Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 12:50 AM JST

PDB ID	:	7VH6
EMDB ID	:	EMD-31988
Title	:	Cryo-EM structure of the hexameric plasma membrane H+-ATPase in the active state (pH 6.0, BeF3-, conformation 1, C1 symmetry)
Authors	:	Zhao, P.; Zhao, C.; Chen, D.; Yun, C.; Li, H.; Bai, L.
Deposited on	:	2021-09-21
Resolution	:	3.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

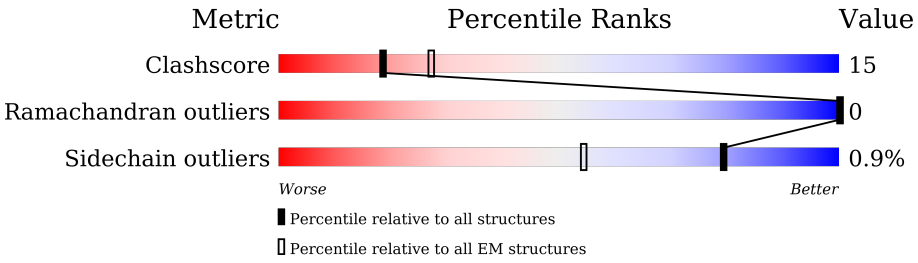
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	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	918	10% 61% 22% • 16%
1	B	918	16% 61% 22% • 16%
1	C	918	29% 61% 22% • 16%
1	D	918	44% 61% 22% • 16%
1	E	918	47% 62% 22% 16%
1	F	918	25% 62% 21% • 16%

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
2	BEF	A	1001	-	-	X	-
2	BEF	B	1001	-	-	X	-
2	BEF	C	1001	-	-	X	-
2	BEF	D	1001	-	-	X	-
2	BEF	E	1001	-	-	X	-
2	BEF	F	1001	-	-	X	-

2 Entry composition (i)

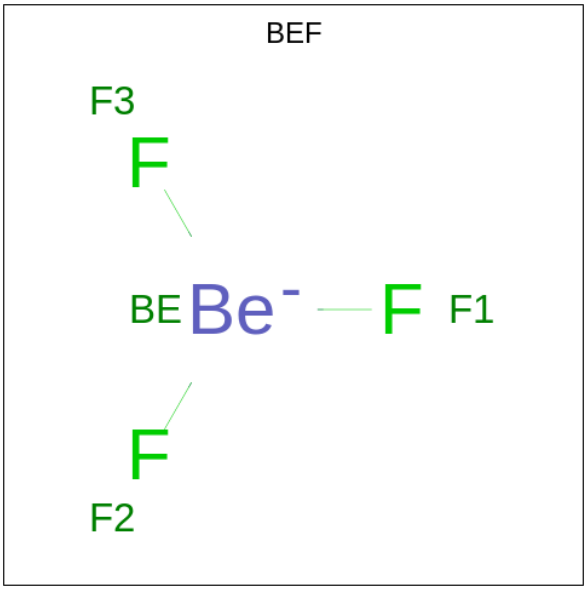
There are 3 unique types of molecules in this entry. The entry contains 38202 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Plasma membrane ATPase 1.

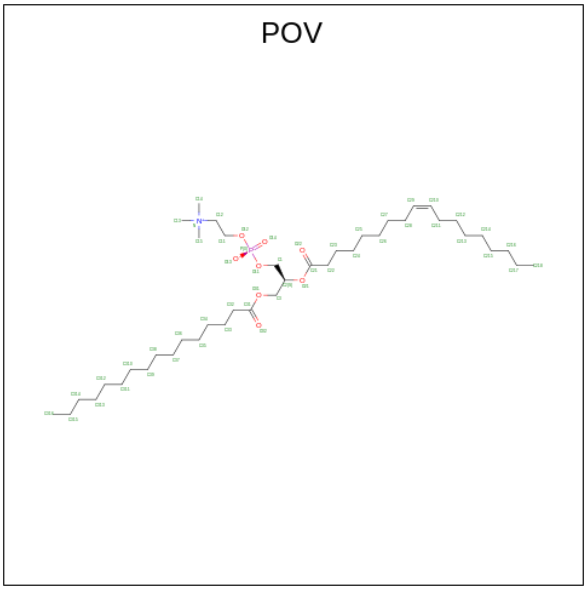
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	768	Total	C	N	O	S	0	0
			5869	3802	967	1073	27		
1	B	768	Total	C	N	O	S	0	0
			5869	3802	967	1073	27		
1	C	768	Total	C	N	O	S	0	0
			5869	3802	967	1073	27		
1	D	768	Total	C	N	O	S	0	0
			5869	3802	967	1073	27		
1	E	768	Total	C	N	O	S	0	0
			5869	3802	967	1073	27		
1	F	768	Total	C	N	O	S	0	0
			5869	3802	967	1073	27		

- Molecule 2 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total 4	Be 1	F 3	0
2	B	1	Total 4	Be 1	F 3	0
2	C	1	Total 4	Be 1	F 3	0
2	D	1	Total 4	Be 1	F 3	0
2	E	1	Total 4	Be 1	F 3	0
2	F	1	Total 4	Be 1	F 3	0

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



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 572	C 462	N 11	O 88	P 11	0
3	A	1	Total 572	C 462	N 11	O 88	P 11	0
3	A	1	Total 572	C 462	N 11	O 88	P 11	0
3	A	1	Total 572	C 462	N 11	O 88	P 11	0
3	A	1	Total 572	C 462	N 11	O 88	P 11	0

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Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O P 572 462 11 88 11	0
3	A	1	Total C N O P 572 462 11 88 11	0
3	A	1	Total C N O P 572 462 11 88 11	0
3	A	1	Total C N O P 572 462 11 88 11	0
3	A	1	Total C N O P 572 462 11 88 11	0
3	A	1	Total C N O P 572 462 11 88 11	0
3	B	1	Total C N O P 468 378 9 72 9	0
3	B	1	Total C N O P 468 378 9 72 9	0
3	B	1	Total C N O P 468 378 9 72 9	0
3	B	1	Total C N O P 468 378 9 72 9	0
3	B	1	Total C N O P 468 378 9 72 9	0
3	B	1	Total C N O P 468 378 9 72 9	0
3	B	1	Total C N O P 468 378 9 72 9	0
3	B	1	Total C N O P 468 378 9 72 9	0
3	B	1	Total C N O P 468 378 9 72 9	0
3	C	1	Total C N O P 468 378 9 72 9	0
3	C	1	Total C N O P 468 378 9 72 9	0
3	C	1	Total C N O P 468 378 9 72 9	0
3	C	1	Total C N O P 468 378 9 72 9	0
3	C	1	Total C N O P 468 378 9 72 9	0
3	C	1	Total C N O P 468 378 9 72 9	0

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Mol	Chain	Residues	Atoms	AltConf
3	C	1	Total C N O P 468 378 9 72 9	0
3	C	1	Total C N O P 468 378 9 72 9	0
3	C	1	Total C N O P 468 378 9 72 9	0
3	D	1	Total C N O P 520 420 10 80 10	0
3	D	1	Total C N O P 520 420 10 80 10	0
3	D	1	Total C N O P 520 420 10 80 10	0
3	D	1	Total C N O P 520 420 10 80 10	0
3	D	1	Total C N O P 520 420 10 80 10	0
3	D	1	Total C N O P 520 420 10 80 10	0
3	D	1	Total C N O P 520 420 10 80 10	0
3	D	1	Total C N O P 520 420 10 80 10	0
3	D	1	Total C N O P 520 420 10 80 10	0
3	D	1	Total C N O P 520 420 10 80 10	0
3	E	1	Total C N O P 468 378 9 72 9	0
3	E	1	Total C N O P 468 378 9 72 9	0
3	E	1	Total C N O P 468 378 9 72 9	0
3	E	1	Total C N O P 468 378 9 72 9	0
3	E	1	Total C N O P 468 378 9 72 9	0
3	E	1	Total C N O P 468 378 9 72 9	0
3	E	1	Total C N O P 468 378 9 72 9	0
3	E	1	Total C N O P 468 378 9 72 9	0

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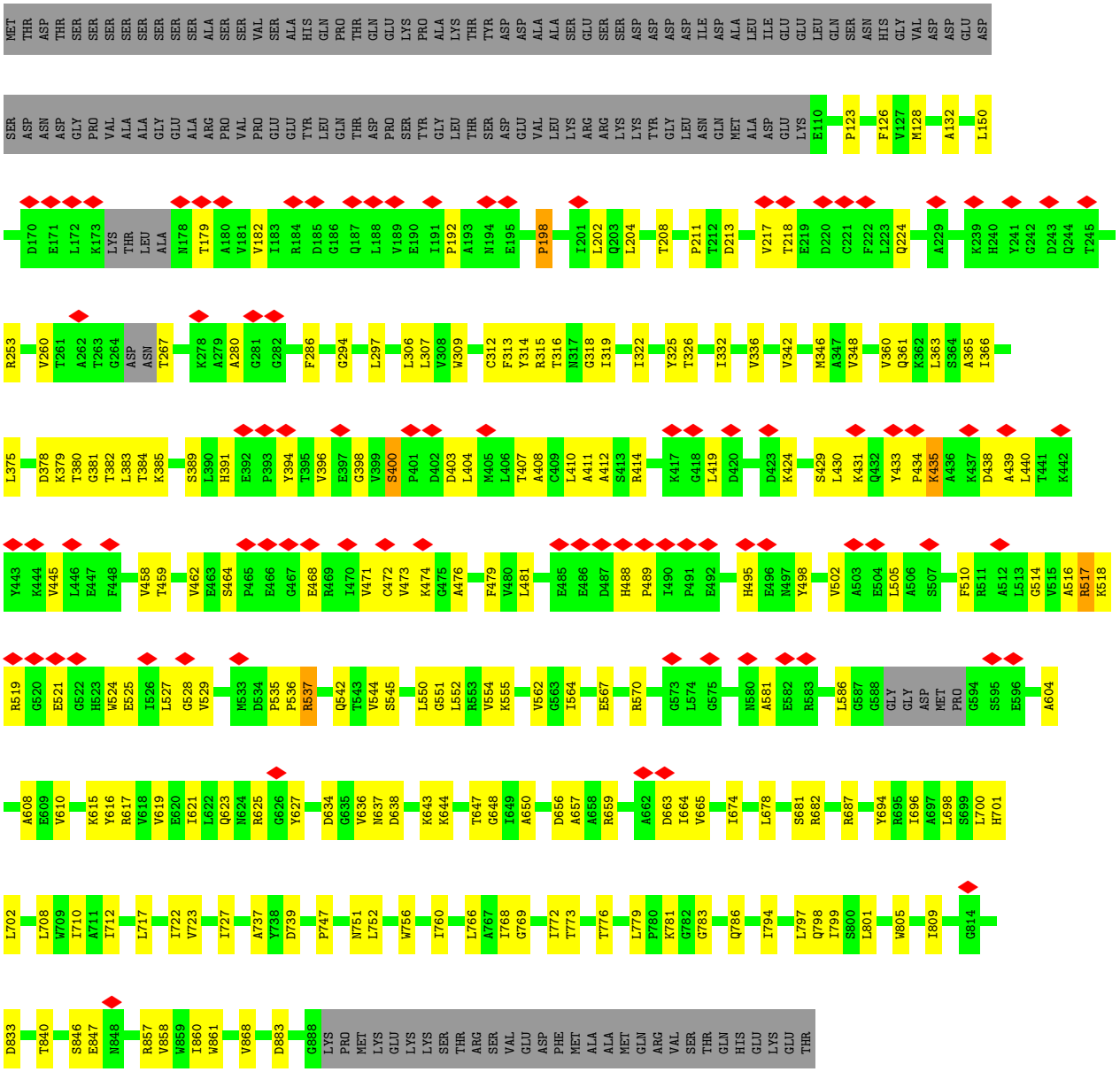
Mol	Chain	Residues	Atoms	AltConf
3	E	1	Total C N O P 468 378 9 72 9	0
3	F	1	Total C N O P 468 378 9 72 9	0
3	F	1	Total C N O P 468 378 9 72 9	0
3	F	1	Total C N O P 468 378 9 72 9	0
3	F	1	Total C N O P 468 378 9 72 9	0
3	F	1	Total C N O P 468 378 9 72 9	0
3	F	1	Total C N O P 468 378 9 72 9	0
3	F	1	Total C N O P 468 378 9 72 9	0
3	F	1	Total C N O P 468 378 9 72 9	0
3	F	1	Total C N O P 468 378 9 72 9	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

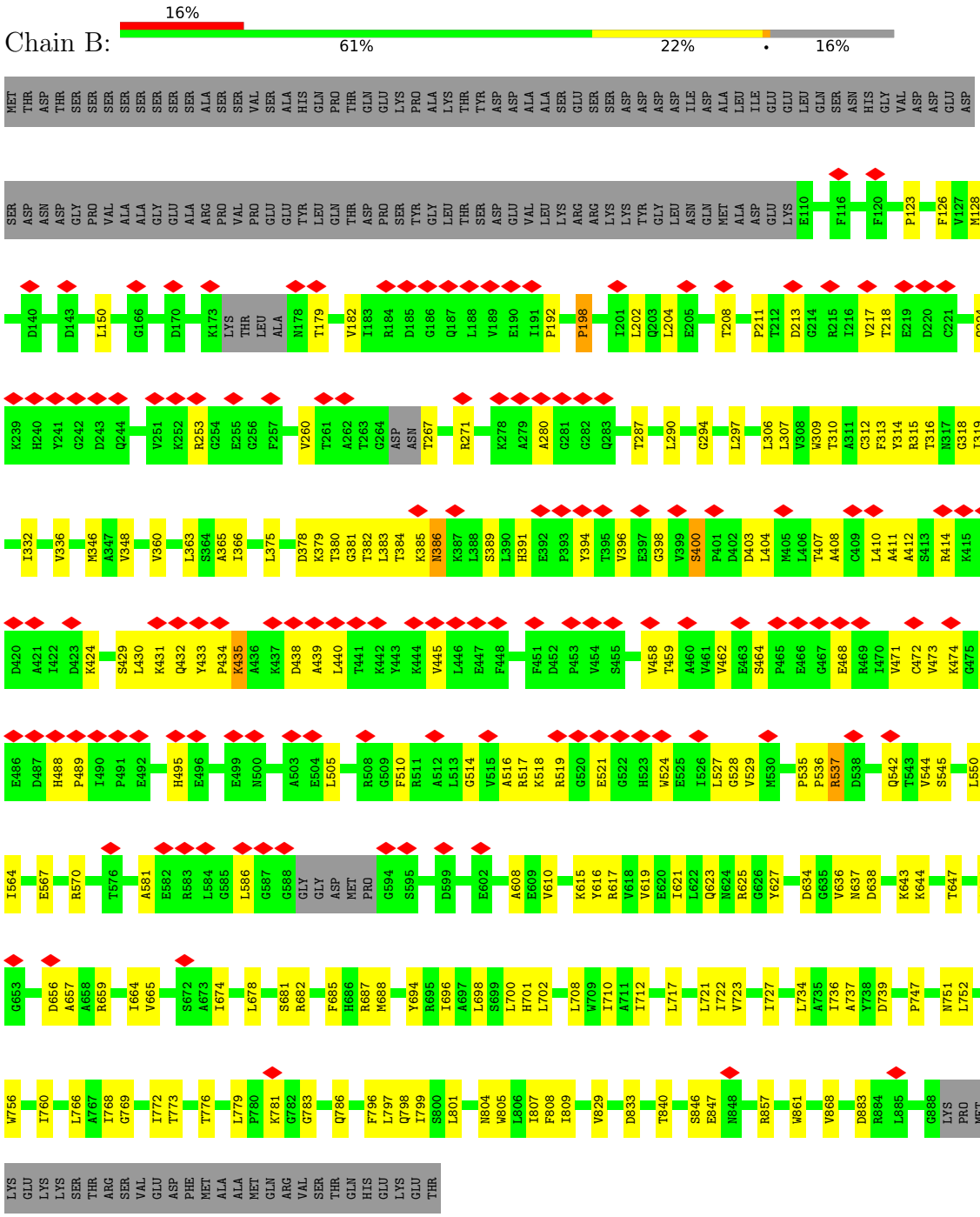
- Molecule 1: Plasma membrane ATPase 1

Chain A:



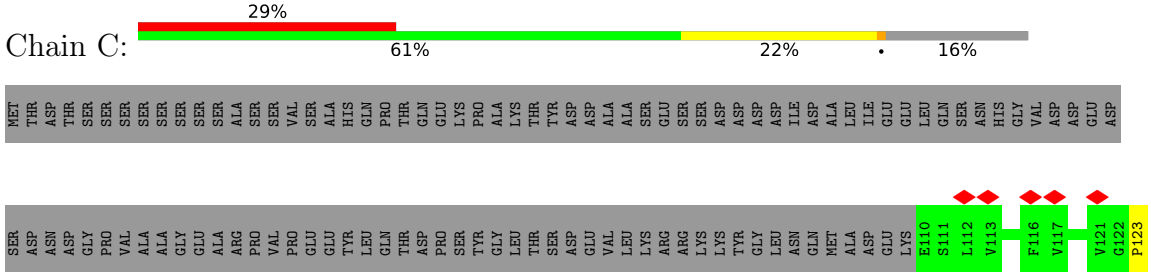
• Molecule 1: Plasma membrane ATPase 1

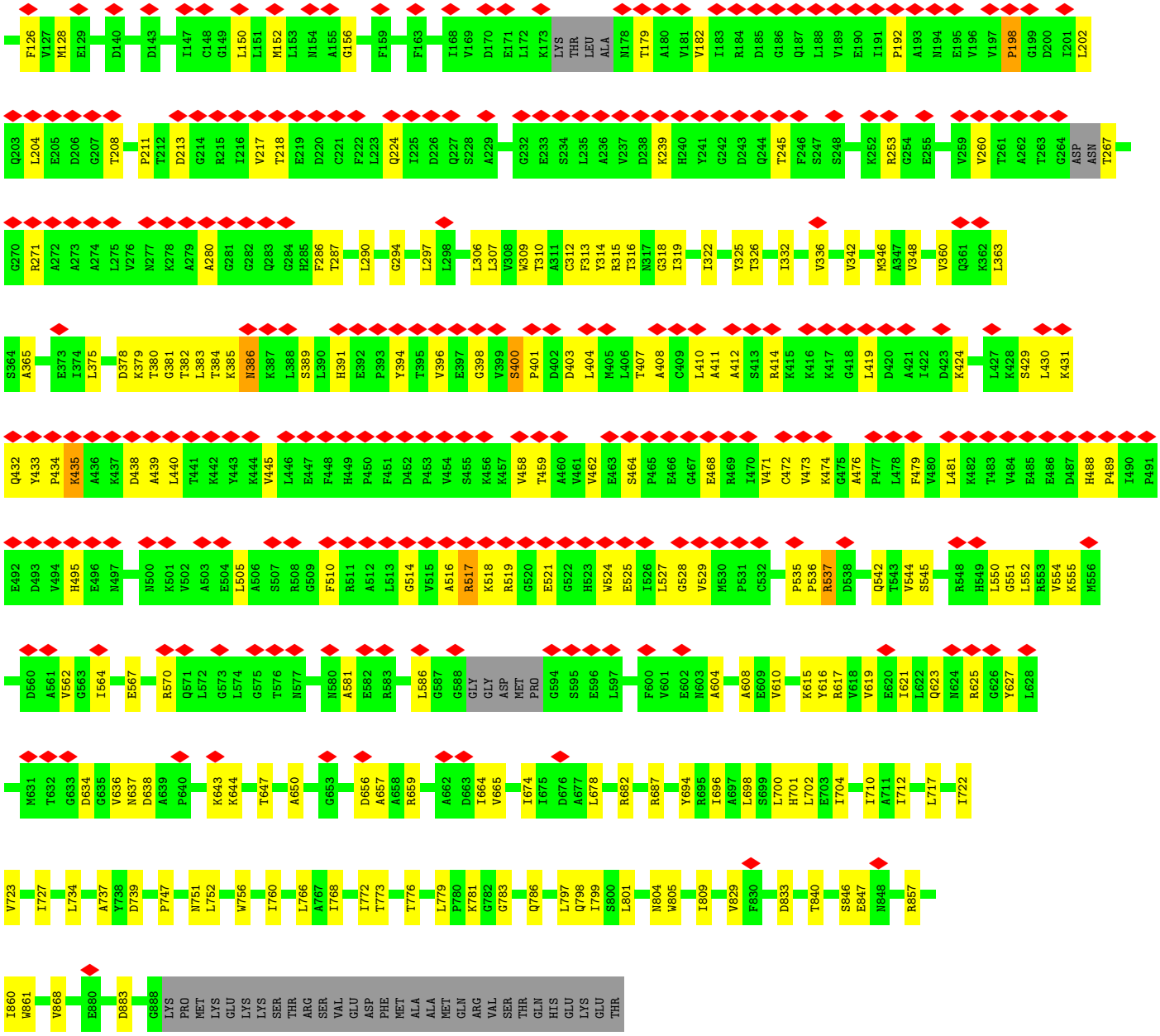
Chain B:



• Molecule 1: Plasma membrane ATPase 1

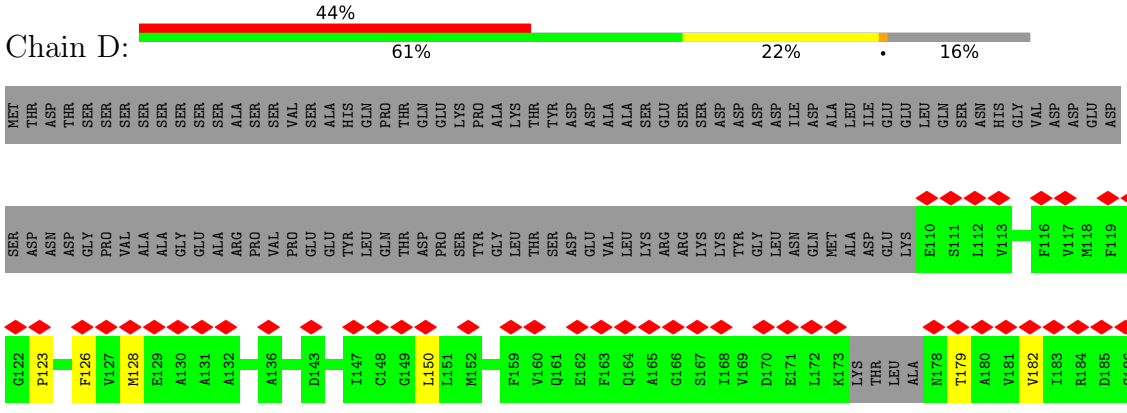
Chain C:





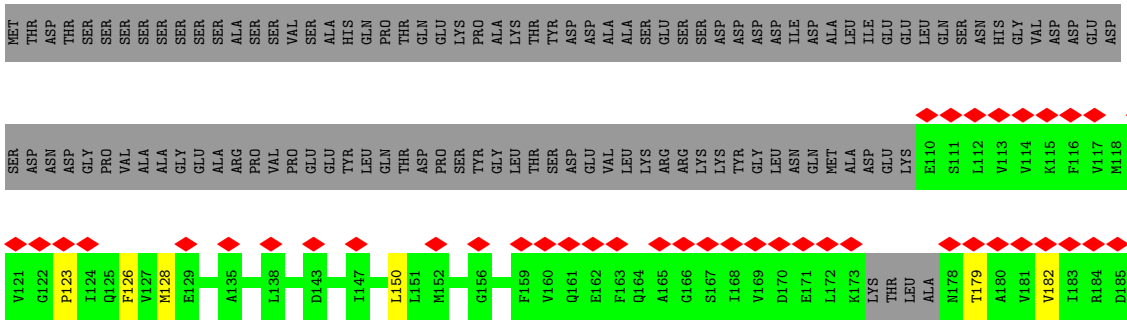
• Molecule 1: Plasma membrane ATPase 1

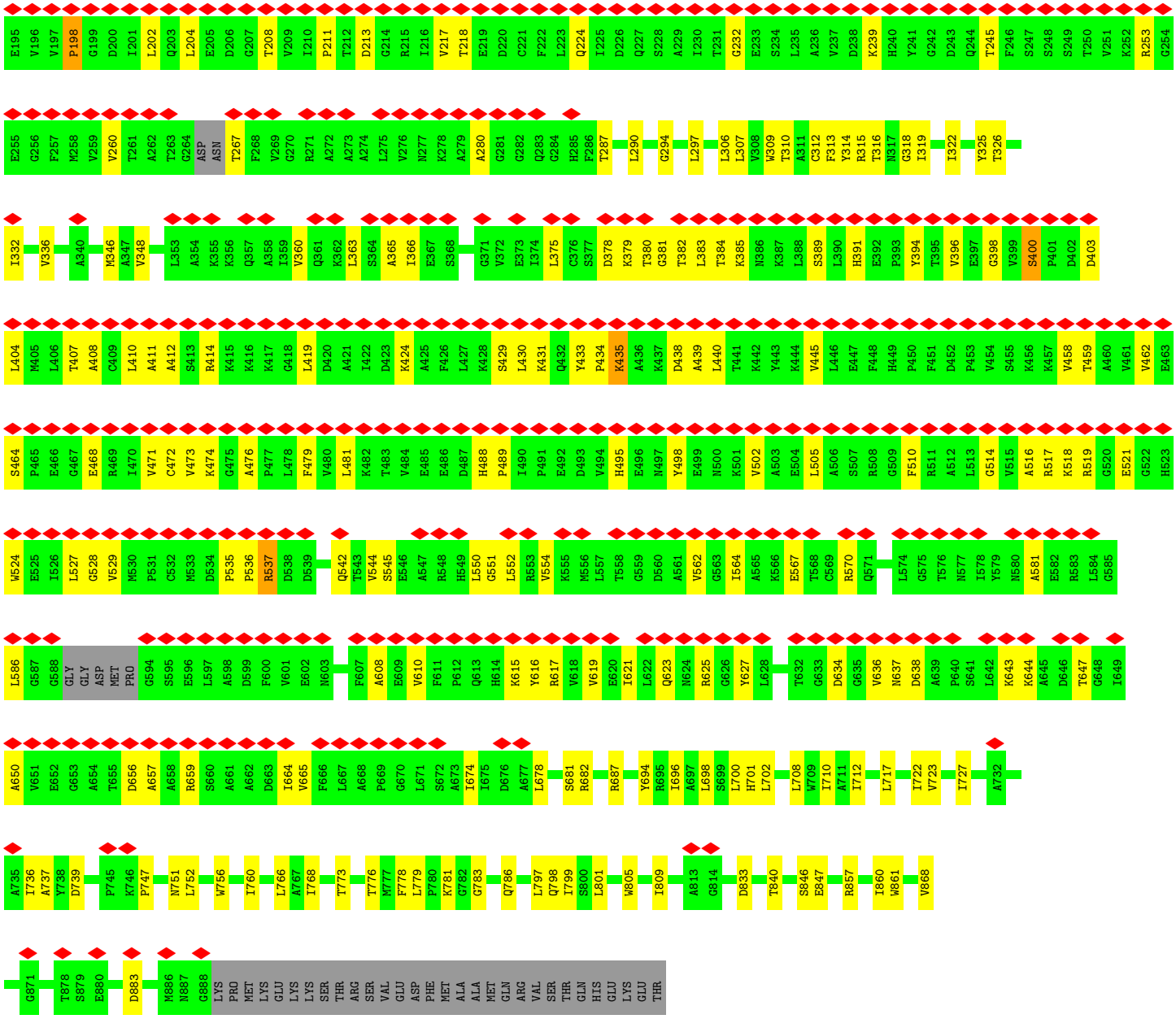
Chain D:



- Molecule 1: Plasma membrane ATPase 1

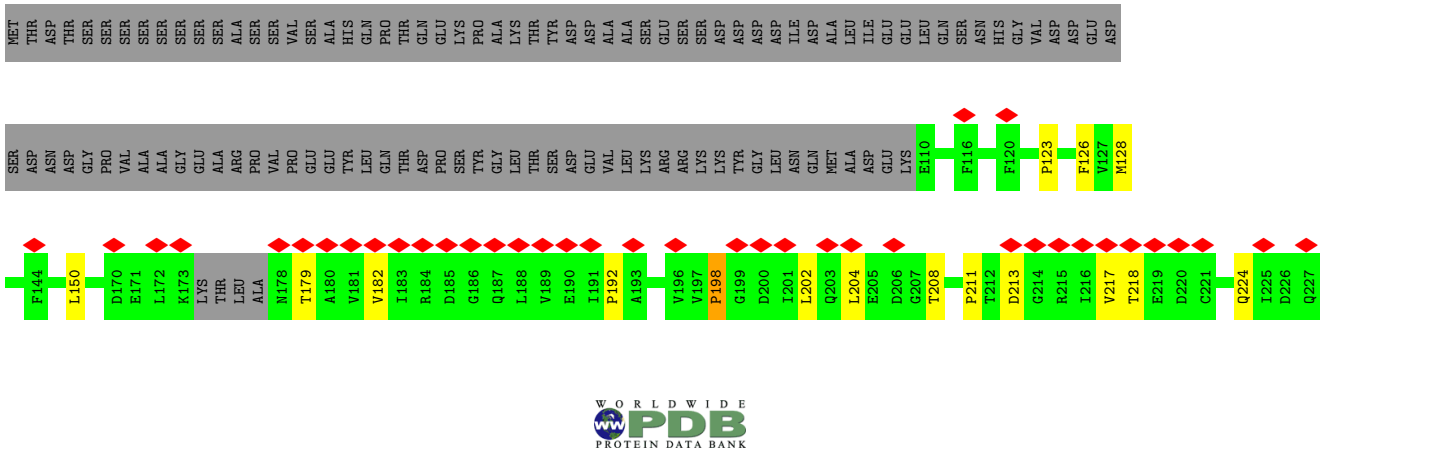
Chain E:

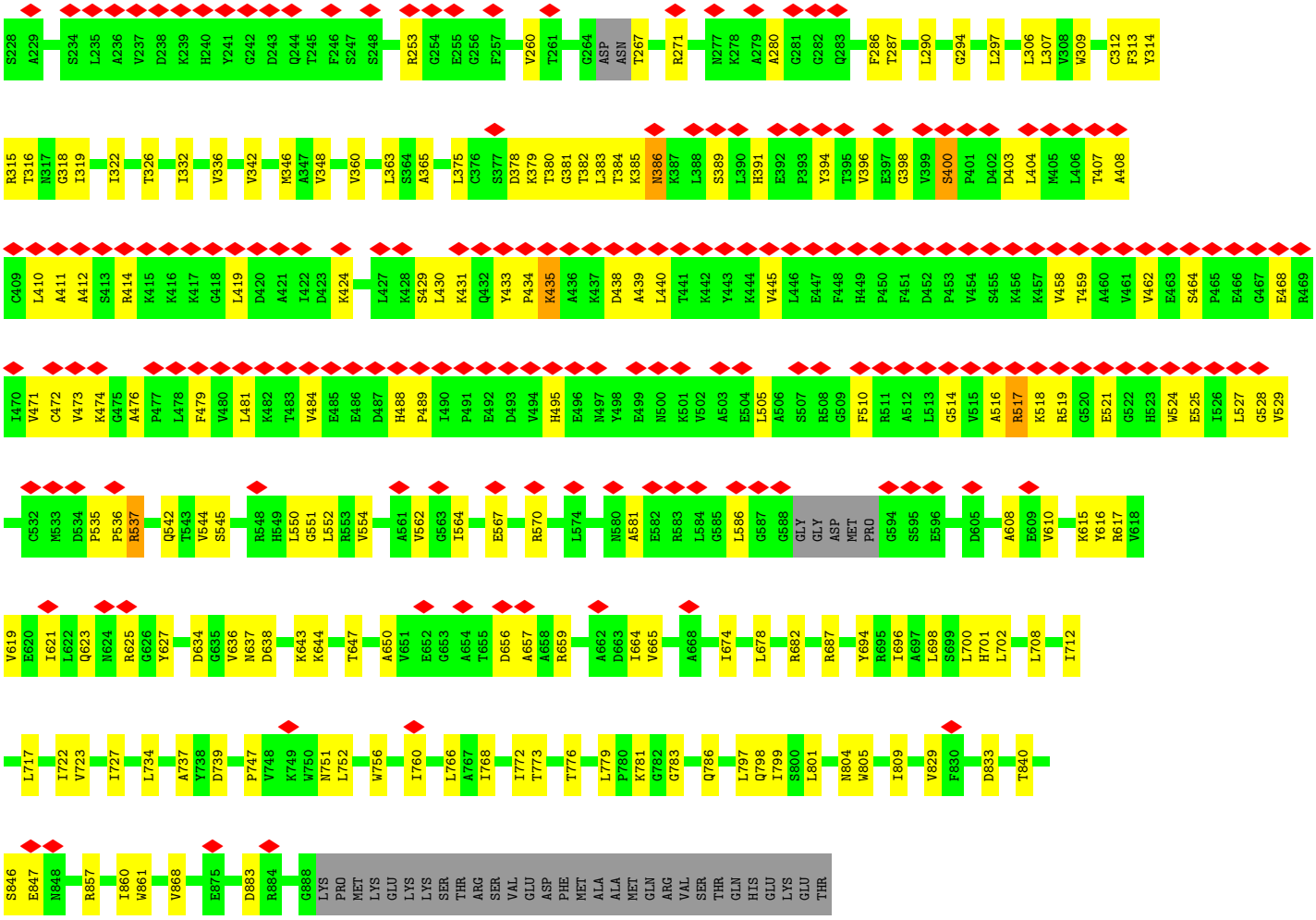




• Molecule 1: Plasma membrane ATPase 1

Chain F:




S228 A229 S234 L235 A236 V237 D238 K239 H240 Y241 G242 D243 Q244 T245 F246 S247 S248 R253 G254 E255 G256 F257 V260 T261 C264 ASP ASN T267 R271 N277 K278 A279 A280 G281 G282 Q283 F286 T287 L290 G294 L297 L306 L307 V308 W309 C312 F313 Y314
R315 T316 N317 G318 I319 I322 T326 I332 V336 V342 M346 A347 V348 V360 L363 S364 A365 L375 C376 S377 D378 K379 T380 G381 T382 L383 T384 K385 N386 K387 L388 S389 L390 H391 E392 P393 Y394 T395 V396 E397 G398 V399 S400 P401 D402 D403 L404 M405 L406 T407 A408
C409 L410 A411 A412 S413 R414 K415 K416 K417 G418 L419 D420 A421 I422 D423 K424 L427 K428 S429 L430 K431 Q432 Y433 P434 K435 A436 K437 D438 A439 L440 T441 K442 Y443 K444 V445 L446 E447 F448 H449 P450 F451 D452 P453 V454 S455 K456 K457 V458 T459 A460 V461 V462 E463 S464 P465 E466 G467 E468 R469
I470 V471 C472 V473 K474 G475 A476 P477 L478 F479 V480 L481 K482 T483 V484 E485 E486 D487 H488 P489 I490 P491 E492 D493 V494 H495 E496 N497 Y498 E499 N500 K501 V502 A503 E504 L505 A506 S507 R508 G509 F510 R511 A512 L513 G514 V515 A516 R517 K518 R519 G520 E521 G522 H523 W524 E525 I526 L527 G528 V529
C532 M533 D534 P535 P536 R537 Q542 T543 V544 S545 R548 H549 L550 G551 L552 R553 V554 A561 V562 G563 I564 E567 R570 L574 N580 A581 E582 R583 L584 G585 L586 G587 G588 GLY GLY ASP MET PRO G594 S595 E596 D605 A608 E609 V610 K615 Y616 R617 V618
V619 E620 I621 L622 Q623 N624 R625 G626 Y627 D634 G635 V636 N637 D638 K643 K644 T647 A650 V651 E652 G653 A654 T655 D656 A657 A658 R659 A662 D663 I664 V665 A668 I674 L678 R682 R687 Y694 R695 I696 A697 L698 S699 L700 H701 L702 L708 I712
L717 I722 V723 I727 L734 A737 Y738 D739 P747 V748 K749 W750 N751 L752 W756 I760 L766 A767 I768 I772 T773 T776 L779 P780 K781 G782 G783 Q786 L797 Q798 I799 S800 L801 N804 W805 I809 V829 F830 D833 T840
S846 E847 N848 R857 I860 W861 V868 E875 D883 R884 G888 LYS PRO MET LYS GLU LYS LYS SER THR ARG SER VAL GLU ASP PHE MET ALA ALA MET GLN ARG VAL SER THR GLN HIS GLU LYS GLU THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63661	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 ($e^-/Å^2$)	1.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.34	1/5989 (0.0%)	0.57	5/8141 (0.1%)
1	B	0.34	1/5989 (0.0%)	0.57	5/8141 (0.1%)
1	C	0.34	1/5989 (0.0%)	0.57	5/8141 (0.1%)
1	D	0.34	1/5989 (0.0%)	0.57	5/8141 (0.1%)
1	E	0.34	1/5989 (0.0%)	0.57	5/8141 (0.1%)
1	F	0.34	1/5989 (0.0%)	0.57	5/8141 (0.1%)
All	All	0.34	6/35934 (0.0%)	0.57	30/48846 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	PRO	CG-CD	-11.21	1.13	1.50
1	F	198	PRO	CG-CD	-11.21	1.13	1.50
1	D	198	PRO	CG-CD	-11.20	1.13	1.50
1	E	198	PRO	CG-CD	-11.19	1.13	1.50
1	A	198	PRO	CG-CD	-11.19	1.13	1.50
1	C	198	PRO	CG-CD	-11.16	1.13	1.50

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	198	PRO	N-CD-CG	-12.83	83.96	103.20
1	A	198	PRO	N-CD-CG	-12.82	83.97	103.20
1	F	198	PRO	N-CD-CG	-12.81	83.98	103.20
1	E	198	PRO	N-CD-CG	-12.81	83.99	103.20
1	B	198	PRO	N-CD-CG	-12.80	84.00	103.20
1	D	198	PRO	N-CD-CG	-12.78	84.04	103.20
1	D	198	PRO	CA-N-CD	-8.29	99.90	111.50
1	A	198	PRO	CA-N-CD	-8.28	99.91	111.50
1	B	198	PRO	CA-N-CD	-8.28	99.91	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	198	PRO	CA-N-CD	-8.27	99.92	111.50
1	F	198	PRO	CA-N-CD	-8.26	99.93	111.50
1	C	198	PRO	CA-N-CD	-8.23	99.98	111.50
1	F	211	PRO	CA-N-CD	-7.26	101.33	111.50
1	A	211	PRO	CA-N-CD	-7.26	101.34	111.50
1	C	211	PRO	CA-N-CD	-7.26	101.34	111.50
1	B	211	PRO	CA-N-CD	-7.26	101.34	111.50
1	D	211	PRO	CA-N-CD	-7.25	101.35	111.50
1	E	211	PRO	CA-N-CD	-7.24	101.36	111.50
1	B	198	PRO	CA-CB-CG	-7.10	90.52	104.00
1	A	198	PRO	CA-CB-CG	-7.08	90.54	104.00
1	D	198	PRO	CA-CB-CG	-7.08	90.54	104.00
1	C	198	PRO	CA-CB-CG	-7.07	90.56	104.00
1	F	198	PRO	CA-CB-CG	-7.07	90.56	104.00
1	E	198	PRO	CA-CB-CG	-7.07	90.58	104.00
1	A	552	LEU	CA-CB-CG	5.14	127.12	115.30
1	E	552	LEU	CA-CB-CG	5.14	127.12	115.30
1	C	552	LEU	CA-CB-CG	5.13	127.11	115.30
1	D	552	LEU	CA-CB-CG	5.13	127.11	115.30
1	B	552	LEU	CA-CB-CG	5.13	127.10	115.30
1	F	552	LEU	CA-CB-CG	5.13	127.09	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	5869	0	5973	181	0
1	B	5869	0	5973	180	0
1	C	5869	0	5973	194	0
1	D	5869	0	5973	188	0
1	E	5869	0	5973	171	0
1	F	5869	0	5973	186	0
2	A	4	0	0	3	0
2	B	4	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	4	0	0	3	0
2	D	4	0	0	3	0
2	E	4	0	0	3	0
2	F	4	0	0	3	0
3	A	572	0	900	67	0
3	B	468	0	736	48	0
3	C	468	0	734	58	0
3	D	520	0	818	55	0
3	E	468	0	736	45	0
3	F	468	0	736	45	0
All	All	38202	0	40498	1143	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 15.

All (1143) 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:C:400:SER:O	1:C:404:LEU:HG	1.23	1.32
1:F:400:SER:O	1:F:404:LEU:HG	1.21	1.30
1:D:400:SER:O	1:D:404:LEU:HG	1.23	1.29
1:B:400:SER:O	1:B:404:LEU:HG	1.24	1.28
1:F:315:ARG:NE	3:F:1002:POV:O13	1.67	1.28
1:A:400:SER:O	1:A:404:LEU:HG	1.23	1.27
1:E:400:SER:O	1:E:404:LEU:HG	1.23	1.26
1:B:315:ARG:NE	3:B:1004:POV:O13	1.68	1.25
1:A:315:ARG:NE	3:A:1003:POV:O13	1.70	1.22
1:E:316:THR:CG2	1:F:783:GLY:H	1.52	1.20
1:C:316:THR:CG2	1:D:783:GLY:H	1.58	1.16
1:E:315:ARG:NE	3:E:1003:POV:O13	1.80	1.14
1:A:316:THR:CG2	1:B:783:GLY:H	1.60	1.13
1:D:768:ILE:HD12	3:D:1004:POV:H21J	1.16	1.10
1:C:768:ILE:HD12	3:C:1004:POV:H21J	1.28	1.09
1:A:781:LYS:O	1:F:316:THR:HG21	1.51	1.09
1:A:783:GLY:H	1:F:316:THR:CG2	1.66	1.07
1:E:316:THR:HG21	1:F:781:LYS:O	1.55	1.05
1:B:316:THR:HG21	1:C:781:LYS:O	1.57	1.03
1:D:316:THR:HG21	1:E:781:LYS:O	1.60	1.02
1:D:316:THR:CG2	1:E:783:GLY:H	1.74	1.00
1:B:316:THR:CG2	1:C:783:GLY:H	1.74	1.00
1:D:400:SER:HB3	1:D:403:ASP:HB3	1.44	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:400:SER:HB3	1:F:403:ASP:HB3	1.46	0.98
1:C:400:SER:HB3	1:C:403:ASP:HB3	1.43	0.96
1:E:316:THR:CG2	1:F:783:GLY:N	2.30	0.95
1:E:768:ILE:HD13	3:E:1004:POV:H31D	1.50	0.93
1:A:400:SER:HB3	1:A:403:ASP:HB3	1.46	0.93
1:A:316:THR:HG21	1:B:781:LYS:O	1.67	0.92
1:E:768:ILE:CD1	3:E:1004:POV:H31D	2.00	0.92
1:C:316:THR:HG21	1:D:781:LYS:O	1.68	0.92
1:C:306:LEU:CD1	1:D:868:VAL:CG2	2.48	0.92
1:D:315:ARG:HB3	3:D:1002:POV:H14B	1.50	0.90
1:E:400:SER:HB3	1:E:403:ASP:HB3	1.53	0.90
1:C:315:ARG:NH1	3:C:1003:POV:O13	2.05	0.90
1:E:314:TYR:O	1:F:779:LEU:HD22	1.72	0.89
1:C:316:THR:CG2	1:D:783:GLY:N	2.35	0.89
1:E:313:PHE:O	1:F:783:GLY:O	1.91	0.89
1:A:316:THR:HG22	1:B:783:GLY:H	1.35	0.89
1:D:315:ARG:NH1	3:D:1003:POV:O13	2.05	0.88
1:A:314:TYR:O	1:B:779:LEU:HD22	1.75	0.87
1:A:779:LEU:HD22	1:F:314:TYR:O	1.73	0.87
1:B:768:ILE:CD1	3:B:1005:POV:H31D	2.05	0.86
1:C:712:ILE:HG13	3:C:1003:POV:H32A	1.55	0.86
1:F:400:SER:CB	1:F:403:ASP:HB3	2.04	0.86
1:B:768:ILE:HD13	3:B:1005:POV:H31D	1.58	0.86
1:F:768:ILE:HD13	3:F:1003:POV:H31D	1.57	0.86
1:C:315:ARG:HB3	3:C:1002:POV:H14B	1.56	0.86
1:A:783:GLY:H	1:F:316:THR:HG22	1.41	0.85
1:C:306:LEU:HD11	1:D:868:VAL:HG23	1.58	0.85
1:E:316:THR:HG22	1:F:783:GLY:N	1.92	0.85
1:C:768:ILE:CD1	3:C:1004:POV:H31D	2.06	0.85
1:E:400:SER:CB	1:E:403:ASP:HB3	2.07	0.84
1:A:768:ILE:CD1	3:A:1004:POV:H31D	2.08	0.84
1:A:316:THR:CG2	1:B:783:GLY:N	2.41	0.83
1:A:314:TYR:O	1:B:779:LEU:CD2	2.27	0.83
1:A:783:GLY:O	1:F:313:PHE:O	1.97	0.83
1:B:400:SER:HB3	1:B:403:ASP:HB3	1.58	0.83
1:C:400:SER:CB	1:C:403:ASP:HB3	2.08	0.82
1:A:316:THR:HG22	1:B:783:GLY:N	1.92	0.82
1:A:400:SER:CB	1:A:403:ASP:HB3	2.08	0.82
1:E:306:LEU:CD1	1:F:868:VAL:CG2	2.57	0.82
1:C:314:TYR:O	1:D:779:LEU:HD22	1.77	0.82
1:F:768:ILE:CD1	3:F:1003:POV:H31D	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:THR:HG23	1:F:783:GLY:H	1.44	0.82
1:A:768:ILE:HD13	3:A:1004:POV:H31D	1.62	0.82
1:D:400:SER:CB	1:D:403:ASP:HB3	2.09	0.81
1:A:772:ILE:HD13	3:A:1010:POV:H31C	1.63	0.81
1:B:400:SER:CB	1:B:403:ASP:HB3	2.10	0.81
3:B:1003:POV:H31C	1:C:772:ILE:HD13	1.63	0.80
1:C:316:THR:HG22	1:D:783:GLY:N	1.97	0.80
3:D:1005:POV:H34A	3:D:1005:POV:H27	1.61	0.80
1:A:779:LEU:CD2	1:F:314:TYR:O	2.30	0.80
1:C:313:PHE:O	1:D:783:GLY:O	1.99	0.80
1:F:400:SER:O	1:F:404:LEU:CG	2.18	0.80
3:F:1004:POV:H34A	3:F:1004:POV:H27	1.64	0.78
1:E:708:LEU:HD21	3:E:1003:POV:H312	1.64	0.78
1:A:783:GLY:N	1:F:316:THR:CG2	2.47	0.78
1:D:307:LEU:HD12	3:D:1002:POV:H36A	1.65	0.78
1:A:783:GLY:N	1:F:316:THR:HG22	1.99	0.77
1:C:307:LEU:HD12	3:C:1002:POV:H36A	1.65	0.77
1:B:313:PHE:O	1:C:783:GLY:O	2.01	0.77
1:A:781:LYS:C	1:F:316:THR:HG21	2.04	0.77
1:E:319:ILE:HD13	1:F:857:ARG:HG2	1.67	0.77
1:D:430:LEU:O	1:D:435:LYS:HE2	1.85	0.77
1:E:306:LEU:HD11	1:F:868:VAL:HG23	1.66	0.77
1:D:768:ILE:HD12	3:D:1004:POV:C218	2.08	0.76
3:B:1006:POV:H27	3:B:1006:POV:H34A	1.66	0.76
1:F:708:LEU:HD21	3:F:1002:POV:H312	1.67	0.76
1:A:319:ILE:HD13	1:B:857:ARG:HG2	1.67	0.75
3:C:1005:POV:H27	3:C:1005:POV:H34A	1.66	0.75
1:C:768:ILE:HD11	3:C:1004:POV:H31D	1.66	0.75
1:D:316:THR:HG22	1:E:783:GLY:H	1.50	0.75
3:E:1005:POV:H27	3:E:1005:POV:H34A	1.66	0.75
3:A:1005:POV:H27	3:A:1005:POV:H34A	1.69	0.74
3:A:1002:POV:H31C	1:B:772:ILE:HD13	1.69	0.74
1:C:307:LEU:CD1	3:C:1002:POV:H36A	2.18	0.74
1:B:314:TYR:O	1:C:779:LEU:HD22	1.86	0.74
1:D:314:TYR:O	1:E:779:LEU:HD22	1.88	0.74
1:C:306:LEU:HD11	1:D:868:VAL:CG2	2.15	0.73
1:E:314:TYR:O	1:F:779:LEU:CD2	2.36	0.73
1:E:306:LEU:HD11	1:F:868:VAL:CG2	2.18	0.73
1:D:768:ILE:CD1	3:D:1004:POV:H31D	2.18	0.73
1:F:550:LEU:HD23	1:F:678:LEU:HD22	1.70	0.73
1:C:550:LEU:HD23	1:C:678:LEU:HD22	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:LEU:CD1	1:D:868:VAL:HG21	2.19	0.73
1:A:550:LEU:HD23	1:A:678:LEU:HD22	1.70	0.72
1:D:550:LEU:HD23	1:D:678:LEU:HD22	1.70	0.72
3:E:1002:POV:H31C	1:F:772:ILE:HD13	1.71	0.72
1:E:400:SER:O	1:E:404:LEU:CG	2.19	0.72
1:B:316:THR:HG22	1:C:783:GLY:H	1.51	0.72
1:A:700:LEU:HD11	1:A:760:ILE:HD13	1.70	0.72
1:D:313:PHE:O	1:E:783:GLY:O	2.08	0.72
1:B:430:LEU:O	1:B:435:LYS:HE2	1.89	0.72
1:E:700:LEU:HD11	1:E:760:ILE:HD13	1.70	0.72
1:D:768:ILE:CD1	3:D:1004:POV:H21J	2.08	0.72
1:C:700:LEU:HD11	1:C:760:ILE:HD13	1.70	0.72
1:B:700:LEU:HD11	1:B:760:ILE:HD13	1.70	0.71
1:E:550:LEU:HD23	1:E:678:LEU:HD22	1.70	0.71
1:F:700:LEU:HD11	1:F:760:ILE:HD13	1.70	0.71
1:B:550:LEU:HD23	1:B:678:LEU:HD22	1.70	0.71
1:D:700:LEU:HD11	1:D:760:ILE:HD13	1.70	0.71
1:C:314:TYR:O	1:D:779:LEU:CD2	2.39	0.71
1:A:857:ARG:HG2	1:F:319:ILE:HD13	1.71	0.71
1:C:314:TYR:CD1	1:D:776:THR:HG22	2.26	0.70
1:C:430:LEU:HB2	1:C:435:LYS:HB3	1.73	0.70
1:B:319:ILE:HD13	1:C:857:ARG:HG2	1.73	0.70
1:C:306:LEU:HD13	1:D:868:VAL:HG21	1.73	0.70
1:F:430:LEU:HB2	1:F:435:LYS:HB3	1.73	0.70
3:D:1005:POV:H27A	3:D:1006:POV:H27A	1.74	0.70
1:E:314:TYR:CD1	1:F:776:THR:HG22	2.27	0.70
1:C:400:SER:O	1:C:404:LEU:CG	2.20	0.69
1:C:319:ILE:HD13	1:D:857:ARG:HG2	1.75	0.69
1:B:316:THR:HG22	1:C:783:GLY:N	2.08	0.69
1:D:307:LEU:CD1	3:D:1002:POV:H36A	2.22	0.69
1:C:768:ILE:CD1	3:C:1004:POV:C313	2.71	0.69
1:D:316:THR:CG2	1:E:783:GLY:N	2.54	0.69
1:D:316:THR:HG22	1:E:783:GLY:N	2.08	0.69
1:B:398:GLY:HA3	1:B:404:LEU:HD11	1.75	0.69
1:D:314:TYR:O	1:E:779:LEU:CD2	2.40	0.69
1:E:316:THR:HG21	1:F:781:LYS:C	2.14	0.69
1:B:314:TYR:O	1:C:779:LEU:CD2	2.41	0.68
1:C:398:GLY:HA3	1:C:404:LEU:HD11	1.75	0.68
1:D:398:GLY:HA3	1:D:404:LEU:HD11	1.75	0.68
1:D:315:ARG:HD3	3:D:1002:POV:H13A	1.75	0.68
1:E:430:LEU:HB2	1:E:435:LYS:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:THR:CG2	1:C:783:GLY:N	2.54	0.68
1:F:398:GLY:HA3	1:F:404:LEU:HD11	1.74	0.68
1:B:306:LEU:CD1	1:C:868:VAL:CG2	2.72	0.68
1:E:398:GLY:HA3	1:E:404:LEU:HD11	1.75	0.68
1:D:319:ILE:HD13	1:E:857:ARG:HG2	1.74	0.68
1:A:316:THR:HG21	1:B:781:LYS:C	2.13	0.68
1:A:398:GLY:HA3	1:A:404:LEU:HD11	1.75	0.68
3:A:1005:POV:H27A	3:A:1006:POV:H27A	1.75	0.67
1:A:306:LEU:CD1	1:B:868:VAL:CG2	2.71	0.67
3:C:1005:POV:H27A	3:C:1006:POV:H27A	1.75	0.67
1:D:701:HIS:ND1	1:D:766:LEU:HB3	2.10	0.67
1:E:712:ILE:HG13	3:E:1003:POV:H34	1.77	0.67
1:C:768:ILE:HD11	3:C:1004:POV:C313	2.24	0.67
1:C:701:HIS:ND1	1:C:766:LEU:HB3	2.10	0.67
3:C:1004:POV:H38	3:C:1005:POV:H311	1.76	0.67
1:A:701:HIS:ND1	1:A:766:LEU:HB3	2.10	0.67
1:B:430:LEU:HB2	1:B:435:LYS:HB3	1.76	0.67
1:E:701:HIS:ND1	1:E:766:LEU:HB3	2.10	0.67
1:F:701:HIS:ND1	1:F:766:LEU:HB3	2.10	0.67
1:B:701:HIS:ND1	1:B:766:LEU:HB3	2.10	0.66
1:E:634:ASP:OD1	2:E:1001:BEF:F3	2.03	0.66
1:E:306:LEU:CD1	1:F:868:VAL:HG21	2.25	0.66
1:B:316:THR:HG21	1:C:781:LYS:C	2.15	0.66
1:E:318:GLY:HA2	1:F:786:GLN:NE2	2.11	0.66
1:A:314:TYR:CE2	3:A:1002:POV:H27A	2.31	0.66
1:A:400:SER:O	1:A:404:LEU:CG	2.20	0.66
3:F:1004:POV:H27A	3:F:1005:POV:H27A	1.77	0.66
3:B:1006:POV:H27A	3:B:1007:POV:H27A	1.77	0.65
1:B:314:TYR:CE2	3:B:1003:POV:H27A	2.31	0.65
1:B:712:ILE:HG13	3:B:1004:POV:H34	1.78	0.65
1:D:400:SER:O	1:D:404:LEU:CG	2.20	0.65
1:D:316:THR:HG21	1:E:781:LYS:C	2.16	0.65
1:C:751:ASN:ND2	1:C:883:ASP:OD1	2.30	0.64
1:A:751:ASN:ND2	1:A:883:ASP:OD1	2.30	0.64
1:E:773:THR:HG21	1:E:798:GLN:HG3	1.79	0.64
1:C:316:THR:HG23	1:D:783:GLY:H	1.55	0.64
1:F:751:ASN:ND2	1:F:883:ASP:OD1	2.30	0.64
1:B:773:THR:HG21	1:B:798:GLN:HG3	1.79	0.64
1:D:773:THR:HG21	1:D:798:GLN:HG3	1.79	0.64
1:A:313:PHE:O	1:B:783:GLY:O	2.15	0.64
1:A:773:THR:HG21	1:A:798:GLN:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:768:ILE:HD11	3:D:1004:POV:H31D	1.78	0.64
1:D:751:ASN:ND2	1:D:883:ASP:OD1	2.30	0.64
1:C:404:LEU:HD22	1:C:527:LEU:HB3	1.80	0.64
1:A:306:LEU:HD11	1:B:868:VAL:CG2	2.28	0.64
1:B:751:ASN:ND2	1:B:883:ASP:OD1	2.30	0.64
1:E:751:ASN:ND2	1:E:883:ASP:OD1	2.30	0.64
1:F:404:LEU:HD22	1:F:527:LEU:HB3	1.80	0.64
3:F:1003:POV:H38	3:F:1004:POV:H311	1.80	0.64
1:D:360:VAL:HG12	1:D:664:ILE:HG12	1.81	0.63
1:B:404:LEU:HD22	1:B:527:LEU:HB3	1.80	0.63
1:A:360:VAL:HG12	1:A:664:ILE:HG12	1.81	0.63
1:E:360:VAL:HG12	1:E:664:ILE:HG12	1.81	0.63
1:E:404:LEU:HD22	1:E:527:LEU:HB3	1.80	0.63
1:F:773:THR:HG21	1:F:798:GLN:HG3	1.79	0.63
1:D:430:LEU:HB2	1:D:435:LYS:HB3	1.81	0.63
3:B:1005:POV:H24	3:B:1006:POV:H23	1.79	0.63
1:C:773:THR:HG21	1:C:798:GLN:HG3	1.79	0.62
1:A:306:LEU:HD11	1:B:868:VAL:HG23	1.81	0.62
1:D:404:LEU:HD22	1:D:527:LEU:HB3	1.81	0.62
1:A:404:LEU:HD22	1:A:527:LEU:HB3	1.80	0.62
1:C:768:ILE:HD13	3:C:1004:POV:H312	1.80	0.62
1:B:360:VAL:HG12	1:B:664:ILE:HG12	1.81	0.62
1:B:768:ILE:HD11	3:B:1005:POV:H31D	1.82	0.62
1:A:868:VAL:CG2	1:F:306:LEU:CD1	2.77	0.62
1:C:360:VAL:HG12	1:C:664:ILE:HG12	1.81	0.62
1:D:306:LEU:CD1	1:E:868:VAL:CG2	2.78	0.62
1:E:429:SER:O	1:E:431:LYS:NZ	2.33	0.62
1:A:776:THR:HG22	1:F:314:TYR:CD1	2.35	0.61
3:A:1004:POV:H38	3:A:1005:POV:H311	1.82	0.61
1:F:360:VAL:HG12	1:F:664:ILE:HG12	1.80	0.61
1:D:429:SER:O	1:D:431:LYS:NZ	2.33	0.61
1:E:314:TYR:CE2	3:E:1002:POV:H27A	2.36	0.61
1:A:429:SER:O	1:A:431:LYS:NZ	2.33	0.61
1:C:316:THR:HG21	1:D:783:GLY:H	1.63	0.61
1:C:429:SER:O	1:C:431:LYS:NZ	2.33	0.61
1:E:182:VAL:HG12	1:E:202:LEU:HG	1.83	0.61
1:B:182:VAL:HG12	1:B:202:LEU:HG	1.83	0.60
1:B:306:LEU:HD11	1:C:868:VAL:HG23	1.83	0.60
1:F:389:SER:HB3	1:F:535:PRO:HG3	1.84	0.60
1:F:429:SER:O	1:F:431:LYS:NZ	2.33	0.60
1:A:389:SER:HB3	1:A:535:PRO:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:SER:O	1:B:431:LYS:NZ	2.33	0.60
1:D:389:SER:HB3	1:D:535:PRO:HG3	1.83	0.60
1:E:309:TRP:CH2	1:F:860:ILE:HG21	2.36	0.60
1:C:389:SER:HB3	1:C:535:PRO:HG3	1.84	0.60
1:A:378:ASP:O	1:A:382:THR:OG1	2.20	0.60
1:C:636:VAL:HG12	1:C:657:ALA:HB3	1.83	0.60
1:D:636:VAL:HG12	1:D:657:ALA:HB3	1.83	0.60
1:F:636:VAL:HG12	1:F:657:ALA:HB3	1.84	0.60
1:A:636:VAL:HG12	1:A:657:ALA:HB3	1.84	0.60
3:B:1005:POV:H38	3:B:1006:POV:H311	1.83	0.60
1:F:378:ASP:O	1:F:382:THR:OG1	2.20	0.60
1:B:385:LYS:O	1:B:386:ASN:ND2	2.35	0.60
1:B:389:SER:HB3	1:B:535:PRO:HG3	1.84	0.60
1:D:182:VAL:HG12	1:D:202:LEU:HG	1.83	0.60
1:D:712:ILE:HG13	3:D:1003:POV:H32A	1.83	0.60
1:A:182:VAL:HG12	1:A:202:LEU:HG	1.83	0.60
1:E:389:SER:HB3	1:E:535:PRO:HG3	1.84	0.60
1:F:182:VAL:HG12	1:F:202:LEU:HG	1.83	0.60
1:B:797:LEU:HD22	1:B:840:THR:HG21	1.84	0.59
1:C:182:VAL:HG12	1:C:202:LEU:HG	1.83	0.59
1:C:315:ARG:HD3	3:C:1002:POV:H13A	1.83	0.59
1:C:615:LYS:HD3	1:C:638:ASP:HB3	1.84	0.59
1:C:768:ILE:HD13	3:C:1004:POV:H31D	1.81	0.59
1:D:378:ASP:O	1:D:382:THR:OG1	2.20	0.59
1:A:694:TYR:CZ	1:A:698:LEU:HD11	2.37	0.59
1:C:297:LEU:HD21	1:C:696:ILE:HG23	1.85	0.59
1:C:378:ASP:O	1:C:382:THR:OG1	2.20	0.59
1:C:410:LEU:HA	1:C:414:ARG:HH12	1.68	0.59
1:D:694:TYR:CZ	1:D:698:LEU:HD11	2.37	0.59
1:A:768:ILE:HD11	3:A:1004:POV:H31D	1.84	0.59
1:B:694:TYR:CZ	1:B:698:LEU:HD11	2.37	0.59
1:D:410:LEU:HA	1:D:414:ARG:HH12	1.68	0.59
1:F:297:LEU:HD21	1:F:696:ILE:HG23	1.85	0.59
1:E:797:LEU:HD22	1:E:840:THR:HG21	1.85	0.59
1:F:410:LEU:HA	1:F:414:ARG:HH12	1.68	0.59
1:A:382:THR:O	1:A:537:ARG:NH2	2.36	0.59
1:A:410:LEU:HA	1:A:414:ARG:HH12	1.68	0.59
1:B:297:LEU:HD21	1:B:696:ILE:HG23	1.85	0.59
1:E:297:LEU:HD21	1:E:696:ILE:HG23	1.85	0.59
1:F:615:LYS:HD3	1:F:638:ASP:HB3	1.84	0.59
3:D:1004:POV:H38	3:D:1005:POV:H311	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:797:LEU:HD22	1:F:840:THR:HG21	1.85	0.59
1:A:772:ILE:CD1	3:A:1010:POV:H31C	2.31	0.59
1:B:410:LEU:HA	1:B:414:ARG:HH12	1.68	0.59
1:C:385:LYS:O	1:C:386:ASN:ND2	2.35	0.59
1:C:797:LEU:HD22	1:C:840:THR:HG21	1.85	0.59
1:E:636:VAL:HG12	1:E:657:ALA:HB3	1.84	0.59
1:A:783:GLY:H	1:F:316:THR:HG23	1.62	0.59
1:B:378:ASP:O	1:B:382:THR:OG1	2.20	0.59
1:C:315:ARG:CZ	3:C:1003:POV:O13	2.50	0.59
1:D:615:LYS:HD3	1:D:638:ASP:HB3	1.84	0.59
1:E:410:LEU:HA	1:E:414:ARG:HH12	1.68	0.59
1:E:694:TYR:CZ	1:E:698:LEU:HD11	2.38	0.59
1:F:694:TYR:CZ	1:F:698:LEU:HD11	2.38	0.59
1:A:712:ILE:HG13	3:A:1003:POV:H34	1.83	0.59
1:A:615:LYS:HD3	1:A:638:ASP:HB3	1.84	0.58
1:B:400:SER:O	1:B:404:LEU:CG	2.21	0.58
1:E:615:LYS:HD3	1:E:638:ASP:HB3	1.84	0.58
1:F:385:LYS:O	1:F:386:ASN:ND2	2.35	0.58
1:A:797:LEU:HD22	1:A:840:THR:HG21	1.85	0.58
1:D:382:THR:O	1:D:537:ARG:NH2	2.36	0.58
1:B:636:VAL:HG12	1:B:657:ALA:HB3	1.84	0.58
1:D:315:ARG:NE	3:D:1003:POV:O13	2.36	0.58
1:B:708:LEU:HD21	3:B:1004:POV:H312	1.84	0.58
1:D:306:LEU:HD11	1:E:868:VAL:CG2	2.34	0.58
1:D:768:ILE:CD1	3:D:1004:POV:C313	2.82	0.58
1:D:773:THR:O	1:D:776:THR:OG1	2.22	0.58
1:F:773:THR:O	1:F:776:THR:OG1	2.21	0.58
1:C:694:TYR:CZ	1:C:698:LEU:HD11	2.37	0.58
1:D:797:LEU:HD22	1:D:840:THR:HG21	1.85	0.58
1:E:382:THR:O	1:E:537:ARG:NH2	2.36	0.58
1:A:297:LEU:HD21	1:A:696:ILE:HG23	1.85	0.58
1:B:382:THR:O	1:B:537:ARG:NH2	2.36	0.58
1:D:297:LEU:HD21	1:D:696:ILE:HG23	1.85	0.58
1:D:307:LEU:CD1	3:D:1002:POV:C36	2.81	0.58
1:E:768:ILE:HD11	3:E:1004:POV:H31D	1.81	0.58
1:A:772:ILE:HD13	3:A:1010:POV:C312	2.33	0.58
1:B:306:LEU:HD11	1:C:868:VAL:CG2	2.33	0.58
1:F:430:LEU:O	1:F:435:LYS:HE2	2.04	0.58
1:C:309:TRP:HE1	1:C:326:THR:HG1	1.51	0.58
1:C:773:THR:O	1:C:776:THR:OG1	2.22	0.58
1:D:315:ARG:CZ	3:D:1003:POV:O13	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:768:ILE:HD11	3:D:1004:POV:C313	2.34	0.58
1:A:773:THR:O	1:A:776:THR:OG1	2.22	0.58
1:B:615:LYS:HD3	1:B:638:ASP:HB3	1.84	0.58
1:E:306:LEU:HD13	1:F:868:VAL:HG21	1.84	0.58
1:E:378:ASP:O	1:E:382:THR:OG1	2.20	0.58
1:E:773:THR:O	1:E:776:THR:OG1	2.21	0.58
1:C:316:THR:HG21	1:D:781:LYS:C	2.24	0.57
3:E:1010:POV:H32	3:E:1010:POV:H22A	1.86	0.57
1:A:708:LEU:HD21	3:A:1003:POV:H312	1.86	0.57
1:C:306:LEU:CD1	1:D:868:VAL:HG23	2.21	0.57
1:E:396:VAL:HG21	1:E:528:GLY:HA3	1.86	0.57
1:C:315:ARG:NE	3:C:1003:POV:O13	2.36	0.57
1:B:396:VAL:HG21	1:B:528:GLY:HA3	1.86	0.57
1:C:396:VAL:HG21	1:C:528:GLY:HA3	1.86	0.57
3:B:1003:POV:C312	1:C:772:ILE:HD13	2.34	0.57
1:F:382:THR:O	1:F:537:ARG:NH2	2.36	0.57
1:C:768:ILE:CD1	3:C:1004:POV:H21J	2.19	0.57
3:E:1004:POV:H38	3:E:1005:POV:H311	1.85	0.57
3:A:1011:POV:H32	3:A:1011:POV:H22A	1.87	0.57
1:B:773:THR:O	1:B:776:THR:OG1	2.22	0.57
1:C:382:THR:O	1:C:537:ARG:NH2	2.36	0.57
1:F:396:VAL:HG21	1:F:528:GLY:HA3	1.86	0.57
1:C:309:TRP:CH2	1:D:860:ILE:HG21	2.39	0.56
3:E:1005:POV:H27A	3:E:1006:POV:H27A	1.87	0.56
1:F:805:TRP:NE1	1:F:833:ASP:OD2	2.38	0.56
3:A:1004:POV:H1	3:A:1004:POV:H14B	1.87	0.56
1:B:224:GLN:HB2	1:B:253:ARG:HB2	1.87	0.56
1:C:768:ILE:HD12	3:C:1004:POV:C218	2.19	0.56
3:C:1002:POV:H13	3:C:1003:POV:H15A	1.87	0.56
1:E:434:PRO:O	1:E:438:ASP:HB2	2.05	0.56
1:B:434:PRO:O	1:B:438:ASP:HB2	2.05	0.56
1:C:224:GLN:HB2	1:C:253:ARG:HB2	1.87	0.56
1:C:567:GLU:OE1	1:C:570:ARG:NH1	2.39	0.56
1:C:805:TRP:NE1	1:C:833:ASP:OD2	2.38	0.56
1:E:224:GLN:HB2	1:E:253:ARG:HB2	1.87	0.56
3:E:1002:POV:H314	1:F:772:ILE:CD1	2.35	0.56
3:E:1006:POV:H32	3:E:1008:POV:H32A	1.87	0.56
1:F:567:GLU:OE1	1:F:570:ARG:NH1	2.39	0.56
1:D:306:LEU:HD11	1:E:868:VAL:HG23	1.87	0.56
1:F:224:GLN:HB2	1:F:253:ARG:HB2	1.87	0.56
1:A:805:TRP:NE1	1:A:833:ASP:OD2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:GLU:OE1	1:B:570:ARG:NH1	2.39	0.56
1:D:567:GLU:OE1	1:D:570:ARG:NH1	2.39	0.56
3:D:1002:POV:H13	3:D:1003:POV:H15A	1.85	0.56
1:C:307:LEU:CD1	3:C:1002:POV:C36	2.84	0.56
1:D:396:VAL:HG21	1:D:528:GLY:HA3	1.86	0.56
1:D:434:PRO:O	1:D:438:ASP:HB2	2.05	0.56
1:A:567:GLU:OE1	1:A:570:ARG:NH1	2.39	0.56
1:C:519:ARG:NH1	1:C:521:GLU:OE2	2.39	0.56
1:F:434:PRO:O	1:F:438:ASP:HB2	2.05	0.56
1:A:868:VAL:HG23	1:F:306:LEU:HD11	1.88	0.56
1:E:567:GLU:OE1	1:E:570:ARG:NH1	2.39	0.56
1:F:519:ARG:NH1	1:F:521:GLU:OE2	2.39	0.56
1:D:224:GLN:HB2	1:D:253:ARG:HB2	1.87	0.55
1:E:805:TRP:NE1	1:E:833:ASP:OD2	2.38	0.55
3:E:1002:POV:H31C	1:F:772:ILE:CD1	2.36	0.55
1:F:610:VAL:HG11	1:F:615:LYS:HG3	1.89	0.55
1:A:224:GLN:HB2	1:A:253:ARG:HB2	1.87	0.55
1:A:519:ARG:NH1	1:A:521:GLU:OE2	2.39	0.55
3:A:1002:POV:H212	3:A:1002:POV:H39A	1.88	0.55
1:B:438:ASP:OD1	1:B:438:ASP:O	2.25	0.55
1:B:519:ARG:NH1	1:B:521:GLU:OE2	2.39	0.55
3:B:1002:POV:H32	3:B:1002:POV:H22A	1.88	0.55
1:C:434:PRO:O	1:C:438:ASP:HB2	2.06	0.55
1:D:805:TRP:NE1	1:D:833:ASP:OD2	2.38	0.55
1:F:380:THR:OG1	2:F:1001:BEF:F3	2.15	0.55
1:F:701:HIS:HD2	1:F:702:LEU:HG	1.72	0.55
3:B:1007:POV:H32	3:B:1009:POV:H32A	1.89	0.55
1:F:419:LEU:O	1:F:424:LYS:NZ	2.39	0.55
1:A:396:VAL:HG21	1:A:528:GLY:HA3	1.86	0.55
1:C:610:VAL:HG11	1:C:615:LYS:HG3	1.88	0.55
1:E:519:ARG:NH1	1:E:521:GLU:OE2	2.39	0.55
1:A:434:PRO:O	1:A:438:ASP:HB2	2.06	0.55
1:D:519:ARG:NH1	1:D:521:GLU:OE2	2.39	0.55
3:D:1004:POV:H24	3:D:1005:POV:H23	1.88	0.55
1:F:712:ILE:HG13	3:F:1002:POV:H34	1.86	0.55
1:C:701:HIS:HD2	1:C:702:LEU:HG	1.72	0.55
1:C:768:ILE:HD13	3:C:1004:POV:C313	2.34	0.55
1:E:438:ASP:OD1	1:E:438:ASP:O	2.25	0.55
1:A:438:ASP:OD1	1:A:438:ASP:O	2.25	0.55
1:B:314:TYR:CD1	1:C:776:THR:HG22	2.42	0.55
1:B:380:THR:OG1	2:B:1001:BEF:F3	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:LEU:O	1:B:424:LYS:NZ	2.39	0.55
1:D:380:THR:OG1	2:D:1001:BEF:F3	2.15	0.55
1:A:610:VAL:HG11	1:A:615:LYS:HG3	1.88	0.55
1:B:805:TRP:NE1	1:B:833:ASP:OD2	2.38	0.55
1:D:309:TRP:NE1	1:D:326:THR:OG1	2.40	0.55
1:D:438:ASP:OD1	1:D:438:ASP:O	2.24	0.55
1:E:610:VAL:HG11	1:E:615:LYS:HG3	1.89	0.55
3:A:1010:POV:H39A	3:A:1010:POV:H212	1.87	0.55
1:C:380:THR:OG1	2:C:1001:BEF:F3	2.15	0.55
1:A:586:LEU:O	1:A:617:ARG:NH2	2.40	0.55
1:C:419:LEU:O	1:C:424:LYS:NZ	2.39	0.55
1:D:514:GLY:HA2	1:D:529:VAL:HA	1.89	0.55
1:B:701:HIS:HD2	1:B:702:LEU:HG	1.72	0.54
1:C:586:LEU:O	1:C:617:ARG:NH2	2.40	0.54
1:D:610:VAL:HG11	1:D:615:LYS:HG3	1.89	0.54
1:A:306:LEU:CD1	1:B:868:VAL:HG21	2.37	0.54
1:A:514:GLY:HA2	1:A:529:VAL:HA	1.89	0.54
1:B:400:SER:OG	1:B:403:ASP:HB3	2.07	0.54
1:B:610:VAL:HG11	1:B:615:LYS:HG3	1.88	0.54
1:D:419:LEU:O	1:D:424:LYS:NZ	2.39	0.54
3:D:1007:POV:H3	3:E:1010:POV:H15B	1.89	0.54
1:D:768:ILE:HD13	3:D:1004:POV:H31D	1.90	0.54
1:F:309:TRP:NE1	1:F:326:THR:OG1	2.40	0.54
1:F:586:LEU:O	1:F:617:ARG:NH2	2.40	0.54
1:A:701:HIS:HD2	1:A:702:LEU:HG	1.72	0.54
1:B:318:GLY:HA2	1:C:786:GLN:NE2	2.22	0.54
1:C:438:ASP:O	1:C:438:ASP:OD1	2.24	0.54
1:D:586:LEU:O	1:D:617:ARG:NH2	2.40	0.54
1:F:438:ASP:OD1	1:F:438:ASP:O	2.24	0.54
1:A:786:GLN:NE2	1:F:318:GLY:HA2	2.23	0.54
1:B:634:ASP:OD1	2:B:1001:BEF:F3	2.16	0.54
1:A:380:THR:OG1	2:A:1001:BEF:F3	2.15	0.54
1:A:414:ARG:NH1	1:A:439:ALA:O	2.41	0.54
1:B:306:LEU:CD1	1:C:868:VAL:HG21	2.37	0.54
3:F:1005:POV:H32	3:F:1007:POV:H32A	1.88	0.54
1:E:419:LEU:O	1:E:424:LYS:NZ	2.39	0.54
1:B:586:LEU:O	1:B:617:ARG:NH2	2.40	0.54
1:D:179:THR:HA	1:D:192:PRO:HA	1.90	0.54
1:A:179:THR:HA	1:A:192:PRO:HA	1.90	0.54
1:B:514:GLY:HA2	1:B:529:VAL:HA	1.89	0.54
1:A:781:LYS:O	1:F:316:THR:CG2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1006:POV:H32	3:A:1008:POV:H32A	1.89	0.54
1:D:701:HIS:HD2	1:D:702:LEU:HG	1.72	0.54
1:E:586:LEU:O	1:E:617:ARG:NH2	2.40	0.54
1:A:419:LEU:O	1:A:424:LYS:NZ	2.39	0.53
1:D:384:THR:HA	1:D:536:PRO:HA	1.90	0.53
1:D:634:ASP:OD1	2:D:1001:BEF:F3	2.16	0.53
1:E:701:HIS:HD2	1:E:702:LEU:HG	1.72	0.53
1:A:430:LEU:HB2	1:A:435:LYS:HB3	1.90	0.53
1:A:768:ILE:HG21	3:A:1010:POV:H217	1.90	0.53
1:C:309:TRP:NE1	1:C:326:THR:OG1	2.40	0.53
3:D:1002:POV:H13B	3:D:1003:POV:H13B	1.89	0.53
1:A:384:THR:HA	1:A:536:PRO:HA	1.90	0.53
1:C:514:GLY:HA2	1:C:529:VAL:HA	1.89	0.53
3:C:1002:POV:H13B	3:C:1003:POV:H13B	1.91	0.53
1:D:414:ARG:NH1	1:D:439:ALA:O	2.41	0.53
1:F:414:ARG:NH1	1:F:439:ALA:O	2.41	0.53
1:B:414:ARG:NH1	1:B:439:ALA:O	2.41	0.53
1:C:414:ARG:NH1	1:C:439:ALA:O	2.41	0.53
3:C:1010:POV:H22A	3:C:1010:POV:H32	1.90	0.53
1:F:514:GLY:HA2	1:F:529:VAL:HA	1.89	0.53
1:B:309:TRP:NE1	1:B:326:THR:OG1	2.40	0.53
1:C:634:ASP:OD1	2:C:1001:BEF:F3	2.16	0.53
1:E:414:ARG:NH1	1:E:439:ALA:O	2.41	0.53
1:B:798:GLN:HE21	1:B:861:TRP:HE1	1.57	0.53
3:E:1002:POV:H210	3:F:1003:POV:H216	1.90	0.53
1:F:634:ASP:OD1	2:F:1001:BEF:F3	2.16	0.53
1:C:798:GLN:HE21	1:C:861:TRP:HE1	1.57	0.53
1:E:309:TRP:NE1	1:E:326:THR:OG1	2.40	0.53
1:E:514:GLY:HA2	1:E:529:VAL:HA	1.89	0.53
1:E:798:GLN:HE21	1:E:861:TRP:HE1	1.57	0.53
1:F:798:GLN:HE21	1:F:861:TRP:HE1	1.57	0.53
1:B:384:THR:HA	1:B:536:PRO:HA	1.90	0.53
1:E:313:PHE:O	1:F:783:GLY:C	2.47	0.53
3:F:1004:POV:H21C	3:F:1005:POV:H21B	1.90	0.53
1:A:634:ASP:OD1	2:A:1001:BEF:F3	2.16	0.53
1:C:384:THR:HA	1:C:536:PRO:HA	1.90	0.53
1:E:400:SER:OG	1:E:403:ASP:HB3	2.08	0.53
1:F:708:LEU:CD2	3:F:1002:POV:H312	2.38	0.53
1:F:656:ASP:OD1	1:F:659:ARG:NH1	2.42	0.53
3:A:1002:POV:H31C	1:B:772:ILE:CD1	2.38	0.52
3:A:1010:POV:H27A	1:F:314:TYR:CE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1011:POV:H15B	3:F:1006:POV:H3	1.91	0.52
1:B:674:ILE:O	1:B:678:LEU:N	2.36	0.52
3:B:1003:POV:H314	1:C:772:ILE:CD1	2.39	0.52
1:C:656:ASP:OD1	1:C:659:ARG:NH1	2.42	0.52
1:F:179:THR:HA	1:F:192:PRO:HA	1.90	0.52
3:B:1010:POV:H37A	3:C:1009:POV:H27A	1.90	0.52
1:F:581:ALA:HB2	1:F:610:VAL:HG22	1.91	0.52
3:B:1008:POV:H3	3:C:1010:POV:H15B	1.90	0.52
1:C:581:ALA:HB2	1:C:610:VAL:HG22	1.91	0.52
1:F:384:THR:HA	1:F:536:PRO:HA	1.90	0.52
1:A:581:ALA:HB2	1:A:610:VAL:HG22	1.91	0.52
1:A:772:ILE:CD1	3:A:1010:POV:H314	2.39	0.52
1:B:179:THR:HA	1:B:192:PRO:HA	1.90	0.52
1:E:384:THR:HA	1:E:536:PRO:HA	1.90	0.52
3:E:1002:POV:C312	1:F:772:ILE:HD13	2.37	0.52
1:A:656:ASP:OD1	1:A:659:ARG:NH1	2.43	0.52
1:B:315:ARG:CZ	3:B:1004:POV:O13	2.50	0.52
1:D:656:ASP:OD1	1:D:659:ARG:NH1	2.43	0.52
1:E:656:ASP:OD1	1:E:659:ARG:NH1	2.42	0.52
1:B:656:ASP:OD1	1:B:659:ARG:NH1	2.43	0.52
1:C:198:PRO:HA	1:C:260:VAL:HG23	1.92	0.52
1:E:179:THR:HA	1:E:192:PRO:HA	1.90	0.52
1:E:198:PRO:HA	1:E:260:VAL:HG23	1.92	0.52
1:B:198:PRO:HA	1:B:260:VAL:HG23	1.92	0.52
3:B:1004:POV:H29	3:B:1007:POV:H310	1.92	0.52
1:F:204:LEU:HD12	1:F:208:THR:HG21	1.92	0.52
1:C:179:THR:HA	1:C:192:PRO:HA	1.90	0.52
1:D:674:ILE:O	1:D:678:LEU:N	2.36	0.52
1:E:414:ARG:HE	1:E:440:LEU:HD13	1.75	0.52
1:B:414:ARG:HE	1:B:440:LEU:HD13	1.75	0.52
3:B:1006:POV:H21C	3:B:1007:POV:H21B	1.91	0.52
1:D:204:LEU:HD12	1:D:208:THR:HG21	1.92	0.52
1:D:318:GLY:HA2	1:E:786:GLN:NE2	2.25	0.52
1:B:312:CYS:HB3	1:B:322:ILE:HG12	1.92	0.52
1:C:414:ARG:HE	1:C:440:LEU:HD13	1.75	0.52
1:E:408:ALA:HB1	1:E:474:LYS:HD3	1.92	0.52
1:D:414:ARG:HE	1:D:440:LEU:HD13	1.75	0.51
1:F:198:PRO:HA	1:F:260:VAL:HG23	1.92	0.51
1:F:309:TRP:HE1	1:F:326:THR:HG1	1.58	0.51
1:A:204:LEU:HD12	1:A:208:THR:HG21	1.92	0.51
1:B:408:ALA:HB1	1:B:474:LYS:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:ALA:HB2	1:B:610:VAL:HG22	1.91	0.51
1:C:204:LEU:HD12	1:C:208:THR:HG21	1.92	0.51
1:E:312:CYS:HB3	1:E:322:ILE:HG12	1.92	0.51
1:A:408:ALA:HB1	1:A:474:LYS:HD3	1.92	0.51
1:C:459:THR:HB	1:C:473:VAL:HG23	1.93	0.51
1:C:768:ILE:HD13	3:C:1004:POV:C312	2.40	0.51
1:D:312:CYS:HB3	1:D:322:ILE:HG12	1.92	0.51
1:D:408:ALA:HB1	1:D:474:LYS:HD3	1.92	0.51
1:D:581:ALA:HB2	1:D:610:VAL:HG22	1.91	0.51
1:E:204:LEU:HD12	1:E:208:THR:HG21	1.92	0.51
3:E:1002:POV:H39A	3:E:1002:POV:H212	1.92	0.51
1:F:414:ARG:HE	1:F:440:LEU:HD13	1.75	0.51
1:F:459:THR:HB	1:F:473:VAL:HG23	1.93	0.51
1:A:459:THR:HB	1:A:473:VAL:HG23	1.93	0.51
3:A:1007:POV:H3	3:B:1002:POV:H15B	1.93	0.51
1:D:459:THR:HB	1:D:473:VAL:HG23	1.93	0.51
1:E:459:THR:HB	1:E:473:VAL:HG23	1.93	0.51
3:E:1002:POV:H217	1:F:768:ILE:HG21	1.92	0.51
1:A:312:CYS:HB3	1:A:322:ILE:HG12	1.92	0.51
3:B:1005:POV:H1	3:B:1005:POV:H14B	1.92	0.51
1:A:309:TRP:NE1	1:A:326:THR:OG1	2.40	0.51
1:A:798:GLN:HE21	1:A:861:TRP:HE1	1.57	0.51
1:C:674:ILE:O	1:C:678:LEU:N	2.37	0.51
1:A:414:ARG:HE	1:A:440:LEU:HD13	1.75	0.51
1:F:674:ILE:O	1:F:678:LEU:N	2.36	0.51
1:F:518:LYS:HD3	1:F:524:TRP:CE2	2.46	0.51
1:A:314:TYR:OH	3:A:1002:POV:H29	2.11	0.51
1:A:518:LYS:HD3	1:A:524:TRP:CE2	2.46	0.51
1:B:459:THR:HB	1:B:473:VAL:HG23	1.93	0.51
1:D:198:PRO:HA	1:D:260:VAL:HG23	1.92	0.51
1:D:798:GLN:HE21	1:D:861:TRP:HE1	1.57	0.51
1:E:217:VAL:HG12	1:E:218:THR:HG23	1.93	0.51
1:E:581:ALA:HB2	1:E:610:VAL:HG22	1.91	0.51
1:A:380:THR:OG1	1:A:381:GLY:N	2.44	0.51
1:B:217:VAL:HG12	1:B:218:THR:HG23	1.93	0.51
1:C:217:VAL:HG12	1:C:218:THR:HG23	1.93	0.51
1:D:380:THR:OG1	1:D:381:GLY:N	2.44	0.51
1:F:312:CYS:HB3	1:F:322:ILE:HG12	1.92	0.51
1:A:198:PRO:HA	1:A:260:VAL:HG23	1.92	0.50
1:E:307:LEU:HD23	3:E:1003:POV:H31E	1.92	0.50
3:F:1003:POV:H24	3:F:1004:POV:H23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:518:LYS:HD3	1:D:524:TRP:CE2	2.46	0.50
1:F:380:THR:OG1	1:F:381:GLY:N	2.44	0.50
3:A:1010:POV:H13B	3:F:1002:POV:H13B	1.94	0.50
1:B:204:LEU:HD12	1:B:208:THR:HG21	1.92	0.50
1:C:380:THR:OG1	1:C:381:GLY:N	2.44	0.50
1:C:518:LYS:HD3	1:C:524:TRP:CE2	2.46	0.50
3:C:1006:POV:H37A	3:D:1011:POV:H27A	1.93	0.50
3:C:1007:POV:H1	3:D:1011:POV:H15B	1.94	0.50
1:E:518:LYS:HD3	1:E:524:TRP:CE2	2.46	0.50
1:F:408:ALA:HB1	1:F:474:LYS:HD3	1.92	0.50
1:C:408:ALA:HB1	1:C:474:LYS:HD3	1.92	0.50
1:E:380:THR:OG1	1:E:381:GLY:N	2.44	0.50
1:F:217:VAL:HG12	1:F:218:THR:HG23	1.93	0.50
1:B:518:LYS:HD3	1:B:524:TRP:CE2	2.46	0.50
3:D:1011:POV:H32	3:D:1011:POV:H22A	1.94	0.50
1:F:550:LEU:O	1:F:682:ARG:NH2	2.41	0.50
3:A:1007:POV:H25	3:A:1007:POV:H32	1.93	0.50
1:C:312:CYS:HB3	1:C:322:ILE:HG12	1.92	0.50
1:C:318:GLY:HA2	1:D:786:GLN:NE2	2.26	0.50
1:F:379:LYS:HA	1:F:383:LEU:HD12	1.94	0.50
1:A:769:GLY:HA2	3:A:1010:POV:H31H	1.94	0.50
1:C:379:LYS:HA	1:C:383:LEU:HD12	1.94	0.50
3:C:1002:POV:H39A	3:C:1002:POV:H212	1.94	0.50
1:A:150:LEU:HD23	1:A:336:VAL:HG12	1.94	0.49
1:A:786:GLN:HE22	1:F:319:ILE:H	1.59	0.49
1:B:309:TRP:HE1	1:B:326:THR:HG1	1.60	0.49
1:B:380:THR:O	1:B:384:THR:OG1	2.29	0.49
1:C:150:LEU:HD23	1:C:336:VAL:HG12	1.94	0.49
3:D:1009:POV:H31F	3:D:1010:POV:H21G	1.94	0.49
1:A:315:ARG:CZ	3:A:1003:POV:O13	2.54	0.49
1:D:306:LEU:CD1	1:E:868:VAL:HG21	2.42	0.49
1:A:217:VAL:HG12	1:A:218:THR:HG23	1.93	0.49
3:A:1004:POV:H24	3:A:1005:POV:H23	1.93	0.49
3:C:1009:POV:H35	3:D:1008:POV:H27	1.94	0.49
1:E:379:LYS:HA	1:E:383:LEU:HD12	1.94	0.49
1:E:846:SER:OG	1:E:847:GLU:N	2.45	0.49
3:F:1006:POV:H25	3:F:1006:POV:H32	1.94	0.49
1:B:380:THR:OG1	1:B:381:GLY:N	2.44	0.49
3:C:1007:POV:H3	3:D:1011:POV:H15B	1.95	0.49
1:D:217:VAL:HG12	1:D:218:THR:HG23	1.93	0.49
1:A:674:ILE:O	1:A:678:LEU:N	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:GLY:HA2	1:F:313:PHE:O	2.13	0.49
1:B:150:LEU:HD23	1:B:336:VAL:HG12	1.94	0.49
1:B:379:LYS:HA	1:B:383:LEU:HD12	1.94	0.49
1:B:846:SER:OG	1:B:847:GLU:N	2.45	0.49
1:D:150:LEU:HD23	1:D:336:VAL:HG12	1.94	0.49
1:A:551:GLY:HA3	1:A:747:PRO:HD3	1.95	0.49
1:B:551:GLY:HA3	1:B:747:PRO:HD3	1.95	0.49
1:D:380:THR:O	1:D:384:THR:OG1	2.29	0.49
1:F:846:SER:OG	1:F:847:GLU:N	2.45	0.49
1:D:551:GLY:HA3	1:D:747:PRO:HD3	1.95	0.49
1:D:846:SER:OG	1:D:847:GLU:N	2.45	0.49
1:E:380:THR:O	1:E:384:THR:OG1	2.29	0.49
1:A:846:SER:OG	1:A:847:GLU:N	2.45	0.49
1:E:708:LEU:CD2	3:E:1003:POV:H312	2.38	0.49
1:E:551:GLY:HA3	1:E:747:PRO:HD3	1.95	0.49
1:A:366:ILE:O	1:A:681:SER:OG	2.23	0.49
3:A:1002:POV:H314	1:B:772:ILE:CD1	2.43	0.49
1:C:846:SER:OG	1:C:847:GLU:N	2.45	0.49
1:E:150:LEU:HD23	1:E:336:VAL:HG12	1.94	0.49
3:E:1007:POV:H1	3:F:1010:POV:H15B	1.95	0.49
3:E:1007:POV:H3	3:F:1010:POV:H15B	1.95	0.49
1:F:150:LEU:HD23	1:F:336:VAL:HG12	1.94	0.49
3:A:1003:POV:H29	3:A:1006:POV:H310	1.94	0.48
3:A:1012:POV:H31F	3:B:1010:POV:H21G	1.95	0.48
3:A:1012:POV:H33A	3:D:1009:POV:H23A	1.94	0.48
1:C:332:ILE:HG21	1:C:702:LEU:HB2	1.95	0.48
1:A:783:GLY:C	1:F:313:PHE:O	2.52	0.48
1:B:391:HIS:HB3	1:B:394:TYR:HD2	1.78	0.48
1:C:430:LEU:O	1:C:435:LYS:HE2	2.13	0.48
1:C:550:LEU:O	1:C:682:ARG:NH2	2.41	0.48
1:E:306:LEU:CD1	1:F:868:VAL:HG23	2.35	0.48
1:A:379:LYS:HA	1:A:383:LEU:HD12	1.94	0.48
3:D:1007:POV:H1	3:E:1010:POV:H15B	1.94	0.48
1:F:332:ILE:HG21	1:F:702:LEU:HB2	1.95	0.48
3:F:1004:POV:H29	3:F:1004:POV:H26	1.53	0.48
1:C:551:GLY:HA3	1:C:747:PRO:HD3	1.95	0.48
1:E:309:TRP:HE1	1:E:326:THR:HG1	1.62	0.48
1:E:391:HIS:HB3	1:E:394:TYR:HD2	1.78	0.48
1:B:309:TRP:CH2	1:C:860:ILE:HG21	2.49	0.48
1:C:637:ASN:OD1	1:C:638:ASP:N	2.47	0.48
1:D:379:LYS:HA	1:D:383:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:HIS:HB3	1:D:394:TYR:HD2	1.78	0.48
1:E:550:LEU:O	1:E:682:ARG:NH2	2.41	0.48
1:F:637:ASN:OD1	1:F:638:ASP:N	2.47	0.48
3:B:1003:POV:H217	1:C:768:ILE:HG21	1.95	0.48
1:A:307:LEU:HD23	3:A:1003:POV:H31E	1.95	0.48
3:A:1007:POV:H1	3:B:1002:POV:H15B	1.96	0.48
1:C:391:HIS:HB3	1:C:394:TYR:HD2	1.78	0.48
3:F:1008:POV:H31F	3:F:1009:POV:H21G	1.96	0.48
1:C:280:ALA:HB2	1:C:643:LYS:HD2	1.96	0.48
3:D:1005:POV:H26	3:D:1005:POV:H29	1.57	0.48
1:F:280:ALA:HB2	1:F:643:LYS:HD2	1.96	0.48
1:F:391:HIS:HB3	1:F:394:TYR:HD2	1.78	0.48
1:F:551:GLY:HA3	1:F:747:PRO:HD3	1.95	0.48
3:A:1002:POV:C312	1:B:772:ILE:HD13	2.41	0.47
1:B:280:ALA:HB2	1:B:643:LYS:HD2	1.96	0.47
1:C:380:THR:O	1:C:384:THR:OG1	2.29	0.47
1:E:307:LEU:CD2	3:E:1003:POV:H31E	2.44	0.47
1:E:332:ILE:HG21	1:E:702:LEU:HB2	1.95	0.47
3:A:1008:POV:H212	3:F:1009:POV:H39A	1.96	0.47
1:D:366:ILE:O	1:D:681:SER:OG	2.23	0.47
1:A:550:LEU:O	1:A:682:ARG:NH2	2.41	0.47
1:A:868:VAL:CG2	1:F:306:LEU:HD11	2.44	0.47
1:B:332:ILE:HG21	1:B:702:LEU:HB2	1.95	0.47
1:B:378:ASP:OD2	2:B:1001:BEF:F2	2.22	0.47
3:B:1003:POV:H39A	3:B:1003:POV:H212	1.96	0.47
1:A:391:HIS:HB3	1:A:394:TYR:HD2	1.78	0.47
3:A:1010:POV:H13A	3:A:1010:POV:H11A	1.52	0.47
1:E:280:ALA:HB2	1:E:643:LYS:HD2	1.96	0.47
1:E:481:LEU:HD21	1:E:495:HIS:HA	1.97	0.47
1:A:637:ASN:OD1	1:A:638:ASP:N	2.47	0.47
1:B:307:LEU:HD23	3:B:1004:POV:H31E	1.96	0.47
1:B:481:LEU:HD21	1:B:495:HIS:HA	1.97	0.47
3:C:1003:POV:H29	3:C:1006:POV:H310	1.96	0.47
1:D:378:ASP:OD2	2:D:1001:BEF:F2	2.22	0.47
1:A:280:ALA:HB2	1:A:643:LYS:HD2	1.96	0.47
3:B:1008:POV:H1	3:C:1010:POV:H15B	1.96	0.47
3:C:1006:POV:H32	3:C:1008:POV:H32A	1.97	0.47
1:D:314:TYR:CD1	1:E:776:THR:HG22	2.50	0.47
1:D:332:ILE:HG21	1:D:702:LEU:HB2	1.95	0.47
1:F:380:THR:O	1:F:384:THR:OG1	2.29	0.47
1:C:378:ASP:OD2	2:C:1001:BEF:F2	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:ALA:HB2	1:D:643:LYS:HD2	1.96	0.47
1:A:332:ILE:HG21	1:A:702:LEU:HB2	1.95	0.47
1:C:809:ILE:HD12	1:C:809:ILE:H	1.80	0.47
1:D:365:ALA:HB1	1:D:647:THR:HG23	1.97	0.47
1:A:378:ASP:OD2	2:A:1001:BEF:F2	2.22	0.47
1:C:481:LEU:HD21	1:C:495:HIS:HA	1.97	0.47
3:C:1006:POV:H210	3:C:1008:POV:H39	1.96	0.47
1:D:309:TRP:HE1	1:D:326:THR:HG1	1.61	0.47
1:A:868:VAL:HG21	1:F:306:LEU:CD1	2.44	0.46
3:A:1002:POV:H13	3:A:1003:POV:H15A	1.97	0.46
1:A:380:THR:O	1:A:384:THR:OG1	2.29	0.46
3:A:1011:POV:H15B	3:F:1006:POV:H1	1.98	0.46
1:B:550:LEU:O	1:B:682:ARG:NH2	2.41	0.46
3:D:1004:POV:H34	3:D:1004:POV:H210	1.97	0.46
1:F:378:ASP:OD2	2:F:1001:BEF:F2	2.22	0.46
1:F:481:LEU:HD21	1:F:495:HIS:HA	1.97	0.46
3:F:1002:POV:H29	3:F:1005:POV:H310	1.97	0.46
1:A:701:HIS:CD2	1:A:702:LEU:HG	2.50	0.46
1:C:701:HIS:CD2	1:C:702:LEU:HG	2.50	0.46
1:E:701:HIS:CD2	1:E:702:LEU:HG	2.50	0.46
1:F:809:ILE:H	1:F:809:ILE:HD12	1.80	0.46
3:B:1007:POV:H11	3:B:1007:POV:H15A	1.62	0.46
3:C:1008:POV:H14A	3:C:1008:POV:H11	1.62	0.46
1:D:637:ASN:OD1	1:D:638:ASP:N	2.47	0.46
3:D:1010:POV:H3	3:D:1010:POV:O13	2.16	0.46
1:F:365:ALA:HB1	1:F:647:THR:HG23	1.97	0.46
1:F:701:HIS:CD2	1:F:702:LEU:HG	2.50	0.46
1:A:365:ALA:HB1	1:A:647:THR:HG23	1.97	0.46
3:B:1003:POV:H31C	1:C:772:ILE:CD1	2.39	0.46
1:D:768:ILE:HD13	3:D:1004:POV:C313	2.45	0.46
3:F:1005:POV:H11	3:F:1005:POV:H15A	1.59	0.46
1:D:701:HIS:CD2	1:D:702:LEU:HG	2.50	0.46
1:D:809:ILE:H	1:D:809:ILE:HD12	1.81	0.46
1:A:213:ASP:OD1	1:A:267:THR:N	2.49	0.46
1:A:860:ILE:HG21	1:F:309:TRP:CH2	2.51	0.46
1:D:316:THR:HG23	1:E:783:GLY:H	1.73	0.46
3:F:1009:POV:H3	3:F:1009:POV:O13	2.16	0.46
1:B:365:ALA:HB1	1:B:647:THR:HG23	1.97	0.46
1:B:650:ALA:HB3	1:B:665:VAL:HA	1.98	0.46
1:D:650:ALA:HB3	1:D:665:VAL:HA	1.98	0.46
1:E:458:VAL:HG23	1:E:474:LYS:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1006:POV:H15A	3:E:1006:POV:H11	1.59	0.46
1:F:458:VAL:HG23	1:F:474:LYS:HB2	1.98	0.46
1:C:458:VAL:HG23	1:C:474:LYS:HB2	1.98	0.46
1:E:365:ALA:HB1	1:E:647:THR:HG23	1.97	0.46
1:E:674:ILE:O	1:E:678:LEU:N	2.36	0.46
3:F:1008:POV:H28	3:F:1008:POV:H211	1.73	0.46
1:A:458:VAL:HG23	1:A:474:LYS:HB2	1.98	0.46
1:B:348:VAL:HB	1:B:737:ALA:HB1	1.98	0.46
1:B:458:VAL:HG23	1:B:474:LYS:HB2	1.98	0.46
3:B:1010:POV:O13	3:B:1010:POV:H3	2.15	0.46
3:D:1002:POV:H13A	3:D:1002:POV:H11A	1.50	0.46
3:D:1006:POV:H11	3:D:1006:POV:H15A	1.60	0.46
1:E:348:VAL:HB	1:E:737:ALA:HB1	1.98	0.46
1:F:213:ASP:OD1	1:F:267:THR:N	2.49	0.46
1:A:481:LEU:HD21	1:A:495:HIS:HA	1.97	0.45
1:A:650:ALA:HB3	1:A:665:VAL:HA	1.98	0.45
1:C:365:ALA:HB1	1:C:647:THR:HG23	1.97	0.45
1:C:385:LYS:NZ	1:C:536:PRO:O	2.50	0.45
1:A:430:LEU:HB2	1:A:435:LYS:CB	2.47	0.45
1:B:385:LYS:NZ	1:B:536:PRO:O	2.49	0.45
1:D:213:ASP:OD1	1:D:267:THR:N	2.49	0.45
1:E:650:ALA:HB3	1:E:665:VAL:HA	1.98	0.45
3:A:1005:POV:H29	3:A:1005:POV:H26	1.61	0.45
1:B:213:ASP:OD1	1:B:267:THR:N	2.49	0.45
1:B:701:HIS:CD2	1:B:702:LEU:HG	2.50	0.45
1:D:458:VAL:HG23	1:D:474:LYS:HB2	1.98	0.45
3:A:1012:POV:H37	3:C:1009:POV:H27	1.99	0.45
1:C:310:THR:HG23	1:D:772:ILE:CG2	2.46	0.45
3:D:1009:POV:H28	3:D:1009:POV:H211	1.79	0.45
1:F:385:LYS:NZ	1:F:536:PRO:O	2.49	0.45
3:A:1002:POV:H21E	3:A:1007:POV:H31H	1.98	0.45
1:C:213:ASP:OD1	1:C:267:THR:N	2.49	0.45
1:C:517:ARG:O	1:C:525:GLU:N	2.36	0.45
1:D:481:LEU:HD21	1:D:495:HIS:HA	1.97	0.45
1:E:637:ASN:OD1	1:E:638:ASP:N	2.47	0.45
1:E:809:ILE:HD12	1:E:809:ILE:H	1.80	0.45
1:A:809:ILE:HD12	1:A:809:ILE:H	1.81	0.45
3:A:1010:POV:H13	3:F:1002:POV:H15A	1.98	0.45
1:E:385:LYS:NZ	1:E:536:PRO:O	2.49	0.45
1:A:385:LYS:NZ	1:A:536:PRO:O	2.49	0.45
3:C:1007:POV:H29	3:C:1007:POV:H26A	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:ASP:OD1	1:E:267:THR:N	2.49	0.45
3:F:1010:POV:H32	3:F:1010:POV:H22A	1.98	0.45
1:B:809:ILE:HD12	1:B:809:ILE:H	1.80	0.45
3:C:1009:POV:H211	3:C:1009:POV:H28	1.76	0.45
1:F:315:ARG:CZ	3:F:1002:POV:O13	2.54	0.45
3:B:1002:POV:H312	3:B:1002:POV:H214	1.99	0.45
1:C:562:VAL:HG22	1:C:608:ALA:HB3	1.99	0.45
1:D:385:LYS:NZ	1:D:536:PRO:O	2.50	0.45
1:D:411:ALA:HB3	1:D:474:LYS:HG3	1.99	0.45
1:D:550:LEU:O	1:D:682:ARG:NH2	2.41	0.45
1:F:464:SER:HB2	1:F:468:GLU:HB2	1.99	0.45
3:F:1005:POV:H21J	3:F:1010:POV:H31F	1.98	0.45
1:B:316:THR:HG23	1:C:783:GLY:H	1.70	0.45
1:B:637:ASN:OD1	1:B:638:ASP:N	2.47	0.45
1:D:464:SER:HB2	1:D:468:GLU:HB2	1.99	0.45
1:F:650:ALA:HB3	1:F:665:VAL:HA	1.98	0.45
1:A:464:SER:HB2	1:A:468:GLU:HB2	1.99	0.44
1:A:776:THR:HG22	1:F:314:TYR:CE1	2.52	0.44
1:C:316:THR:HG22	1:D:783:GLY:CA	2.47	0.44
1:C:464:SER:HB2	1:C:468:GLU:HB2	1.99	0.44
3:C:1002:POV:H21D	1:D:768:ILE:HG21	1.99	0.44
3:C:1005:POV:H21C	3:C:1006:POV:H21B	2.00	0.44
3:C:1006:POV:H15A	3:C:1006:POV:H11	1.59	0.44
3:D:1007:POV:H25	3:D:1007:POV:H32	1.97	0.44
1:E:562:VAL:HG22	1:E:608:ALA:HB3	2.00	0.44
3:E:1002:POV:H314	1:F:772:ILE:HD11	1.99	0.44
1:B:306:LEU:HD13	1:C:868:VAL:HG21	1.98	0.44
1:B:562:VAL:HG22	1:B:608:ALA:HB3	1.99	0.44
3:E:1009:POV:H3	3:E:1009:POV:O13	2.18	0.44
1:A:309:TRP:HE1	1:A:326:THR:HG1	1.62	0.44
1:A:411:ALA:HB3	1:A:474:LYS:HG3	1.99	0.44
1:A:702:LEU:HD21	1:A:799:ILE:HD13	1.99	0.44
1:C:650:ALA:HB3	1:C:665:VAL:HA	1.98	0.44
1:D:768:ILE:HD13	3:D:1004:POV:H312	1.99	0.44
1:F:562:VAL:HG22	1:F:608:ALA:HB3	1.99	0.44
3:F:1002:POV:H21E	3:F:1002:POV:H39	2.00	0.44
1:A:314:TYR:CD1	1:B:776:THR:HG22	2.53	0.44
1:A:510:PHE:HE1	1:A:567:GLU:HG2	1.83	0.44
1:C:400:SER:HA	1:C:401:PRO:HD2	1.91	0.44
1:D:348:VAL:HB	1:D:737:ALA:HB1	1.99	0.44
1:D:702:LEU:HD21	1:D:799:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:ALA:O	1:E:414:ARG:NH2	2.51	0.44
1:F:346:MET:SD	1:F:363:LEU:HB3	2.58	0.44
1:A:346:MET:SD	1:A:363:LEU:HB3	2.58	0.44
1:B:412:ALA:O	1:B:414:ARG:NH2	2.51	0.44
1:C:346:MET:SD	1:C:363:LEU:HB3	2.58	0.44
1:F:348:VAL:HB	1:F:737:ALA:HB1	1.98	0.44
3:A:1009:POV:H3	3:A:1009:POV:O13	2.16	0.44
1:B:464:SER:HB2	1:B:468:GLU:HB2	1.98	0.44
1:B:510:PHE:HE1	1:B:567:GLU:HG2	1.83	0.44
1:C:704:ILE:HG12	3:C:1003:POV:H31D	1.99	0.44
1:D:346:MET:SD	1:D:363:LEU:HB3	2.58	0.44
3:E:1002:POV:H13B	3:E:1003:POV:H13B	2.00	0.44
1:A:412:ALA:O	1:A:414:ARG:NH2	2.51	0.44
3:A:1002:POV:H31H	1:B:769:GLY:HA2	1.99	0.44
3:B:1009:POV:H11	3:B:1009:POV:H14A	1.60	0.44
3:C:1008:POV:H28	3:C:1008:POV:H211	1.79	0.44
3:C:1010:POV:H15A	3:C:1010:POV:H11	1.75	0.44
1:D:375:LEU:HB3	1:D:554:VAL:HG12	2.00	0.44
1:D:510:PHE:HE1	1:D:567:GLU:HG2	1.83	0.44
1:E:510:PHE:HE1	1:E:567:GLU:HG2	1.83	0.44
1:F:411:ALA:HB3	1:F:474:LYS:HG3	1.99	0.44
1:A:348:VAL:HB	1:A:737:ALA:HB1	1.98	0.44
3:A:1002:POV:H13B	3:A:1003:POV:H13B	2.00	0.44
1:B:702:LEU:HD21	1:B:799:ILE:HD13	1.99	0.44
3:B:1006:POV:H26	3:B:1006:POV:H29	1.54	0.44
1:C:348:VAL:HB	1:C:737:ALA:HB1	1.98	0.44
1:C:411:ALA:HB3	1:C:474:LYS:HG3	1.99	0.44
3:F:1007:POV:H14A	3:F:1007:POV:H11	1.60	0.44
1:A:717:LEU:HB3	1:A:722:ILE:HD11	2.00	0.43
3:B:1008:POV:H37	3:C:1005:POV:H210	2.00	0.43
1:D:717:LEU:HB3	1:D:722:ILE:HD11	2.00	0.43
1:E:346:MET:SD	1:E:363:LEU:HB3	2.58	0.43
1:E:464:SER:HB2	1:E:468:GLU:HB2	1.99	0.43
1:E:702:LEU:HD21	1:E:799:ILE:HD13	1.99	0.43
1:A:375:LEU:HB3	1:A:554:VAL:HG12	2.00	0.43
1:B:123:PRO:HA	1:B:126:PHE:HD2	1.83	0.43
1:D:412:ALA:O	1:D:414:ARG:NH2	2.51	0.43
1:A:123:PRO:HG2	1:A:294:GLY:HA3	2.01	0.43
1:A:562:VAL:HG22	1:A:608:ALA:HB3	1.99	0.43
1:B:123:PRO:HG2	1:B:294:GLY:HA3	2.01	0.43
1:D:562:VAL:HG22	1:D:608:ALA:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:PRO:HA	1:E:126:PHE:HD2	1.84	0.43
1:E:717:LEU:HB3	1:E:722:ILE:HD11	2.00	0.43
1:F:768:ILE:HD11	3:F:1003:POV:H31D	1.96	0.43
1:A:123:PRO:HA	1:A:126:PHE:HD2	1.83	0.43
3:B:1006:POV:H21E	3:B:1007:POV:H21D	2.00	0.43
1:C:412:ALA:O	1:C:414:ARG:NH2	2.51	0.43
1:D:123:PRO:HA	1:D:126:PHE:HD2	1.83	0.43
1:F:517:ARG:O	1:F:525:GLU:N	2.36	0.43
1:F:717:LEU:HB3	1:F:722:ILE:HD11	2.00	0.43
1:A:306:LEU:HD13	1:B:868:VAL:HG21	1.99	0.43
1:D:128:MET:HE3	1:D:336:VAL:HA	2.01	0.43
1:F:702:LEU:HD21	1:F:799:ILE:HD13	1.99	0.43
1:B:346:MET:SD	1:B:363:LEU:HB3	2.58	0.43
1:B:488:HIS:ND1	1:B:489:PRO:O	2.52	0.43
1:C:309:TRP:CZ3	1:D:860:ILE:CG2	3.02	0.43
1:C:717:LEU:HB3	1:C:722:ILE:HD11	2.00	0.43
3:C:1009:POV:H3	3:C:1009:POV:O13	2.18	0.43
1:D:407:THR:HG23	1:D:472:CYS:SG	2.59	0.43
1:E:634:ASP:OD1	2:E:1001:BEF:F1	2.26	0.43
1:F:510:PHE:HE1	1:F:567:GLU:HG2	1.83	0.43
3:A:1006:POV:H15A	3:A:1006:POV:H11	1.60	0.43
3:B:1003:POV:H13A	3:B:1003:POV:H11A	1.55	0.43
1:C:616:TYR:CE2	1:C:644:LYS:HD2	2.54	0.43
1:C:702:LEU:HD21	1:C:799:ILE:HD13	1.99	0.43
1:D:123:PRO:HG2	1:D:294:GLY:HA3	2.01	0.43
1:E:123:PRO:HG2	1:E:294:GLY:HA3	2.01	0.43
1:E:309:TRP:CZ3	1:F:860:ILE:CG2	3.01	0.43
3:E:1005:POV:H21C	3:E:1006:POV:H21B	2.00	0.43
1:A:488:HIS:ND1	1:A:489:PRO:O	2.52	0.43
1:A:616:TYR:CE2	1:A:644:LYS:HD2	2.54	0.43
1:D:518:LYS:HB3	1:D:524:TRP:HA	2.01	0.43
3:D:1007:POV:H35	3:E:1005:POV:H210	1.99	0.43
1:E:316:THR:HG22	1:F:783:GLY:CA	2.49	0.43
1:E:411:ALA:HB3	1:E:474:LYS:HG3	1.99	0.43
1:E:445:VAL:HG22	1:E:462:VAL:HG12	2.01	0.43
1:E:488:HIS:ND1	1:E:489:PRO:O	2.52	0.43
3:E:1008:POV:H211	3:E:1008:POV:H28	1.81	0.43
1:F:412:ALA:O	1:F:414:ARG:NH2	2.51	0.43
1:A:128:MET:HE3	1:A:336:VAL:HA	2.01	0.43
1:A:318:GLY:HA2	1:B:786:GLN:NE2	2.34	0.43
3:A:1008:POV:H11	3:A:1008:POV:H14A	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ALA:HB3	1:B:474:LYS:HG3	1.99	0.43
1:C:375:LEU:HB3	1:C:554:VAL:HG12	2.00	0.43
1:D:517:ARG:O	1:D:525:GLU:N	2.36	0.43
1:D:704:ILE:HG12	3:D:1003:POV:H31D	2.00	0.43
1:F:616:TYR:CE2	1:F:644:LYS:HD2	2.54	0.43
1:F:625:ARG:HD3	1:F:627:TYR:CE2	2.54	0.43
1:A:625:ARG:HD3	1:A:627:TYR:CE2	2.54	0.43
3:A:1006:POV:H37A	3:B:1002:POV:H27A	2.01	0.43
1:B:616:TYR:CE2	1:B:644:LYS:HD2	2.54	0.43
1:D:488:HIS:ND1	1:D:489:PRO:O	2.52	0.43
1:E:616:TYR:CE2	1:E:644:LYS:HD2	2.54	0.43
1:E:625:ARG:HD3	1:E:627:TYR:CE2	2.54	0.43
1:F:123:PRO:HA	1:F:126:PHE:HD2	1.83	0.43
1:F:407:THR:HG23	1:F:472:CYS:SG	2.59	0.43
1:A:518:LYS:HB3	1:A:524:TRP:HA	2.01	0.42
1:B:407:THR:HG23	1:B:472:CYS:SG	2.59	0.42
1:B:717:LEU:HB3	1:B:722:ILE:HD11	2.00	0.42
1:C:123:PRO:HG2	1:C:294:GLY:HA3	2.01	0.42
1:C:510:PHE:HE1	1:C:567:GLU:HG2	1.83	0.42
1:C:687:ARG:NH1	1:C:739:ASP:O	2.52	0.42
1:E:498:TYR:O	1:E:502:VAL:N	2.43	0.42
1:F:400:SER:OG	1:F:403:ASP:HB3	2.17	0.42
1:A:407:THR:HG23	1:A:472:CYS:SG	2.59	0.42
1:A:868:VAL:HG21	1:F:306:LEU:HD13	2.01	0.42
1:B:625:ARG:HD3	1:B:627:TYR:CE2	2.54	0.42
1:C:625:ARG:HD3	1:C:627:TYR:CE2	2.54	0.42
1:D:430:LEU:HB2	1:D:435:LYS:CB	2.47	0.42
1:D:616:TYR:CE2	1:D:644:LYS:HD2	2.54	0.42
3:D:1002:POV:H39A	3:D:1002:POV:H212	2.00	0.42
1:E:366:ILE:O	1:E:681:SER:OG	2.23	0.42
3:E:1010:POV:H312	3:E:1010:POV:H214	2.00	0.42
1:F:128:MET:HE3	1:F:336:VAL:HA	2.02	0.42
1:F:375:LEU:HB3	1:F:554:VAL:HG12	2.00	0.42
1:B:375:LEU:HB3	1:B:554:VAL:HG12	2.00	0.42
1:B:752:LEU:HG	1:B:756:TRP:CD1	2.55	0.42
1:D:625:ARG:HD3	1:D:627:TYR:CE2	2.54	0.42
1:F:123:PRO:HG2	1:F:294:GLY:HA3	2.01	0.42
3:F:1006:POV:H26A	3:F:1006:POV:H29	1.79	0.42
3:A:1012:POV:H14A	3:A:1012:POV:O14	2.19	0.42
3:A:1012:POV:H28	3:A:1012:POV:H211	1.76	0.42
1:B:518:LYS:HB3	1:B:524:TRP:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:VAL:HG22	1:C:462:VAL:HG12	2.01	0.42
3:D:1005:POV:H21C	3:D:1006:POV:H21B	2.01	0.42
3:D:1006:POV:H32	3:D:1008:POV:H32A	2.00	0.42
1:C:407:THR:HG23	1:C:472:CYS:SG	2.59	0.42
1:C:488:HIS:ND1	1:C:489:PRO:O	2.52	0.42
1:D:445:VAL:HG22	1:D:462:VAL:HG12	2.00	0.42
1:D:471:VAL:HB	1:D:518:LYS:HG3	2.02	0.42
1:E:375:LEU:HB3	1:E:554:VAL:HG12	2.00	0.42
1:E:407:THR:HG23	1:E:472:CYS:SG	2.59	0.42
1:E:619:VAL:O	1:E:623:GLN:HG2	2.20	0.42
3:E:1009:POV:H32	3:E:1009:POV:H24A	2.00	0.42
1:F:619:VAL:O	1:F:623:GLN:HG2	2.20	0.42
1:F:687:ARG:NH1	1:F:739:ASP:O	2.52	0.42
1:A:471:VAL:HB	1:A:518:LYS:HG3	2.02	0.42
1:A:498:TYR:O	1:A:502:VAL:N	2.43	0.42
1:A:772:ILE:HD11	3:A:1010:POV:H314	2.02	0.42
1:B:445:VAL:HG22	1:B:462:VAL:HG12	2.01	0.42
1:C:313:PHE:O	1:D:783:GLY:C	2.56	0.42
1:C:314:TYR:CE1	1:D:776:THR:HG22	2.53	0.42
1:D:723:VAL:O	1:D:727:ILE:HG13	2.20	0.42
3:D:1003:POV:H21E	3:D:1003:POV:H39	2.01	0.42
1:E:309:TRP:CH2	1:F:860:ILE:CG2	3.02	0.42
1:E:314:TYR:CE1	1:F:776:THR:HG22	2.52	0.42
1:E:471:VAL:HB	1:E:518:LYS:HG3	2.02	0.42
1:E:752:LEU:HG	1:E:756:TRP:CD1	2.55	0.42
3:E:1005:POV:H29	3:E:1005:POV:H26	1.56	0.42
1:A:723:VAL:O	1:A:727:ILE:HG13	2.20	0.42
1:A:752:LEU:HG	1:A:756:TRP:CD1	2.55	0.42
3:A:1006:POV:H28	3:A:1006:POV:H211	1.84	0.42
1:B:723:VAL:O	1:B:727:ILE:HG13	2.20	0.42
3:B:1010:POV:H211	3:B:1010:POV:H28	1.75	0.42
1:C:123:PRO:HA	1:C:126:PHE:HD2	1.84	0.42
1:C:752:LEU:HG	1:C:756:TRP:CD1	2.55	0.42
3:C:1004:POV:H210	3:C:1004:POV:H34	2.01	0.42
3:C:1004:POV:H2	3:C:1004:POV:H25	2.02	0.42
1:D:315:ARG:HB3	3:D:1002:POV:C14	2.36	0.42
1:E:518:LYS:HB3	1:E:524:TRP:HA	2.01	0.42
1:E:723:VAL:O	1:E:727:ILE:HG13	2.20	0.42
1:E:736:ILE:HD13	1:E:736:ILE:HA	1.90	0.42
3:E:1009:POV:H39A	3:F:1007:POV:H212	2.01	0.42
1:F:723:VAL:O	1:F:727:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:752:LEU:HG	1:F:756:TRP:CD1	2.55	0.42
1:A:307:LEU:CD2	3:A:1003:POV:H31E	2.50	0.42
3:A:1011:POV:H28	3:A:1011:POV:H21A	1.75	0.42
1:B:471:VAL:HB	1:B:518:LYS:HG3	2.02	0.42
3:B:1010:POV:H37	3:C:1008:POV:H27	2.00	0.42
1:C:128:MET:HE3	1:C:336:VAL:HA	2.02	0.42
1:C:518:LYS:HB3	1:C:524:TRP:HA	2.01	0.42
1:C:723:VAL:O	1:C:727:ILE:HG13	2.20	0.42
1:D:619:VAL:O	1:D:623:GLN:HG2	2.20	0.42
1:D:687:ARG:NH1	1:D:739:ASP:O	2.52	0.42
1:D:752:LEU:HG	1:D:756:TRP:CD1	2.55	0.42
1:E:310:THR:HG23	1:F:772:ILE:CG2	2.50	0.42
3:E:1005:POV:H11A	3:E:1005:POV:H15B	1.88	0.42
1:F:445:VAL:HG22	1:F:462:VAL:HG12	2.01	0.42
1:F:518:LYS:HB3	1:F:524:TRP:HA	2.01	0.42
3:F:1007:POV:H37A	3:F:1009:POV:H28A	2.01	0.42
3:A:1011:POV:H27A	3:F:1005:POV:H37A	2.00	0.42
1:B:307:LEU:CD2	3:B:1004:POV:H31E	2.50	0.42
1:B:314:TYR:CE1	1:C:776:THR:HG22	2.55	0.42
3:B:1006:POV:H11A	3:B:1006:POV:H15B	1.88	0.42
1:C:267:THR:O	1:C:271:ARG:N	2.44	0.42
1:C:471:VAL:HB	1:C:518:LYS:HG3	2.02	0.42
1:C:505:LEU:HG	1:C:510:PHE:HB2	2.01	0.42
1:E:476:ALA:HB3	1:E:479:PHE:HD2	1.85	0.42
1:F:267:THR:O	1:F:271:ARG:N	2.44	0.42
3:F:1003:POV:H210	3:F:1003:POV:H34	2.01	0.42
1:A:445:VAL:HG22	1:A:462:VAL:HG12	2.01	0.42
1:A:619:VAL:O	1:A:623:GLN:HG2	2.20	0.42
3:A:1004:POV:H34	3:A:1004:POV:H210	2.02	0.42
1:B:542:GLN:O	1:B:545:SER:N	2.53	0.42
1:B:619:VAL:O	1:B:623:GLN:HG2	2.20	0.42
3:B:1002:POV:H11	3:B:1002:POV:H15A	1.73	0.42
1:D:505:LEU:HG	1:D:510:PHE:HB2	2.01	0.42
1:E:505:LEU:HG	1:E:510:PHE:HB2	2.01	0.42
1:E:542:GLN:O	1:E:545:SER:N	2.53	0.42
1:F:488:HIS:ND1	1:F:489:PRO:O	2.52	0.42
1:F:734:LEU:HD23	1:F:734:LEU:HA	1.90	0.42
1:A:555:LYS:NZ	1:A:604:ALA:O	2.41	0.41
3:B:1004:POV:H11A	3:B:1004:POV:H14B	1.82	0.41
1:C:619:VAL:O	1:C:623:GLN:HG2	2.20	0.41
3:C:1002:POV:H31F	1:D:868:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:617:ARG:O	1:D:621:ILE:HG12	2.20	0.41
1:E:128:MET:HE3	1:E:336:VAL:HA	2.02	0.41
1:F:797:LEU:O	1:F:801:LEU:HD23	2.20	0.41
1:A:617:ARG:O	1:A:621:ILE:HG12	2.20	0.41
3:A:1008:POV:H27	3:F:1009:POV:H35	2.02	0.41
3:A:1010:POV:H31G	3:A:1010:POV:H31D	1.81	0.41
1:B:128:MET:HE3	1:B:336:VAL:HA	2.02	0.41
1:B:366:ILE:O	1:B:681:SER:OG	2.23	0.41
1:B:505:LEU:HG	1:B:510:PHE:HB2	2.01	0.41
1:B:734:LEU:HD23	1:B:734:LEU:HA	1.89	0.41
1:B:797:LEU:O	1:B:801:LEU:HD23	2.20	0.41
1:C:797:LEU:O	1:C:801:LEU:HD23	2.20	0.41
3:E:1003:POV:H21E	3:E:1003:POV:H39	2.02	0.41
1:F:471:VAL:HB	1:F:518:LYS:HG3	2.02	0.41
3:F:1008:POV:H15B	3:F:1008:POV:H11	1.78	0.41
1:A:542:GLN:O	1:A:545:SER:N	2.53	0.41
3:A:1007:POV:H13B	3:A:1007:POV:H11A	1.73	0.41
1:B:476:ALA:HB3	1:B:479:PHE:HD2	1.85	0.41
3:C:1006:POV:H37	3:C:1007:POV:H28	2.02	0.41
3:E:1002:POV:H13A	3:E:1002:POV:H11A	1.55	0.41
1:F:505:LEU:HG	1:F:510:PHE:HB2	2.01	0.41
1:A:316:THR:HG23	1:B:783:GLY:H	1.68	0.41
1:A:505:LEU:HG	1:A:510:PHE:HB2	2.01	0.41
1:C:152:MET:O	1:C:156:GLY:N	2.51	0.41
1:D:704:ILE:HG21	3:D:1004:POV:H314	2.02	0.41
3:D:1010:POV:H28	3:D:1010:POV:H211	1.75	0.41
1:E:617:ARG:O	1:E:621:ILE:HG12	2.20	0.41
1:E:797:LEU:O	1:E:801:LEU:HD23	2.20	0.41
1:A:128:MET:O	1:A:132:ALA:N	2.48	0.41
1:A:316:THR:HG22	1:B:783:GLY:CA	2.49	0.41
3:A:1002:POV:H13A	3:A:1002:POV:H11A	1.53	0.41
3:A:1002:POV:H31G	3:A:1002:POV:H31D	1.80	0.41
1:B:516:ALA:HA	1:B:527:LEU:H	1.86	0.41
1:C:476:ALA:HB3	1:C:479:PHE:HD2	1.85	0.41
1:D:542:GLN:O	1:D:545:SER:N	2.53	0.41
1:E:516:ALA:HA	1:E:527:LEU:H	1.86	0.41
1:F:379:LYS:NZ	1:F:564:ILE:HG23	2.36	0.41
1:A:361:GLN:NE2	1:A:659:ARG:O	2.52	0.41
1:A:544:VAL:HG13	1:A:554:VAL:HG21	2.03	0.41
1:C:297:LEU:HD23	1:C:297:LEU:HA	1.91	0.41
1:C:544:VAL:HG13	1:C:554:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:544:VAL:HG13	1:E:554:VAL:HG21	2.03	0.41
1:F:297:LEU:HD23	1:F:297:LEU:HA	1.92	0.41
1:F:617:ARG:O	1:F:621:ILE:HG12	2.20	0.41
3:F:1009:POV:H11	3:F:1009:POV:H14A	1.82	0.41
1:A:687:ARG:NH1	1:A:739:ASP:O	2.52	0.41
1:C:734:LEU:HD23	1:C:734:LEU:HA	1.90	0.41
3:E:1007:POV:H29	3:E:1007:POV:H26A	1.85	0.41
3:A:1010:POV:H21A	3:A:1010:POV:H28A	1.85	0.41
1:B:379:LYS:NZ	1:B:564:ILE:HG23	2.36	0.41
1:C:379:LYS:NZ	1:C:564:ILE:HG23	2.36	0.41
1:C:516:ALA:HA	1:C:527:LEU:H	1.86	0.41
3:D:1005:POV:H15B	3:D:1005:POV:H11A	1.83	0.41
1:F:307:LEU:HD23	3:F:1002:POV:H31E	2.03	0.41
1:F:476:ALA:HB3	1:F:479:PHE:HD2	1.85	0.41
3:F:1004:POV:H21E	3:F:1005:POV:H21D	2.03	0.41
1:A:286:PHE:HZ	1:A:342:VAL:HG11	1.86	0.41
3:A:1011:POV:H312	3:A:1011:POV:H214	2.03	0.41
1:B:267:THR:O	1:B:271:ARG:N	2.44	0.41
1:B:310:THR:OG1	3:B:1003:POV:H312	2.21	0.41
1:B:313:PHE:O	1:C:783:GLY:C	2.60	0.41
1:B:325:TYR:HB3	1:B:710:ILE:HD13	2.03	0.41
1:B:544:VAL:HG13	1:B:554:VAL:HG21	2.03	0.41
1:B:617:ARG:O	1:B:621:ILE:HG12	2.20	0.41
1:C:617:ARG:O	1:C:621:ILE:HG12	2.20	0.41
3:C:1005:POV:H28A	3:C:1005:POV:H211	1.81	0.41
1:D:307:LEU:HD13	3:D:1002:POV:C36	2.51	0.41
1:D:567:GLU:HA	1:D:570:ARG:NH1	2.35	0.41
1:E:379:LYS:NZ	1:E:564:ILE:HG23	2.36	0.41
1:E:687:ARG:NH1	1:E:739:ASP:O	2.52	0.41
1:F:430:LEU:HB2	1:F:435:LYS:CB	2.47	0.41
1:F:516:ALA:HA	1:F:527:LEU:H	1.86	0.41
1:F:544:VAL:HG13	1:F:554:VAL:HG21	2.03	0.41
1:F:804:ASN:HB3	1:F:829:VAL:HG13	2.03	0.41
1:A:325:TYR:HB3	1:A:710:ILE:HD13	2.03	0.41
1:A:797:LEU:O	1:A:801:LEU:HD23	2.20	0.41
1:B:287:THR:HA	1:B:290:LEU:HB3	2.03	0.41
1:C:804:ASN:HB3	1:C:829:VAL:HG13	2.03	0.41
1:D:516:ALA:HA	1:D:527:LEU:H	1.86	0.41
1:D:797:LEU:O	1:D:801:LEU:HD23	2.20	0.41
1:F:542:GLN:O	1:F:545:SER:N	2.53	0.41
1:A:476:ALA:HB3	1:A:479:PHE:HD2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:LYS:NZ	1:C:604:ALA:O	2.41	0.40
1:D:544:VAL:HG13	1:D:554:VAL:HG21	2.03	0.40
1:D:648:GLY:H	1:D:663:ASP:HB2	1.86	0.40
1:F:287:THR:HA	1:F:290:LEU:HB3	2.03	0.40
1:F:567:GLU:HA	1:F:570:ARG:NH1	2.35	0.40
1:A:379:LYS:NZ	1:A:564:ILE:HG23	2.36	0.40
1:A:407:THR:HG21	1:A:527:LEU:HD12	2.03	0.40
1:A:516:ALA:HA	1:A:527:LEU:H	1.86	0.40
1:B:400:SER:OG	1:B:403:ASP:CB	2.69	0.40
3:B:1003:POV:H13B	3:B:1004:POV:H13B	2.03	0.40
1:C:286:PHE:HZ	1:C:342:VAL:HG11	1.86	0.40
1:C:287:THR:HA	1:C:290:LEU:HB3	2.03	0.40
1:C:325:TYR:HB3	1:C:710:ILE:HD13	2.03	0.40
1:C:542:GLN:O	1:C:545:SER:N	2.53	0.40
3:C:1002:POV:H13A	3:C:1002:POV:H11A	1.51	0.40
3:C:1005:POV:H15B	3:C:1005:POV:H11A	1.85	0.40
1:D:286:PHE:HZ	1:D:342:VAL:HG11	1.86	0.40
1:D:325:TYR:HB3	1:D:710:ILE:HD13	2.03	0.40
3:D:1007:POV:H23	3:E:1010:POV:H22	2.02	0.40
1:E:325:TYR:HB3	1:E:710:ILE:HD13	2.03	0.40
1:B:687:ARG:NH1	1:B:739:ASP:O	2.52	0.40
1:B:752:LEU:HD12	1:B:752:LEU:HA	1.93	0.40
3:B:1010:POV:H11	3:B:1010:POV:H14A	1.87	0.40
1:D:476:ALA:HB3	1:D:479:PHE:HD2	1.85	0.40
1:D:721:LEU:HD23	1:D:796:PHE:HB2	2.04	0.40
1:D:808:PHE:HE1	1:D:829:VAL:HG11	1.87	0.40
3:D:1005:POV:H28A	3:D:1005:POV:H211	1.84	0.40
3:D:1010:POV:H39A	3:E:1008:POV:H212	2.02	0.40
1:E:778:PHE:O	3:E:1004:POV:H14A	2.21	0.40
1:F:286:PHE:HZ	1:F:342:VAL:HG11	1.86	0.40
1:A:794:ILE:HG23	1:A:858:VAL:HG21	2.04	0.40
1:B:736:ILE:HD11	1:B:807:ILE:HG12	2.03	0.40
1:B:808:PHE:HE1	1:B:829:VAL:HG11	1.87	0.40
1:C:239:LYS:NZ	1:C:245:THR:HA	2.37	0.40
3:C:1002:POV:H28A	3:C:1002:POV:H21A	1.82	0.40
1:E:232:GLY:HA3	1:E:380:THR:HG21	2.03	0.40
1:E:239:LYS:NZ	1:E:245:THR:HA	2.37	0.40
1:E:287:THR:HA	1:E:290:LEU:HB3	2.03	0.40
1:E:567:GLU:HA	1:E:570:ARG:NH1	2.35	0.40
1:F:484:VAL:HG23	1:F:524:TRP:HD1	1.86	0.40
3:F:1004:POV:H3A	3:F:1005:POV:H2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1010:POV:H15A	3:F:1010:POV:H11	1.75	0.40
1:A:517:ARG:O	1:A:525:GLU:N	2.36	0.40
1:A:648:GLY:H	1:A:663:ASP:HB2	1.86	0.40
1:B:567:GLU:HA	1:B:570:ARG:NH1	2.35	0.40
1:B:685:PHE:HA	1:B:688:MET:HE2	2.03	0.40
1:B:721:LEU:HD23	1:B:796:PHE:HB2	2.04	0.40
1:B:804:ASN:HB3	1:B:829:VAL:HG13	2.03	0.40
1:D:287:THR:HA	1:D:290:LEU:HB3	2.03	0.40
1:D:309:TRP:CH2	1:E:860:ILE:HG21	2.56	0.40
1:D:379:LYS:NZ	1:D:564:ILE:HG23	2.36	0.40
1:D:407:THR:HG21	1:D:527:LEU:HD12	2.03	0.40
1:E:378:ASP:OD2	2:E:1001:BEF:F2	2.29	0.40
3:E:1007:POV:H28	3:E:1007:POV:H211	1.94	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	760/918 (83%)	734 (97%)	26 (3%)	0	100	100
1	B	760/918 (83%)	734 (97%)	26 (3%)	0	100	100
1	C	760/918 (83%)	734 (97%)	26 (3%)	0	100	100
1	D	760/918 (83%)	734 (97%)	26 (3%)	0	100	100
1	E	760/918 (83%)	734 (97%)	26 (3%)	0	100	100
1	F	760/918 (83%)	734 (97%)	26 (3%)	0	100	100
All	All	4560/5508 (83%)	4404 (97%)	156 (3%)	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	622/752 (83%)	617 (99%)	5 (1%)	81 89
1	B	622/752 (83%)	615 (99%)	7 (1%)	73 85
1	C	622/752 (83%)	615 (99%)	7 (1%)	73 85
1	D	622/752 (83%)	617 (99%)	5 (1%)	81 89
1	E	622/752 (83%)	617 (99%)	5 (1%)	81 89
1	F	622/752 (83%)	616 (99%)	6 (1%)	76 86
All	All	3732/4512 (83%)	3697 (99%)	35 (1%)	79 88

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	400	SER
1	A	433	TYR
1	A	435	LYS
1	A	517	ARG
1	A	537	ARG
1	B	386	ASN
1	B	400	SER
1	B	432	GLN
1	B	433	TYR
1	B	435	LYS
1	B	517	ARG
1	B	537	ARG
1	C	386	ASN
1	C	400	SER
1	C	432	GLN
1	C	433	TYR
1	C	435	LYS
1	C	517	ARG
1	C	537	ARG
1	D	400	SER
1	D	433	TYR
1	D	435	LYS

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Mol	Chain	Res	Type
1	D	517	ARG
1	D	537	ARG
1	E	400	SER
1	E	433	TYR
1	E	435	LYS
1	E	517	ARG
1	E	537	ARG
1	F	386	ASN
1	F	400	SER
1	F	433	TYR
1	F	435	LYS
1	F	517	ARG
1	F	537	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	701	HIS
1	B	386	ASN
1	B	701	HIS
1	C	386	ASN
1	C	701	HIS
1	D	701	HIS
1	E	701	HIS
1	F	386	ASN
1	F	701	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

63 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	$\#\|Z\| > 2$
3	POV	C	1006	-	51,51,51	1.18	4 (7%)	57,59,59	1.22	3 (5%)
3	POV	C	1008	-	51,51,51	1.19	4 (7%)	57,59,59	1.17	3 (5%)
3	POV	E	1006	-	51,51,51	1.19	4 (7%)	57,59,59	1.17	3 (5%)
3	POV	F	1010	3	51,51,51	1.21	6 (11%)	57,59,59	1.15	2 (3%)
3	POV	D	1007	3	51,51,51	1.22	5 (9%)	57,59,59	1.24	3 (5%)
3	POV	F	1008	-	51,51,51	1.19	4 (7%)	57,59,59	1.22	3 (5%)
3	POV	B	1004	-	51,51,51	1.20	4 (7%)	57,59,59	1.20	3 (5%)
3	POV	B	1008	3	51,51,51	1.21	5 (9%)	57,59,59	1.25	3 (5%)
3	POV	D	1005	-	51,51,51	1.18	4 (7%)	57,59,59	1.18	3 (5%)
3	POV	B	1006	-	51,51,51	1.19	5 (9%)	57,59,59	1.17	3 (5%)
3	POV	C	1003	-	51,51,51	1.23	5 (9%)	57,59,59	1.17	3 (5%)
3	POV	D	1008	-	51,51,51	1.19	4 (7%)	57,59,59	1.16	2 (3%)
3	POV	C	1005	-	51,51,51	1.18	4 (7%)	57,59,59	1.18	3 (5%)
3	POV	E	1003	-	51,51,51	1.22	6 (11%)	57,59,59	1.15	3 (5%)
3	POV	E	1007	3	51,51,51	1.22	5 (9%)	57,59,59	1.25	3 (5%)
3	POV	A	1002	-	51,51,51	1.20	4 (7%)	57,59,59	1.14	2 (3%)
3	POV	C	1009	-	51,51,51	1.18	4 (7%)	57,59,59	1.19	3 (5%)
3	POV	D	1010	-	51,51,51	1.18	4 (7%)	57,59,59	1.17	3 (5%)
3	POV	A	1011	3	51,51,51	1.21	5 (9%)	57,59,59	1.14	2 (3%)
3	POV	E	1002	-	51,51,51	1.20	4 (7%)	57,59,59	1.13	2 (3%)
3	POV	C	1007	3	51,51,51	1.22	5 (9%)	57,59,59	1.26	3 (5%)
3	POV	D	1004	-	51,51,51	1.18	5 (9%)	57,59,59	1.16	2 (3%)
3	POV	E	1005	-	51,51,51	1.18	4 (7%)	57,59,59	1.17	4 (7%)
3	POV	D	1006	-	51,51,51	1.19	4 (7%)	57,59,59	1.21	2 (3%)
3	POV	A	1003	-	51,51,51	1.21	4 (7%)	57,59,59	1.20	2 (3%)
3	POV	E	1009	-	51,51,51	1.19	4 (7%)	57,59,59	1.17	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	POV	C	1004	1	51,51,51	1.19	4 (7%)	57,59,59	1.12	2 (3%)
3	POV	A	1005	-	51,51,51	1.19	4 (7%)	57,59,59	1.17	3 (5%)
3	POV	A	1006	-	51,51,51	1.19	4 (7%)	57,59,59	1.18	2 (3%)
3	POV	A	1008	-	51,51,51	1.19	4 (7%)	57,59,59	1.13	2 (3%)
3	POV	A	1004	-	51,51,51	1.19	5 (9%)	57,59,59	1.10	2 (3%)
2	BEF	C	1001	-	0,3,3	-	-	-		
3	POV	B	1009	-	51,51,51	1.19	4 (7%)	57,59,59	1.15	3 (5%)
3	POV	B	1007	-	51,51,51	1.19	4 (7%)	57,59,59	1.18	2 (3%)
3	POV	C	1010	3	51,51,51	1.19	5 (9%)	57,59,59	1.19	2 (3%)
3	POV	F	1003	-	51,51,51	1.19	4 (7%)	57,59,59	1.11	2 (3%)
3	POV	D	1003	-	51,51,51	1.24	6 (11%)	57,59,59	1.16	3 (5%)
3	POV	D	1009	-	51,51,51	1.18	4 (7%)	57,59,59	1.21	3 (5%)
3	POV	F	1004	-	51,51,51	1.19	5 (9%)	57,59,59	1.18	3 (5%)
3	POV	F	1005	-	51,51,51	1.19	4 (7%)	57,59,59	1.19	2 (3%)
3	POV	F	1002	-	51,51,51	1.20	4 (7%)	57,59,59	1.17	2 (3%)
3	POV	A	1009	-	51,51,51	1.18	4 (7%)	57,59,59	1.18	3 (5%)
3	POV	D	1002	-	51,51,51	1.20	4 (7%)	57,59,59	1.10	2 (3%)
3	POV	A	1007	3	51,51,51	1.22	5 (9%)	57,59,59	1.23	3 (5%)
2	BEF	E	1001	-	0,3,3	-	-	-		
3	POV	B	1005	-	51,51,51	1.19	5 (9%)	57,59,59	1.12	2 (3%)
3	POV	B	1010	-	51,51,51	1.18	4 (7%)	57,59,59	1.18	3 (5%)
3	POV	D	1011	3	51,51,51	1.19	4 (7%)	57,59,59	1.16	2 (3%)
2	BEF	A	1001	-	0,3,3	-	-	-		
3	POV	F	1006	3	51,51,51	1.23	6 (11%)	57,59,59	1.25	3 (5%)
2	BEF	B	1001	-	0,3,3	-	-	-		
3	POV	E	1008	-	51,51,51	1.19	4 (7%)	57,59,59	1.14	2 (3%)
2	BEF	F	1001	-	0,3,3	-	-	-		
3	POV	A	1012	-	51,51,51	1.19	4 (7%)	57,59,59	1.18	2 (3%)
3	POV	C	1002	-	51,51,51	1.20	4 (7%)	57,59,59	1.10	2 (3%)
3	POV	A	1010	-	51,51,51	1.20	4 (7%)	57,59,59	1.16	3 (5%)
3	POV	B	1003	-	51,51,51	1.19	4 (7%)	57,59,59	1.17	2 (3%)
3	POV	F	1009	-	51,51,51	1.18	4 (7%)	57,59,59	1.15	3 (5%)
3	POV	F	1007	-	51,51,51	1.20	4 (7%)	57,59,59	1.15	3 (5%)
3	POV	E	1010	3	51,51,51	1.20	5 (9%)	57,59,59	1.15	2 (3%)
2	BEF	D	1001	-	0,3,3	-	-	-		
3	POV	B	1002	3	51,51,51	1.21	5 (9%)	57,59,59	1.15	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	POV	E	1004	-	51,51,51	1.21	5 (9%)	57,59,59	1.07	2 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	C	1006	-	-	30/55/55/55	-
3	POV	C	1008	-	-	25/55/55/55	-
3	POV	E	1006	-	-	29/55/55/55	-
3	POV	F	1010	3	-	24/55/55/55	-
3	POV	D	1007	3	-	24/55/55/55	-
3	POV	F	1008	-	-	20/55/55/55	-
3	POV	B	1004	-	-	24/55/55/55	-
3	POV	B	1008	3	-	23/55/55/55	-
3	POV	D	1005	-	-	26/55/55/55	-
3	POV	B	1006	-	-	27/55/55/55	-
3	POV	C	1003	-	-	26/55/55/55	-
3	POV	D	1008	-	-	28/55/55/55	-
3	POV	C	1005	-	-	27/55/55/55	-
3	POV	E	1003	-	-	27/55/55/55	-
3	POV	E	1007	3	-	21/55/55/55	-
3	POV	A	1002	-	-	26/55/55/55	-
3	POV	C	1009	-	-	23/55/55/55	-
3	POV	D	1010	-	-	22/55/55/55	-
3	POV	A	1011	3	-	21/55/55/55	-
3	POV	E	1002	-	-	25/55/55/55	-
3	POV	C	1007	3	-	24/55/55/55	-
3	POV	D	1004	-	-	24/55/55/55	-
3	POV	E	1005	-	-	27/55/55/55	-
3	POV	D	1006	-	-	29/55/55/55	-
3	POV	A	1003	-	-	24/55/55/55	-
3	POV	E	1009	-	-	23/55/55/55	-
3	POV	C	1004	1	-	23/55/55/55	-
3	POV	A	1005	-	-	26/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	A	1006	-	-	28/55/55/55	-
3	POV	A	1008	-	-	29/55/55/55	-
3	POV	A	1004	-	-	24/55/55/55	-
3	POV	B	1009	-	-	28/55/55/55	-
3	POV	B	1007	-	-	28/55/55/55	-
3	POV	C	1010	3	-	22/55/55/55	-
3	POV	F	1003	-	-	24/55/55/55	-
3	POV	D	1003	-	-	26/55/55/55	-
3	POV	D	1009	-	-	20/55/55/55	-
3	POV	F	1004	-	-	27/55/55/55	-
3	POV	F	1005	-	-	27/55/55/55	-
3	POV	F	1002	-	-	26/55/55/55	-
3	POV	A	1009	-	-	25/55/55/55	-
3	POV	D	1002	-	-	26/55/55/55	-
3	POV	A	1007	3	-	23/55/55/55	-
3	POV	B	1005	-	-	25/55/55/55	-
3	POV	B	1010	-	-	23/55/55/55	-
3	POV	D	1011	3	-	22/55/55/55	-
3	POV	F	1006	3	-	22/55/55/55	-
3	POV	E	1008	-	-	26/55/55/55	-
3	POV	C	1002	-	-	27/55/55/55	-
3	POV	A	1012	-	-	21/55/55/55	-
3	POV	A	1010	-	-	26/55/55/55	-
3	POV	B	1003	-	-	30/55/55/55	-
3	POV	F	1009	-	-	22/55/55/55	-
3	POV	F	1007	-	-	32/55/55/55	-
3	POV	E	1010	3	-	24/55/55/55	-
3	POV	B	1002	3	-	26/55/55/55	-
3	POV	E	1004	-	-	27/55/55/55	-

All (252) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1004	POV	O31-C31	3.83	1.44	1.33
3	D	1003	POV	O31-C31	3.81	1.44	1.33
3	D	1002	POV	O31-C31	3.79	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1003	POV	O31-C31	3.78	1.44	1.33
3	A	1005	POV	O31-C31	3.78	1.44	1.33
3	A	1008	POV	O31-C31	3.78	1.44	1.33
3	E	1003	POV	O31-C31	3.78	1.44	1.33
3	C	1002	POV	O31-C31	3.77	1.44	1.33
3	E	1005	POV	O31-C31	3.76	1.44	1.33
3	C	1005	POV	O31-C31	3.76	1.44	1.33
3	B	1002	POV	O31-C31	3.76	1.44	1.33
3	B	1006	POV	O31-C31	3.75	1.44	1.33
3	A	1002	POV	O31-C31	3.75	1.44	1.33
3	E	1008	POV	O31-C31	3.75	1.44	1.33
3	A	1011	POV	O31-C31	3.74	1.44	1.33
3	E	1006	POV	O31-C31	3.73	1.44	1.33
3	B	1007	POV	O31-C31	3.73	1.44	1.33
3	F	1006	POV	O31-C31	3.73	1.44	1.33
3	E	1007	POV	O31-C31	3.72	1.44	1.33
3	F	1002	POV	O31-C31	3.72	1.44	1.33
3	F	1007	POV	O31-C31	3.72	1.44	1.33
3	B	1004	POV	O31-C31	3.72	1.44	1.33
3	D	1005	POV	O31-C31	3.72	1.44	1.33
3	F	1005	POV	O31-C31	3.72	1.44	1.33
3	A	1012	POV	O31-C31	3.71	1.44	1.33
3	E	1010	POV	O31-C31	3.71	1.44	1.33
3	F	1009	POV	O31-C31	3.71	1.44	1.33
3	D	1007	POV	O31-C31	3.70	1.44	1.33
3	B	1009	POV	O31-C31	3.70	1.44	1.33
3	F	1010	POV	O31-C31	3.70	1.44	1.33
3	E	1002	POV	O31-C31	3.70	1.44	1.33
3	A	1010	POV	O31-C31	3.70	1.44	1.33
3	A	1006	POV	O31-C31	3.70	1.44	1.33
3	D	1006	POV	O31-C31	3.70	1.44	1.33
3	D	1008	POV	O31-C31	3.69	1.44	1.33
3	B	1008	POV	O31-C31	3.69	1.44	1.33
3	E	1009	POV	O31-C31	3.69	1.44	1.33
3	B	1003	POV	O31-C31	3.68	1.44	1.33
3	A	1003	POV	O31-C31	3.68	1.44	1.33
3	C	1006	POV	O31-C31	3.68	1.44	1.33
3	D	1011	POV	O31-C31	3.68	1.44	1.33
3	F	1008	POV	O31-C31	3.68	1.44	1.33
3	C	1008	POV	O31-C31	3.67	1.44	1.33
3	A	1009	POV	O31-C31	3.67	1.44	1.33
3	A	1007	POV	O31-C31	3.66	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1010	POV	O31-C31	3.65	1.44	1.33
3	C	1007	POV	O31-C31	3.65	1.44	1.33
3	C	1010	POV	O31-C31	3.65	1.44	1.33
3	E	1004	POV	O31-C31	3.65	1.44	1.33
3	D	1009	POV	O31-C31	3.63	1.43	1.33
3	C	1009	POV	O31-C31	3.62	1.43	1.33
3	D	1010	POV	O31-C31	3.62	1.43	1.33
3	F	1003	POV	O31-C31	3.61	1.43	1.33
3	D	1004	POV	O31-C31	3.59	1.43	1.33
3	C	1004	POV	O31-C31	3.59	1.43	1.33
3	B	1005	POV	O31-C31	3.57	1.43	1.33
3	A	1004	POV	O31-C31	3.51	1.43	1.33
3	F	1006	POV	O21-C21	3.07	1.43	1.34
3	E	1007	POV	O21-C21	3.05	1.42	1.34
3	D	1007	POV	O21-C21	3.03	1.42	1.34
3	A	1007	POV	O21-C21	3.02	1.42	1.34
3	B	1008	POV	O21-C21	3.00	1.42	1.34
3	C	1007	POV	O21-C21	2.99	1.42	1.34
3	E	1009	POV	O21-C21	2.95	1.42	1.34
3	B	1010	POV	O21-C21	2.91	1.42	1.34
3	C	1009	POV	O21-C21	2.91	1.42	1.34
3	F	1010	POV	O21-C21	2.90	1.42	1.34
3	E	1003	POV	O21-C21	2.90	1.42	1.34
3	C	1010	POV	O21-C21	2.89	1.42	1.34
3	B	1002	POV	O21-C21	2.89	1.42	1.34
3	D	1010	POV	O21-C21	2.87	1.42	1.34
3	F	1004	POV	O21-C21	2.87	1.42	1.34
3	F	1009	POV	O21-C21	2.86	1.42	1.34
3	A	1005	POV	O21-C21	2.86	1.42	1.34
3	A	1009	POV	O21-C21	2.85	1.42	1.34
3	E	1010	POV	O21-C21	2.85	1.42	1.34
3	A	1011	POV	O21-C21	2.84	1.42	1.34
3	D	1003	POV	O21-C21	2.84	1.42	1.34
3	C	1005	POV	O21-C21	2.83	1.42	1.34
3	D	1005	POV	O21-C21	2.83	1.42	1.34
3	E	1005	POV	O21-C21	2.83	1.42	1.34
3	F	1008	POV	O21-C21	2.82	1.42	1.34
3	D	1006	POV	O21-C21	2.82	1.42	1.34
3	D	1011	POV	O21-C21	2.82	1.42	1.34
3	A	1010	POV	O21-C21	2.82	1.42	1.34
3	D	1005	POV	P-O12	2.81	1.70	1.59
3	E	1004	POV	O21-C21	2.81	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1004	POV	O21-C21	2.81	1.42	1.34
3	C	1006	POV	O21-C21	2.81	1.42	1.34
3	F	1002	POV	O21-C21	2.81	1.42	1.34
3	D	1009	POV	O21-C21	2.80	1.42	1.34
3	A	1012	POV	O21-C21	2.79	1.42	1.34
3	D	1002	POV	O21-C21	2.79	1.42	1.34
3	B	1006	POV	O21-C21	2.79	1.42	1.34
3	B	1007	POV	O21-C21	2.78	1.42	1.34
3	B	1006	POV	P-O12	2.78	1.70	1.59
3	A	1002	POV	O21-C21	2.78	1.42	1.34
3	F	1005	POV	O21-C21	2.78	1.42	1.34
3	C	1004	POV	O21-C21	2.77	1.42	1.34
3	F	1004	POV	P-O12	2.77	1.70	1.59
3	E	1008	POV	P-O12	2.77	1.70	1.59
3	C	1003	POV	O21-C21	2.76	1.42	1.34
3	A	1006	POV	O21-C21	2.76	1.42	1.34
3	C	1005	POV	P-O12	2.76	1.70	1.59
3	A	1005	POV	P-O12	2.75	1.70	1.59
3	F	1003	POV	O21-C21	2.75	1.42	1.34
3	C	1008	POV	P-O12	2.75	1.70	1.59
3	C	1002	POV	O21-C21	2.75	1.42	1.34
3	A	1004	POV	O21-C21	2.74	1.42	1.34
3	B	1005	POV	O21-C21	2.74	1.42	1.34
3	E	1006	POV	O21-C21	2.74	1.42	1.34
3	A	1003	POV	O21-C21	2.73	1.42	1.34
3	B	1009	POV	P-O12	2.73	1.70	1.59
3	D	1008	POV	P-O12	2.73	1.70	1.59
3	F	1007	POV	P-O12	2.73	1.70	1.59
3	A	1008	POV	P-O12	2.73	1.70	1.59
3	E	1005	POV	P-O12	2.73	1.70	1.59
3	A	1003	POV	P-O12	2.72	1.70	1.59
3	E	1002	POV	O21-C21	2.71	1.42	1.34
3	B	1003	POV	O21-C21	2.70	1.41	1.34
3	C	1003	POV	P-O12	2.69	1.70	1.59
3	D	1004	POV	O21-C21	2.68	1.41	1.34
3	C	1004	POV	P-O12	2.68	1.70	1.59
3	C	1008	POV	O21-C21	2.68	1.41	1.34
3	D	1003	POV	P-O12	2.67	1.70	1.59
3	E	1004	POV	P-O12	2.67	1.70	1.59
3	D	1004	POV	P-O12	2.66	1.70	1.59
3	D	1008	POV	O21-C21	2.66	1.41	1.34
3	B	1005	POV	P-O12	2.66	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1008	POV	O21-C21	2.65	1.41	1.34
3	E	1003	POV	P-O12	2.64	1.70	1.59
3	F	1002	POV	P-O12	2.64	1.70	1.59
3	F	1007	POV	O21-C21	2.64	1.41	1.34
3	B	1004	POV	P-O12	2.63	1.70	1.59
3	A	1008	POV	O21-C21	2.63	1.41	1.34
3	B	1009	POV	O21-C21	2.62	1.41	1.34
3	A	1004	POV	P-O12	2.61	1.69	1.59
3	F	1003	POV	P-O12	2.60	1.69	1.59
3	A	1011	POV	P-O12	2.59	1.69	1.59
3	A	1007	POV	P-O12	2.58	1.69	1.59
3	E	1007	POV	P-O12	2.58	1.69	1.59
3	B	1002	POV	P-O12	2.57	1.69	1.59
3	B	1008	POV	P-O12	2.57	1.69	1.59
3	F	1010	POV	P-O12	2.57	1.69	1.59
3	F	1006	POV	P-O12	2.57	1.69	1.59
3	D	1007	POV	P-O12	2.55	1.69	1.59
3	C	1007	POV	P-O12	2.55	1.69	1.59
3	C	1010	POV	P-O12	2.55	1.69	1.59
3	D	1003	POV	C12-C11	2.55	1.59	1.51
3	C	1003	POV	C12-C11	2.54	1.59	1.51
3	E	1009	POV	P-O12	2.53	1.69	1.59
3	A	1009	POV	P-O12	2.53	1.69	1.59
3	A	1012	POV	P-O12	2.52	1.69	1.59
3	E	1010	POV	P-O12	2.52	1.69	1.59
3	B	1005	POV	C12-C11	2.51	1.59	1.51
3	B	1007	POV	P-O12	2.51	1.69	1.59
3	F	1008	POV	P-O12	2.50	1.69	1.59
3	D	1011	POV	P-O12	2.50	1.69	1.59
3	D	1009	POV	P-O12	2.50	1.69	1.59
3	E	1004	POV	C12-C11	2.49	1.59	1.51
3	C	1009	POV	P-O12	2.49	1.69	1.59
3	A	1006	POV	P-O12	2.49	1.69	1.59
3	E	1006	POV	P-O12	2.48	1.69	1.59
3	B	1010	POV	P-O12	2.48	1.69	1.59
3	D	1004	POV	C12-C11	2.48	1.59	1.51
3	D	1006	POV	P-O12	2.47	1.69	1.59
3	D	1010	POV	P-O12	2.47	1.69	1.59
3	C	1004	POV	C12-C11	2.47	1.59	1.51
3	F	1005	POV	P-O12	2.46	1.69	1.59
3	C	1006	POV	P-O12	2.46	1.69	1.59
3	C	1002	POV	P-O12	2.46	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1009	POV	P-O12	2.45	1.69	1.59
3	A	1004	POV	C12-C11	2.44	1.59	1.51
3	D	1002	POV	P-O12	2.44	1.69	1.59
3	E	1002	POV	P-O12	2.42	1.69	1.59
3	B	1003	POV	P-O12	2.42	1.69	1.59
3	F	1003	POV	C12-C11	2.41	1.58	1.51
3	A	1002	POV	P-O12	2.40	1.69	1.59
3	A	1010	POV	P-O12	2.40	1.69	1.59
3	F	1010	POV	C12-C11	2.37	1.58	1.51
3	A	1003	POV	C12-C11	2.36	1.58	1.51
3	B	1002	POV	C12-C11	2.36	1.58	1.51
3	A	1011	POV	C12-C11	2.35	1.58	1.51
3	C	1007	POV	C12-C11	2.34	1.58	1.51
3	D	1002	POV	C12-C11	2.33	1.58	1.51
3	C	1010	POV	C12-C11	2.33	1.58	1.51
3	F	1006	POV	C12-C11	2.32	1.58	1.51
3	E	1007	POV	C12-C11	2.31	1.58	1.51
3	A	1007	POV	C12-C11	2.31	1.58	1.51
3	B	1007	POV	C12-C11	2.31	1.58	1.51
3	C	1006	POV	C12-C11	2.31	1.58	1.51
3	B	1009	POV	C12-C11	2.30	1.58	1.51
3	D	1007	POV	C12-C11	2.30	1.58	1.51
3	D	1006	POV	C12-C11	2.30	1.58	1.51
3	E	1006	POV	C12-C11	2.30	1.58	1.51
3	A	1006	POV	C12-C11	2.30	1.58	1.51
3	F	1007	POV	C12-C11	2.30	1.58	1.51
3	E	1008	POV	C12-C11	2.29	1.58	1.51
3	A	1005	POV	C12-C11	2.29	1.58	1.51
3	E	1010	POV	C12-C11	2.29	1.58	1.51
3	F	1004	POV	C12-C11	2.29	1.58	1.51
3	C	1008	POV	C12-C11	2.29	1.58	1.51
3	F	1008	POV	C12-C11	2.29	1.58	1.51
3	F	1002	POV	C12-C11	2.29	1.58	1.51
3	B	1008	POV	C12-C11	2.29	1.58	1.51
3	F	1005	POV	C12-C11	2.29	1.58	1.51
3	B	1004	POV	C12-C11	2.29	1.58	1.51
3	A	1008	POV	C12-C11	2.28	1.58	1.51
3	A	1012	POV	C12-C11	2.28	1.58	1.51
3	D	1009	POV	C12-C11	2.28	1.58	1.51
3	B	1006	POV	C12-C11	2.28	1.58	1.51
3	C	1002	POV	C12-C11	2.28	1.58	1.51
3	D	1008	POV	C12-C11	2.27	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1002	POV	C12-C11	2.27	1.58	1.51
3	A	1010	POV	C12-C11	2.27	1.58	1.51
3	D	1011	POV	C12-C11	2.26	1.58	1.51
3	A	1002	POV	C12-C11	2.26	1.58	1.51
3	C	1005	POV	C12-C11	2.26	1.58	1.51
3	D	1005	POV	C12-C11	2.25	1.58	1.51
3	E	1005	POV	C12-C11	2.24	1.58	1.51
3	B	1003	POV	C12-C11	2.24	1.58	1.51
3	E	1009	POV	C12-C11	2.22	1.58	1.51
3	C	1009	POV	C12-C11	2.22	1.58	1.51
3	E	1003	POV	C12-C11	2.22	1.58	1.51
3	A	1009	POV	C12-C11	2.21	1.58	1.51
3	D	1010	POV	C12-C11	2.17	1.58	1.51
3	B	1010	POV	C12-C11	2.16	1.58	1.51
3	F	1009	POV	C12-C11	2.13	1.58	1.51
3	F	1006	POV	C22-C21	2.12	1.56	1.50
3	B	1008	POV	C22-C21	2.09	1.56	1.50
3	A	1007	POV	C22-C21	2.08	1.56	1.50
3	E	1007	POV	C22-C21	2.08	1.56	1.50
3	E	1004	POV	P-O11	2.06	1.67	1.59
3	B	1002	POV	C22-C21	2.06	1.56	1.50
3	C	1003	POV	P-O11	2.05	1.67	1.59
3	D	1003	POV	P-O11	2.05	1.67	1.59
3	F	1004	POV	C22-C21	2.05	1.56	1.50
3	E	1003	POV	C22-C21	2.04	1.56	1.50
3	A	1011	POV	C22-C21	2.04	1.56	1.50
3	F	1010	POV	C22-C21	2.03	1.56	1.50
3	C	1010	POV	C22-C21	2.03	1.56	1.50
3	E	1010	POV	C22-C21	2.03	1.56	1.50
3	C	1007	POV	C22-C21	2.03	1.56	1.50
3	D	1007	POV	C22-C21	2.03	1.56	1.50
3	E	1003	POV	P-O11	2.02	1.67	1.59
3	B	1005	POV	P-O11	2.02	1.67	1.59
3	F	1006	POV	P-O11	2.01	1.67	1.59
3	B	1006	POV	C22-C21	2.01	1.56	1.50
3	D	1004	POV	P-O11	2.01	1.67	1.59
3	D	1003	POV	C22-C21	2.01	1.56	1.50
3	A	1004	POV	P-O11	2.01	1.67	1.59
3	F	1010	POV	P-O11	2.00	1.67	1.59

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1006	POV	O21-C21-C22	5.07	122.43	111.50
3	E	1007	POV	O21-C21-C22	4.87	122.00	111.50
3	A	1007	POV	O21-C21-C22	4.80	121.85	111.50
3	D	1007	POV	O21-C21-C22	4.78	121.81	111.50
3	C	1007	POV	O21-C21-C22	4.73	121.69	111.50
3	B	1008	POV	O21-C21-C22	4.70	121.64	111.50
3	D	1006	POV	O21-C21-C22	4.40	120.99	111.50
3	C	1006	POV	O21-C21-C22	4.37	120.91	111.50
3	D	1004	POV	O21-C21-C22	4.33	120.84	111.50
3	F	1005	POV	O21-C21-C22	4.29	120.75	111.50
3	B	1005	POV	O21-C21-C22	4.28	120.72	111.50
3	B	1007	POV	O21-C21-C22	4.23	120.61	111.50
3	A	1006	POV	O21-C21-C22	4.21	120.58	111.50
3	B	1002	POV	O21-C21-C22	4.21	120.57	111.50
3	C	1010	POV	O21-C21-C22	4.21	120.56	111.50
3	F	1010	POV	O21-C21-C22	4.20	120.55	111.50
3	E	1006	POV	O21-C21-C22	4.17	120.48	111.50
3	E	1003	POV	O21-C21-C22	4.13	120.41	111.50
3	E	1010	POV	O21-C21-C22	4.13	120.41	111.50
3	A	1004	POV	O21-C21-C22	4.09	120.31	111.50
3	A	1011	POV	O21-C21-C22	4.07	120.27	111.50
3	E	1004	POV	O21-C21-C22	4.06	120.26	111.50
3	F	1003	POV	O21-C21-C22	4.05	120.22	111.50
3	A	1003	POV	O21-C21-C22	4.04	120.21	111.50
3	E	1009	POV	O21-C21-C22	4.03	120.19	111.50
3	D	1011	POV	O21-C21-C22	3.96	120.03	111.50
3	C	1009	POV	O21-C21-C22	3.94	119.99	111.50
3	D	1003	POV	O21-C21-C22	3.93	119.96	111.50
3	A	1012	POV	O21-C21-C22	3.92	119.96	111.50
3	D	1009	POV	O21-C21-C22	3.89	119.89	111.50
3	B	1006	POV	O21-C21-C22	3.89	119.87	111.50
3	A	1002	POV	O21-C21-C22	3.88	119.86	111.50
3	F	1008	POV	O21-C21-C22	3.87	119.85	111.50
3	C	1003	POV	O21-C21-C22	3.86	119.83	111.50
3	C	1004	POV	O21-C21-C22	3.85	119.80	111.50
3	D	1010	POV	O21-C21-C22	3.85	119.80	111.50
3	B	1003	POV	O21-C21-C22	3.85	119.79	111.50
3	F	1004	POV	O21-C21-C22	3.85	119.79	111.50
3	C	1005	POV	O21-C21-C22	3.83	119.75	111.50
3	B	1004	POV	O21-C21-C22	3.82	119.73	111.50
3	B	1010	POV	O21-C21-C22	3.80	119.70	111.50
3	F	1002	POV	O21-C21-C22	3.77	119.63	111.50
3	E	1002	POV	O21-C21-C22	3.76	119.61	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1005	POV	O21-C21-C22	3.72	119.52	111.50
3	F	1009	POV	O21-C21-C22	3.72	119.51	111.50
3	A	1009	POV	O21-C21-C22	3.71	119.50	111.50
3	C	1008	POV	O21-C21-C22	3.71	119.49	111.50
3	D	1005	POV	O21-C21-C22	3.68	119.42	111.50
3	F	1007	POV	O21-C21-C22	3.67	119.42	111.50
3	B	1009	POV	O21-C21-C22	3.65	119.37	111.50
3	D	1002	POV	O21-C21-C22	3.62	119.30	111.50
3	D	1008	POV	O21-C21-C22	3.60	119.26	111.50
3	E	1008	POV	O21-C21-C22	3.60	119.25	111.50
3	C	1002	POV	O21-C21-C22	3.59	119.25	111.50
3	A	1008	POV	O21-C21-C22	3.56	119.17	111.50
3	A	1010	POV	O21-C21-C22	3.53	119.11	111.50
3	E	1005	POV	O21-C21-C22	3.46	118.96	111.50
3	A	1010	POV	O31-C31-C32	3.31	122.29	111.91
3	D	1003	POV	O31-C31-C32	3.23	122.06	111.91
3	A	1003	POV	O31-C31-C32	3.19	121.91	111.91
3	B	1004	POV	O31-C31-C32	3.10	121.64	111.91
3	C	1003	POV	O31-C31-C32	3.09	121.59	111.91
3	B	1003	POV	O31-C31-C32	2.96	121.19	111.91
3	A	1002	POV	O31-C31-C32	2.94	121.12	111.91
3	F	1002	POV	O31-C31-C32	2.93	121.09	111.91
3	B	1008	POV	C3-C2-C1	-2.91	104.91	111.79
3	D	1007	POV	O31-C31-C32	2.91	121.03	111.91
3	E	1002	POV	O31-C31-C32	2.89	120.99	111.91
3	C	1007	POV	O31-C31-C32	2.88	120.95	111.91
3	A	1007	POV	C3-C2-C1	-2.87	104.99	111.79
3	C	1007	POV	C3-C2-C1	-2.87	105.01	111.79
3	E	1003	POV	O31-C31-C32	2.84	120.82	111.91
3	B	1008	POV	O31-C31-C32	2.82	120.76	111.91
3	E	1007	POV	C3-C2-C1	-2.80	105.16	111.79
3	C	1002	POV	O31-C31-C32	2.79	120.66	111.91
3	F	1006	POV	C3-C2-C1	-2.78	105.21	111.79
3	D	1002	POV	O31-C31-C32	2.76	120.57	111.91
3	A	1007	POV	O31-C31-C32	2.73	120.48	111.91
3	F	1006	POV	O31-C31-C32	2.73	120.46	111.91
3	E	1007	POV	O31-C31-C32	2.72	120.44	111.91
3	F	1007	POV	O31-C31-C32	2.70	120.37	111.91
3	F	1010	POV	O31-C31-C32	2.68	120.31	111.91
3	C	1008	POV	O31-C31-C32	2.67	120.29	111.91
3	B	1002	POV	O31-C31-C32	2.66	120.26	111.91
3	E	1008	POV	O31-C31-C32	2.65	120.22	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1011	POV	O31-C31-C32	2.63	120.15	111.91
3	E	1010	POV	O31-C31-C32	2.59	120.05	111.91
3	A	1011	POV	O31-C31-C32	2.59	120.05	111.91
3	B	1009	POV	O31-C31-C32	2.58	120.01	111.91
3	D	1007	POV	C3-C2-C1	-2.57	105.71	111.79
3	D	1008	POV	O31-C31-C32	2.54	119.89	111.91
3	C	1010	POV	O31-C31-C32	2.54	119.87	111.91
3	A	1008	POV	O31-C31-C32	2.53	119.86	111.91
3	C	1009	POV	O31-C31-C32	2.53	119.84	111.91
3	A	1009	POV	O31-C31-C32	2.51	119.79	111.91
3	E	1009	POV	O31-C31-C32	2.50	119.75	111.91
3	B	1010	POV	O31-C31-C32	2.48	119.70	111.91
3	F	1009	POV	O31-C31-C32	2.47	119.66	111.91
3	F	1004	POV	O31-C31-C32	2.47	119.65	111.91
3	D	1010	POV	O31-C31-C32	2.47	119.65	111.91
3	D	1009	POV	O31-C31-C32	2.46	119.64	111.91
3	F	1008	POV	O31-C31-C32	2.43	119.52	111.91
3	F	1003	POV	O31-C31-C32	2.42	119.50	111.91
3	C	1005	POV	C11-C12-N	-2.39	107.81	115.78
3	A	1012	POV	O31-C31-C32	2.38	119.38	111.91
3	D	1005	POV	C11-C12-N	-2.37	107.86	115.78
3	C	1006	POV	O31-C31-C32	2.36	119.32	111.91
3	E	1006	POV	O31-C31-C32	2.35	119.29	111.91
3	A	1006	POV	O31-C31-C32	2.35	119.29	111.91
3	B	1007	POV	O31-C31-C32	2.34	119.25	111.91
3	E	1005	POV	C11-C12-N	-2.33	108.01	115.78
3	F	1007	POV	C2-O21-C21	-2.33	112.06	117.79
3	D	1006	POV	O31-C31-C32	2.32	119.18	111.91
3	A	1004	POV	O31-C31-C32	2.31	119.17	111.91
3	F	1005	POV	O31-C31-C32	2.31	119.16	111.91
3	B	1006	POV	O31-C31-C32	2.30	119.14	111.91
3	C	1004	POV	O31-C31-C32	2.30	119.12	111.91
3	D	1004	POV	O31-C31-C32	2.29	119.11	111.91
3	A	1005	POV	C11-C12-N	-2.29	108.13	115.78
3	B	1006	POV	C11-C12-N	-2.28	108.18	115.78
3	C	1005	POV	O31-C31-C32	2.27	119.04	111.91
3	C	1009	POV	C3-C2-C1	-2.25	106.46	111.79
3	A	1005	POV	O31-C31-C32	2.21	118.84	111.91
3	B	1005	POV	O31-C31-C32	2.21	118.83	111.91
3	E	1004	POV	O31-C31-C32	2.20	118.83	111.91
3	F	1004	POV	C11-C12-N	-2.20	108.44	115.78
3	D	1010	POV	C3-C2-C1	-2.19	106.60	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1005	POV	O31-C31-C32	2.19	118.77	111.91
3	B	1010	POV	C3-C2-C1	-2.17	106.66	111.79
3	D	1009	POV	C3-C2-C1	-2.13	106.75	111.79
3	B	1004	POV	C24-C23-C22	-2.13	105.53	113.19
3	E	1009	POV	C3-C2-C1	-2.12	106.76	111.79
3	B	1009	POV	C2-O21-C21	-2.10	112.61	117.79
3	F	1008	POV	C3-C2-C1	-2.09	106.84	111.79
3	D	1003	POV	C24-C23-C22	-2.08	105.70	113.19
3	E	1003	POV	C24-C23-C22	-2.08	105.71	113.19
3	E	1005	POV	O31-C31-C32	2.07	118.40	111.91
3	A	1009	POV	C3-C2-C1	-2.06	106.92	111.79
3	C	1003	POV	C24-C23-C22	-2.06	105.80	113.19
3	C	1006	POV	C3-C2-C1	-2.05	106.95	111.79
3	F	1009	POV	C3-C2-C1	-2.03	106.97	111.79
3	C	1008	POV	C2-O21-C21	-2.01	112.84	117.79
3	E	1005	POV	C2-O21-C21	-2.01	112.84	117.79
3	A	1010	POV	O31-C31-O32	-2.01	118.52	123.59
3	E	1006	POV	C2-O21-C21	-2.00	112.86	117.79

There are no chirality outliers.

All (1434) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	POV	C1-O11-P-O14
3	A	1003	POV	C12-C11-O12-P
3	A	1004	POV	C1-O11-P-O13
3	A	1005	POV	C22-C21-O21-C2
3	A	1006	POV	C1-O11-P-O14
3	A	1006	POV	C11-O12-P-O13
3	A	1006	POV	C11-O12-P-O14
3	A	1006	POV	O12-C11-C12-N
3	A	1007	POV	C11-O12-P-O11
3	A	1007	POV	C11-O12-P-O13
3	A	1007	POV	C11-O12-P-O14
3	A	1007	POV	O12-C11-C12-N
3	A	1007	POV	C22-C21-O21-C2
3	A	1007	POV	O22-C21-O21-C2
3	A	1008	POV	C1-O11-P-O12
3	A	1008	POV	C1-O11-P-O13
3	A	1008	POV	C1-O11-P-O14
3	A	1008	POV	O12-C11-C12-N
3	A	1008	POV	C12-C11-O12-P

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Mol	Chain	Res	Type	Atoms
3	A	1008	POV	C22-C21-O21-C2
3	A	1010	POV	C1-O11-P-O14
3	A	1011	POV	C1-O11-P-O14
3	A	1011	POV	C11-O12-P-O14
3	A	1011	POV	C22-C21-O21-C2
3	A	1011	POV	O22-C21-O21-C2
3	A	1012	POV	O12-C11-C12-N
3	B	1002	POV	C11-O12-P-O11
3	B	1002	POV	C11-O12-P-O14
3	B	1002	POV	C22-C21-O21-C2
3	B	1002	POV	O22-C21-O21-C2
3	B	1003	POV	C1-O11-P-O14
3	B	1004	POV	C11-O12-P-O13
3	B	1004	POV	C12-C11-O12-P
3	B	1005	POV	C1-O11-P-O13
3	B	1006	POV	C22-C21-O21-C2
3	B	1007	POV	C1-O11-P-O14
3	B	1007	POV	C11-O12-P-O13
3	B	1007	POV	C11-O12-P-O14
3	B	1007	POV	O12-C11-C12-N
3	B	1008	POV	C11-O12-P-O13
3	B	1008	POV	C11-O12-P-O14
3	B	1008	POV	O12-C11-C12-N
3	B	1008	POV	C22-C21-O21-C2
3	B	1008	POV	O22-C21-O21-C2
3	B	1009	POV	C1-O11-P-O12
3	B	1009	POV	C1-O11-P-O13
3	B	1009	POV	C1-O11-P-O14
3	B	1009	POV	O12-C11-C12-N
3	B	1009	POV	C12-C11-O12-P
3	B	1009	POV	C22-C21-O21-C2
3	C	1002	POV	C1-O11-P-O14
3	C	1003	POV	C1-O11-P-O12
3	C	1003	POV	C1-O11-P-O13
3	C	1003	POV	C1-O11-P-O14
3	C	1003	POV	O12-C11-C12-N
3	C	1003	POV	C12-C11-O12-P
3	C	1004	POV	C1-O11-P-O13
3	C	1004	POV	C22-C21-O21-C2
3	C	1005	POV	C22-C21-O21-C2
3	C	1006	POV	C1-O11-P-O14
3	C	1006	POV	C11-O12-P-O13

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Mol	Chain	Res	Type	Atoms
3	C	1006	POV	C11-O12-P-O14
3	C	1006	POV	O12-C11-C12-N
3	C	1007	POV	C11-O12-P-O13
3	C	1007	POV	C11-O12-P-O14
3	C	1007	POV	O12-C11-C12-N
3	C	1007	POV	C22-C21-O21-C2
3	C	1007	POV	O22-C21-O21-C2
3	C	1008	POV	C1-O11-P-O13
3	C	1008	POV	C1-O11-P-O14
3	C	1008	POV	O12-C11-C12-N
3	C	1008	POV	C12-C11-O12-P
3	C	1008	POV	C22-C21-O21-C2
3	C	1010	POV	C1-O11-P-O14
3	C	1010	POV	C22-C21-O21-C2
3	C	1010	POV	O22-C21-O21-C2
3	D	1002	POV	C1-O11-P-O14
3	D	1003	POV	C1-O11-P-O12
3	D	1003	POV	C1-O11-P-O13
3	D	1003	POV	C1-O11-P-O14
3	D	1003	POV	O12-C11-C12-N
3	D	1003	POV	C12-C11-O12-P
3	D	1004	POV	C1-O11-P-O13
3	D	1004	POV	C22-C21-O21-C2
3	D	1005	POV	C22-C21-O21-C2
3	D	1006	POV	C1-O11-P-O14
3	D	1006	POV	C11-O12-P-O13
3	D	1006	POV	C11-O12-P-O14
3	D	1006	POV	O12-C11-C12-N
3	D	1007	POV	C11-O12-P-O13
3	D	1007	POV	C11-O12-P-O14
3	D	1007	POV	O12-C11-C12-N
3	D	1007	POV	C22-C21-O21-C2
3	D	1007	POV	O22-C21-O21-C2
3	D	1008	POV	C1-O11-P-O13
3	D	1008	POV	C1-O11-P-O14
3	D	1008	POV	O12-C11-C12-N
3	D	1008	POV	C12-C11-O12-P
3	D	1008	POV	C22-C21-O21-C2
3	D	1009	POV	O12-C11-C12-N
3	D	1011	POV	C11-O12-P-O14
3	D	1011	POV	C22-C21-O21-C2
3	D	1011	POV	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
3	E	1002	POV	C1-O11-P-O14
3	E	1003	POV	C1-O11-P-O14
3	E	1003	POV	C11-O12-P-O13
3	E	1003	POV	C11-O12-P-O14
3	E	1004	POV	C1-O11-P-O13
3	E	1004	POV	C1-O11-P-O14
3	E	1004	POV	C22-C21-O21-C2
3	E	1005	POV	C22-C21-O21-C2
3	E	1006	POV	C1-O11-P-O14
3	E	1006	POV	C11-O12-P-O13
3	E	1006	POV	C11-O12-P-O14
3	E	1006	POV	O12-C11-C12-N
3	E	1007	POV	C11-O12-P-O11
3	E	1007	POV	C11-O12-P-O13
3	E	1007	POV	C11-O12-P-O14
3	E	1007	POV	O12-C11-C12-N
3	E	1007	POV	C22-C21-O21-C2
3	E	1007	POV	O22-C21-O21-C2
3	E	1008	POV	C1-O11-P-O12
3	E	1008	POV	C1-O11-P-O13
3	E	1008	POV	C1-O11-P-O14
3	E	1008	POV	O12-C11-C12-N
3	E	1008	POV	C12-C11-O12-P
3	E	1008	POV	C22-C21-O21-C2
3	E	1010	POV	C11-O12-P-O14
3	E	1010	POV	C22-C21-O21-C2
3	E	1010	POV	O22-C21-O21-C2
3	F	1002	POV	C11-O12-P-O13
3	F	1002	POV	C11-O12-P-O14
3	F	1002	POV	C12-C11-O12-P
3	F	1003	POV	C1-O11-P-O13
3	F	1003	POV	C1-O11-P-O14
3	F	1003	POV	C22-C21-O21-C2
3	F	1004	POV	C22-C21-O21-C2
3	F	1005	POV	C1-O11-P-O14
3	F	1005	POV	C11-O12-P-O13
3	F	1005	POV	C11-O12-P-O14
3	F	1005	POV	O12-C11-C12-N
3	F	1006	POV	C11-O12-P-O13
3	F	1006	POV	C11-O12-P-O14
3	F	1006	POV	O12-C11-C12-N
3	F	1006	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
3	F	1006	POV	O22-C21-O21-C2
3	F	1007	POV	C1-O11-P-O12
3	F	1007	POV	C1-O11-P-O13
3	F	1007	POV	C1-O11-P-O14
3	F	1007	POV	O12-C11-C12-N
3	F	1007	POV	C12-C11-O12-P
3	F	1007	POV	C22-C21-O21-C2
3	F	1008	POV	O12-C11-C12-N
3	F	1010	POV	C11-O12-P-O14
3	F	1010	POV	C22-C21-O21-C2
3	F	1010	POV	O22-C21-O21-C2
3	A	1011	POV	O32-C31-O31-C3
3	B	1002	POV	O32-C31-O31-C3
3	C	1010	POV	O32-C31-O31-C3
3	E	1010	POV	O32-C31-O31-C3
3	F	1010	POV	O32-C31-O31-C3
3	A	1004	POV	O22-C21-O21-C2
3	A	1005	POV	O22-C21-O21-C2
3	A	1008	POV	O22-C21-O21-C2
3	B	1005	POV	O22-C21-O21-C2
3	B	1006	POV	O22-C21-O21-C2
3	B	1009	POV	O22-C21-O21-C2
3	C	1004	POV	O22-C21-O21-C2
3	C	1008	POV	O22-C21-O21-C2
3	D	1004	POV	O22-C21-O21-C2
3	D	1005	POV	O22-C21-O21-C2
3	D	1008	POV	O22-C21-O21-C2
3	E	1004	POV	O22-C21-O21-C2
3	E	1005	POV	O22-C21-O21-C2
3	E	1008	POV	O22-C21-O21-C2
3	F	1003	POV	O22-C21-O21-C2
3	F	1007	POV	O22-C21-O21-C2
3	A	1007	POV	C32-C31-O31-C3
3	D	1007	POV	C32-C31-O31-C3
3	F	1006	POV	C32-C31-O31-C3
3	A	1004	POV	C22-C21-O21-C2
3	B	1005	POV	C22-C21-O21-C2
3	D	1011	POV	O32-C31-O31-C3
3	A	1011	POV	C32-C31-O31-C3
3	B	1002	POV	C32-C31-O31-C3
3	B	1008	POV	C32-C31-O31-C3
3	C	1007	POV	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
3	C	1010	POV	C32-C31-O31-C3
3	D	1011	POV	C32-C31-O31-C3
3	E	1007	POV	C32-C31-O31-C3
3	E	1010	POV	C32-C31-O31-C3
3	F	1010	POV	C32-C31-O31-C3
3	C	1005	POV	O22-C21-O21-C2
3	F	1004	POV	O22-C21-O21-C2
3	F	1006	POV	O32-C31-O31-C3
3	A	1007	POV	O32-C31-O31-C3
3	D	1007	POV	O32-C31-O31-C3
3	E	1007	POV	O32-C31-O31-C3
3	E	1006	POV	C22-C21-O21-C2
3	B	1008	POV	O32-C31-O31-C3
3	C	1007	POV	O32-C31-O31-C3
3	C	1008	POV	C32-C31-O31-C3
3	A	1002	POV	C22-C21-O21-C2
3	B	1003	POV	C22-C21-O21-C2
3	C	1002	POV	C22-C21-O21-C2
3	E	1006	POV	O22-C21-O21-C2
3	D	1004	POV	C11-C12-N-C13
3	D	1004	POV	C11-C12-N-C14
3	A	1008	POV	C32-C31-O31-C3
3	A	1009	POV	C32-C31-O31-C3
3	B	1009	POV	C32-C31-O31-C3
3	B	1010	POV	C32-C31-O31-C3
3	C	1009	POV	C32-C31-O31-C3
3	D	1008	POV	C32-C31-O31-C3
3	D	1010	POV	C32-C31-O31-C3
3	E	1009	POV	C32-C31-O31-C3
3	F	1009	POV	C32-C31-O31-C3
3	B	1002	POV	C31-C32-C33-C34
3	A	1006	POV	C22-C21-O21-C2
3	A	1010	POV	C22-C21-O21-C2
3	B	1007	POV	C22-C21-O21-C2
3	D	1002	POV	C22-C21-O21-C2
3	E	1002	POV	C22-C21-O21-C2
3	A	1010	POV	C21-C22-C23-C24
3	C	1010	POV	C21-C22-C23-C24
3	C	1010	POV	C31-C32-C33-C34
3	D	1006	POV	C31-C32-C33-C34
3	D	1009	POV	C31-C32-C33-C34
3	E	1009	POV	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	E	1010	POV	C31-C32-C33-C34
3	A	1009	POV	O32-C31-O31-C3
3	E	1008	POV	C32-C31-O31-C3
3	A	1002	POV	C21-C22-C23-C24
3	A	1006	POV	C31-C32-C33-C34
3	A	1007	POV	C21-C22-C23-C24
3	A	1012	POV	C31-C32-C33-C34
3	B	1006	POV	C31-C32-C33-C34
3	B	1007	POV	C31-C32-C33-C34
3	C	1002	POV	C21-C22-C23-C24
3	C	1006	POV	C31-C32-C33-C34
3	C	1009	POV	C21-C22-C23-C24
3	D	1010	POV	C21-C22-C23-C24
3	D	1011	POV	C21-C22-C23-C24
3	F	1004	POV	C31-C32-C33-C34
3	C	1009	POV	O32-C31-O31-C3
3	F	1009	POV	O32-C31-O31-C3
3	A	1005	POV	C31-C32-C33-C34
3	A	1009	POV	C21-C22-C23-C24
3	A	1011	POV	C31-C32-C33-C34
3	A	1012	POV	C21-C22-C23-C24
3	B	1005	POV	C21-C22-C23-C24
3	B	1008	POV	C21-C22-C23-C24
3	B	1010	POV	C21-C22-C23-C24
3	C	1005	POV	C31-C32-C33-C34
3	C	1007	POV	C21-C22-C23-C24
3	D	1005	POV	C31-C32-C33-C34
3	D	1006	POV	C21-C22-C23-C24
3	D	1007	POV	C21-C22-C23-C24
3	D	1009	POV	C21-C22-C23-C24
3	D	1011	POV	C31-C32-C33-C34
3	E	1002	POV	C21-C22-C23-C24
3	E	1004	POV	C21-C22-C23-C24
3	E	1005	POV	C31-C32-C33-C34
3	E	1006	POV	C31-C32-C33-C34
3	E	1007	POV	C21-C22-C23-C24
3	F	1005	POV	C31-C32-C33-C34
3	F	1006	POV	C21-C22-C23-C24
3	F	1008	POV	C31-C32-C33-C34
3	F	1009	POV	C21-C22-C23-C24
3	F	1010	POV	C31-C32-C33-C34
3	A	1002	POV	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
3	C	1004	POV	C21-C22-C23-C24
3	D	1002	POV	C21-C22-C23-C24
3	D	1004	POV	C21-C22-C23-C24
3	F	1003	POV	C21-C22-C23-C24
3	F	1008	POV	C21-C22-C23-C24
3	C	1006	POV	C22-C21-O21-C2
3	F	1005	POV	C22-C21-O21-C2
3	A	1008	POV	O32-C31-O31-C3
3	B	1010	POV	O32-C31-O31-C3
3	D	1008	POV	O32-C31-O31-C3
3	E	1009	POV	O32-C31-O31-C3
3	A	1004	POV	C21-C22-C23-C24
3	B	1003	POV	C21-C22-C23-C24
3	D	1010	POV	O32-C31-O31-C3
3	B	1002	POV	C21-C22-C23-C24
3	E	1010	POV	C21-C22-C23-C24
3	A	1010	POV	O22-C21-O21-C2
3	B	1003	POV	O22-C21-O21-C2
3	C	1002	POV	O22-C21-O21-C2
3	F	1007	POV	C32-C31-O31-C3
3	F	1008	POV	C32-C31-O31-C3
3	B	1009	POV	O32-C31-O31-C3
3	C	1008	POV	O32-C31-O31-C3
3	E	1008	POV	O32-C31-O31-C3
3	B	1010	POV	C22-C21-O21-C2
3	D	1006	POV	C22-C21-O21-C2
3	F	1009	POV	C22-C21-O21-C2
3	A	1003	POV	C1-O11-P-O12
3	A	1004	POV	C1-O11-P-O12
3	A	1005	POV	C11-O12-P-O11
3	A	1006	POV	C11-O12-P-O11
3	A	1011	POV	C1-O11-P-O12
3	A	1011	POV	C11-O12-P-O11
3	A	1012	POV	C11-O12-P-O11
3	B	1002	POV	C1-O11-P-O12
3	B	1004	POV	C1-O11-P-O12
3	B	1004	POV	C11-O12-P-O11
3	B	1005	POV	C1-O11-P-O12
3	B	1006	POV	C11-O12-P-O11
3	B	1007	POV	C11-O12-P-O11
3	B	1008	POV	C11-O12-P-O11
3	C	1004	POV	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
3	C	1005	POV	C11-O12-P-O11
3	C	1006	POV	C11-O12-P-O11
3	C	1007	POV	C11-O12-P-O11
3	C	1008	POV	C1-O11-P-O12
3	C	1010	POV	C11-O12-P-O11
3	D	1002	POV	C1-O11-P-O12
3	D	1004	POV	C1-O11-P-O12
3	D	1005	POV	C11-O12-P-O11
3	D	1006	POV	C11-O12-P-O11
3	D	1007	POV	C11-O12-P-O11
3	D	1008	POV	C1-O11-P-O12
3	D	1009	POV	C11-O12-P-O11
3	D	1011	POV	C1-O11-P-O12
3	D	1011	POV	C11-O12-P-O11
3	E	1003	POV	C1-O11-P-O12
3	E	1003	POV	C11-O12-P-O11
3	E	1004	POV	C1-O11-P-O12
3	E	1005	POV	C11-O12-P-O11
3	E	1006	POV	C11-O12-P-O11
3	E	1010	POV	C1-O11-P-O12
3	E	1010	POV	C11-O12-P-O11
3	F	1002	POV	C1-O11-P-O12
3	F	1002	POV	C11-O12-P-O11
3	F	1003	POV	C1-O11-P-O12
3	F	1004	POV	C11-O12-P-O11
3	F	1005	POV	C11-O12-P-O11
3	F	1006	POV	C11-O12-P-O11
3	F	1008	POV	C11-O12-P-O11
3	F	1010	POV	C1-O11-P-O12
3	F	1010	POV	C11-O12-P-O11
3	A	1006	POV	C32-C31-O31-C3
3	C	1006	POV	C32-C31-O31-C3
3	D	1009	POV	C32-C31-O31-C3
3	F	1005	POV	C21-C22-C23-C24
3	A	1006	POV	O22-C21-O21-C2
3	A	1009	POV	O22-C21-O21-C2
3	B	1007	POV	O22-C21-O21-C2
3	B	1010	POV	O22-C21-O21-C2
3	C	1006	POV	O22-C21-O21-C2
3	D	1002	POV	O22-C21-O21-C2
3	D	1006	POV	O22-C21-O21-C2
3	E	1002	POV	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
3	F	1005	POV	O22-C21-O21-C2
3	F	1009	POV	O22-C21-O21-C2
3	A	1012	POV	C32-C31-O31-C3
3	C	1005	POV	C33-C34-C35-C36
3	A	1009	POV	C22-C21-O21-C2
3	D	1010	POV	C22-C21-O21-C2
3	E	1009	POV	C22-C21-O21-C2
3	A	1010	POV	C39-C310-C311-C312
3	B	1006	POV	C33-C34-C35-C36
3	B	1010	POV	C22-C23-C24-C25
3	D	1003	POV	C310-C311-C312-C313
3	D	1009	POV	C310-C311-C312-C313
3	E	1002	POV	C24-C25-C26-C27
3	E	1008	POV	C24-C25-C26-C27
3	E	1010	POV	C212-C213-C214-C215
3	F	1002	POV	C312-C313-C314-C315
3	F	1004	POV	C33-C34-C35-C36
3	F	1010	POV	C212-C213-C214-C215
3	A	1002	POV	C39-C310-C311-C312
3	A	1003	POV	C310-C311-C312-C313
3	A	1011	POV	C212-C213-C214-C215
3	A	1012	POV	C310-C311-C312-C313
3	B	1006	POV	C22-C23-C24-C25
3	C	1002	POV	C24-C25-C26-C27
3	D	1002	POV	C24-C25-C26-C27
3	E	1002	POV	C39-C310-C311-C312
3	F	1002	POV	C311-C310-C39-C38
3	D	1010	POV	O22-C21-O21-C2
3	E	1009	POV	O22-C21-O21-C2
3	A	1003	POV	C31-C32-C33-C34
3	A	1008	POV	C24-C25-C26-C27
3	A	1010	POV	C24-C25-C26-C27
3	B	1003	POV	C24-C25-C26-C27
3	C	1003	POV	C39-C310-C311-C312
3	C	1010	POV	C212-C213-C214-C215
3	D	1003	POV	C311-C310-C39-C38
3	D	1005	POV	C22-C23-C24-C25
3	E	1005	POV	C33-C34-C35-C36
3	A	1003	POV	C32-C33-C34-C35
3	A	1005	POV	C22-C23-C24-C25
3	A	1005	POV	C33-C34-C35-C36
3	B	1003	POV	C39-C310-C311-C312

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Mol	Chain	Res	Type	Atoms
3	D	1005	POV	C33-C34-C35-C36
3	D	1006	POV	C32-C33-C34-C35
3	D	1011	POV	C212-C213-C214-C215
3	F	1009	POV	C22-C23-C24-C25
3	A	1003	POV	C39-C310-C311-C312
3	A	1009	POV	C22-C23-C24-C25
3	B	1004	POV	C39-C310-C311-C312
3	C	1002	POV	C39-C310-C311-C312
3	C	1003	POV	C311-C310-C39-C38
3	E	1003	POV	C39-C310-C311-C312
3	F	1002	POV	C39-C310-C311-C312
3	A	1011	POV	C21-C22-C23-C24
3	D	1003	POV	C31-C32-C33-C34
3	F	1010	POV	C21-C22-C23-C24
3	A	1010	POV	C212-C213-C214-C215
3	B	1002	POV	C212-C213-C214-C215
3	D	1002	POV	C39-C310-C311-C312
3	D	1010	POV	C22-C23-C24-C25
3	E	1009	POV	C22-C23-C24-C25
3	F	1008	POV	C22-C23-C24-C25
3	F	1007	POV	O32-C31-O31-C3
3	F	1008	POV	O32-C31-O31-C3
3	B	1004	POV	C310-C311-C312-C313
3	C	1003	POV	C310-C311-C312-C313
3	E	1002	POV	C212-C213-C214-C215
3	E	1003	POV	C310-C311-C312-C313
3	E	1010	POV	C22-C23-C24-C25
3	F	1004	POV	C22-C23-C24-C25
3	A	1002	POV	C24-C25-C26-C27
3	A	1006	POV	C22-C23-C24-C25
3	A	1008	POV	C211-C212-C213-C214
3	A	1012	POV	C311-C312-C313-C314
3	B	1003	POV	C212-C213-C214-C215
3	C	1005	POV	C22-C23-C24-C25
3	C	1006	POV	C32-C33-C34-C35
3	C	1008	POV	C212-C213-C214-C215
3	D	1002	POV	C212-C213-C214-C215
3	D	1003	POV	C32-C33-C34-C35
3	D	1009	POV	C311-C312-C313-C314
3	E	1006	POV	C32-C33-C34-C35
3	F	1005	POV	C22-C23-C24-C25
3	F	1005	POV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
3	F	1007	POV	C212-C213-C214-C215
3	C	1002	POV	C212-C213-C214-C215
3	D	1003	POV	C39-C310-C311-C312
3	E	1003	POV	C311-C310-C39-C38
3	F	1010	POV	C22-C23-C24-C25
3	C	1009	POV	O22-C21-O21-C2
3	C	1009	POV	C22-C21-O21-C2
3	A	1012	POV	C22-C23-C24-C25
3	B	1005	POV	C23-C24-C25-C26
3	B	1007	POV	C32-C33-C34-C35
3	C	1008	POV	C211-C212-C213-C214
3	C	1009	POV	C22-C23-C24-C25
3	D	1008	POV	C24-C25-C26-C27
3	D	1009	POV	C22-C23-C24-C25
3	C	1003	POV	C26-C27-C28-C29
3	D	1002	POV	C210-C211-C212-C213
3	E	1007	POV	C210-C211-C212-C213
3	A	1003	POV	C311-C310-C39-C38
3	A	1006	POV	C32-C33-C34-C35
3	B	1002	POV	C22-C23-C24-C25
3	B	1004	POV	C32-C33-C34-C35
3	B	1009	POV	C212-C213-C214-C215
3	B	1009	POV	C36-C37-C38-C39
3	C	1008	POV	C36-C37-C38-C39
3	C	1010	POV	C22-C23-C24-C25
3	D	1008	POV	C211-C212-C213-C214
3	E	1003	POV	C24-C25-C26-C27
3	E	1003	POV	C32-C33-C34-C35
3	E	1004	POV	C23-C24-C25-C26
3	E	1008	POV	C212-C213-C214-C215
3	F	1002	POV	C24-C25-C26-C27
3	F	1003	POV	C23-C24-C25-C26
3	F	1008	POV	C310-C311-C312-C313
3	F	1008	POV	C311-C312-C313-C314
3	D	1004	POV	C11-C12-N-C15
3	B	1003	POV	C311-C310-C39-C38
3	D	1002	POV	C311-C310-C39-C38
3	D	1008	POV	C212-C213-C214-C215
3	A	1002	POV	C212-C213-C214-C215
3	B	1004	POV	C311-C310-C39-C38
3	B	1009	POV	C211-C212-C213-C214
3	C	1003	POV	C312-C313-C314-C315

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Mol	Chain	Res	Type	Atoms
3	C	1007	POV	C312-C313-C314-C315
3	C	1008	POV	C24-C25-C26-C27
3	E	1008	POV	C211-C212-C213-C214
3	E	1008	POV	C36-C37-C38-C39
3	F	1007	POV	C211-C212-C213-C214
3	A	1006	POV	C21-C22-C23-C24
3	C	1006	POV	O32-C31-O31-C3
3	A	1008	POV	C36-C37-C38-C39
3	B	1007	POV	C22-C23-C24-C25
3	C	1002	POV	C311-C310-C39-C38
3	C	1003	POV	C32-C33-C34-C35
3	D	1008	POV	C36-C37-C38-C39
3	E	1003	POV	C312-C313-C314-C315
3	F	1007	POV	C36-C37-C38-C39
3	F	1005	POV	C32-C31-O31-C3
3	B	1009	POV	C24-C25-C26-C27
3	D	1004	POV	C23-C24-C25-C26
3	F	1006	POV	C312-C313-C314-C315
3	A	1011	POV	C22-C23-C24-C25
3	C	1008	POV	C37-C38-C39-C310
3	E	1006	POV	C24-C25-C26-C27
3	A	1006	POV	O32-C31-O31-C3
3	D	1009	POV	O32-C31-O31-C3
3	F	1002	POV	C32-C33-C34-C35
3	F	1007	POV	C24-C25-C26-C27
3	A	1002	POV	C311-C310-C39-C38
3	C	1004	POV	C23-C24-C25-C26
3	C	1006	POV	C24-C25-C26-C27
3	C	1006	POV	C21-C22-C23-C24
3	B	1007	POV	C24-C25-C26-C27
3	B	1007	POV	C32-C31-O31-C3
3	D	1006	POV	C32-C31-O31-C3
3	C	1009	POV	C211-C212-C213-C214
3	B	1009	POV	C37-C38-C39-C310
3	D	1006	POV	C22-C23-C24-C25
3	D	1011	POV	C22-C23-C24-C25
3	F	1009	POV	C310-C311-C312-C313
3	A	1002	POV	C210-C211-C212-C213
3	A	1005	POV	C210-C211-C212-C213
3	B	1008	POV	C210-C211-C212-C213
3	C	1002	POV	C210-C211-C212-C213
3	C	1007	POV	C210-C211-C212-C213

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Mol	Chain	Res	Type	Atoms
3	D	1007	POV	C210-C211-C212-C213
3	E	1005	POV	C210-C211-C212-C213
3	F	1006	POV	C210-C211-C212-C213
3	D	1010	POV	C211-C212-C213-C214
3	C	1003	POV	C311-C312-C313-C314
3	C	1009	POV	C310-C311-C312-C313
3	A	1012	POV	O32-C31-O31-C3
3	A	1008	POV	C212-C213-C214-C215
3	A	1009	POV	C310-C311-C312-C313
3	B	1004	POV	C312-C313-C314-C315
3	E	1009	POV	C212-C213-C214-C215
3	F	1007	POV	C37-C38-C39-C310
3	A	1010	POV	C311-C310-C39-C38
3	C	1005	POV	C311-C312-C313-C314
3	F	1003	POV	C311-C312-C313-C314
3	F	1008	POV	C32-C33-C34-C35
3	A	1003	POV	C24-C25-C26-C27
3	B	1010	POV	C211-C212-C213-C214
3	D	1005	POV	C311-C312-C313-C314
3	D	1007	POV	C312-C313-C314-C315
3	D	1009	POV	C32-C33-C34-C35
3	E	1004	POV	C11-C12-N-C14
3	B	1007	POV	C21-C22-C23-C24
3	A	1008	POV	C37-C38-C39-C310
3	E	1004	POV	C311-C312-C313-C314
3	E	1008	POV	C37-C38-C39-C310
3	E	1006	POV	C32-C31-O31-C3
3	A	1012	POV	C22-C21-O21-C2
3	F	1002	POV	C310-C311-C312-C313
3	B	1004	POV	C31-C32-C33-C34
3	A	1005	POV	C24-C25-C26-C27
3	B	1004	POV	C24-C25-C26-C27
3	E	1002	POV	C311-C310-C39-C38
3	E	1006	POV	C22-C23-C24-C25
3	E	1009	POV	C211-C212-C213-C214
3	E	1010	POV	C33-C34-C35-C36
3	D	1003	POV	C311-C312-C313-C314
3	E	1005	POV	C311-C312-C313-C314
3	E	1005	POV	C24-C25-C26-C27
3	B	1007	POV	O32-C31-O31-C3
3	D	1006	POV	O32-C31-O31-C3
3	F	1005	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
3	A	1003	POV	C26-C27-C28-C29
3	A	1007	POV	C210-C211-C212-C213
3	A	1011	POV	C26-C27-C28-C29
3	B	1002	POV	C26-C27-C28-C29
3	B	1003	POV	C210-C211-C212-C213
3	B	1004	POV	C26-C27-C28-C29
3	C	1010	POV	C26-C27-C28-C29
3	D	1003	POV	C26-C27-C28-C29
3	D	1005	POV	C210-C211-C212-C213
3	D	1011	POV	C26-C27-C28-C29
3	E	1002	POV	C210-C211-C212-C213
3	F	1002	POV	C26-C27-C28-C29
3	F	1008	POV	O22-C21-O21-C2
3	C	1003	POV	C31-C32-C33-C34
3	E	1003	POV	C31-C32-C33-C34
3	A	1007	POV	C312-C313-C314-C315
3	A	1012	POV	C32-C33-C34-C35
3	A	1003	POV	C312-C313-C314-C315
3	A	1012	POV	C39-C310-C311-C312
3	D	1003	POV	C24-C25-C26-C27
3	A	1004	POV	C311-C312-C313-C314
3	A	1011	POV	C33-C34-C35-C36
3	B	1002	POV	C33-C34-C35-C36
3	B	1006	POV	C311-C312-C313-C314
3	B	1010	POV	C212-C213-C214-C215
3	E	1007	POV	C312-C313-C314-C315
3	F	1007	POV	C22-C23-C24-C25
3	B	1003	POV	C25-C26-C27-C28
3	C	1008	POV	C35-C36-C37-C38
3	D	1010	POV	C310-C311-C312-C313
3	E	1002	POV	C25-C26-C27-C28
3	D	1003	POV	C312-C313-C314-C315
3	D	1004	POV	C311-C312-C313-C314
3	D	1005	POV	C24-C25-C26-C27
3	D	1006	POV	C24-C25-C26-C27
3	D	1008	POV	C37-C38-C39-C310
3	E	1009	POV	C311-C312-C313-C314
3	F	1010	POV	C33-C34-C35-C36
3	D	1009	POV	C22-C21-O21-C2
3	F	1008	POV	C22-C21-O21-C2
3	A	1004	POV	C23-C24-C25-C26
3	B	1009	POV	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
3	A	1008	POV	C22-C23-C24-C25
3	A	1009	POV	C211-C212-C213-C214
3	A	1012	POV	O22-C21-O21-C2
3	A	1009	POV	C212-C213-C214-C215
3	F	1009	POV	C212-C213-C214-C215
3	D	1011	POV	C33-C34-C35-C36
3	A	1010	POV	C210-C211-C212-C213
3	E	1003	POV	C26-C27-C28-C29
3	E	1010	POV	C26-C27-C28-C29
3	F	1010	POV	C26-C27-C28-C29
3	B	1005	POV	C311-C312-C313-C314
3	A	1006	POV	C24-C25-C26-C27
3	A	1008	POV	C35-C36-C37-C38
3	D	1008	POV	C35-C36-C37-C38
3	F	1009	POV	C211-C212-C213-C214
3	F	1007	POV	C35-C36-C37-C38
3	E	1006	POV	O32-C31-O31-C3
3	B	1004	POV	C36-C37-C38-C39
3	C	1008	POV	C22-C23-C24-C25
3	C	1009	POV	C212-C213-C214-C215
3	D	1003	POV	C36-C37-C38-C39
3	D	1006	POV	C214-C215-C216-C217
3	E	1009	POV	C310-C311-C312-C313
3	A	1010	POV	C1-O11-P-O12
3	B	1003	POV	C1-O11-P-O12
3	C	1002	POV	C1-O11-P-O12
3	E	1002	POV	C1-O11-P-O12
3	C	1002	POV	C310-C311-C312-C313
3	D	1002	POV	C310-C311-C312-C313
3	D	1010	POV	C39-C310-C311-C312
3	B	1003	POV	C313-C314-C315-C316
3	D	1008	POV	C22-C23-C24-C25
3	F	1005	POV	C24-C25-C26-C27
3	F	1009	POV	C311-C312-C313-C314
3	A	1002	POV	C25-C26-C27-C28
3	B	1004	POV	C214-C215-C216-C217
3	B	1009	POV	C22-C23-C24-C25
3	C	1010	POV	C214-C215-C216-C217
3	B	1006	POV	C24-C25-C26-C27
3	C	1005	POV	C24-C25-C26-C27
3	D	1009	POV	C39-C310-C311-C312
3	E	1006	POV	C214-C215-C216-C217

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Mol	Chain	Res	Type	Atoms
3	F	1004	POV	C24-C25-C26-C27
3	F	1009	POV	C39-C310-C311-C312
3	C	1005	POV	C210-C211-C212-C213
3	A	1005	POV	C311-C312-C313-C314
3	B	1005	POV	C37-C38-C39-C310
3	C	1009	POV	C39-C310-C311-C312
3	E	1004	POV	C22-C23-C24-C25
3	C	1002	POV	C25-C26-C27-C28
3	C	1006	POV	C22-C23-C24-C25
3	C	1003	POV	C214-C215-C216-C217
3	C	1010	POV	C33-C34-C35-C36
3	F	1002	POV	C31-C32-C33-C34
3	A	1003	POV	C36-C37-C38-C39
3	C	1003	POV	C36-C37-C38-C39
3	A	1005	POV	C1-C2-C3-O31
3	A	1008	POV	C1-C2-C3-O31
3	A	1010	POV	C1-C2-C3-O31
3	B	1006	POV	C1-C2-C3-O31
3	B	1009	POV	C1-C2-C3-O31
3	C	1004	POV	C311-C312-C313-C314
3	C	1005	POV	C1-C2-C3-O31
3	C	1008	POV	C1-C2-C3-O31
3	D	1005	POV	C1-C2-C3-O31
3	D	1008	POV	C1-C2-C3-O31
3	F	1007	POV	C1-C2-C3-O31
3	A	1007	POV	C313-C314-C315-C316
3	A	1009	POV	C311-C312-C313-C314
3	B	1006	POV	C23-C24-C25-C26
3	B	1008	POV	C313-C314-C315-C316
3	A	1006	POV	C39-C310-C311-C312
3	B	1004	POV	C311-C312-C313-C314
3	E	1006	POV	C21-C22-C23-C24
3	A	1003	POV	C214-C215-C216-C217
3	A	1004	POV	C24-C25-C26-C27
3	A	1004	POV	C37-C38-C39-C310
3	B	1008	POV	C312-C313-C314-C315
3	F	1008	POV	C39-C310-C311-C312
3	B	1006	POV	C210-C211-C212-C213
3	D	1003	POV	C210-C211-C212-C213
3	F	1004	POV	C210-C211-C212-C213
3	C	1003	POV	C24-C25-C26-C27
3	C	1006	POV	C214-C215-C216-C217

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Mol	Chain	Res	Type	Atoms
3	D	1004	POV	C22-C23-C24-C25
3	D	1010	POV	C212-C213-C214-C215
3	D	1007	POV	C313-C314-C315-C316
3	E	1010	POV	C214-C215-C216-C217
3	B	1010	POV	C39-C310-C311-C312
3	E	1002	POV	C313-C314-C315-C316
3	A	1002	POV	C31-C32-C33-C34
3	C	1006	POV	C39-C310-C311-C312
3	C	1004	POV	C37-C38-C39-C310
3	E	1008	POV	C35-C36-C37-C38
3	F	1005	POV	C214-C215-C216-C217
3	D	1009	POV	O22-C21-O21-C2
3	B	1010	POV	C310-C311-C312-C313
3	A	1010	POV	C25-C26-C27-C28
3	C	1007	POV	C313-C314-C315-C316
3	E	1003	POV	C311-C312-C313-C314
3	F	1004	POV	C23-C24-C25-C26
3	A	1009	POV	C39-C310-C311-C312
3	A	1005	POV	O11-C1-C2-O21
3	E	1004	POV	O11-C1-C2-O21
3	F	1003	POV	O11-C1-C2-O21
3	F	1004	POV	O11-C1-C2-O21
3	D	1002	POV	C36-C37-C38-C39
3	E	1007	POV	C313-C314-C315-C316
3	D	1003	POV	C214-C215-C216-C217
3	A	1006	POV	C210-C211-C212-C213
3	D	1006	POV	C210-C211-C212-C213
3	B	1002	POV	C214-C215-C216-C217
3	F	1006	POV	C313-C314-C315-C316
3	A	1008	POV	O21-C2-C3-O31
3	F	1005	POV	C39-C310-C311-C312
3	F	1002	POV	C36-C37-C38-C39
3	A	1003	POV	C311-C312-C313-C314
3	D	1005	POV	C23-C24-C25-C26
3	E	1002	POV	C32-C33-C34-C35
3	E	1004	POV	C37-C38-C39-C310
3	E	1008	POV	C34-C35-C36-C37
3	E	1003	POV	C214-C215-C216-C217
3	F	1002	POV	C214-C215-C216-C217
3	A	1010	POV	C310-C311-C312-C313
3	B	1003	POV	C310-C311-C312-C313
3	F	1008	POV	C312-C313-C314-C315

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Mol	Chain	Res	Type	Atoms
3	D	1010	POV	C311-C312-C313-C314
3	F	1002	POV	C210-C211-C212-C213
3	B	1006	POV	C32-C33-C34-C35
3	E	1004	POV	C11-C12-N-C15
3	B	1009	POV	C34-C35-C36-C37
3	C	1009	POV	C311-C312-C313-C314
3	D	1008	POV	C34-C35-C36-C37
3	E	1002	POV	C310-C311-C312-C313
3	E	1003	POV	C36-C37-C38-C39
3	D	1002	POV	C25-C26-C27-C28
3	C	1002	POV	C313-C314-C315-C316
3	C	1005	POV	C23-C24-C25-C26
3	E	1008	POV	C311-C310-C39-C38
3	A	1005	POV	C32-C31-O31-C3
3	B	1006	POV	C32-C31-O31-C3
3	E	1002	POV	C32-C31-O31-C3
3	B	1003	POV	C31-C32-C33-C34
3	A	1002	POV	C313-C314-C315-C316
3	A	1011	POV	C214-C215-C216-C217
3	F	1007	POV	C34-C35-C36-C37
3	A	1002	POV	C310-C311-C312-C313
3	E	1002	POV	C35-C36-C37-C38
3	F	1004	POV	C311-C312-C313-C314
3	A	1005	POV	C23-C24-C25-C26
3	F	1007	POV	C32-C33-C34-C35
3	A	1002	POV	C32-C33-C34-C35
3	E	1005	POV	C32-C33-C34-C35
3	F	1010	POV	C214-C215-C216-C217
3	C	1002	POV	C1-C2-C3-O31
3	E	1005	POV	C1-C2-C3-O31
3	E	1008	POV	C1-C2-C3-O31
3	F	1004	POV	C1-C2-C3-O31
3	B	1010	POV	C311-C312-C313-C314
3	A	1002	POV	C213-C214-C215-C216
3	A	1006	POV	C211-C212-C213-C214
3	D	1006	POV	C39-C310-C311-C312
3	A	1010	POV	C313-C314-C315-C316
3	B	1009	POV	C32-C33-C34-C35
3	F	1004	POV	C32-C33-C34-C35
3	F	1007	POV	C311-C310-C39-C38
3	D	1004	POV	C37-C38-C39-C310
3	C	1010	POV	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
3	D	1002	POV	C31-C32-C33-C34
3	A	1006	POV	C311-C310-C39-C38
3	A	1002	POV	O11-C1-C2-O21
3	A	1010	POV	O11-C1-C2-O21
3	A	1011	POV	O11-C1-C2-O21
3	B	1003	POV	O11-C1-C2-O21
3	C	1002	POV	O11-C1-C2-O21
3	C	1005	POV	O11-C1-C2-O21
3	D	1005	POV	O11-C1-C2-O21
3	D	1011	POV	O11-C1-C2-O21
3	E	1010	POV	O11-C1-C2-O21
3	C	1004	POV	C32-C31-O31-C3
3	F	1003	POV	C32-C31-O31-C3
3	A	1004	POV	C22-C23-C24-C25
3	A	1006	POV	C214-C215-C216-C217
3	B	1009	POV	C312-C313-C314-C315
3	E	1008	POV	C32-C33-C34-C35
3	F	1005	POV	C211-C212-C213-C214
3	E	1006	POV	C39-C310-C311-C312
3	D	1008	POV	O21-C2-C3-O31
3	E	1008	POV	O21-C2-C3-O31
3	A	1008	POV	C34-C35-C36-C37
3	E	1002	POV	C213-C214-C215-C216
3	E	1008	POV	C312-C313-C314-C315
3	B	1010	POV	C311-C310-C39-C38
3	D	1009	POV	C312-C313-C314-C315
3	E	1006	POV	C211-C212-C213-C214
3	A	1005	POV	C212-C213-C214-C215
3	D	1005	POV	C212-C213-C214-C215
3	F	1005	POV	C311-C310-C39-C38
3	A	1009	POV	C31-C32-C33-C34
3	C	1002	POV	C213-C214-C215-C216
3	B	1003	POV	C213-C214-C215-C216
3	E	1005	POV	C23-C24-C25-C26
3	A	1012	POV	C211-C212-C213-C214
3	E	1008	POV	C22-C23-C24-C25
3	F	1003	POV	C37-C38-C39-C310
3	F	1008	POV	C211-C212-C213-C214
3	A	1007	POV	C212-C213-C214-C215
3	C	1006	POV	C211-C212-C213-C214
3	E	1009	POV	C39-C310-C311-C312
3	C	1003	POV	C215-C216-C217-C218

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Mol	Chain	Res	Type	Atoms
3	E	1004	POV	C35-C36-C37-C38
3	A	1005	POV	C312-C313-C314-C315
3	A	1006	POV	C310-C311-C312-C313
3	C	1002	POV	C36-C37-C38-C39
3	E	1003	POV	C215-C216-C217-C218
3	F	1002	POV	C215-C216-C217-C218
3	A	1003	POV	C215-C216-C217-C218
3	B	1007	POV	C39-C310-C311-C312
3	D	1003	POV	C35-C36-C37-C38
3	E	1004	POV	C310-C311-C312-C313
3	A	1005	POV	C32-C33-C34-C35
3	F	1009	POV	C23-C24-C25-C26
3	A	1011	POV	O11-C1-C2-C3
3	E	1004	POV	O11-C1-C2-C3
3	F	1003	POV	O11-C1-C2-C3
3	D	1005	POV	C311-C310-C39-C38
3	D	1010	POV	C32-C33-C34-C35
3	B	1007	POV	C210-C211-C212-C213
3	C	1004	POV	C210-C211-C212-C213
3	A	1008	POV	C311-C310-C39-C38
3	A	1010	POV	C213-C214-C215-C216
3	B	1003	POV	C32-C33-C34-C35
3	B	1003	POV	C36-C37-C38-C39
3	F	1002	POV	C313-C314-C315-C316
3	C	1005	POV	C212-C213-C214-C215
3	D	1002	POV	C213-C214-C215-C216
3	F	1004	POV	C212-C213-C214-C215
3	C	1005	POV	C32-C31-O31-C3
3	C	1009	POV	C23-C24-C25-C26
3	F	1002	POV	C35-C36-C37-C38
3	A	1004	POV	C32-C33-C34-C35
3	E	1009	POV	C312-C313-C314-C315
3	A	1008	POV	C32-C33-C34-C35
3	B	1004	POV	C215-C216-C217-C218
3	E	1004	POV	C32-C31-O31-C3
3	E	1005	POV	C32-C31-O31-C3
3	D	1005	POV	C312-C313-C314-C315
3	A	1003	POV	C210-C211-C212-C213
3	E	1003	POV	C210-C211-C212-C213
3	A	1003	POV	C2-C1-O11-P
3	D	1002	POV	C1-C2-C3-O31
3	B	1002	POV	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
3	B	1006	POV	O11-C1-C2-O21
3	C	1004	POV	O11-C1-C2-O21
3	C	1010	POV	O11-C1-C2-O21
3	D	1002	POV	O11-C1-C2-O21
3	E	1002	POV	O11-C1-C2-O21
3	E	1005	POV	O11-C1-C2-O21
3	F	1009	POV	O11-C1-C2-O21
3	F	1010	POV	O11-C1-C2-O21
3	B	1007	POV	C214-C215-C216-C217
3	D	1006	POV	C34-C35-C36-C37
3	C	1004	POV	O32-C31-O31-C3
3	A	1002	POV	C36-C37-C38-C39
3	C	1006	POV	C310-C311-C312-C313
3	D	1009	POV	C23-C24-C25-C26
3	A	1005	POV	O32-C31-O31-C3
3	B	1006	POV	O32-C31-O31-C3
3	C	1006	POV	C311-C310-C39-C38
3	A	1005	POV	O21-C2-C3-O31
3	A	1010	POV	O21-C2-C3-O31
3	A	1011	POV	O21-C2-C3-O31
3	B	1007	POV	O21-C2-C3-O31
3	B	1009	POV	O21-C2-C3-O31
3	C	1008	POV	O21-C2-C3-O31
3	D	1005	POV	O21-C2-C3-O31
3	E	1006	POV	O21-C2-C3-O31
3	F	1007	POV	O21-C2-C3-O31
3	C	1004	POV	C22-C23-C24-C25
3	B	1010	POV	C23-C24-C25-C26
3	F	1005	POV	C210-C211-C212-C213
3	A	1002	POV	C35-C36-C37-C38
3	C	1004	POV	C311-C310-C39-C38
3	D	1003	POV	C215-C216-C217-C218
3	D	1004	POV	C39-C310-C311-C312
3	E	1002	POV	O32-C31-O31-C3
3	F	1003	POV	O32-C31-O31-C3
3	A	1007	POV	C35-C36-C37-C38
3	B	1006	POV	C311-C310-C39-C38
3	D	1009	POV	C211-C212-C213-C214
3	E	1005	POV	C22-C23-C24-C25
3	E	1005	POV	O32-C31-O31-C3
3	B	1009	POV	C311-C310-C39-C38
3	D	1011	POV	C214-C215-C216-C217

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Mol	Chain	Res	Type	Atoms
3	A	1006	POV	C213-C214-C215-C216
3	B	1003	POV	C35-C36-C37-C38
3	C	1005	POV	O32-C31-O31-C3
3	E	1009	POV	C31-C32-C33-C34
3	B	1003	POV	C214-C215-C216-C217
3	C	1004	POV	C24-C25-C26-C27
3	D	1005	POV	C32-C31-O31-C3
3	C	1003	POV	C35-C36-C37-C38
3	F	1004	POV	C26-C27-C28-C29
3	A	1002	POV	C1-O11-P-O12
3	A	1003	POV	C11-O12-P-O11
3	A	1006	POV	C1-O11-P-O12
3	B	1007	POV	C1-O11-P-O12
3	C	1006	POV	C1-O11-P-O12
3	D	1006	POV	C1-O11-P-O12
3	E	1006	POV	C1-O11-P-O12
3	F	1005	POV	C1-O11-P-O12
3	C	1003	POV	C2-C1-O11-P
3	B	1006	POV	C37-C38-C39-C310
3	E	1002	POV	C36-C37-C38-C39
3	A	1002	POV	C1-O11-P-O13
3	A	1002	POV	C11-O12-P-O13
3	A	1003	POV	C1-O11-P-O13
3	A	1003	POV	C1-O11-P-O14
3	A	1004	POV	C1-O11-P-O14
3	A	1005	POV	C11-O12-P-O13
3	A	1005	POV	C11-O12-P-O14
3	A	1010	POV	C1-O11-P-O13
3	A	1010	POV	C11-O12-P-O13
3	A	1012	POV	C11-O12-P-O13
3	B	1002	POV	C1-O11-P-O13
3	B	1002	POV	C1-O11-P-O14
3	B	1003	POV	C1-O11-P-O13
3	B	1003	POV	C11-O12-P-O13
3	B	1004	POV	C1-O11-P-O13
3	B	1004	POV	C1-O11-P-O14
3	B	1005	POV	C1-O11-P-O14
3	B	1006	POV	C11-O12-P-O13
3	B	1006	POV	C11-O12-P-O14
3	C	1002	POV	C1-O11-P-O13
3	C	1002	POV	C11-O12-P-O13
3	C	1004	POV	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
3	C	1005	POV	C11-O12-P-O13
3	C	1005	POV	C11-O12-P-O14
3	C	1010	POV	C11-O12-P-O14
3	D	1002	POV	C1-O11-P-O13
3	D	1002	POV	C11-O12-P-O13
3	D	1004	POV	C1-O11-P-O14
3	D	1004	POV	C11-O12-P-O14
3	D	1005	POV	C11-O12-P-O13
3	D	1005	POV	C11-O12-P-O14
3	D	1009	POV	C11-O12-P-O13
3	D	1011	POV	C1-O11-P-O13
3	D	1011	POV	C1-O11-P-O14
3	E	1002	POV	C1-O11-P-O13
3	E	1002	POV	C11-O12-P-O13
3	E	1005	POV	C11-O12-P-O13
3	E	1005	POV	C11-O12-P-O14
3	E	1010	POV	C1-O11-P-O13
3	E	1010	POV	C1-O11-P-O14
3	F	1002	POV	C1-O11-P-O13
3	F	1002	POV	C1-O11-P-O14
3	F	1004	POV	C11-O12-P-O13
3	F	1004	POV	C11-O12-P-O14
3	F	1008	POV	C11-O12-P-O13
3	F	1010	POV	C1-O11-P-O13
3	F	1010	POV	C1-O11-P-O14
3	D	1006	POV	C211-C212-C213-C214
3	F	1003	POV	C35-C36-C37-C38
3	B	1005	POV	C32-C31-O31-C3
3	A	1005	POV	O11-C1-C2-C3
3	B	1002	POV	O11-C1-C2-C3
3	B	1006	POV	O11-C1-C2-C3
3	C	1010	POV	O11-C1-C2-C3
3	D	1005	POV	O11-C1-C2-C3
3	D	1011	POV	O11-C1-C2-C3
3	E	1005	POV	O11-C1-C2-C3
3	E	1010	POV	O11-C1-C2-C3
3	F	1004	POV	O11-C1-C2-C3
3	F	1010	POV	O11-C1-C2-C3
3	A	1005	POV	C311-C310-C39-C38
3	C	1007	POV	C33-C34-C35-C36
3	C	1008	POV	C34-C35-C36-C37
3	D	1004	POV	C310-C311-C312-C313

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Mol	Chain	Res	Type	Atoms
3	F	1003	POV	C22-C23-C24-C25
3	C	1003	POV	C313-C314-C315-C316
3	D	1008	POV	C32-C33-C34-C35
3	E	1005	POV	C212-C213-C214-C215
3	A	1007	POV	C12-C11-O12-P
3	B	1008	POV	C12-C11-O12-P
3	C	1007	POV	C12-C11-O12-P
3	D	1007	POV	C12-C11-O12-P
3	E	1003	POV	C12-C11-O12-P
3	E	1007	POV	C12-C11-O12-P
3	F	1006	POV	C12-C11-O12-P
3	D	1006	POV	C311-C310-C39-C38
3	E	1002	POV	C31-C32-C33-C34
3	E	1003	POV	C35-C36-C37-C38
3	E	1005	POV	C311-C310-C39-C38
3	D	1004	POV	C32-C31-O31-C3
3	D	1008	POV	C311-C310-C39-C38
3	D	1011	POV	C310-C311-C312-C313
3	A	1012	POV	C312-C313-C314-C315
3	C	1009	POV	C25-C26-C27-C28
3	E	1009	POV	C23-C24-C25-C26
3	D	1005	POV	O32-C31-O31-C3
3	E	1004	POV	O32-C31-O31-C3
3	B	1010	POV	C25-C26-C27-C28
3	A	1007	POV	C11-C12-N-C13
3	B	1005	POV	C11-C12-N-C14
3	F	1006	POV	C11-C12-N-C13
3	E	1006	POV	C310-C311-C312-C313
3	F	1003	POV	C212-C213-C214-C215
3	E	1005	POV	O21-C21-C22-C23
3	A	1003	POV	O12-C11-C12-N
3	A	1005	POV	O12-C11-C12-N
3	A	1009	POV	O12-C11-C12-N
3	A	1011	POV	O12-C11-C12-N
3	B	1002	POV	O12-C11-C12-N
3	B	1004	POV	O12-C11-C12-N
3	B	1006	POV	O12-C11-C12-N
3	C	1005	POV	O12-C11-C12-N
3	C	1010	POV	O12-C11-C12-N
3	D	1005	POV	O12-C11-C12-N
3	D	1011	POV	O12-C11-C12-N
3	E	1003	POV	O12-C11-C12-N

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Mol	Chain	Res	Type	Atoms
3	E	1005	POV	O12-C11-C12-N
3	E	1007	POV	C36-C37-C38-C39
3	E	1010	POV	O12-C11-C12-N
3	F	1002	POV	O12-C11-C12-N
3	F	1004	POV	O12-C11-C12-N
3	F	1010	POV	O12-C11-C12-N
3	B	1006	POV	O21-C2-C3-O31
3	C	1002	POV	O21-C2-C3-O31
3	C	1005	POV	O21-C2-C3-O31
3	D	1011	POV	O21-C2-C3-O31
3	E	1005	POV	O21-C2-C3-O31
3	E	1010	POV	O21-C2-C3-O31
3	F	1004	POV	O21-C2-C3-O31
3	D	1010	POV	C311-C310-C39-C38
3	A	1012	POV	C23-C24-C25-C26
3	B	1004	POV	C35-C36-C37-C38
3	D	1002	POV	C313-C314-C315-C316
3	D	1003	POV	C2-C1-O11-P
3	E	1010	POV	C310-C311-C312-C313
3	E	1009	POV	C25-C26-C27-C28
3	F	1008	POV	C23-C24-C25-C26
3	B	1005	POV	O32-C31-O31-C3
3	D	1004	POV	O32-C31-O31-C3
3	F	1007	POV	C312-C313-C314-C315
3	A	1006	POV	C23-C24-C25-C26
3	F	1003	POV	C310-C311-C312-C313
3	B	1010	POV	C31-C32-C33-C34
3	B	1005	POV	C11-C12-N-C15
3	B	1008	POV	C11-C12-N-C13
3	C	1006	POV	C11-C12-N-C15
3	C	1007	POV	C11-C12-N-C13
3	D	1005	POV	C32-C33-C34-C35
3	E	1004	POV	C211-C212-C213-C214
3	A	1002	POV	C214-C215-C216-C217
3	E	1006	POV	C311-C310-C39-C38
3	E	1010	POV	C25-C26-C27-C28
3	F	1004	POV	C312-C313-C314-C315
3	B	1006	POV	C212-C213-C214-C215
3	D	1007	POV	C36-C37-C38-C39
3	F	1009	POV	C25-C26-C27-C28
3	B	1004	POV	C213-C214-C215-C216
3	D	1010	POV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
3	A	1004	POV	C211-C212-C213-C214
3	F	1003	POV	C39-C310-C311-C312
3	C	1002	POV	C214-C215-C216-C217
3	E	1005	POV	C312-C313-C314-C315
3	E	1006	POV	C34-C35-C36-C37
3	D	1006	POV	C213-C214-C215-C216
3	C	1004	POV	O11-C1-C2-C3
3	C	1005	POV	O11-C1-C2-C3
3	E	1002	POV	C214-C215-C216-C217
3	D	1006	POV	C310-C311-C312-C313
3	F	1006	POV	C35-C36-C37-C38
3	A	1005	POV	C37-C38-C39-C310
3	C	1005	POV	C34-C35-C36-C37
3	B	1004	POV	C2-C1-O11-P
3	E	1003	POV	C2-C1-O11-P
3	F	1002	POV	C2-C1-O11-P
3	F	1009	POV	C2-C1-O11-P
3	C	1008	POV	C312-C313-C314-C315
3	E	1004	POV	C212-C213-C214-C215
3	E	1004	POV	C11-C12-N-C13
3	A	1007	POV	C22-C23-C24-C25
3	B	1005	POV	C24-C25-C26-C27
3	E	1010	POV	C24-C25-C26-C27
3	B	1002	POV	C36-C37-C38-C39
3	A	1002	POV	C11-O12-P-O11
3	A	1007	POV	C1-O11-P-O12
3	A	1008	POV	C11-O12-P-O11
3	A	1009	POV	C11-O12-P-O11
3	B	1003	POV	C11-O12-P-O11
3	B	1008	POV	C1-O11-P-O12
3	B	1009	POV	C11-O12-P-O11
3	B	1010	POV	C11-O12-P-O11
3	C	1002	POV	C11-O12-P-O11
3	C	1003	POV	C11-O12-P-O11
3	C	1007	POV	C1-O11-P-O12
3	C	1008	POV	C11-O12-P-O11
3	C	1009	POV	C11-O12-P-O11
3	D	1002	POV	C11-O12-P-O11
3	D	1003	POV	C11-O12-P-O11
3	D	1007	POV	C1-O11-P-O12
3	D	1008	POV	C11-O12-P-O11
3	D	1010	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
3	E	1007	POV	C1-O11-P-O12
3	E	1008	POV	C11-O12-P-O11
3	E	1009	POV	C11-O12-P-O11
3	F	1006	POV	C1-O11-P-O12
3	F	1007	POV	C11-O12-P-O11
3	F	1009	POV	C11-O12-P-O11
3	F	1003	POV	C24-C25-C26-C27
3	A	1009	POV	C311-C310-C39-C38
3	C	1009	POV	C214-C215-C216-C217
3	E	1010	POV	C1-C2-C3-O31
3	C	1002	POV	C35-C36-C37-C38
3	E	1006	POV	C23-C24-C25-C26
3	D	1004	POV	C35-C36-C37-C38
3	F	1010	POV	C24-C25-C26-C27
3	D	1007	POV	C11-C12-N-C13
3	E	1007	POV	C11-C12-N-C13
3	B	1005	POV	C210-C211-C212-C213
3	A	1010	POV	C36-C37-C38-C39
3	A	1004	POV	C32-C31-O31-C3
3	F	1009	POV	C311-C310-C39-C38
3	C	1005	POV	C32-C33-C34-C35
3	E	1004	POV	C32-C33-C34-C35
3	A	1003	POV	C35-C36-C37-C38
3	A	1004	POV	C311-C310-C39-C38
3	B	1010	POV	C32-C33-C34-C35
3	E	1005	POV	C37-C38-C39-C310
3	A	1012	POV	C2-C1-O11-P
3	D	1009	POV	C2-C1-O11-P
3	F	1008	POV	C2-C1-O11-P
3	A	1010	POV	C35-C36-C37-C38
3	B	1005	POV	C211-C212-C213-C214
3	C	1002	POV	C31-C32-C33-C34
3	C	1008	POV	C32-C33-C34-C35
3	C	1006	POV	C210-C211-C212-C213
3	D	1006	POV	C26-C27-C28-C29
3	E	1006	POV	C210-C211-C212-C213
3	A	1004	POV	O32-C31-O31-C3
3	B	1007	POV	C211-C212-C213-C214
3	F	1005	POV	C310-C311-C312-C313
3	F	1004	POV	C32-C31-O31-C3
3	A	1002	POV	O11-C1-C2-C3
3	A	1003	POV	C213-C214-C215-C216

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Mol	Chain	Res	Type	Atoms
3	A	1009	POV	C23-C24-C25-C26
3	B	1006	POV	C310-C311-C312-C313
3	A	1009	POV	O11-C1-C2-O21
3	B	1005	POV	C32-C33-C34-C35
3	D	1003	POV	C37-C38-C39-C310
3	D	1002	POV	C35-C36-C37-C38
3	B	1002	POV	O21-C2-C3-O31
3	C	1010	POV	O21-C2-C3-O31
3	D	1002	POV	O21-C2-C3-O31
3	C	1006	POV	C213-C214-C215-C216
3	C	1005	POV	C311-C310-C39-C38
3	B	1010	POV	C2-C1-O11-P
3	D	1010	POV	C2-C1-O11-P
3	C	1005	POV	O21-C21-C22-C23
3	B	1005	POV	C310-C311-C312-C313
3	C	1007	POV	C36-C37-C38-C39
3	B	1006	POV	C26-C27-C28-C29
3	D	1004	POV	C210-C211-C212-C213
3	B	1007	POV	C23-C24-C25-C26
3	F	1009	POV	C312-C313-C314-C315
3	A	1003	POV	C33-C34-C35-C36
3	A	1004	POV	C35-C36-C37-C38
3	A	1009	POV	C32-C33-C34-C35
3	B	1003	POV	C22-C23-C24-C25
3	C	1004	POV	C32-C33-C34-C35
3	D	1010	POV	C23-C24-C25-C26
3	E	1003	POV	C313-C314-C315-C316
3	B	1005	POV	C22-C23-C24-C25
3	B	1007	POV	C310-C311-C312-C313
3	F	1004	POV	C311-C310-C39-C38
3	F	1004	POV	O32-C31-O31-C3
3	A	1009	POV	C25-C26-C27-C28
3	A	1012	POV	C210-C211-C212-C213
3	A	1012	POV	C26-C27-C28-C29
3	D	1009	POV	C210-C211-C212-C213
3	D	1009	POV	C26-C27-C28-C29
3	E	1009	POV	C26-C27-C28-C29
3	A	1007	POV	C11-C12-N-C14
3	A	1007	POV	C11-C12-N-C15
3	B	1005	POV	C11-C12-N-C13
3	F	1006	POV	C11-C12-N-C15
3	C	1009	POV	C312-C313-C314-C315

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Mol	Chain	Res	Type	Atoms
3	E	1008	POV	C21-C22-C23-C24
3	C	1004	POV	C35-C36-C37-C38
3	A	1007	POV	C33-C34-C35-C36
3	C	1007	POV	C35-C36-C37-C38
3	C	1009	POV	C31-C32-C33-C34
3	D	1008	POV	C312-C313-C314-C315
3	C	1009	POV	C32-C33-C34-C35
3	A	1009	POV	C26-C27-C28-C29
3	B	1010	POV	C26-C27-C28-C29
3	B	1006	POV	C312-C313-C314-C315
3	A	1008	POV	C21-C22-C23-C24
3	D	1002	POV	C214-C215-C216-C217
3	D	1007	POV	C212-C213-C214-C215
3	B	1010	POV	C312-C313-C314-C315
3	B	1008	POV	C33-C34-C35-C36
3	D	1007	POV	C33-C34-C35-C36
3	A	1012	POV	O21-C2-C3-O31
3	D	1003	POV	O21-C2-C3-O31
3	D	1006	POV	O21-C2-C3-O31
3	F	1005	POV	O21-C2-C3-O31
3	F	1005	POV	C213-C214-C215-C216
3	B	1004	POV	C210-C211-C212-C213
3	C	1003	POV	C210-C211-C212-C213
3	C	1006	POV	C26-C27-C28-C29
3	A	1008	POV	C31-C32-C33-C34
3	B	1006	POV	C34-C35-C36-C37
3	F	1002	POV	C213-C214-C215-C216
3	F	1006	POV	C33-C34-C35-C36
3	B	1005	POV	C35-C36-C37-C38
3	A	1004	POV	C39-C310-C311-C312
3	E	1004	POV	C312-C313-C314-C315
3	D	1003	POV	C313-C314-C315-C316
3	F	1003	POV	C313-C314-C315-C316
3	A	1009	POV	C2-C1-O11-P
3	B	1008	POV	C35-C36-C37-C38
3	C	1007	POV	C212-C213-C214-C215
3	E	1006	POV	C213-C214-C215-C216
3	D	1003	POV	C213-C214-C215-C216
3	A	1008	POV	C312-C313-C314-C315
3	E	1004	POV	C24-C25-C26-C27
3	A	1006	POV	C34-C35-C36-C37
3	B	1005	POV	C27-C28-C29-C210

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Mol	Chain	Res	Type	Atoms
3	D	1004	POV	C27-C28-C29-C210
3	E	1004	POV	C27-C28-C29-C210
3	B	1010	POV	O11-C1-C2-O21
3	C	1009	POV	O11-C1-C2-O21
3	D	1010	POV	O11-C1-C2-O21
3	E	1005	POV	C310-C311-C312-C313
3	F	1006	POV	C22-C23-C24-C25
3	D	1003	POV	O21-C21-C22-C23
3	C	1007	POV	C22-C23-C24-C25
3	F	1007	POV	C11-C12-N-C14
3	D	1004	POV	C311-C310-C39-C38
3	A	1009	POV	O11-C1-C2-C3
3	B	1003	POV	O11-C1-C2-C3
3	B	1010	POV	O11-C1-C2-C3
3	C	1009	POV	O11-C1-C2-C3
3	D	1010	POV	O11-C1-C2-C3
3	E	1002	POV	O11-C1-C2-C3
3	F	1009	POV	O11-C1-C2-C3
3	F	1004	POV	O21-C21-C22-C23
3	A	1011	POV	C310-C311-C312-C313
3	C	1003	POV	C213-C214-C215-C216
3	C	1002	POV	O32-C31-O31-C3
3	F	1007	POV	C31-C32-C33-C34
3	F	1002	POV	C311-C312-C313-C314
3	E	1009	POV	C2-C1-O11-P
3	A	1006	POV	C26-C27-C28-C29
3	F	1008	POV	C26-C27-C28-C29
3	C	1006	POV	O21-C2-C3-O31
3	F	1010	POV	O21-C2-C3-O31
3	B	1004	POV	O21-C21-C22-C23
3	E	1008	POV	O21-C21-C22-C23
3	C	1002	POV	C32-C31-O31-C3
3	F	1003	POV	C27-C28-C29-C210
3	A	1008	POV	C313-C314-C315-C316
3	B	1002	POV	C24-C25-C26-C27
3	C	1008	POV	C311-C310-C39-C38
3	D	1002	POV	C37-C38-C39-C310
3	E	1004	POV	C39-C310-C311-C312
3	F	1010	POV	C25-C26-C27-C28
3	D	1005	POV	C37-C38-C39-C310
3	B	1008	POV	C11-C12-N-C15
3	C	1006	POV	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
3	E	1006	POV	C11-C12-N-C15
3	F	1006	POV	C11-C12-N-C14
3	C	1008	POV	O21-C21-C22-C23
3	E	1009	POV	C32-C33-C34-C35
3	A	1004	POV	C210-C211-C212-C213
3	A	1009	POV	C210-C211-C212-C213
3	B	1007	POV	C26-C27-C28-C29
3	B	1009	POV	C210-C211-C212-C213
3	C	1010	POV	C310-C311-C312-C313
3	A	1007	POV	C27-C28-C29-C210
3	E	1007	POV	C27-C28-C29-C210
3	F	1005	POV	C34-C35-C36-C37
3	A	1005	POV	C34-C35-C36-C37
3	A	1008	POV	O21-C21-C22-C23
3	B	1009	POV	O21-C21-C22-C23
3	E	1003	POV	O21-C21-C22-C23
3	B	1007	POV	C311-C310-C39-C38
3	B	1003	POV	C32-C31-O31-C3
3	E	1003	POV	C33-C34-C35-C36
3	D	1008	POV	O21-C21-C22-C23
3	B	1002	POV	C310-C311-C312-C313
3	A	1004	POV	C27-C28-C29-C210
3	B	1008	POV	C27-C28-C29-C210
3	C	1004	POV	C27-C28-C29-C210
3	D	1010	POV	C26-C27-C28-C29
3	A	1010	POV	C214-C215-C216-C217
3	A	1011	POV	C1-C2-C3-O31
3	B	1002	POV	C1-C2-C3-O31
3	C	1009	POV	C2-C1-O11-P
3	C	1010	POV	C1-C2-C3-O31
3	D	1011	POV	C1-C2-C3-O31
3	F	1010	POV	C1-C2-C3-O31
3	E	1009	POV	O11-C1-C2-O21
3	F	1007	POV	O21-C21-C22-C23
3	C	1006	POV	C11-C12-N-C13
3	C	1007	POV	C11-C12-N-C15
3	D	1006	POV	C11-C12-N-C15
3	D	1008	POV	C11-C12-N-C14
3	E	1007	POV	C11-C12-N-C15
3	F	1005	POV	C11-C12-N-C15
3	B	1003	POV	O32-C31-O31-C3
3	B	1008	POV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
3	C	1003	POV	O21-C21-C22-C23
3	B	1009	POV	C27-C28-C29-C210
3	C	1007	POV	C27-C28-C29-C210
3	F	1004	POV	C27-C28-C29-C210
3	D	1007	POV	C22-C23-C24-C25
3	A	1005	POV	C26-C27-C28-C29
3	E	1009	POV	C210-C211-C212-C213
3	F	1008	POV	C210-C211-C212-C213
3	A	1010	POV	O11-C1-C2-C3
3	C	1002	POV	O11-C1-C2-C3
3	E	1009	POV	O11-C1-C2-C3
3	F	1005	POV	C23-C24-C25-C26
3	C	1006	POV	C311-C312-C313-C314
3	A	1006	POV	O21-C2-C3-O31
3	A	1002	POV	C29-C210-C211-C212
3	A	1010	POV	C29-C210-C211-C212
3	C	1004	POV	C29-C210-C211-C212
3	F	1010	POV	C36-C37-C38-C39
3	B	1007	POV	C34-C35-C36-C37
3	A	1006	POV	C11-C12-N-C15
3	C	1007	POV	C11-C12-N-C14
3	D	1007	POV	C11-C12-N-C15
3	C	1005	POV	C310-C311-C312-C313
3	D	1007	POV	C35-C36-C37-C38
3	D	1007	POV	C27-C28-C29-C210
3	D	1008	POV	C27-C28-C29-C210
3	F	1006	POV	C27-C28-C29-C210
3	B	1005	POV	C311-C310-C39-C38
3	F	1009	POV	C214-C215-C216-C217
3	A	1010	POV	C32-C33-C34-C35
3	F	1003	POV	C211-C212-C213-C214
3	B	1009	POV	O22-C21-C22-C23
3	E	1003	POV	C213-C214-C215-C216
3	D	1004	POV	C29-C210-C211-C212
3	D	1005	POV	C26-C27-C28-C29
3	D	1008	POV	O22-C21-C22-C23
3	F	1007	POV	O22-C21-C22-C23
3	A	1004	POV	O11-C1-C2-O21
3	D	1010	POV	C312-C313-C314-C315
3	C	1005	POV	C312-C313-C314-C315
3	A	1008	POV	O22-C21-C22-C23
3	E	1008	POV	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
3	F	1009	POV	C32-C33-C34-C35
3	C	1008	POV	O22-C21-C22-C23
3	A	1009	POV	C214-C215-C216-C217
3	A	1004	POV	C11-C12-N-C14
3	A	1004	POV	C11-O12-P-O14
3	A	1007	POV	C1-O11-P-O14
3	A	1009	POV	C11-O12-P-O14
3	B	1003	POV	C11-O12-P-O14
3	B	1005	POV	C11-O12-P-O14
3	B	1007	POV	C11-C12-N-C15
3	B	1008	POV	C11-C12-N-C14
3	B	1008	POV	C1-O11-P-O14
3	B	1009	POV	C11-C12-N-C14
3	B	1010	POV	C11-O12-P-O14
3	C	1004	POV	C11-O12-P-O14
3	C	1007	POV	C1-O11-P-O14
3	C	1009	POV	C11-O12-P-O14
3	D	1007	POV	C11-C12-N-C14
3	D	1007	POV	C1-O11-P-O14
3	D	1010	POV	C11-O12-P-O14
3	E	1003	POV	C1-O11-P-O13
3	E	1004	POV	C11-O12-P-O14
3	E	1007	POV	C1-O11-P-O14
3	E	1009	POV	C11-O12-P-O14
3	F	1006	POV	C1-O11-P-O14
3	F	1007	POV	C11-O12-P-O14
3	F	1009	POV	C11-O12-P-O14
3	D	1002	POV	O11-C1-C2-C3
3	D	1004	POV	C24-C25-C26-C27
3	C	1005	POV	C26-C27-C28-C29
3	B	1003	POV	C29-C210-C211-C212
3	D	1006	POV	C27-C28-C29-C210
3	B	1002	POV	C34-C35-C36-C37
3	F	1004	POV	C313-C314-C315-C316
3	A	1002	POV	C37-C38-C39-C310
3	C	1003	POV	C211-C212-C213-C214
3	D	1008	POV	C11-C12-N-C15
3	E	1007	POV	C11-C12-N-C14
3	F	1003	POV	C11-C12-N-C14
3	F	1007	POV	C11-C12-N-C13
3	F	1007	POV	C11-C12-N-C15
3	A	1008	POV	C27-C28-C29-C210

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Mol	Chain	Res	Type	Atoms
3	D	1005	POV	C27-C28-C29-C210
3	F	1005	POV	O31-C31-C32-C33
3	C	1003	POV	C37-C38-C39-C310
3	A	1010	POV	C37-C38-C39-C310
3	B	1003	POV	C37-C38-C39-C310
3	B	1007	POV	C213-C214-C215-C216
3	C	1010	POV	C24-C25-C26-C27
3	B	1007	POV	O31-C31-C32-C33
3	D	1006	POV	O31-C31-C32-C33
3	E	1006	POV	O31-C31-C32-C33
3	B	1005	POV	O11-C1-C2-O21
3	C	1009	POV	O21-C21-C22-C23
3	E	1005	POV	C27-C28-C29-C210
3	F	1007	POV	C27-C28-C29-C210
3	C	1004	POV	C39-C310-C311-C312
3	B	1002	POV	C39-C310-C311-C312
3	F	1002	POV	O21-C21-C22-C23
3	F	1007	POV	C210-C211-C212-C213
3	D	1006	POV	O32-C31-C32-C33
3	E	1007	POV	C35-C36-C37-C38
3	A	1003	POV	O21-C21-C22-C23
3	A	1006	POV	O31-C31-C32-C33
3	C	1006	POV	O31-C31-C32-C33
3	E	1006	POV	C11-C12-N-C13
3	F	1003	POV	C11-C12-N-C13
3	C	1006	POV	C27-C28-C29-C210
3	A	1004	POV	C310-C311-C312-C313
3	B	1008	POV	C212-C213-C214-C215
3	E	1006	POV	O32-C31-C32-C33

There are no ring outliers.

63 monomers are involved in 305 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1006	POV	8	0
3	C	1008	POV	5	0
3	E	1006	POV	4	0
3	F	1010	POV	5	0
3	D	1007	POV	5	0
3	F	1008	POV	3	0
3	B	1004	POV	9	0
3	B	1008	POV	3	0

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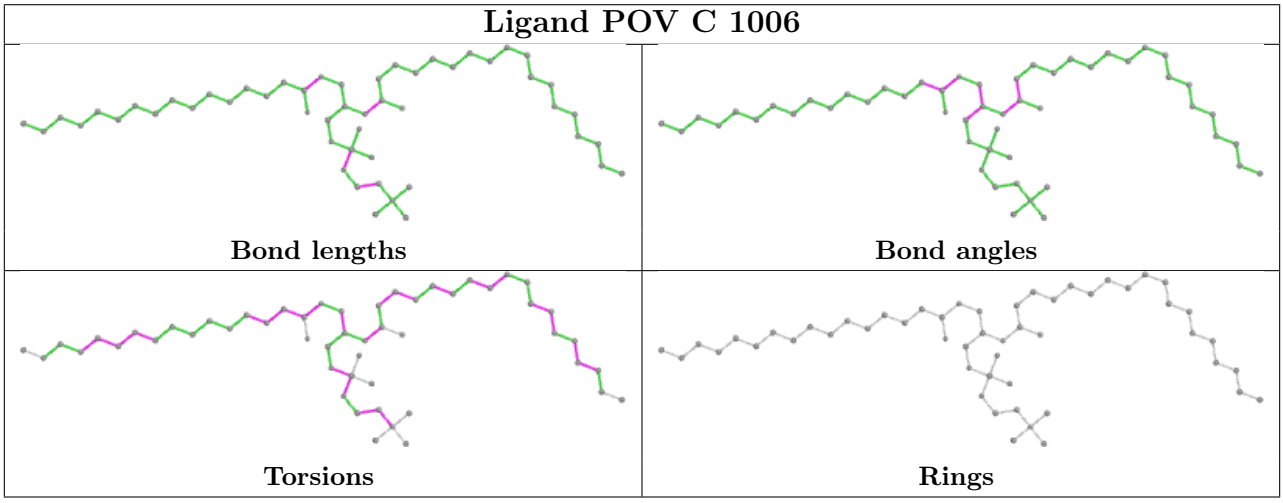
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1005	POV	8	0
3	B	1006	POV	8	0
3	C	1003	POV	8	0
3	D	1008	POV	2	0
3	C	1005	POV	7	0
3	E	1003	POV	8	0
3	E	1007	POV	4	0
3	A	1002	POV	13	0
3	C	1009	POV	5	0
3	D	1010	POV	4	0
3	A	1011	POV	6	0
3	E	1002	POV	11	0
3	C	1007	POV	4	0
3	D	1004	POV	14	0
3	E	1005	POV	7	0
3	D	1006	POV	4	0
3	A	1003	POV	9	0
3	E	1009	POV	3	0
3	C	1004	POV	14	0
3	A	1005	POV	5	0
3	A	1006	POV	6	0
3	A	1008	POV	4	0
3	A	1004	POV	7	0
2	C	1001	BEF	3	0
3	B	1009	POV	2	0
3	B	1007	POV	6	0
3	C	1010	POV	4	0
3	F	1003	POV	7	0
3	D	1003	POV	8	0
3	D	1009	POV	3	0
3	F	1004	POV	8	0
3	F	1005	POV	9	0
3	F	1002	POV	10	0
3	A	1009	POV	1	0
3	D	1002	POV	11	0
3	A	1007	POV	5	0
2	E	1001	BEF	3	0
3	B	1005	POV	6	0
3	B	1010	POV	6	0
3	D	1011	POV	4	0
2	A	1001	BEF	3	0
3	F	1006	POV	4	0

Continued on next page...

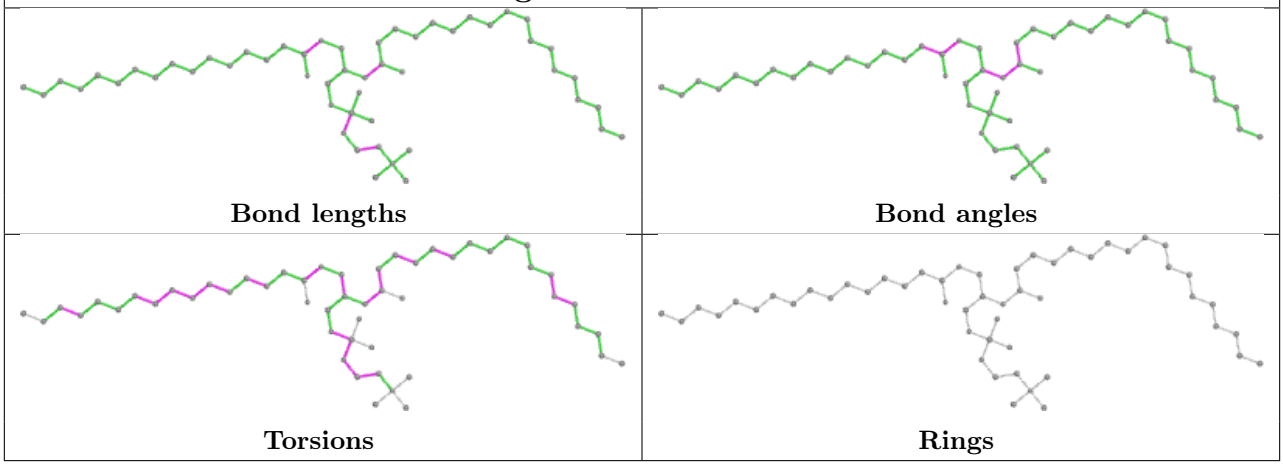
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	BEF	3	0
3	E	1008	POV	3	0
2	F	1001	BEF	3	0
3	A	1012	POV	5	0
3	C	1002	POV	12	0
3	A	1010	POV	14	0
3	B	1003	POV	10	0
3	F	1009	POV	6	0
3	F	1007	POV	4	0
3	E	1010	POV	5	0
2	D	1001	BEF	3	0
3	B	1002	POV	6	0
3	E	1004	POV	5	0

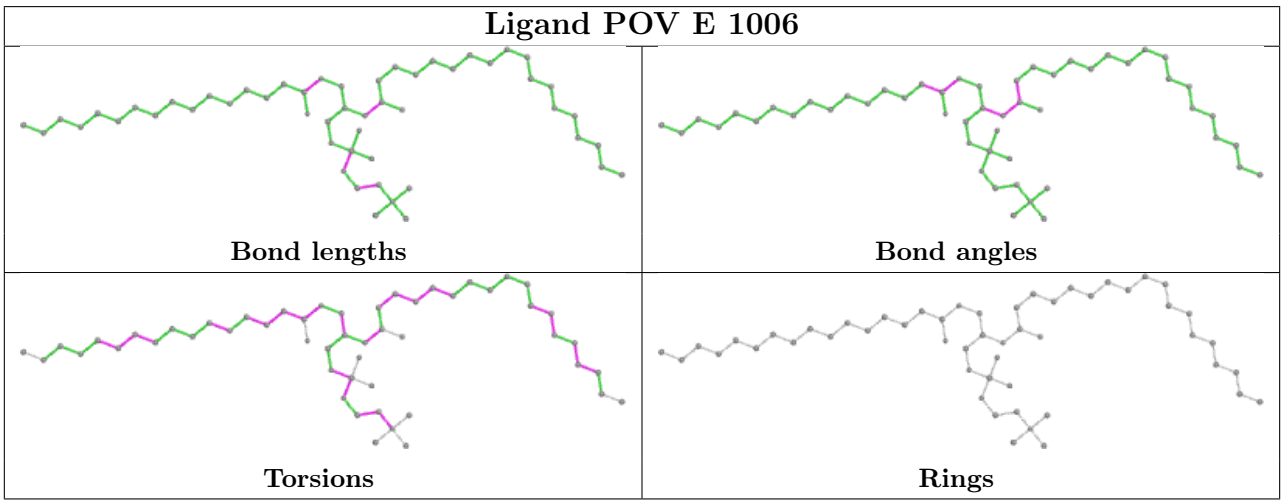
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



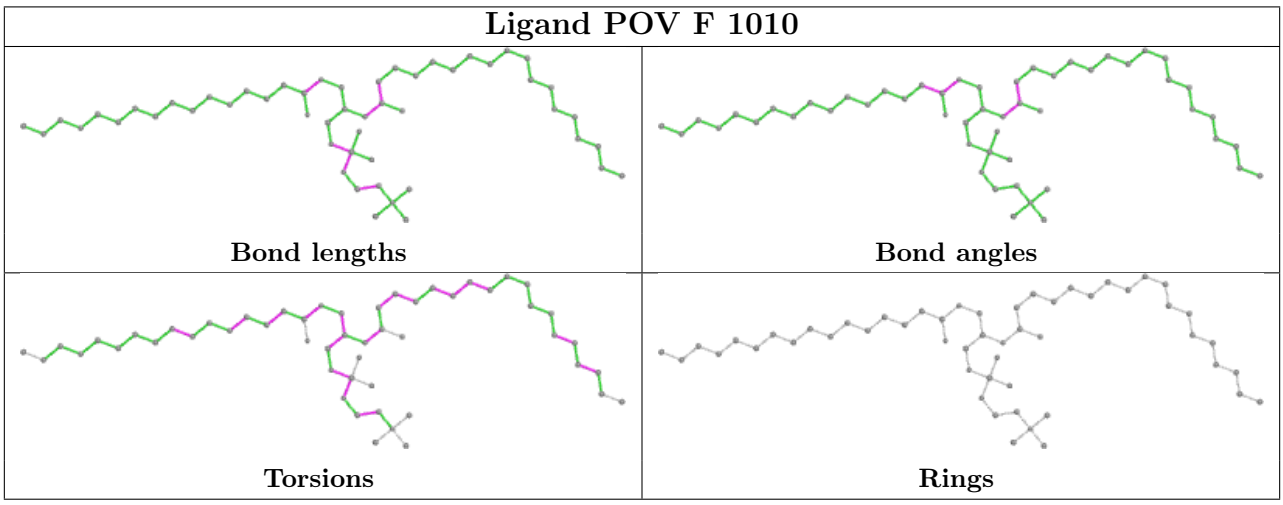
Ligand POV C 1008



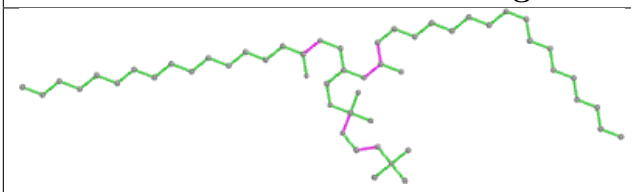
Ligand POV E 1006



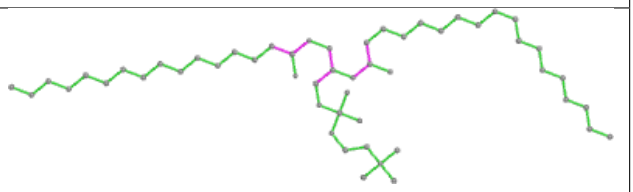
Ligand POV F 1010



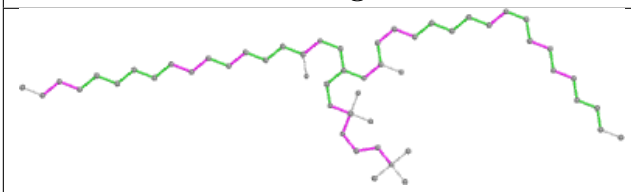
Ligand POV D 1007



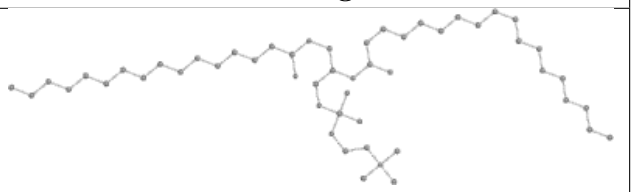
Bond lengths



Bond angles

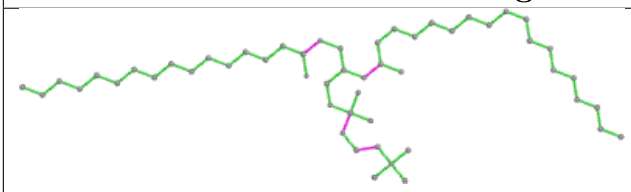


Torsions

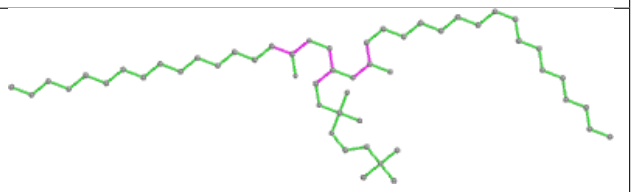


Rings

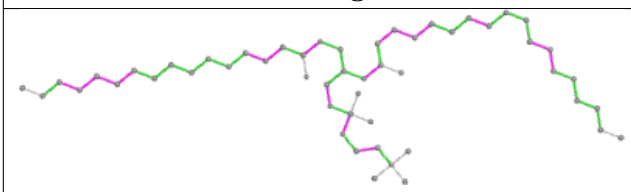
Ligand POV F 1008



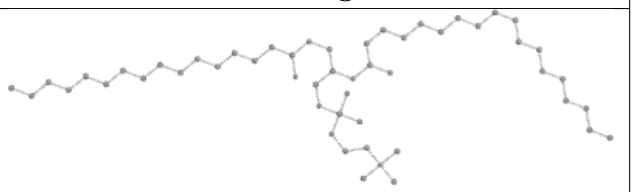
Bond lengths



Bond angles

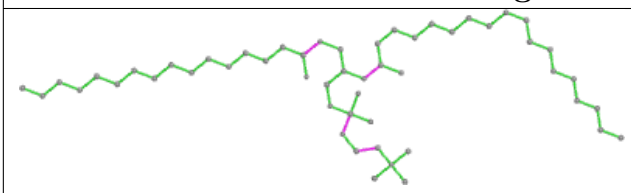


Torsions

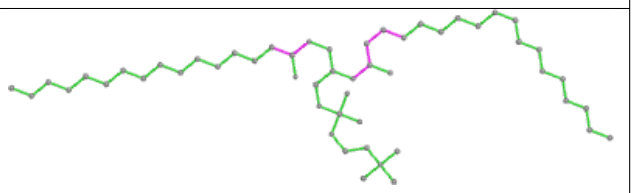


Rings

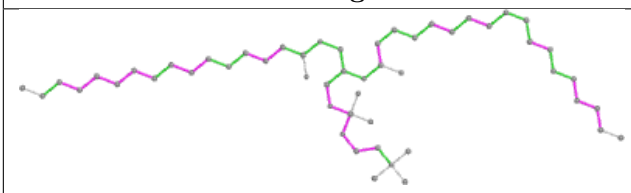
Ligand POV B 1004



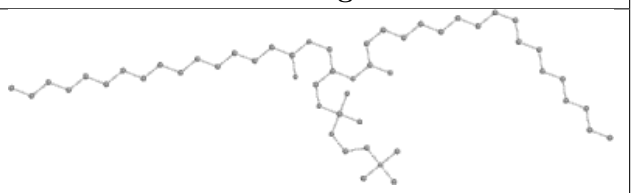
Bond lengths



Bond angles

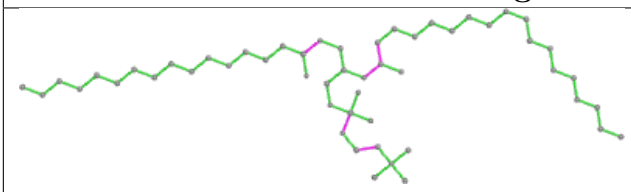


Torsions

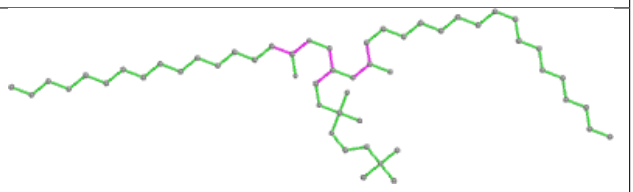


Rings

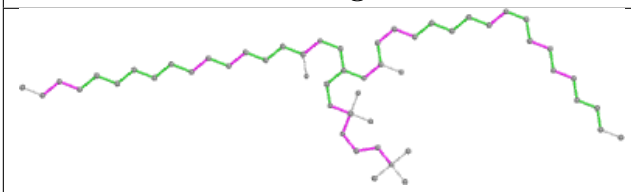
Ligand POV B 1008



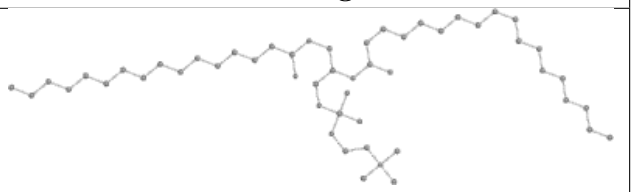
Bond lengths



Bond angles

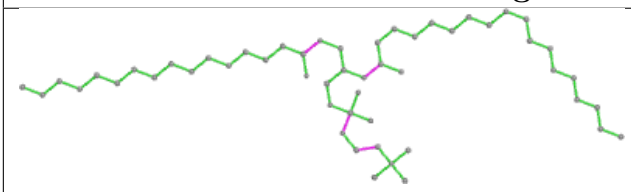


Torsions

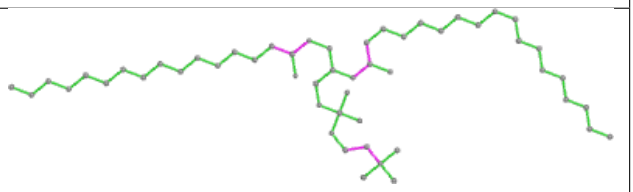


Rings

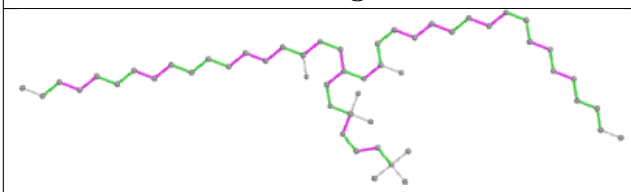
Ligand POV D 1005



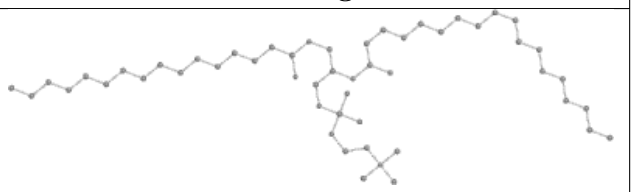
Bond lengths



Bond angles

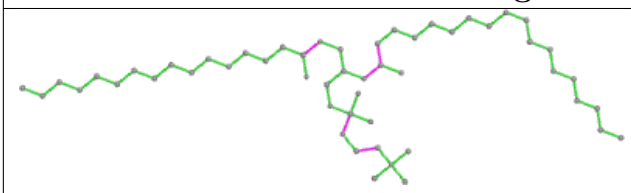


Torsions

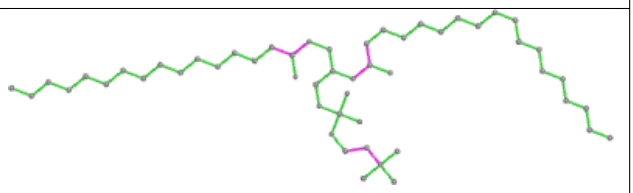


Rings

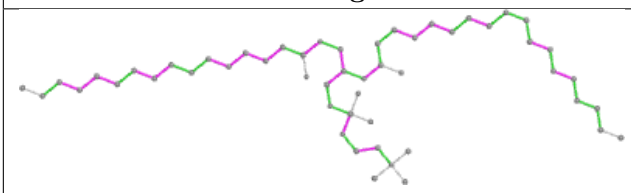
Ligand POV B 1006



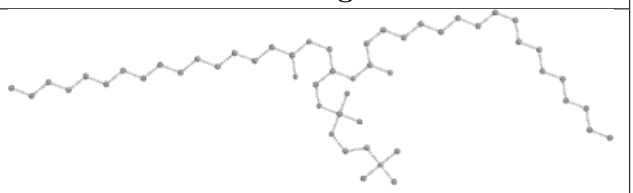
Bond lengths



Bond angles

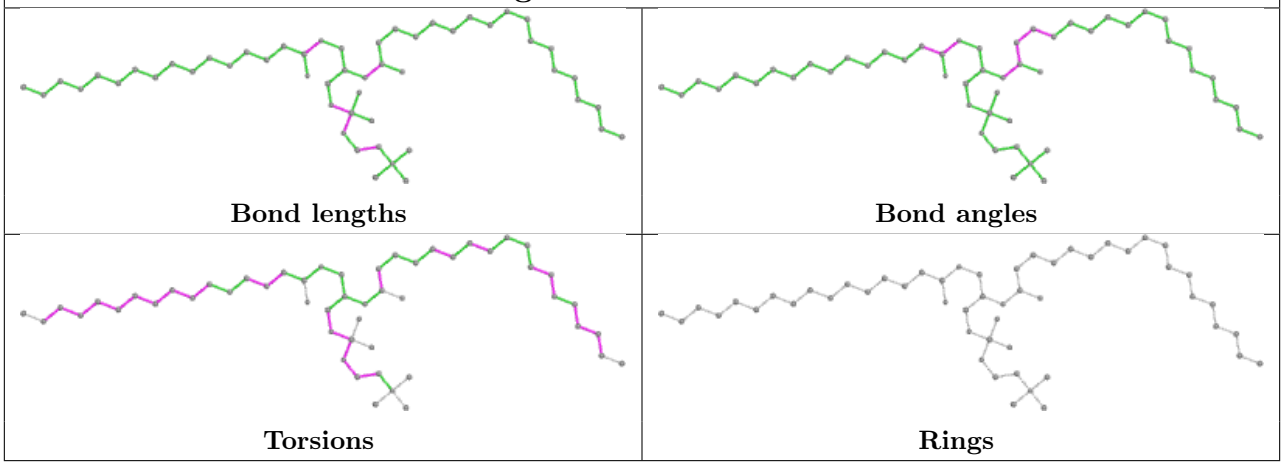


Torsions

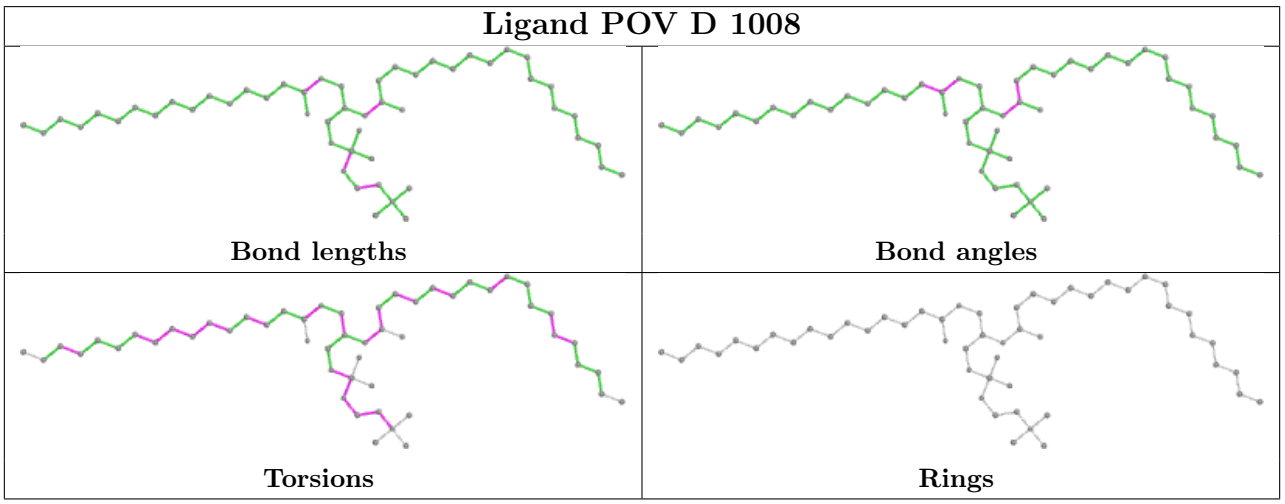


Rings

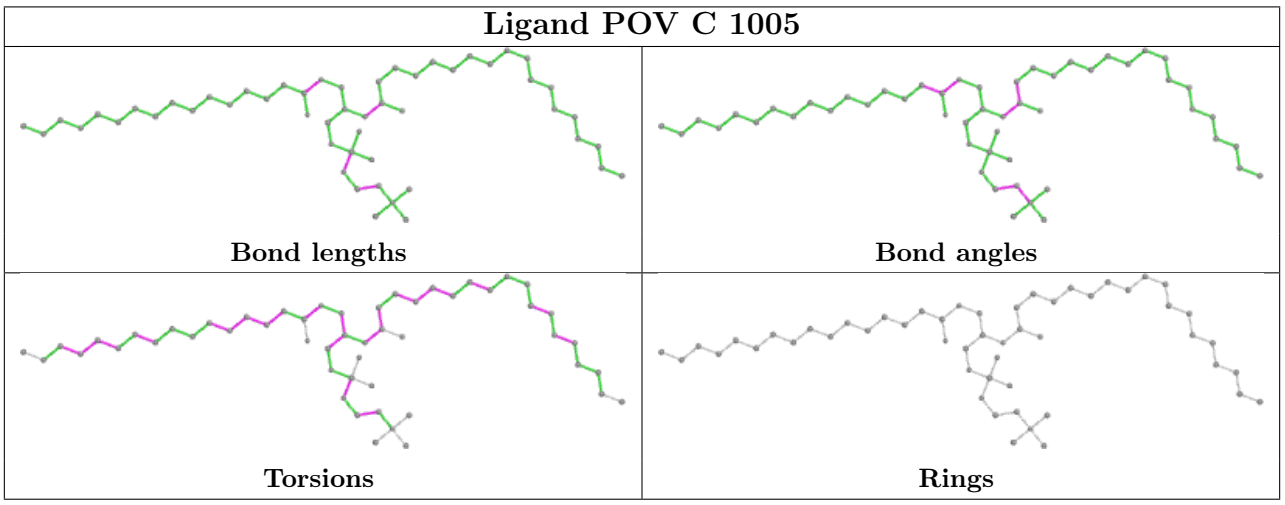
Ligand POV C 1003



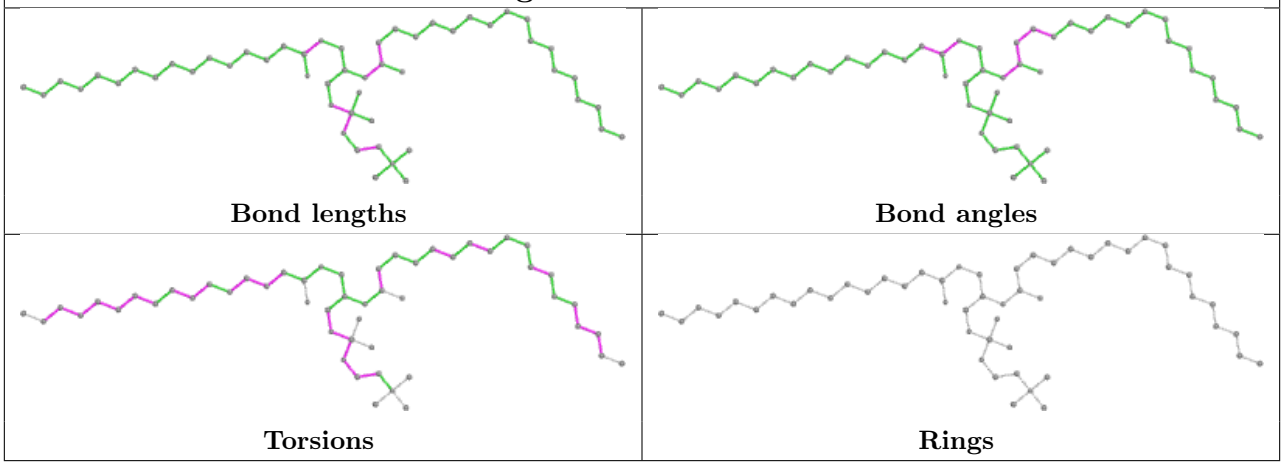
Ligand POV D 1008



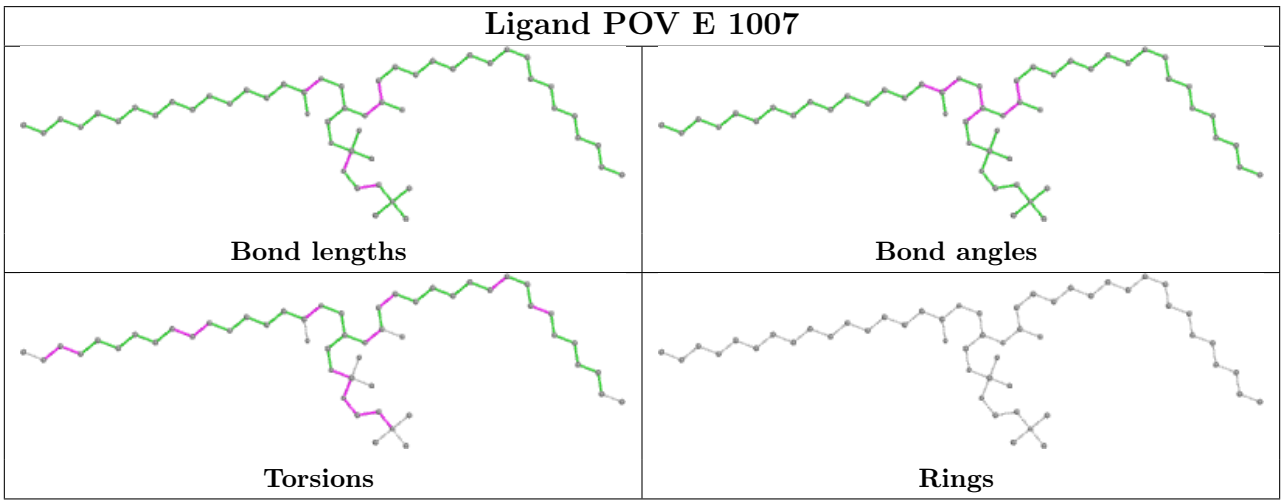
Ligand POV C 1005



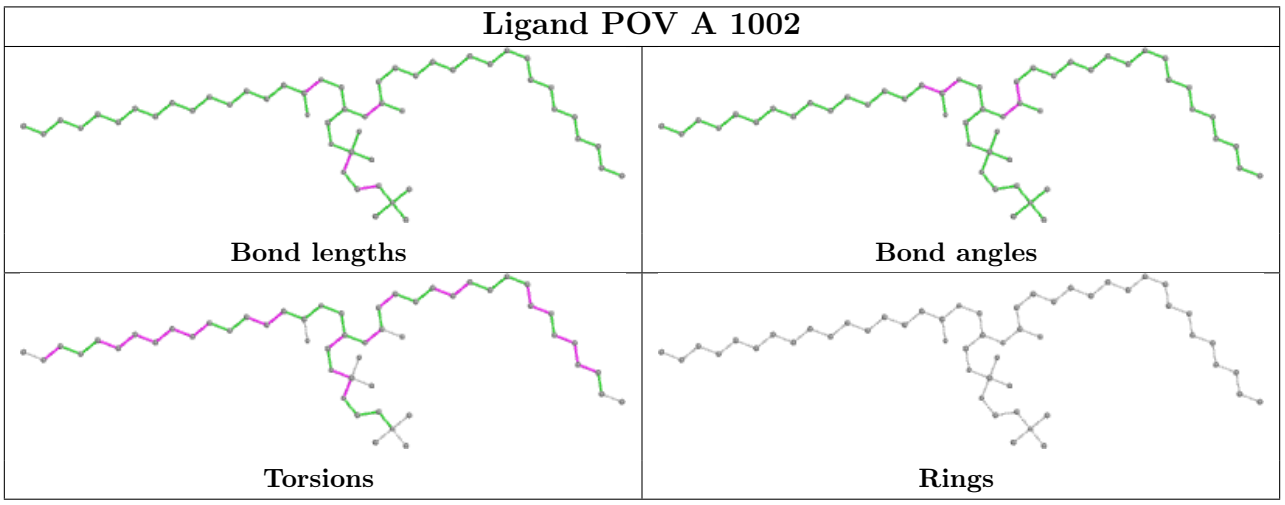
Ligand POV E 1003



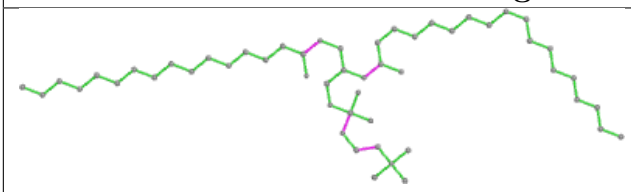
Ligand POV E 1007



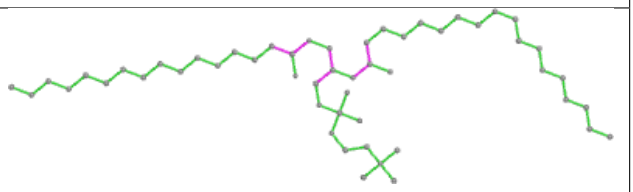
Ligand POV A 1002



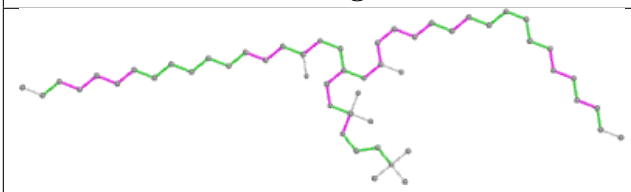
Ligand POV C 1009



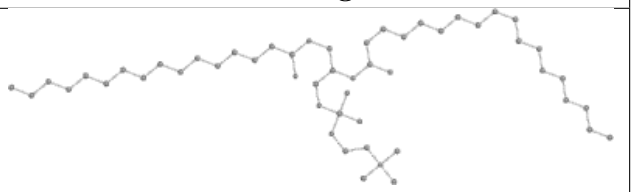
Bond lengths



Bond angles

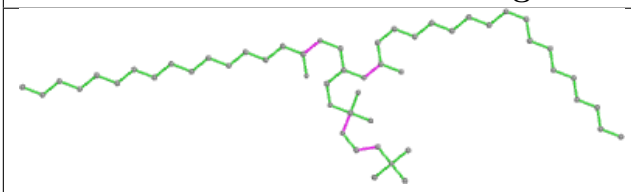


Torsions

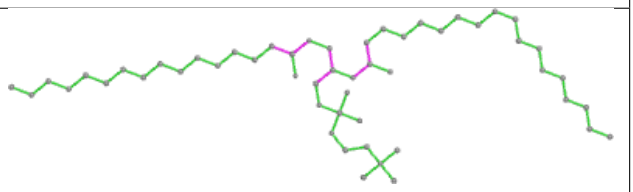


Rings

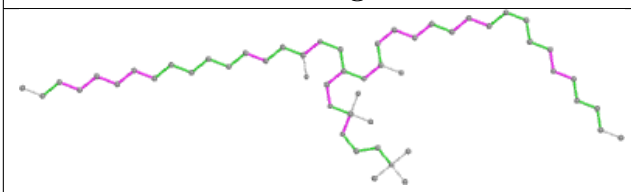
Ligand POV D 1010



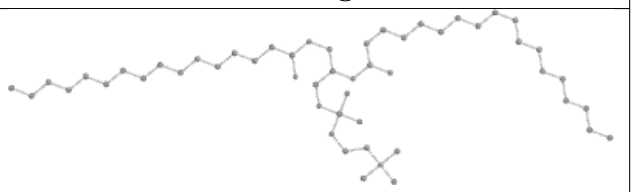
Bond lengths



Bond angles

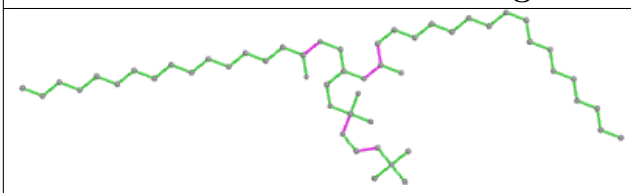


Torsions

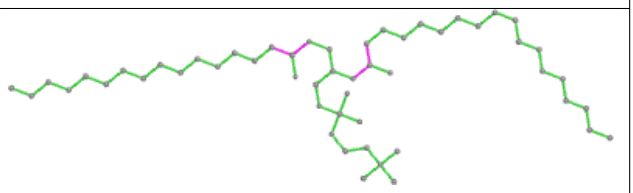


Rings

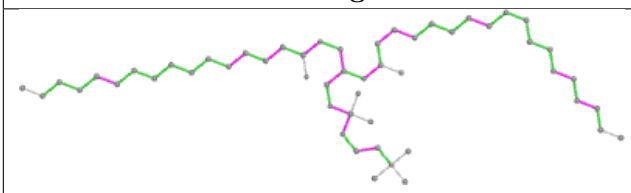
Ligand POV A 1011



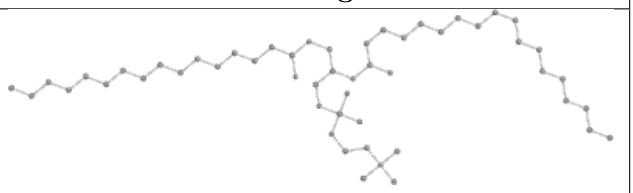
Bond lengths



Bond angles

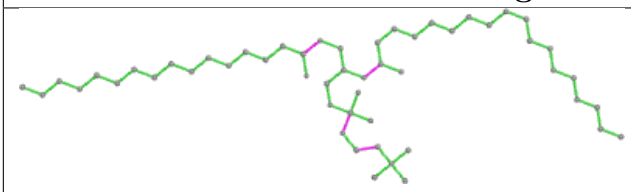


Torsions

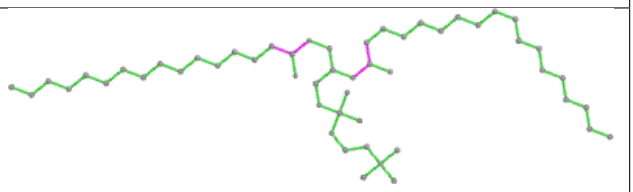


Rings

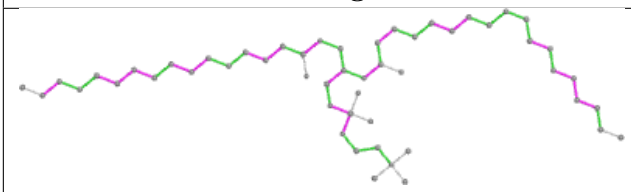
Ligand POV E 1002



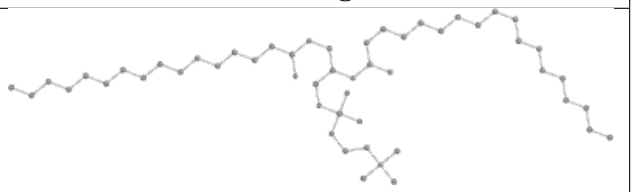
Bond lengths



Bond angles

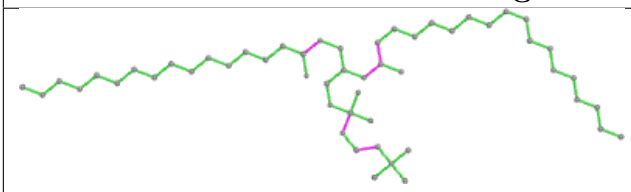


Torsions

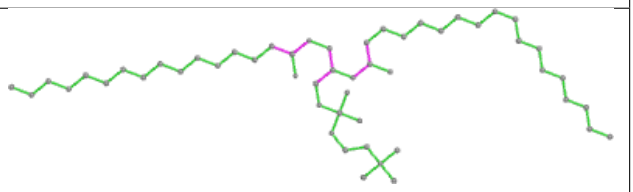


Rings

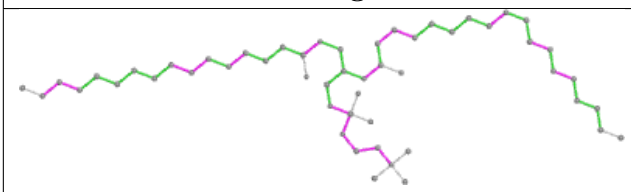
Ligand POV C 1007



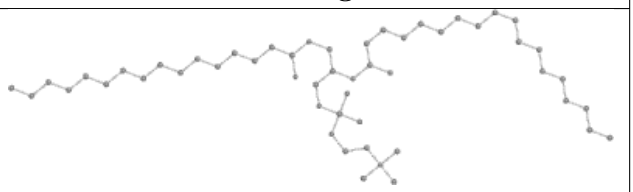
Bond lengths



Bond angles

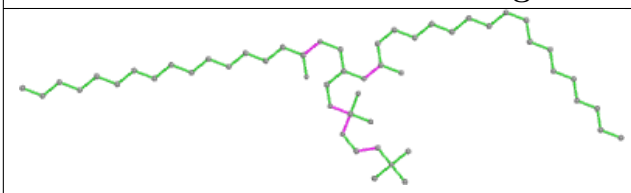


Torsions

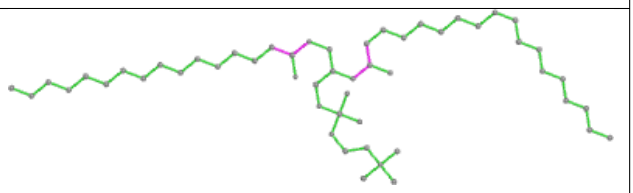


Rings

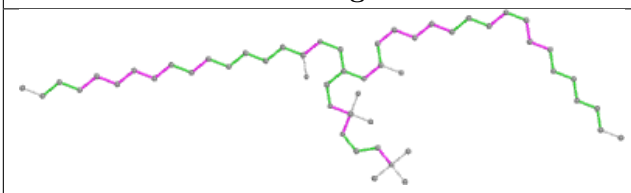
Ligand POV D 1004



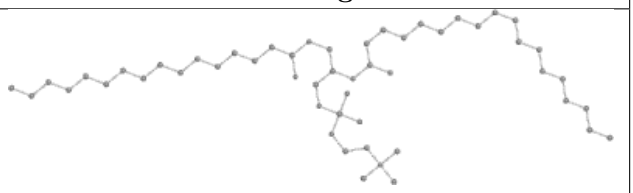
Bond lengths



Bond angles

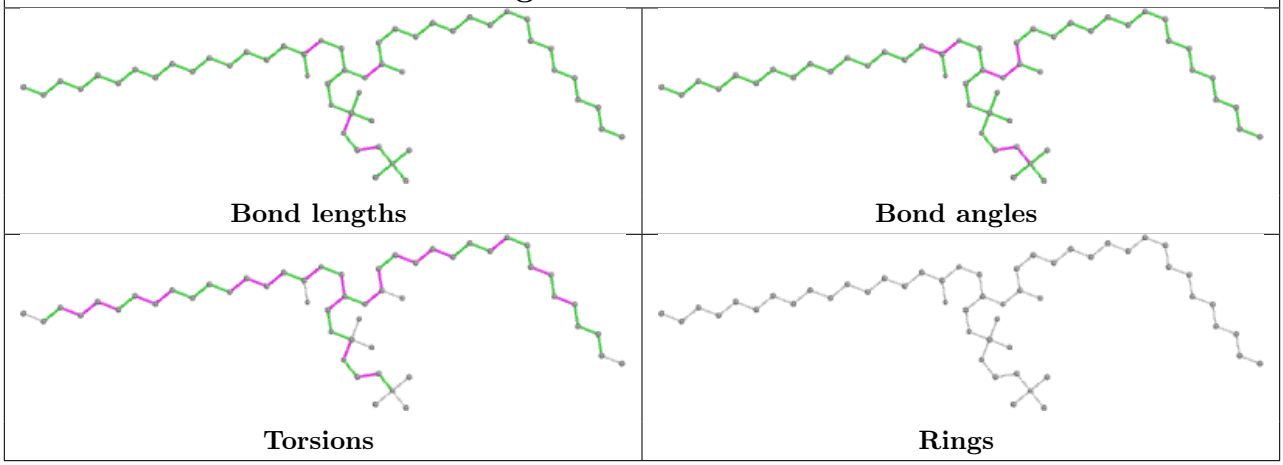


Torsions

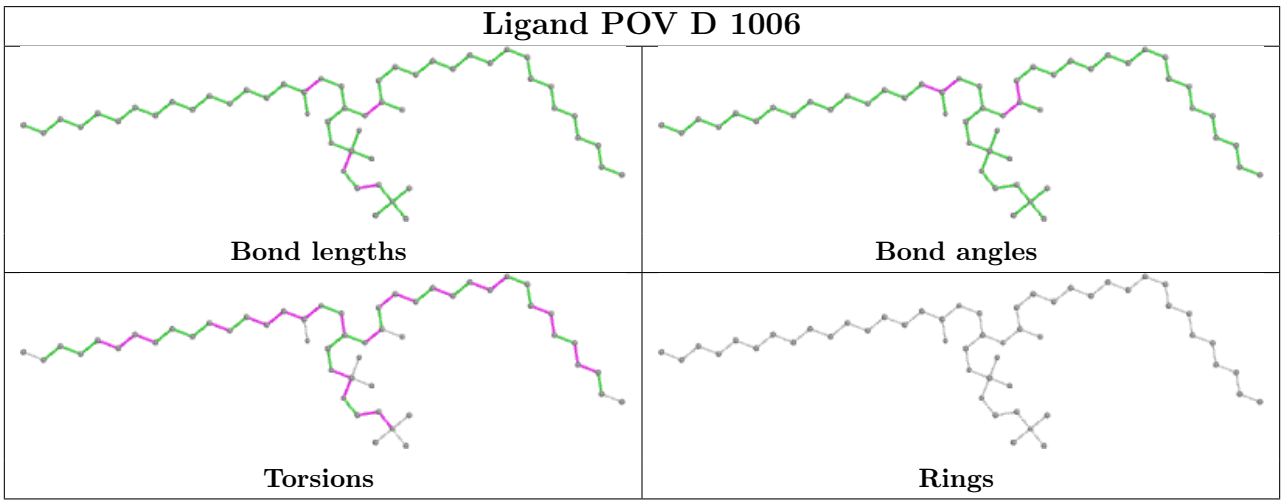


Rings

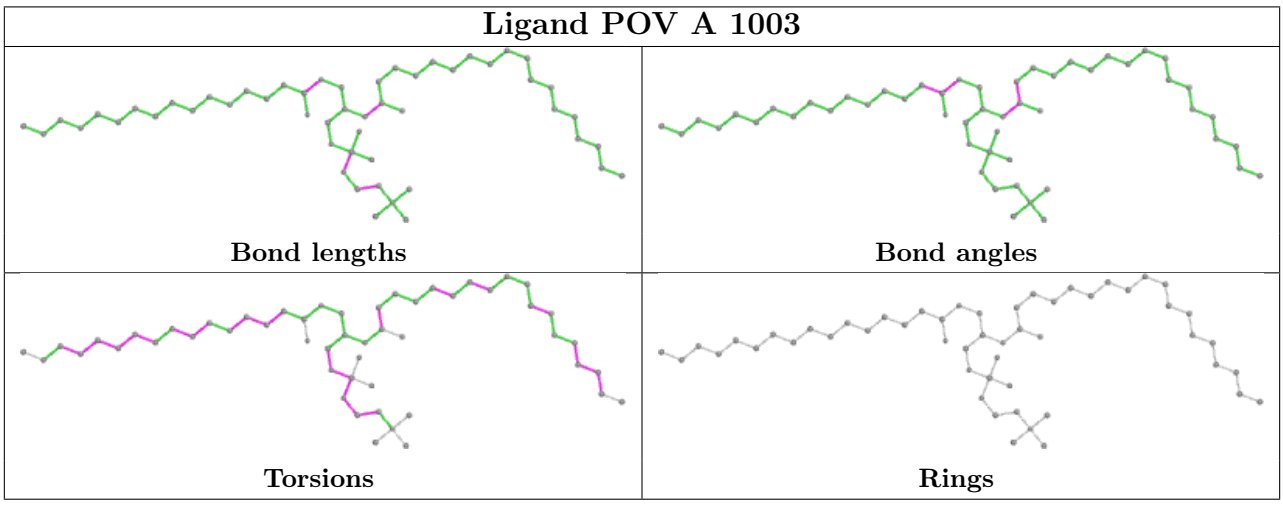
Ligand POV E 1005



Ligand POV D 1006



Ligand POV A 1003



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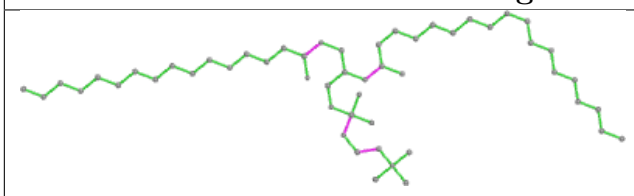
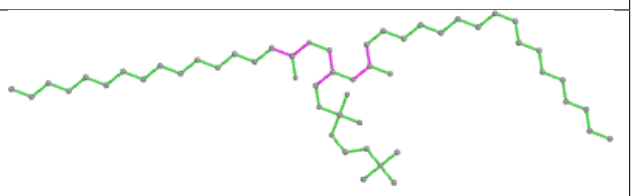
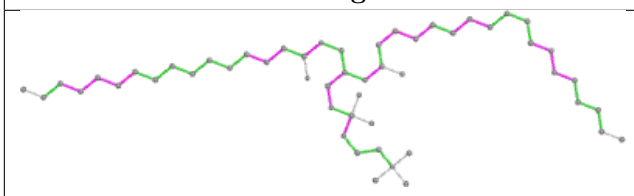
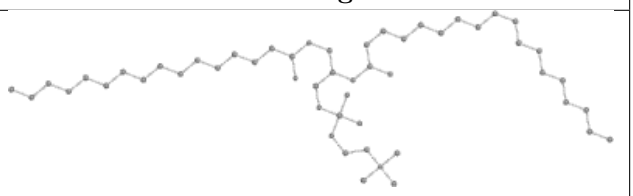
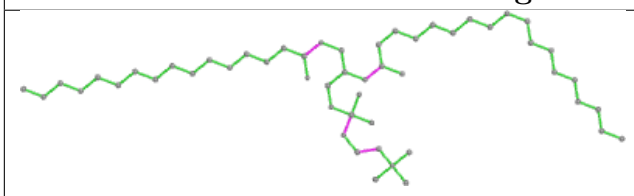

Bond lengths


Bond angles


Torsions


Rings

Ligand POV C 1004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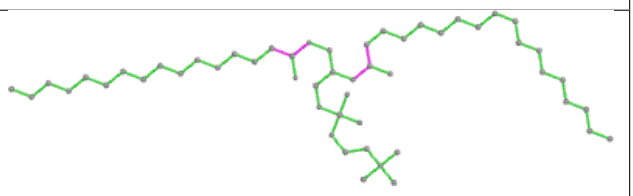
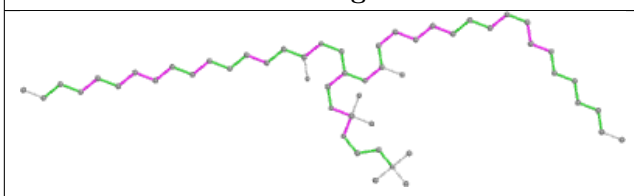

Bond angles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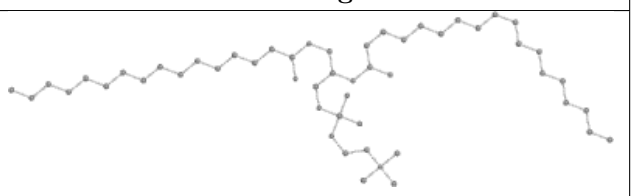
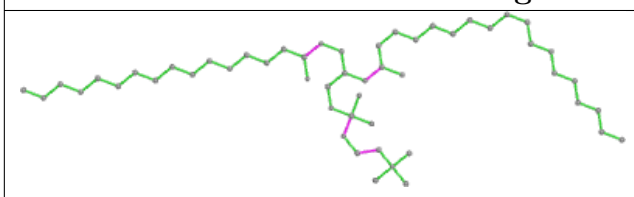
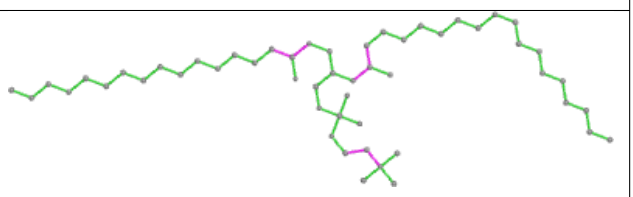
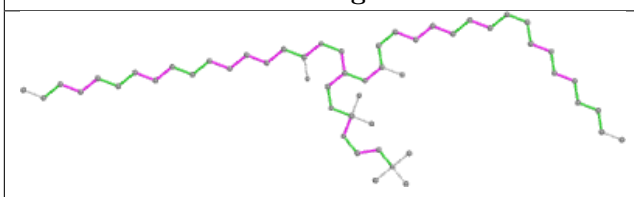
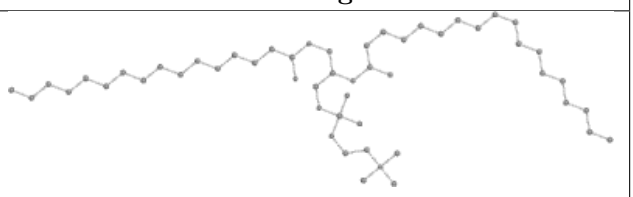

Rings

Ligand POV A 1005

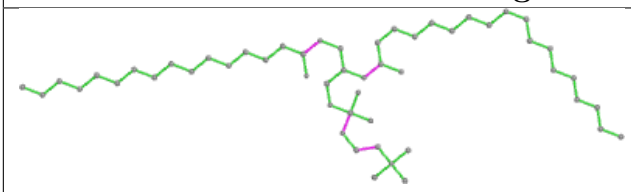

Bond lengths


Bond angles

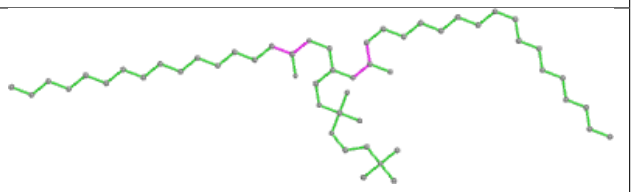

Torsions


Rings

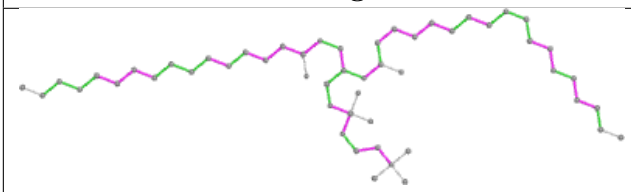
Ligand POV A 1006



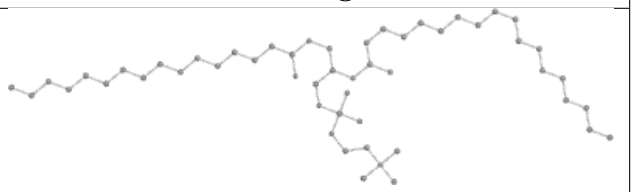
Bond lengths



Bond angles

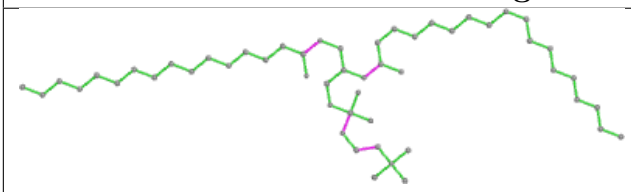


Torsions



Rings

Ligand POV A 1008



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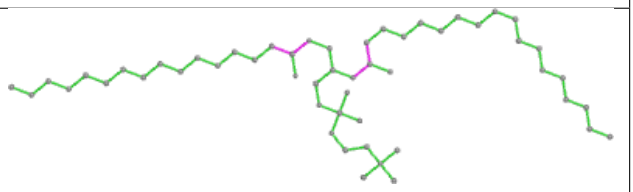
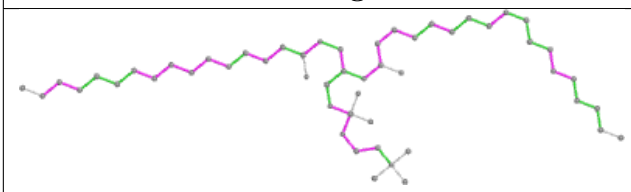
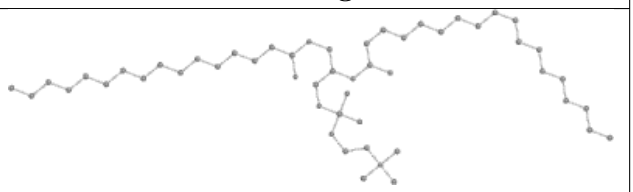


Bond angles

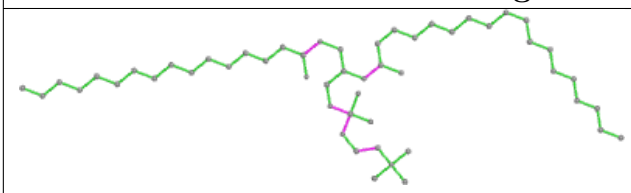


Torsions

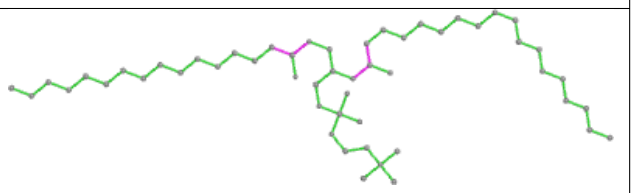


Rings

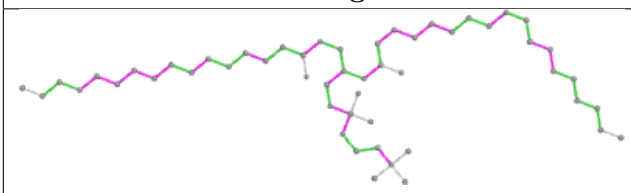
Ligand POV A 1004



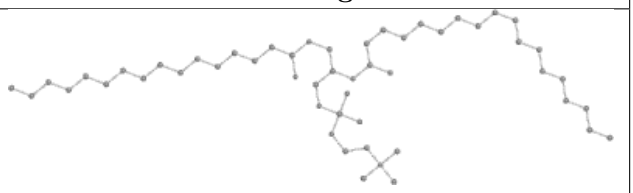
Bond lengths



Bond angles

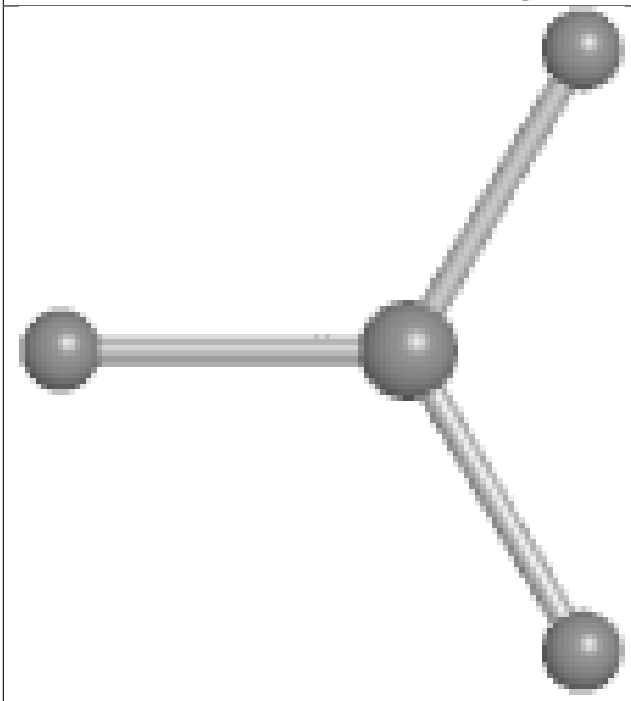


Torsions



Rings

Ligand BEF C 1001



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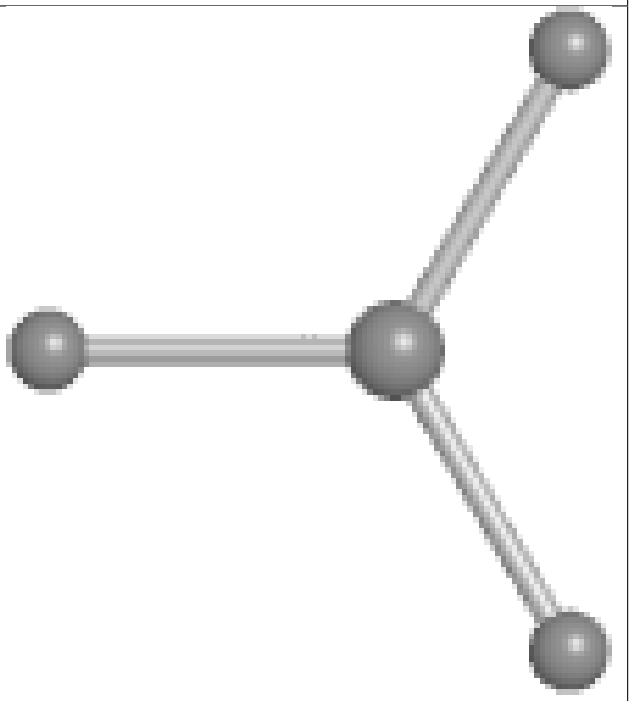
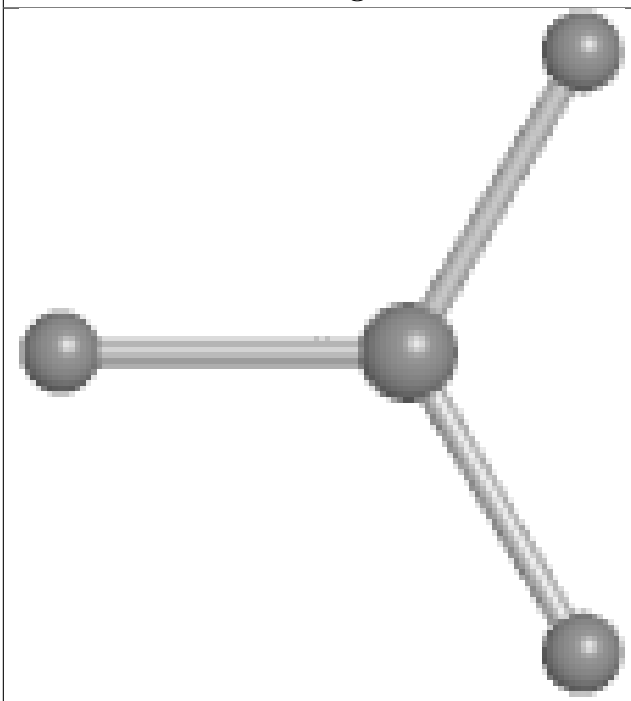
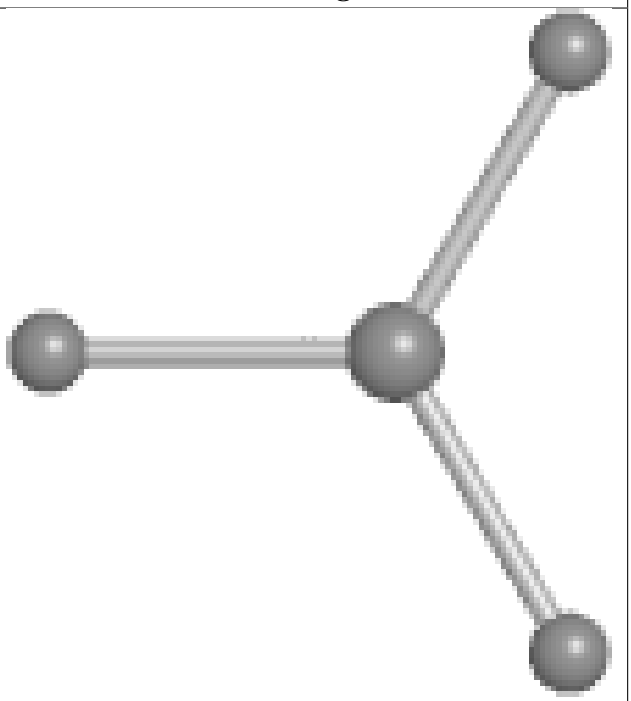


Bond angles

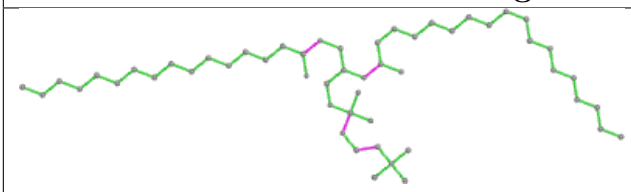


Torsions

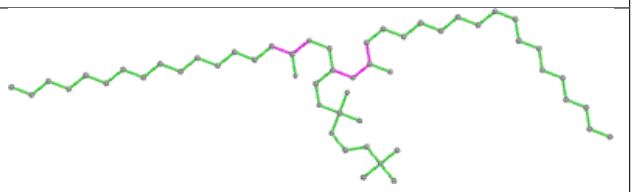


Rings

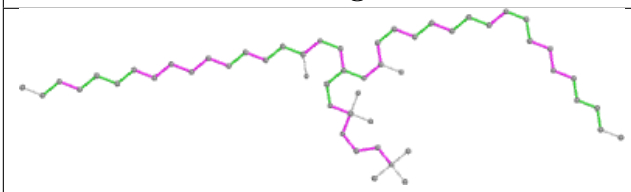
Ligand POV B 1009



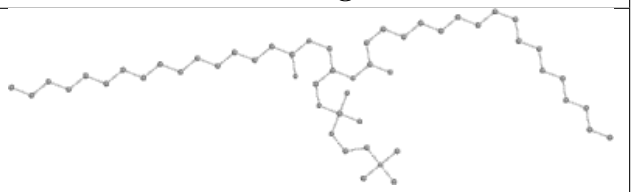
Bond lengths



Bond angles

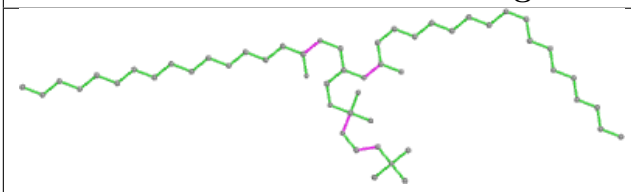


Torsions

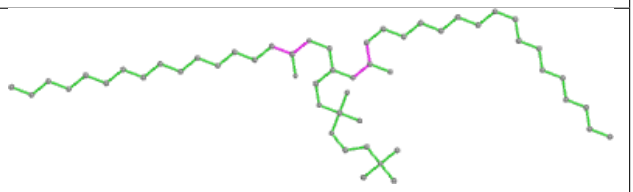


Rings

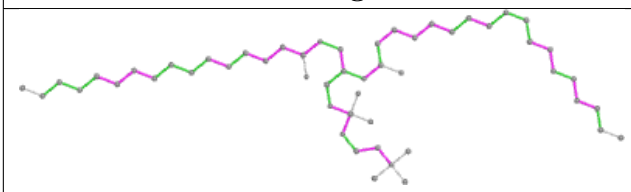
Ligand POV B 1007



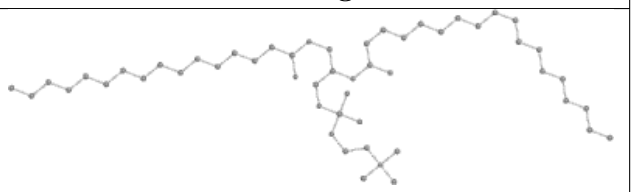
Bond lengths



Bond angles

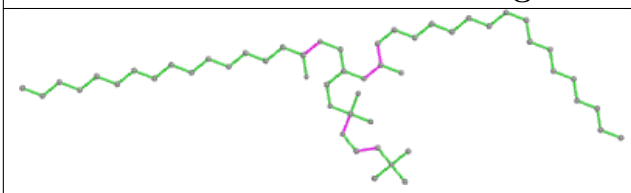


Torsions

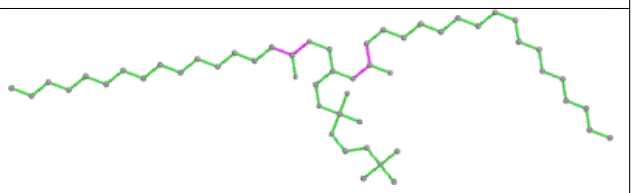


Rings

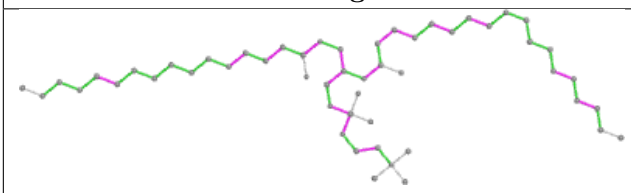
Ligand POV C 1010



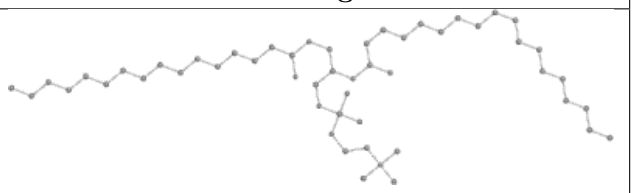
Bond lengths



Bond angles

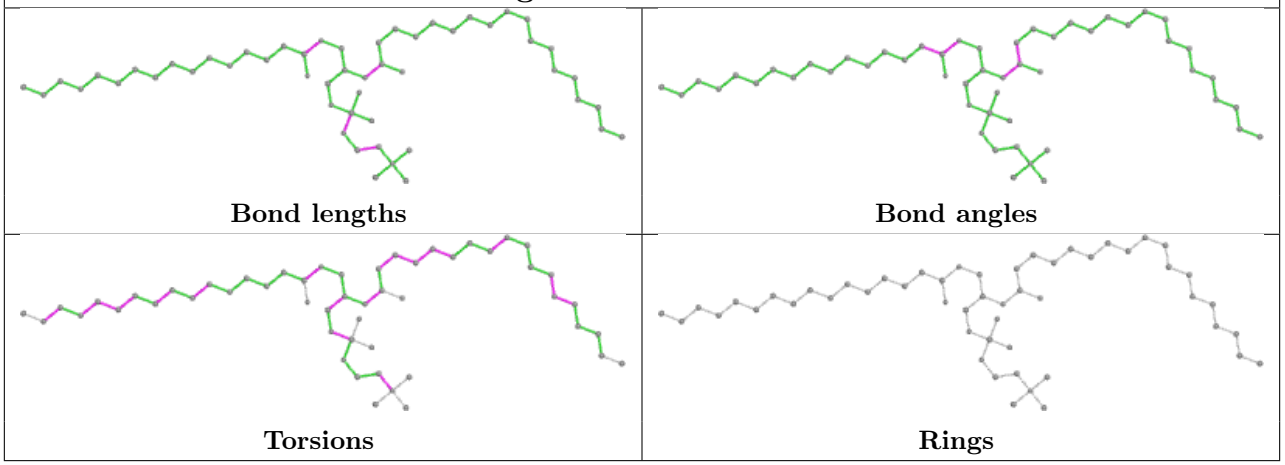


Torsions

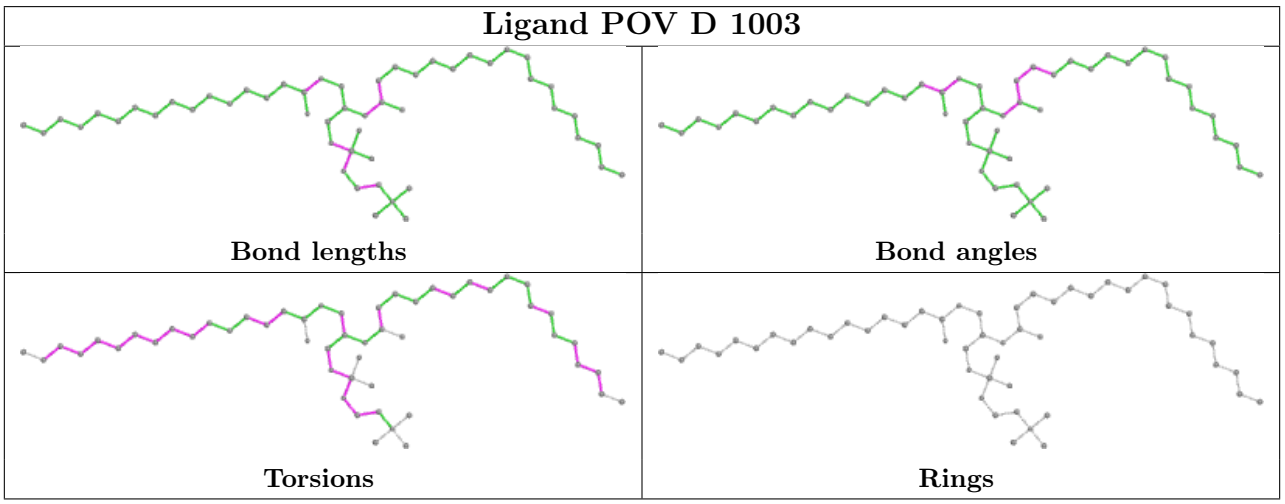


Rings

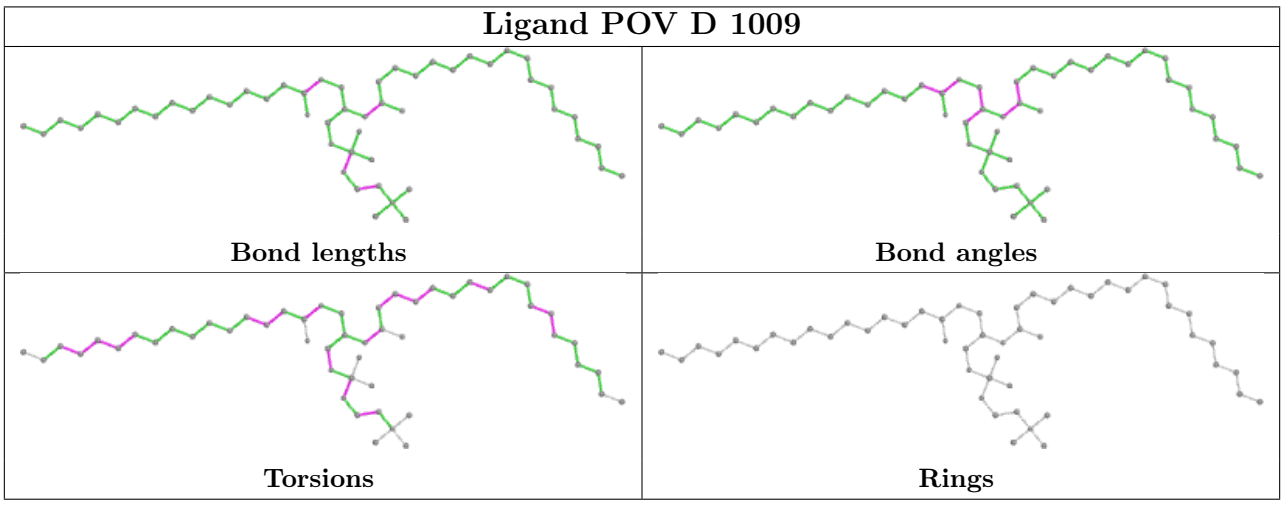
Ligand POV F 1003



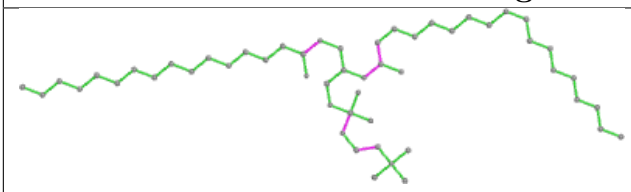
Ligand POV D 1003



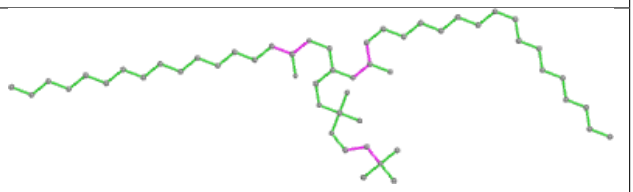
Ligand POV D 1009



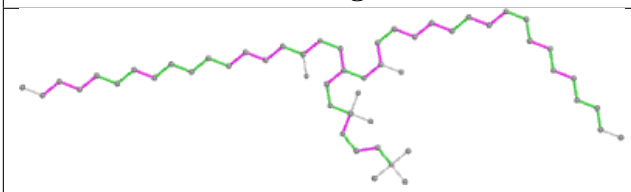
Ligand POV F 1004



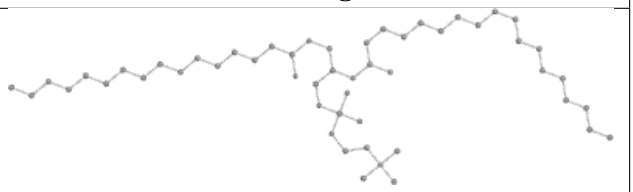
Bond lengths



Bond angles

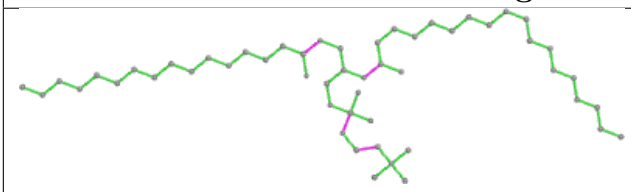


Torsions

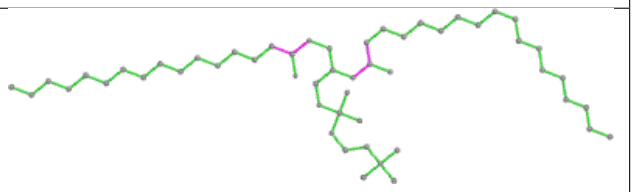


Rings

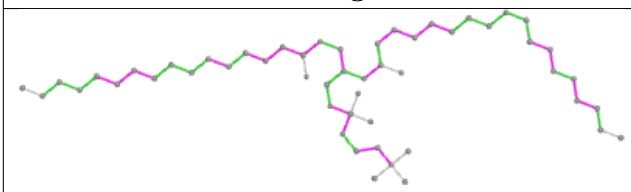
Ligand POV F 1005



Bond lengths



Bond angles



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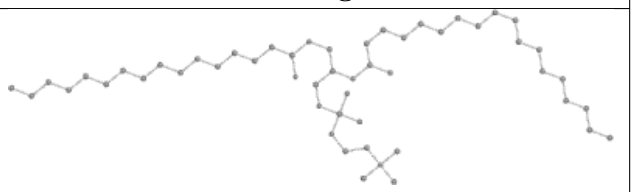
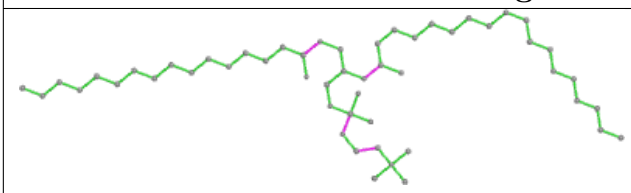


Rings

Ligand POV F 1002



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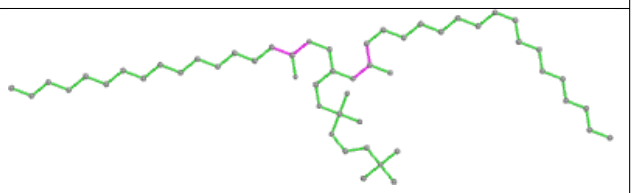

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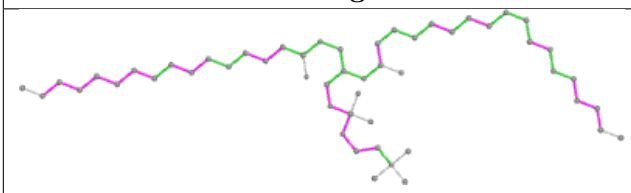
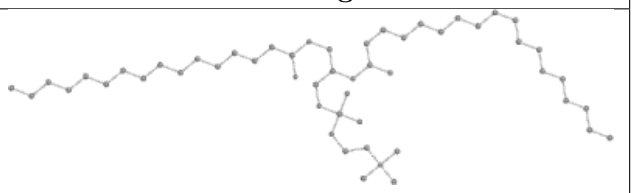
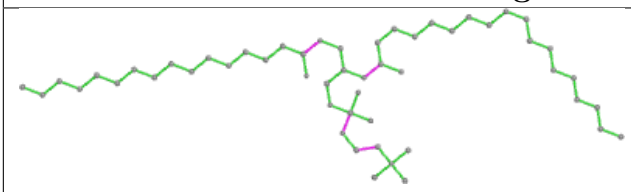


Torsions



Rings

Ligand POV A 1009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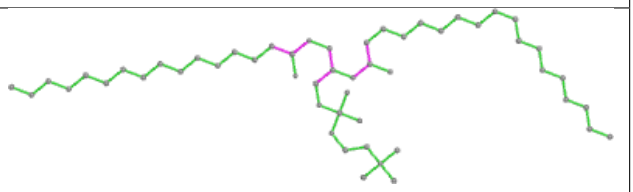
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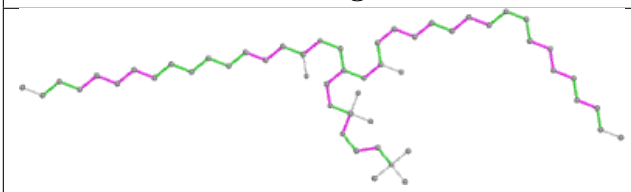
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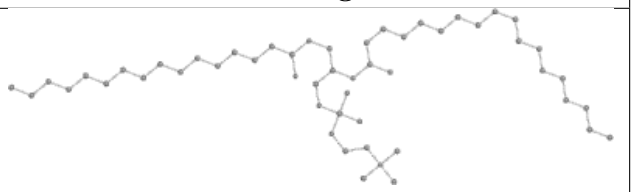
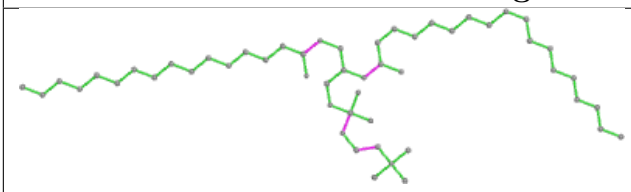

Rings

Ligand POV D 1002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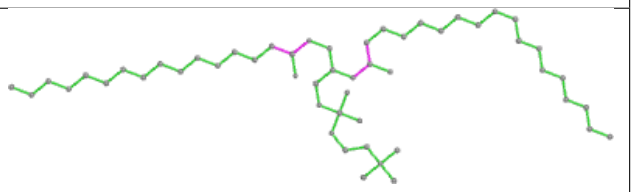
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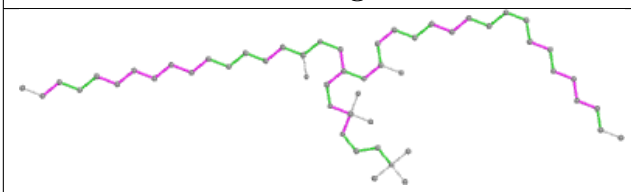
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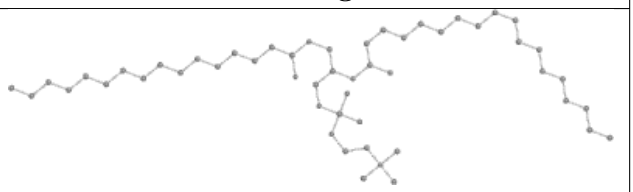
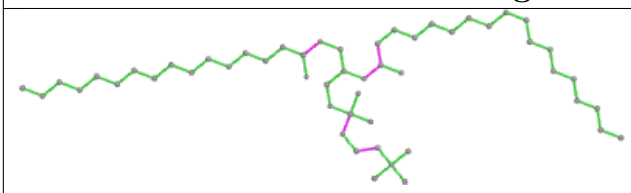

Rings

Ligand POV A 1007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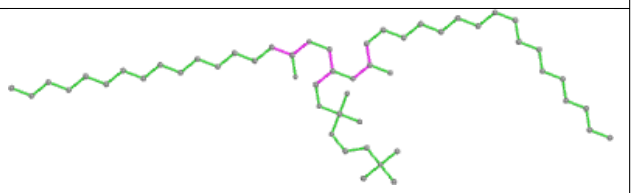
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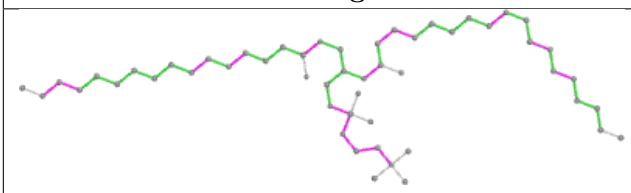
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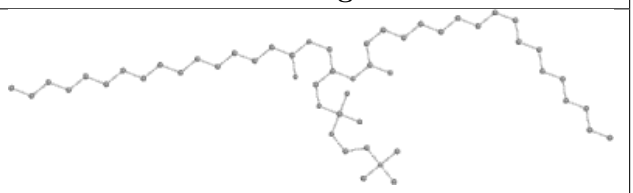
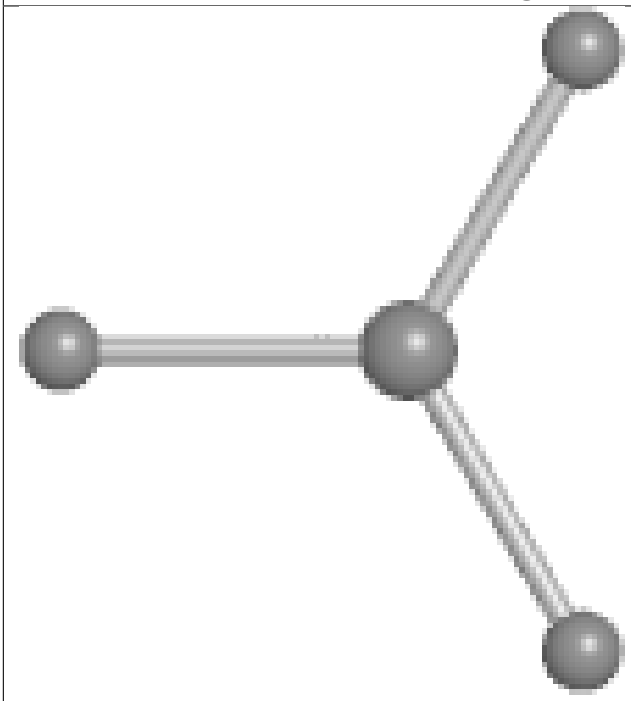

Rings

Ligand BEF E 1001



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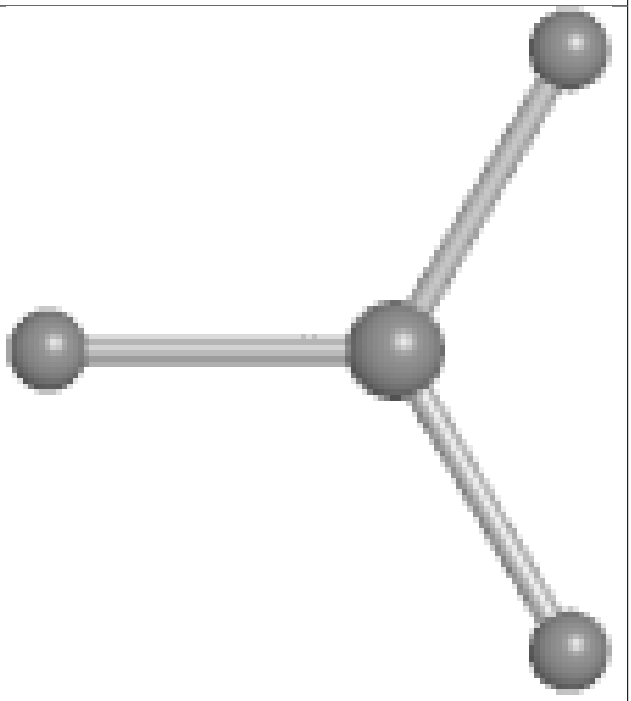
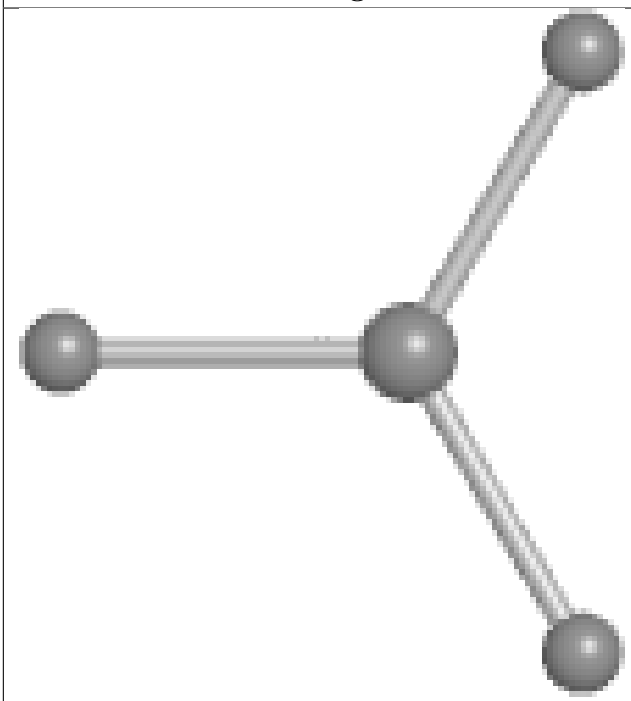


Bond angles



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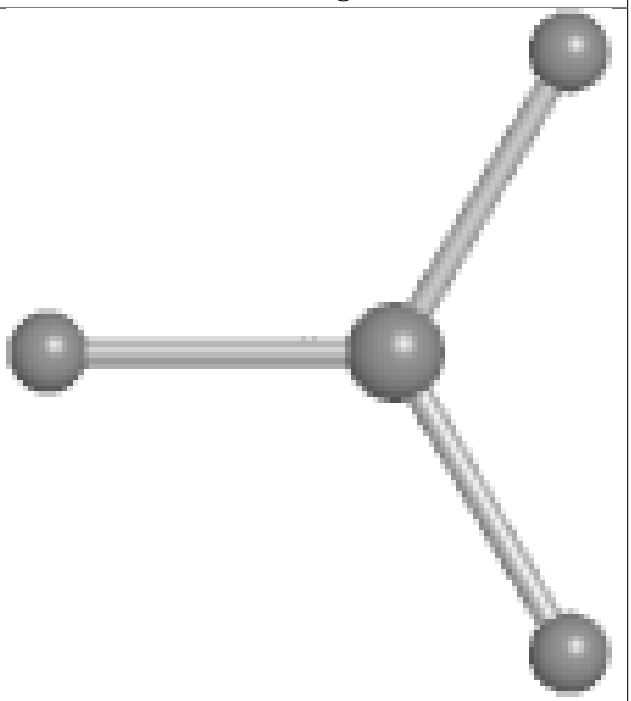
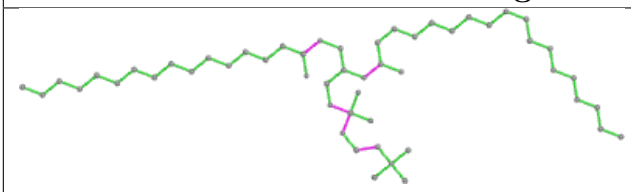


Rings

Ligand POV B 1005



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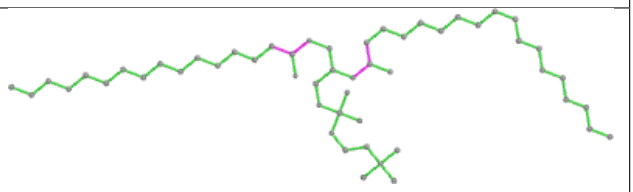
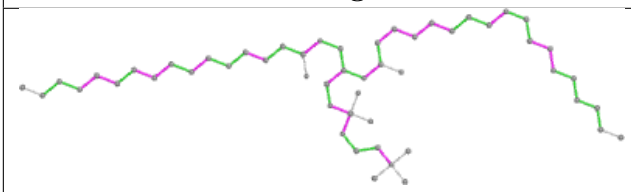


Bond angles



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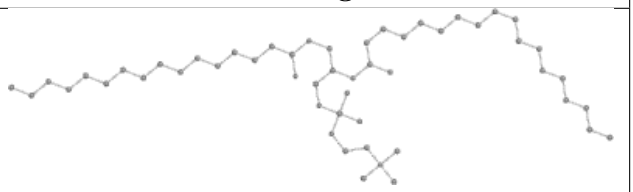
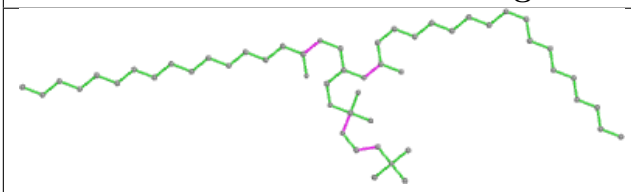


Rings

Ligand POV B 1010



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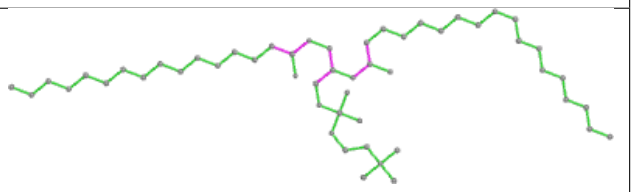
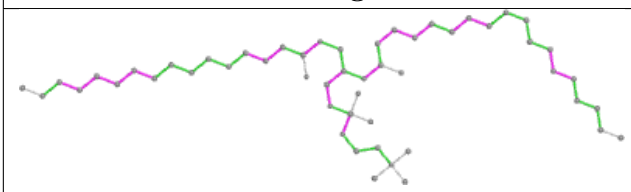


Bond angles



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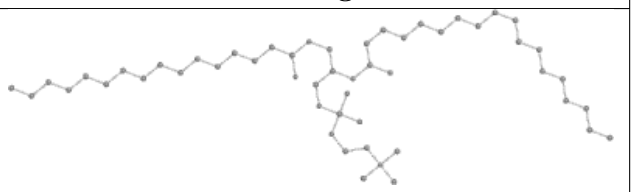
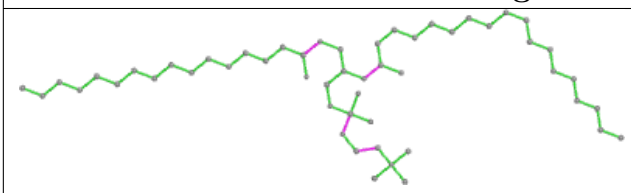


Rings

Ligand POV D 1011



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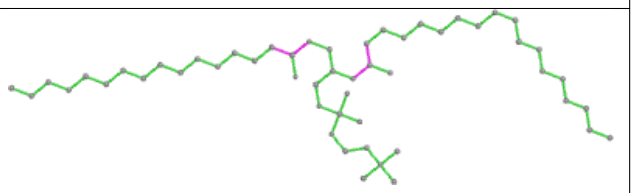
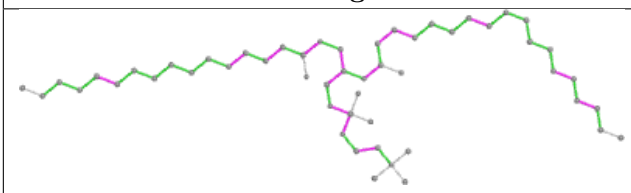


Bond angles



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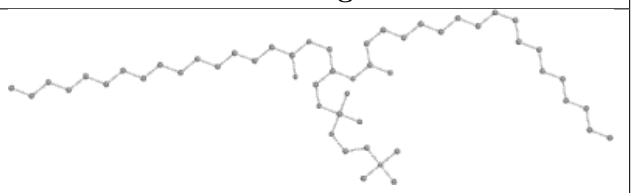
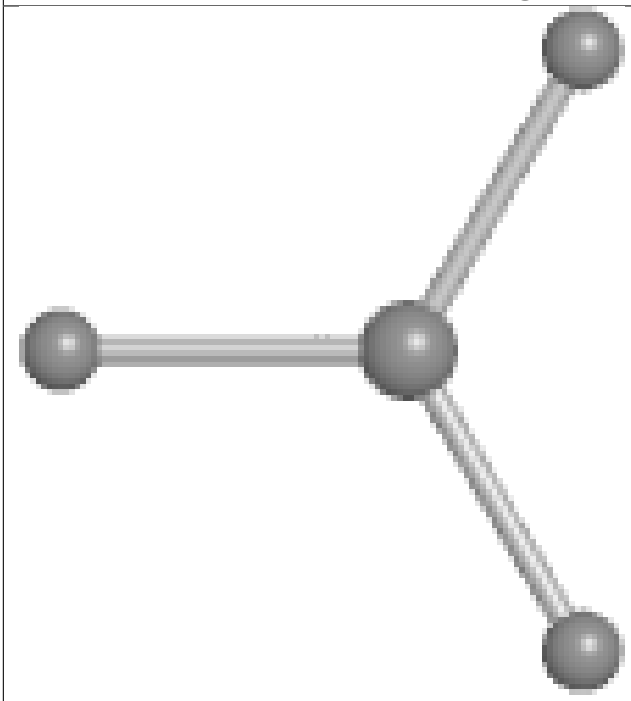


Rings

Ligand BEF A 1001



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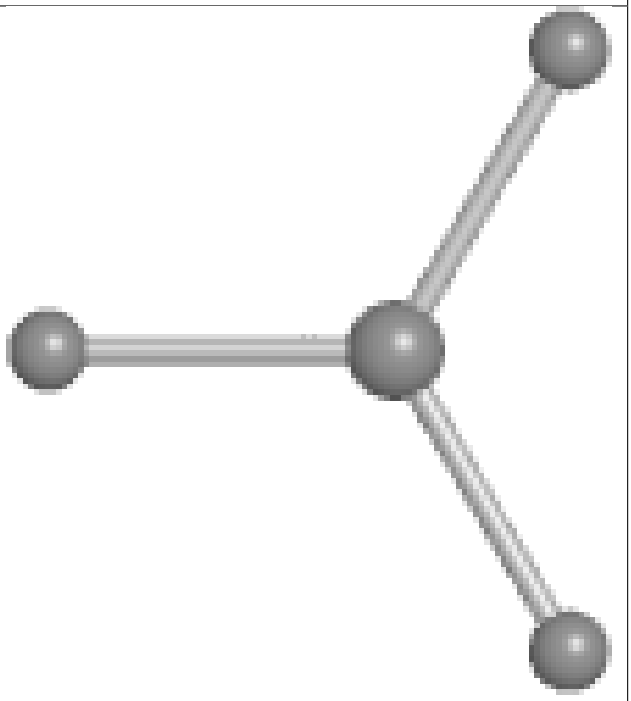
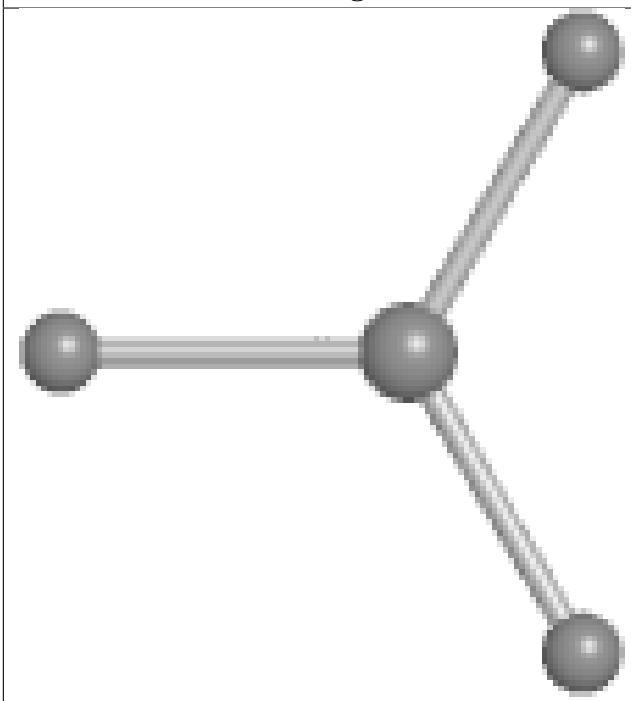


Bond angles



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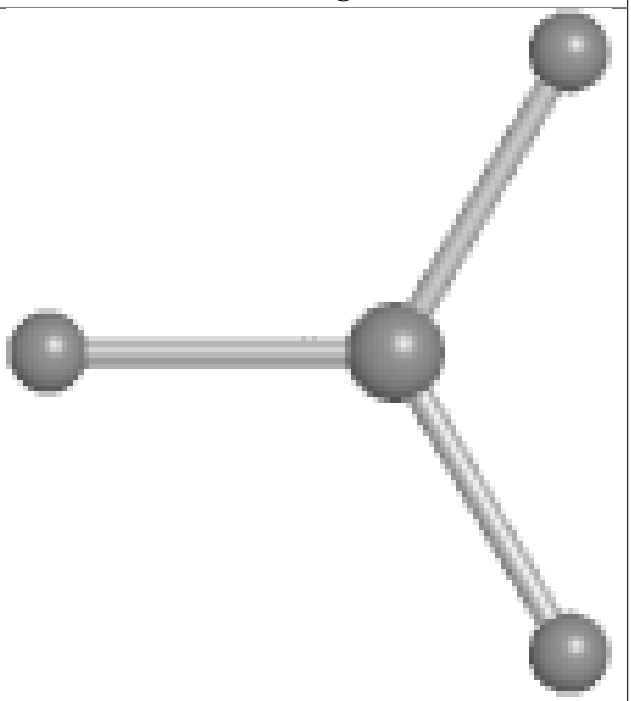
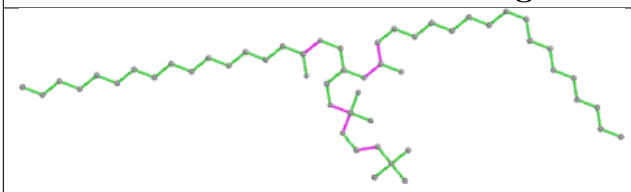


Rings

Ligand POV F 1006



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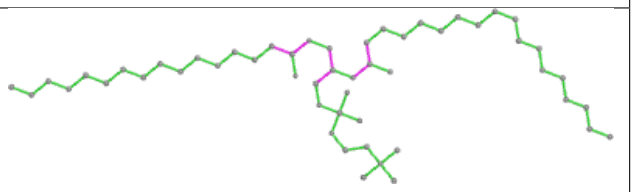
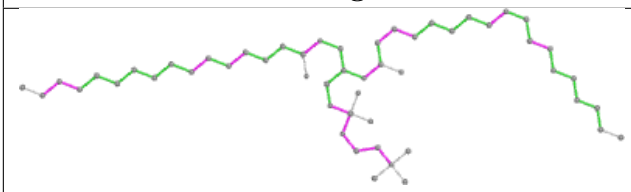


Bond angles



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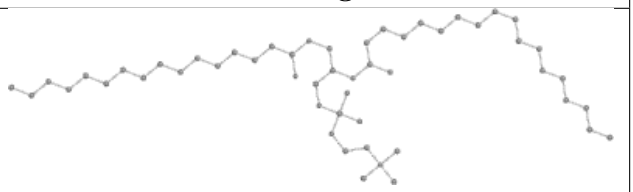
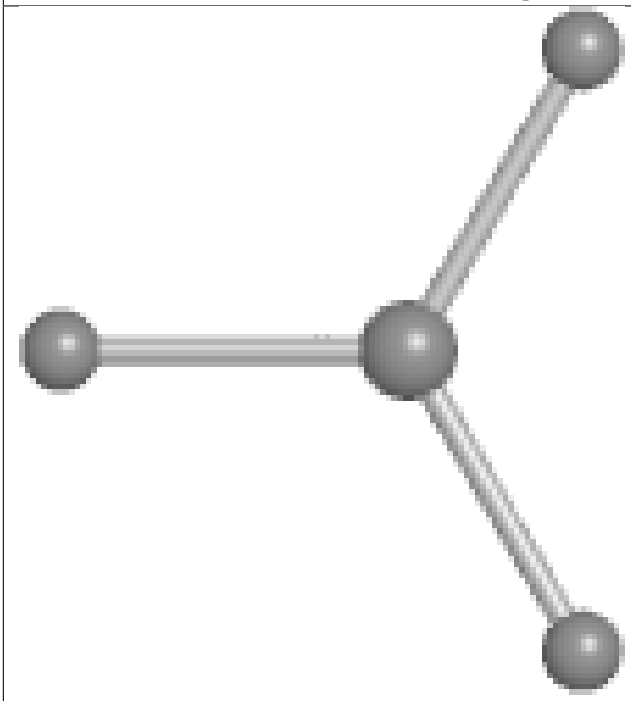


Rings

Ligand BEF B 1001



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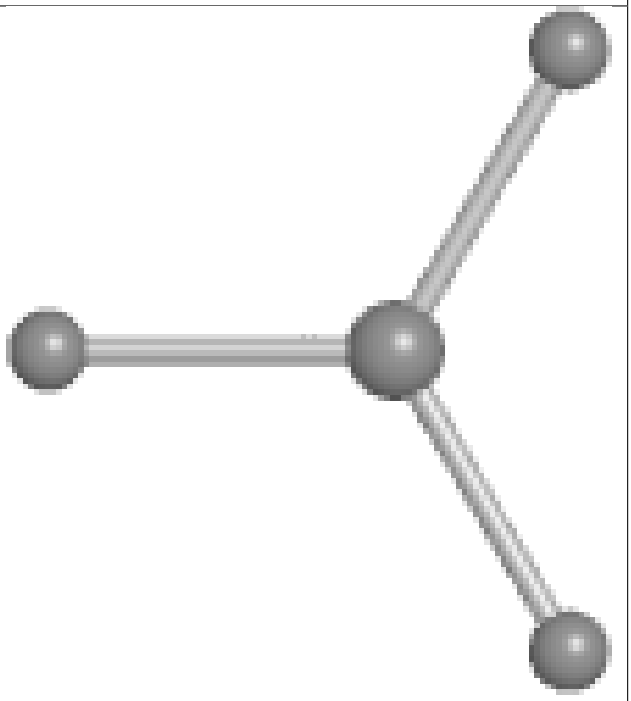
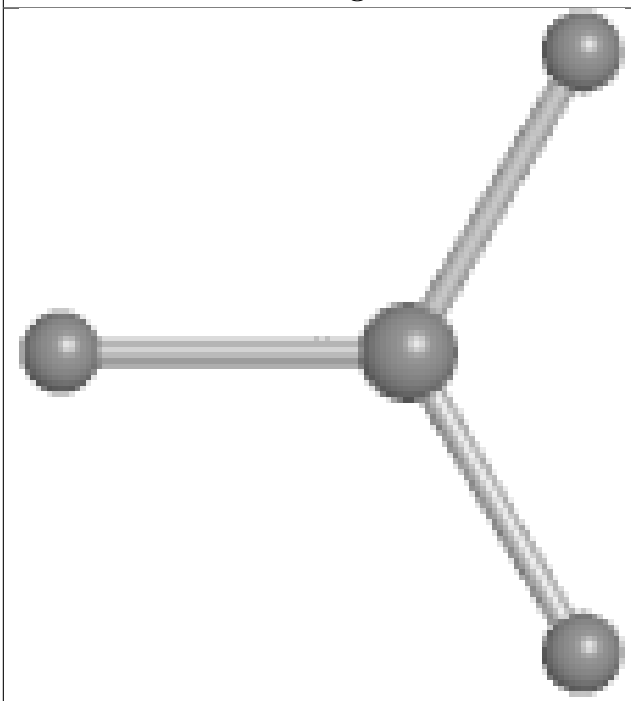


Bond angles



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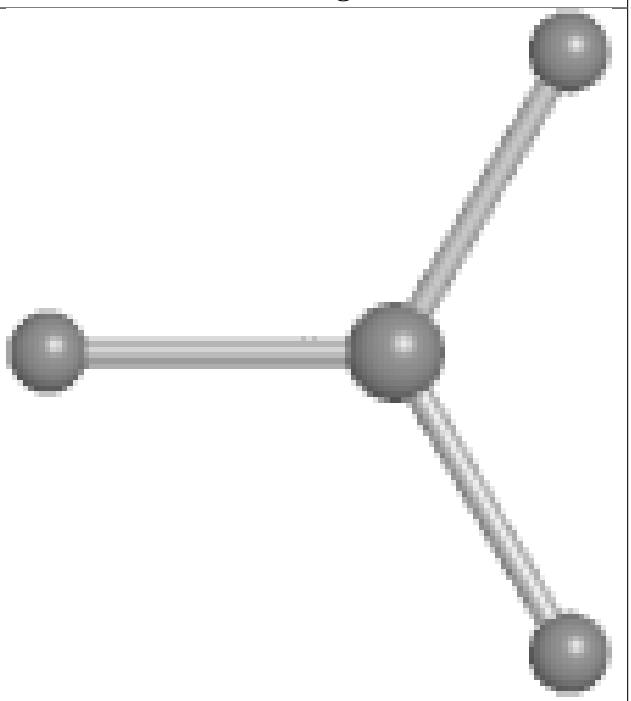
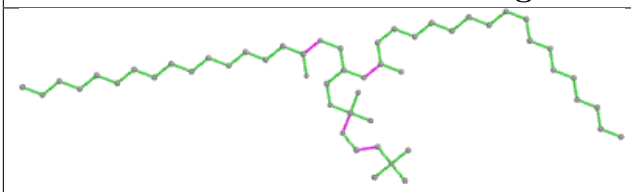


Rings

Ligand POV E 1008



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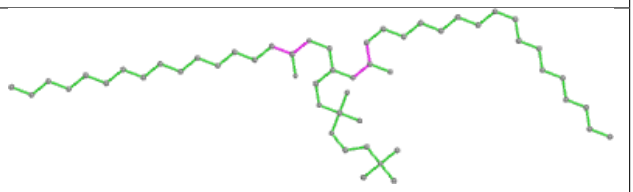
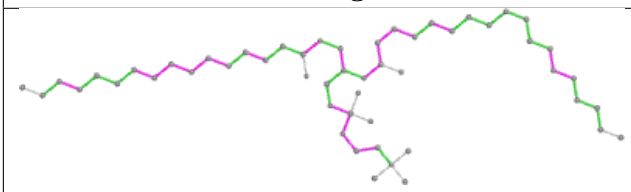
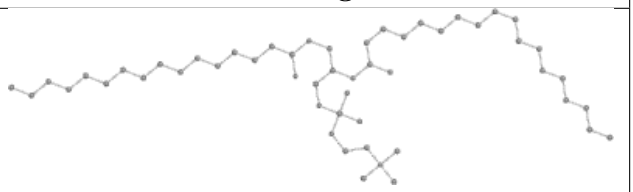


Bond angles

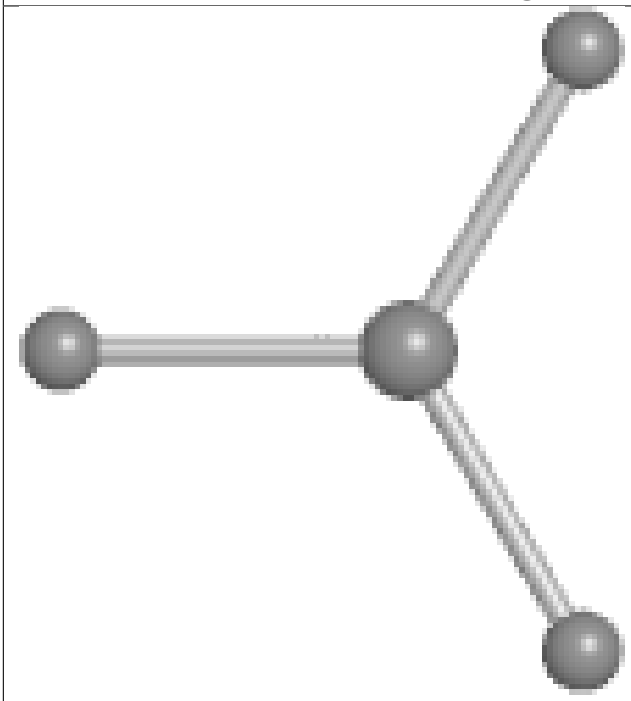


Torsions



Rings

Ligand BEF F 1001



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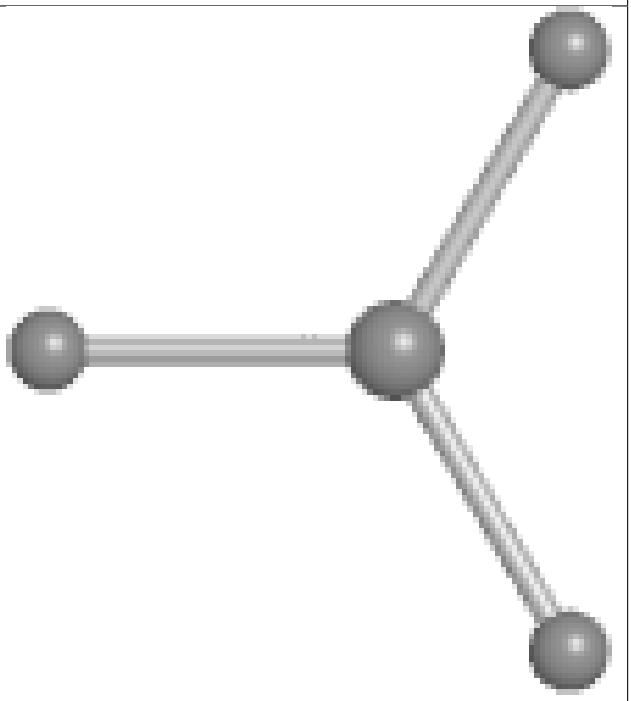
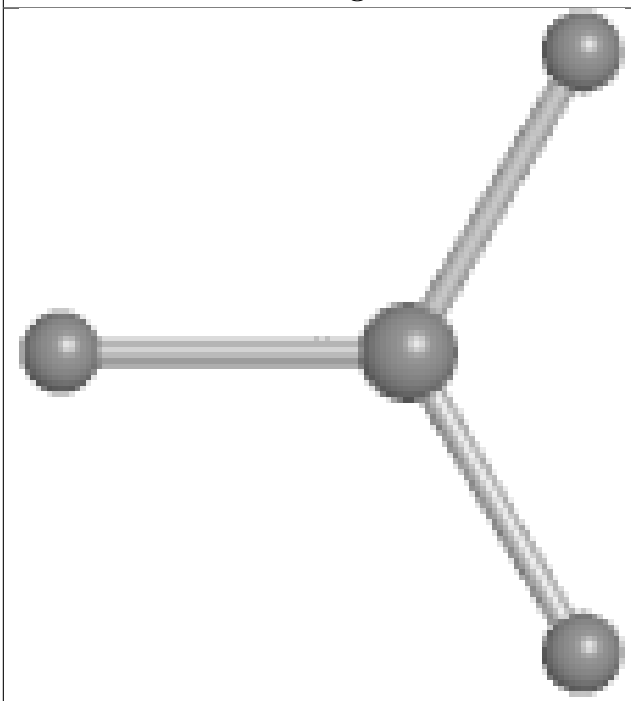


Bond angles



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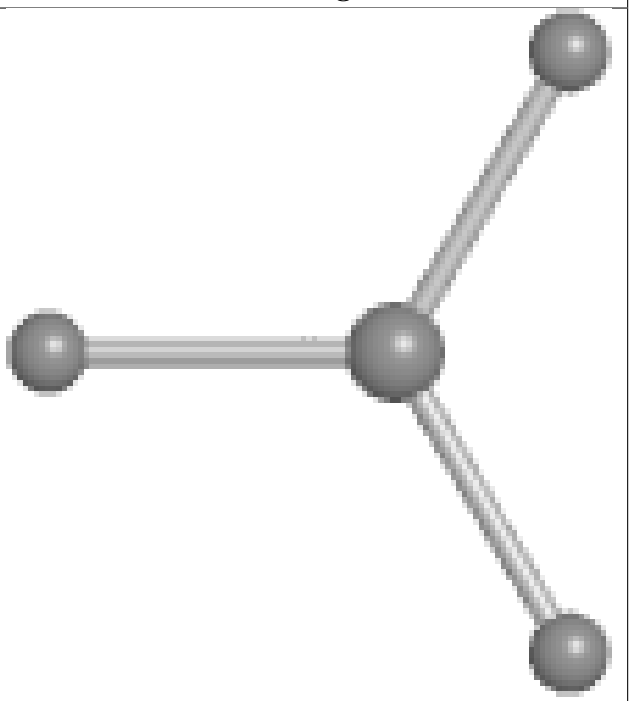
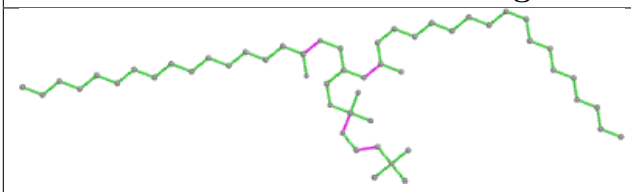


Rings

Ligand POV A 1012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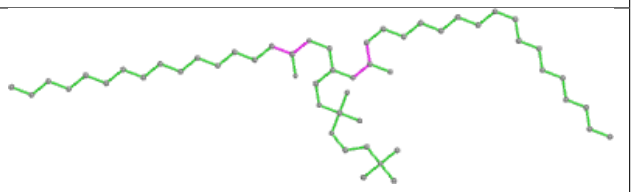
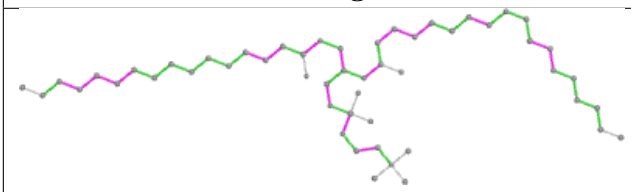

Bond angles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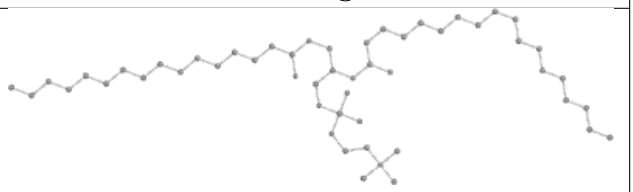
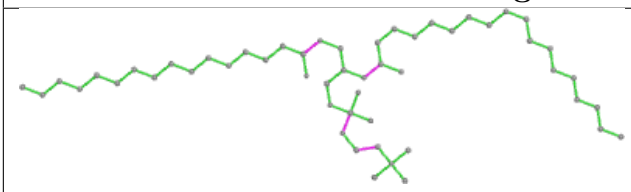
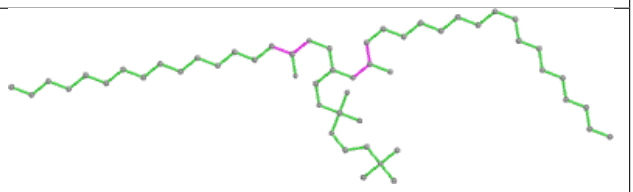
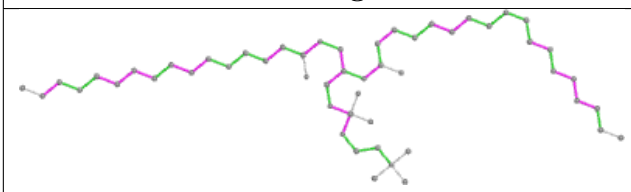
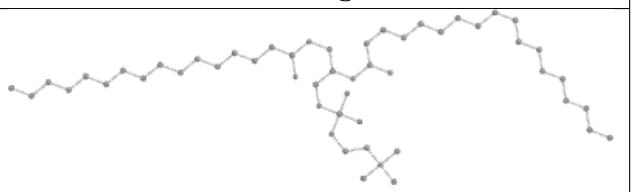

Rings

Ligand POV C 1002

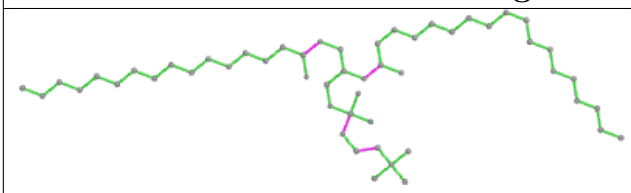

Bond lengths

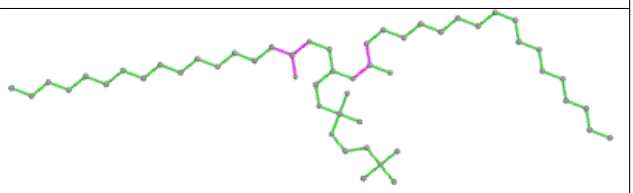

Bond angles

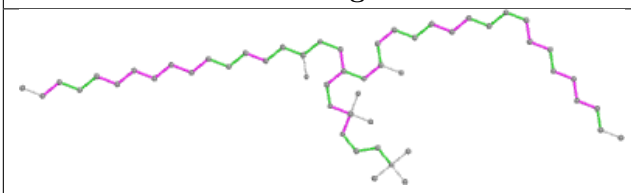

Torsions

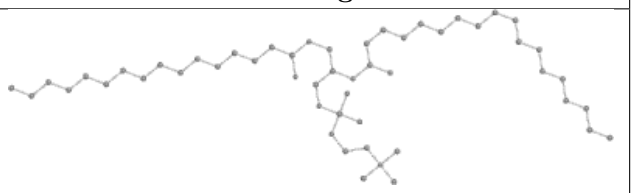

Rings

Ligand POV A 1010

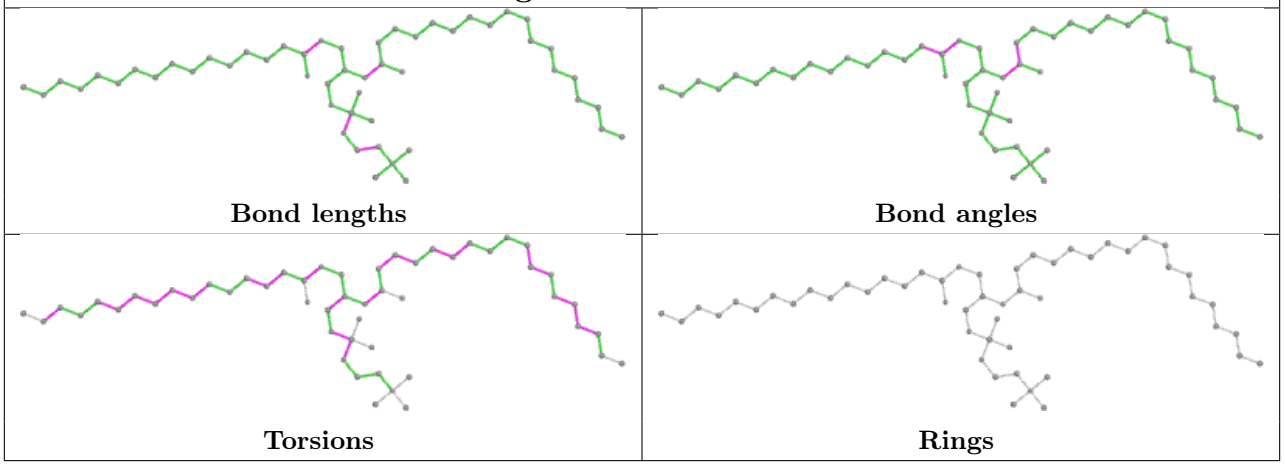

Bond lengths


Bond angles

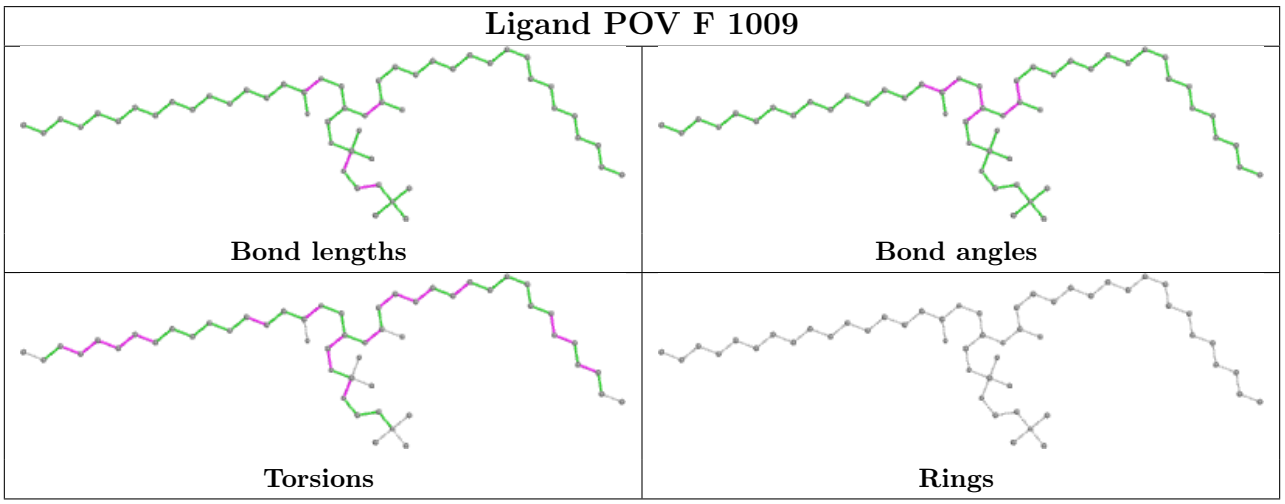

Torsions


Rings

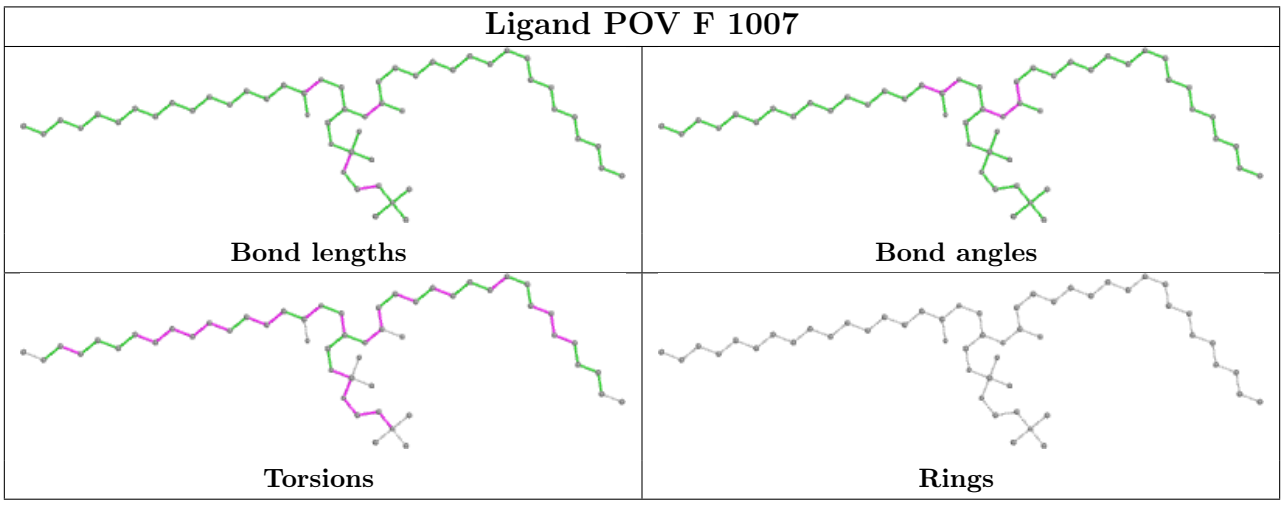
Ligand POV B 1003



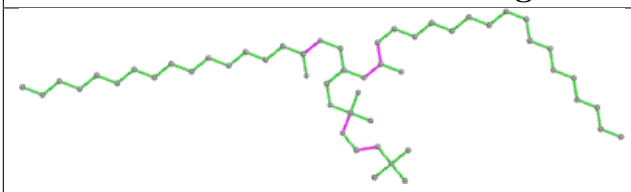
Ligand POV F 1009



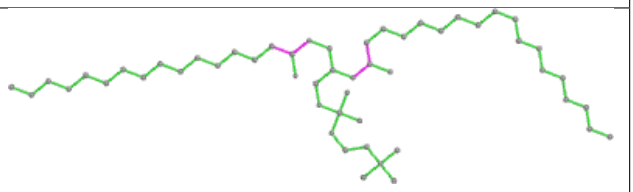
Ligand POV F 1007



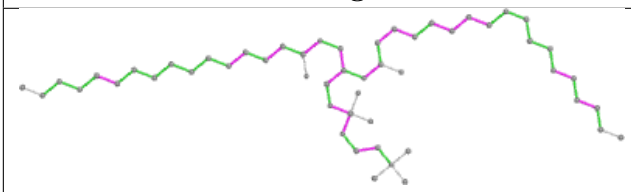
Ligand POV E 1010



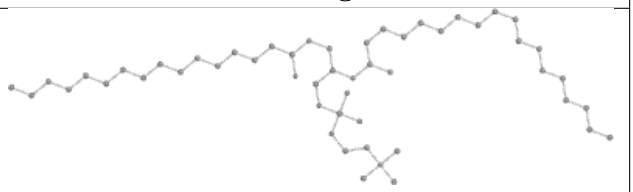
Bond lengths



Bond angles

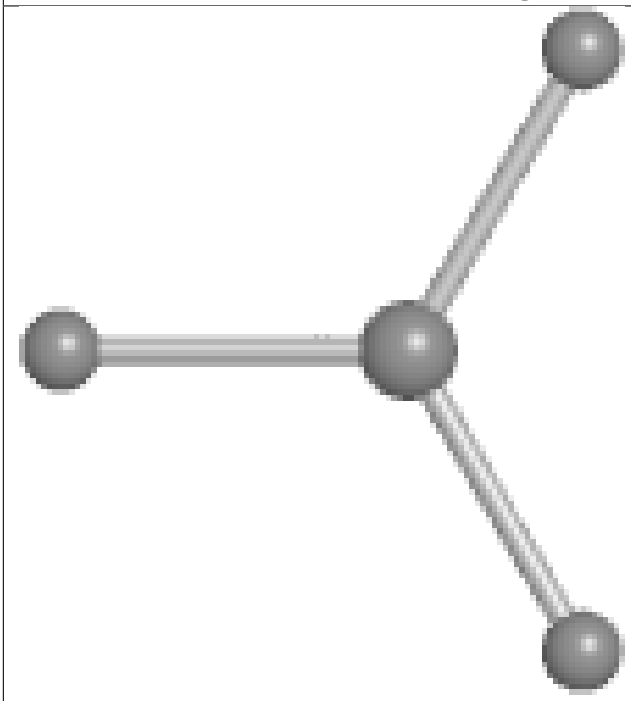


Torsions

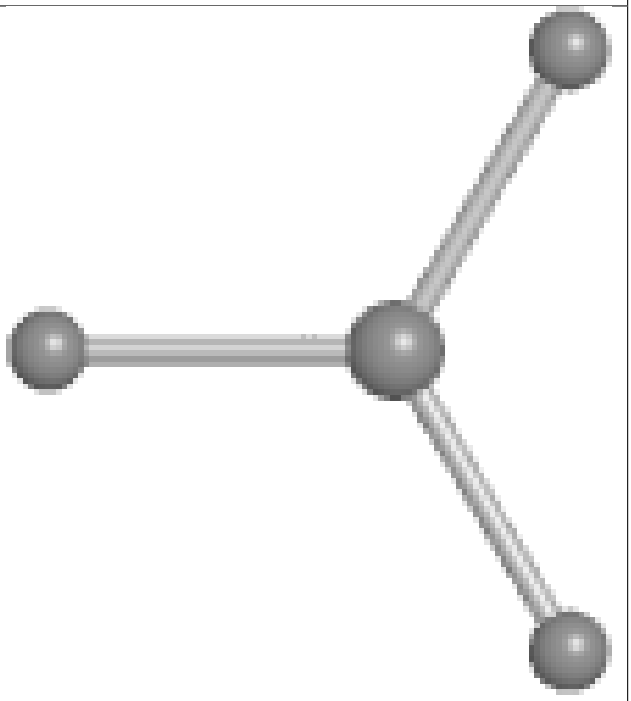


Rings

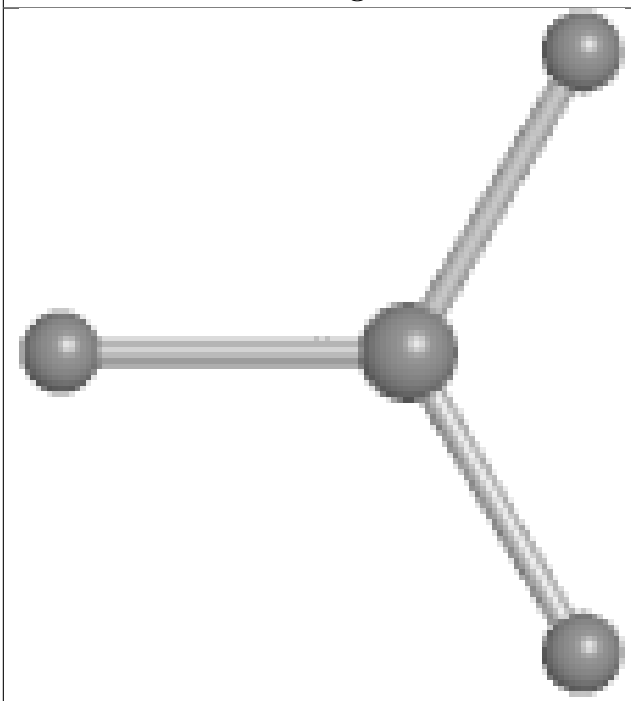
Ligand BEF D 1001



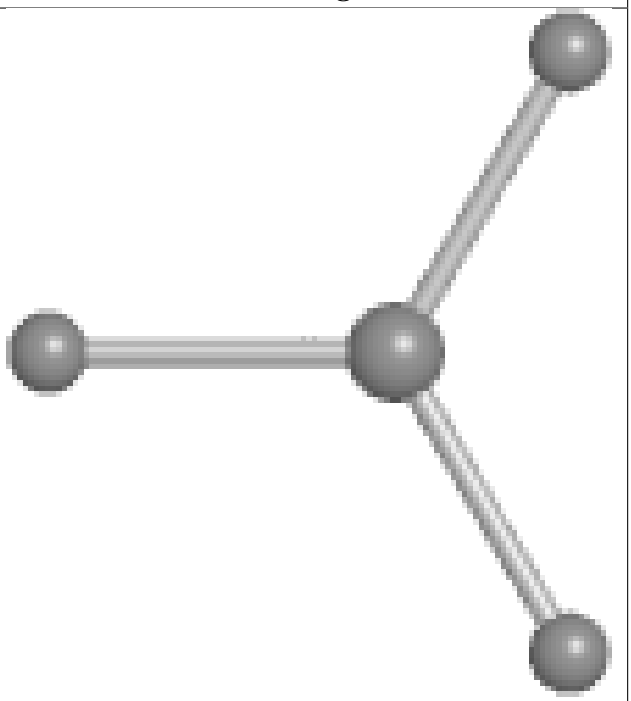
Bond lengths



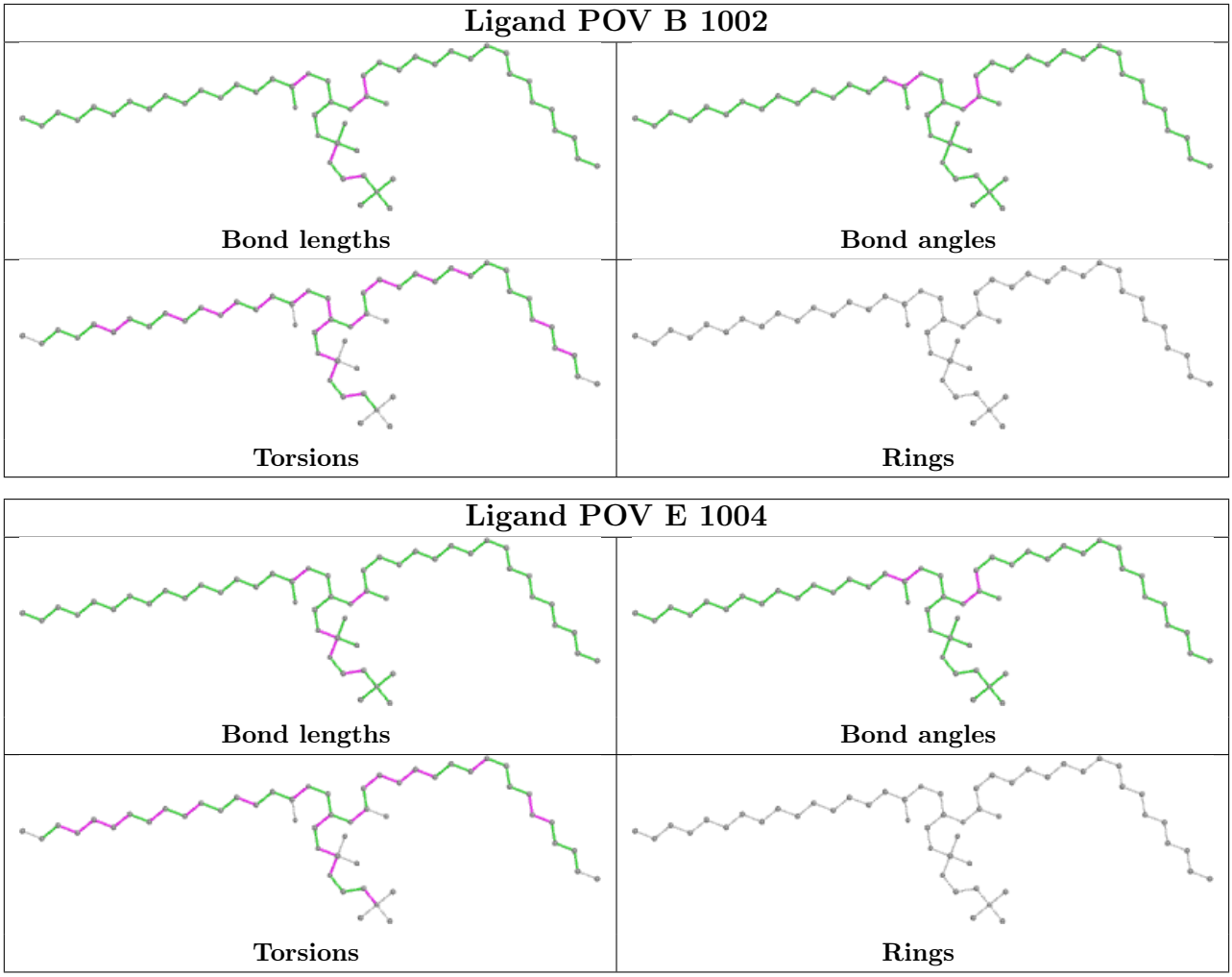
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

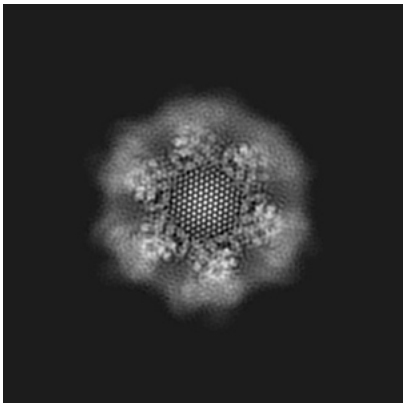
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31988. These allow visual inspection of the internal detail of the map and identification of artifacts.

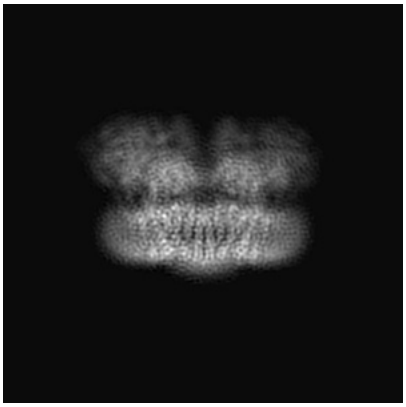
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

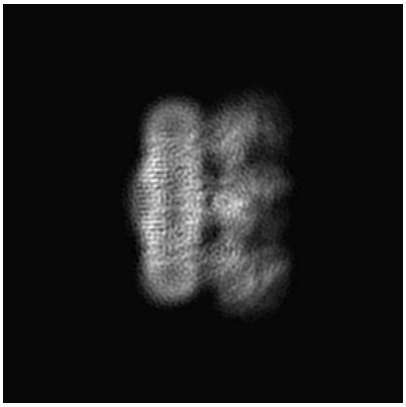
6.1.1 Primary map



X



Y

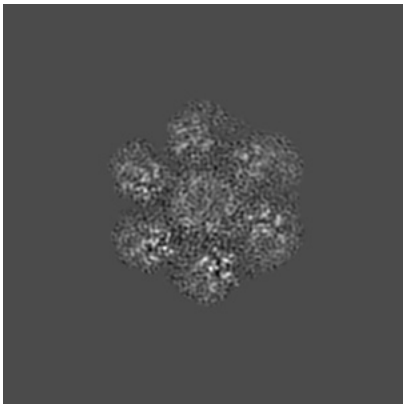


Z

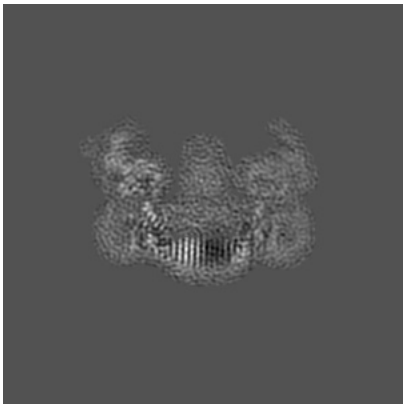
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 150



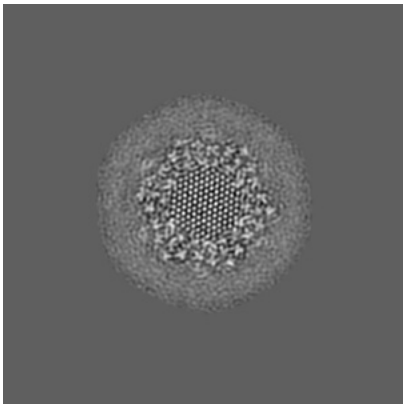
Y Index: 150

Z Index: 150

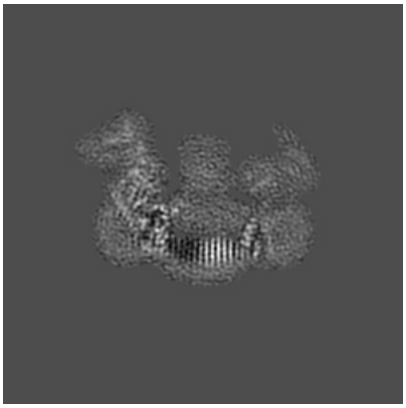
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 116



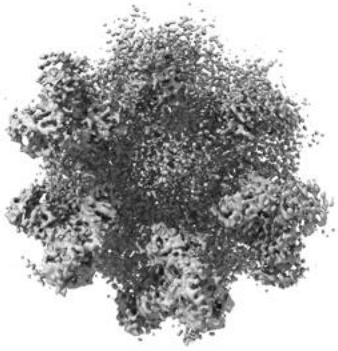
Y Index: 156

Z Index: 121

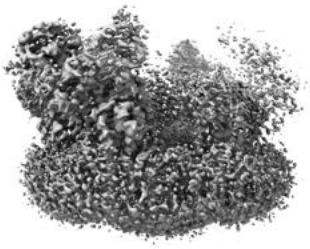
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

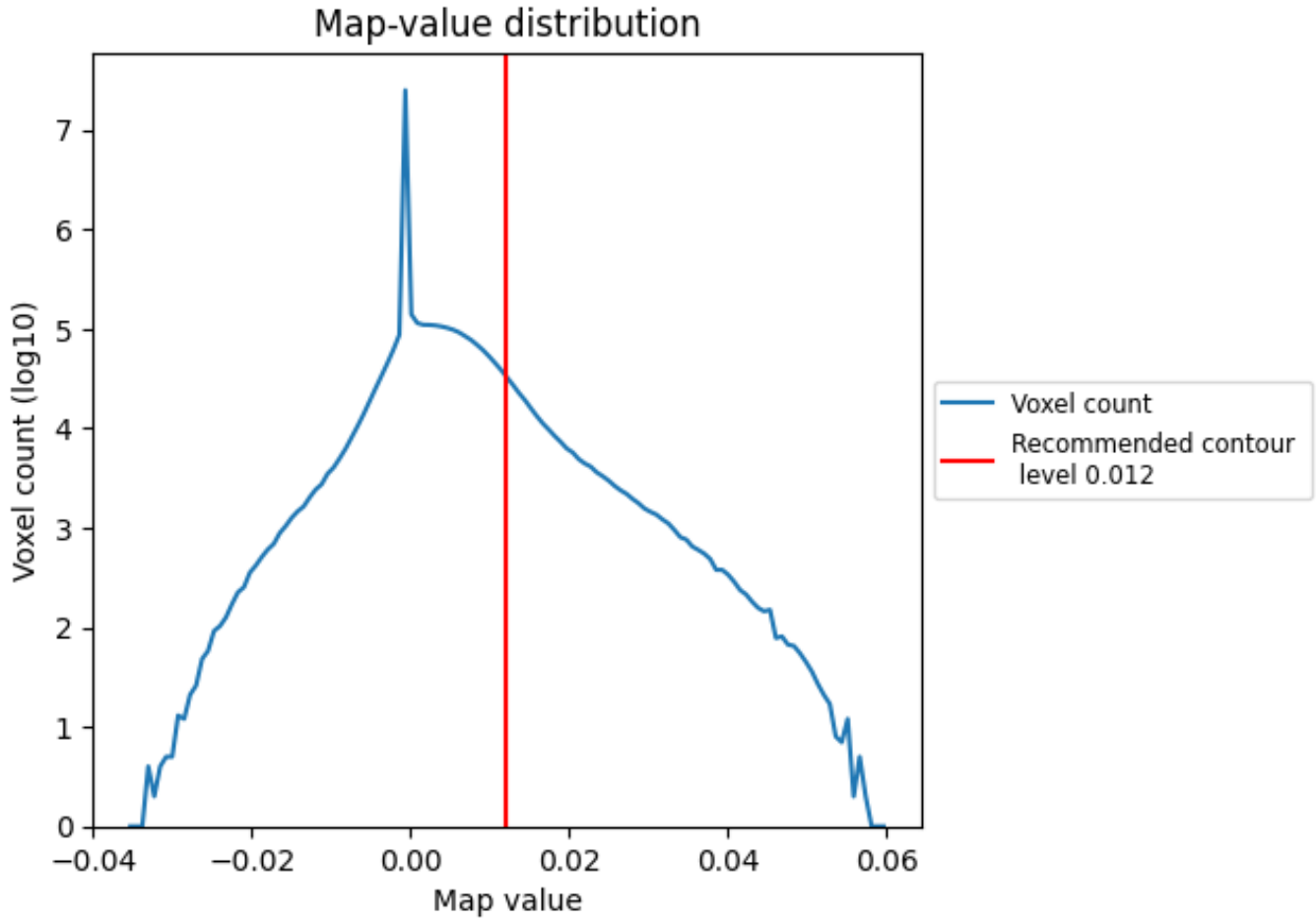
6.5 Mask visualisation (i)

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

7 Map analysis

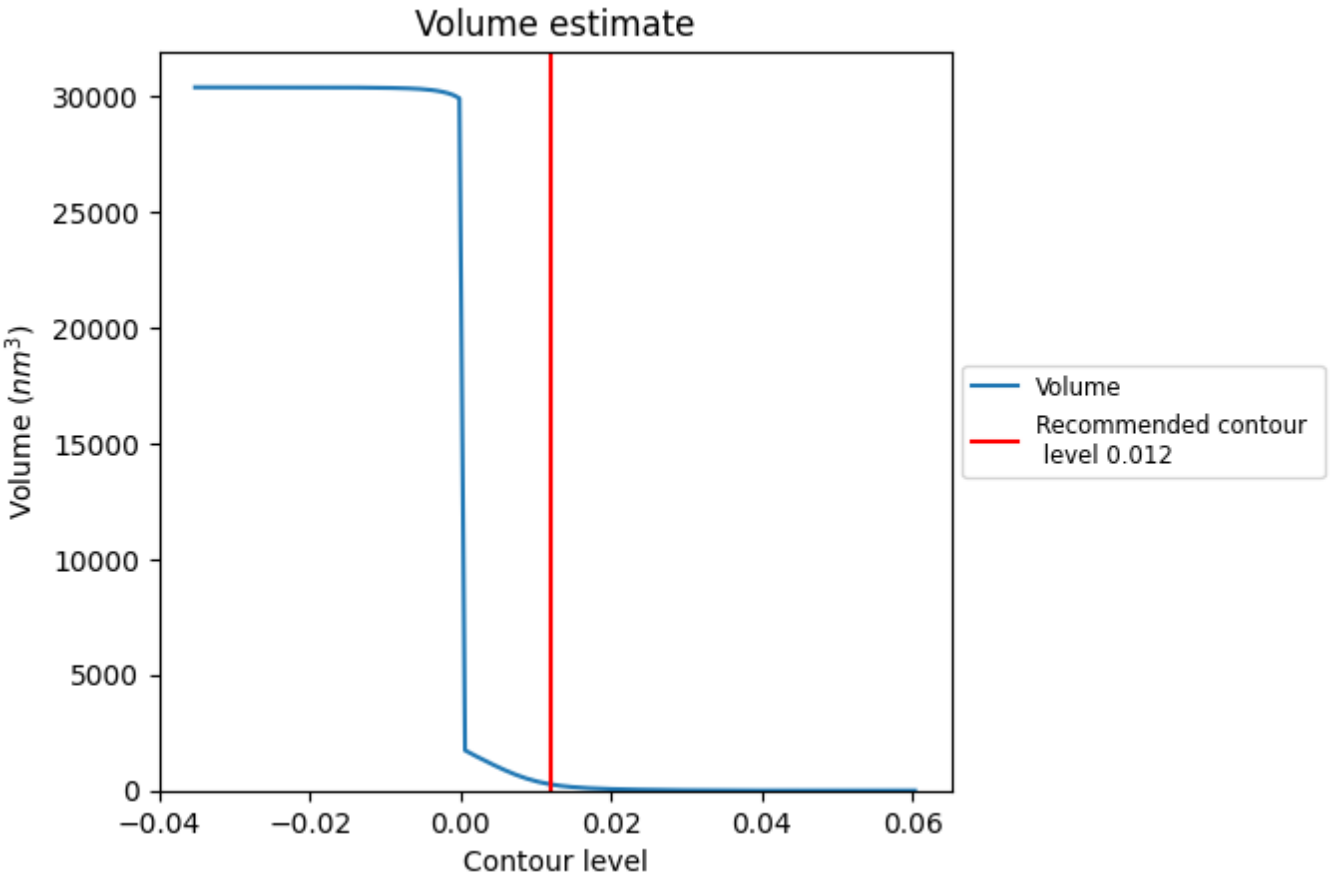
This section contains the results of statistical analysis of the map.

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.

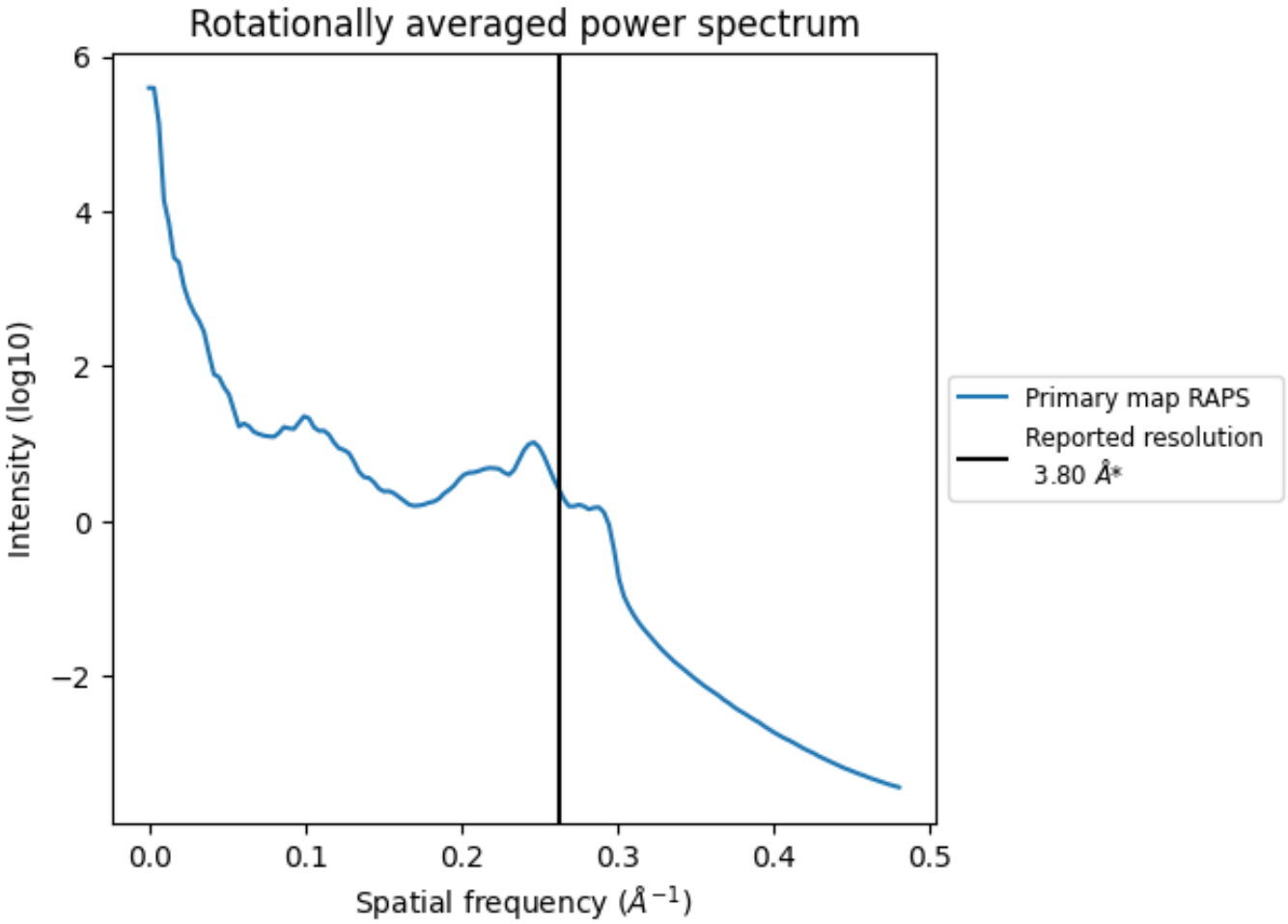
7.2 Volume estimate



The volume at the recommended contour level is 267 nm^3; this corresponds to an approximate mass of 241 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 0.263 Å^{-1}

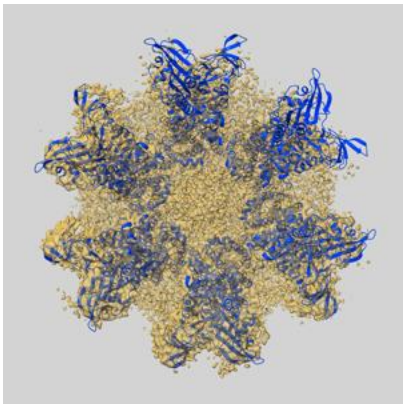
8 Fourier-Shell correlation (i)

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

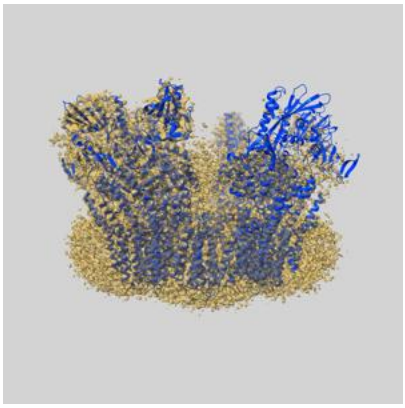
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31988 and PDB model 7VH6. Per-residue inclusion information can be found in section 3 on page 9.

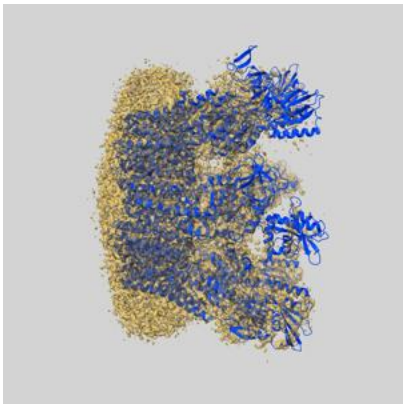
9.1 Map-model overlay



X



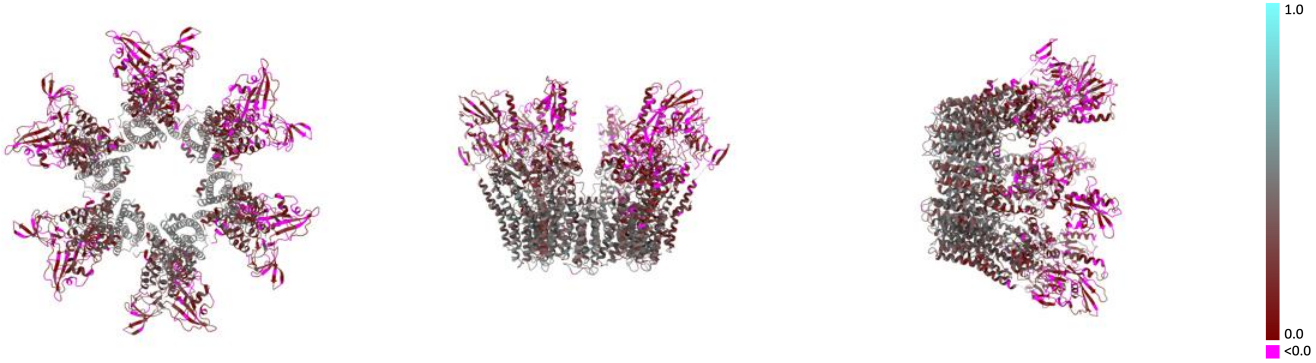
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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.

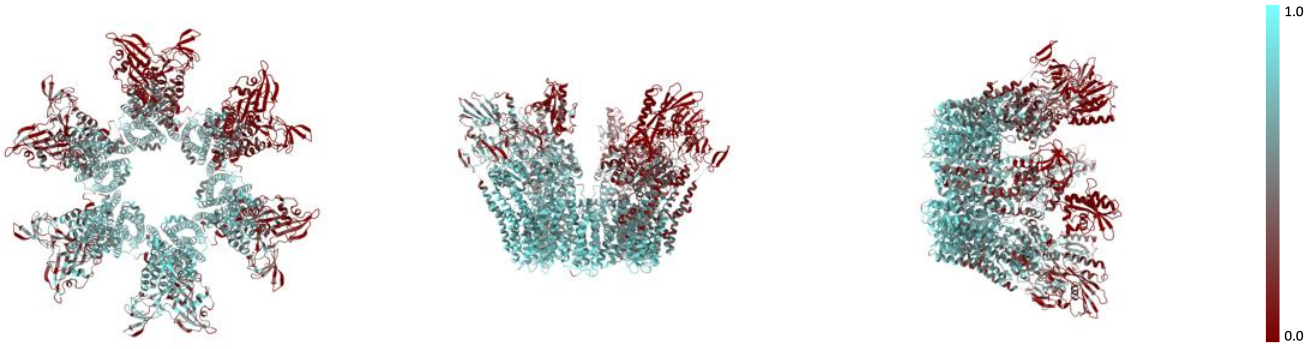
9.2 Q-score mapped to coordinate model



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.

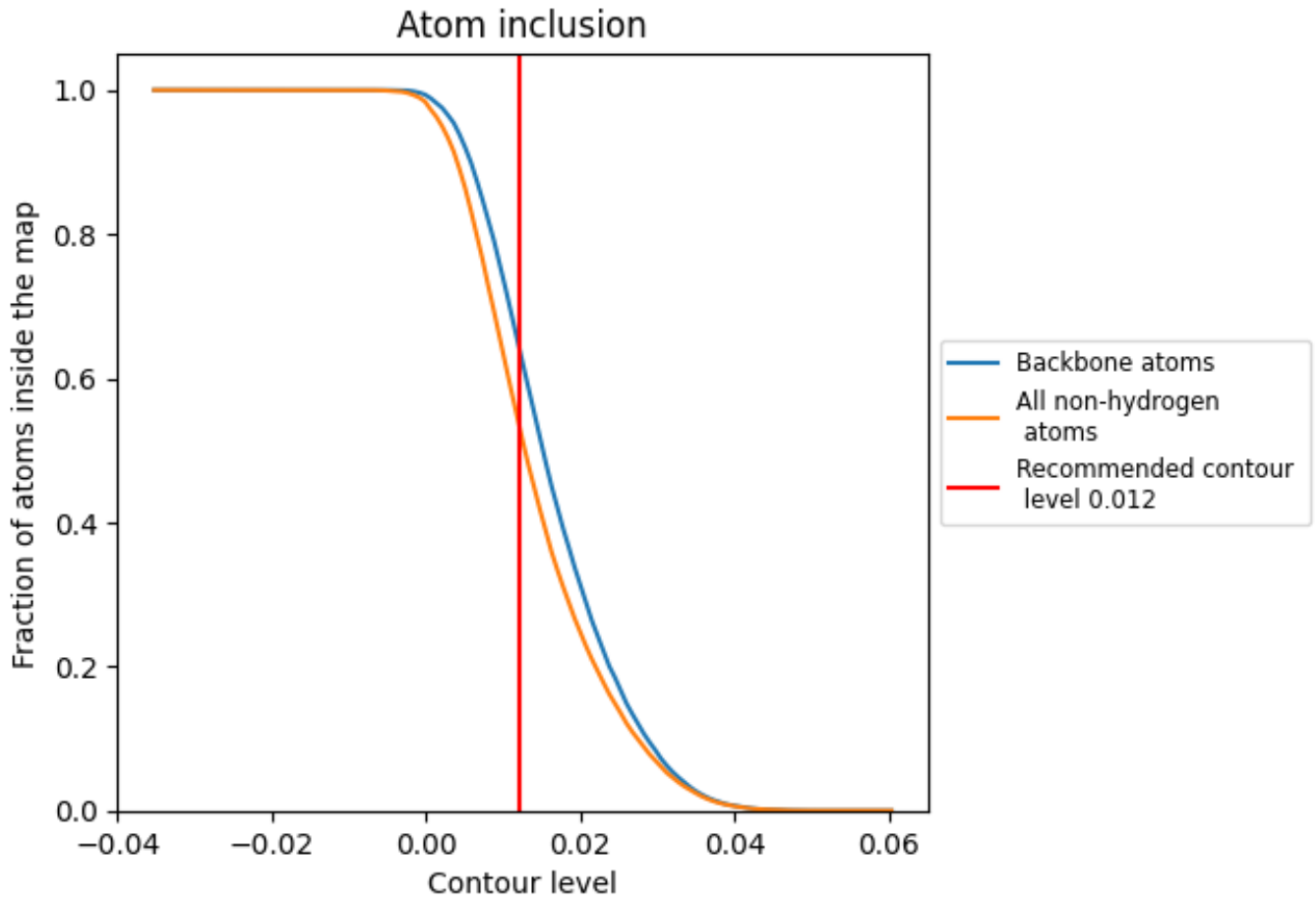
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5378	0.2890
A	0.6943	0.3680
B	0.6392	0.3170
C	0.5325	0.2870
D	0.4088	0.2460
E	0.3855	0.2290
F	0.5651	0.2870