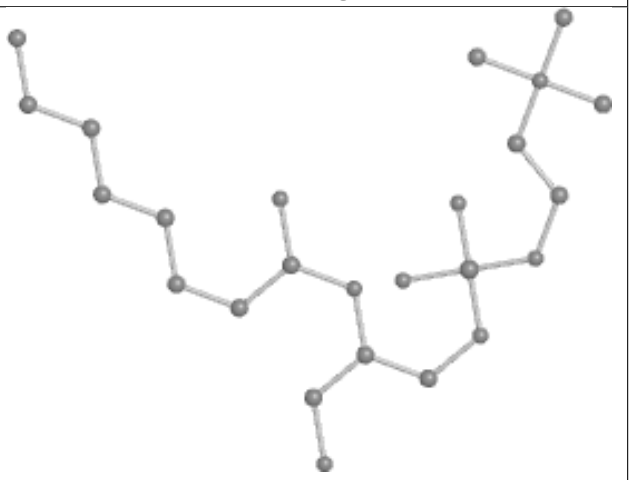
Bond lengths



Bond angles

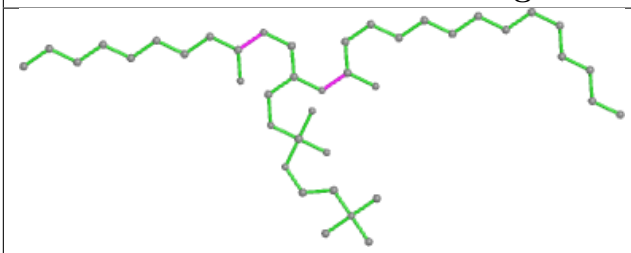


Torsions

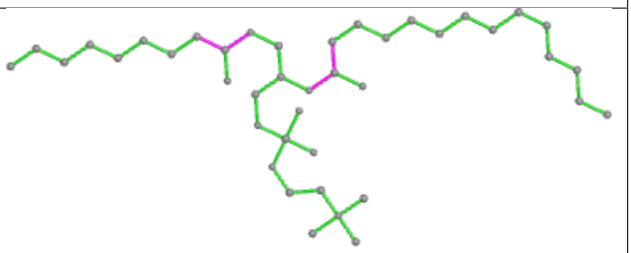


Rings

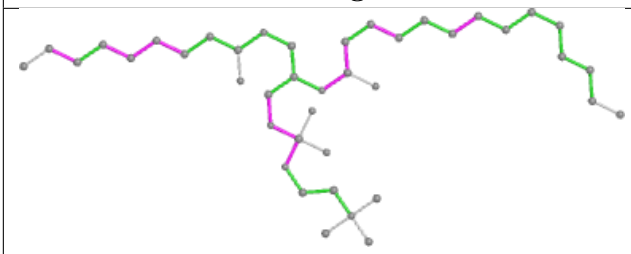
Ligand POV B 1605



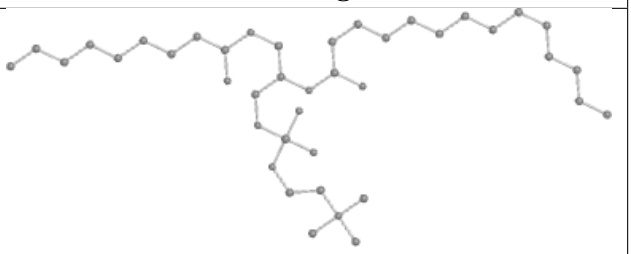
Bond lengths



Bond angles

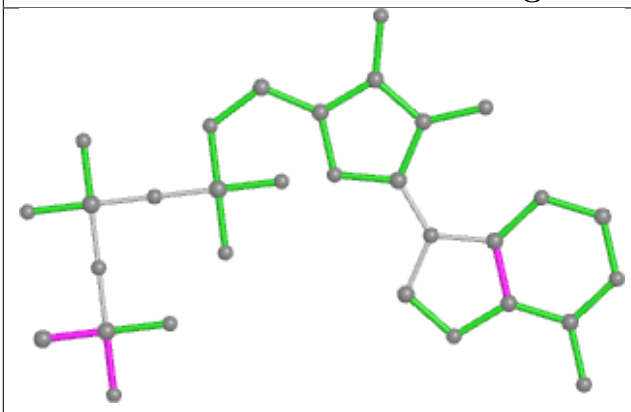


Torsions



Rings

Ligand AGS A 402



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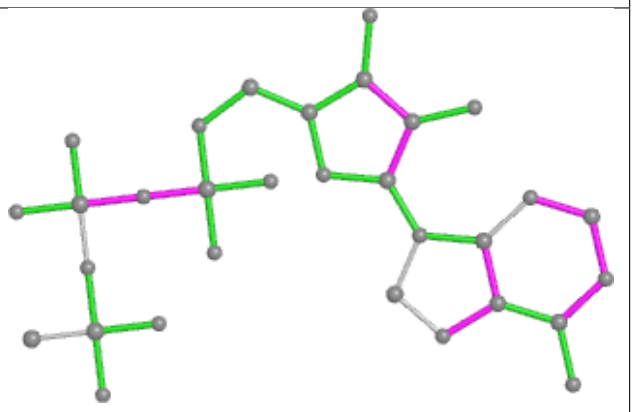
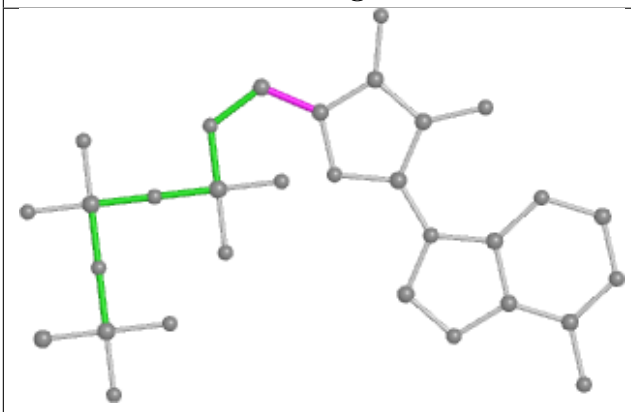
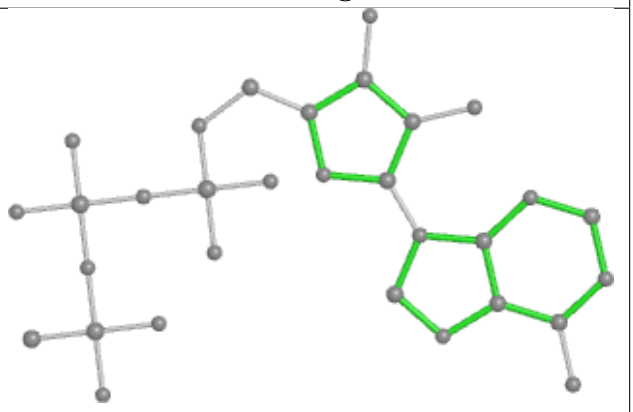


Bond angles

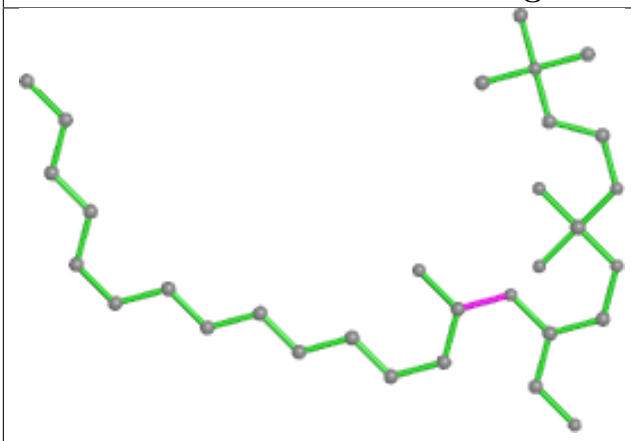


Torsions

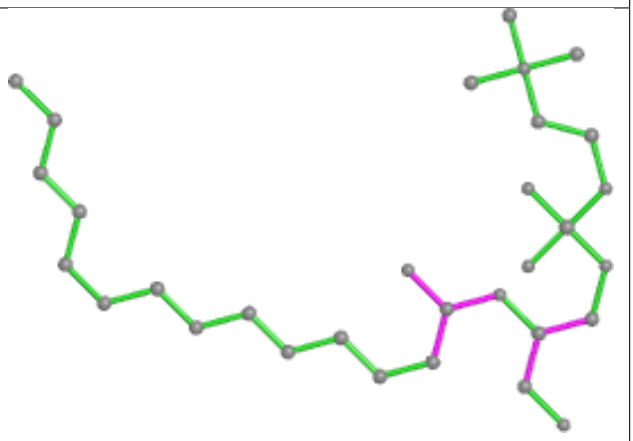


Rings

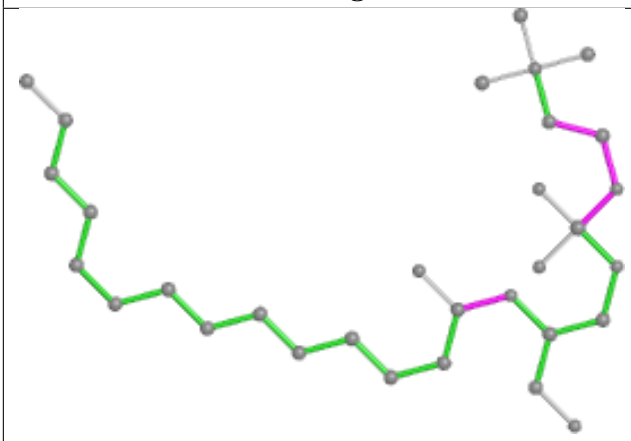
Ligand POV E 402



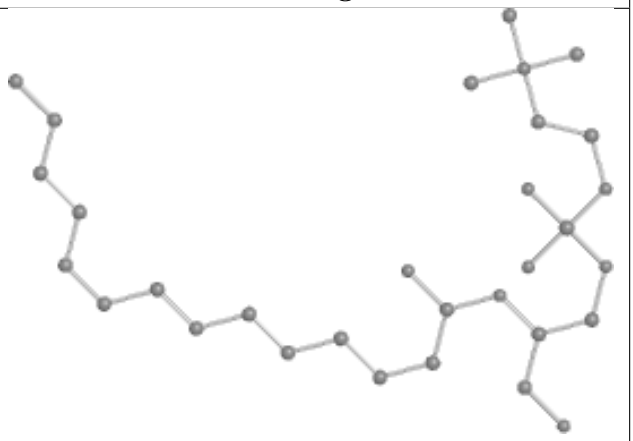
Bond lengths



Bond angles

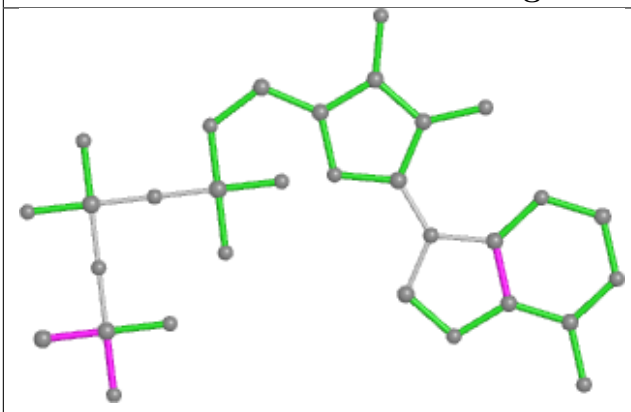


Torsions

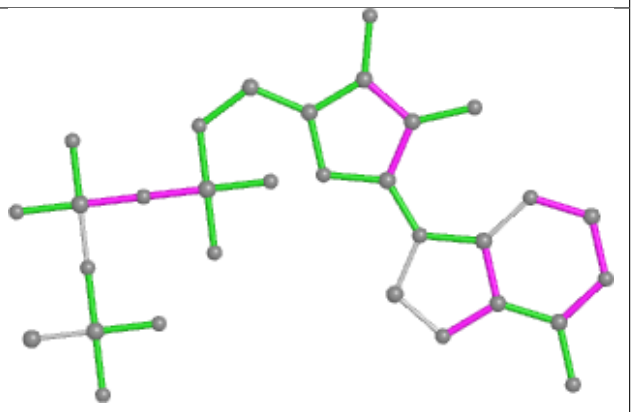


Rings

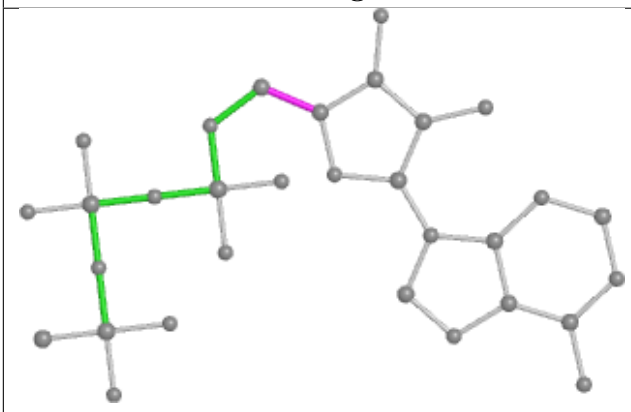
Ligand AGS G 401



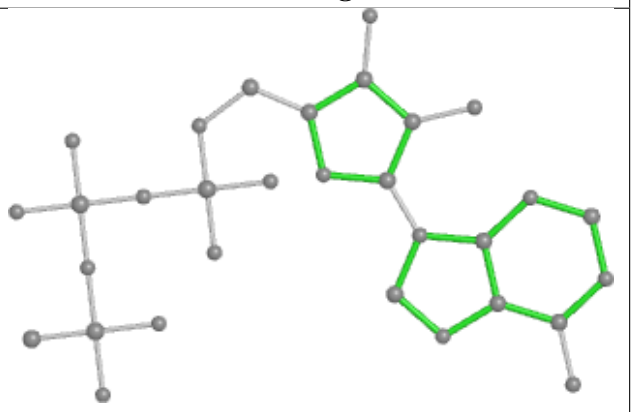
Bond lengths



Bond angles

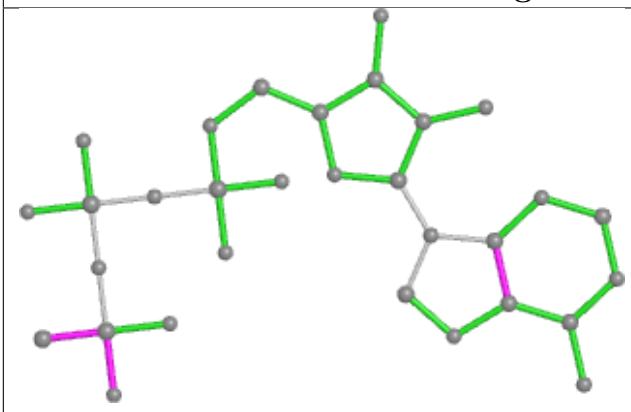


Torsions



Rings

Ligand AGS H 1602



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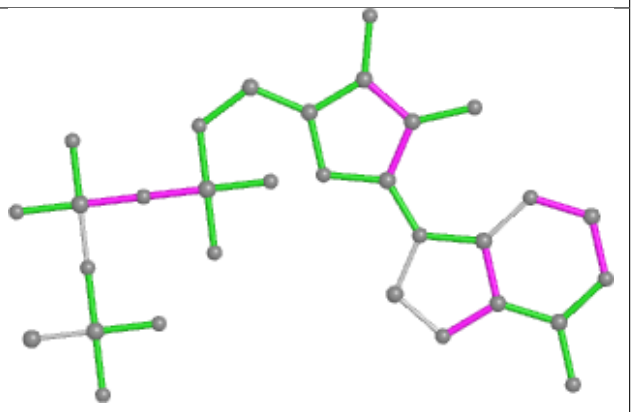
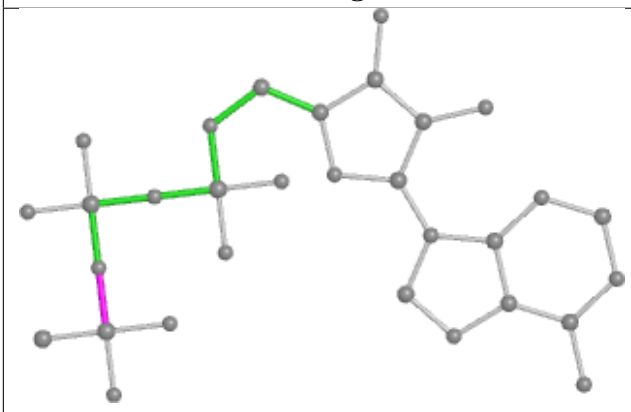
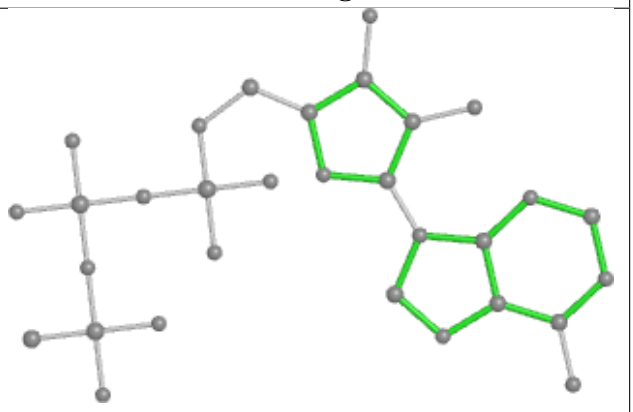


Bond angles

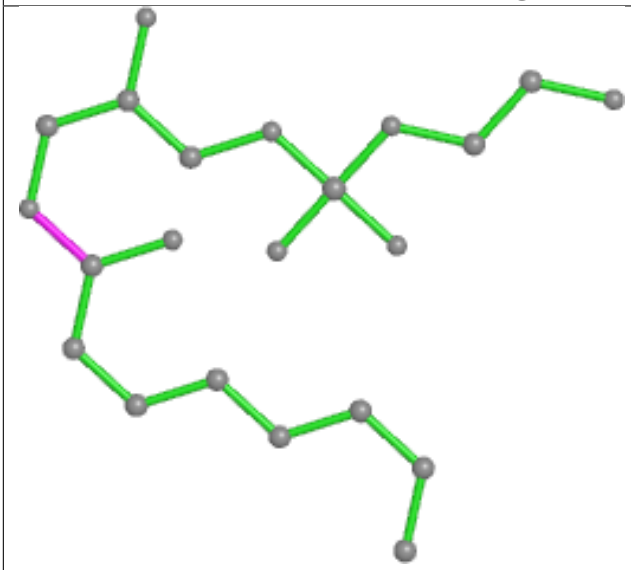


Torsions



Rings

Ligand PTY D 1614



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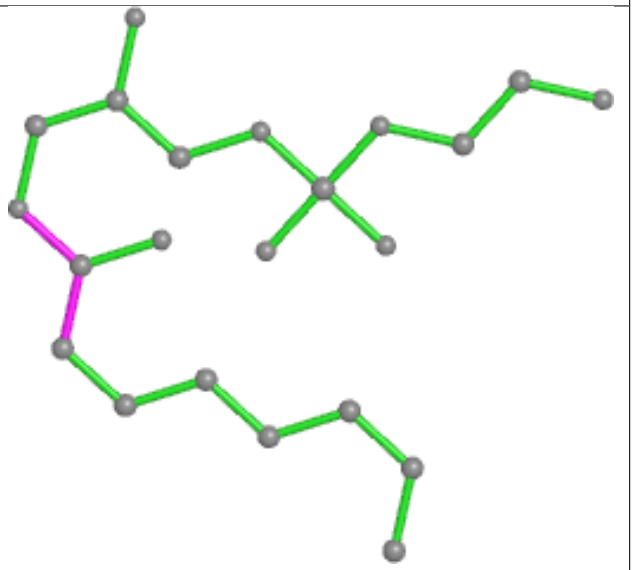
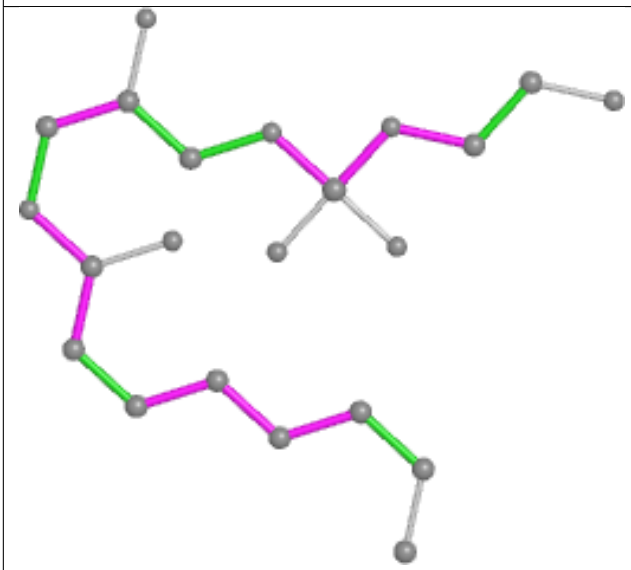


Bond angles



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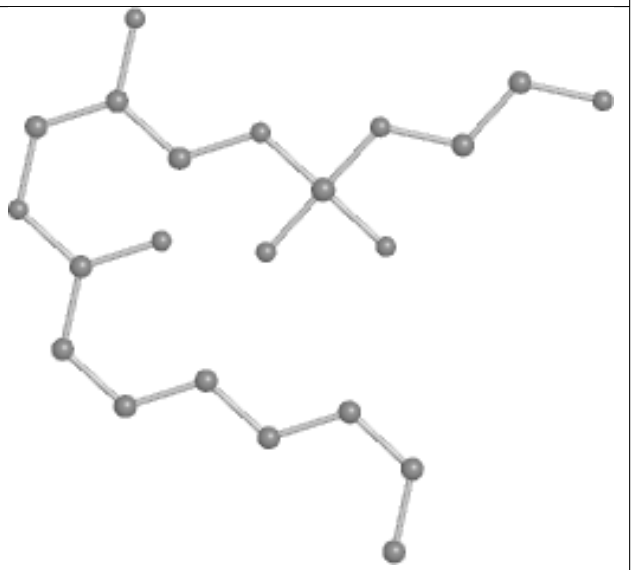
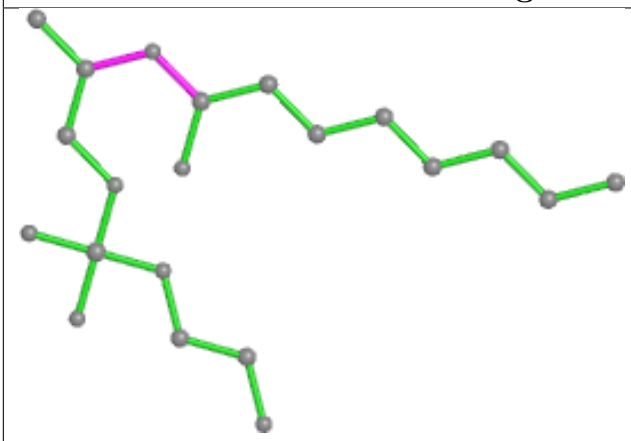
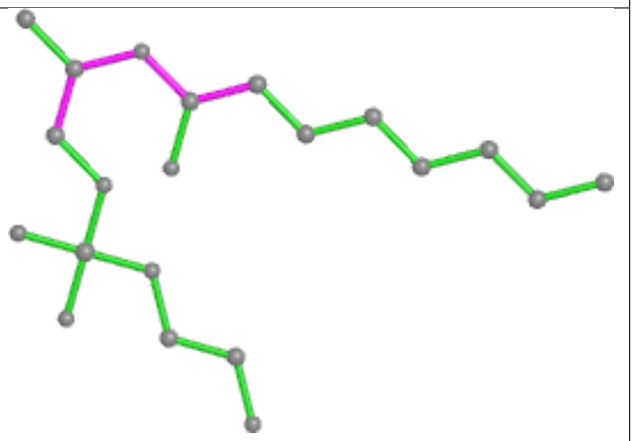


Rings

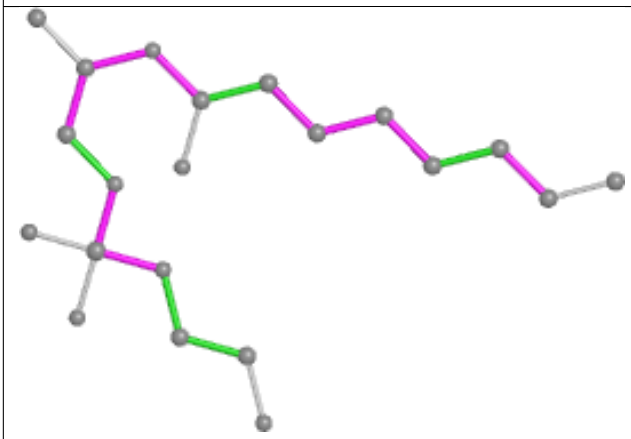
Ligand PTY F 1615



Bond lengths



Bond angles



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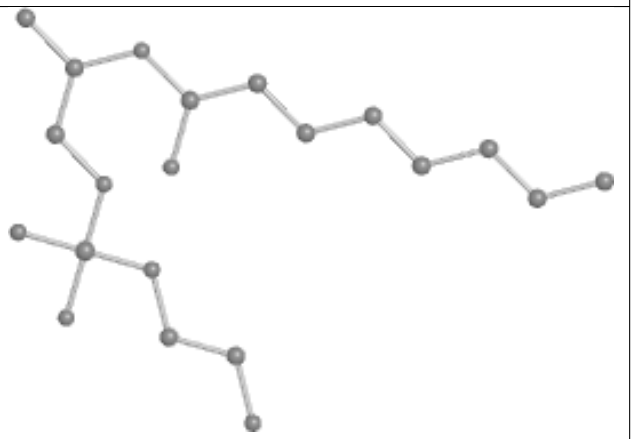
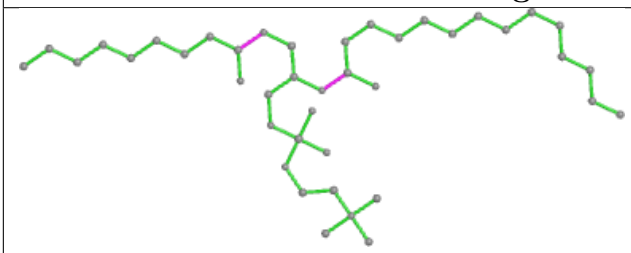


Rings

Ligand POV H 1607



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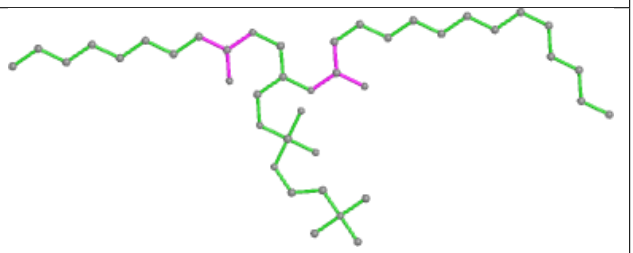
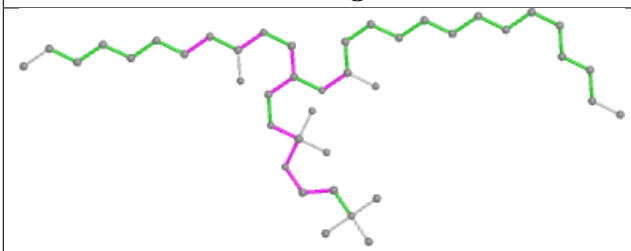
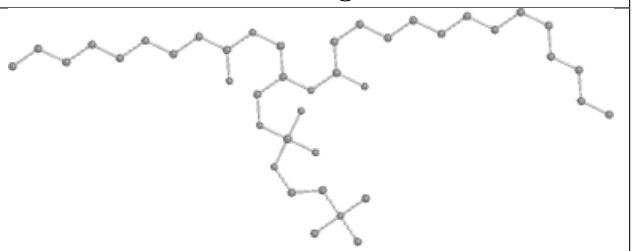


Bond angles

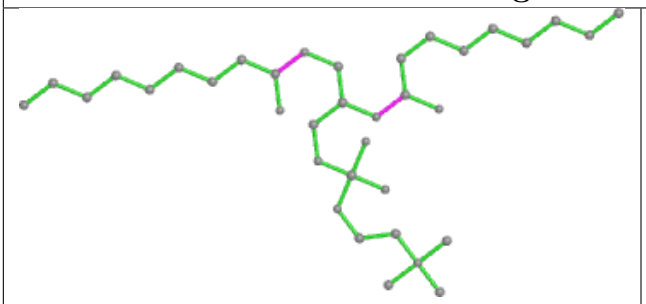


Torsions

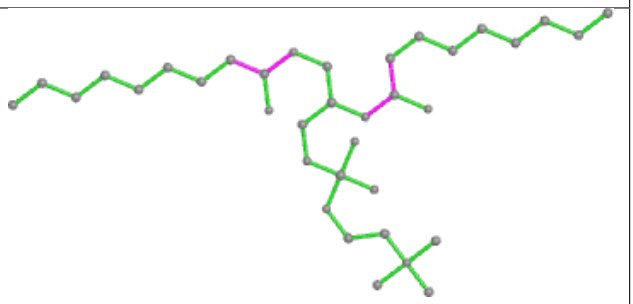


Rings

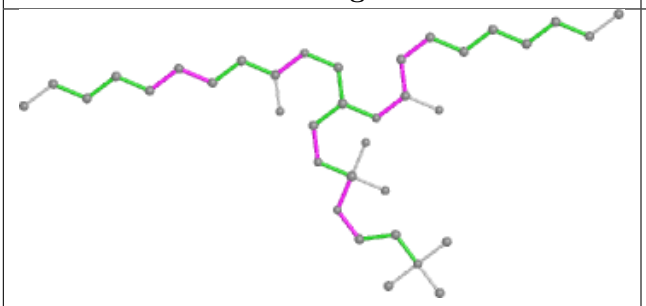
Ligand POV H 1604



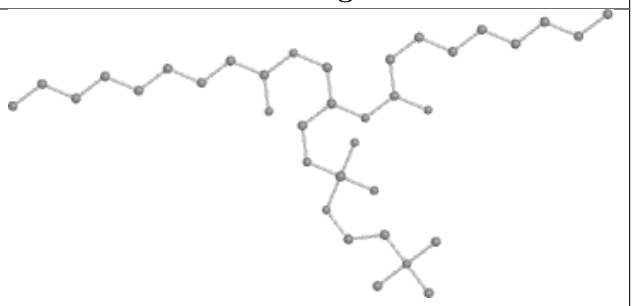
Bond lengths



Bond angles

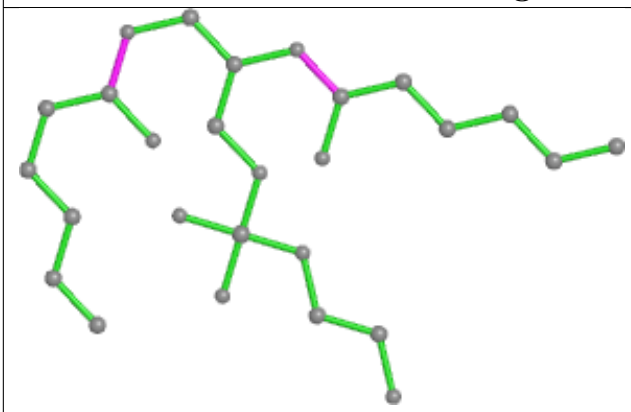


Torsions



Rings

Ligand PTY H 1613



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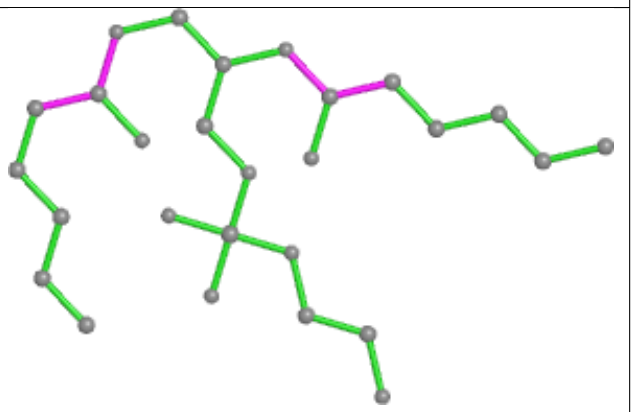
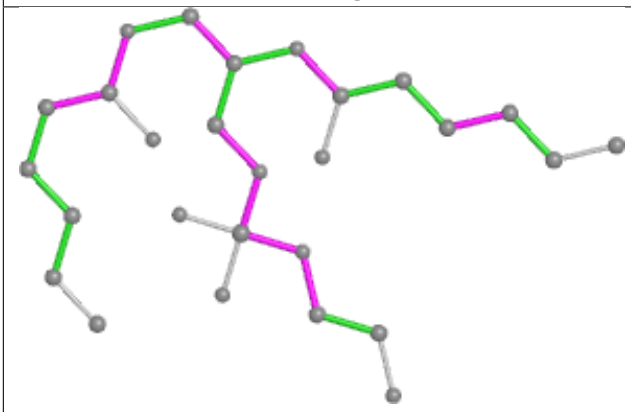
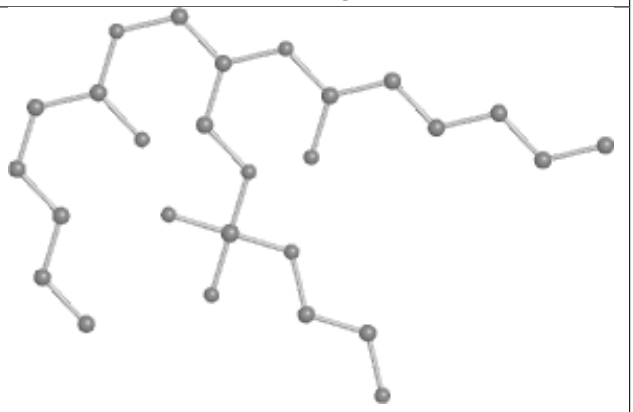


Bond angles

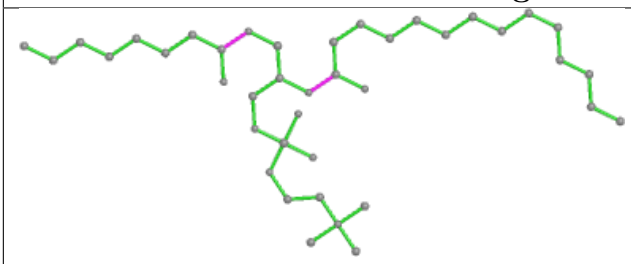


Torsions



Rings

Ligand POV H 1606



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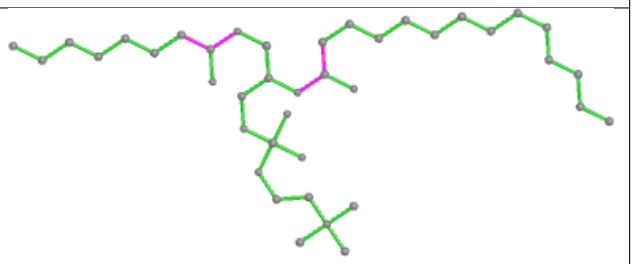
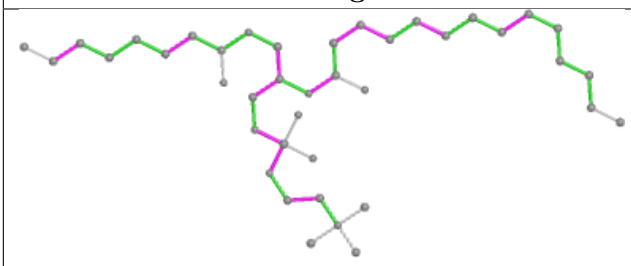
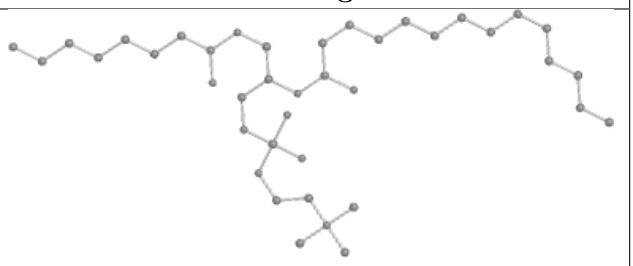


Bond angles

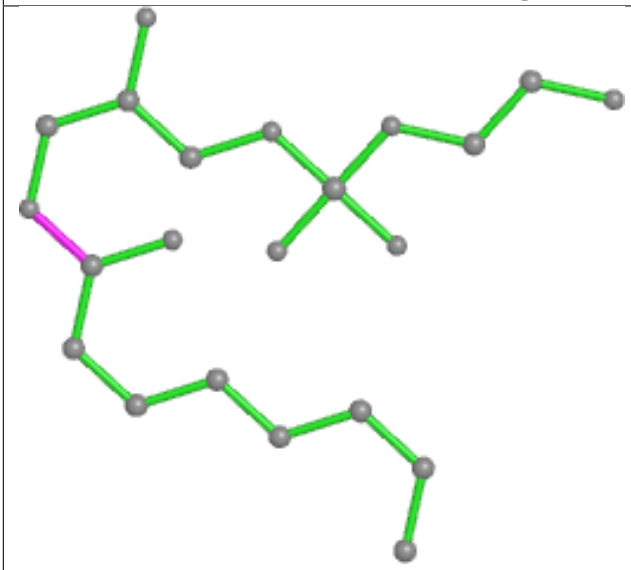


Torsions

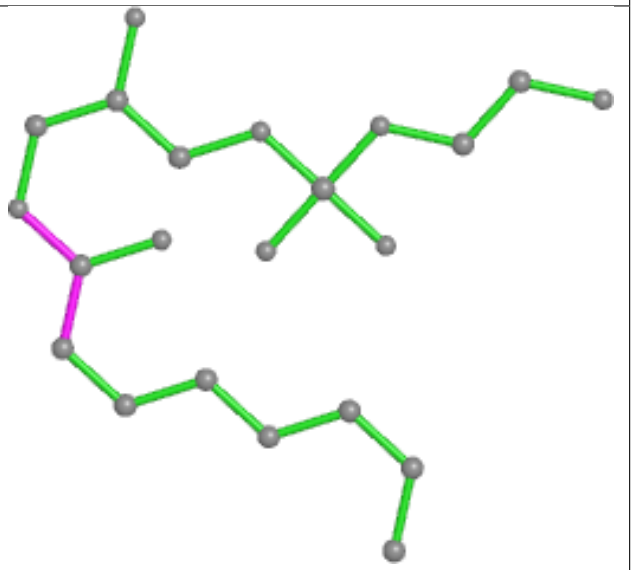


Rings

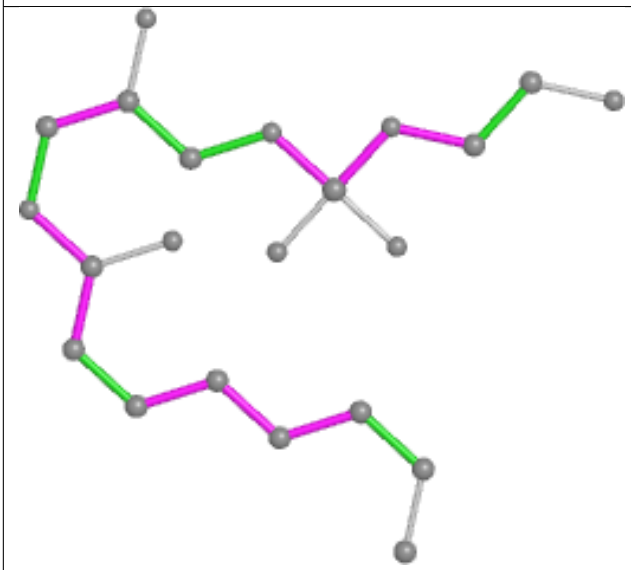
Ligand PTY F 1614



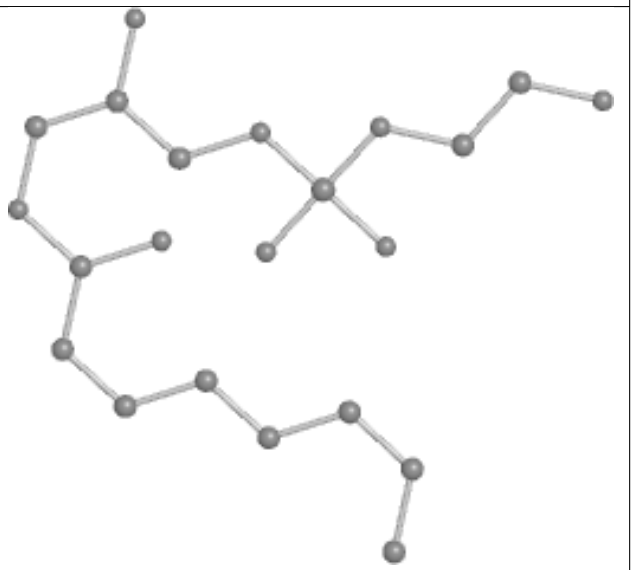
Bond lengths



Bond angles

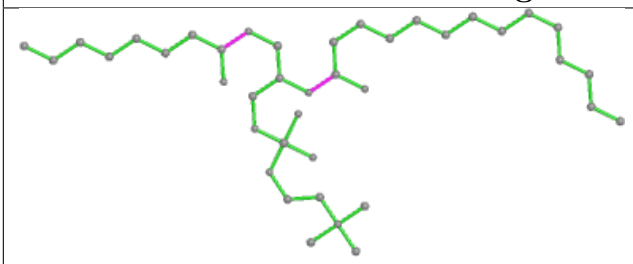


Torsions



Rings

Ligand POV F 1606



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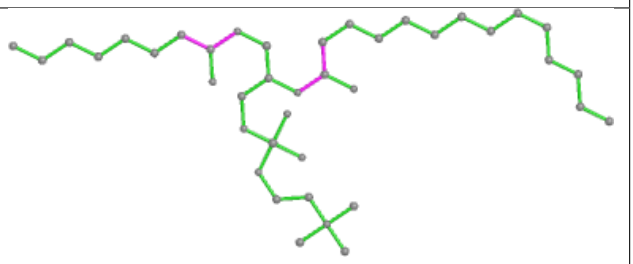
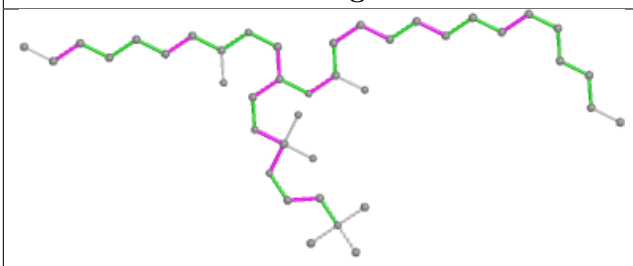
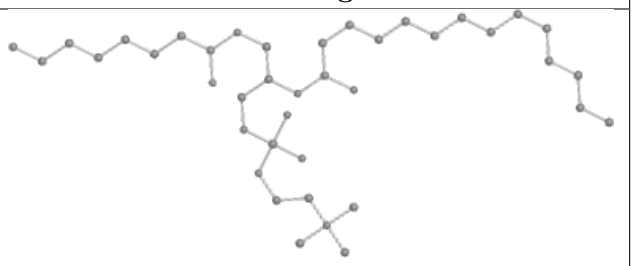


Bond angles

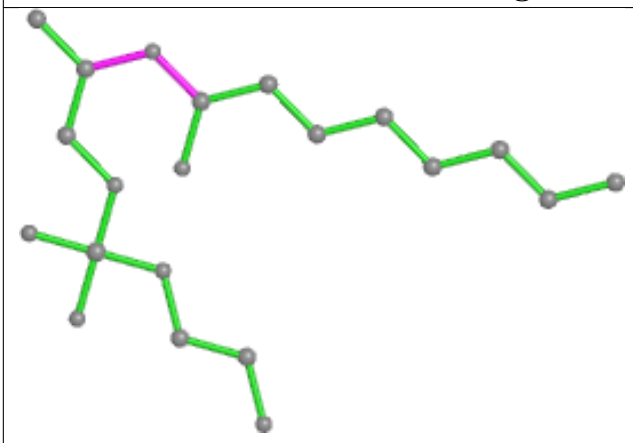


Torsions



Rings

Ligand PTY H 1615



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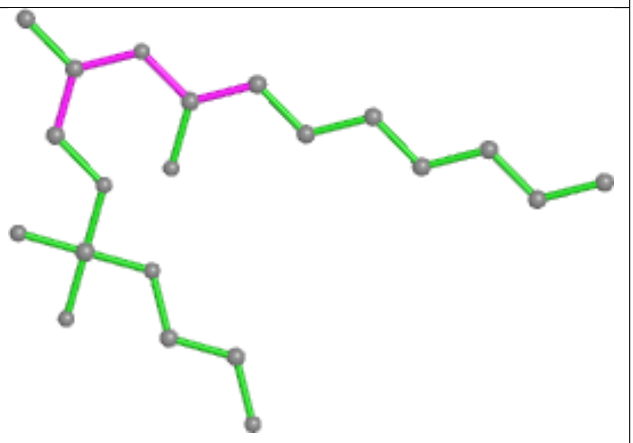
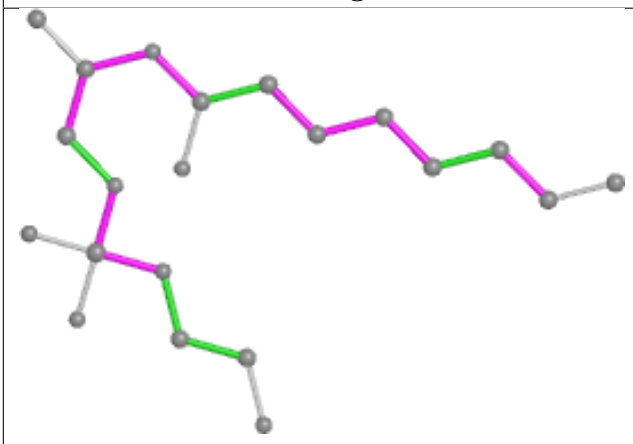
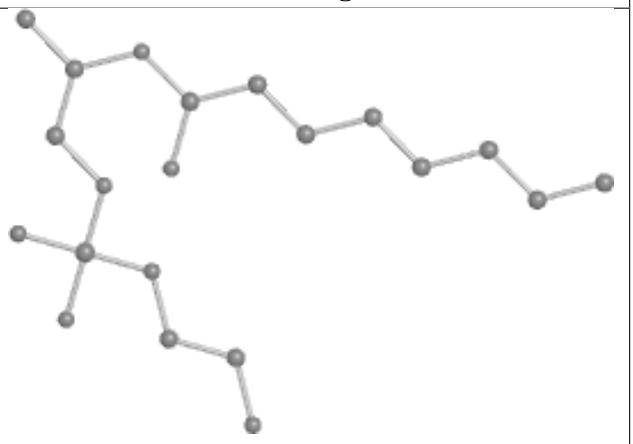


Bond angles

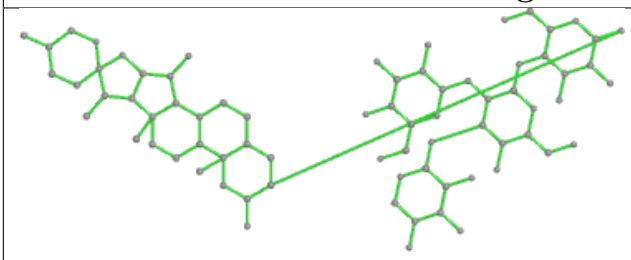


Torsions



Rings

Ligand AJP D 1601



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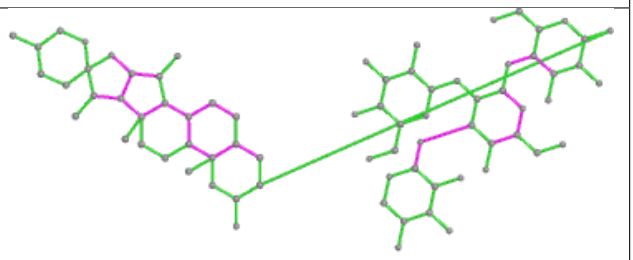
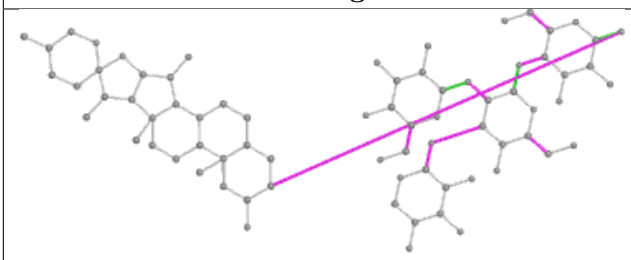
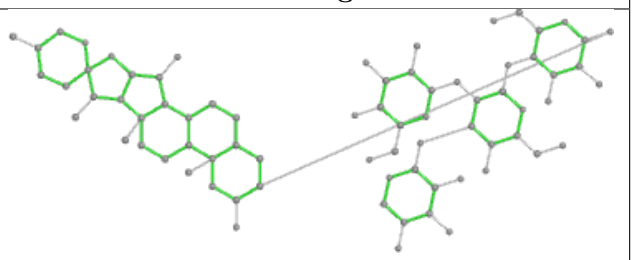


Bond angles

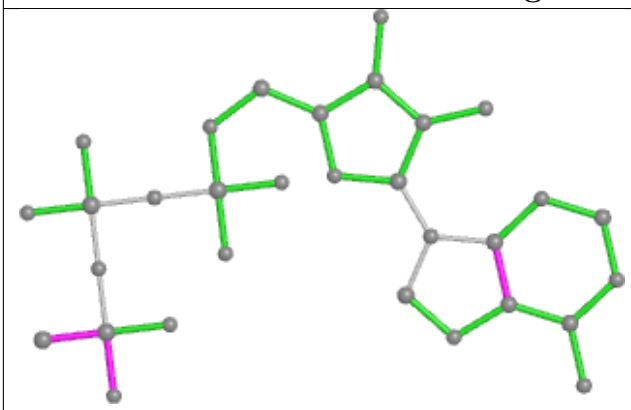


Torsions



Rings

Ligand AGS C 401



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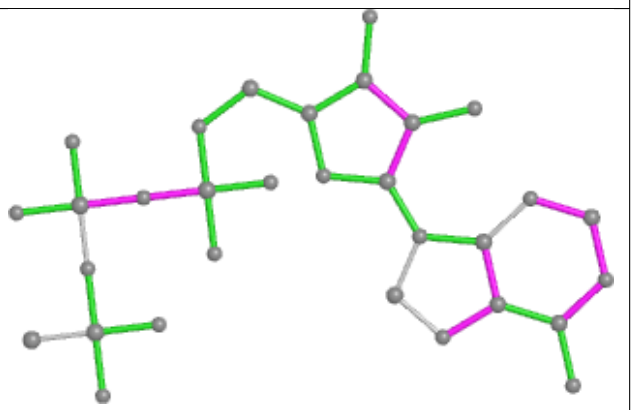
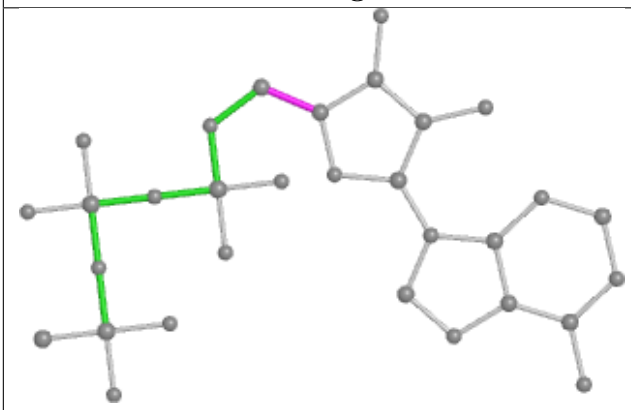
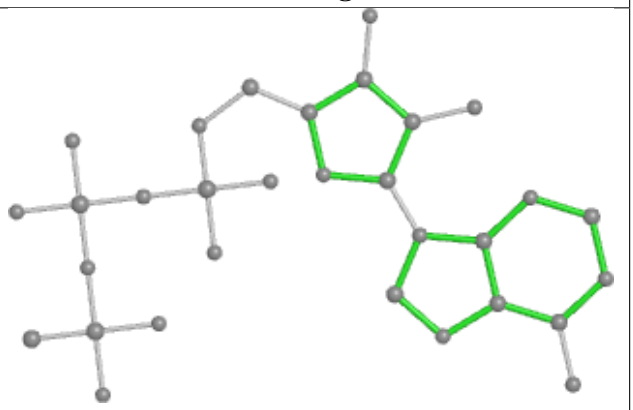


Bond angles

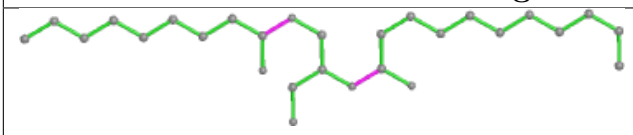


Torsions

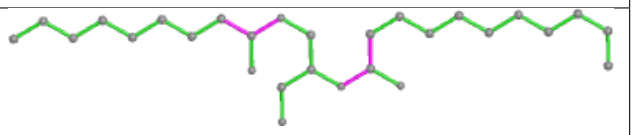


Rings

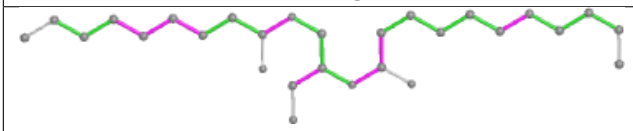
Ligand POV D 1611



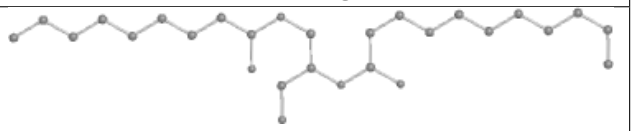
Bond lengths



Bond angles

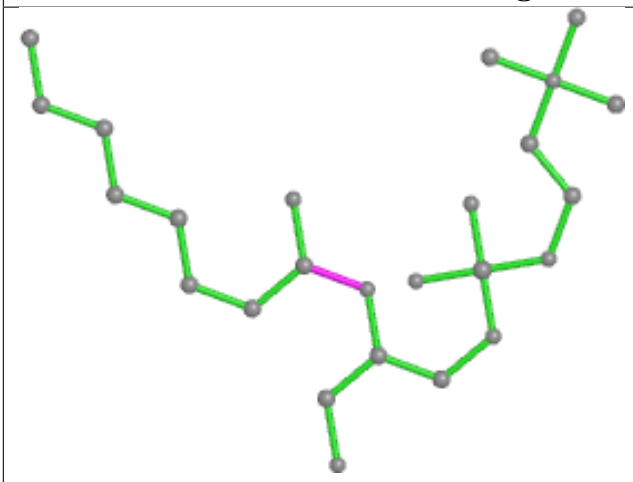


Torsions

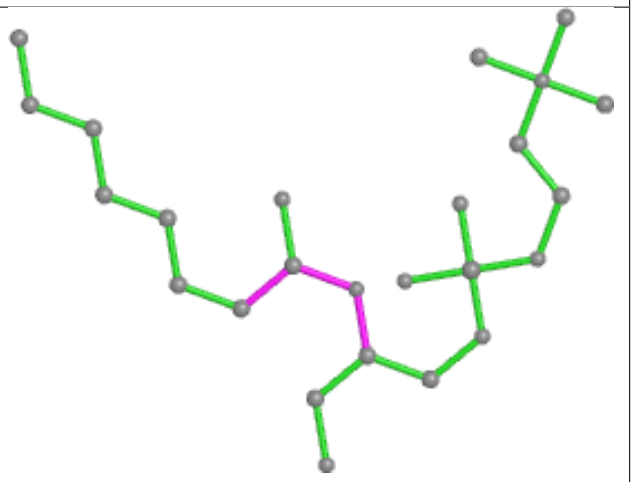


Rings

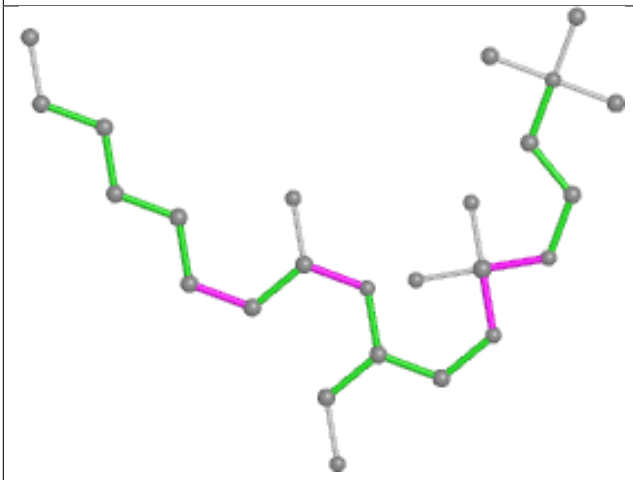
Ligand POV F 1610



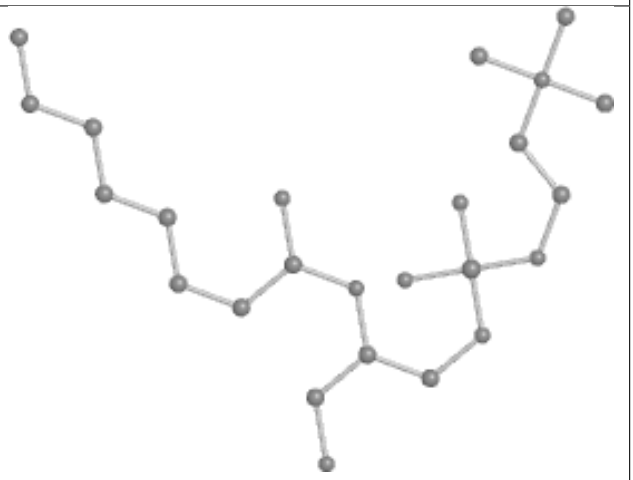
Bond lengths



Bond angles

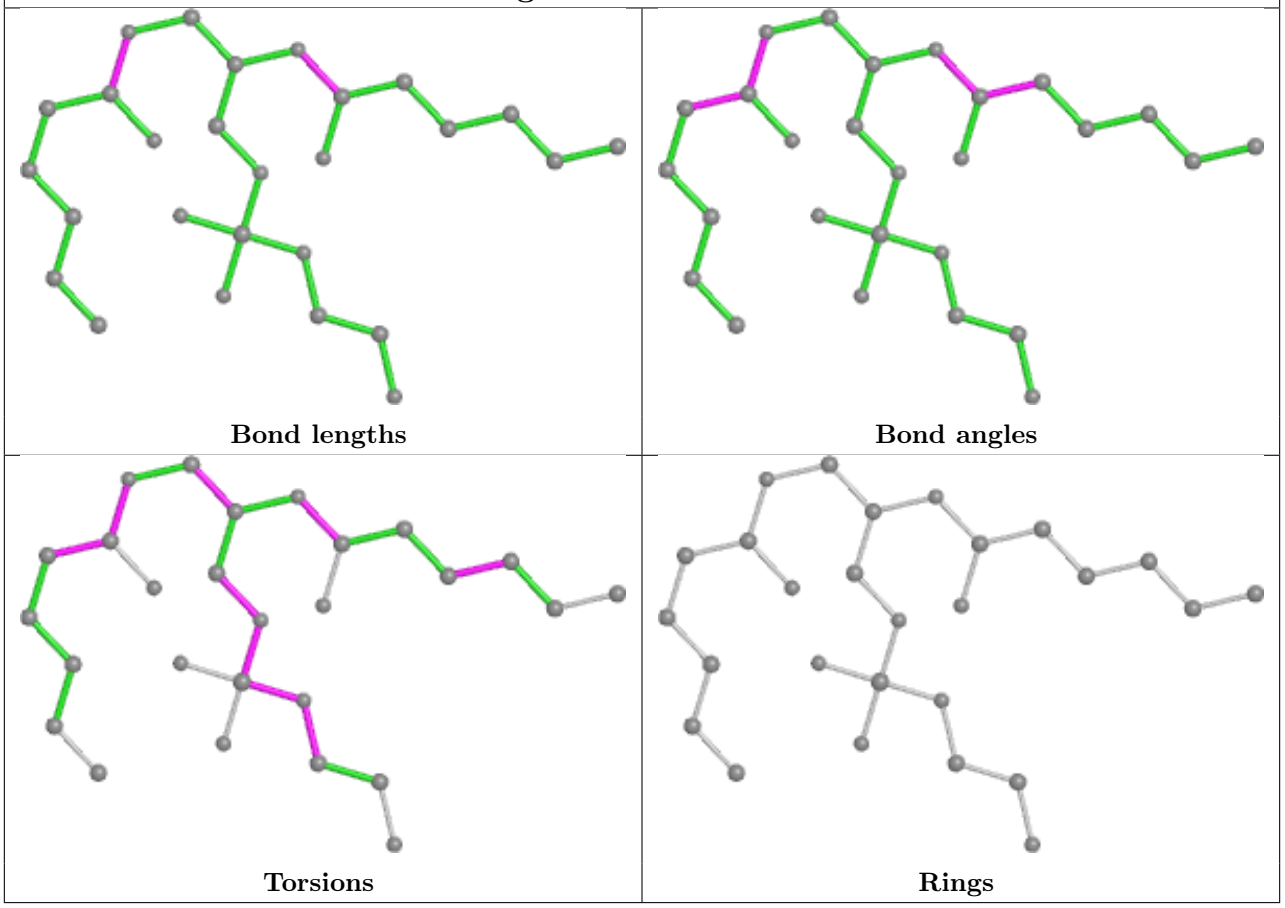


Torsions

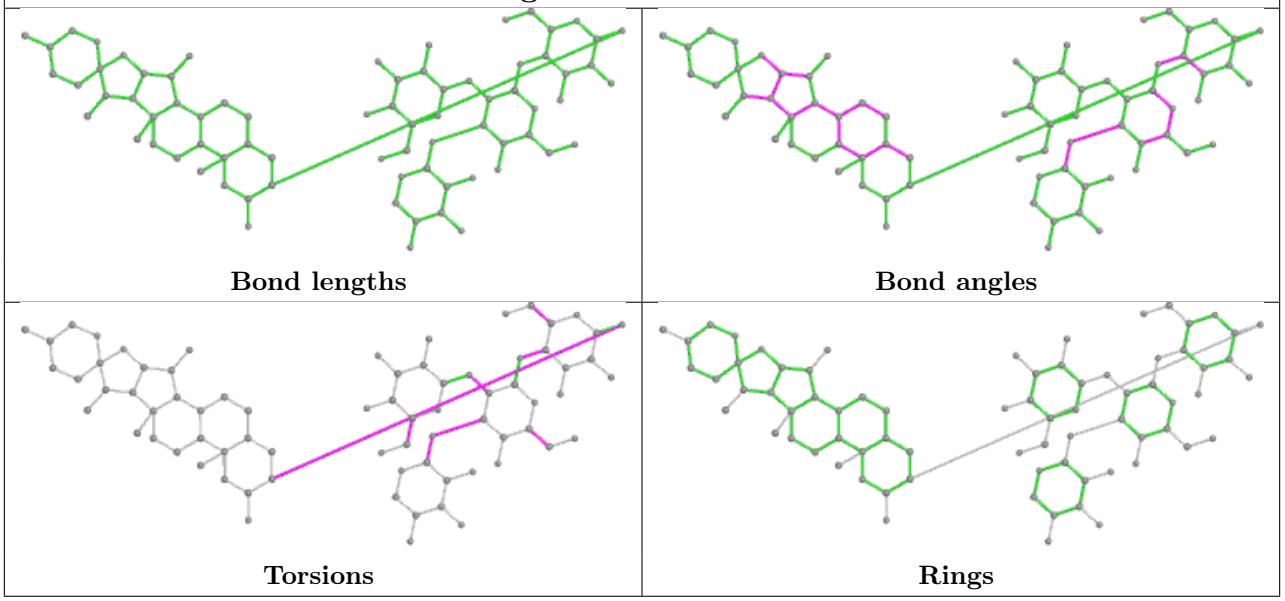


Rings

Ligand PTY F 1613



Ligand AJP F 1601



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.

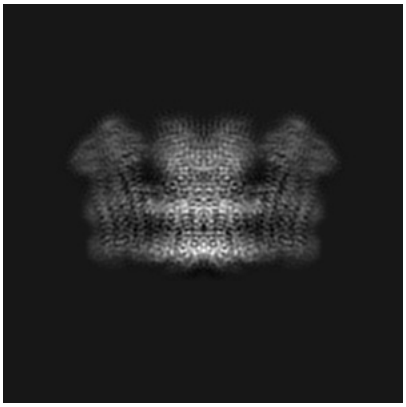
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9787. These allow visual inspection of the internal detail of the map and identification of artifacts.

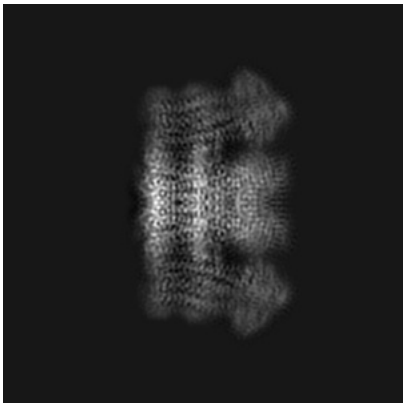
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

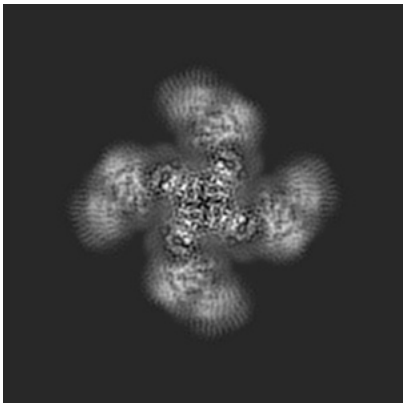
6.1.1 Primary map



X



Y

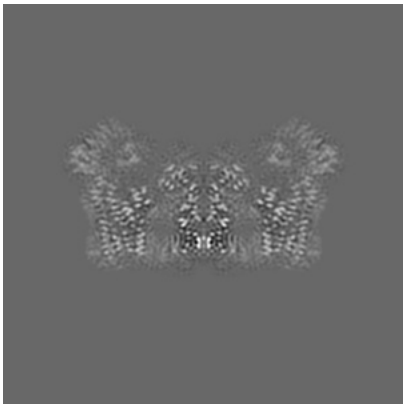


Z

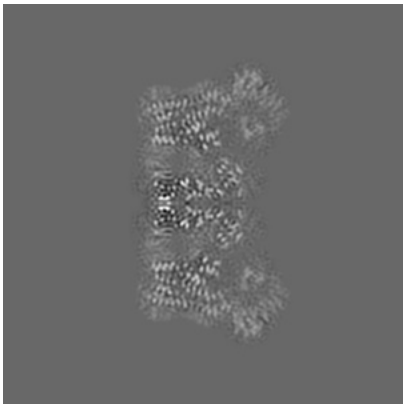
The images above show the map projected in three orthogonal directions.

6.2 Central slices

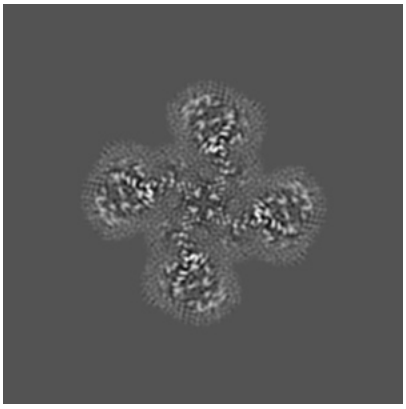
6.2.1 Primary map



X Index: 128



Y Index: 128

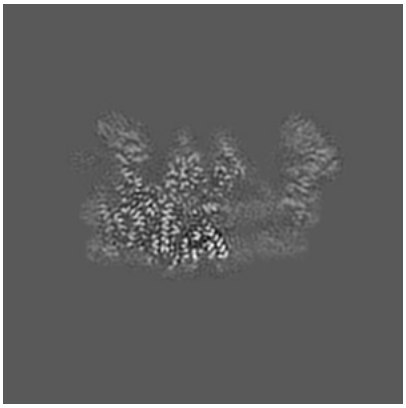


Z Index: 128

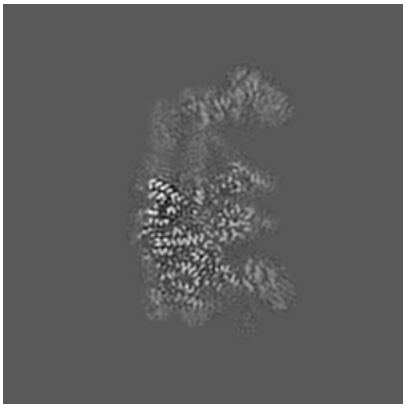
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

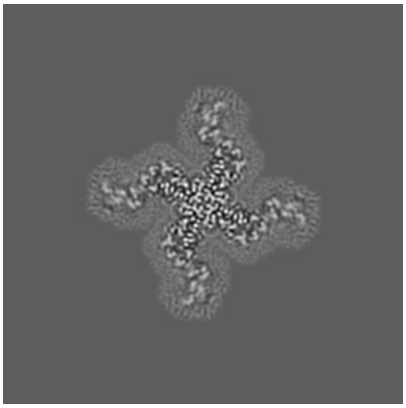
6.3.1 Primary map



X Index: 117



Y Index: 139

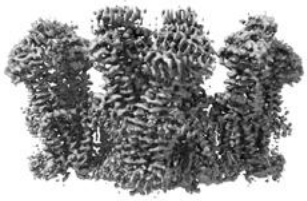


Z Index: 98

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

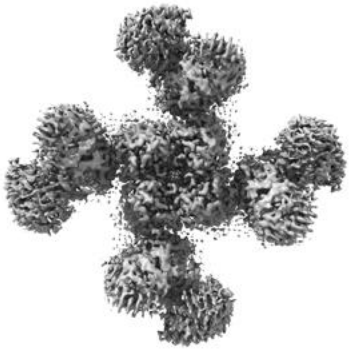
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

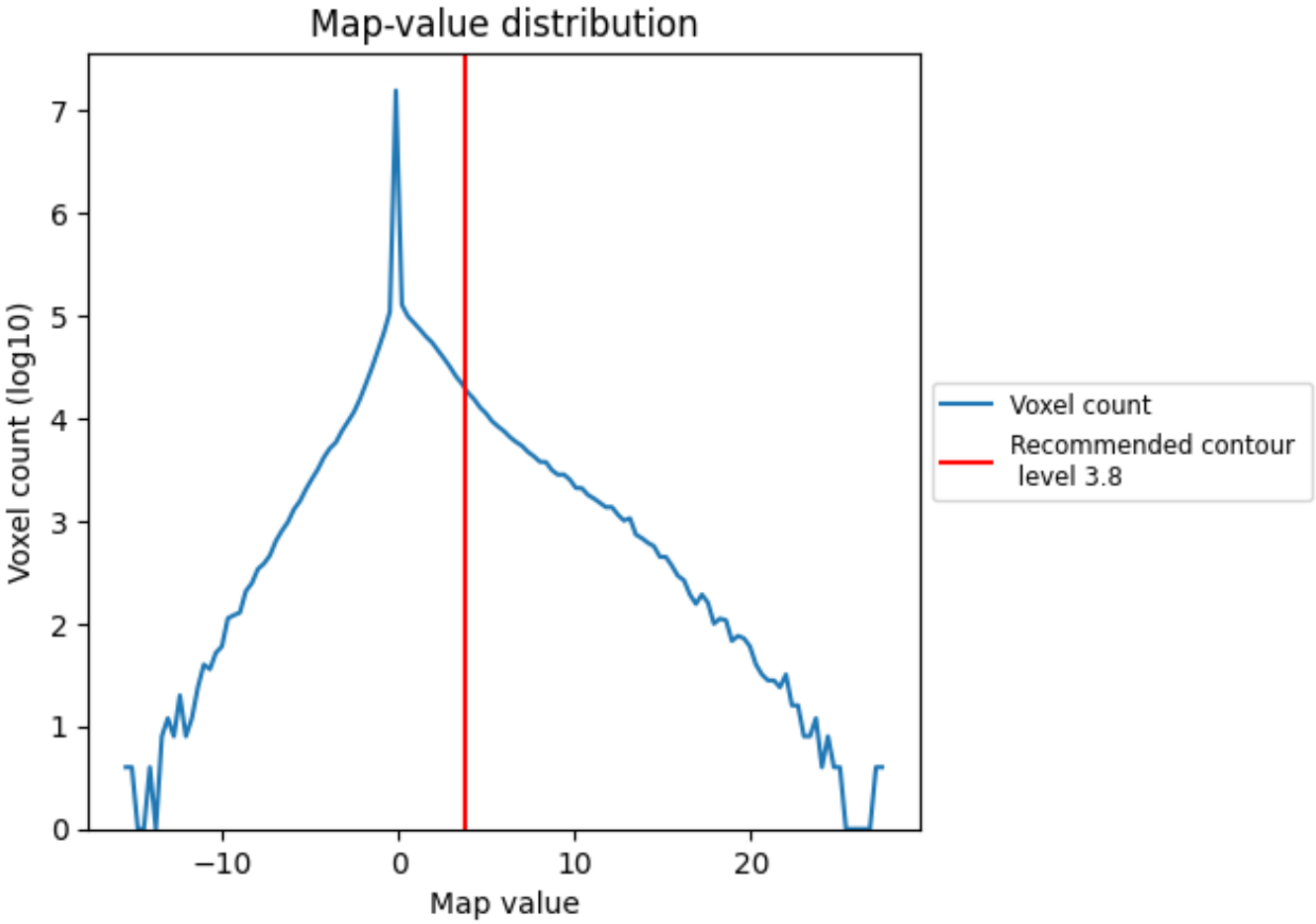
6.5 Mask visualisation (i)

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

7 Map analysis

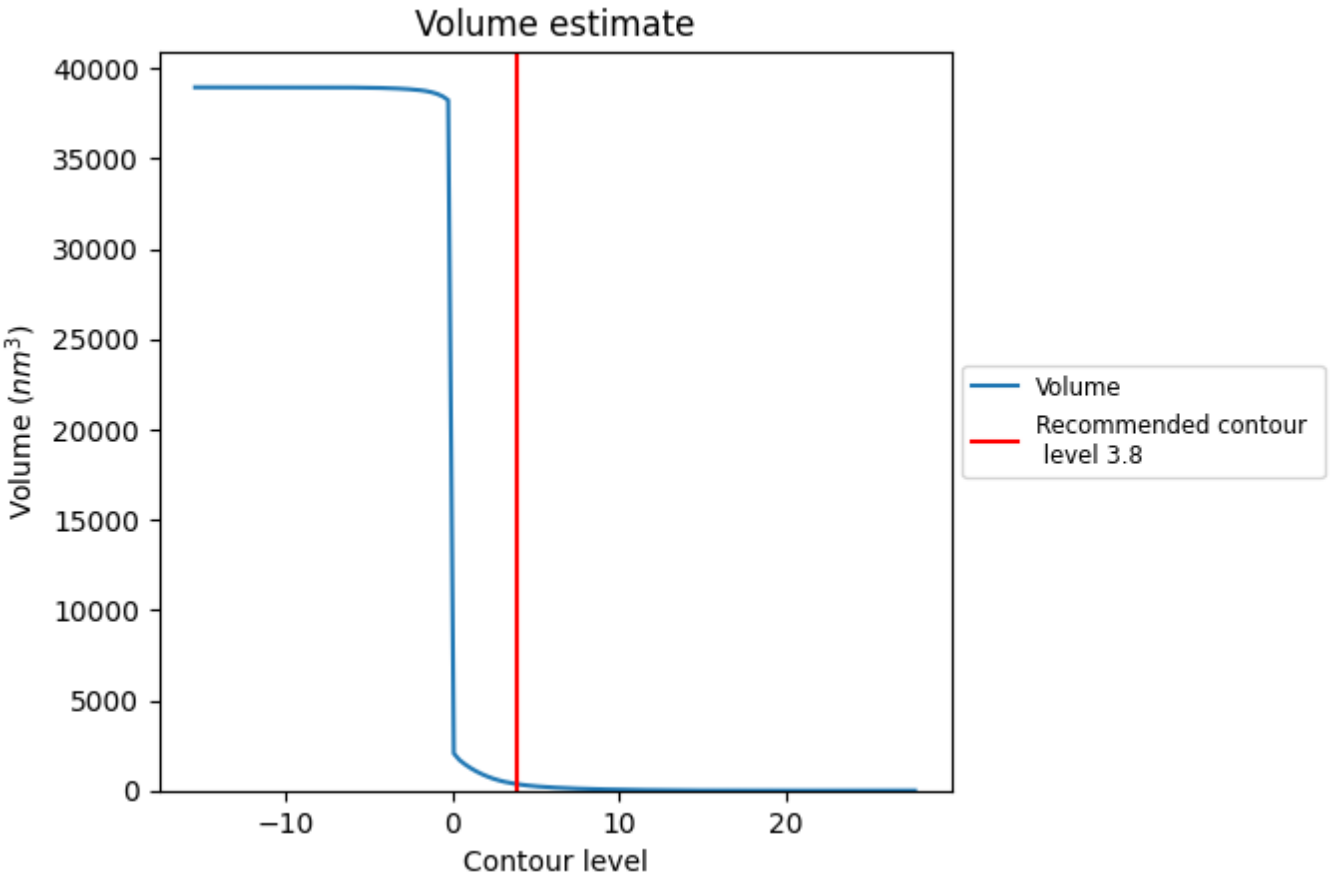
This section contains the results of statistical analysis of the map.

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.

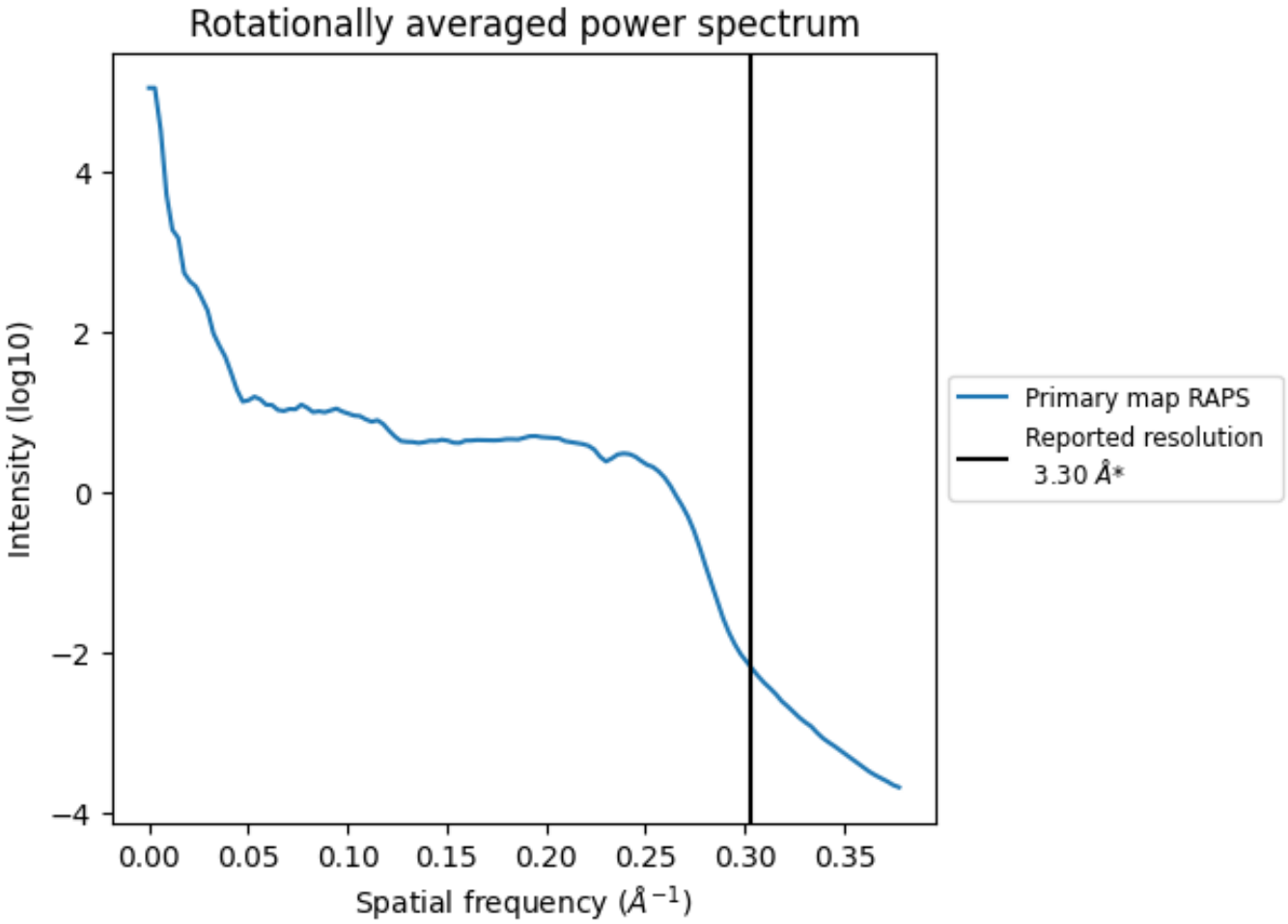
7.2 Volume estimate



The volume at the recommended contour level is 365 nm^3; this corresponds to an approximate mass of 330 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 0.303 Å^{-1}

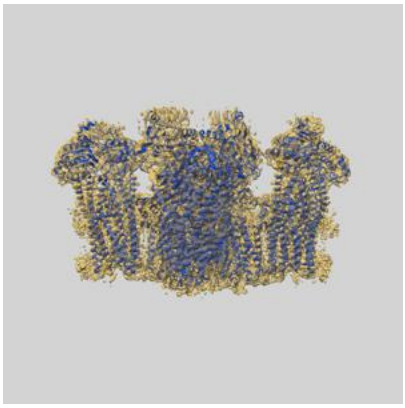
8 Fourier-Shell correlation

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

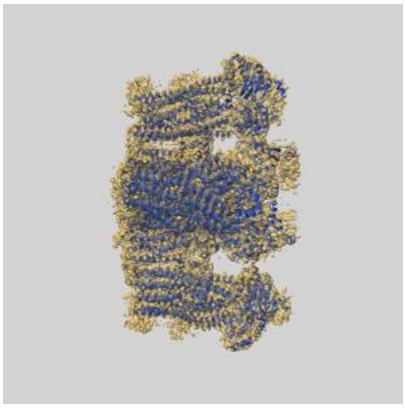
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9787 and PDB model 6JB1. Per-residue inclusion information can be found in section 3 on page 11.

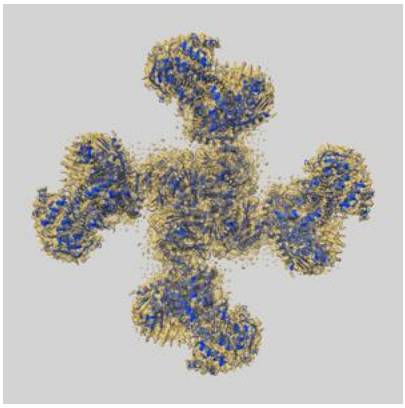
9.1 Map-model overlay



X



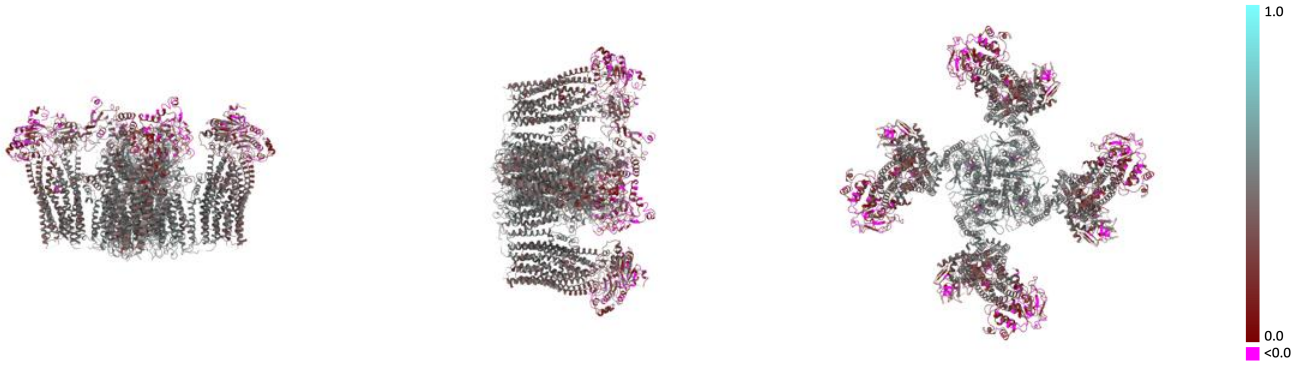
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.8 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.

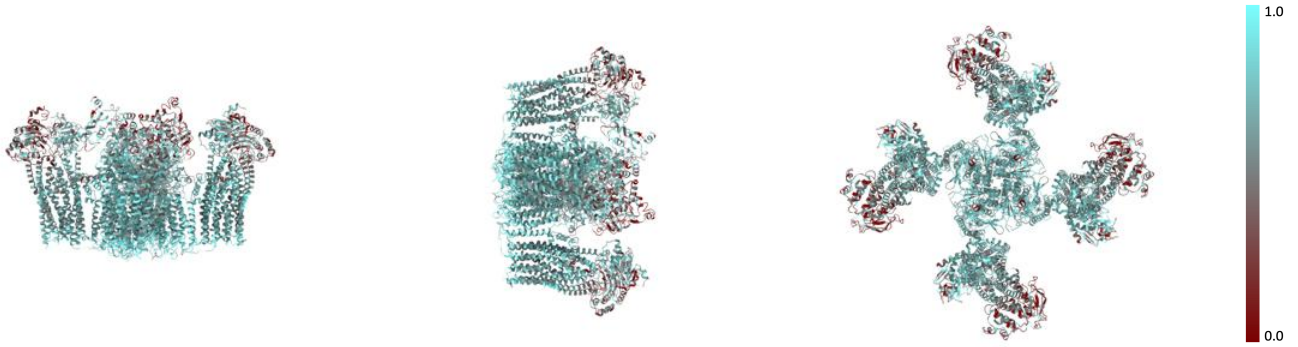
9.2 Q-score mapped to coordinate model (i)



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.

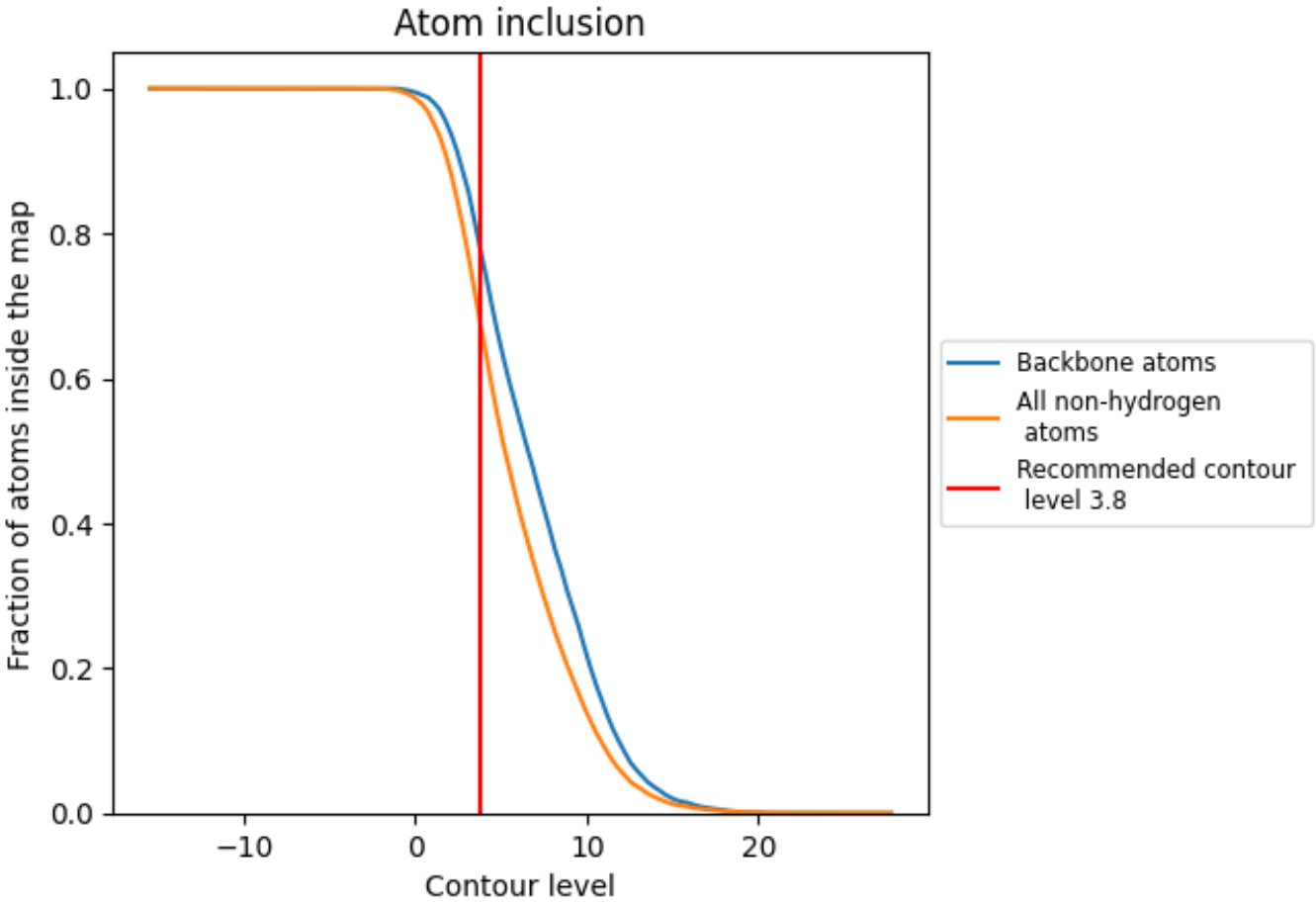
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.8).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 67% 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 (3.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6745	0.4060
A	0.7532	0.5010
B	0.6548	0.3820
C	0.7532	0.5000
D	0.6548	0.3820
E	0.7532	0.5010
F	0.6548	0.3830
G	0.7532	0.5000
H	0.6548	0.3820