Full wwPDB EM Validation Report ⓘ

Oct 30, 2023 – 05:57 PM EDT

PDB ID	:	8TKG
EMDB ID	:	EMD-41350
Title	:	Human Type 3 IP3 Receptor - Resting State (+IP3/ATP)
Authors	:	Paknejad, N.; Sapuru, V.; Hite, R.K.
Deposited on	:	2023-07-25
Resolution	:	2.50 Å(reported)

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

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

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

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

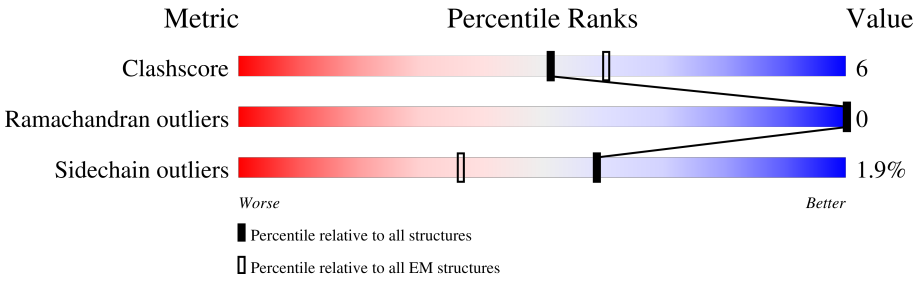
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2671	12% 73% 9% 17%
1	B	2671	13% 73% 9% 17%
1	C	2671	13% 73% 9% 17%
1	D	2671	12% 73% 9% 17%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 146960 atoms, of which 73560 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.

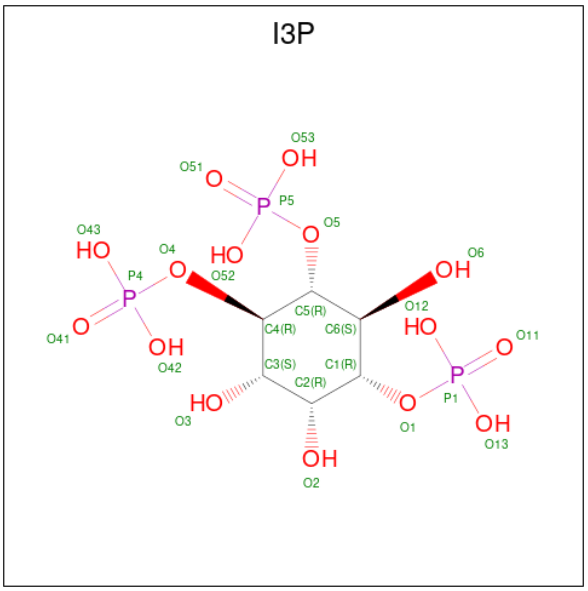
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2210	Total 35839	C 11398	H 17984	N 3057	O 3286	S 114	0	0
1	B	2210	Total 35839	C 11398	H 17984	N 3057	O 3286	S 114	0	0
1	C	2210	Total 35839	C 11398	H 17984	N 3057	O 3286	S 114	0	0
1	D	2210	Total 35839	C 11398	H 17984	N 3057	O 3286	S 114	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Zn 1	0
2	B	1	Total 1	Zn 1	0
2	C	1	Total 1	Zn 1	0
2	D	1	Total 1	Zn 1	0

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).

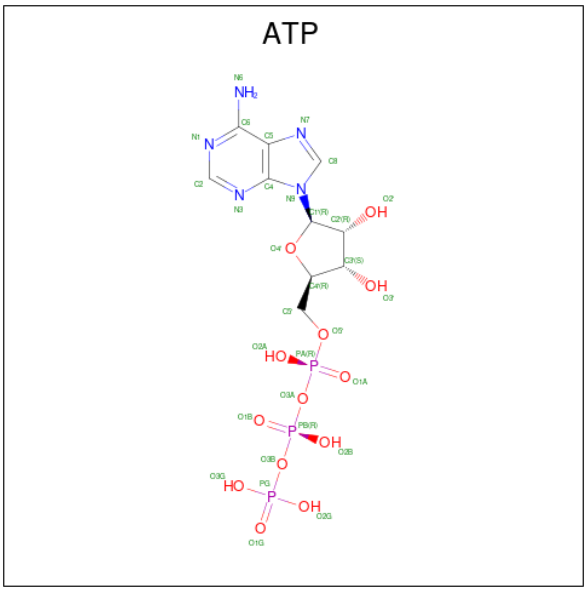


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	

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

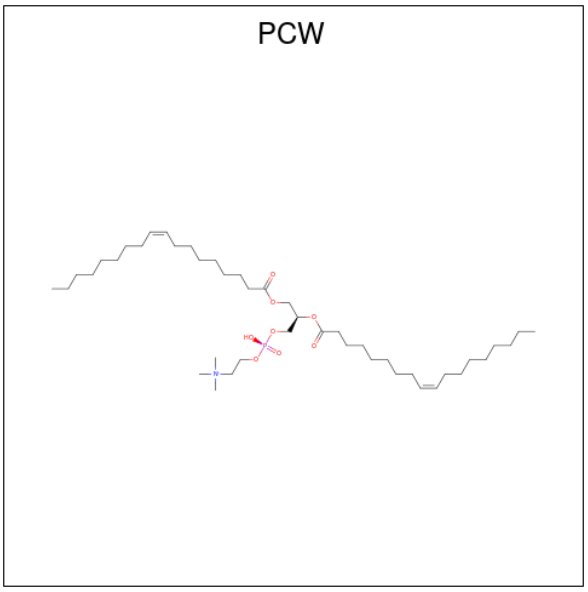
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Ca	0
			2	2	
4	B	2	Total	Ca	0
			2	2	
4	C	2	Total	Ca	0
			2	2	
4	D	2	Total	Ca	0
			2	2	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 6 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	H	N	O	P	0
			101	33	58	1	8	1	
6	A	1	Total	C	H	N	O	P	0
			117	38	69	1	8	1	
6	A	1	Total	C	H	N	O	P	0
			98	31	57	1	8	1	
6	A	1	Total	C	H	N	O	P	0
			112	38	64	1	8	1	
6	A	1	Total	C	H	N	O	P	0
			108	36	62	1	8	1	
6	A	1	Total	C	H	N	O	P	0
			126	41	75	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			126	41	75	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			101	33	58	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			117	38	69	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			98	31	57	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			112	38	64	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			108	36	62	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			126	41	75	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			101	33	58	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			117	38	69	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			98	31	57	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			112	38	64	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			108	36	62	1	8	1	
6	D	1	Total	C	H	N	O	P	0
			112	38	64	1	8	1	
6	D	1	Total	C	H	N	O	P	0
			108	36	62	1	8	1	
6	D	1	Total	C	H	N	O	P	0
			126	41	75	1	8	1	
6	D	1	Total	C	H	N	O	P	0
			101	33	58	1	8	1	

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Mol	Chain	Residues	Atoms						AltConf
6	D	1	Total	C	H	N	O	P	0
			117	38	69	1	8	1	
6	D	1	Total	C	H	N	O	P	0
			98	31	57	1	8	1	

- Molecule 7 is water.

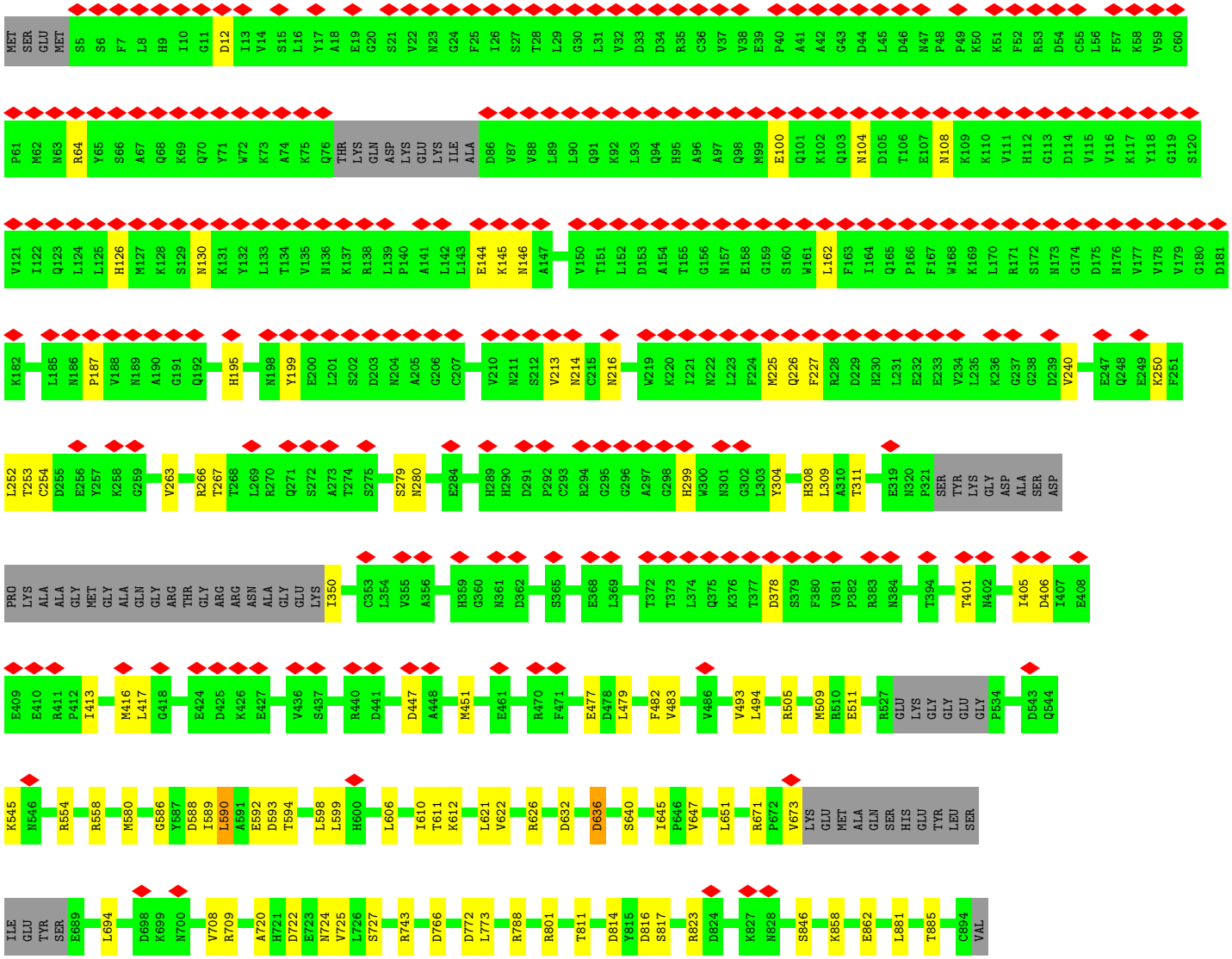
Mol	Chain	Residues	Atoms		AltConf
7	A	160	Total	O	0
			160	160	
7	B	160	Total	O	0
			160	160	
7	C	160	Total	O	0
			160	160	
7	D	160	Total	O	0
			160	160	

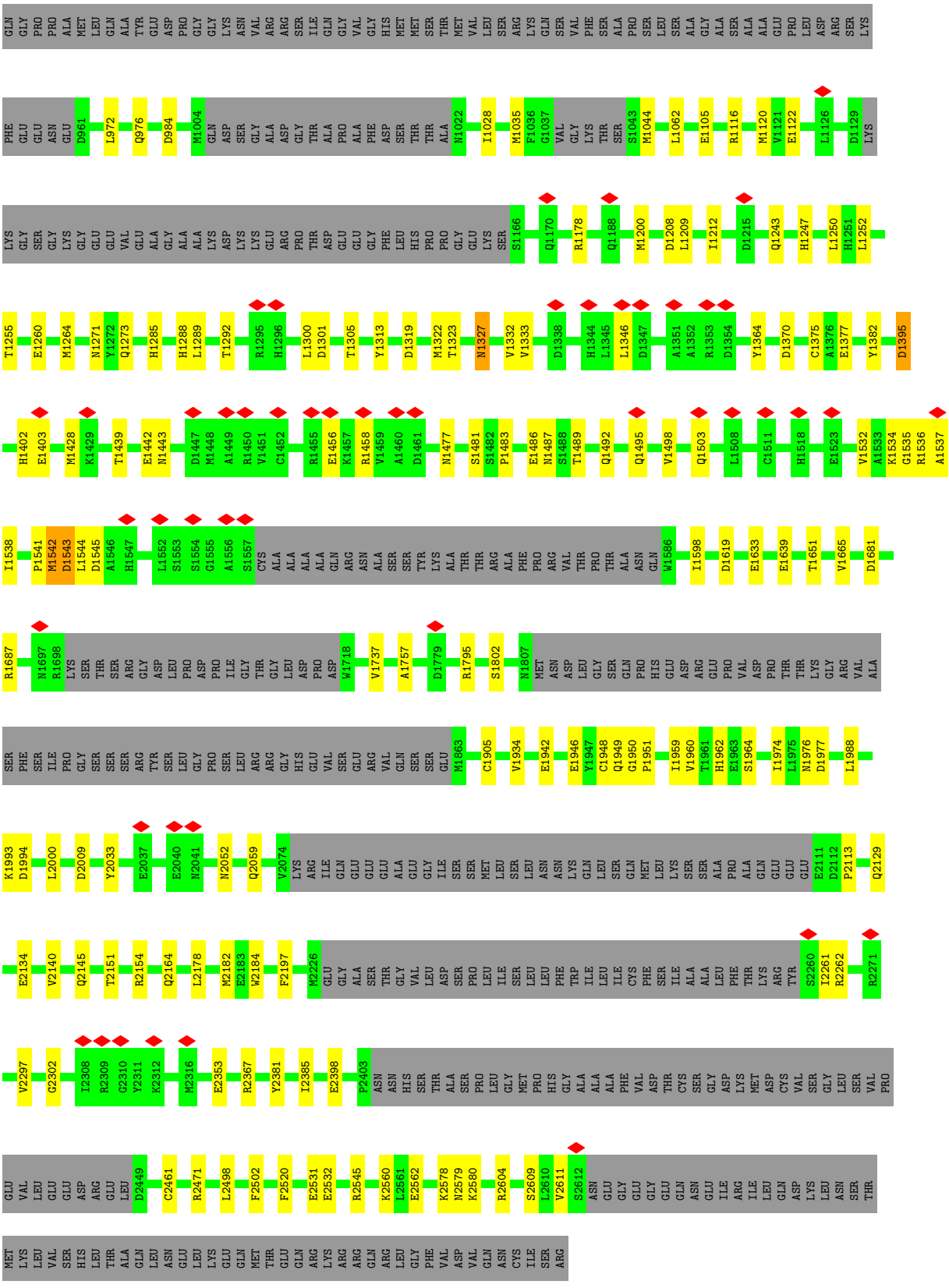
3 Residue-property plots (i)

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: Inositol 1,4,5-trisphosphate receptor type 3

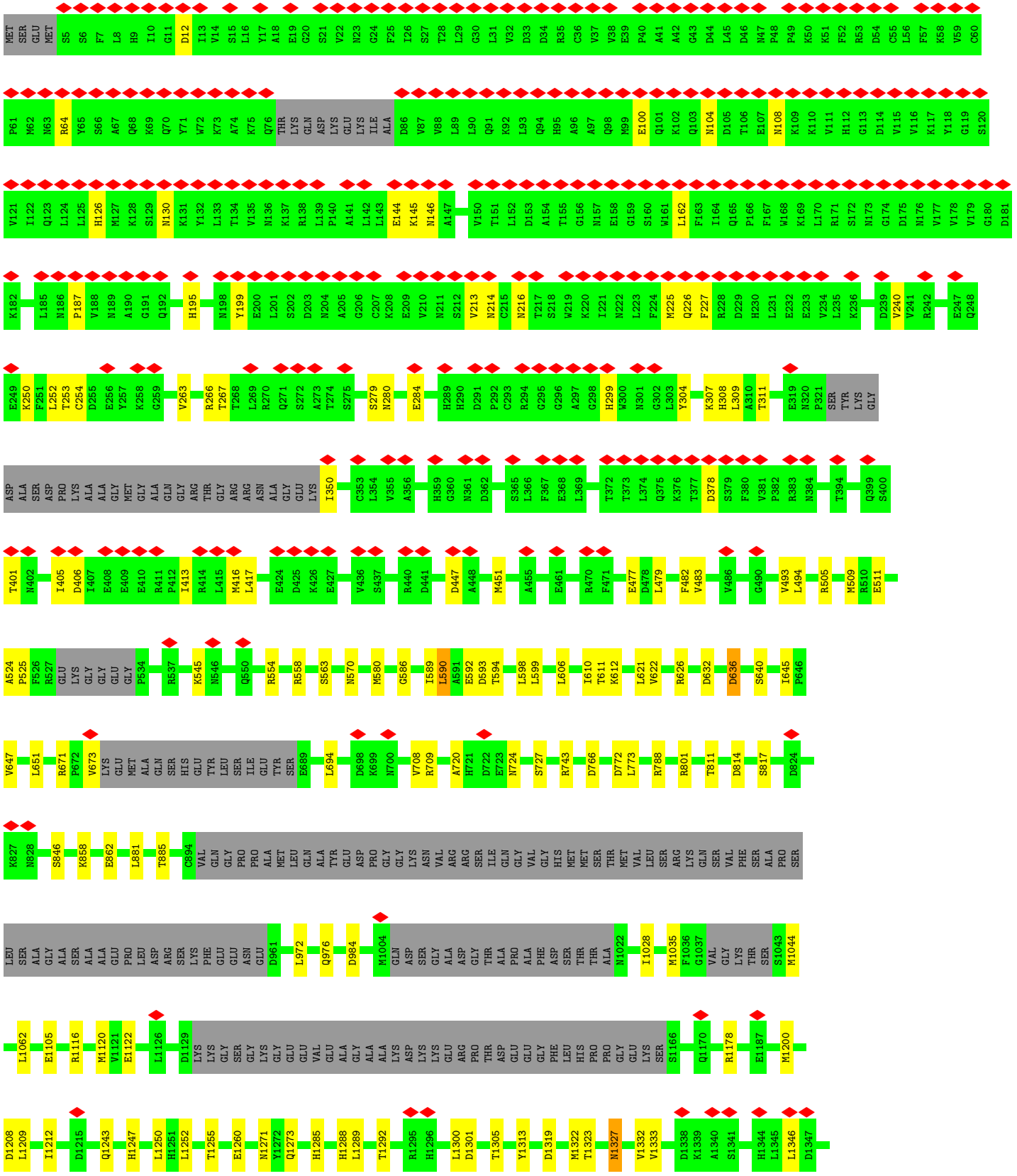
Chain A:

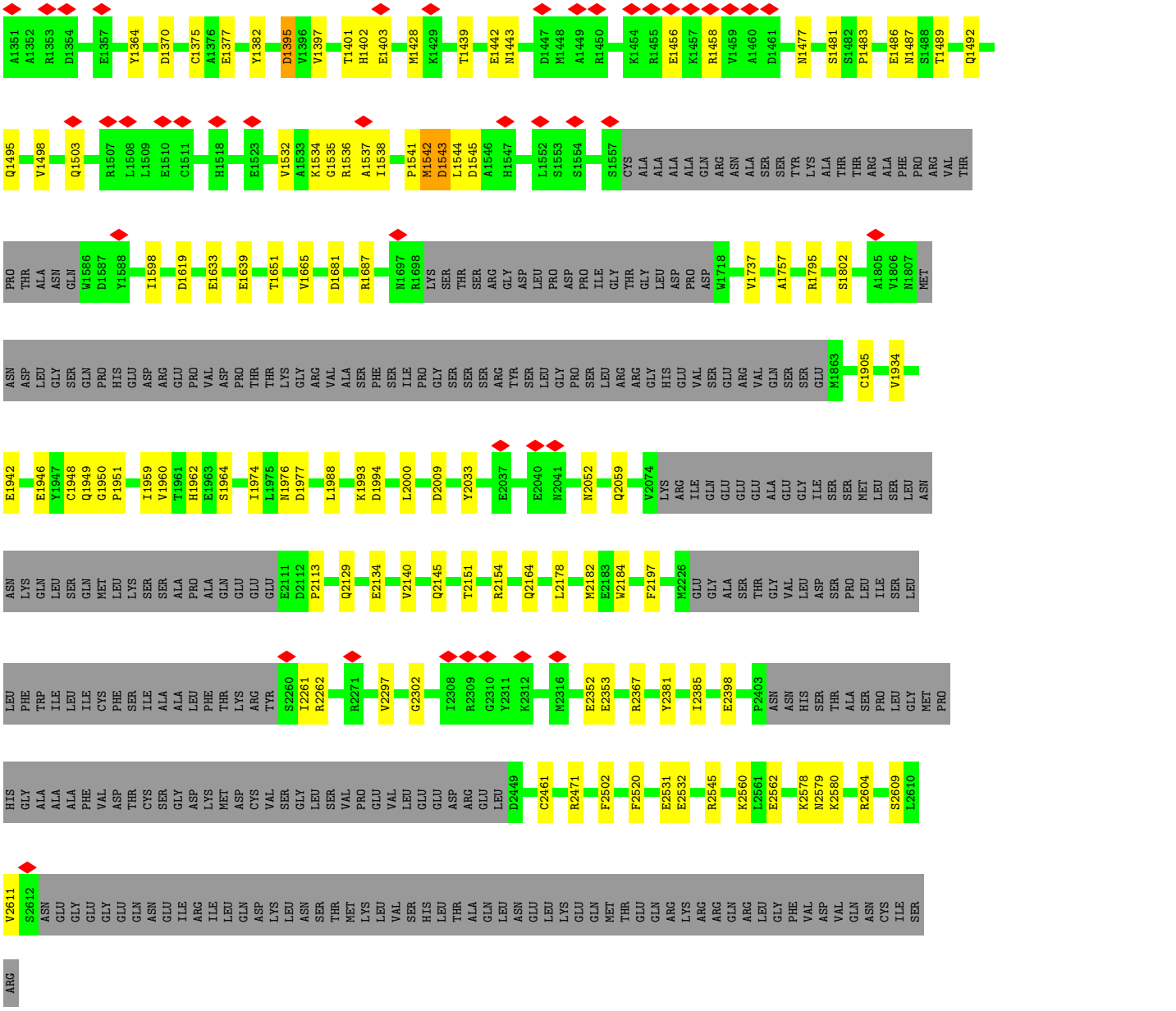




• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

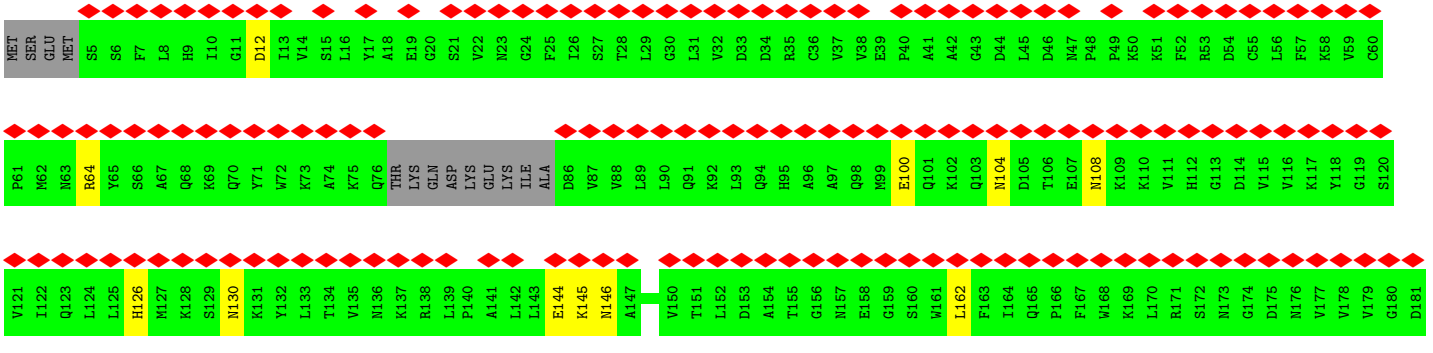
Chain B:

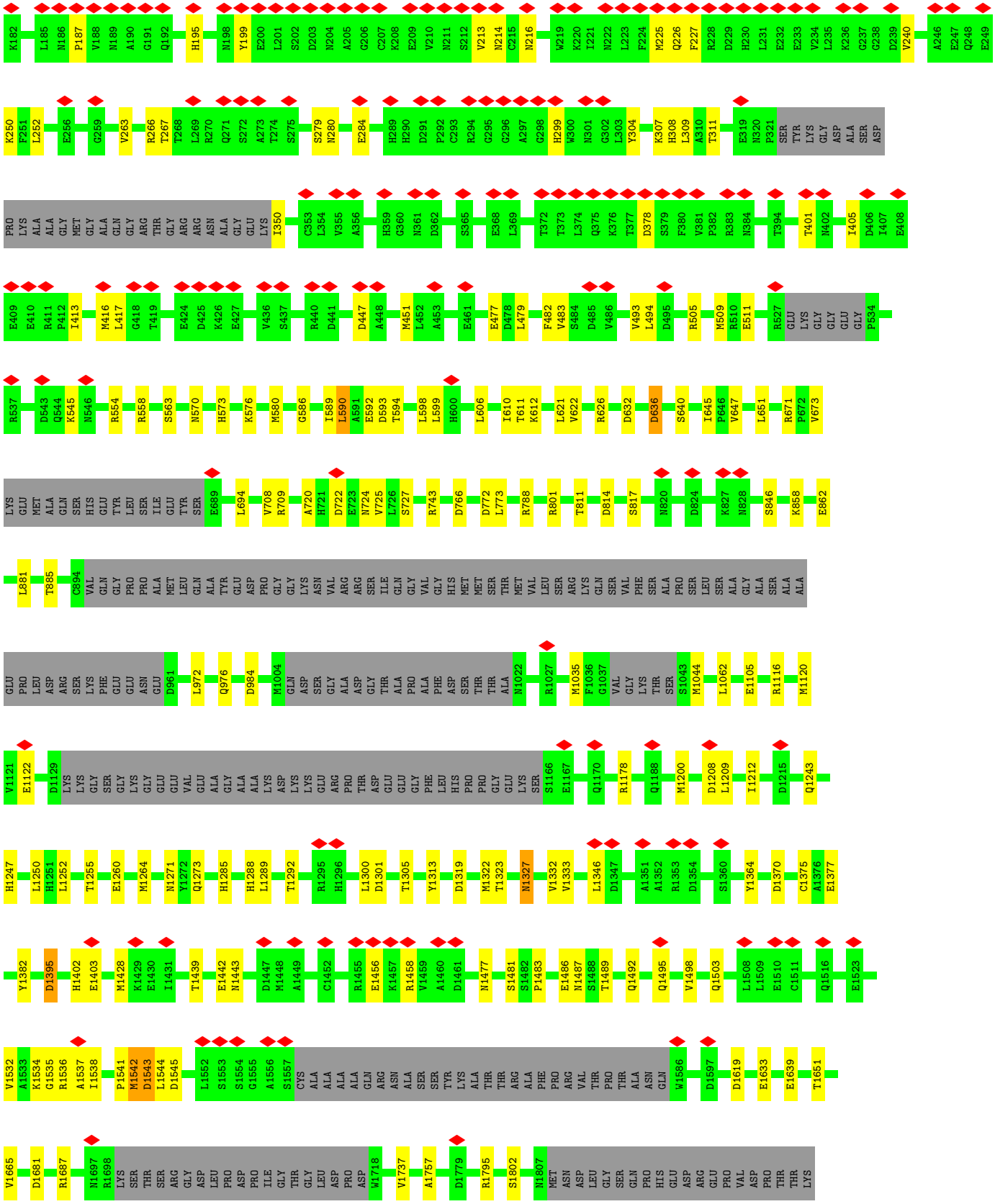

MET SER GLU MET S5 S6 F7 L8 H9 I10 G11 D12 I13 V14 S15 L16 Y17 A18 E19 G20 S21 V22 N23 G24 F25 I26 S27 T28 L29 G30 L31 V32 D33 D34 R35 C36 V37 V38 E39 P40 A41 A42 G43 D44 L45 D46 N47 P48 P49 K50 K51 F52 R53 D54 C55 L56 F57 K58 V59 C60
P61 M62 M63 R64 Y65 S66 A67 Q68 K69 Q70 Y71 W72 K73 A74 K75 Q76 THR LYS GLN ASP LYS GLU LYS ILE ALA D86 V87 V88 L89 L90 Q91 K92 L93 Q94 H95 A96 A97 Q98 M99 E100 Q101 K102 Q103 N104 D105 T106 E107 N108 K109 K110 V111 H112 G113 D114 V115 V116 K117 Y118 G119 S120
V121 I122 Q123 L124 L125 H126 M127 K128 S129 N130 K131 Y132 L133 T134 V135 N136 K137 R138 L139 P140 A141 L142 L143 E144 K145 N146 A147 V150 T151 L152 D153 A154 T155 G156 N157 E158 G159 S160 W161 L162 F163 I164 Q165 P166 F167 W168 K169 L170 R171 S172 N173 G174 D175 N176 V177 V178 V179 G180 D181
K182 L185 N186 P187 V188 N189 A190 G191 Q192 H195 N198 Y199 E200 L201 S202 D203 N204 A205 G206 C207 K208 E209 V210 N211 S212 V213 N214 C215 N216 T217 S218 W219 K220 I221 N222 L223 F224 M225 Q226 F227 R228 D229 H230 L231 E232 E233 V234 L235 K236 D239 V240 V241 R242 E247 Q248
E249 K250 F251 L252 T253 C254 D255 E256 Y257 K258 G259 V263 R266 T267 T268 L269 R270 Q271 S272 A273 T274 S275 S279 N280 E284 H289 H290 D291 P292 C293 R294 G295 G296 A297 G298 H299 W300 N301 G302 L303 Y304 K307 H308 L309 A310 T311 E319 N320 P321 SER TYR LYS GLY
ASP ALA SER ASP PRO LYS ALA ALA GLY MET GLY GLY ALA GLN GLY ARG THR GLY ARG ARG ASN ALA GLY GLU LYS I350 C353 L354 V355 A356 H359 G360 N361 D362 S365 L366 F367 E368 L369 T372 T373 L374 Q375 K376 T377 D378 S379 F380 V381 P382 R383 N384 T394 Q399 S400
T401 N402 I405 D406 I407 E408 E409 E410 R411 P412 I413 R414 L415 M416 L417 E424 D425 K426 E427 V436 S437 R440 D441 D447 A448 M451 A455 E461 R470 F471 E477 D478 L479 F482 V483 V486 G490 V493 L494 R505 M509 R510 E511
A524 P525 F526 R527 GLU LYS GLY GLY GLU GLY P534 R537 K545 N546 Q550 R554 R558 S563 N570 M580 G586 I589 L590 A591 E592 D593 T594 L598 L599 L606 I610 T611 K612 L621 V622 R626 D632 D636 S640 I645 P646
V647 L651 R671 P672 V673 LYS GLU MET ALA GLN SER HIS GLU TYR LEU SER ILE GLU TYR SER E689 L694 D698 K699 N700 V708 R709 A720 H721 D722 E723 W724 S727 R743 D766 D772 L773 R788 R801 T811 D814 S817 D824
K827 N828 S846 K858 E862 L881 T885 C894 VAL GLN GLY PRO PRO ALA MET LEU GLN ALA TYR GLU ASP PRO GLY GLY LYS ASN VAL ARG ARG SER ILE GLN GLY VAL GLY HIS MET MET SER THR MET VAL LEU SER ARG LYS GLN SER VAL PHE SER ALA PRO SER
LEU SER ALA GLY ALA SER ALA ALA GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961 L972 Q976 D984 M1004 GLN ASP SER GLY ALA ASP GLY THR ALA PRO ALA PHE ASP SER THR THR ALA N1022 I1028 M1035 F1036 G1037 VAL GLY LYS THR SER S1043 M1044
L1062 E1105 R1116 M1120 V1121 E1122 L1126 D1129 LYS LYS GLY SER GLY LYS GLY GLU GLU VAL GLU ALA GLY ALA ALA LYS ASP LYS LYS LYS GLU ARG PRO THR ASP GLU GLU GLU GLY PHE LEU HIS PRO PRO GLY GLU LYS SER S1166 Q1170 R1178 E1187 M1200
D1208 L1209 I1212 D1215 Q1243 H1247 L1250 H1251 L1252 T1255 E1260 N1271 Y1272 Q1273 H1285 H1288 L1289 T1292 R1295 H1296 L1300 D1301 T1305 Y1313 D1319 M1322 T1323 N1327 V1332 V1333 D1338 K1339 A1340 S1341 H1344 L1345 L1346 D1347

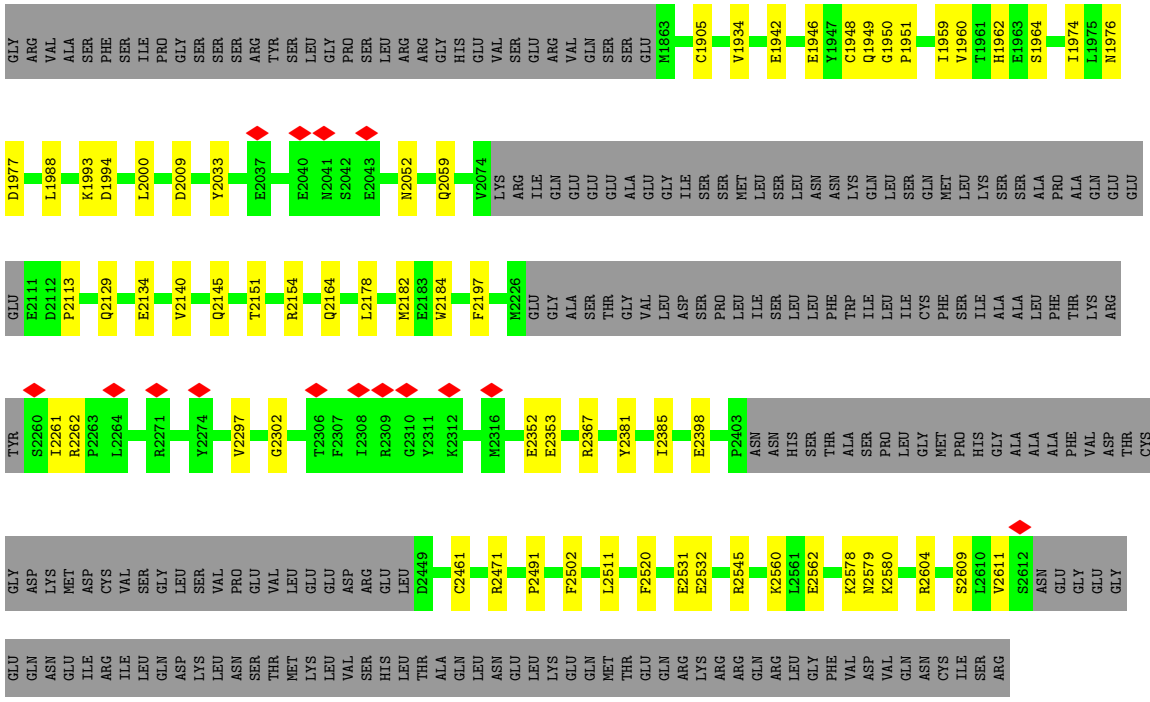


• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

Chain C:

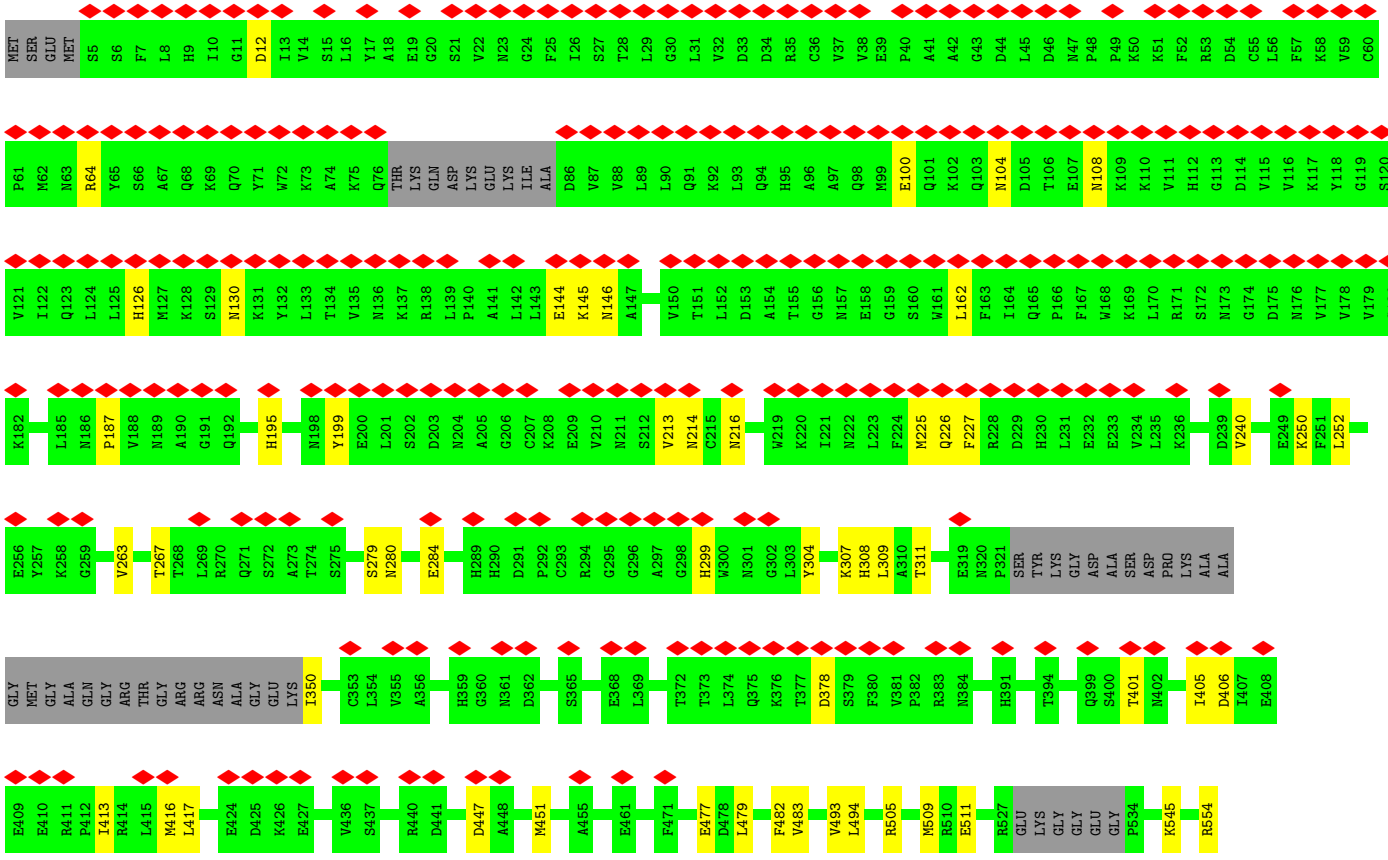


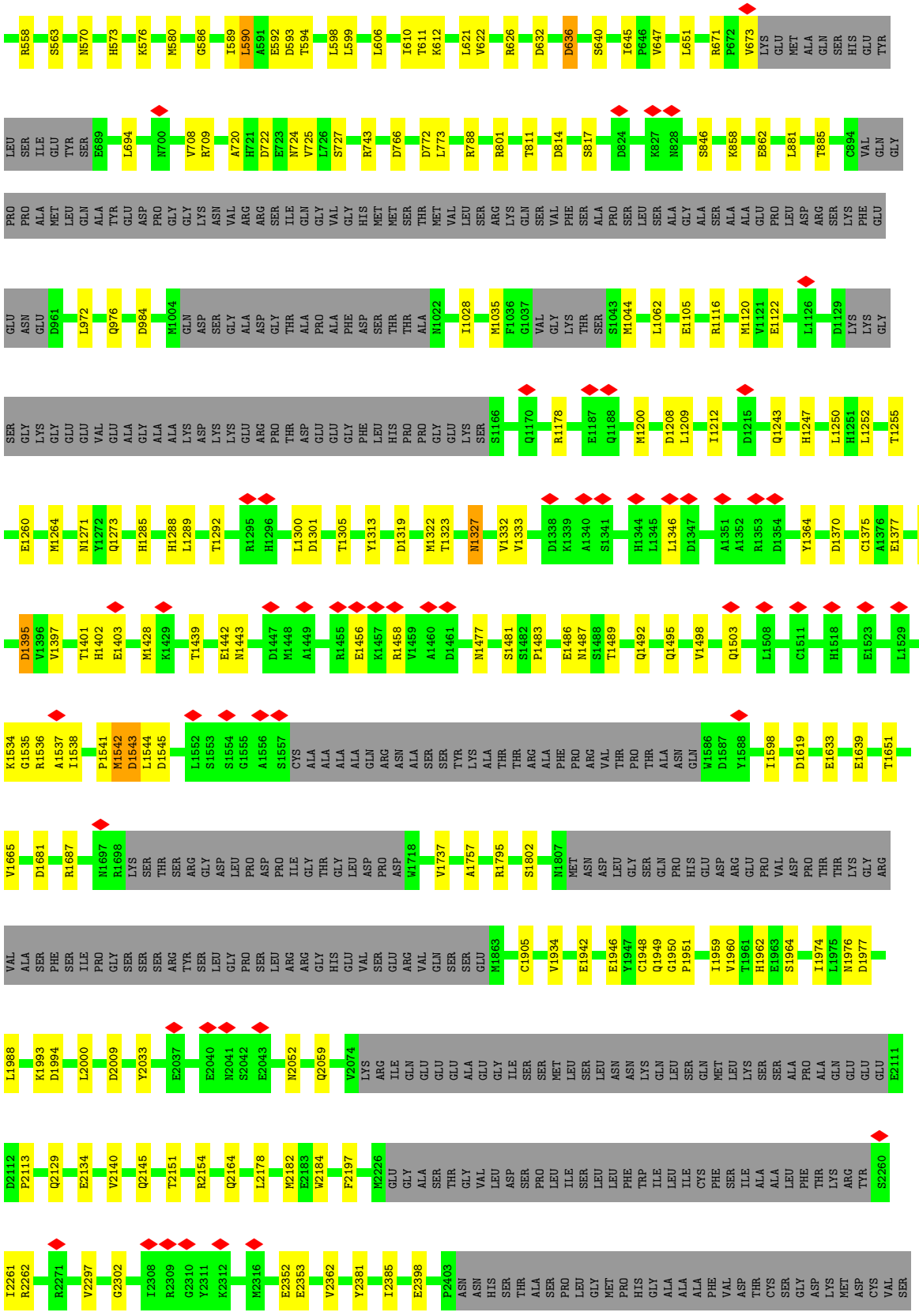

K182 L185 N186 P187 V188 N189 A190 G191 Q192 H195 N198 Y199 E200 L201 S202 D203 N204 A205 G206 C207 K208 E209 V210 N211 S212 V213 N214 C215 N216 W219 K220 I221 N222 L223 F224 M225 Q226 F227 R228 D229 H230 L231 E232 E233 V234 L235 K236 G237 G238 D239 V240 A246 E247 Q248 E249
K250 F251 L252 E256 G259 V263 R266 T267 T268 L269 R270 Q271 S272 A273 T274 S275 S279 N280 E284 H289 H290 D291 P292 C293 R294 C295 G296 A297 G298 H299 W300 N301 G302 L303 Y304 K307 H308 L309 A310 T311 E319 N320 P321 SER TYR LYS GLY ASP ALA SER ASP
PRO LYS ALA ALA GLY MET GLY ALA GLN GLY ARG THR GLY ARG ARG ASN ALA GLY GLU LYS I350 C353 L354 V355 A356 H359 G360 N361 D362 S365 E368 L369 T372 T373 L374 Q375 K376 T377 D378 S379 F380 V381 P382 R383 N384 T394 T401 N402 I405 D406 I407 E408
E409 E410 R411 P412 I413 M416 L417 G418 T419 E424 D425 K426 E427 V436 S437 R440 D441 D447 A448 M451 L452 A453 E461 E477 D478 L479 F482 V483 S484 D485 V486 V493 L494 D495 R505 M509 R510 E511 R527 GLU LYS GLY GLY GLU GLY P534
R537 D543 Q544 K545 N546 R554 R558 S563 N570 H573 K576 M580 G586 I589 L590 A591 E592 D593 T594 L598 L599 H600 L606 I610 T611 K612 L621 V622 R626 D632 D636 S640 I645 P646 V647 L651 R671 P672 V673
LYS GLU MET ALA GLN SER HIS GLU TYR LEU SER ILE GLU TYR SER E689 L694 V708 R709 A720 H721 D722 E723 N724 V725 L726 S727 R743 D766 D772 L773 R788 R801 T811 D814 S817 N820 D824 K827 N828 S846 K858 E862
L881 T885 C894 VAL GLN GLY PRO PRO ALA MET LEU GLN ALA TYR GLU ASP PRO GLY GLY LYS ASN VAL ARG ARG SER ILE GLN GLY VAL GLY HIS MET MET SER THR MET VAL LEU SER ARG LYS GLN SER VAL PHE SER ALA PRO SER LEU SER ALA GLY ALA SER ALA ALA
GLU PRO LEU ASP ARG SER LYS PHE GLU GLU ASN GLU D961 L972 Q976 D984 M1004 GLN ASP SER GLY ALA ASP GLY THR ALA PRO ALA PHE ASP SER THR THR ALA N1022 R1027 M1035 F1036 G1037 VAL GLY LYS THR SER S1043 M1044 L1062 E1105 R1116 M1120
V1121 E1122 D1129 LYS LYS GLY SER GLY LYS GLY GLU GLU VAL GLU ALA GLY ALA ALA LYS ASP LYS LYS GLU ARG PRO THR ASP GLU GLU GLY PHE LEU HIS PRO PRO GLY GLU LYS SER S1166 E1167 Q1170 R1178 Q1188 M1200 D1208 L1209 I1212 D1215 Q1243
H1247 L1250 H1251 L1252 T1255 E1260 M1264 N1271 Y1272 Q1273 H1285 H1288 L1289 T1292 R1295 H1296 L1300 D1301 T1305 Y1313 D1319 M1322 T1323 N1327 V1332 V1333 L1346 D1347 A1351 A1352 R1353 D1354 S1360 Y1364 D1370 C1375 A1376 E1377
Y1382 D1396 H1402 E1403 M1428 K1429 E1430 I1431 T1439 E1442 N1443 D1447 M1448 A1449 C1452 R1455 E1456 K1457 R1458 V1459 A1460 D1461 N1477 S1481 S1482 P1483 E1486 N1487 S1488 T1489 Q1492 Q1495 V1498 Q1503 L1508 L1509 E1510 C1511 Q1516 E1523
V1532 A1533 K1534 G1535 R1536 A1537 I1538 P1541 M1542 D1543 L1544 D1545 L1552 S1553 S1554 G1555 A1556 S1557 CYS ALA ALA ALA ALA GLN ARG ASN ALA SER SER TYR LYS ALA THR THR ARG ALA PHE PRO ARG VAL THR PRO THR ALA ASN GLN W1586 D1597 D1619 E1633 E1639 T1651
V1665 D1681 R1687 N1697 R1698 LYS SER THR SER ARG GLY ASP LEU PRO ASP PRO ILE GLY THR GLY LEU ASP PRO ASP W1718 V1737 A1757 D1779 R1795 S1802 N1807 MET ASN ASP LEU GLY SER GLN PRO HIS GLU ASP ARG GLU PRO VAL ASP PRO THR THR LYS

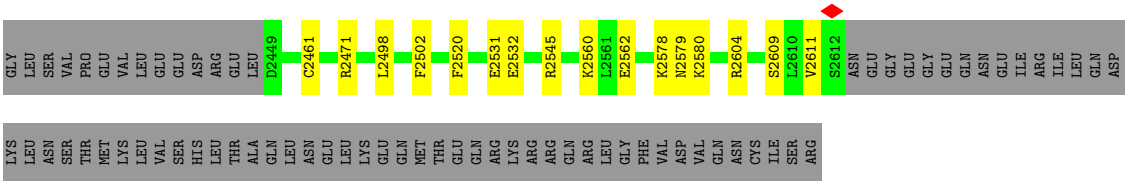


• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

Chain D:






GLY LEU SER VAL PRO GLU VAL LEU GLU GLU ASP ARG GLU LEU D2449 C2461 R2471 L2498 F2502 F2520 E2531 E2532 R2545 K2560 L2561 E2562 K2578 N2579 K2580 R2604 S2609 L2610 V2611 S2612 ASN GLU GLY GLU GLY GLU GLN ASN GLU ILE ARG ILE LEU GLN ASP
LYS LEU ASN SER THR MET LYS LEU VAL SER HIS LEU THR ALA GLN LEU ASN GLU LEU LYS GLU GLN MET THR GLU GLN ARG LYS ARG ARG GLN ARG LEU GLY PHE VAL ASP VAL GLN ASN CYS ILE SER ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3668312	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	66	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4300	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	113.116	Depositor
Minimum map value	-57.161	Depositor
Average map value	0.146	Depositor
Map value standard deviation	1.901	Depositor
Recommended contour level	6.0	Depositor
Map size (Å)	422.68802, 422.68802, 422.68802	wwPDB
Map dimensions	672, 672, 672	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.629, 0.629, 0.629	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, I3P, ZN, ATP, PCW

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	0.24	0/18187	0.45	0/24569
1	B	0.24	0/18187	0.45	0/24569
1	C	0.24	0/18187	0.45	0/24569
1	D	0.24	0/18187	0.45	0/24569
All	All	0.24	0/72748	0.45	0/98276

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17855	17984	17979	278	0
1	B	17855	17984	17978	280	0
1	C	17855	17984	17978	280	0
1	D	17855	17984	17978	280	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	9	9	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	9	9	1	0
3	C	24	9	9	1	0
3	D	24	9	9	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	31	12	12	2	0
5	B	31	12	12	2	0
5	C	31	12	12	2	0
5	D	31	12	12	2	0
6	A	277	385	388	5	0
6	B	277	385	388	5	0
6	C	277	385	388	7	0
6	D	277	385	388	4	0
7	A	160	0	0	14	0
7	B	160	0	0	14	0
7	C	160	0	0	14	0
7	D	160	0	0	14	0
All	All	73400	73560	73549	848	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 6.

All (848) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1483:PRO:HA	1:D:214:ASN:ND2	1.17	1.48
1:A:1535:GLY:C	1:D:144:GLU:HG3	1.33	1.48
1:B:144:GLU:HG3	1:C:1535:GLY:C	1.32	1.44
1:C:214:ASN:ND2	1:D:1483:PRO:HA	1.18	1.43
1:A:144:GLU:HG3	1:B:1535:GLY:C	1.34	1.43
1:A:144:GLU:CG	1:B:1535:GLY:O	1.67	1.43
1:B:144:GLU:CG	1:C:1535:GLY:O	1.67	1.42
1:A:199:TYR:CZ	1:B:1537:ALA:N	1.74	1.42
1:B:214:ASN:ND2	1:C:1483:PRO:HA	1.23	1.42
1:A:214:ASN:ND2	1:B:1483:PRO:HA	1.22	1.40
1:C:144:GLU:HG3	1:D:1535:GLY:C	1.38	1.38
1:B:199:TYR:CZ	1:C:1537:ALA:N	1.75	1.38
1:A:1535:GLY:O	1:D:144:GLU:CG	1.68	1.38
1:C:199:TYR:CZ	1:D:1537:ALA:N	1.84	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:GLU:CG	1:D:1535:GLY:O	1.74	1.35
1:A:1535:GLY:CA	1:D:144:GLU:HG3	1.62	1.29
1:C:144:GLU:HG3	1:D:1535:GLY:CA	1.63	1.28
1:B:144:GLU:HG3	1:C:1535:GLY:O	1.09	1.26
1:B:144:GLU:HG3	1:C:1535:GLY:CA	1.64	1.26
1:A:1483:PRO:CA	1:D:214:ASN:ND2	1.99	1.25
1:B:199:TYR:CE2	1:C:1537:ALA:N	2.04	1.25
1:C:144:GLU:HG3	1:D:1535:GLY:O	1.16	1.25
1:A:144:GLU:HG3	1:B:1535:GLY:O	1.08	1.24
1:A:1535:GLY:O	1:D:144:GLU:HG3	1.12	1.24
1:C:214:ASN:ND2	1:D:1483:PRO:CA	2.01	1.24
1:A:199:TYR:CE2	1:B:1537:ALA:N	2.02	1.23
1:A:1537:ALA:N	1:D:199:TYR:CE2	2.07	1.23
1:A:214:ASN:ND2	1:B:1483:PRO:CA	2.02	1.23
1:B:214:ASN:ND2	1:C:1483:PRO:CA	2.03	1.21
1:A:144:GLU:HG3	1:B:1535:GLY:CA	1.68	1.20
1:B:199:TYR:CE1	1:C:1537:ALA:N	2.09	1.20
1:A:144:GLU:HA	1:B:1535:GLY:CA	1.72	1.20
1:A:1534:LYS:HB3	1:D:145:LYS:N	1.15	1.19
1:A:1535:GLY:CA	1:D:144:GLU:HA	1.71	1.19
1:A:214:ASN:CG	1:B:1483:PRO:O	1.80	1.19
1:B:144:GLU:HA	1:C:1535:GLY:CA	1.71	1.18
1:C:145:LYS:N	1:D:1534:LYS:HB3	1.17	1.18
1:A:1483:PRO:O	1:D:214:ASN:CG	1.81	1.18
1:A:1534:LYS:CB	1:D:145:LYS:N	2.02	1.18
1:B:214:ASN:CG	1:C:1483:PRO:O	1.81	1.18
1:A:1537:ALA:N	1:D:199:TYR:CZ	1.81	1.18
1:C:144:GLU:HA	1:D:1535:GLY:HA3	1.21	1.17
1:C:199:TYR:CE2	1:D:1537:ALA:N	2.12	1.17
1:C:214:ASN:CG	1:D:1483:PRO:O	1.84	1.16
1:A:1483:PRO:CA	1:D:214:ASN:HD21	1.58	1.15
1:A:145:LYS:N	1:B:1534:LYS:HB3	1.25	1.15
1:B:145:LYS:N	1:C:1534:LYS:HB3	1.23	1.14
1:A:199:TYR:CE1	1:B:1537:ALA:N	2.11	1.14
1:C:145:LYS:N	1:D:1534:LYS:CB	2.05	1.14
1:C:144:GLU:HA	1:D:1535:GLY:CA	1.77	1.13
1:C:214:ASN:HD21	1:D:1483:PRO:CA	1.60	1.13
1:B:144:GLU:CA	1:C:1535:GLY:HA3	1.79	1.11
1:A:1535:GLY:O	1:D:144:GLU:CD	1.86	1.11
1:A:1535:GLY:HA3	1:D:144:GLU:CA	1.80	1.11
1:B:144:GLU:HA	1:C:1535:GLY:HA3	1.12	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLU:HA	1:B:1535:GLY:HA3	1.10	1.10
1:B:144:GLU:CD	1:C:1535:GLY:O	1.88	1.10
1:A:144:GLU:CA	1:B:1535:GLY:HA3	1.80	1.10
1:A:1535:GLY:HA3	1:D:144:GLU:HA	1.16	1.09
1:C:199:TYR:CE1	1:D:1537:ALA:N	2.15	1.09
1:B:214:ASN:HD21	1:C:1483:PRO:CA	1.60	1.08
1:C:144:GLU:CD	1:D:1535:GLY:O	1.91	1.08
1:A:145:LYS:N	1:B:1534:LYS:CB	2.10	1.07
1:A:214:ASN:HD21	1:B:1483:PRO:CA	1.59	1.06
1:A:144:GLU:CD	1:B:1535:GLY:O	1.91	1.06
1:B:145:LYS:N	1:C:1534:LYS:CB	2.08	1.05
1:C:144:GLU:CA	1:D:1535:GLY:HA3	1.87	1.04
1:A:1535:GLY:CA	1:D:144:GLU:CG	2.38	1.02
1:B:144:GLU:CG	1:C:1535:GLY:CA	2.39	0.99
1:C:144:GLU:CG	1:D:1535:GLY:CA	2.40	0.98
1:A:144:GLU:CG	1:B:1535:GLY:CA	2.42	0.97
1:A:1536:ARG:HH12	1:D:195:HIS:CE1	1.88	0.90
1:C:145:LYS:H	1:D:1534:LYS:HB3	1.36	0.90
1:A:1535:GLY:N	1:D:144:GLU:HA	1.86	0.89
1:A:214:ASN:ND2	1:B:1483:PRO:C	2.26	0.88
1:A:1534:LYS:HB3	1:D:145:LYS:H	1.37	0.87
1:B:214:ASN:ND2	1:C:1483:PRO:C	2.28	0.86
1:A:1534:LYS:N	1:D:146:ASN:HD22	1.74	0.86
1:C:146:ASN:HD22	1:D:1534:LYS:N	1.74	0.86
1:C:195:HIS:CE1	1:D:1536:ARG:HH12	1.95	0.85
1:A:214:ASN:ND2	1:B:1483:PRO:O	2.08	0.85
1:A:1535:GLY:HA3	1:D:144:GLU:CB	2.06	0.85
1:B:144:GLU:HA	1:C:1535:GLY:N	1.92	0.85
1:A:1483:PRO:C	1:D:214:ASN:ND2	2.29	0.84
1:A:199:TYR:CE1	1:B:1536:ARG:C	2.23	0.84
1:C:214:ASN:ND2	1:D:1483:PRO:C	2.30	0.84
1:B:144:GLU:CB	1:C:1535:GLY:HA3	2.08	0.84
1:B:195:HIS:CE1	1:C:1536:ARG:HH12	1.95	0.84
1:B:214:ASN:ND2	1:C:1483:PRO:O	2.10	0.83
1:C:144:GLU:HA	1:D:1535:GLY:N	1.91	0.83
1:A:1536:ARG:NH1	1:D:195:HIS:HE1	1.76	0.83
1:A:2471:ARG:NH2	7:A:3107:HOH:O	2.13	0.82
1:B:146:ASN:HB3	1:C:1534:LYS:H	1.44	0.82
1:A:144:GLU:HA	1:B:1535:GLY:N	1.94	0.82
1:A:1536:ARG:NH1	1:D:195:HIS:CE1	2.48	0.81
1:A:145:LYS:H	1:B:1534:LYS:HB3	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:TYR:CE1	1:D:1536:ARG:C	2.26	0.81
1:B:146:ASN:HD22	1:C:1534:LYS:N	1.79	0.81
1:A:2059:GLN:OE1	7:A:3101:HOH:O	1.99	0.81
1:C:2059:GLN:OE1	7:C:2801:HOH:O	1.99	0.80
1:C:144:GLU:CB	1:D:1535:GLY:HA3	2.11	0.80
1:C:214:ASN:ND2	1:D:1483:PRO:O	2.15	0.80
1:A:144:GLU:CB	1:B:1535:GLY:HA3	2.11	0.80
1:A:195:HIS:CE1	1:B:1536:ARG:HH12	1.98	0.79
1:B:199:TYR:CE1	1:C:1536:ARG:C	2.21	0.79
1:A:146:ASN:HB3	1:B:1534:LYS:H	1.46	0.79
1:D:2059:GLN:OE1	7:D:2801:HOH:O	1.99	0.79
1:B:2059:GLN:OE1	7:B:2801:HOH:O	1.99	0.79
1:A:1483:PRO:O	1:D:214:ASN:ND2	2.16	0.79
1:B:145:LYS:H	1:C:1534:LYS:HB3	1.43	0.78
1:A:1534:LYS:H	1:D:146:ASN:HB3	1.48	0.77
1:C:195:HIS:HE1	1:D:1536:ARG:NH1	1.81	0.77
1:A:1532:VAL:O	1:D:146:ASN:ND2	2.18	0.77
1:C:195:HIS:CE1	1:D:1536:ARG:NH1	2.53	0.77
1:B:195:HIS:HE1	1:C:1536:ARG:NH1	1.84	0.76
1:A:146:ASN:HD22	1:B:1534:LYS:N	1.83	0.76
1:C:146:ASN:HB3	1:D:1534:LYS:H	1.49	0.75
1:B:195:HIS:CE1	1:C:1536:ARG:NH1	2.55	0.75
1:C:144:GLU:HG3	1:D:1535:GLY:HA3	1.68	0.74
1:B:1319:ASP:O	1:B:1323:THR:HG23	1.88	0.74
1:A:1319:ASP:O	1:A:1323:THR:HG23	1.88	0.74
1:C:743:ARG:NH1	1:C:1122:GLU:OE2	2.21	0.74
1:A:743:ARG:NH1	1:A:1122:GLU:OE2	2.21	0.74
1:A:1942:GLU:OE1	7:A:3103:HOH:O	2.06	0.74
1:D:1946:GLU:OE2	7:D:2802:HOH:O	2.06	0.74
1:B:1946:GLU:OE2	7:B:2802:HOH:O	2.06	0.74
1:D:1319:ASP:O	1:D:1323:THR:HG23	1.88	0.74
1:D:2471:ARG:NH2	7:D:2812:HOH:O	2.21	0.73
1:B:743:ARG:NH1	1:B:1122:GLU:OE2	2.21	0.73
1:C:1319:ASP:O	1:C:1323:THR:HG23	1.88	0.73
1:A:195:HIS:HE1	1:B:1536:ARG:NH1	1.86	0.73
1:B:144:GLU:HG3	1:C:1535:GLY:HA3	1.69	0.73
1:D:743:ARG:NH1	1:D:1122:GLU:OE2	2.21	0.73
1:B:146:ASN:ND2	1:C:1532:VAL:O	2.22	0.73
1:A:1946:GLU:OE2	7:A:3102:HOH:O	2.06	0.73
1:B:1942:GLU:OE1	7:B:2803:HOH:O	2.06	0.72
1:A:1535:GLY:H	1:D:144:GLU:HG2	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:GLU:CG	1:C:1535:GLY:HA3	2.19	0.72
5:C:2706:ATP:O4'	7:C:2804:HOH:O	2.07	0.72
1:D:1942:GLU:OE1	7:D:2803:HOH:O	2.06	0.72
1:C:1946:GLU:OE2	7:C:2802:HOH:O	2.06	0.72
1:A:144:GLU:HG3	1:B:1535:GLY:HA3	1.71	0.72
5:B:2706:ATP:O4'	7:B:2804:HOH:O	2.07	0.72
1:C:214:ASN:C	1:D:1487:ASN:N	2.04	0.72
1:C:1942:GLU:OE1	7:C:2803:HOH:O	2.06	0.72
5:A:3005:ATP:O4'	7:A:3104:HOH:O	2.07	0.71
1:C:2578:LYS:O	7:C:2805:HOH:O	2.09	0.71
1:A:195:HIS:CE1	1:B:1536:ARG:NH1	2.58	0.71
1:B:2578:LYS:O	7:B:2805:HOH:O	2.09	0.71
1:B:1255:THR:OG1	1:B:1260:GLU:OE2	2.09	0.71
1:C:146:ASN:ND2	1:D:1532:VAL:O	2.23	0.71
1:A:1535:GLY:HA3	1:D:144:GLU:HG3	1.70	0.71
1:C:2471:ARG:NH2	7:C:2813:HOH:O	2.23	0.71
1:A:1532:VAL:CA	1:D:146:ASN:CB	2.68	0.70
1:B:299:HIS:ND1	1:B:378:ASP:O	2.25	0.70
1:A:1532:VAL:HA	1:D:146:ASN:HB2	1.73	0.70
1:A:1538:ILE:HG12	1:D:199:TYR:OH	1.91	0.70
1:C:144:GLU:HG2	1:D:1535:GLY:H	1.56	0.70
5:D:2708:ATP:O4'	7:D:2804:HOH:O	2.07	0.70
1:A:146:ASN:HB2	1:B:1532:VAL:HA	1.71	0.70
1:D:299:HIS:ND1	1:D:378:ASP:O	2.25	0.70
1:D:2578:LYS:O	7:D:2805:HOH:O	2.09	0.70
1:A:146:ASN:ND2	1:B:1532:VAL:O	2.22	0.70
1:C:1255:THR:OG1	1:C:1260:GLU:OE2	2.09	0.70
1:A:1255:THR:OG1	1:A:1260:GLU:OE2	2.09	0.70
1:B:479:LEU:O	1:B:483:VAL:HG23	1.92	0.69
1:A:144:GLU:CG	1:B:1535:GLY:HA3	2.22	0.69
1:B:146:ASN:HB2	1:C:1532:VAL:HA	1.72	0.69
1:A:1535:GLY:N	1:D:144:GLU:CG	2.55	0.69
1:A:299:HIS:ND1	1:A:378:ASP:O	2.25	0.69
1:A:2578:LYS:O	7:A:3105:HOH:O	2.09	0.69
1:B:146:ASN:HB2	1:C:1532:VAL:CA	2.15	0.69
1:B:199:TYR:CE2	1:C:1537:ALA:H	1.50	0.69
1:C:299:HIS:ND1	1:C:378:ASP:O	2.25	0.69
1:C:479:LEU:O	1:C:483:VAL:HG23	1.92	0.69
1:A:479:LEU:O	1:A:483:VAL:HG23	1.92	0.69
1:A:199:TYR:CZ	1:B:1537:ALA:H	1.38	0.69
1:A:1483:PRO:O	1:D:214:ASN:CB	2.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ASN:CB	1:C:1532:VAL:CA	2.71	0.69
1:D:479:LEU:O	1:D:483:VAL:HG23	1.92	0.68
1:D:1255:THR:OG1	1:D:1260:GLU:OE2	2.09	0.68
1:B:144:GLU:HG2	1:C:1535:GLY:H	1.59	0.68
1:A:146:ASN:HB2	1:B:1532:VAL:CA	2.16	0.68
1:A:199:TYR:CE2	1:B:1537:ALA:CA	2.76	0.68
1:A:214:ASN:CB	1:B:1483:PRO:O	2.42	0.68
1:C:144:GLU:CG	1:D:1535:GLY:N	2.57	0.67
1:B:199:TYR:CE2	1:C:1537:ALA:CA	2.77	0.67
1:B:2009:ASP:OD1	7:B:2806:HOH:O	2.13	0.67
1:B:593:ASP:OD1	1:B:594:THR:N	2.28	0.67
1:D:2009:ASP:OD1	7:D:2806:HOH:O	2.12	0.67
1:C:1960:VAL:O	7:C:2807:HOH:O	2.13	0.67
1:A:1960:VAL:O	7:A:3108:HOH:O	2.13	0.67
1:B:1948:CYS:SG	1:B:1959:ILE:HD12	2.35	0.67
1:C:214:ASN:CB	1:D:1483:PRO:O	2.42	0.67
1:D:1960:VAL:O	7:D:2807:HOH:O	2.13	0.67
1:B:199:TYR:OH	1:C:1538:ILE:HG12	1.96	0.66
1:B:214:ASN:C	1:C:1487:ASN:N	2.00	0.66
1:A:1332:VAL:HG23	1:A:1333:VAL:HG13	1.77	0.66
1:C:593:ASP:OD1	1:C:594:THR:N	2.28	0.66
1:C:1948:CYS:SG	1:C:1959:ILE:HD12	2.35	0.66
1:B:1960:VAL:O	7:B:2807:HOH:O	2.13	0.66
1:D:1948:CYS:SG	1:D:1959:ILE:HD12	2.35	0.66
1:C:104:ASN:O	1:C:108:ASN:ND2	2.29	0.66
1:A:593:ASP:OD1	1:A:594:THR:N	2.28	0.66
1:A:1948:CYS:SG	1:A:1959:ILE:HD12	2.35	0.66
1:C:1332:VAL:HG23	1:C:1333:VAL:HG13	1.77	0.66
1:D:104:ASN:O	1:D:108:ASN:ND2	2.29	0.66
1:A:214:ASN:HD21	1:B:1483:PRO:HA	0.66	0.66
1:B:214:ASN:CB	1:C:1483:PRO:O	2.44	0.66
1:B:606:LEU:HD23	1:B:645:ILE:HD12	1.78	0.66
1:C:2009:ASP:OD1	7:C:2806:HOH:O	2.13	0.66
1:A:1243:GLN:OE1	1:A:1271:ASN:ND2	2.29	0.65
1:A:104:ASN:O	1:A:108:ASN:ND2	2.29	0.65
1:C:146:ASN:HB2	1:D:1532:VAL:HA	1.77	0.65
1:C:199:TYR:OH	1:D:1538:ILE:HG12	1.96	0.65
1:A:145:LYS:HB2	1:B:1534:LYS:HA	1.79	0.65
1:D:593:ASP:OD1	1:D:594:THR:N	2.28	0.65
1:D:972:LEU:HD11	1:D:1062:LEU:HD13	1.79	0.65
1:A:1535:GLY:H	1:D:144:GLU:CG	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2009:ASP:OD1	7:A:3106:HOH:O	2.13	0.65
1:B:145:LYS:HB2	1:C:1534:LYS:HA	1.79	0.65
1:B:104:ASN:O	1:B:108:ASN:ND2	2.29	0.65
1:A:1456:GLU:O	1:A:1458:ARG:NH1	2.30	0.65
1:B:1243:GLN:OE1	1:B:1271:ASN:ND2	2.29	0.65
1:B:1456:GLU:O	1:B:1458:ARG:NH1	2.30	0.65
1:C:146:ASN:HB2	1:D:1532:VAL:CA	2.19	0.65
1:C:1456:GLU:O	1:C:1458:ARG:NH1	2.30	0.65
1:D:1243:GLN:OE1	1:D:1271:ASN:ND2	2.29	0.65
1:A:146:ASN:CB	1:B:1532:VAL:CA	2.72	0.65
1:B:1332:VAL:HG23	1:B:1333:VAL:HG13	1.77	0.65
1:C:972:LEU:HD11	1:C:1062:LEU:HD13	1.79	0.65
1:A:972:LEU:HD11	1:A:1062:LEU:HD13	1.79	0.64
1:C:146:ASN:CB	1:D:1532:VAL:CA	2.73	0.64
1:A:743:ARG:NH1	1:A:788:ARG:O	2.31	0.64
1:A:1532:VAL:CA	1:D:146:ASN:HB2	2.14	0.64
1:D:1332:VAL:HG23	1:D:1333:VAL:HG13	1.77	0.64
1:A:1537:ALA:H	1:D:199:TYR:CE2	1.55	0.64
1:C:606:LEU:HD23	1:C:645:ILE:HD12	1.78	0.64
1:C:1243:GLN:OE1	1:C:1271:ASN:ND2	2.29	0.64
1:D:1456:GLU:O	1:D:1458:ARG:NH1	2.30	0.64
1:C:881:LEU:O	1:C:885:THR:HG23	1.98	0.64
1:A:1535:GLY:N	1:D:144:GLU:CA	2.59	0.64
1:D:606:LEU:HD23	1:D:645:ILE:HD12	1.78	0.64
1:D:743:ARG:NH1	1:D:788:ARG:O	2.31	0.64
1:A:144:GLU:HG2	1:B:1535:GLY:H	1.63	0.64
1:B:881:LEU:O	1:B:885:THR:HG23	1.98	0.64
1:C:144:GLU:CG	1:D:1535:GLY:HA3	2.20	0.64
1:A:881:LEU:O	1:A:885:THR:HG23	1.98	0.64
1:A:1535:GLY:CA	1:D:144:GLU:CA	2.54	0.64
1:A:214:ASN:C	1:B:1487:ASN:N	2.01	0.64
1:B:743:ARG:NH1	1:B:788:ARG:O	2.31	0.64
1:A:606:LEU:HD23	1:A:645:ILE:HD12	1.78	0.63
1:B:144:GLU:CG	1:C:1535:GLY:N	2.60	0.63
1:C:1619:ASP:OD2	1:C:1687:ARG:NH2	2.31	0.63
1:D:881:LEU:O	1:D:885:THR:HG23	1.98	0.63
1:D:1619:ASP:OD2	1:D:1687:ARG:NH2	2.31	0.63
1:A:1619:ASP:OD2	1:A:1687:ARG:NH2	2.31	0.63
1:B:2471:ARG:NH2	7:B:2817:HOH:O	2.30	0.63
1:C:743:ARG:NH1	1:C:788:ARG:O	2.31	0.63
1:B:972:LEU:HD11	1:B:1062:LEU:HD13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:801:ARG:NH2	1:C:984:ASP:OD1	2.32	0.63
1:A:144:GLU:CA	1:B:1535:GLY:CA	2.56	0.63
1:B:1619:ASP:OD2	1:B:1687:ARG:NH2	2.31	0.63
1:B:2262:ARG:NH1	6:B:2701:PCW:O1P	2.31	0.63
1:A:1537:ALA:CA	1:D:199:TYR:CE2	2.81	0.63
1:A:2140:VAL:O	7:A:3109:HOH:O	2.16	0.63
1:D:801:ARG:NH2	1:D:984:ASP:OD1	2.32	0.63
1:A:199:TYR:OH	1:B:1538:ILE:HG12	1.99	0.62
1:B:801:ARG:NH2	1:B:984:ASP:OD1	2.32	0.62
1:A:2262:ARG:NH1	6:A:3011:PCW:O1P	2.32	0.62
1:C:299:HIS:O	1:C:304:TYR:OH	2.16	0.62
1:A:801:ARG:NH2	1:A:984:ASP:OD1	2.32	0.62
1:C:144:GLU:CG	1:D:1535:GLY:H	2.11	0.62
1:D:252:LEU:HD11	1:D:263:VAL:HG12	1.82	0.62
1:A:1534:LYS:CA	1:D:145:LYS:HB2	2.21	0.62
1:A:1534:LYS:HA	1:D:145:LYS:HB2	1.81	0.61
1:B:483:VAL:HG22	1:B:509:MET:SD	2.41	0.61
1:A:252:LEU:HD11	1:A:263:VAL:HG12	1.82	0.61
1:B:214:ASN:HD21	1:C:1483:PRO:HA	0.66	0.61
1:B:1492:GLN:OE1	1:B:1492:GLN:N	2.32	0.61
1:C:252:LEU:HD11	1:C:263:VAL:HG12	1.82	0.61
1:C:199:TYR:CD1	1:D:1537:ALA:N	2.63	0.61
1:A:640:SER:HB3	1:A:645:ILE:HD11	1.83	0.61
1:D:483:VAL:HG22	1:D:509:MET:SD	2.40	0.61
1:A:483:VAL:HG22	1:A:509:MET:SD	2.41	0.61
1:B:199:TYR:CD1	1:C:1537:ALA:N	2.60	0.60
1:B:252:LEU:HD11	1:B:263:VAL:HG12	1.82	0.60
1:B:640:SER:HB3	1:B:645:ILE:HD11	1.83	0.60
1:C:483:VAL:HG22	1:C:509:MET:SD	2.41	0.60
1:C:2262:ARG:NH1	6:C:2701:PCW:O1P	2.34	0.60
1:C:144:GLU:CA	1:D:1535:GLY:CA	2.60	0.60
1:C:2140:VAL:O	7:C:2808:HOH:O	2.16	0.60
1:D:2140:VAL:O	7:D:2808:HOH:O	2.16	0.60
1:A:144:GLU:CG	1:B:1535:GLY:N	2.64	0.60
1:D:640:SER:HB3	1:D:645:ILE:HD11	1.83	0.60
1:B:145:LYS:H	1:C:1534:LYS:C	2.05	0.60
1:A:199:TYR:CD1	1:B:1537:ALA:N	2.63	0.59
1:A:1477:ASN:O	1:A:1481:SER:OG	2.12	0.59
1:B:2140:VAL:O	7:B:2808:HOH:O	2.16	0.59
1:A:145:LYS:H	1:B:1534:LYS:C	2.06	0.59
1:A:1534:LYS:C	1:D:145:LYS:H	2.04	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:640:SER:HB3	1:C:645:ILE:HD11	1.83	0.59
1:D:1492:GLN:N	1:D:1492:GLN:OE1	2.32	0.59
1:A:1535:GLY:HA3	1:D:144:GLU:CG	2.20	0.59
1:B:144:GLU:CA	1:C:1535:GLY:N	2.65	0.59
1:B:1477:ASN:O	1:B:1481:SER:OG	2.12	0.59
1:B:2052:ASN:OD1	7:B:2809:HOH:O	2.17	0.59
1:C:1542:MET:N	1:C:1542:MET:SD	2.76	0.59
1:A:2052:ASN:OD1	7:A:3110:HOH:O	2.17	0.59
1:C:2052:ASN:OD1	7:C:2809:HOH:O	2.17	0.59
1:C:1492:GLN:N	1:C:1492:GLN:OE1	2.32	0.58
1:A:1492:GLN:N	1:A:1492:GLN:OE1	2.32	0.58
1:A:1542:MET:SD	1:A:1542:MET:N	2.76	0.58
1:A:1535:GLY:N	1:D:144:GLU:HG3	2.16	0.58
1:A:308:HIS:ND1	1:A:311:THR:OG1	2.31	0.58
1:B:252:LEU:HD11	1:B:263:VAL:CG1	2.34	0.58
1:C:199:TYR:CE2	1:D:1537:ALA:CA	2.86	0.58
1:C:632:ASP:O	1:C:636:ASP:OD1	2.21	0.58
1:D:308:HIS:ND1	1:D:311:THR:OG1	2.31	0.58
1:D:632:ASP:O	1:D:636:ASP:OD1	2.21	0.58
1:A:126:HIS:O	1:A:130:ASN:N	2.36	0.58
1:B:632:ASP:O	1:B:636:ASP:OD1	2.21	0.58
1:B:1542:MET:SD	1:B:1542:MET:N	2.76	0.58
1:C:144:GLU:HG3	1:D:1535:GLY:N	2.16	0.58
1:A:252:LEU:HD11	1:A:263:VAL:CG1	2.34	0.58
1:A:632:ASP:O	1:A:636:ASP:OD1	2.21	0.58
1:D:2052:ASN:OD1	7:D:2809:HOH:O	2.17	0.58
1:A:1633:GLU:OE1	1:A:1633:GLU:N	2.27	0.57
1:B:144:GLU:CG	1:C:1535:GLY:H	2.16	0.57
1:C:252:LEU:HD11	1:C:263:VAL:CG1	2.34	0.57
1:C:1477:ASN:O	1:C:1481:SER:OG	2.12	0.57
1:B:225:MET:SD	1:B:226:GLN:N	2.78	0.57
1:D:1542:MET:SD	1:D:1542:MET:N	2.76	0.57
1:C:145:LYS:HB2	1:D:1534:LYS:HA	1.86	0.57
1:A:1976:ASN:O	1:A:1993:LYS:NZ	2.38	0.57
1:B:2502:PHE:CD2	6:B:2710:PCW:H471	2.29	0.57
1:A:225:MET:SD	1:A:226:GLN:N	2.78	0.57
1:D:2604:ARG:NH1	7:D:2822:HOH:O	2.38	0.57
1:A:2502:PHE:CD2	6:A:3009:PCW:H471	2.30	0.57
1:C:225:MET:SD	1:C:226:GLN:N	2.78	0.57
1:C:1976:ASN:O	1:C:1993:LYS:NZ	2.38	0.57
1:D:1976:ASN:O	1:D:1993:LYS:NZ	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:HIS:O	1:D:130:ASN:N	2.36	0.56
1:D:299:HIS:O	1:D:304:TYR:OH	2.16	0.56
1:A:1537:ALA:N	1:D:199:TYR:CD2	2.53	0.56
1:D:225:MET:SD	1:D:226:GLN:N	2.78	0.56
1:A:1532:VAL:C	1:D:146:ASN:CG	2.64	0.56
1:C:1332:VAL:O	1:C:1364:TYR:OH	2.24	0.56
1:D:252:LEU:HD11	1:D:263:VAL:CG1	2.34	0.56
1:B:1976:ASN:O	1:B:1993:LYS:NZ	2.38	0.56
1:C:126:HIS:O	1:C:130:ASN:N	2.36	0.56
1:D:599:LEU:HD13	1:D:610:ILE:HD11	1.88	0.56
1:A:1332:VAL:O	1:A:1364:TYR:OH	2.24	0.55
1:B:299:HIS:O	1:B:304:TYR:OH	2.16	0.55
1:B:2398:GLU:HG2	7:B:2891:HOH:O	2.06	0.55
1:C:2398:GLU:HG2	7:C:2891:HOH:O	2.06	0.55
1:A:1537:ALA:N	1:D:199:TYR:CD1	2.57	0.55
1:A:1934:VAL:HG11	1:A:1988:LEU:HD13	1.88	0.55
1:A:2604:ARG:NH1	7:A:3122:HOH:O	2.38	0.55
1:C:1934:VAL:HG11	1:C:1988:LEU:HD13	1.88	0.55
1:C:599:LEU:HD13	1:C:610:ILE:HD11	1.88	0.55
1:C:308:HIS:ND1	1:C:311:THR:OG1	2.31	0.55
1:C:2604:ARG:NH1	7:C:2822:HOH:O	2.38	0.55
1:A:145:LYS:HB2	1:B:1534:LYS:CA	2.16	0.55
1:A:146:ASN:CB	1:B:1532:VAL:HA	2.36	0.55
1:B:126:HIS:O	1:B:130:ASN:N	2.36	0.55
1:A:144:GLU:CG	1:B:1535:GLY:H	2.20	0.55
1:A:1534:LYS:H	1:D:146:ASN:HD22	1.53	0.55
1:D:2398:GLU:HG2	7:D:2891:HOH:O	2.06	0.55
1:A:599:LEU:HD13	1:A:610:ILE:HD11	1.88	0.54
1:A:1532:VAL:HA	1:D:146:ASN:CB	2.35	0.54
1:C:144:GLU:CA	1:D:1535:GLY:N	2.65	0.54
1:D:1934:VAL:HG11	1:D:1988:LEU:HD13	1.88	0.54
1:B:599:LEU:HD13	1:B:610:ILE:HD11	1.88	0.54
1:B:2604:ARG:NH1	7:B:2822:HOH:O	2.38	0.54
1:D:2134:GLU:OE2	7:D:2810:HOH:O	2.18	0.54
1:B:1934:VAL:HG11	1:B:1988:LEU:HD13	1.88	0.54
1:D:1332:VAL:O	1:D:1364:TYR:OH	2.24	0.54
1:B:146:ASN:CB	1:C:1532:VAL:HA	2.36	0.54
1:B:162:LEU:HD23	1:B:187:PRO:HA	1.89	0.54
1:C:145:LYS:H	1:D:1534:LYS:C	2.11	0.54
1:A:350:ILE:HD11	1:A:401:THR:HG21	1.90	0.53
1:B:199:TYR:CE1	1:C:1537:ALA:H	1.65	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:ILE:HD11	1:D:401:THR:HG21	1.90	0.53
1:A:2398:GLU:HG2	7:A:3191:HOH:O	2.06	0.53
1:C:144:GLU:CG	1:D:1535:GLY:C	2.33	0.53
1:C:162:LEU:HD23	1:C:187:PRO:HA	1.89	0.53
1:B:350:ILE:HD11	1:B:401:THR:HG21	1.90	0.53
1:D:162:LEU:HD23	1:D:187:PRO:HA	1.89	0.53
1:C:1633:GLU:OE1	1:C:1633:GLU:N	2.27	0.53
1:A:1532:VAL:C	1:D:146:ASN:CB	2.77	0.53
1:B:284:GLU:OE1	1:B:307:LYS:NZ	2.36	0.53
1:D:2262:ARG:NH1	6:D:2703:PCW:O1P	2.42	0.53
1:A:162:LEU:HD23	1:A:187:PRO:HA	1.89	0.53
1:A:772:ASP:OD1	1:A:773:LEU:N	2.42	0.53
1:C:772:ASP:OD1	1:C:773:LEU:N	2.42	0.53
1:C:12:ASP:OD1	1:C:227:PHE:N	2.40	0.53
1:B:1332:VAL:O	1:B:1364:TYR:OH	2.24	0.53
1:A:144:GLU:CA	1:B:1535:GLY:N	2.67	0.52
1:B:2134:GLU:OE2	7:B:2810:HOH:O	2.18	0.52
1:C:146:ASN:CB	1:D:1532:VAL:HA	2.38	0.52
1:C:350:ILE:HD11	1:C:401:THR:HG21	1.90	0.52
1:C:199:TYR:CD2	1:D:1537:ALA:N	2.61	0.52
1:C:2562:GLU:OE2	1:C:2609:SER:OG	2.28	0.52
1:C:146:ASN:HD22	1:D:1534:LYS:H	1.53	0.52
1:B:214:ASN:OD1	1:C:1483:PRO:O	2.25	0.52
1:C:214:ASN:HD21	1:D:1483:PRO:HA	0.66	0.52
1:C:2134:GLU:OE2	7:C:2810:HOH:O	2.18	0.52
1:A:554:ARG:HG3	1:A:590:LEU:HD13	1.91	0.52
1:B:146:ASN:CB	1:C:1532:VAL:C	2.78	0.52
1:B:308:HIS:ND1	1:B:311:THR:OG1	2.31	0.52
1:B:772:ASP:OD1	1:B:773:LEU:N	2.42	0.52
1:C:2579:ASN:OD1	1:C:2580:LYS:N	2.43	0.52
1:D:2560:LYS:NZ	5:D:2708:ATP:O3A	2.43	0.52
1:D:2579:ASN:OD1	1:D:2580:LYS:N	2.43	0.52
1:A:2560:LYS:NZ	5:A:3005:ATP:O3A	2.43	0.52
1:A:1483:PRO:O	1:D:214:ASN:OD1	2.24	0.51
1:A:2579:ASN:OD1	1:A:2580:LYS:N	2.43	0.51
1:B:621:LEU:HD12	1:B:622:VAL:N	2.26	0.51
1:B:1397:VAL:O	1:B:1401:THR:OG1	2.21	0.51
1:C:2560:LYS:NZ	5:C:2706:ATP:O3A	2.43	0.51
1:A:146:ASN:CB	1:B:1532:VAL:C	2.79	0.51
1:A:621:LEU:HD12	1:A:622:VAL:N	2.26	0.51
1:A:2134:GLU:OE2	7:A:3111:HOH:O	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ASP:OD1	1:B:227:PHE:N	2.40	0.51
1:C:447:ASP:O	1:C:451:MET:HG2	2.11	0.51
1:D:1477:ASN:O	1:D:1481:SER:OG	2.12	0.51
1:A:1532:VAL:C	1:D:146:ASN:ND2	2.64	0.51
1:B:554:ARG:HG3	1:B:590:LEU:HD13	1.91	0.51
1:C:2502:PHE:CD2	6:C:2710:PCW:H471	2.30	0.51
1:D:772:ASP:OD1	1:D:773:LEU:N	2.42	0.51
1:A:252:LEU:HD13	1:A:417:LEU:HD12	1.93	0.51
1:D:554:ARG:HG3	1:D:590:LEU:HD13	1.91	0.51
1:A:1300:LEU:HD11	1:A:1364:TYR:CE1	2.46	0.51
1:B:447:ASP:O	1:B:451:MET:HG2	2.11	0.51
1:C:554:ARG:HG3	1:C:590:LEU:HD13	1.91	0.51
1:D:252:LEU:HD13	1:D:417:LEU:HD12	1.93	0.51
1:D:447:ASP:O	1:D:451:MET:HG2	2.11	0.51
1:D:622:VAL:O	1:D:626:ARG:N	2.41	0.51
1:B:145:LYS:HB2	1:C:1534:LYS:CA	2.17	0.51
1:B:972:LEU:HD11	1:B:1062:LEU:CD1	2.41	0.51
1:B:1651:THR:OG1	1:B:1665:VAL:HG11	2.11	0.51
1:B:1962:HIS:ND1	1:B:1964:SER:OG	2.40	0.51
1:D:1633:GLU:OE1	1:D:1633:GLU:N	2.27	0.51
1:C:622:VAL:O	1:C:626:ARG:N	2.41	0.51
1:A:1483:PRO:O	1:D:214:ASN:HB3	2.11	0.51
1:B:199:TYR:CD2	1:C:1537:ALA:HA	2.46	0.51
1:C:214:ASN:HB3	1:D:1483:PRO:O	2.11	0.51
1:C:972:LEU:HD11	1:C:1062:LEU:CD1	2.41	0.51
1:C:1300:LEU:HD11	1:C:1364:TYR:CE1	2.46	0.51
1:B:2560:LYS:NZ	5:B:2706:ATP:O3A	2.43	0.51
1:B:2562:GLU:OE2	1:B:2609:SER:OG	2.28	0.51
1:D:1300:LEU:HD11	1:D:1364:TYR:CE1	2.46	0.51
1:A:267:THR:HG23	1:A:413:ILE:O	2.12	0.50
1:A:1495:GLN:O	1:A:1498:VAL:HG22	2.12	0.50
1:B:482:PHE:O	1:B:505:ARG:NH1	2.42	0.50
1:C:267:THR:HG23	1:C:413:ILE:O	2.11	0.50
1:D:267:THR:HG23	1:D:413:ILE:O	2.12	0.50
1:A:12:ASP:OD1	1:A:227:PHE:N	2.40	0.50
1:B:267:THR:HG23	1:B:413:ILE:O	2.11	0.50
1:C:1288:HIS:CE1	1:C:1292:THR:HG21	2.47	0.50
1:C:1651:THR:OG1	1:C:1665:VAL:HG11	2.11	0.50
1:B:1300:LEU:HD11	1:B:1364:TYR:CE1	2.46	0.50
1:B:2579:ASN:OD1	1:B:2580:LYS:N	2.43	0.50
1:D:1495:GLN:O	1:D:1498:VAL:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASP:O	1:A:451:MET:HG2	2.11	0.50
1:A:972:LEU:HD11	1:A:1062:LEU:CD1	2.41	0.50
1:B:622:VAL:O	1:B:626:ARG:N	2.41	0.50
1:C:146:ASN:CG	1:D:1532:VAL:C	2.70	0.50
1:C:252:LEU:HD13	1:C:417:LEU:HD12	1.93	0.50
1:D:621:LEU:HD12	1:D:622:VAL:N	2.26	0.50
1:A:482:PHE:O	1:A:505:ARG:NH1	2.42	0.50
1:A:1313:TYR:OH	1:A:1377:GLU:OE1	2.30	0.50
1:B:146:ASN:CG	1:C:1532:VAL:C	2.69	0.50
1:C:621:LEU:HD12	1:C:622:VAL:N	2.26	0.50
1:A:1489:THR:HG21	1:D:216:ASN:HD21	1.76	0.50
1:A:1962:HIS:ND1	1:A:1964:SER:OG	2.40	0.50
1:D:647:VAL:O	1:D:651:LEU:HD22	2.12	0.50
1:D:972:LEU:HD11	1:D:1062:LEU:CD1	2.41	0.50
1:D:1288:HIS:CE1	1:D:1292:THR:HG21	2.47	0.50
1:A:199:TYR:CD2	1:B:1537:ALA:HA	2.47	0.50
1:A:647:VAL:O	1:A:651:LEU:HD22	2.12	0.50
1:B:252:LEU:HD13	1:B:417:LEU:HD12	1.93	0.50
1:B:1288:HIS:CE1	1:B:1292:THR:HG21	2.47	0.50
1:B:1633:GLU:OE1	1:B:1633:GLU:N	2.27	0.50
1:A:1535:GLY:O	1:D:199:TYR:CE1	2.52	0.49
1:C:1495:GLN:O	1:C:1498:VAL:HG22	2.12	0.49
1:A:1288:HIS:CE1	1:A:1292:THR:HG21	2.47	0.49
1:A:1532:VAL:O	1:D:146:ASN:CG	2.49	0.49
1:A:1651:THR:OG1	1:A:1665:VAL:HG11	2.11	0.49
1:B:1495:GLN:O	1:B:1498:VAL:HG22	2.12	0.49
1:C:647:VAL:O	1:C:651:LEU:HD22	2.12	0.49
1:D:1651:THR:OG1	1:D:1665:VAL:HG11	2.11	0.49
1:D:2562:GLU:OE2	1:D:2609:SER:OG	2.28	0.49
1:B:146:ASN:CG	1:C:1532:VAL:O	2.51	0.49
1:B:199:TYR:CD2	1:C:1537:ALA:N	2.55	0.49
1:C:199:TYR:CE1	1:D:1537:ALA:H	1.69	0.49
1:A:214:ASN:OD1	1:B:1483:PRO:O	2.26	0.49
1:D:1313:TYR:OH	1:D:1377:GLU:OE1	2.30	0.49
1:D:1974:ILE:CD1	1:D:2000:LEU:HD12	2.43	0.49
1:A:640:SER:CB	1:A:645:ILE:HD11	2.43	0.49
1:C:284:GLU:OE1	1:C:307:LYS:NZ	2.36	0.49
1:B:647:VAL:O	1:B:651:LEU:HD22	2.12	0.49
1:B:1974:ILE:CD1	1:B:2000:LEU:HD12	2.43	0.49
1:C:279:SER:OG	1:C:511:GLU:OE2	2.25	0.49
1:C:405:ILE:HD11	1:C:416:MET:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1974:ILE:CD1	1:C:2000:LEU:HD12	2.43	0.49
1:A:1974:ILE:CD1	1:A:2000:LEU:HD12	2.43	0.49
1:C:213:VAL:HG22	1:D:1486:GLU:HB3	1.94	0.49
1:D:284:GLU:OE1	1:D:307:LYS:NZ	2.36	0.49
1:A:145:LYS:O	1:B:1534:LYS:HG3	1.67	0.48
1:A:213:VAL:HG22	1:B:1486:GLU:HB3	1.94	0.48
1:A:1486:GLU:HB3	1:D:213:VAL:HG22	1.94	0.48
1:B:1949:GLN:OE1	7:B:2811:HOH:O	2.20	0.48
1:C:640:SER:CB	1:C:645:ILE:HD11	2.43	0.48
1:D:482:PHE:O	1:D:505:ARG:NH1	2.42	0.48
1:B:405:ILE:HD11	1:B:416:MET:HA	1.95	0.48
1:D:640:SER:CB	1:D:645:ILE:HD11	2.43	0.48
1:A:1285:HIS:O	1:A:1289:LEU:HD23	2.14	0.48
1:B:640:SER:CB	1:B:645:ILE:HD11	2.43	0.48
1:C:199:TYR:CE1	1:D:1535:GLY:O	2.51	0.48
1:A:146:ASN:CG	1:B:1532:VAL:C	2.72	0.48
1:B:1285:HIS:O	1:B:1289:LEU:HD23	2.13	0.48
1:B:1313:TYR:OH	1:B:1377:GLU:OE1	2.30	0.48
1:B:2262:ARG:NH2	6:B:2701:PCW:O1P	2.46	0.48
1:C:1962:HIS:ND1	1:C:1964:SER:OG	2.40	0.48
1:C:2367:ARG:NH2	1:D:2352:GLU:OE1	2.46	0.48
1:D:405:ILE:HD11	1:D:416:MET:HA	1.95	0.48
1:A:1486:GLU:H	1:D:214:ASN:HB3	1.20	0.48
1:A:1537:ALA:HA	1:D:199:TYR:CD2	2.48	0.48
1:C:1313:TYR:OH	1:C:1377:GLU:OE1	2.30	0.48
1:D:12:ASP:OD1	1:D:227:PHE:N	2.40	0.48
1:B:545:LYS:HE2	1:B:545:LYS:HA	1.96	0.48
1:B:2381:TYR:CZ	1:B:2385:ILE:HD11	2.49	0.48
1:B:216:ASN:HD21	1:C:1489:THR:HG21	1.78	0.47
1:C:146:ASN:CB	1:D:1532:VAL:C	2.82	0.47
1:A:1487:ASN:O	1:D:216:ASN:OD1	2.32	0.47
1:A:2381:TYR:CZ	1:A:2385:ILE:HD11	2.49	0.47
1:A:146:ASN:CG	1:B:1532:VAL:O	2.52	0.47
1:A:611:THR:HG22	1:A:612:LYS:H	1.80	0.47
1:A:2562:GLU:OE2	1:A:2609:SER:OG	2.28	0.47
1:A:545:LYS:HA	1:A:545:LYS:HE2	1.96	0.47
1:A:2184:TRP:NE1	1:A:2302:GLY:O	2.43	0.47
1:C:216:ASN:HD21	1:D:1489:THR:HG21	1.79	0.47
1:D:279:SER:OG	1:D:511:GLU:OE2	2.25	0.47
1:D:1949:GLN:OE1	7:D:2811:HOH:O	2.20	0.47
1:A:720:ALA:O	1:A:724:ASN:ND2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1285:HIS:O	1:C:1289:LEU:HD23	2.13	0.47
1:D:545:LYS:HE2	1:D:545:LYS:HA	1.96	0.47
1:D:611:THR:HG22	1:D:612:LYS:H	1.80	0.47
1:D:2381:TYR:CZ	1:D:2385:ILE:HD11	2.49	0.47
1:A:199:TYR:CD2	1:B:1537:ALA:N	2.55	0.47
1:C:2164:GLN:HG3	1:D:2545:ARG:HH22	1.80	0.47
1:D:589:ILE:C	1:D:590:LEU:HD12	2.35	0.47
1:A:214:ASN:HB3	1:B:1483:PRO:O	2.13	0.47
1:A:405:ILE:HD11	1:A:416:MET:HA	1.95	0.47
1:B:611:THR:HG22	1:B:612:LYS:H	1.80	0.47
1:B:1178:ARG:HB2	1:B:1178:ARG:CZ	2.45	0.47
1:C:2381:TYR:CZ	1:C:2385:ILE:HD11	2.49	0.47
1:A:1535:GLY:CA	1:D:144:GLU:CB	2.77	0.47
1:A:1949:GLN:OE1	7:A:3112:HOH:O	2.20	0.47
1:B:144:GLU:CA	1:C:1535:GLY:CA	2.55	0.47
1:B:213:VAL:HG22	1:C:1486:GLU:HB3	1.96	0.47
1:B:811:THR:OG1	1:B:814:ASP:OD1	2.31	0.47
1:D:1397:VAL:O	1:D:1401:THR:OG1	2.21	0.47
6:D:2701:PCW:H83	6:D:2701:PCW:O4P	2.15	0.47
1:A:1346:LEU:HD21	1:A:1402:HIS:CD2	2.50	0.47
1:C:146:ASN:ND2	1:D:1532:VAL:C	2.68	0.47
1:C:611:THR:HG22	1:C:612:LYS:H	1.80	0.47
1:C:1178:ARG:HB2	1:C:1178:ARG:CZ	2.45	0.47
1:A:2178:LEU:O	1:A:2182:MET:HG3	2.15	0.47
1:B:199:TYR:CD2	1:C:1537:ALA:CA	2.98	0.47
1:A:299:HIS:O	1:A:304:TYR:OH	2.16	0.46
1:A:1178:ARG:HB2	1:A:1178:ARG:CZ	2.45	0.46
1:B:199:TYR:CE1	1:C:1535:GLY:O	2.58	0.46
1:B:1439:THR:HA	1:B:1442:GLU:HG2	1.98	0.46
1:D:2178:LEU:O	1:D:2182:MET:HG3	2.15	0.46
1:A:622:VAL:O	1:A:626:ARG:N	2.41	0.46
1:C:545:LYS:HA	1:C:545:LYS:HE2	1.96	0.46
1:C:2178:LEU:O	1:C:2182:MET:HG3	2.15	0.46
1:D:1178:ARG:CZ	1:D:1178:ARG:HB2	2.45	0.46
1:A:250:LYS:HE2	1:A:267:THR:HG22	1.97	0.46
1:C:589:ILE:C	1:C:590:LEU:HD12	2.35	0.46
1:D:1346:LEU:HD21	1:D:1402:HIS:CD2	2.50	0.46
1:A:252:LEU:HD13	1:A:417:LEU:CD1	2.46	0.46
1:C:1346:LEU:HD21	1:C:1402:HIS:CD2	2.50	0.46
1:C:1949:GLN:OE1	7:C:2811:HOH:O	2.20	0.46
1:B:1948:CYS:HG	1:B:1959:ILE:HD12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1395:ASP:N	1:C:1395:ASP:OD1	2.49	0.46
1:C:2262:ARG:NH2	6:C:2701:PCW:O1P	2.48	0.46
1:A:589:ILE:C	1:A:590:LEU:HD12	2.35	0.46
6:A:3009:PCW:O4P	6:A:3009:PCW:H83	2.15	0.46
1:C:1439:THR:HA	1:C:1442:GLU:HG2	1.98	0.46
1:D:1285:HIS:O	1:D:1289:LEU:HD23	2.14	0.46
1:A:1439:THR:HA	1:A:1442:GLU:HG2	1.98	0.46
1:B:589:ILE:C	1:B:590:LEU:HD12	2.35	0.46
1:B:1346:LEU:HD21	1:B:1402:HIS:CD2	2.50	0.46
1:C:563:SER:O	1:C:570:ASN:ND2	2.44	0.46
1:D:1395:ASP:OD1	1:D:1395:ASP:N	2.49	0.46
1:B:2178:LEU:O	1:B:2182:MET:HG3	2.15	0.46
1:B:214:ASN:HB3	1:C:1483:PRO:O	2.15	0.46
1:B:720:ALA:O	1:B:724:ASN:ND2	2.46	0.46
1:C:250:LYS:HE2	1:C:267:THR:HG22	1.97	0.46
6:C:2710:PCW:H83	6:C:2710:PCW:O4P	2.15	0.46
1:D:406:ASP:OD1	1:D:406:ASP:N	2.49	0.46
1:A:199:TYR:CD2	1:B:1537:ALA:CA	2.99	0.45
1:A:811:THR:OG1	1:A:814:ASP:OD1	2.31	0.45
1:A:1534:LYS:C	1:D:145:LYS:N	2.69	0.45
1:A:1537:ALA:CA	1:D:199:TYR:CD2	2.98	0.45
1:B:1542:MET:CE	1:B:1542:MET:H	2.30	0.45
6:B:2710:PCW:O4P	6:B:2710:PCW:H83	2.15	0.45
1:C:146:ASN:CG	1:D:1532:VAL:O	2.55	0.45
1:C:477:GLU:OE2	1:C:493:VAL:HG11	2.17	0.45
1:D:250:LYS:HE2	1:D:267:THR:HG22	1.97	0.45
1:C:2184:TRP:NE1	1:C:2302:GLY:O	2.43	0.45
1:D:1439:THR:HA	1:D:1442:GLU:HG2	1.98	0.45
1:A:598:LEU:C	1:A:598:LEU:HD23	2.37	0.45
1:B:406:ASP:OD1	1:B:406:ASP:N	2.49	0.45
1:B:598:LEU:HD23	1:B:598:LEU:C	2.37	0.45
1:C:482:PHE:O	1:C:505:ARG:NH1	2.42	0.45
1:C:1542:MET:H	1:C:1542:MET:CE	2.30	0.45
1:D:252:LEU:HD13	1:D:417:LEU:CD1	2.46	0.45
1:D:858:LYS:O	1:D:862:GLU:HG2	2.17	0.45
1:A:477:GLU:OE2	1:A:493:VAL:HG11	2.17	0.45
1:A:671:ARG:HG3	1:A:673:VAL:HG23	1.99	0.45
1:B:250:LYS:HE2	1:B:267:THR:HG22	1.97	0.45
1:B:252:LEU:HD13	1:B:417:LEU:CD1	2.46	0.45
1:B:586:GLY:N	1:B:592:GLU:OE2	2.48	0.45
1:B:671:ARG:HG3	1:B:673:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:858:LYS:O	1:B:862:GLU:HG2	2.17	0.45
1:C:858:LYS:O	1:C:862:GLU:HG2	2.17	0.45
1:A:279:SER:OG	1:A:511:GLU:OE2	2.25	0.45
1:A:1395:ASP:N	1:A:1395:ASP:OD1	2.49	0.45
1:B:1301:ASP:O	1:B:1305:THR:HG23	2.17	0.45
1:C:1950:GLY:N	1:C:1951:PRO:HA	2.32	0.45
1:C:598:LEU:C	1:C:598:LEU:HD23	2.37	0.45
1:D:477:GLU:OE2	1:D:493:VAL:HG11	2.17	0.45
1:A:406:ASP:OD1	1:A:406:ASP:N	2.49	0.45
1:D:671:ARG:HG3	1:D:673:VAL:HG23	1.99	0.45
1:D:972:LEU:O	1:D:976:GLN:HG3	2.17	0.45
1:D:1542:MET:H	1:D:1542:MET:CE	2.29	0.45
1:A:1301:ASP:O	1:A:1305:THR:HG23	2.17	0.45
1:A:1542:MET:H	1:A:1542:MET:CE	2.30	0.45
1:A:1950:GLY:N	1:A:1951:PRO:HA	2.32	0.45
1:D:1247:HIS:NE2	1:D:1250:LEU:HD11	2.33	0.45
1:A:216:ASN:HD21	1:B:1489:THR:HG21	1.82	0.44
1:A:1247:HIS:NE2	1:A:1250:LEU:HD11	2.33	0.44
1:B:1247:HIS:NE2	1:B:1250:LEU:HD11	2.32	0.44
1:C:671:ARG:HG3	1:C:673:VAL:HG23	1.99	0.44
1:C:2502:PHE:CD2	6:C:2710:PCW:C47	2.97	0.44
1:D:1301:ASP:O	1:D:1305:THR:HG23	2.17	0.44
1:D:1543:ASP:N	1:D:1543:ASP:OD1	2.51	0.44
1:D:1950:GLY:N	1:D:1951:PRO:HA	2.32	0.44
1:B:146:ASN:HD22	1:C:1534:LYS:H	1.61	0.44
1:B:709:ARG:NH2	1:B:766:ASP:OD1	2.51	0.44
1:B:972:LEU:O	1:B:976:GLN:HG3	2.17	0.44
1:C:972:LEU:O	1:C:976:GLN:HG3	2.17	0.44
1:D:64:ARG:NH1	1:D:100:GLU:OE2	2.51	0.44
1:B:280:ASN:O	1:B:308:HIS:NE2	2.50	0.44
1:C:216:ASN:OD1	1:D:1487:ASN:O	2.34	0.44
1:C:709:ARG:NH2	1:C:766:ASP:OD1	2.51	0.44
1:C:1301:ASP:O	1:C:1305:THR:HG23	2.17	0.44
1:D:598:LEU:C	1:D:598:LEU:HD23	2.37	0.44
1:D:1962:HIS:ND1	1:D:1964:SER:OG	2.40	0.44
1:A:64:ARG:NH1	1:A:100:GLU:OE2	2.51	0.44
1:A:1402:HIS:ND1	1:A:1403:GLU:N	2.65	0.44
1:A:2545:ARG:HH22	1:D:2164:GLN:HG3	1.83	0.44
1:B:146:ASN:CB	1:C:1534:LYS:H	2.22	0.44
1:B:1288:HIS:HD1	1:B:1288:HIS:C	2.21	0.44
1:B:1950:GLY:N	1:B:1951:PRO:HA	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:ARG:NH1	1:C:100:GLU:OE2	2.51	0.44
1:C:811:THR:OG1	1:C:814:ASP:OD1	2.31	0.44
1:C:1402:HIS:ND1	1:C:1403:GLU:N	2.65	0.44
1:D:720:ALA:O	1:D:724:ASN:ND2	2.46	0.44
1:A:1209:LEU:O	1:A:1212:ILE:HG22	2.18	0.44
1:A:1483:PRO:HA	1:D:214:ASN:HD21	0.62	0.44
1:B:1402:HIS:ND1	1:B:1403:GLU:N	2.66	0.44
1:B:1541:PRO:O	1:B:1545:ASP:N	2.45	0.44
1:B:477:GLU:OE2	1:B:493:VAL:HG11	2.17	0.44
1:C:252:LEU:HD13	1:C:417:LEU:CD1	2.46	0.44
1:A:145:LYS:N	1:B:1534:LYS:C	2.71	0.44
1:A:858:LYS:O	1:A:862:GLU:HG2	2.17	0.44
1:C:586:GLY:N	1:C:592:GLU:OE2	2.48	0.44
1:A:1543:ASP:OD1	1:A:1543:ASP:N	2.51	0.44
1:B:279:SER:OG	1:B:511:GLU:OE2	2.25	0.44
1:C:1543:ASP:OD1	1:C:1543:ASP:N	2.51	0.44
1:D:1209:LEU:O	1:D:1212:ILE:HG22	2.18	0.44
1:B:1543:ASP:OD1	1:B:1543:ASP:N	2.51	0.44
1:C:2531:GLU:OE2	1:C:2531:GLU:HA	2.18	0.44
1:D:606:LEU:HD23	1:D:645:ILE:CD1	2.48	0.44
1:D:1402:HIS:ND1	1:D:1403:GLU:N	2.65	0.44
1:B:1994:ASP:OD1	1:B:2052:ASN:ND2	2.51	0.43
1:B:2531:GLU:HA	1:B:2531:GLU:OE2	2.18	0.43
1:D:240:VAL:HG11	1:D:309:LEU:HD22	2.00	0.43
1:C:240:VAL:HG11	1:C:309:LEU:HD22	2.00	0.43
1:C:1209:LEU:O	1:C:1212:ILE:HG22	2.18	0.43
1:A:709:ARG:NH2	1:A:766:ASP:OD1	2.50	0.43
1:A:972:LEU:O	1:A:976:GLN:HG3	2.17	0.43
1:B:144:GLU:CG	1:C:1535:GLY:C	2.28	0.43
1:B:146:ASN:ND2	1:C:1532:VAL:C	2.71	0.43
1:B:1737:VAL:HG11	1:B:1757:ALA:HB2	2.00	0.43
1:D:709:ARG:NH2	1:D:766:ASP:OD1	2.50	0.43
1:A:1994:ASP:OD1	1:A:2052:ASN:ND2	2.51	0.43
1:B:64:ARG:NH1	1:B:100:GLU:OE2	2.51	0.43
1:B:1209:LEU:O	1:B:1212:ILE:HG22	2.18	0.43
1:B:1395:ASP:OD1	1:B:1395:ASP:N	2.49	0.43
1:A:199:TYR:CE1	1:B:1535:GLY:O	2.59	0.43
1:C:199:TYR:HE1	1:D:1536:ARG:HA	0.73	0.43
1:C:214:ASN:OD1	1:D:1483:PRO:O	2.28	0.43
1:C:1737:VAL:HG11	1:C:1757:ALA:HB2	2.00	0.43
1:A:1541:PRO:O	1:A:1545:ASP:N	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2531:GLU:OE2	1:A:2531:GLU:HA	2.18	0.43
1:B:2184:TRP:NE1	1:B:2302:GLY:O	2.43	0.43
1:C:720:ALA:O	1:C:724:ASN:ND2	2.46	0.43
1:A:1534:LYS:H	1:D:146:ASN:CB	2.23	0.43
1:D:1105:GLU:OE1	1:D:1105:GLU:HA	2.19	0.43
1:D:2184:TRP:NE1	1:D:2302:GLY:O	2.43	0.43
1:B:145:LYS:N	1:C:1534:LYS:C	2.70	0.43
1:C:1105:GLU:HA	1:C:1105:GLU:OE1	2.19	0.43
1:D:1994:ASP:OD1	1:D:2052:ASN:ND2	2.51	0.43
1:A:586:GLY:N	1:A:592:GLU:OE2	2.47	0.43
1:C:1994:ASP:OD1	1:C:2052:ASN:ND2	2.51	0.43
1:D:586:GLY:N	1:D:592:GLU:OE2	2.48	0.43
1:A:2164:GLN:N	1:A:2164:GLN:OE1	2.52	0.43
1:B:1323:THR:O	1:B:1327:ASN:OD1	2.37	0.43
1:B:2164:GLN:HG3	1:C:2545:ARG:HH22	1.82	0.43
1:D:1250:LEU:HD22	1:D:1264:MET:HE1	2.01	0.43
1:B:599:LEU:HB3	1:B:606:LEU:HD12	2.01	0.42
1:B:606:LEU:HD23	1:B:645:ILE:CD1	2.48	0.42
1:B:2151:THR:HG23	1:B:2154:ARG:NH2	2.34	0.42
1:C:199:TYR:CD2	1:D:1537:ALA:HA	2.54	0.42
1:C:266:ARG:NH2	3:C:2703:I3P:O43	2.52	0.42
1:C:1247:HIS:NE2	1:C:1250:LEU:HD11	2.32	0.42
1:D:2502:PHE:CD2	6:D:2701:PCW:H471	2.37	0.42
1:A:599:LEU:HB3	1:A:606:LEU:HD12	2.01	0.42
1:A:2151:THR:HG23	1:A:2154:ARG:NH2	2.34	0.42
1:B:563:SER:O	1:B:570:ASN:ND2	2.44	0.42
1:C:599:LEU:HB3	1:C:606:LEU:HD12	2.01	0.42
1:D:2531:GLU:HA	1:D:2531:GLU:OE2	2.18	0.42
1:A:1503:GLN:CG	1:A:1544:LEU:HD22	2.50	0.42
1:D:2611:VAL:HG12	1:D:2611:VAL:O	2.19	0.42
1:B:240:VAL:HG11	1:B:309:LEU:HD22	2.00	0.42
1:C:225:MET:SD	1:C:226:GLN:O	2.78	0.42
1:C:280:ASN:O	1:C:308:HIS:NE2	2.50	0.42
1:C:1116:ARG:HB3	1:C:1116:ARG:CZ	2.49	0.42
1:C:2164:GLN:N	1:C:2164:GLN:OE1	2.52	0.42
6:C:2710:PCW:H472	6:C:2710:PCW:H431	2.01	0.42
6:D:2701:PCW:H472	6:D:2701:PCW:H431	2.01	0.42
1:A:1737:VAL:HG11	1:A:1757:ALA:HB2	2.00	0.42
1:A:2611:VAL:HG12	1:A:2611:VAL:O	2.19	0.42
1:D:1541:PRO:O	1:D:1545:ASP:N	2.45	0.42
1:A:240:VAL:HG11	1:A:309:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2033:TYR:CD1	1:B:2113:PRO:HG3	2.55	0.42
1:C:2491:PRO:HG2	6:C:2711:PCW:H342	2.01	0.42
1:D:599:LEU:HB3	1:D:606:LEU:HD12	2.01	0.42
1:D:1323:THR:O	1:D:1327:ASN:OD1	2.37	0.42
1:D:1737:VAL:HG11	1:D:1757:ALA:HB2	2.00	0.42
1:D:2151:THR:HG23	1:D:2154:ARG:NH2	2.34	0.42
1:A:225:MET:SD	1:A:226:GLN:O	2.78	0.42
1:A:1323:THR:O	1:A:1327:ASN:OD1	2.37	0.42
1:A:2033:TYR:CD1	1:A:2113:PRO:HG3	2.55	0.42
1:A:2261:ILE:HG22	1:A:2261:ILE:O	2.20	0.42
1:B:1105:GLU:OE1	1:B:1105:GLU:HA	2.19	0.42
1:C:2261:ILE:HG22	1:C:2261:ILE:O	2.20	0.42
1:D:811:THR:OG1	1:D:814:ASP:OD1	2.31	0.42
1:D:1116:ARG:HB3	1:D:1116:ARG:CZ	2.49	0.42
1:D:2164:GLN:N	1:D:2164:GLN:OE1	2.52	0.42
1:A:1105:GLU:OE1	1:A:1105:GLU:HA	2.19	0.42
1:C:1541:PRO:O	1:C:1545:ASP:N	2.45	0.42
1:C:2151:THR:HG23	1:C:2154:ARG:NH2	2.34	0.42
1:C:2511:LEU:HD21	1:D:2362:VAL:HG23	2.01	0.42
1:A:1116:ARG:CZ	1:A:1116:ARG:HB3	2.49	0.42
1:A:2164:GLN:HG3	1:B:2545:ARG:HH22	1.84	0.42
1:B:1116:ARG:CZ	1:B:1116:ARG:HB3	2.49	0.42
1:C:494:LEU:HD21	1:C:554:ARG:HD2	2.02	0.42
6:A:3009:PCW:H472	6:A:3009:PCW:H431	2.01	0.42
1:B:225:MET:SD	1:B:226:GLN:O	2.78	0.42
1:C:1323:THR:O	1:C:1327:ASN:OD1	2.37	0.42
1:C:2033:TYR:CD1	1:C:2113:PRO:HG3	2.55	0.42
1:D:1503:GLN:CG	1:D:1544:LEU:HD22	2.50	0.42
1:D:2033:TYR:CD1	1:D:2113:PRO:HG3	2.55	0.41
1:D:2261:ILE:O	1:D:2261:ILE:HG22	2.20	0.41
1:A:477:GLU:OE1	1:A:493:VAL:HG11	2.21	0.41
1:B:477:GLU:OE1	1:B:493:VAL:HG11	2.21	0.41
1:B:1503:GLN:HG3	1:B:1544:LEU:HD22	2.01	0.41
1:B:2261:ILE:O	1:B:2261:ILE:HG22	2.20	0.41
6:B:2710:PCW:H472	6:B:2710:PCW:H431	2.01	0.41
1:C:1503:GLN:CG	1:C:1544:LEU:HD22	2.50	0.41
1:A:1028:ILE:HG21	1:A:1598:ILE:HD12	2.02	0.41
1:B:694:LEU:HD13	1:B:708:VAL:CG2	2.50	0.41
1:A:146:ASN:ND2	1:B:1532:VAL:C	2.73	0.41
1:A:199:TYR:HE1	1:B:1536:ARG:HA	0.72	0.41
1:C:146:ASN:CB	1:D:1534:LYS:H	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:494:LEU:HD21	1:D:554:ARG:HD2	2.02	0.41
1:D:1503:GLN:HG3	1:D:1544:LEU:HD22	2.01	0.41
1:A:494:LEU:HD21	1:A:554:ARG:HD2	2.02	0.41
1:C:694:LEU:HD13	1:C:708:VAL:CG2	2.50	0.41
1:D:225:MET:SD	1:D:226:GLN:O	2.78	0.41
1:B:1503:GLN:CG	1:B:1544:LEU:HD22	2.50	0.41
1:B:2164:GLN:N	1:B:2164:GLN:OE1	2.52	0.41
1:C:1503:GLN:HG3	1:C:1544:LEU:HD22	2.01	0.41
1:A:2367:ARG:NH2	1:B:2352:GLU:OE1	2.54	0.41
1:A:2262:ARG:NH2	6:A:3011:PCW:O1P	2.53	0.41
1:D:477:GLU:OE1	1:D:493:VAL:HG11	2.21	0.41
1:D:573:HIS:HA	1:D:576:LYS:HE3	2.02	0.41
1:D:1028:ILE:HG21	1:D:1598:ILE:HD12	2.02	0.41
1:A:1250:LEU:HD22	1:A:1264:MET:CE	2.51	0.41
1:A:1333:VAL:HG23	1:A:1333:VAL:O	2.21	0.41
1:A:1535:GLY:O	1:D:144:GLU:OE1	2.33	0.41
1:B:2367:ARG:NH2	1:C:2352:GLU:OE1	2.54	0.41
1:B:2611:VAL:O	1:B:2611:VAL:HG12	2.19	0.41
1:C:606:LEU:HD23	1:C:645:ILE:CD1	2.48	0.41
1:C:1250:LEU:HD22	1:C:1264:MET:HE1	2.03	0.41
1:C:1333:VAL:O	1:C:1333:VAL:HG23	2.21	0.41
1:D:280:ASN:O	1:D:308:HIS:NE2	2.50	0.41
1:D:694:LEU:HD13	1:D:708:VAL:CG2	2.50	0.41
1:A:144:GLU:CB	1:B:1535:GLY:CA	2.83	0.41
1:A:253:THR:HG22	1:A:254:CYS:N	2.36	0.41
1:A:1538:ILE:H	1:D:199:TYR:HE2	1.67	0.41
1:B:199:TYR:HE1	1:C:1536:ARG:HA	0.71	0.41
1:B:214:ASN:HB3	1:C:1486:GLU:H	1.24	0.41
1:B:266:ARG:NH2	3:B:2703:I3P:O43	2.52	0.41
1:C:2611:VAL:O	1:C:2611:VAL:HG12	2.19	0.41
1:A:266:ARG:NH2	3:A:3002:I3P:O43	2.52	0.40
1:A:280:ASN:O	1:A:308:HIS:NE2	2.50	0.40
1:A:722:ASP:HA	1:A:725:VAL:HG12	2.03	0.40
1:A:2498:LEU:HD23	1:A:2498:LEU:HA	1.88	0.40
1:B:494:LEU:HD21	1:B:554:ARG:HD2	2.02	0.40
1:B:524:ALA:HB3	1:B:525:PRO:HD3	2.04	0.40
1:B:1028:ILE:HG21	1:B:1598:ILE:HD12	2.02	0.40
1:C:1327:ASN:OD1	1:C:1327:ASN:N	2.54	0.40
1:D:722:ASP:HA	1:D:725:VAL:HG12	2.03	0.40
1:A:146:ASN:CB	1:B:1534:LYS:H	2.25	0.40
1:A:816:ASP:O	1:A:823:ARG:NH2	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1503:GLN:HG3	1:A:1544:LEU:HD22	2.01	0.40
1:D:494:LEU:HG	1:D:554:ARG:HG2	2.03	0.40
1:D:2498:LEU:HD23	1:D:2498:LEU:HA	1.88	0.40
1:B:253:THR:HG22	1:B:254:CYS:N	2.36	0.40
1:C:477:GLU:OE1	1:C:493:VAL:HG11	2.21	0.40
1:D:563:SER:O	1:D:570:ASN:ND2	2.44	0.40
1:D:1250:LEU:HD22	1:D:1264:MET:CE	2.51	0.40
1:A:494:LEU:HG	1:A:554:ARG:HG2	2.03	0.40
1:A:554:ARG:NH2	1:A:588:ASP:O	2.55	0.40
1:C:573:HIS:HA	1:C:576:LYS:HE3	2.02	0.40
1:D:1247:HIS:CD2	1:D:1250:LEU:HD11	2.57	0.40
1:A:694:LEU:HD13	1:A:708:VAL:CG2	2.50	0.40
1:C:722:ASP:HA	1:C:725:VAL:HG12	2.04	0.40
1:D:1333:VAL:HG23	1:D:1333:VAL:O	2.21	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	2180/2671 (82%)	2136 (98%)	44 (2%)	0	100	100
1	B	2180/2671 (82%)	2136 (98%)	44 (2%)	0	100	100
1	C	2180/2671 (82%)	2136 (98%)	44 (2%)	0	100	100
1	D	2180/2671 (82%)	2136 (98%)	44 (2%)	0	100	100
All	All	8720/10684 (82%)	8544 (98%)	176 (2%)	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	2002/2385 (84%)	1964 (98%)	38 (2%)	57 80
1	B	2002/2385 (84%)	1964 (98%)	38 (2%)	57 80
1	C	2002/2385 (84%)	1964 (98%)	38 (2%)	57 80
1	D	2002/2385 (84%)	1964 (98%)	38 (2%)	57 80
All	All	8008/9540 (84%)	7856 (98%)	152 (2%)	59 80

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	558	ARG
1	A	580	MET
1	A	590	LEU
1	A	636	ASP
1	A	727	SER
1	A	817	SER
1	A	846	SER
1	A	1035	MET
1	A	1044	MET
1	A	1120	MET
1	A	1200	MET
1	A	1208	ASP
1	A	1252	LEU
1	A	1273	GLN
1	A	1322	MET
1	A	1327	ASN
1	A	1370	ASP
1	A	1375	CYS
1	A	1382	TYR
1	A	1395	ASP
1	A	1428	MET
1	A	1443	ASN
1	A	1542	MET
1	A	1543	ASP

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Mol	Chain	Res	Type
1	A	1639	GLU
1	A	1681	ASP
1	A	1795	ARG
1	A	1802	SER
1	A	1905	CYS
1	A	1977	ASP
1	A	2129	GLN
1	A	2145	GLN
1	A	2197	PHE
1	A	2297	VAL
1	A	2353	GLU
1	A	2461	CYS
1	A	2520	PHE
1	A	2532	GLU
1	B	558	ARG
1	B	580	MET
1	B	590	LEU
1	B	636	ASP
1	B	727	SER
1	B	817	SER
1	B	846	SER
1	B	1035	MET
1	B	1044	MET
1	B	1120	MET
1	B	1200	MET
1	B	1208	ASP
1	B	1252	LEU
1	B	1273	GLN
1	B	1322	MET
1	B	1327	ASN
1	B	1370	ASP
1	B	1375	CYS
1	B	1382	TYR
1	B	1395	ASP
1	B	1428	MET
1	B	1443	ASN
1	B	1542	MET
1	B	1543	ASP
1	B	1639	GLU
1	B	1681	ASP
1	B	1795	ARG
1	B	1802	SER

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Mol	Chain	Res	Type
1	B	1905	CYS
1	B	1977	ASP
1	B	2129	GLN
1	B	2145	GLN
1	B	2197	PHE
1	B	2297	VAL
1	B	2353	GLU
1	B	2461	CYS
1	B	2520	PHE
1	B	2532	GLU
1	C	558	ARG
1	C	580	MET
1	C	590	LEU
1	C	636	ASP
1	C	727	SER
1	C	817	SER
1	C	846	SER
1	C	1035	MET
1	C	1044	MET
1	C	1120	MET
1	C	1200	MET
1	C	1208	ASP
1	C	1252	LEU
1	C	1273	GLN
1	C	1322	MET
1	C	1327	ASN
1	C	1370	ASP
1	C	1375	CYS
1	C	1382	TYR
1	C	1395	ASP
1	C	1428	MET
1	C	1443	ASN
1	C	1542	MET
1	C	1543	ASP
1	C	1639	GLU
1	C	1681	ASP
1	C	1795	ARG
1	C	1802	SER
1	C	1905	CYS
1	C	1977	ASP
1	C	2129	GLN
1	C	2145	GLN

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Mol	Chain	Res	Type
1	C	2197	PHE
1	C	2297	VAL
1	C	2353	GLU
1	C	2461	CYS
1	C	2520	PHE
1	C	2532	GLU
1	D	558	ARG
1	D	580	MET
1	D	590	LEU
1	D	636	ASP
1	D	727	SER
1	D	817	SER
1	D	846	SER
1	D	1035	MET
1	D	1044	MET
1	D	1120	MET
1	D	1200	MET
1	D	1208	ASP
1	D	1252	LEU
1	D	1273	GLN
1	D	1322	MET
1	D	1327	ASN
1	D	1370	ASP
1	D	1375	CYS
1	D	1382	TYR
1	D	1395	ASP
1	D	1428	MET
1	D	1443	ASN
1	D	1542	MET
1	D	1543	ASP
1	D	1639	GLU
1	D	1681	ASP
1	D	1795	ARG
1	D	1802	SER
1	D	1905	CYS
1	D	1977	ASP
1	D	2129	GLN
1	D	2145	GLN
1	D	2197	PHE
1	D	2297	VAL
1	D	2353	GLU
1	D	2461	CYS

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Mol	Chain	Res	Type
1	D	2520	PHE
1	D	2532	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	195	HIS
1	B	146	ASN
1	B	195	HIS
1	B	214	ASN
1	C	146	ASN
1	C	195	HIS
1	C	214	ASN
1	D	146	ASN
1	D	195	HIS
1	D	214	ASN
1	D	2550	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 44 ligands modelled in this entry, 12 are monoatomic - leaving 32 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ATP	C	2706	-	26,33,33	0.61	0	31,52,52	1.06	2 (6%)
5	ATP	D	2708	-	26,33,33	0.59	0	31,52,52	1.07	2 (6%)
3	I3P	B	2703	-	24,24,24	2.07	3 (12%)	36,39,39	0.89	0
6	PCW	D	2701	-	47,47,53	0.53	0	52,55,61	0.55	1 (1%)
5	ATP	A	3005	-	26,33,33	0.60	0	31,52,52	1.07	2 (6%)
6	PCW	B	2710	-	47,47,53	0.53	0	52,55,61	0.55	1 (1%)
6	PCW	B	2709	-	40,40,53	0.54	0	46,48,61	0.53	0
5	ATP	B	2706	-	26,33,33	0.61	0	31,52,52	1.06	2 (6%)
6	PCW	B	2707	-	42,42,53	0.53	0	48,50,61	0.50	0
3	I3P	C	2703	-	24,24,24	2.07	3 (12%)	36,39,39	0.89	0
6	PCW	A	3009	-	47,47,53	0.53	0	52,55,61	0.55	1 (1%)
6	PCW	B	2701	-	50,50,53	0.50	0	56,58,61	0.53	0
6	PCW	A	3010	-	45,45,53	0.52	0	50,53,61	0.48	0
6	PCW	A	3011	-	50,50,53	0.50	0	56,58,61	0.53	0
6	PCW	C	2709	-	40,40,53	0.54	0	46,48,61	0.53	0
3	I3P	D	2705	-	24,24,24	2.08	3 (12%)	36,39,39	0.89	0
6	PCW	B	2711	-	45,45,53	0.52	0	50,53,61	0.48	0
6	PCW	A	3006	-	42,42,53	0.53	0	48,50,61	0.50	0
6	PCW	D	2709	-	42,42,53	0.52	0	48,50,61	0.50	0
6	PCW	C	2701	-	50,50,53	0.50	0	56,58,61	0.53	0
6	PCW	A	3008	-	40,40,53	0.54	0	46,48,61	0.53	0
6	PCW	D	2703	-	50,50,53	0.50	0	56,58,61	0.53	0
6	PCW	C	2710	-	47,47,53	0.52	0	52,55,61	0.55	1 (1%)
6	PCW	C	2711	-	45,45,53	0.52	0	50,53,61	0.47	0
6	PCW	D	2711	-	40,40,53	0.55	0	46,48,61	0.53	0
6	PCW	C	2707	-	42,42,53	0.53	0	48,50,61	0.50	0
6	PCW	D	2710	-	47,47,53	0.51	0	52,55,61	0.48	0
6	PCW	A	3007	-	47,47,53	0.51	0	52,55,61	0.48	0
3	I3P	A	3002	-	24,24,24	2.07	3 (12%)	36,39,39	0.89	0
6	PCW	D	2702	-	45,45,53	0.52	0	50,53,61	0.48	0
6	PCW	C	2708	-	47,47,53	0.51	0	52,55,61	0.48	0
6	PCW	B	2708	-	47,47,53	0.51	0	52,55,61	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	C	2706	-	-	11/18/38/38	0/3/3/3
5	ATP	D	2708	-	-	11/18/38/38	0/3/3/3
3	I3P	B	2703	-	-	2/15/39/39	0/1/1/1
6	PCW	D	2701	-	-	12/51/51/57	-
5	ATP	A	3005	-	-	11/18/38/38	0/3/3/3
6	PCW	B	2710	-	-	12/51/51/57	-
6	PCW	B	2709	-	-	10/44/44/57	-
5	ATP	B	2706	-	-	11/18/38/38	0/3/3/3
6	PCW	B	2707	-	-	11/46/46/57	-
3	I3P	C	2703	-	-	2/15/39/39	0/1/1/1
6	PCW	A	3009	-	-	12/51/51/57	-
6	PCW	B	2701	-	-	21/54/54/57	-
6	PCW	A	3010	-	-	13/49/49/57	-
6	PCW	A	3011	-	-	21/54/54/57	-
6	PCW	C	2709	-	-	10/44/44/57	-
3	I3P	D	2705	-	-	2/15/39/39	0/1/1/1
6	PCW	B	2711	-	-	13/49/49/57	-
6	PCW	A	3006	-	-	11/46/46/57	-
6	PCW	D	2709	-	-	11/46/46/57	-
6	PCW	C	2701	-	-	21/54/54/57	-
6	PCW	A	3008	-	-	10/44/44/57	-
6	PCW	D	2703	-	-	21/54/54/57	-
6	PCW	C	2710	-	-	12/51/51/57	-
6	PCW	C	2711	-	-	13/49/49/57	-
6	PCW	D	2711	-	-	10/44/44/57	-
6	PCW	C	2707	-	-	11/46/46/57	-
6	PCW	D	2710	-	-	16/51/51/57	-
6	PCW	A	3007	-	-	16/51/51/57	-
3	I3P	A	3002	-	-	2/15/39/39	0/1/1/1
6	PCW	D	2702	-	-	13/49/49/57	-
6	PCW	C	2708	-	-	16/51/51/57	-
6	PCW	B	2708	-	-	16/51/51/57	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2705	I3P	P4-O4	5.69	1.70	1.59
3	A	3002	I3P	P4-O4	5.69	1.70	1.59
3	D	2705	I3P	P5-O5	5.68	1.70	1.59
3	B	2703	I3P	P4-O4	5.67	1.70	1.59
3	C	2703	I3P	P4-O4	5.67	1.70	1.59
3	A	3002	I3P	P5-O5	5.66	1.70	1.59
3	B	2703	I3P	P5-O5	5.66	1.70	1.59
3	C	2703	I3P	P5-O5	5.66	1.70	1.59
3	D	2705	I3P	P1-O1	5.41	1.69	1.59
3	A	3002	I3P	P1-O1	5.40	1.69	1.59
3	B	2703	I3P	P1-O1	5.37	1.69	1.59
3	C	2703	I3P	P1-O1	5.37	1.69	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	2708	ATP	C5-C6-N6	2.33	123.89	120.35
5	A	3005	ATP	C5-C6-N6	2.32	123.88	120.35
5	B	2706	ATP	C5-C6-N6	2.30	123.85	120.35
5	C	2706	ATP	C5-C6-N6	2.30	123.85	120.35
6	A	3009	PCW	C3-C2-C1	2.15	116.88	111.79
6	B	2710	PCW	C3-C2-C1	2.15	116.88	111.79
6	D	2701	PCW	C3-C2-C1	2.15	116.88	111.79
6	C	2710	PCW	C3-C2-C1	2.15	116.88	111.79
5	B	2706	ATP	PB-O3B-PG	2.04	139.84	132.83
5	C	2706	ATP	PB-O3B-PG	2.04	139.84	132.83
5	A	3005	ATP	PB-O3B-PG	2.04	139.83	132.83
5	D	2708	ATP	PB-O3B-PG	2.02	139.77	132.83

There are no chirality outliers.

All (384) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3002	I3P	C5-O5-P5-O51
3	B	2703	I3P	C5-O5-P5-O51
3	C	2703	I3P	C5-O5-P5-O51
3	D	2705	I3P	C5-O5-P5-O51
5	A	3005	ATP	PB-O3B-PG-O3G
5	A	3005	ATP	C5'-O5'-PA-O1A
5	A	3005	ATP	C5'-O5'-PA-O2A
5	B	2706	ATP	PB-O3B-PG-O3G
5	B	2706	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	B	2706	ATP	C5'-O5'-PA-O2A
5	C	2706	ATP	PB-O3B-PG-O3G
5	C	2706	ATP	C5'-O5'-PA-O1A
5	C	2706	ATP	C5'-O5'-PA-O2A
5	D	2708	ATP	PB-O3B-PG-O3G
5	D	2708	ATP	C5'-O5'-PA-O1A
5	D	2708	ATP	C5'-O5'-PA-O2A
6	A	3006	PCW	C1-O3P-P-O1P
6	A	3006	PCW	C1-O3P-P-O2P
6	A	3006	PCW	C1-O3P-P-O4P
6	A	3007	PCW	C1-O3P-P-O2P
6	A	3008	PCW	C2-C1-O3P-P
6	A	3008	PCW	O4P-C4-C5-N
6	A	3008	PCW	C1-O3P-P-O4P
6	A	3009	PCW	C32-C31-O2-C2
6	A	3009	PCW	C1-O3P-P-O2P
6	A	3010	PCW	O3P-C1-C2-O2
6	A	3010	PCW	O4P-C4-C5-N
6	A	3010	PCW	C32-C31-O2-C2
6	A	3010	PCW	C1-O3P-P-O1P
6	A	3010	PCW	C1-O3P-P-O2P
6	A	3011	PCW	C1-O3P-P-O1P
6	A	3011	PCW	C4-O4P-P-O1P
6	B	2701	PCW	C1-O3P-P-O1P
6	B	2701	PCW	C4-O4P-P-O1P
6	B	2707	PCW	C1-O3P-P-O1P
6	B	2707	PCW	C1-O3P-P-O2P
6	B	2707	PCW	C1-O3P-P-O4P
6	B	2708	PCW	C1-O3P-P-O2P
6	B	2709	PCW	C2-C1-O3P-P
6	B	2709	PCW	O4P-C4-C5-N
6	B	2709	PCW	C1-O3P-P-O4P
6	B	2710	PCW	C32-C31-O2-C2
6	B	2710	PCW	C1-O3P-P-O2P
6	B	2711	PCW	O3P-C1-C2-O2
6	B	2711	PCW	O4P-C4-C5-N
6	B	2711	PCW	C32-C31-O2-C2
6	B	2711	PCW	C1-O3P-P-O1P
6	B	2711	PCW	C1-O3P-P-O2P
6	C	2701	PCW	C1-O3P-P-O1P
6	C	2701	PCW	C4-O4P-P-O1P
6	C	2707	PCW	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
6	C	2707	PCW	C1-O3P-P-O2P
6	C	2707	PCW	C1-O3P-P-O4P
6	C	2708	PCW	C1-O3P-P-O2P
6	C	2709	PCW	C2-C1-O3P-P
6	C	2709	PCW	O4P-C4-C5-N
6	C	2709	PCW	C1-O3P-P-O4P
6	C	2710	PCW	C32-C31-O2-C2
6	C	2710	PCW	C1-O3P-P-O2P
6	C	2711	PCW	O3P-C1-C2-O2
6	C	2711	PCW	O4P-C4-C5-N
6	C	2711	PCW	C32-C31-O2-C2
6	C	2711	PCW	C1-O3P-P-O1P
6	C	2711	PCW	C1-O3P-P-O2P
6	D	2701	PCW	C32-C31-O2-C2
6	D	2701	PCW	C1-O3P-P-O2P
6	D	2702	PCW	O3P-C1-C2-O2
6	D	2702	PCW	O4P-C4-C5-N
6	D	2702	PCW	C32-C31-O2-C2
6	D	2702	PCW	C1-O3P-P-O1P
6	D	2702	PCW	C1-O3P-P-O2P
6	D	2703	PCW	C1-O3P-P-O1P
6	D	2703	PCW	C4-O4P-P-O1P
6	D	2709	PCW	C1-O3P-P-O1P
6	D	2709	PCW	C1-O3P-P-O2P
6	D	2709	PCW	C1-O3P-P-O4P
6	D	2710	PCW	C1-O3P-P-O2P
6	D	2711	PCW	C2-C1-O3P-P
6	D	2711	PCW	O4P-C4-C5-N
6	D	2711	PCW	C1-O3P-P-O4P
6	A	3007	PCW	O11-C11-O3-C3
6	B	2708	PCW	O11-C11-O3-C3
6	C	2708	PCW	O11-C11-O3-C3
6	D	2710	PCW	O11-C11-O3-C3
6	A	3010	PCW	O31-C31-O2-C2
6	B	2711	PCW	O31-C31-O2-C2
6	C	2711	PCW	O31-C31-O2-C2
6	D	2702	PCW	O31-C31-O2-C2
6	A	3006	PCW	C12-C11-O3-C3
6	A	3007	PCW	C12-C11-O3-C3
6	B	2707	PCW	C12-C11-O3-C3
6	B	2708	PCW	C12-C11-O3-C3
6	C	2707	PCW	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
6	C	2708	PCW	C12-C11-O3-C3
6	D	2709	PCW	C12-C11-O3-C3
6	D	2710	PCW	C12-C11-O3-C3
6	A	3009	PCW	O31-C31-O2-C2
6	B	2710	PCW	O31-C31-O2-C2
6	C	2710	PCW	O31-C31-O2-C2
6	D	2701	PCW	O31-C31-O2-C2
6	A	3006	PCW	O11-C11-O3-C3
6	B	2707	PCW	O11-C11-O3-C3
6	C	2707	PCW	O11-C11-O3-C3
6	D	2709	PCW	O11-C11-O3-C3
6	A	3009	PCW	C15-C16-C17-C18
6	B	2710	PCW	C15-C16-C17-C18
6	C	2710	PCW	C15-C16-C17-C18
6	D	2701	PCW	C15-C16-C17-C18
6	C	2710	PCW	C44-C45-C46-C47
6	A	3009	PCW	C44-C45-C46-C47
6	B	2710	PCW	C44-C45-C46-C47
6	D	2701	PCW	C44-C45-C46-C47
6	A	3007	PCW	C1-O3P-P-O4P
6	A	3009	PCW	C1-O3P-P-O4P
6	A	3010	PCW	C1-O3P-P-O4P
6	A	3011	PCW	C1-O3P-P-O4P
6	B	2701	PCW	C1-O3P-P-O4P
6	B	2708	PCW	C1-O3P-P-O4P
6	B	2710	PCW	C1-O3P-P-O4P
6	B	2711	PCW	C1-O3P-P-O4P
6	C	2701	PCW	C1-O3P-P-O4P
6	C	2708	PCW	C1-O3P-P-O4P
6	C	2710	PCW	C1-O3P-P-O4P
6	C	2711	PCW	C1-O3P-P-O4P
6	D	2701	PCW	C1-O3P-P-O4P
6	D	2702	PCW	C1-O3P-P-O4P
6	D	2703	PCW	C1-O3P-P-O4P
6	D	2710	PCW	C1-O3P-P-O4P
6	A	3010	PCW	C12-C11-O3-C3
6	B	2711	PCW	C12-C11-O3-C3
6	C	2711	PCW	C12-C11-O3-C3
6	D	2702	PCW	C12-C11-O3-C3
6	A	3007	PCW	C32-C31-O2-C2
6	B	2708	PCW	C32-C31-O2-C2
6	C	2708	PCW	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
6	D	2710	PCW	C32-C31-O2-C2
6	A	3011	PCW	C35-C36-C37-C38
6	B	2701	PCW	C35-C36-C37-C38
6	C	2701	PCW	C35-C36-C37-C38
6	D	2703	PCW	C35-C36-C37-C38
6	A	3007	PCW	O31-C31-O2-C2
6	B	2708	PCW	O31-C31-O2-C2
6	C	2708	PCW	O31-C31-O2-C2
6	D	2710	PCW	O31-C31-O2-C2
6	A	3007	PCW	C35-C36-C37-C38
6	B	2708	PCW	C35-C36-C37-C38
6	C	2708	PCW	C35-C36-C37-C38
6	D	2710	PCW	C35-C36-C37-C38
6	A	3006	PCW	C20-C21-C22-C23
6	B	2707	PCW	C20-C21-C22-C23
6	C	2707	PCW	C20-C21-C22-C23
6	D	2709	PCW	C20-C21-C22-C23
6	A	3010	PCW	O11-C11-O3-C3
6	B	2711	PCW	O11-C11-O3-C3
6	C	2711	PCW	O11-C11-O3-C3
6	D	2702	PCW	O11-C11-O3-C3
6	B	2701	PCW	C34-C35-C36-C37
6	A	3011	PCW	C34-C35-C36-C37
6	C	2701	PCW	C34-C35-C36-C37
6	D	2703	PCW	C34-C35-C36-C37
6	A	3011	PCW	C32-C31-O2-C2
6	B	2701	PCW	C32-C31-O2-C2
6	C	2701	PCW	C32-C31-O2-C2
6	D	2703	PCW	C32-C31-O2-C2
6	A	3009	PCW	C13-C14-C15-C16
6	B	2710	PCW	C13-C14-C15-C16
6	C	2710	PCW	C13-C14-C15-C16
6	D	2701	PCW	C13-C14-C15-C16
5	A	3005	ATP	C3'-C4'-C5'-O5'
5	B	2706	ATP	C3'-C4'-C5'-O5'
5	C	2706	ATP	C3'-C4'-C5'-O5'
5	D	2708	ATP	C3'-C4'-C5'-O5'
6	A	3011	PCW	O31-C31-O2-C2
6	B	2701	PCW	O31-C31-O2-C2
6	C	2701	PCW	O31-C31-O2-C2
6	D	2703	PCW	O31-C31-O2-C2
6	A	3007	PCW	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
6	B	2708	PCW	C42-C43-C44-C45
6	C	2708	PCW	C42-C43-C44-C45
6	D	2710	PCW	C42-C43-C44-C45
6	A	3007	PCW	O2-C2-C3-O3
6	B	2708	PCW	O2-C2-C3-O3
6	C	2708	PCW	O2-C2-C3-O3
6	D	2710	PCW	O2-C2-C3-O3
5	A	3005	ATP	O4'-C4'-C5'-O5'
5	B	2706	ATP	O4'-C4'-C5'-O5'
5	C	2706	ATP	O4'-C4'-C5'-O5'
5	D	2708	ATP	O4'-C4'-C5'-O5'
6	A	3006	PCW	C13-C14-C15-C16
6	B	2707	PCW	C13-C14-C15-C16
6	C	2707	PCW	C13-C14-C15-C16
6	D	2709	PCW	C13-C14-C15-C16
6	A	3011	PCW	C4-O4P-P-O3P
6	C	2701	PCW	C4-O4P-P-O3P
6	D	2703	PCW	C4-O4P-P-O3P
6	D	2710	PCW	C15-C16-C17-C18
6	A	3007	PCW	C15-C16-C17-C18
6	B	2708	PCW	C15-C16-C17-C18
6	C	2708	PCW	C15-C16-C17-C18
6	A	3010	PCW	O3P-C1-C2-C3
6	B	2711	PCW	O3P-C1-C2-C3
6	C	2711	PCW	O3P-C1-C2-C3
6	D	2702	PCW	O3P-C1-C2-C3
6	B	2701	PCW	C31-C32-C33-C34
6	C	2701	PCW	C31-C32-C33-C34
6	D	2703	PCW	C31-C32-C33-C34
6	B	2701	PCW	C12-C13-C14-C15
6	A	3011	PCW	C12-C13-C14-C15
6	C	2701	PCW	C12-C13-C14-C15
6	D	2703	PCW	C12-C13-C14-C15
6	A	3011	PCW	C31-C32-C33-C34
6	A	3011	PCW	C12-C11-O3-C3
6	B	2701	PCW	C12-C11-O3-C3
6	C	2701	PCW	C12-C11-O3-C3
6	D	2703	PCW	C12-C11-O3-C3
6	A	3008	PCW	C39-C40-C41-C42
6	B	2709	PCW	C39-C40-C41-C42
6	C	2709	PCW	C39-C40-C41-C42
6	D	2711	PCW	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
6	A	3011	PCW	O3P-C1-C2-C3
6	B	2701	PCW	O3P-C1-C2-C3
6	C	2701	PCW	O3P-C1-C2-C3
6	D	2703	PCW	O3P-C1-C2-C3
6	A	3006	PCW	C11-C12-C13-C14
6	B	2707	PCW	C11-C12-C13-C14
6	C	2707	PCW	C11-C12-C13-C14
6	D	2709	PCW	C11-C12-C13-C14
6	A	3006	PCW	C1-C2-C3-O3
6	A	3007	PCW	C1-C2-C3-O3
6	B	2707	PCW	C1-C2-C3-O3
6	B	2708	PCW	C1-C2-C3-O3
6	C	2707	PCW	C1-C2-C3-O3
6	C	2708	PCW	C1-C2-C3-O3
6	D	2709	PCW	C1-C2-C3-O3
6	D	2710	PCW	C1-C2-C3-O3
6	B	2701	PCW	C4-O4P-P-O3P
6	A	3006	PCW	O2-C2-C3-O3
6	B	2707	PCW	O2-C2-C3-O3
6	C	2707	PCW	O2-C2-C3-O3
6	D	2709	PCW	O2-C2-C3-O3
6	A	3009	PCW	C40-C41-C42-C43
6	B	2710	PCW	C40-C41-C42-C43
6	C	2710	PCW	C40-C41-C42-C43
6	D	2701	PCW	C40-C41-C42-C43
6	A	3010	PCW	C19-C20-C21-C22
6	B	2711	PCW	C19-C20-C21-C22
6	C	2711	PCW	C19-C20-C21-C22
6	D	2702	PCW	C19-C20-C21-C22
6	A	3007	PCW	C34-C35-C36-C37
6	B	2708	PCW	C34-C35-C36-C37
6	C	2708	PCW	C34-C35-C36-C37
6	D	2703	PCW	C37-C38-C39-C40
6	D	2710	PCW	C34-C35-C36-C37
6	A	3011	PCW	O11-C11-O3-C3
6	B	2701	PCW	O11-C11-O3-C3
6	C	2701	PCW	O11-C11-O3-C3
6	D	2703	PCW	O11-C11-O3-C3
6	A	3011	PCW	O3P-C1-C2-O2
6	B	2701	PCW	O3P-C1-C2-O2
6	C	2701	PCW	O3P-C1-C2-O2
6	D	2703	PCW	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	A	3011	PCW	C37-C38-C39-C40
6	B	2701	PCW	C37-C38-C39-C40
6	C	2701	PCW	C37-C38-C39-C40
5	A	3005	ATP	PB-O3B-PG-O2G
5	B	2706	ATP	PB-O3B-PG-O2G
5	C	2706	ATP	PB-O3B-PG-O2G
5	D	2708	ATP	PB-O3B-PG-O2G
6	A	3011	PCW	O2-C2-C3-O3
6	B	2701	PCW	O2-C2-C3-O3
6	C	2701	PCW	O2-C2-C3-O3
6	D	2703	PCW	O2-C2-C3-O3
3	A	3002	I3P	C5-O5-P5-O53
3	B	2703	I3P	C5-O5-P5-O53
3	C	2703	I3P	C5-O5-P5-O53
3	D	2705	I3P	C5-O5-P5-O53
5	A	3005	ATP	C5'-O5'-PA-O3A
5	B	2706	ATP	C5'-O5'-PA-O3A
5	C	2706	ATP	C5'-O5'-PA-O3A
5	D	2708	ATP	C5'-O5'-PA-O3A
6	A	3011	PCW	C36-C37-C38-C39
6	B	2701	PCW	C36-C37-C38-C39
6	C	2701	PCW	C36-C37-C38-C39
6	D	2703	PCW	C36-C37-C38-C39
5	A	3005	ATP	PB-O3A-PA-O2A
5	B	2706	ATP	PB-O3A-PA-O2A
5	C	2706	ATP	PB-O3A-PA-O2A
5	D	2708	ATP	PB-O3A-PA-O2A
6	A	3007	PCW	C1-O3P-P-O1P
6	A	3008	PCW	C1-O3P-P-O2P
6	A	3009	PCW	C1-O3P-P-O1P
6	A	3011	PCW	C1-O3P-P-O2P
6	B	2701	PCW	C1-O3P-P-O2P
6	B	2708	PCW	C1-O3P-P-O1P
6	B	2709	PCW	C1-O3P-P-O2P
6	B	2710	PCW	C1-O3P-P-O1P
6	C	2701	PCW	C1-O3P-P-O2P
6	C	2708	PCW	C1-O3P-P-O1P
6	C	2709	PCW	C1-O3P-P-O2P
6	C	2710	PCW	C1-O3P-P-O1P
6	D	2701	PCW	C1-O3P-P-O1P
6	D	2703	PCW	C1-O3P-P-O2P
6	D	2710	PCW	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
6	D	2711	PCW	C1-O3P-P-O2P
6	D	2711	PCW	C32-C33-C34-C35
6	A	3008	PCW	C32-C33-C34-C35
6	B	2709	PCW	C32-C33-C34-C35
6	C	2709	PCW	C32-C33-C34-C35
6	A	3010	PCW	C13-C14-C15-C16
6	B	2711	PCW	C13-C14-C15-C16
6	C	2711	PCW	C13-C14-C15-C16
6	D	2702	PCW	C13-C14-C15-C16
6	A	3006	PCW	O4P-C4-C5-N
6	A	3011	PCW	C1-C2-C3-O3
6	B	2701	PCW	C1-C2-C3-O3
6	B	2707	PCW	O4P-C4-C5-N
6	C	2701	PCW	C1-C2-C3-O3
6	C	2707	PCW	O4P-C4-C5-N
6	D	2703	PCW	C1-C2-C3-O3
6	D	2709	PCW	O4P-C4-C5-N
6	B	2701	PCW	C3-C2-O2-C31
6	C	2701	PCW	C3-C2-O2-C31
6	D	2703	PCW	C3-C2-O2-C31
6	A	3009	PCW	C32-C33-C34-C35
6	B	2710	PCW	C32-C33-C34-C35
6	C	2710	PCW	C32-C33-C34-C35
6	D	2701	PCW	C32-C33-C34-C35
6	A	3009	PCW	C4-O4P-P-O3P
6	B	2710	PCW	C4-O4P-P-O3P
6	C	2710	PCW	C4-O4P-P-O3P
6	D	2701	PCW	C4-O4P-P-O3P
5	A	3005	ATP	PG-O3B-PB-O2B
5	B	2706	ATP	PG-O3B-PB-O2B
5	C	2706	ATP	PG-O3B-PB-O2B
5	D	2708	ATP	PG-O3B-PB-O2B
6	A	3007	PCW	C37-C38-C39-C40
6	B	2708	PCW	C37-C38-C39-C40
6	C	2708	PCW	C37-C38-C39-C40
6	D	2710	PCW	C37-C38-C39-C40
6	A	3008	PCW	O3P-C1-C2-C3
6	B	2709	PCW	O3P-C1-C2-C3
6	C	2709	PCW	O3P-C1-C2-C3
6	D	2711	PCW	O3P-C1-C2-C3
6	A	3011	PCW	C3-C2-O2-C31
6	A	3007	PCW	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	B	2708	PCW	O3P-C1-C2-O2
6	C	2708	PCW	O3P-C1-C2-O2
6	D	2710	PCW	O3P-C1-C2-O2
6	A	3007	PCW	O2-C31-C32-C33
6	B	2708	PCW	O2-C31-C32-C33
6	C	2708	PCW	O2-C31-C32-C33
6	D	2710	PCW	O2-C31-C32-C33
6	A	3008	PCW	C31-C32-C33-C34
6	B	2709	PCW	C31-C32-C33-C34
6	C	2709	PCW	C31-C32-C33-C34
6	D	2711	PCW	C31-C32-C33-C34
6	A	3008	PCW	O31-C31-O2-C2
6	B	2709	PCW	O31-C31-O2-C2
6	C	2709	PCW	O31-C31-O2-C2
6	D	2711	PCW	O31-C31-O2-C2
5	A	3005	ATP	PB-O3A-PA-O1A
5	B	2706	ATP	PB-O3A-PA-O1A
5	C	2706	ATP	PB-O3A-PA-O1A
5	D	2708	ATP	PB-O3A-PA-O1A
6	A	3008	PCW	C32-C31-O2-C2
6	B	2709	PCW	C32-C31-O2-C2
6	C	2709	PCW	C32-C31-O2-C2
6	D	2711	PCW	C32-C31-O2-C2
6	A	3009	PCW	C4-O4P-P-O2P
6	A	3011	PCW	C4-O4P-P-O2P
6	B	2701	PCW	C4-O4P-P-O2P
6	B	2710	PCW	C4-O4P-P-O2P
6	C	2701	PCW	C4-O4P-P-O2P
6	C	2710	PCW	C4-O4P-P-O2P
6	D	2701	PCW	C4-O4P-P-O2P
6	D	2703	PCW	C4-O4P-P-O2P
5	A	3005	ATP	PB-O3B-PG-O1G
5	B	2706	ATP	PB-O3B-PG-O1G
5	C	2706	ATP	PB-O3B-PG-O1G
5	D	2708	ATP	PB-O3B-PG-O1G
6	A	3010	PCW	C3-C2-O2-C31
6	B	2711	PCW	C3-C2-O2-C31
6	C	2711	PCW	C3-C2-O2-C31
6	D	2702	PCW	C3-C2-O2-C31

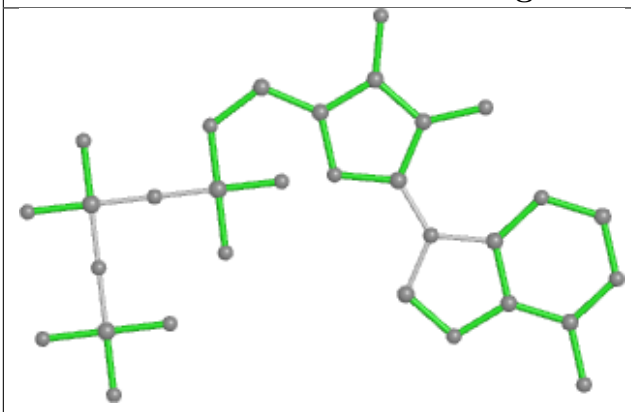
There are no ring outliers.

16 monomers are involved in 32 short contacts:

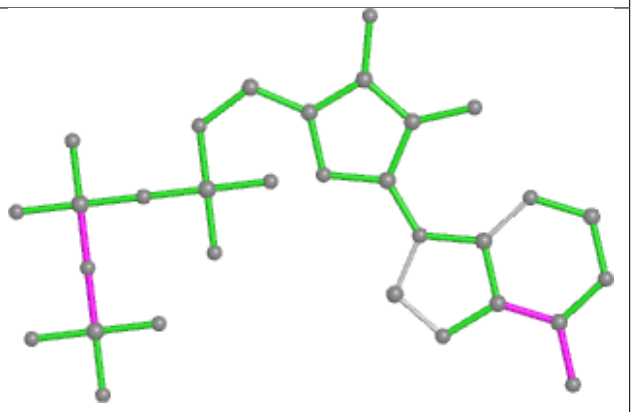
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2706	ATP	2	0
5	D	2708	ATP	2	0
3	B	2703	I3P	1	0
6	D	2701	PCW	3	0
5	A	3005	ATP	2	0
6	B	2710	PCW	3	0
5	B	2706	ATP	2	0
3	C	2703	I3P	1	0
6	A	3009	PCW	3	0
6	B	2701	PCW	2	0
6	A	3011	PCW	2	0
6	C	2701	PCW	2	0
6	D	2703	PCW	1	0
6	C	2710	PCW	4	0
6	C	2711	PCW	1	0
3	A	3002	I3P	1	0

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

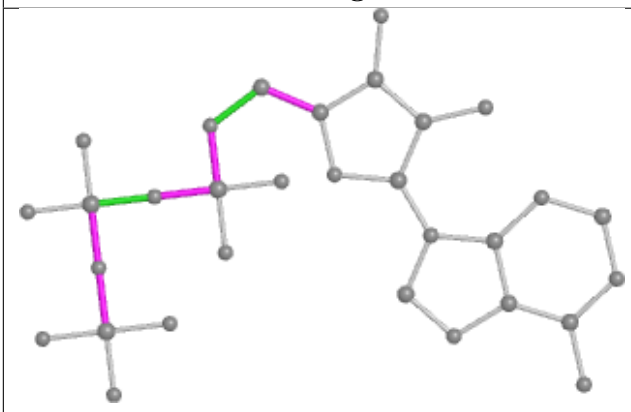
Ligand ATP C 2706



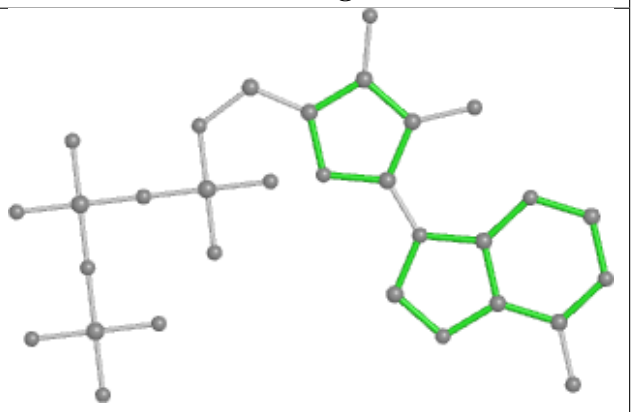
Bond lengths



Bond angles

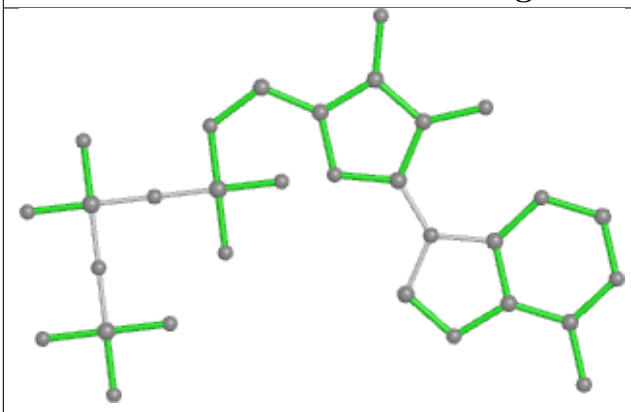


Torsions

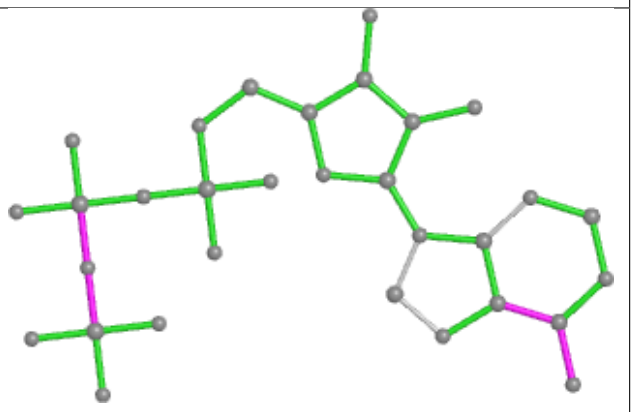


Rings

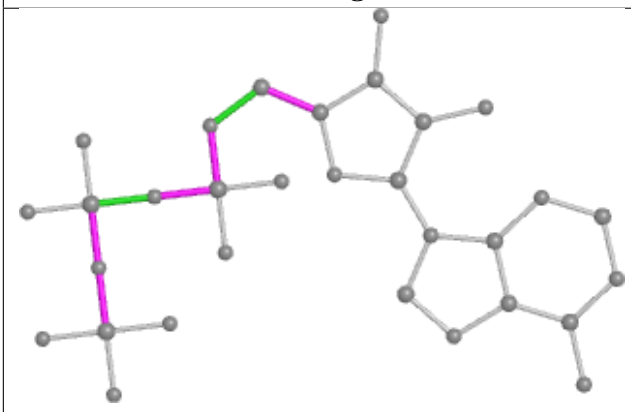
Ligand ATP D 2708



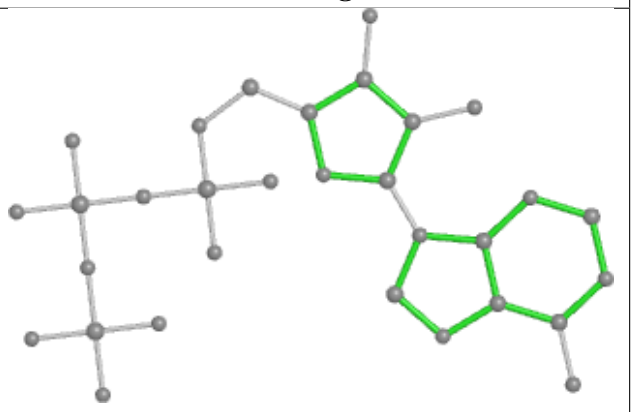
Bond lengths



Bond angles

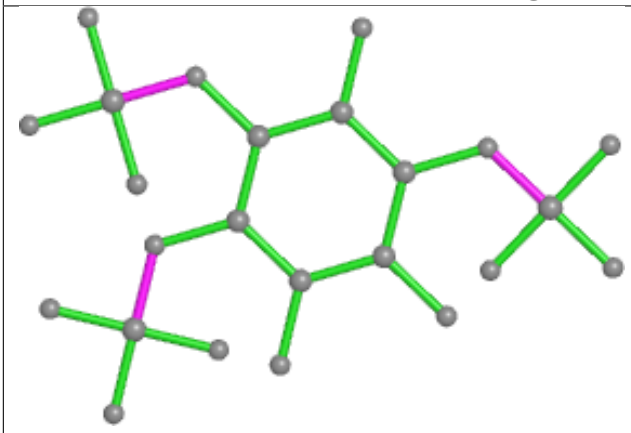


Torsions

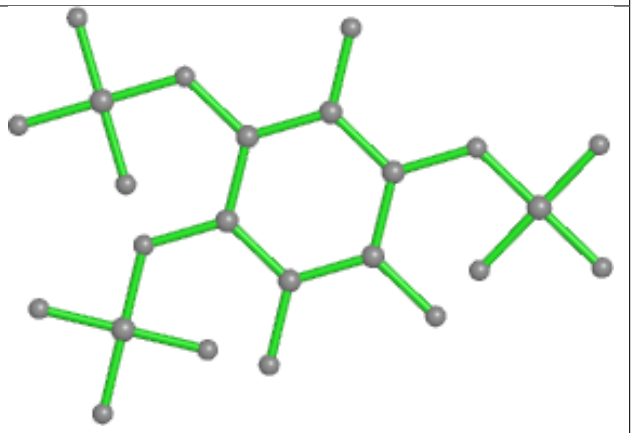


Rings

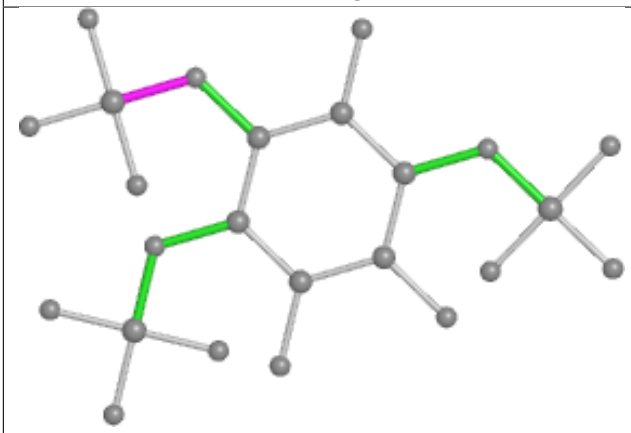
Ligand I3P B 2703



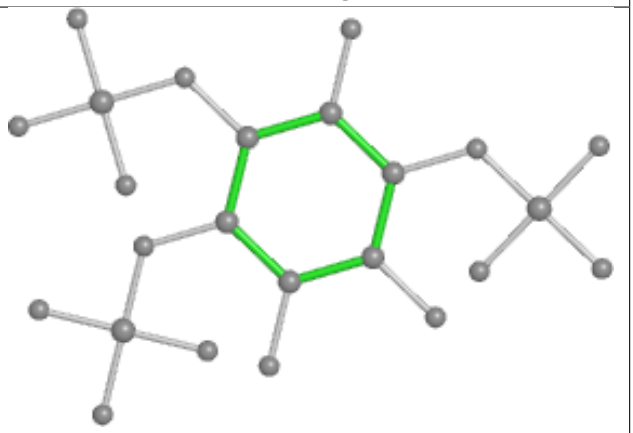
Bond lengths



Bond angles

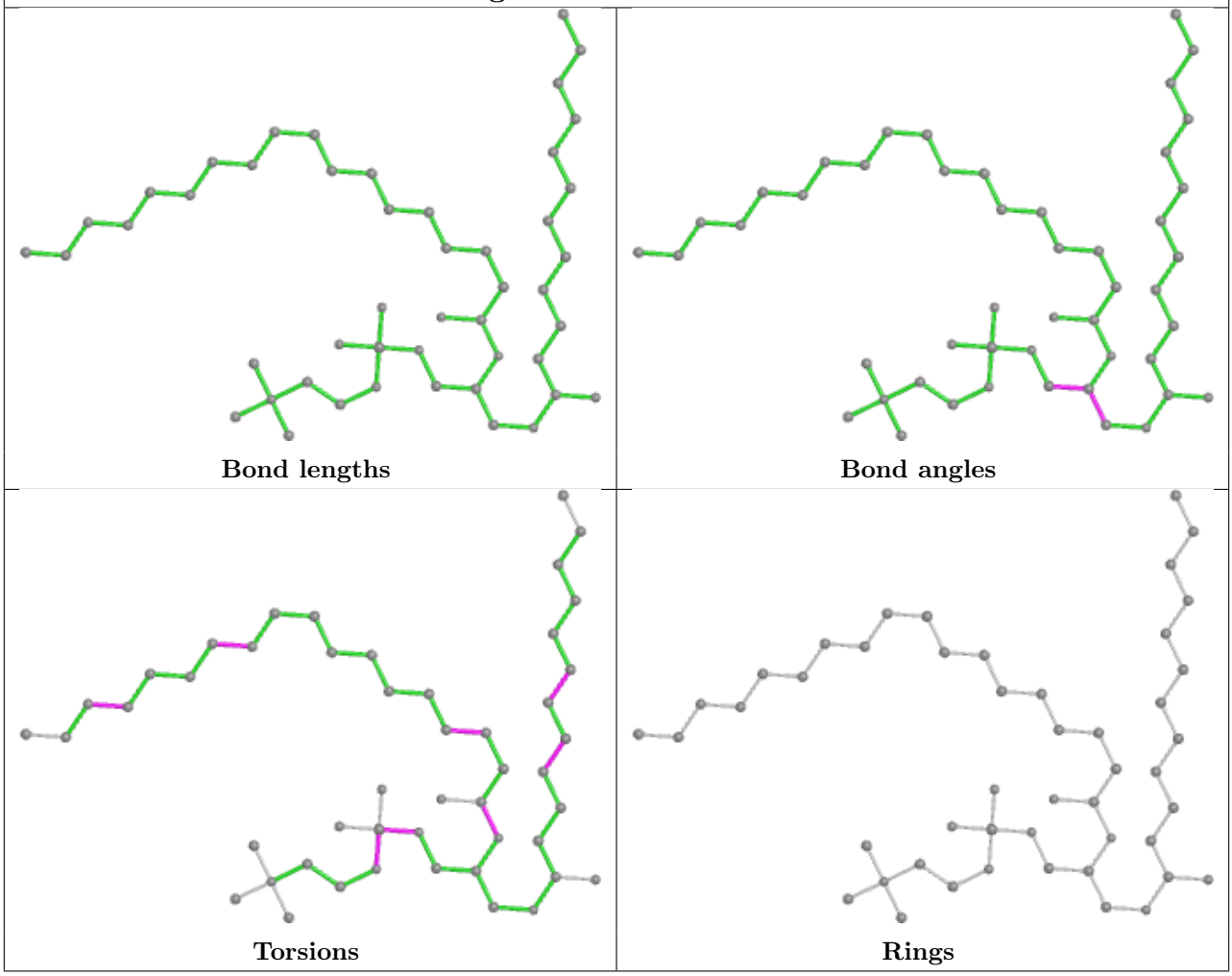


Torsions

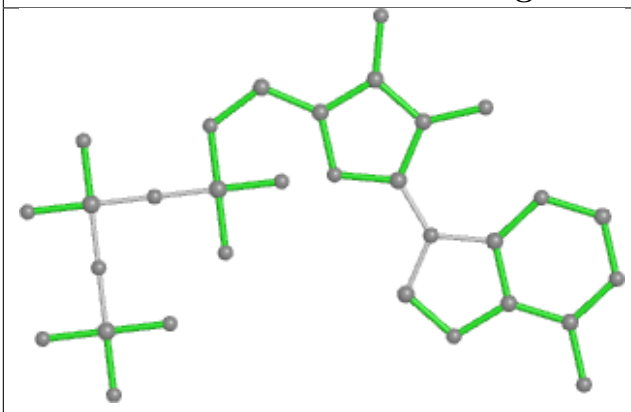


Rings

Ligand PCW D 2701



Ligand ATP A 3005



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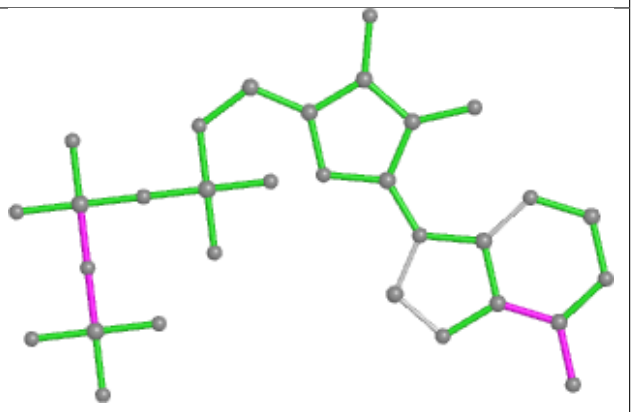
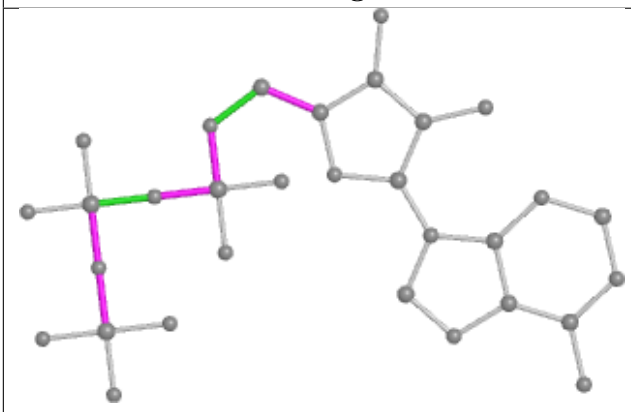


Bond angles



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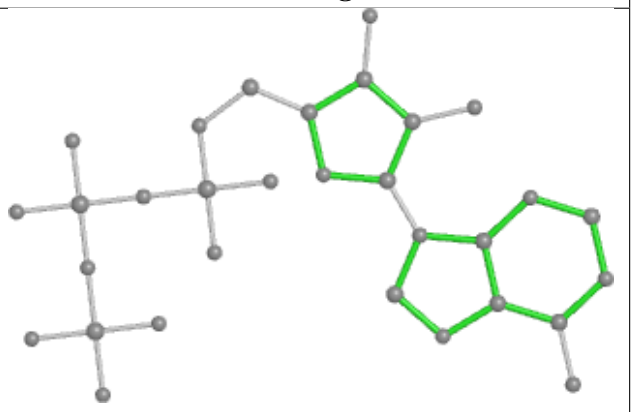
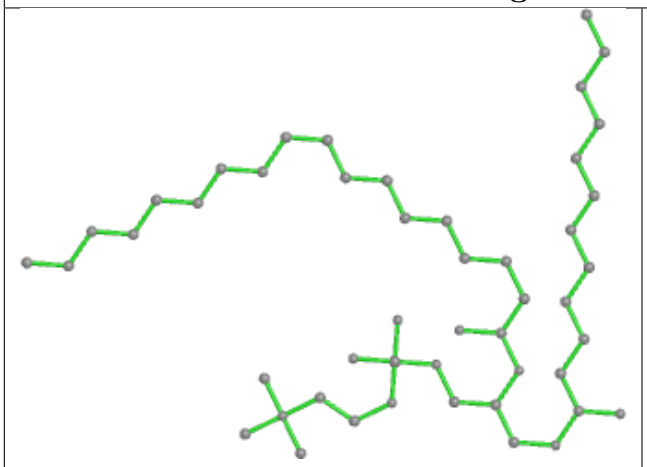
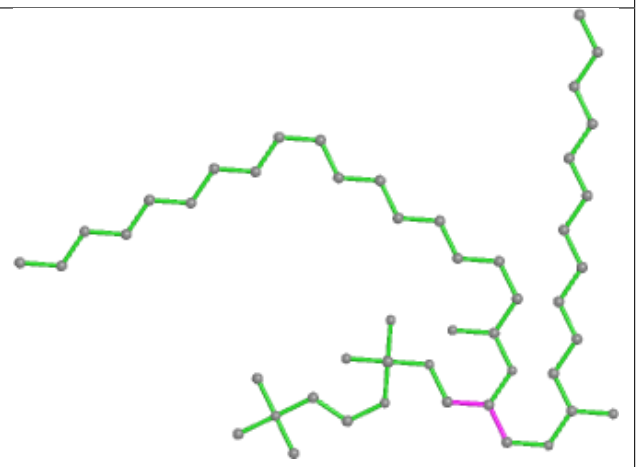


Rings

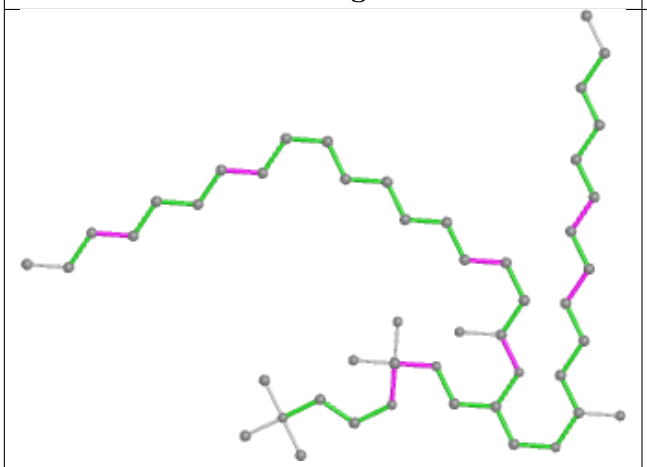
Ligand PCW B 2710



Bond lengths



Bond angles



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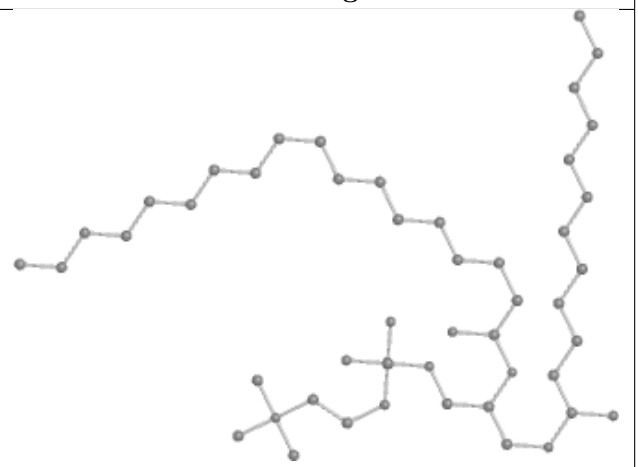
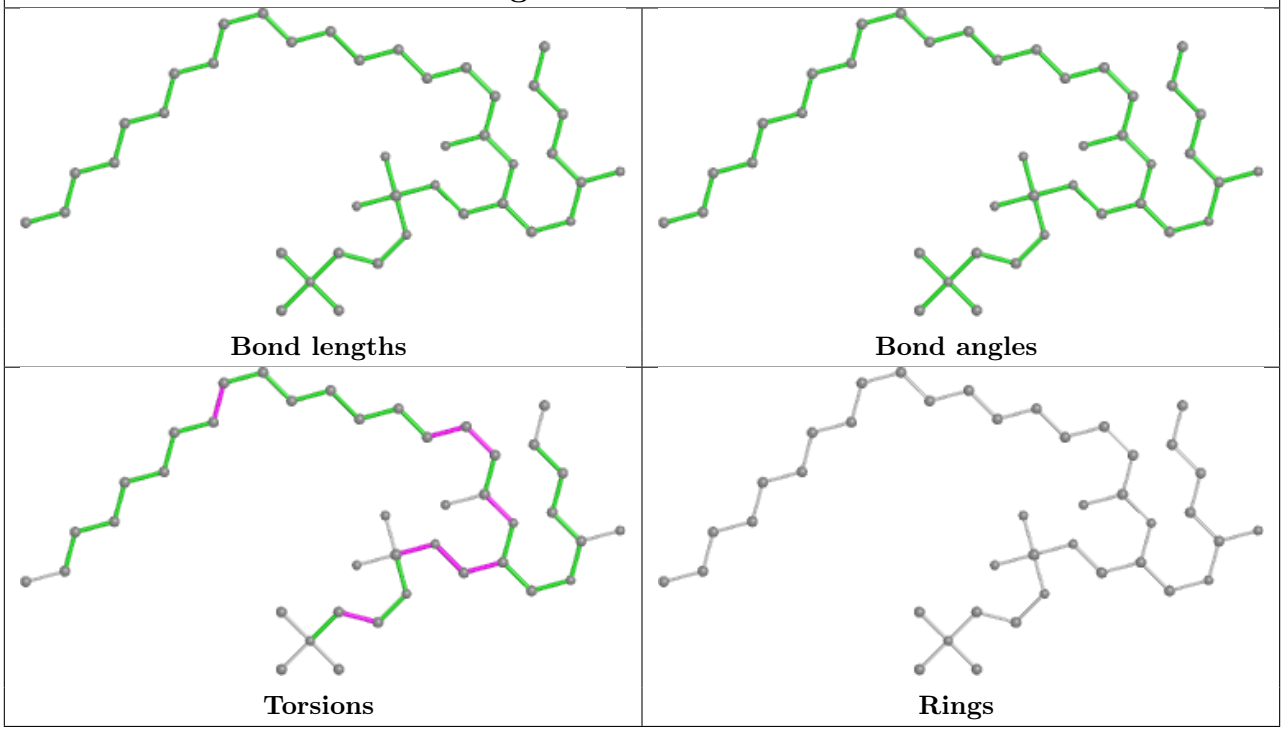
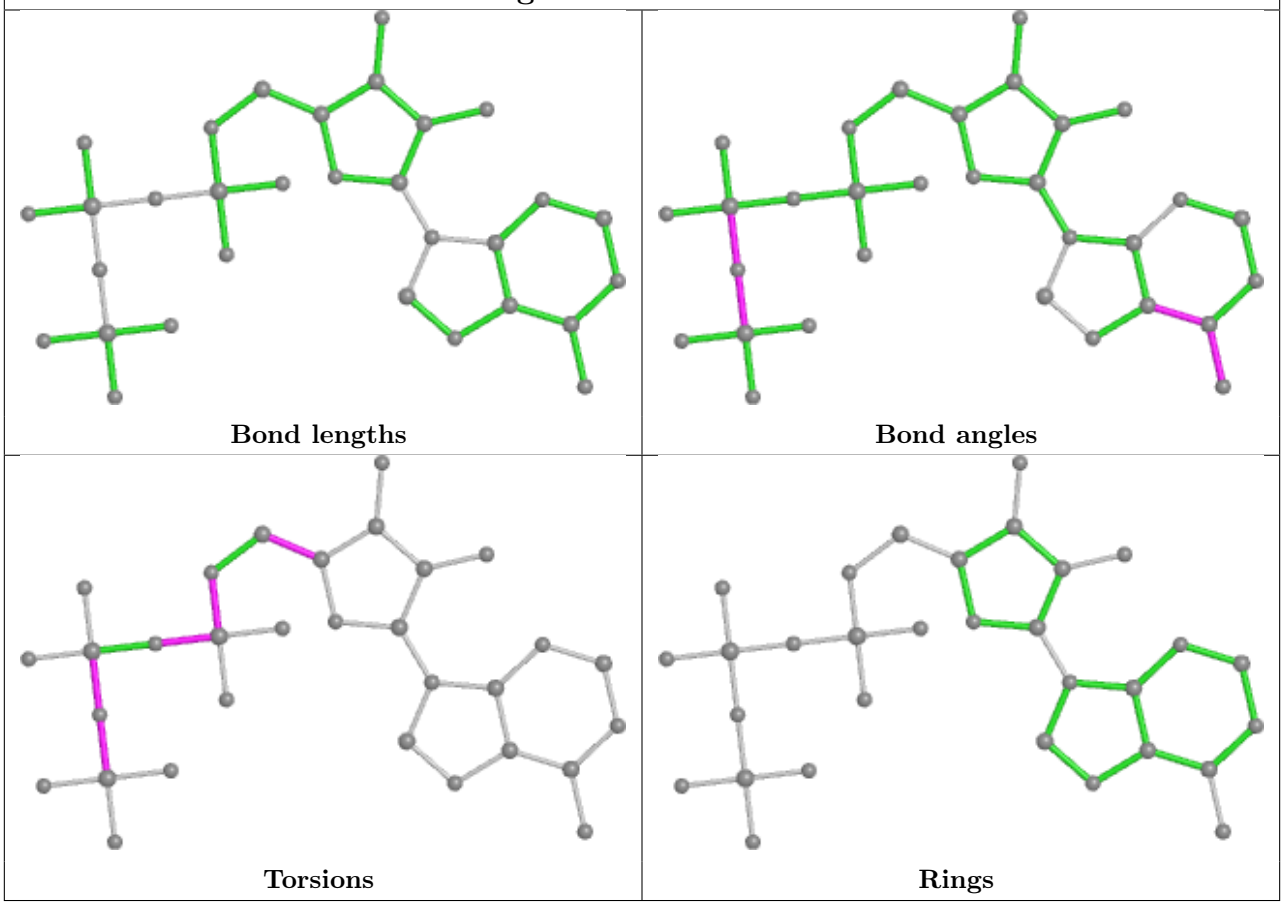


Rings

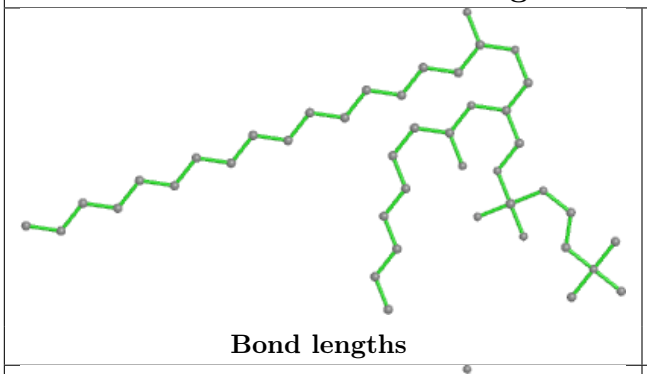
Ligand PCW B 2709



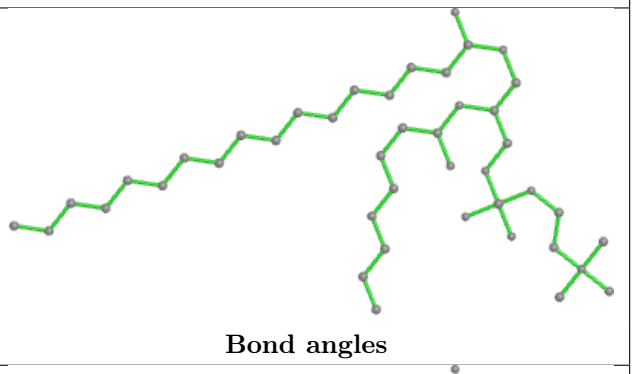
Ligand ATP B 2706



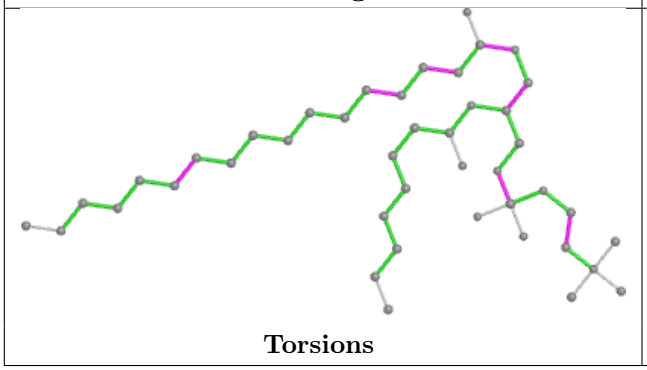
Ligand PCW B 2707



Bond lengths



Bond angles



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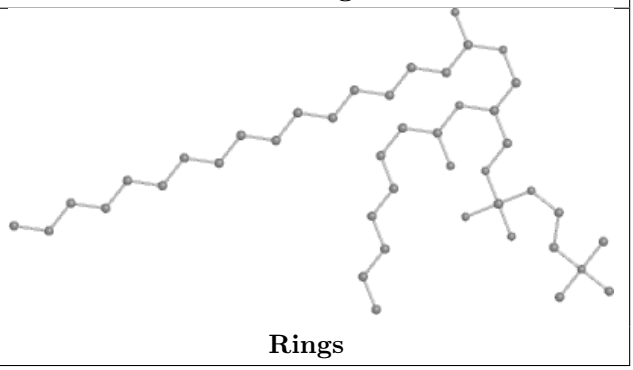
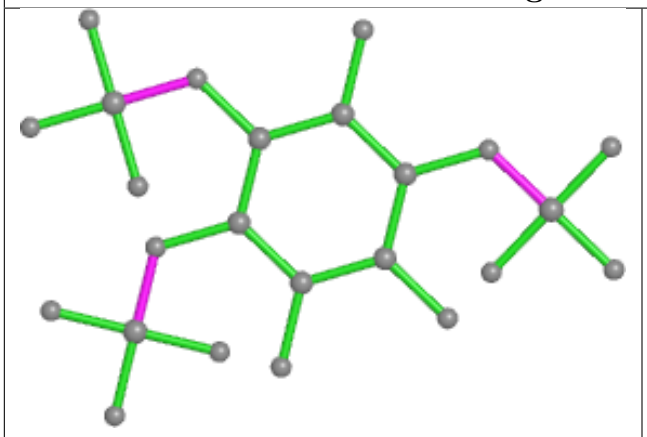
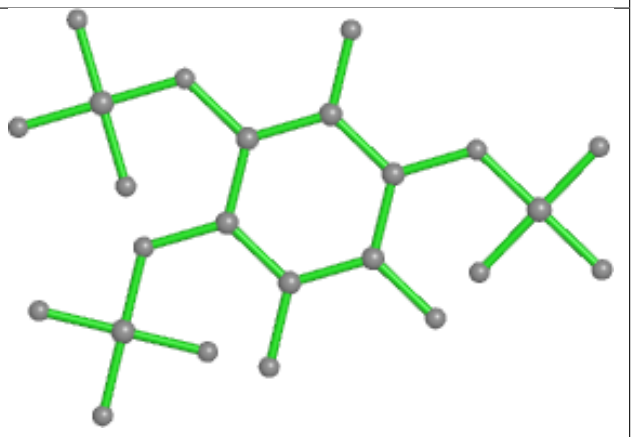


Rings

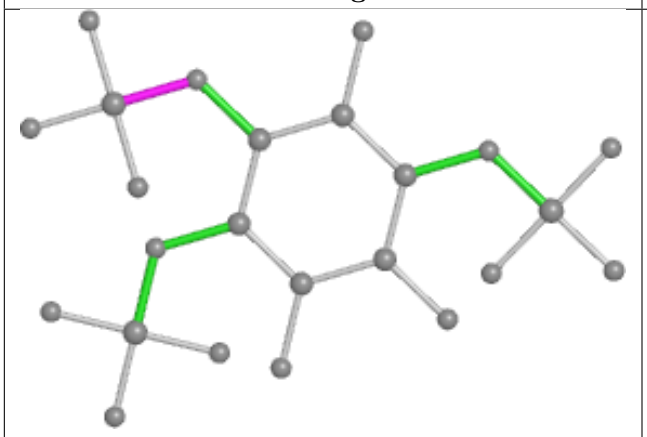
Ligand I3P C 2703



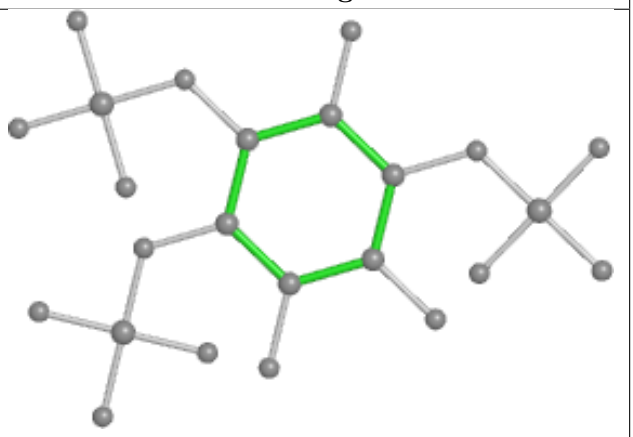
Bond lengths



Bond angles

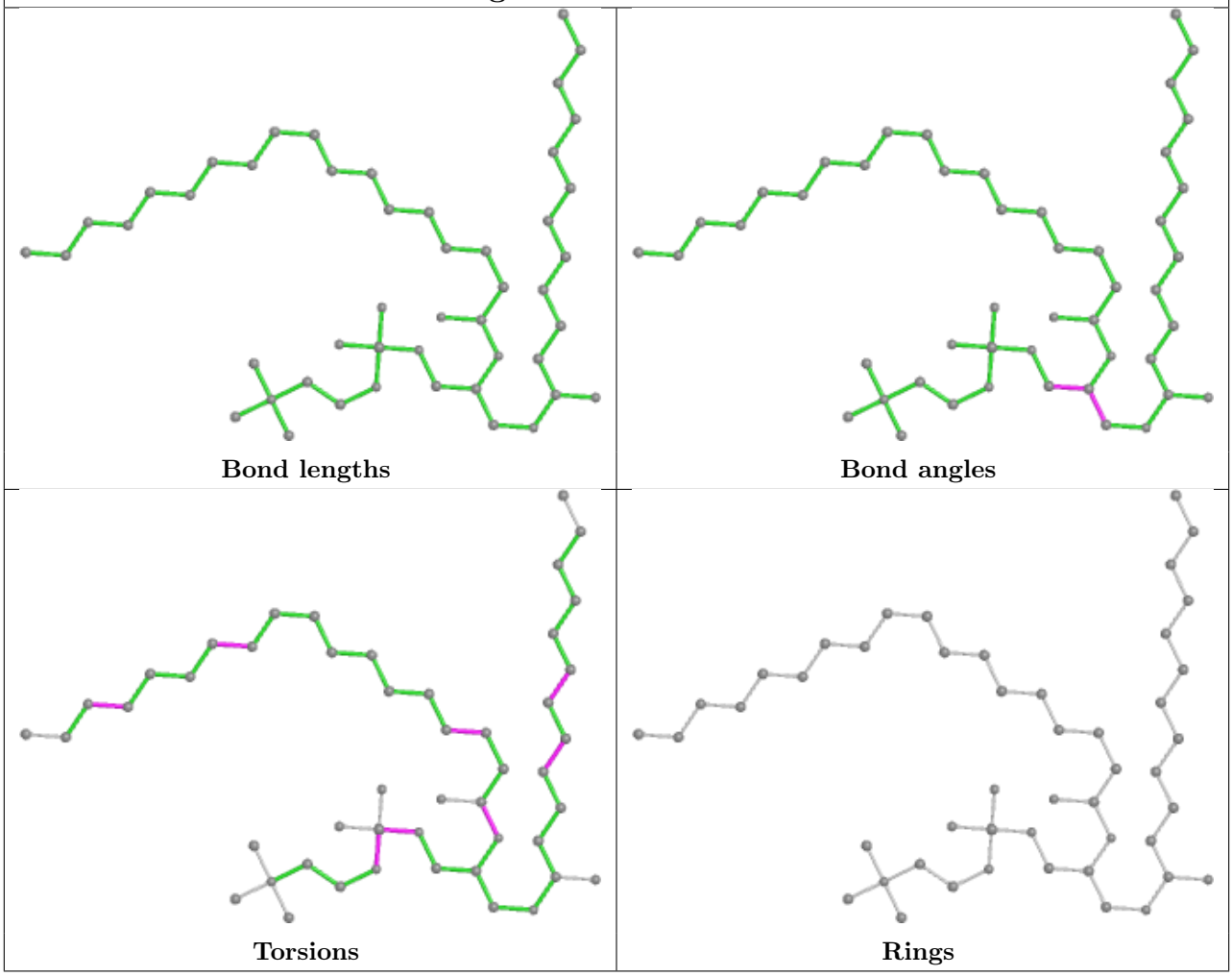


Torsions

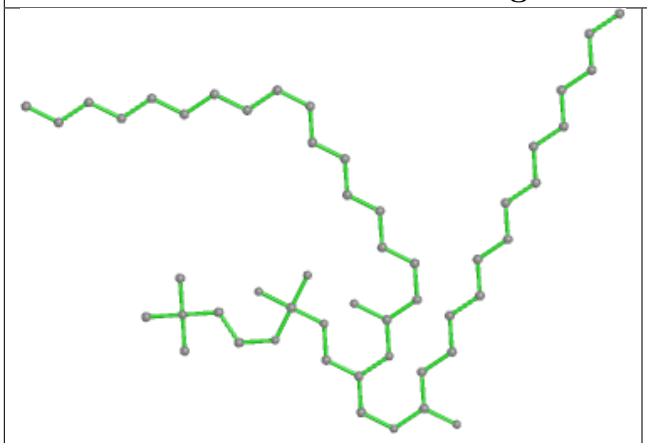


Rings

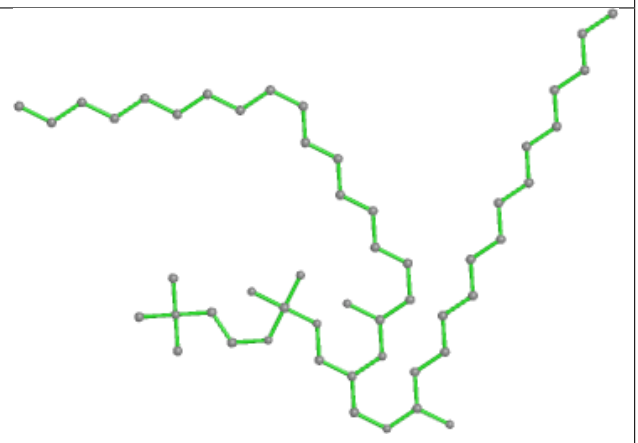
Ligand PCW A 3009



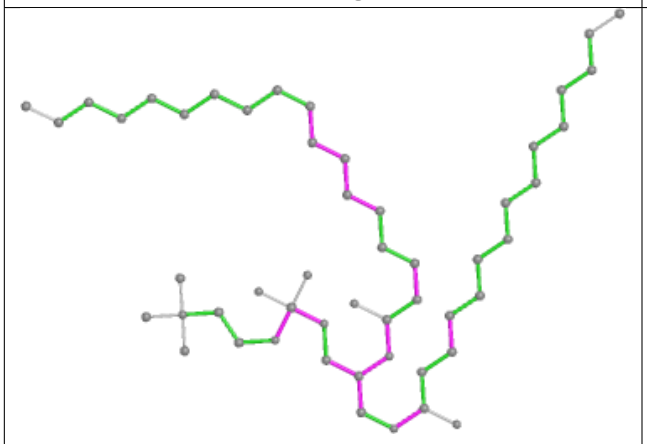
Ligand PCW B 2701



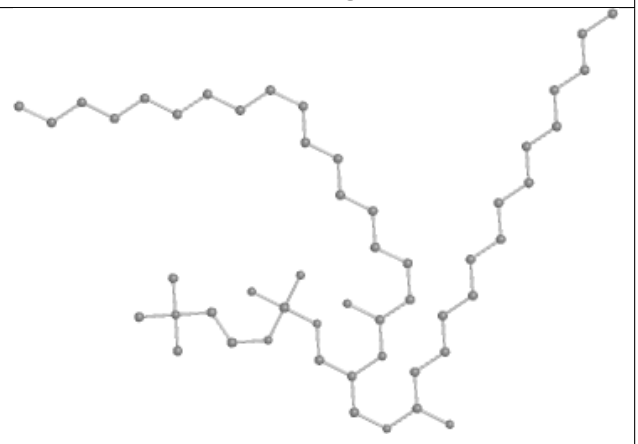
Bond lengths



Bond angles

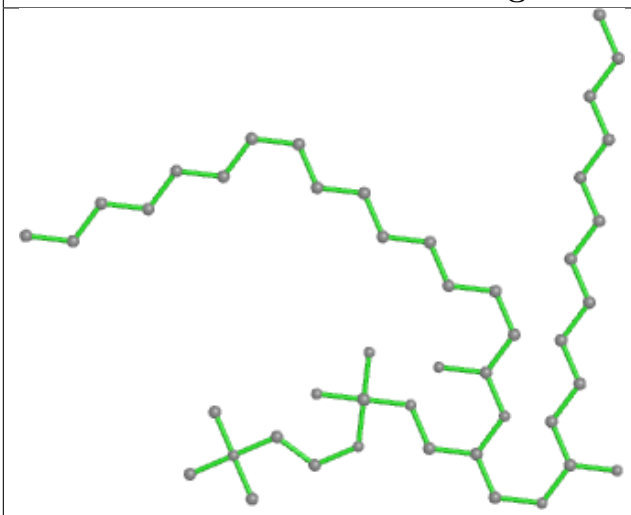


Torsions

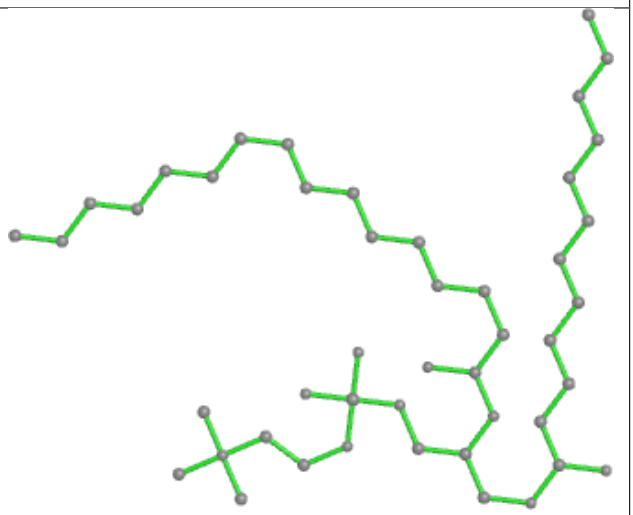


Rings

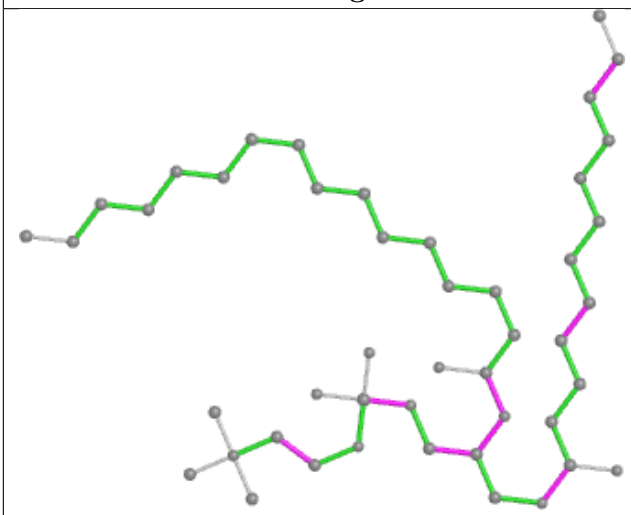
Ligand PCW A 3010



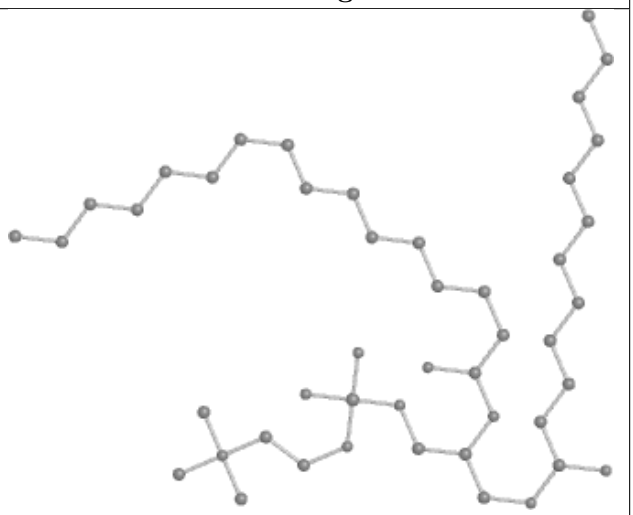
Bond lengths



Bond angles

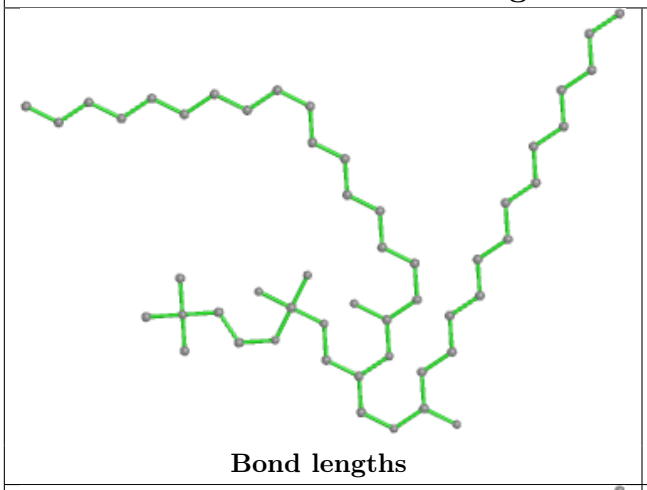


Torsions

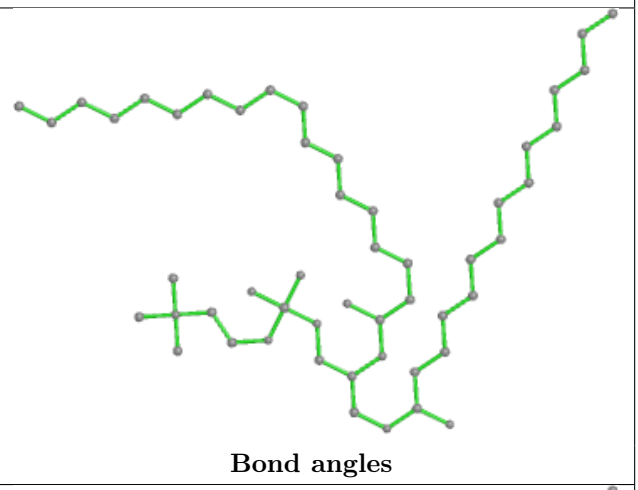


Rings

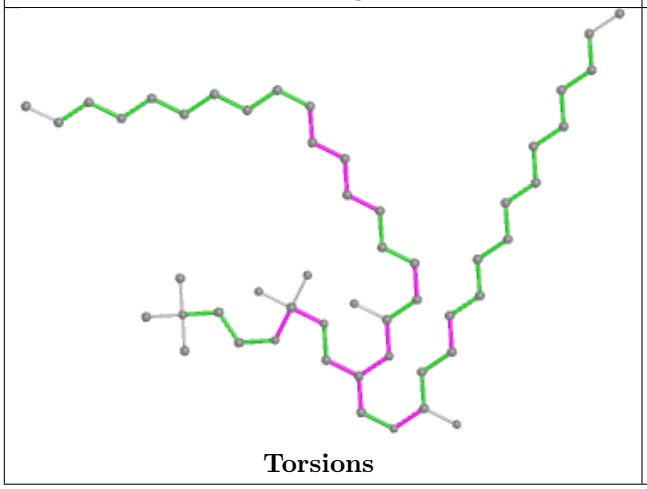
Ligand PCW A 3011



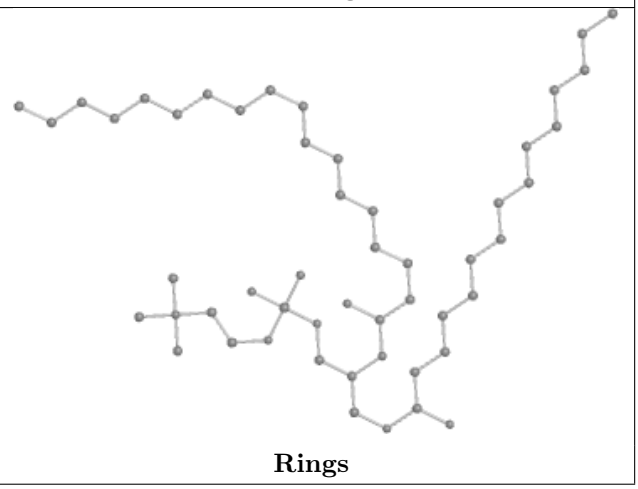
Bond lengths



Bond angles

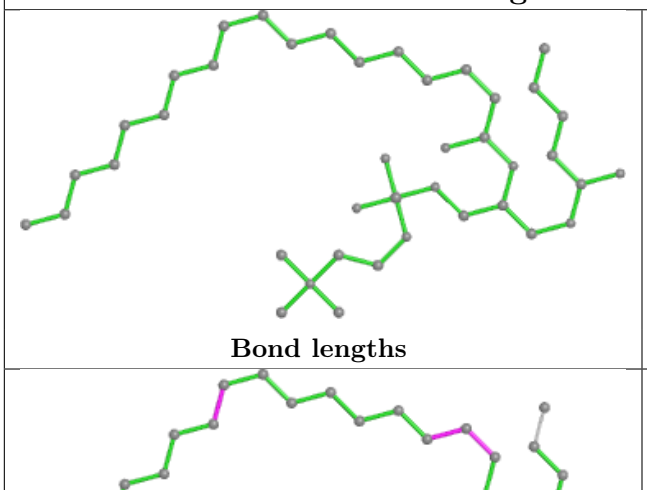


Torsions

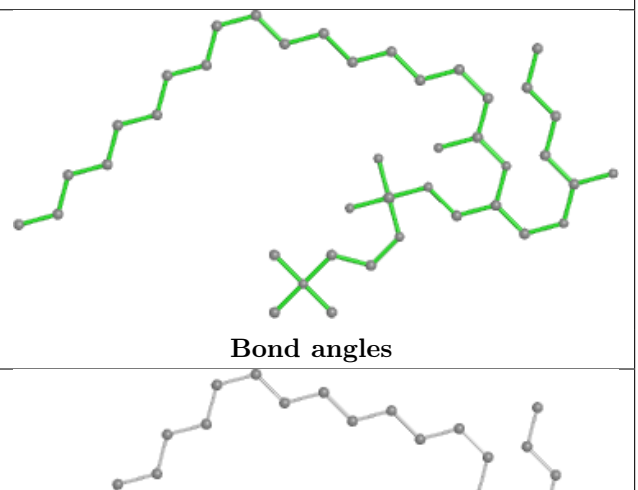


Rings

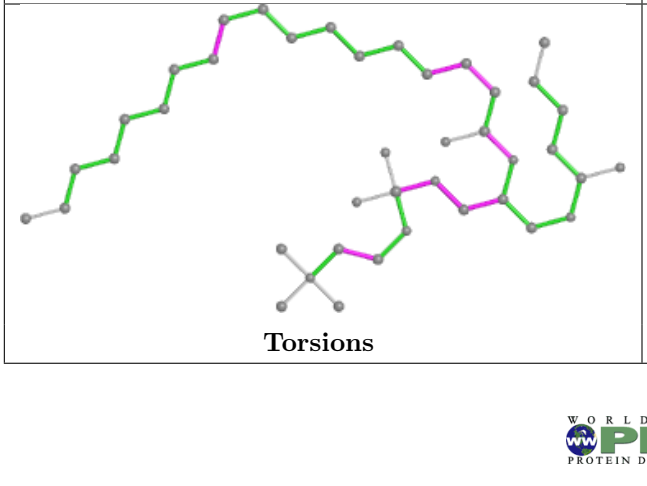
Ligand PCW C 2709



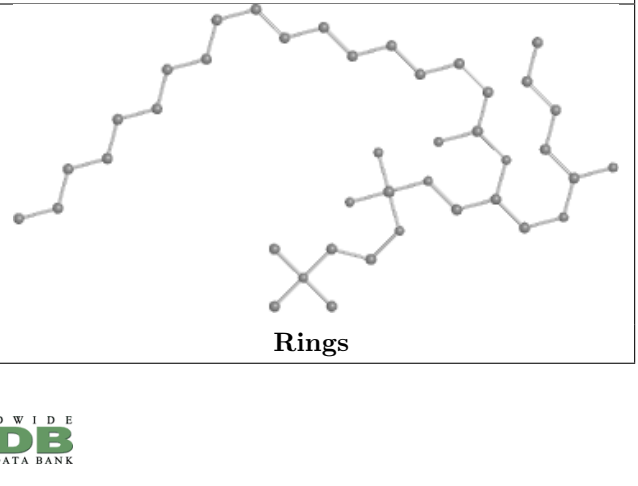
Bond lengths



Bond angles

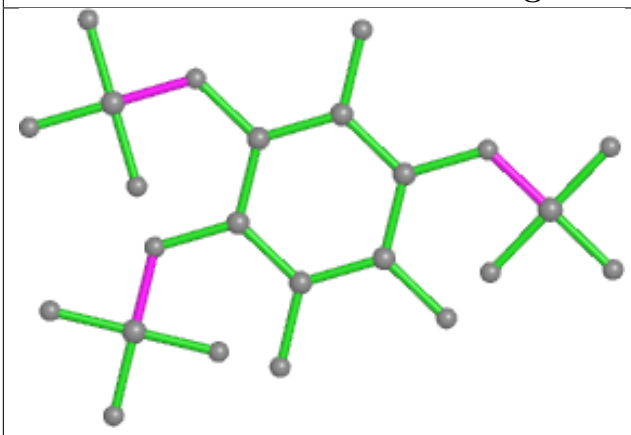


Torsions

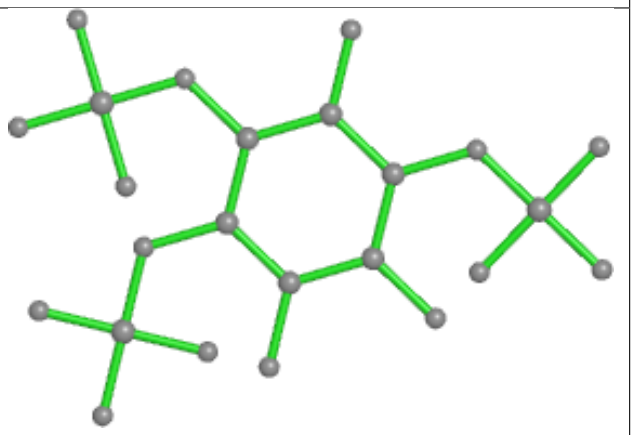


Rings

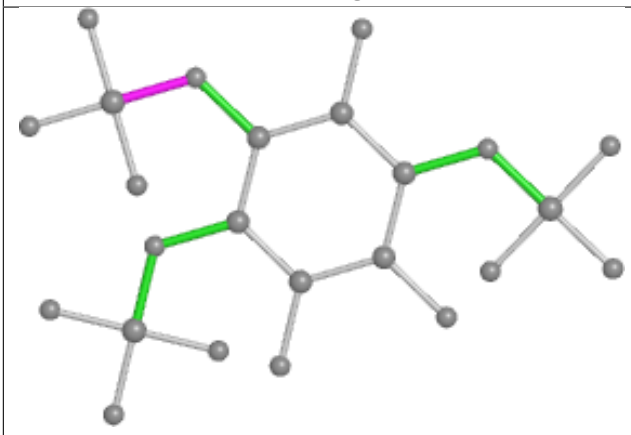
Ligand I3P D 2705



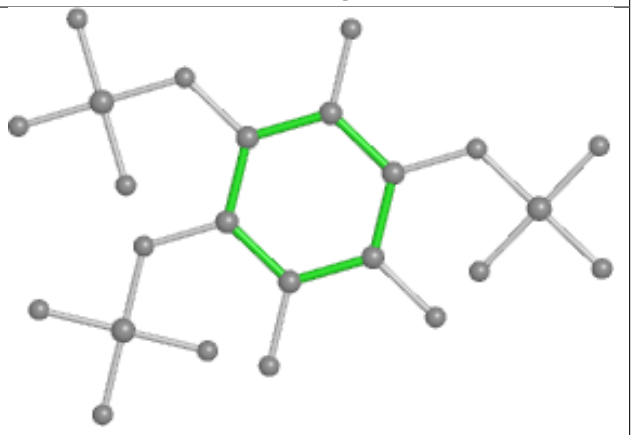
Bond lengths



Bond angles

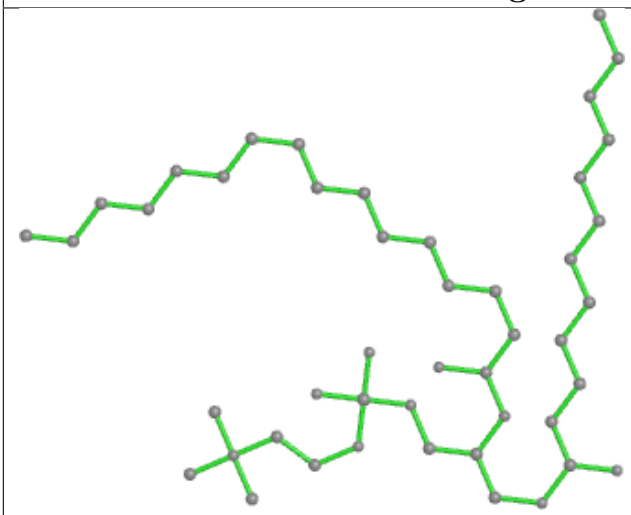


Torsions

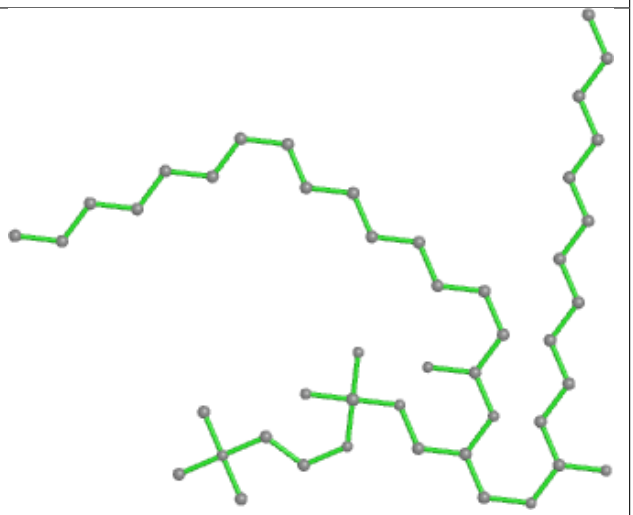


Rings

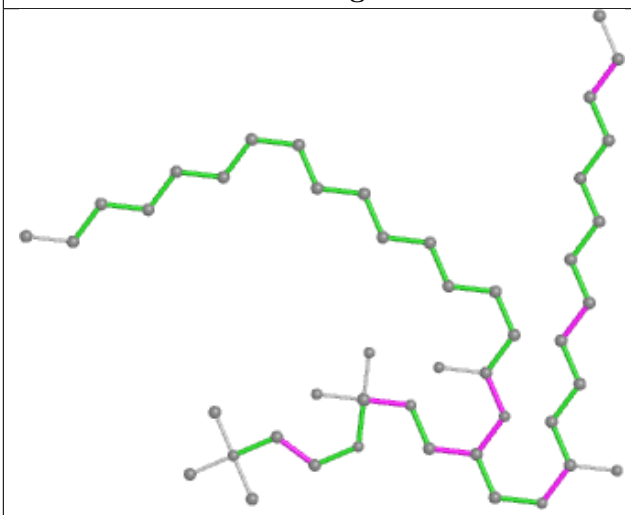
Ligand PCW B 2711



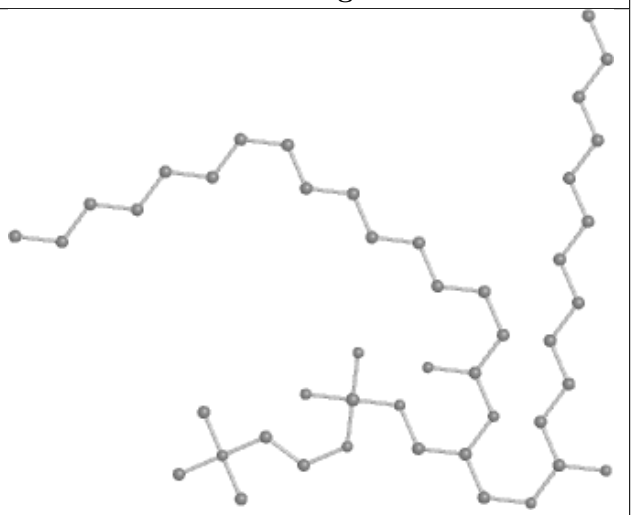
Bond lengths



Bond angles

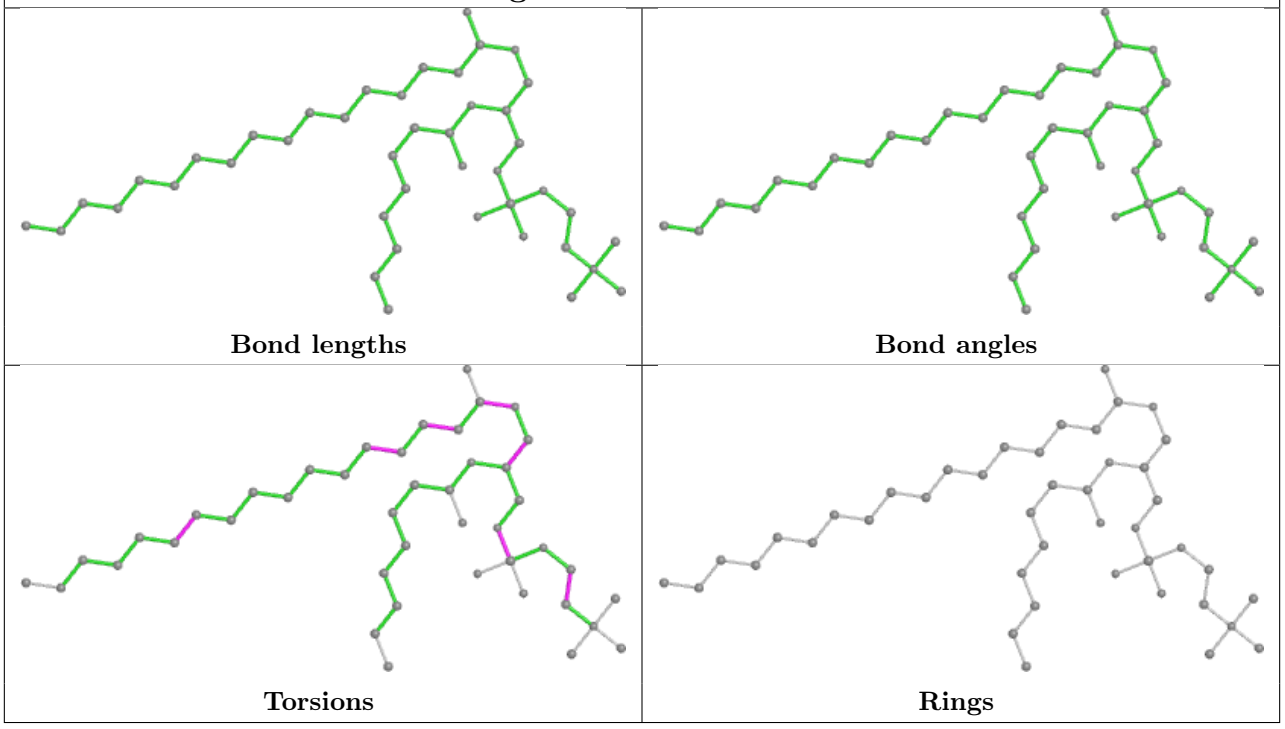


Torsions

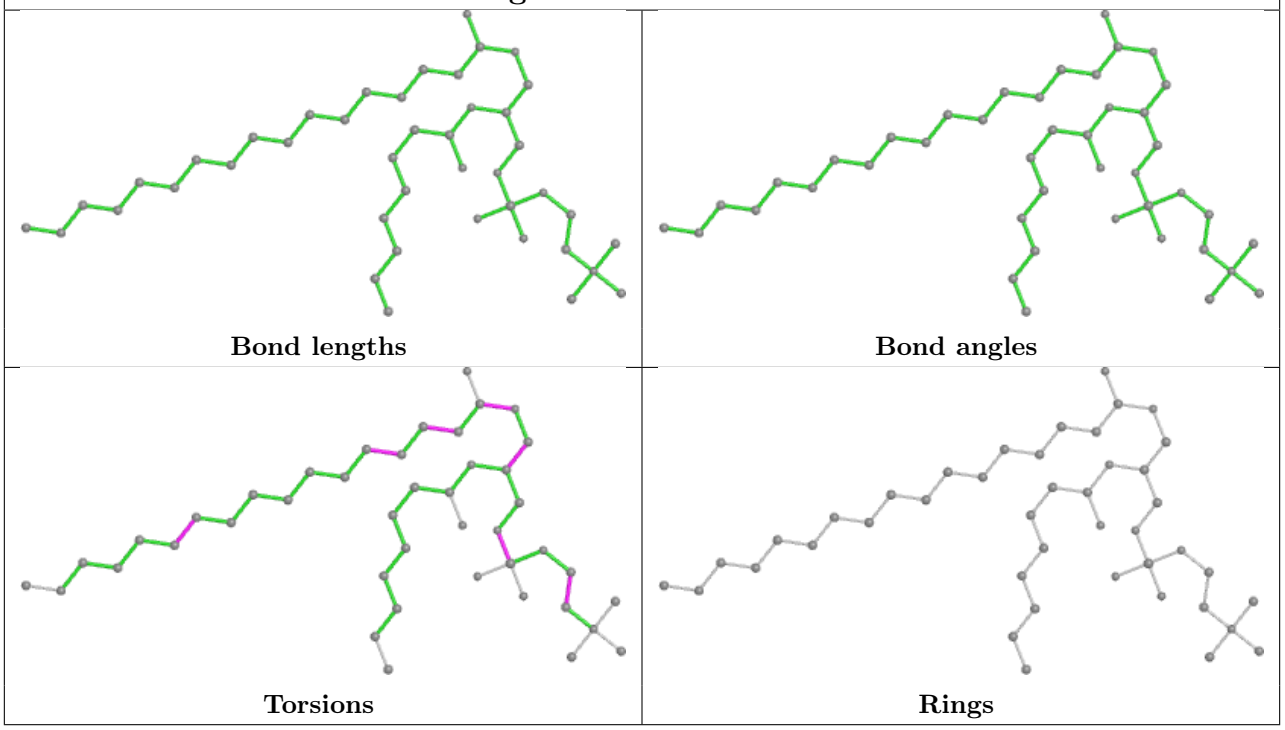


Rings

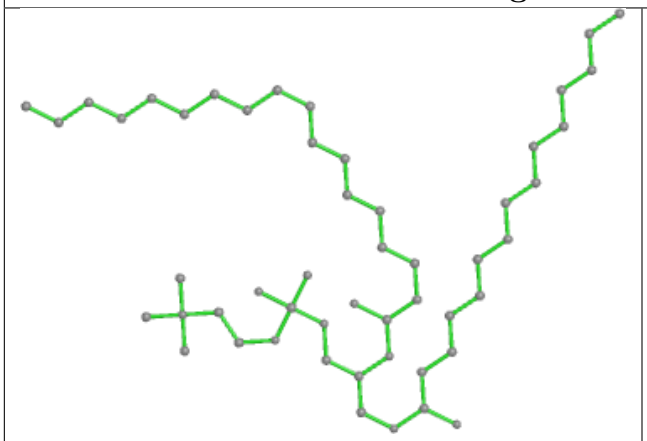
Ligand PCW A 3006



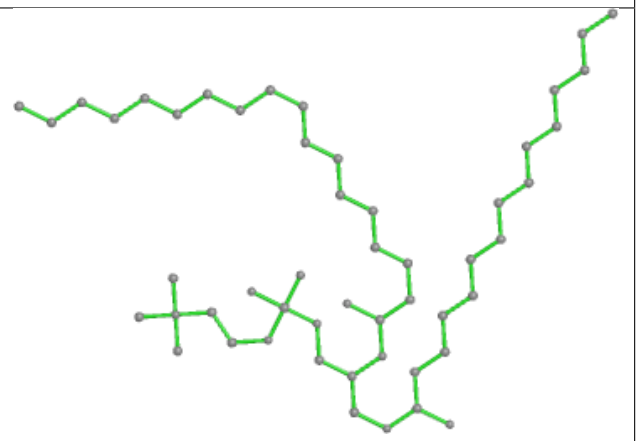
Ligand PCW D 2709



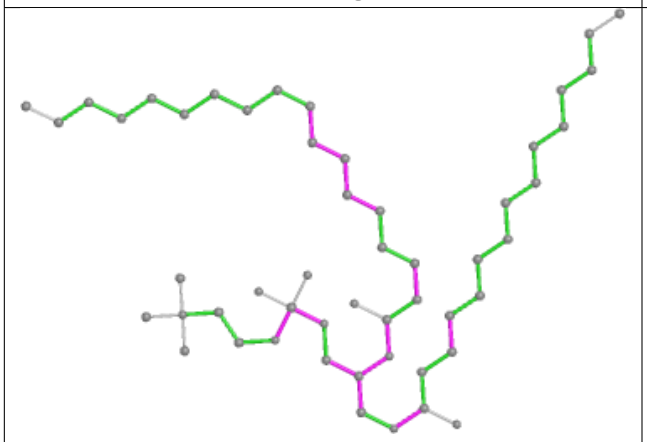
Ligand PCW C 2701



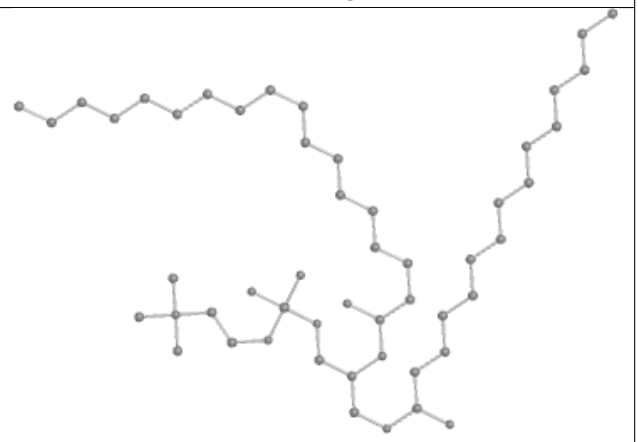
Bond lengths



Bond angles

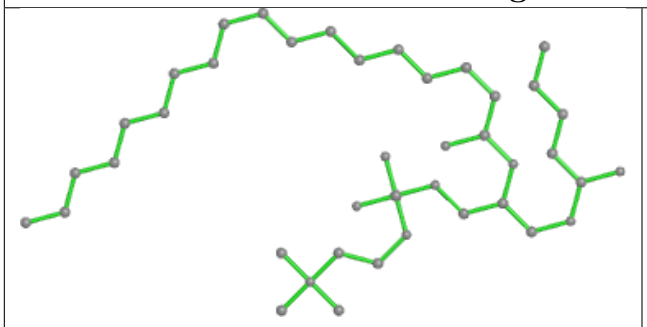


Torsions

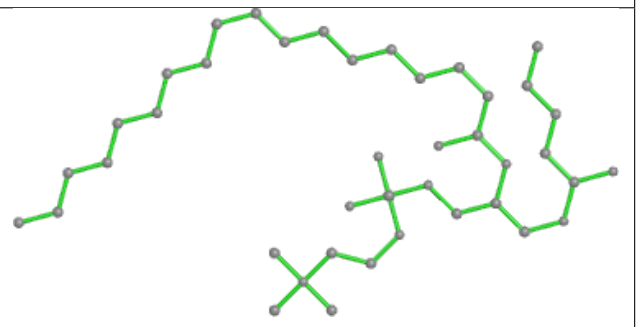


Rings

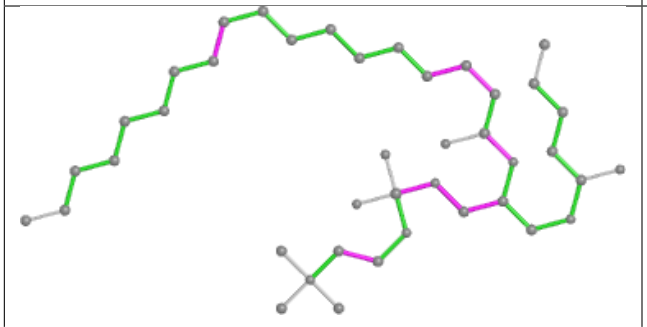
Ligand PCW A 3008



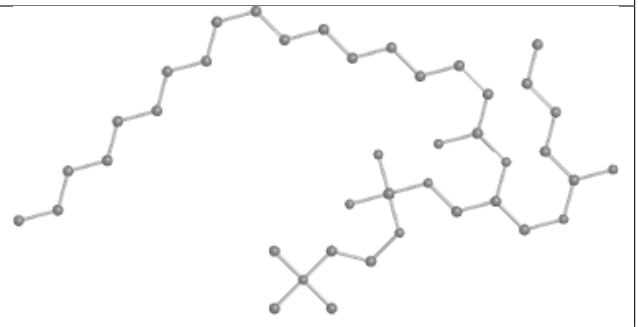
Bond lengths



Bond angles

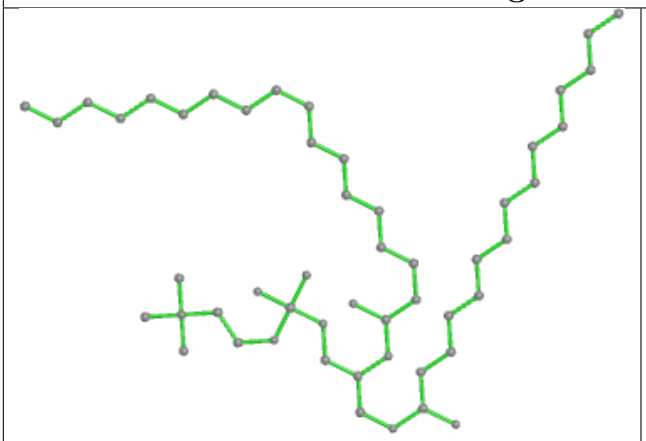


Torsions

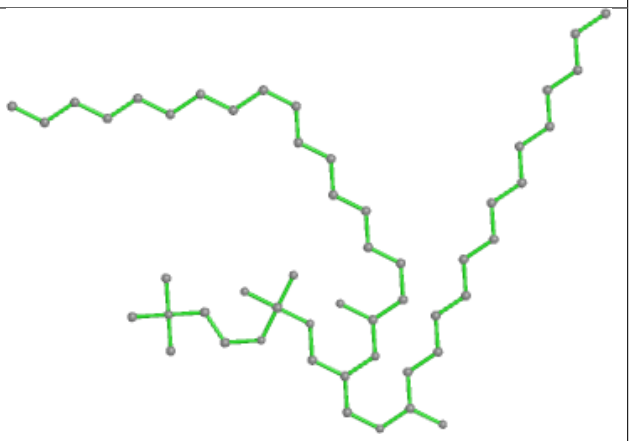


Rings

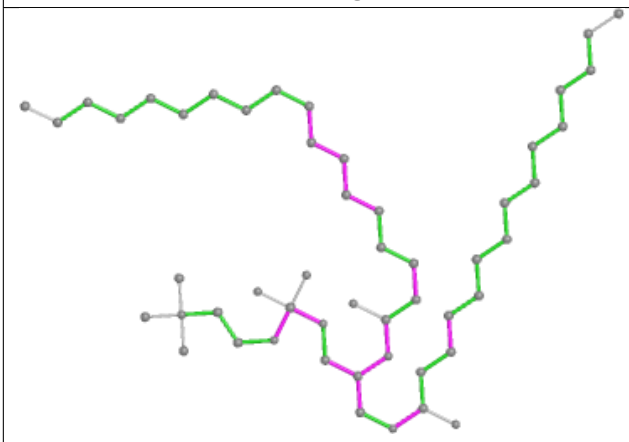
Ligand PCW D 2703



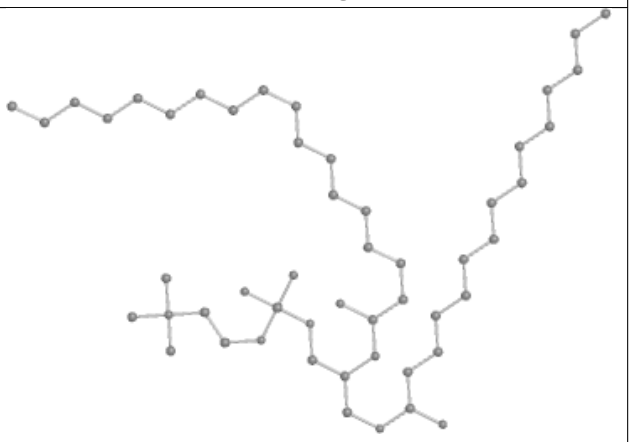
Bond lengths



Bond angles

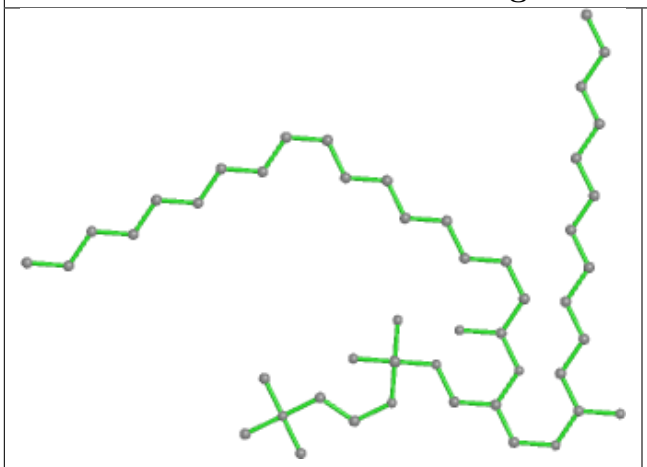


Torsions

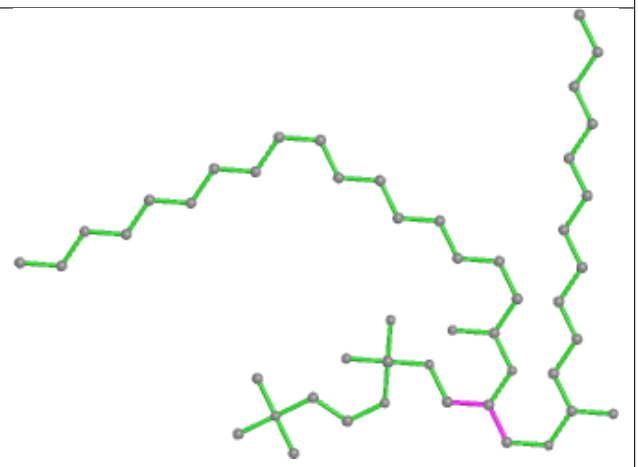


Rings

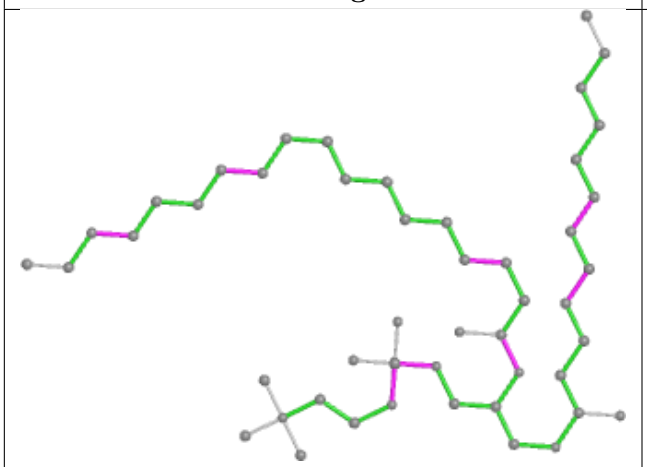
Ligand PCW C 2710



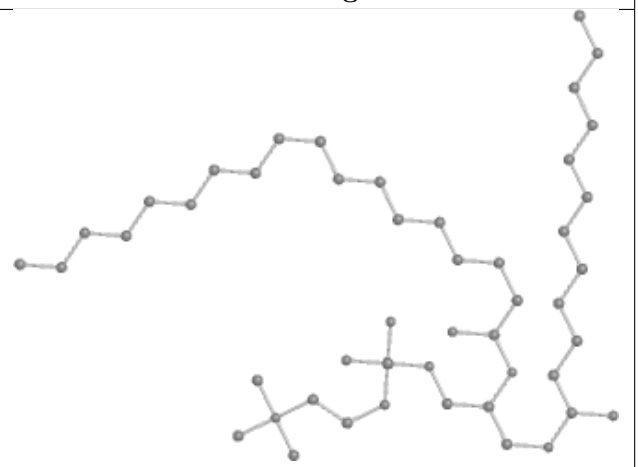
Bond lengths



Bond angles

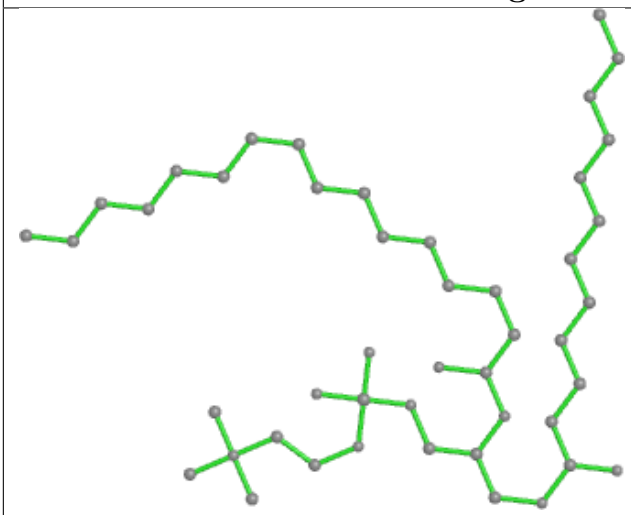


Torsions

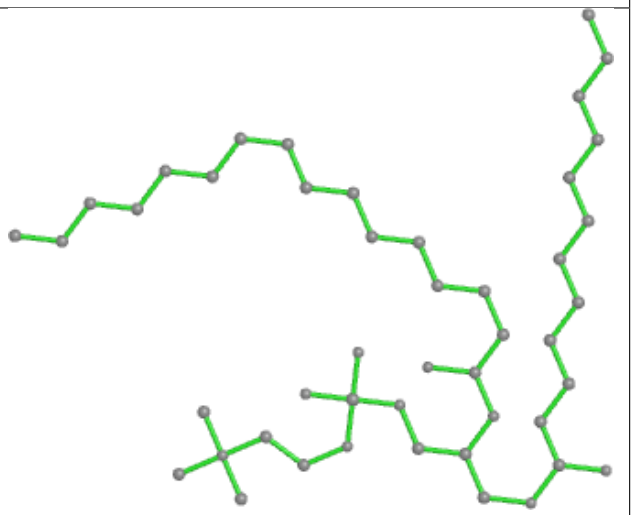


Rings

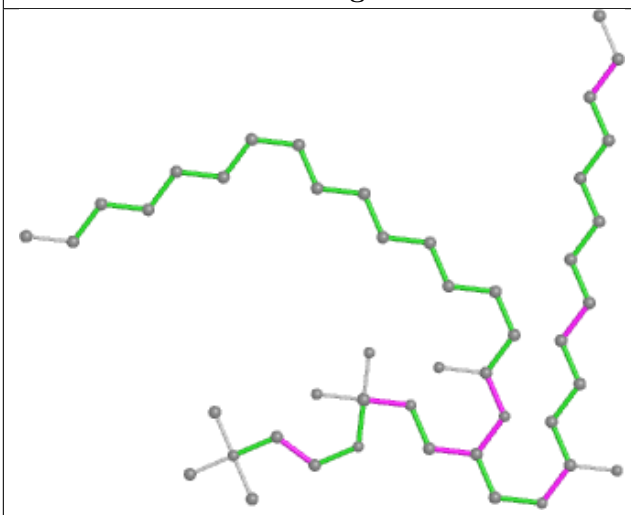
Ligand PCW C 2711



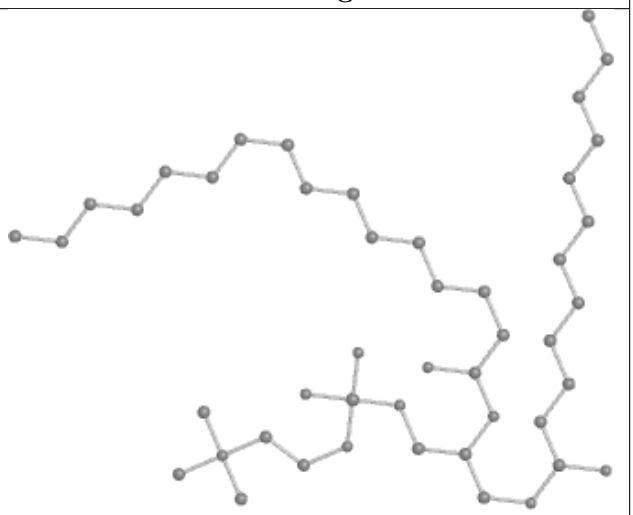
Bond lengths



Bond angles

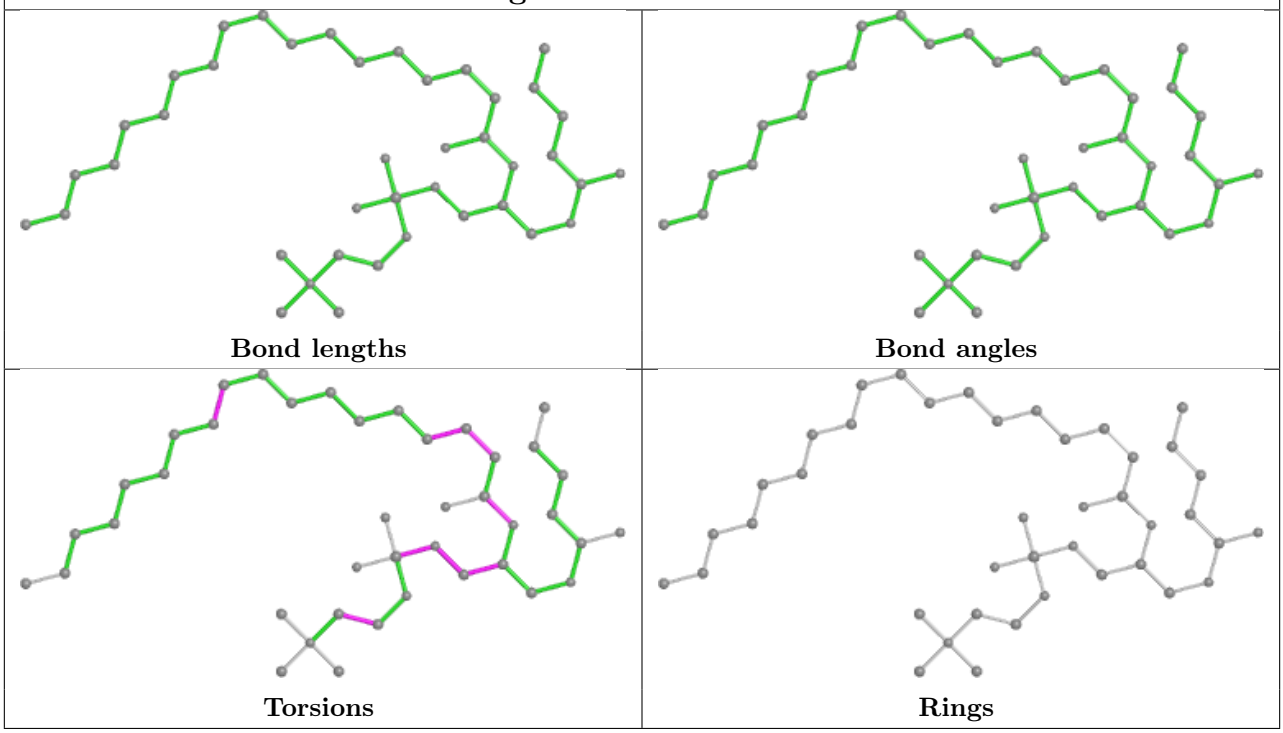


Torsions

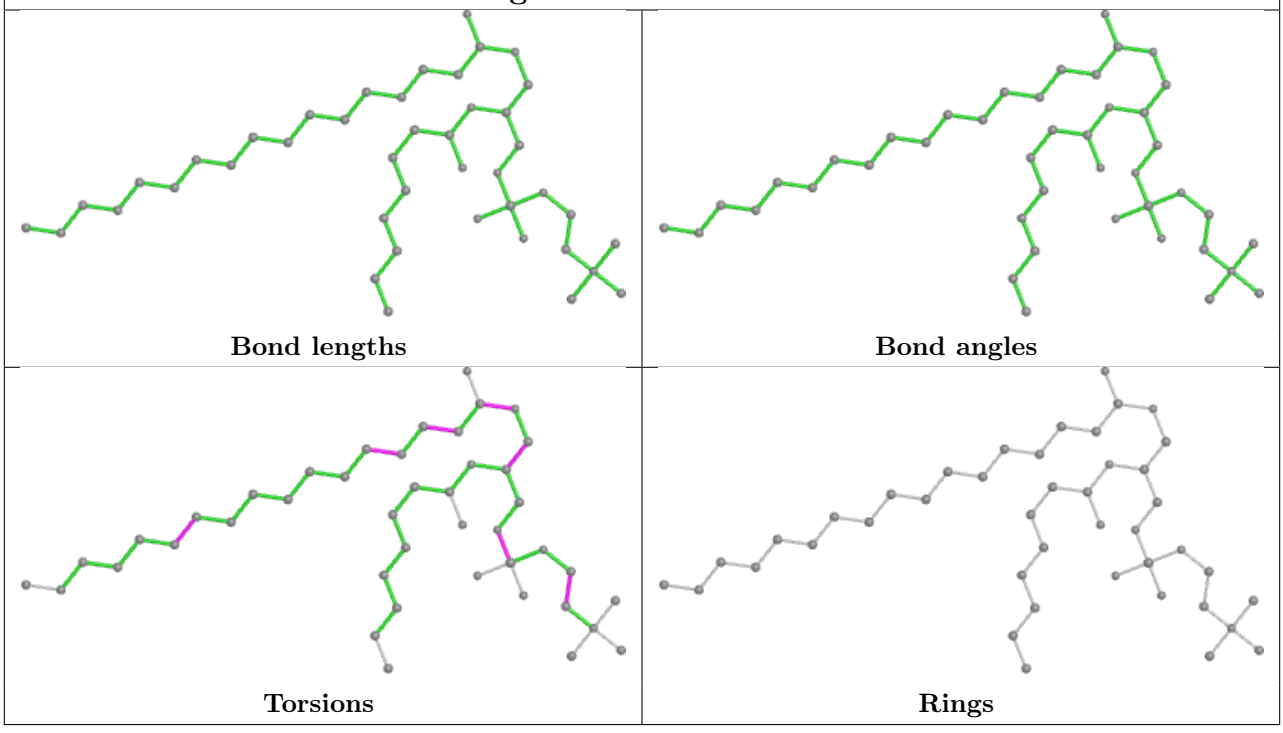


Rings

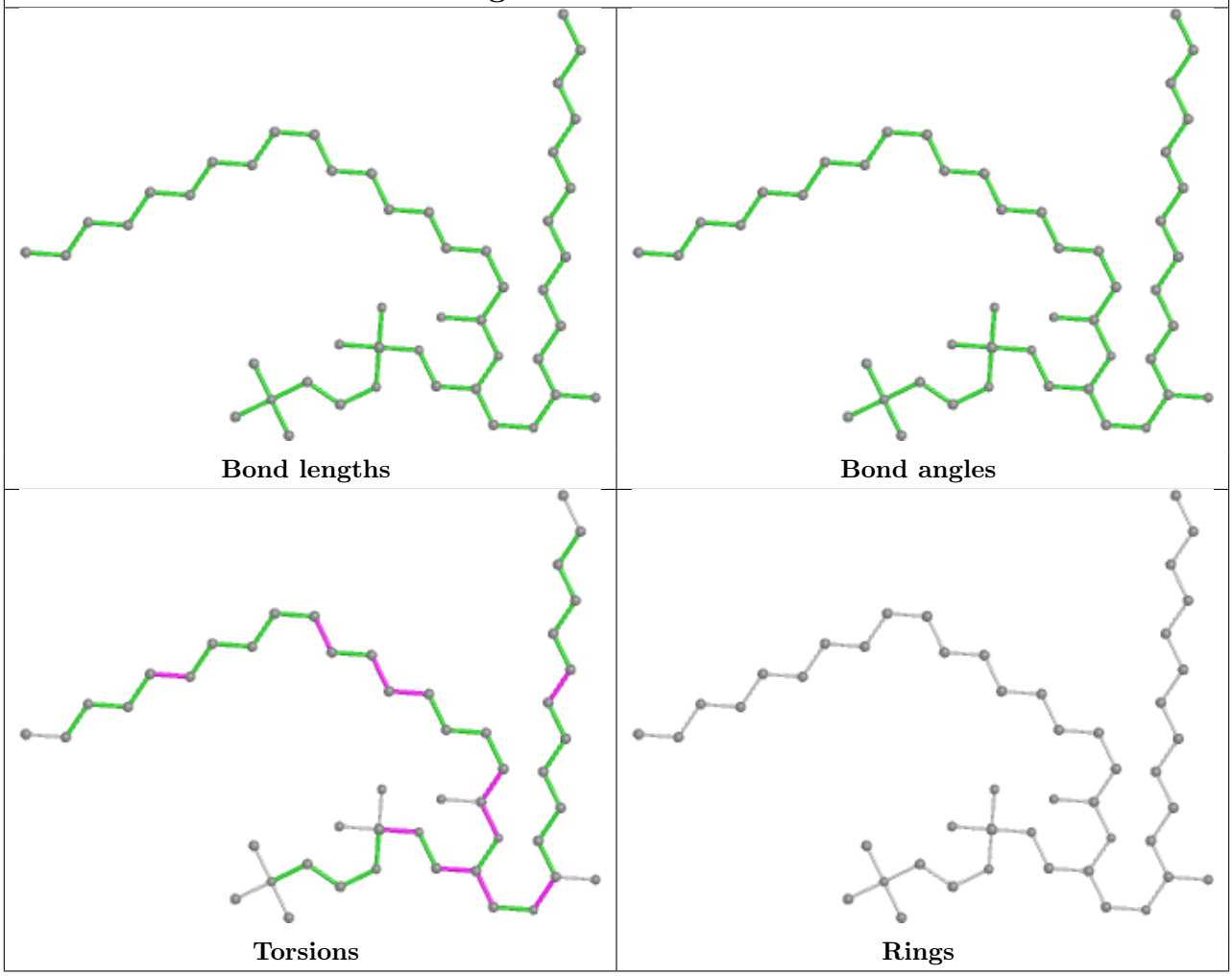
Ligand PCW D 2711



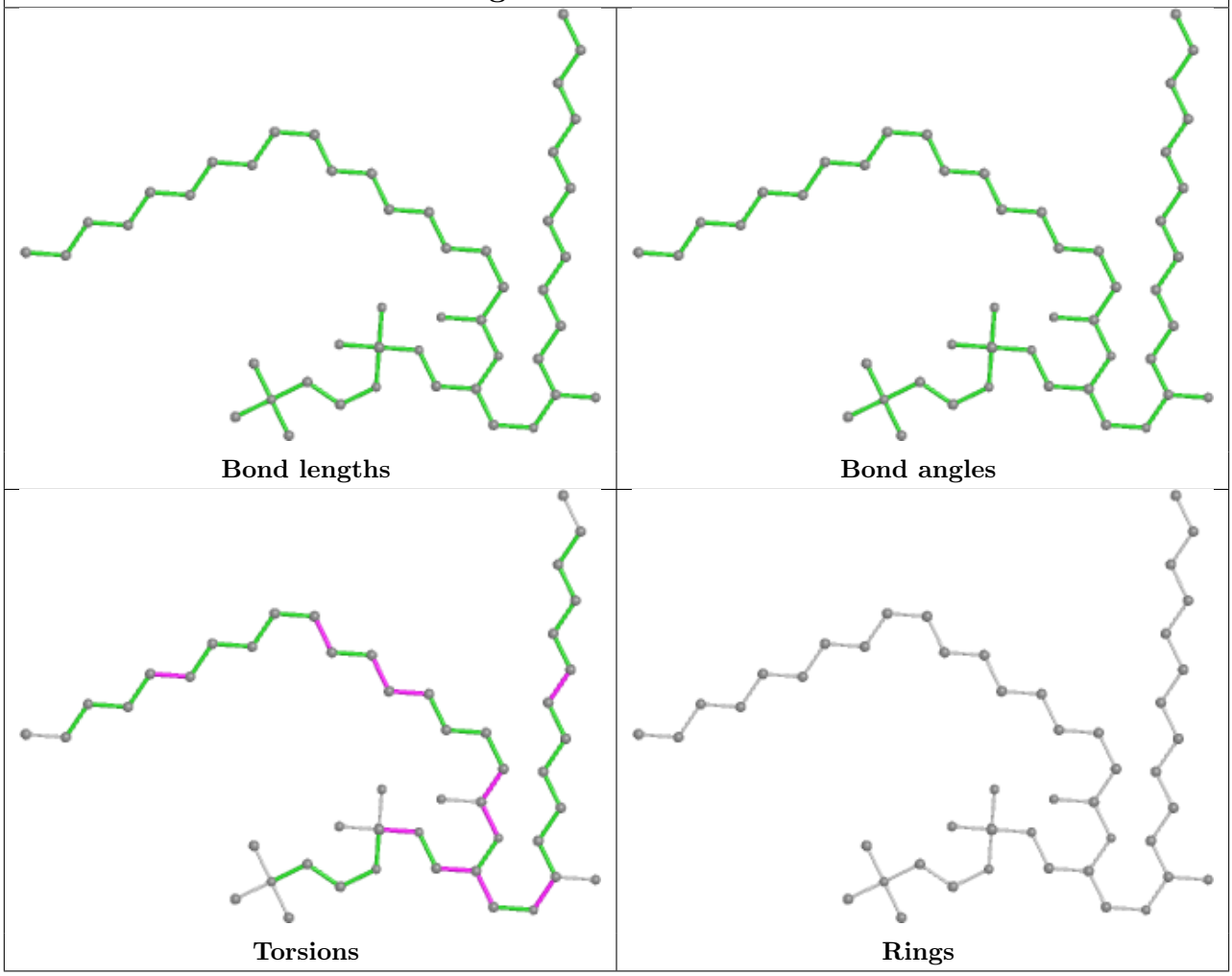
Ligand PCW C 2707



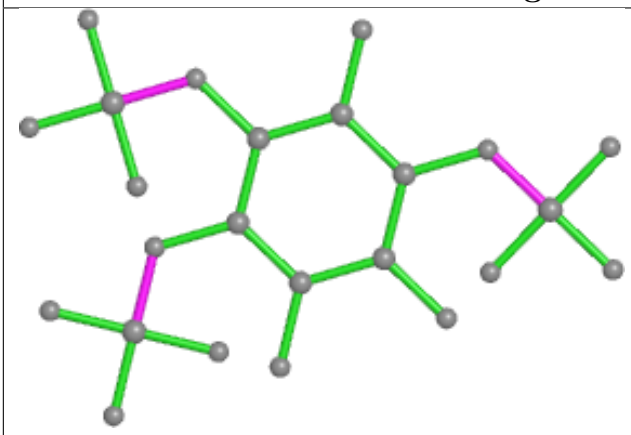
Ligand PCW D 2710



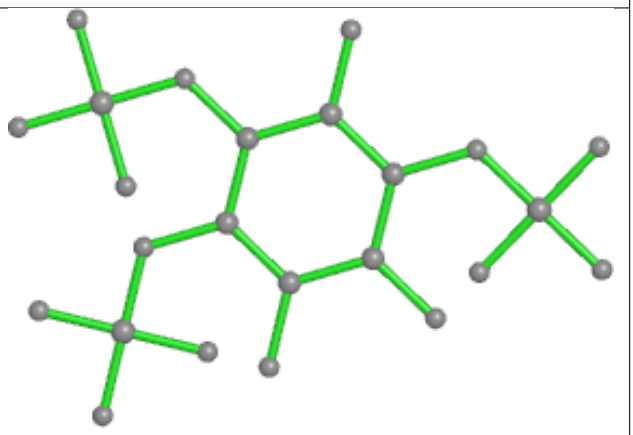
Ligand PCW A 3007



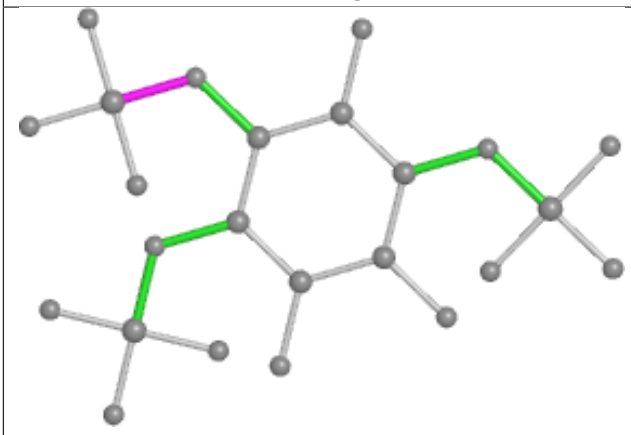
Ligand I3P A 3002



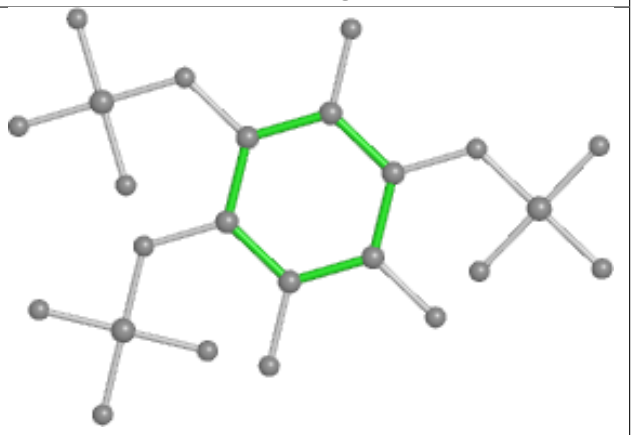
Bond lengths



Bond angles

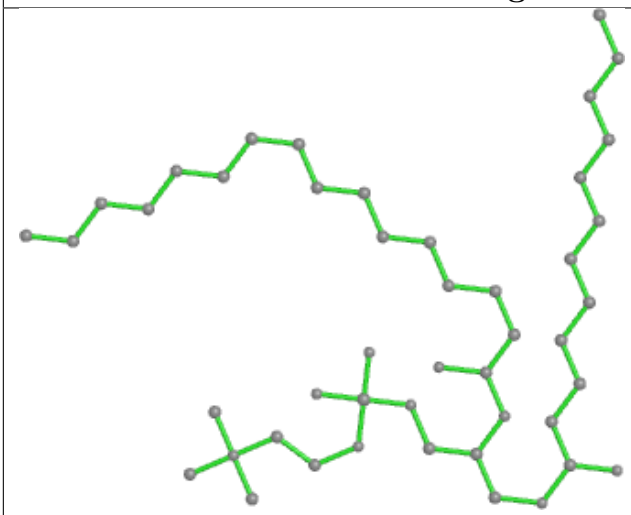


Torsions

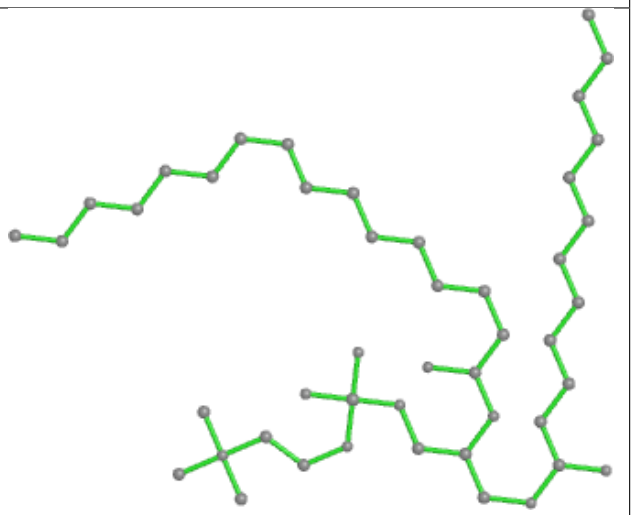


Rings

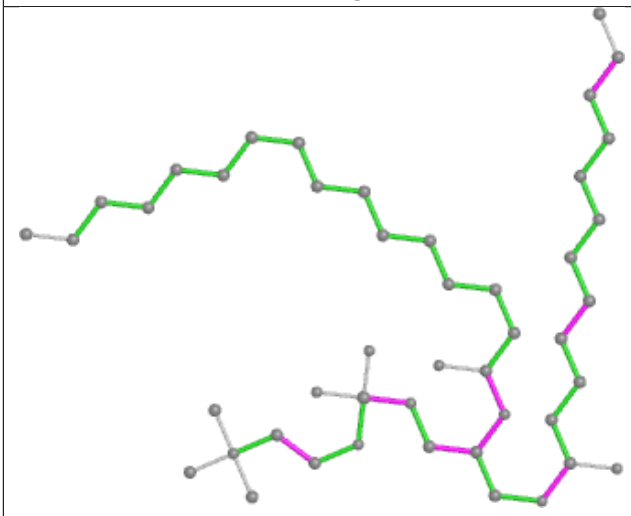
Ligand PCW D 2702



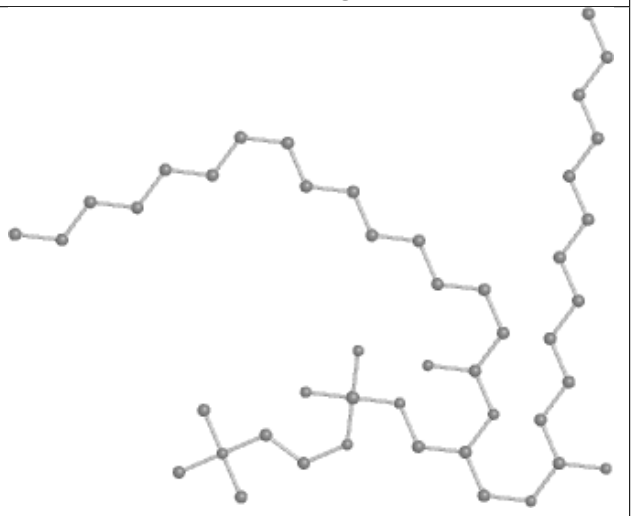
Bond lengths



Bond angles

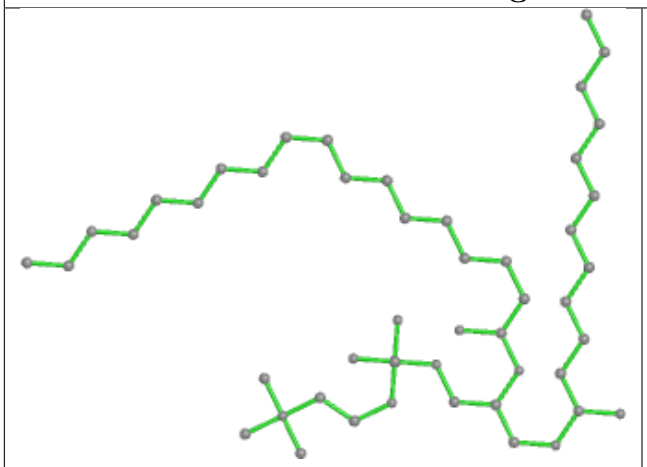


Torsions

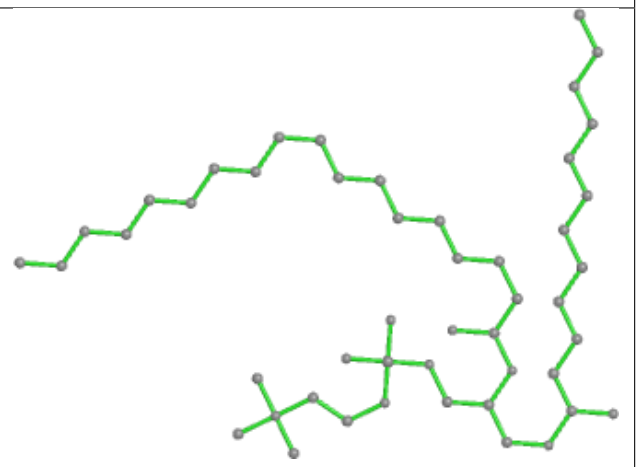


Rings

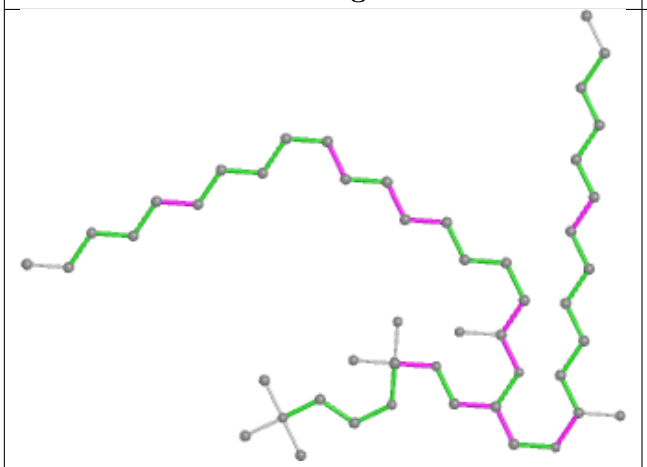
Ligand PCW C 2708



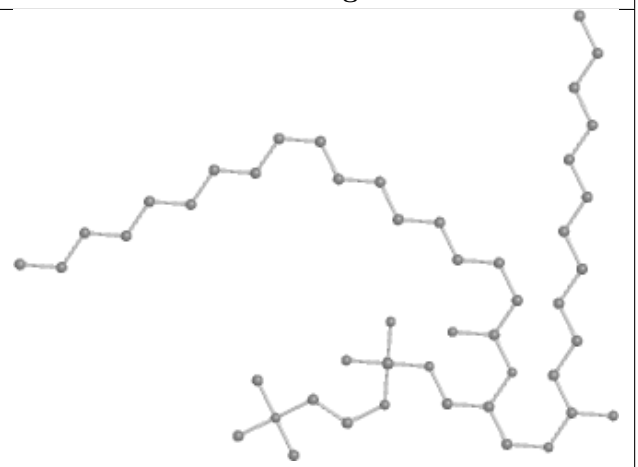
Bond lengths



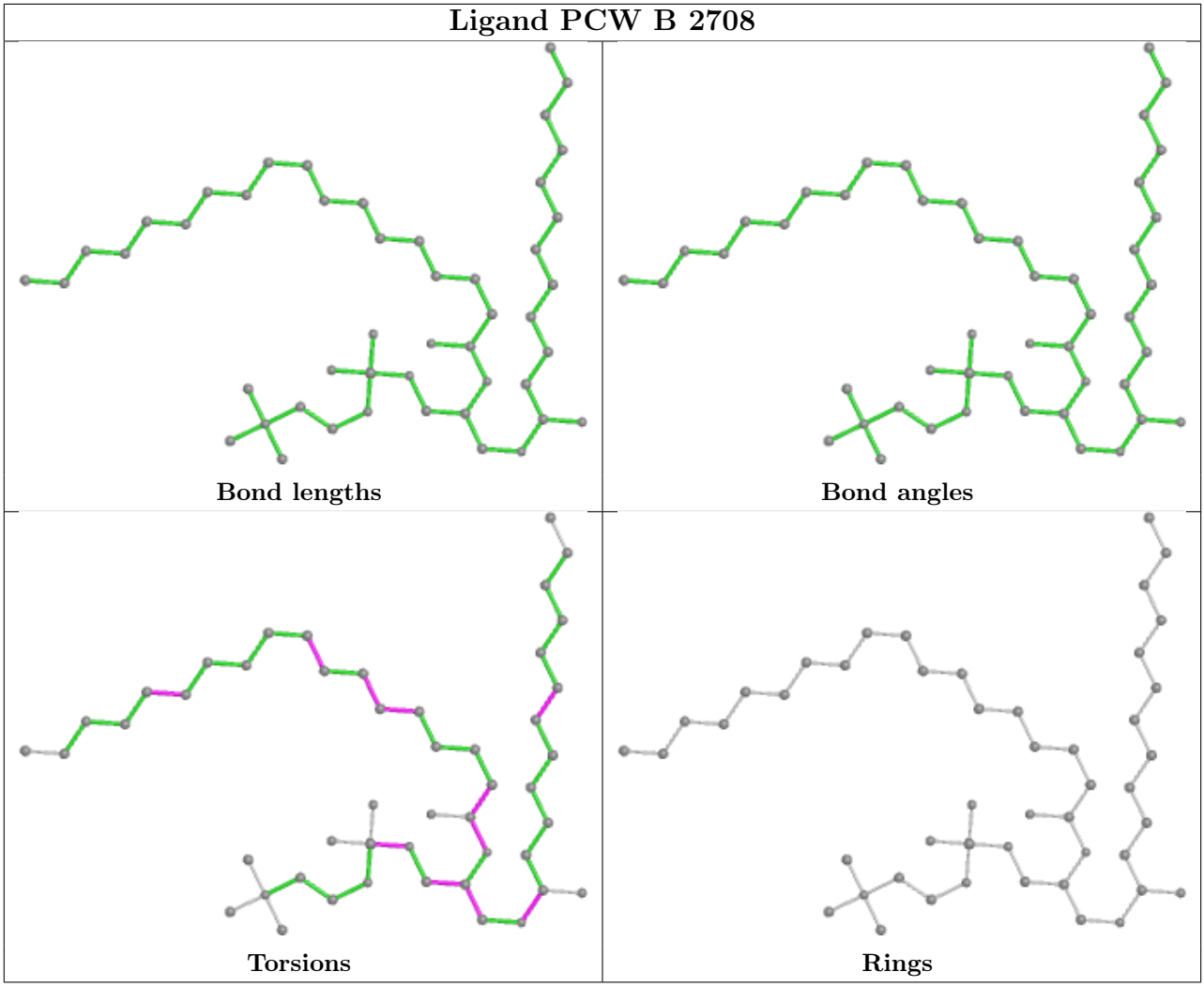
Bond angles



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.

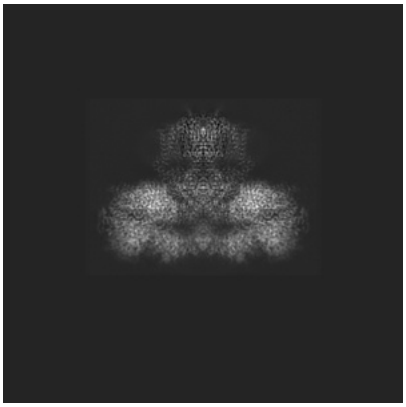
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41350. These allow visual inspection of the internal detail of the map and identification of artifacts.

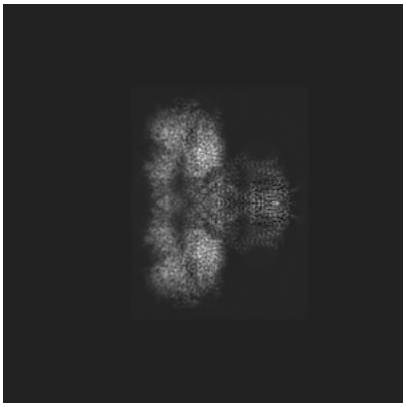
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

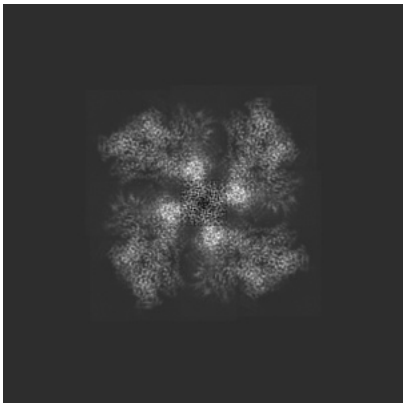
6.1.1 Primary map



X



Y

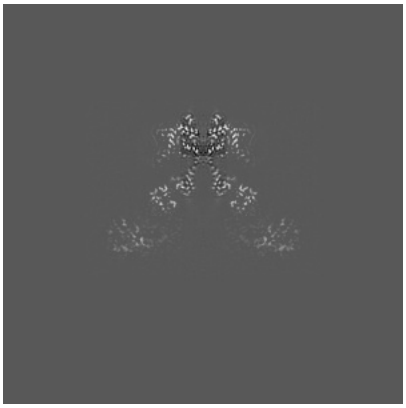


Z

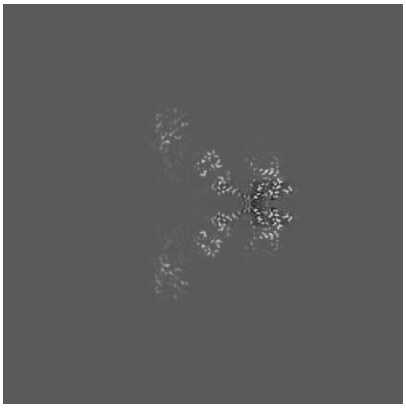
The images above show the map projected in three orthogonal directions.

6.2 Central slices

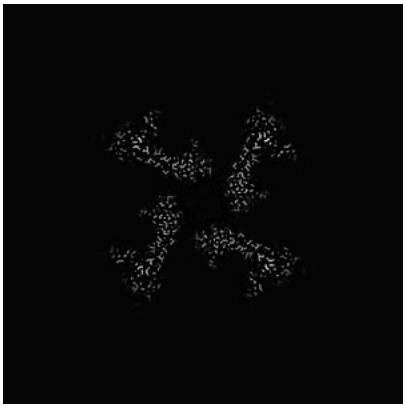
6.2.1 Primary map



X Index: 336



Y Index: 336

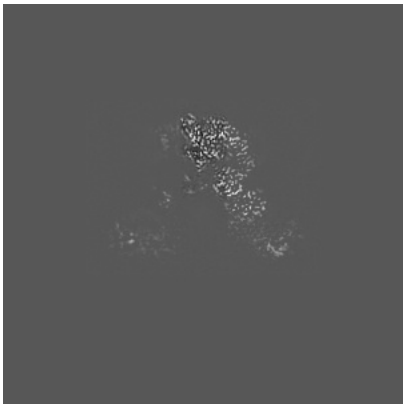


Z Index: 336

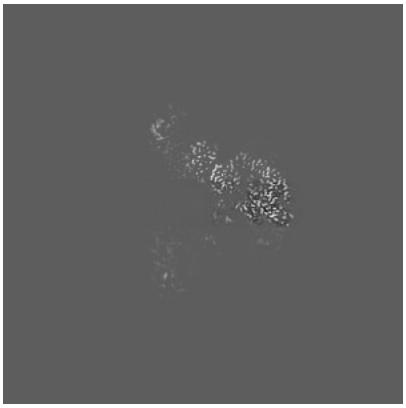
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

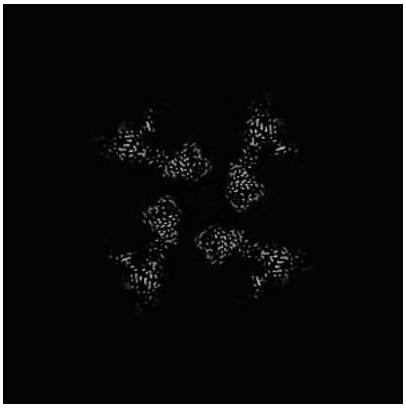
6.3.1 Primary map



X Index: 322



Y Index: 351

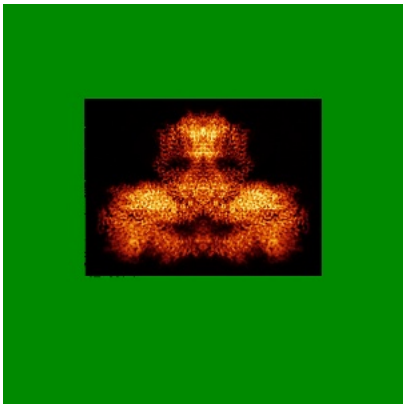


Z Index: 331

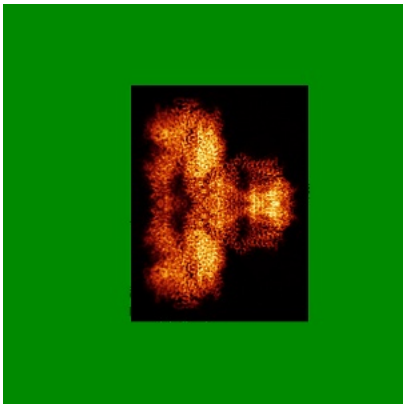
The images above show the largest variance slices of the map in three orthogonal directions.

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

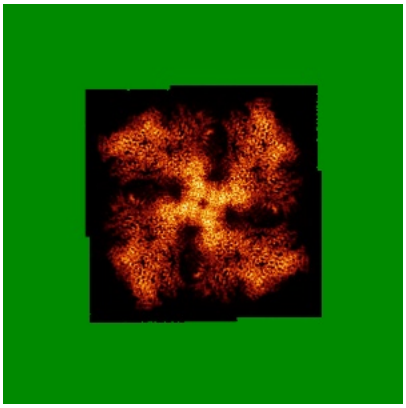
6.4.1 Primary map



X



Y

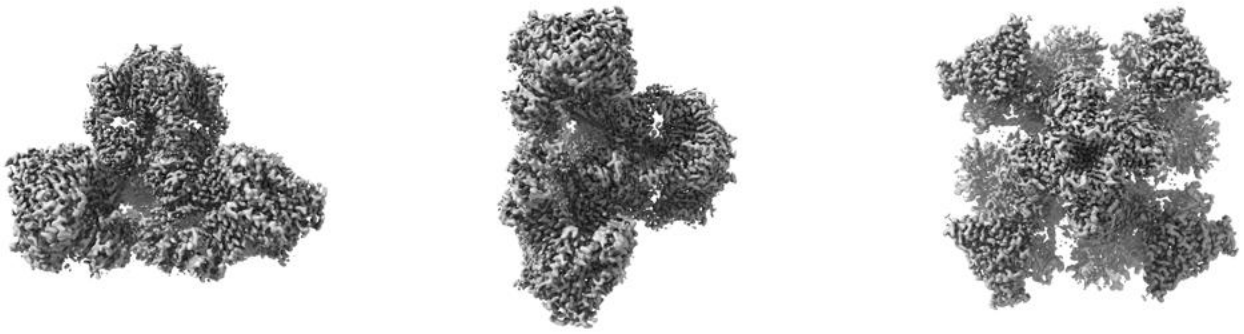


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

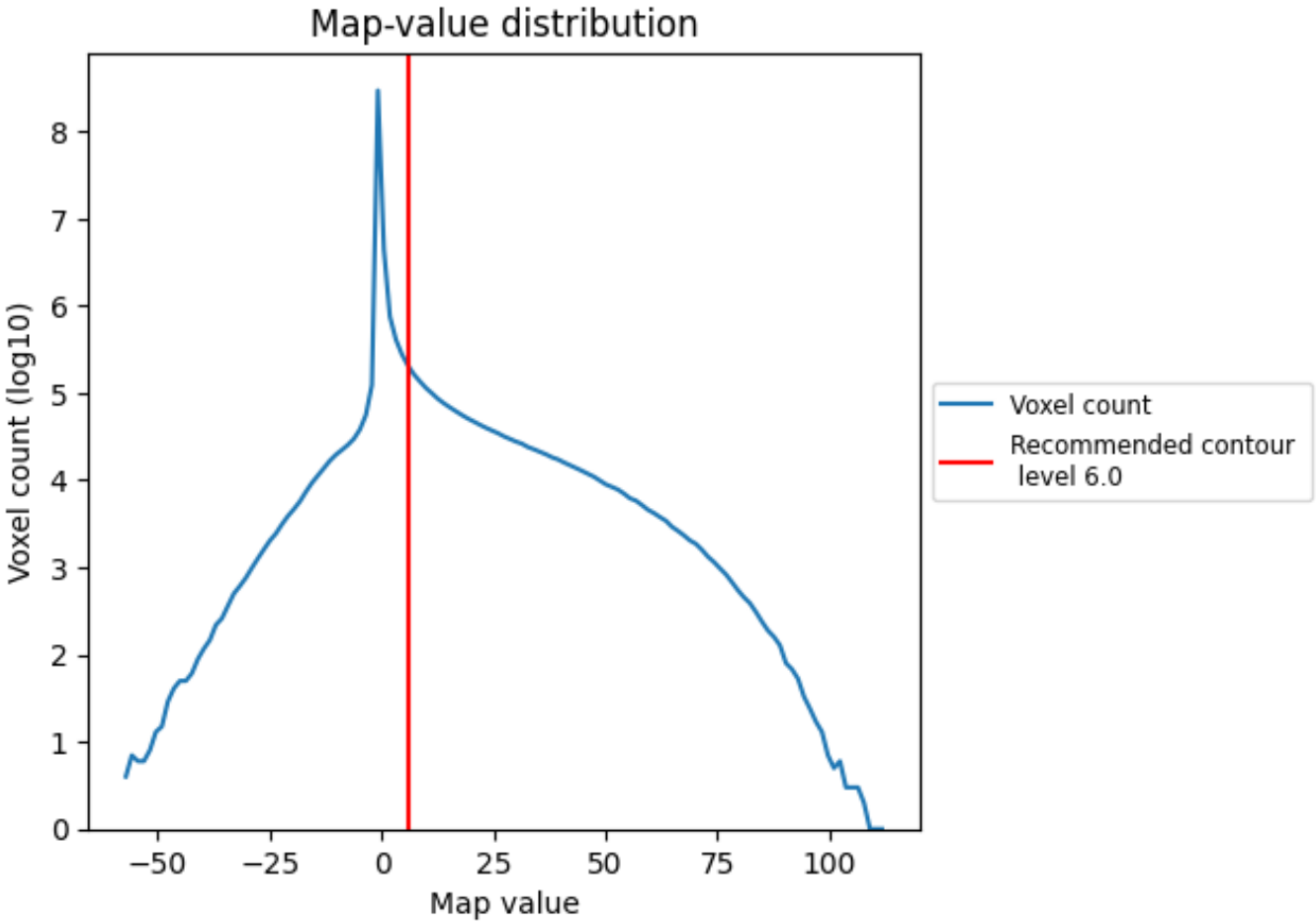
6.6 Mask visualisation (i)

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

7 Map analysis

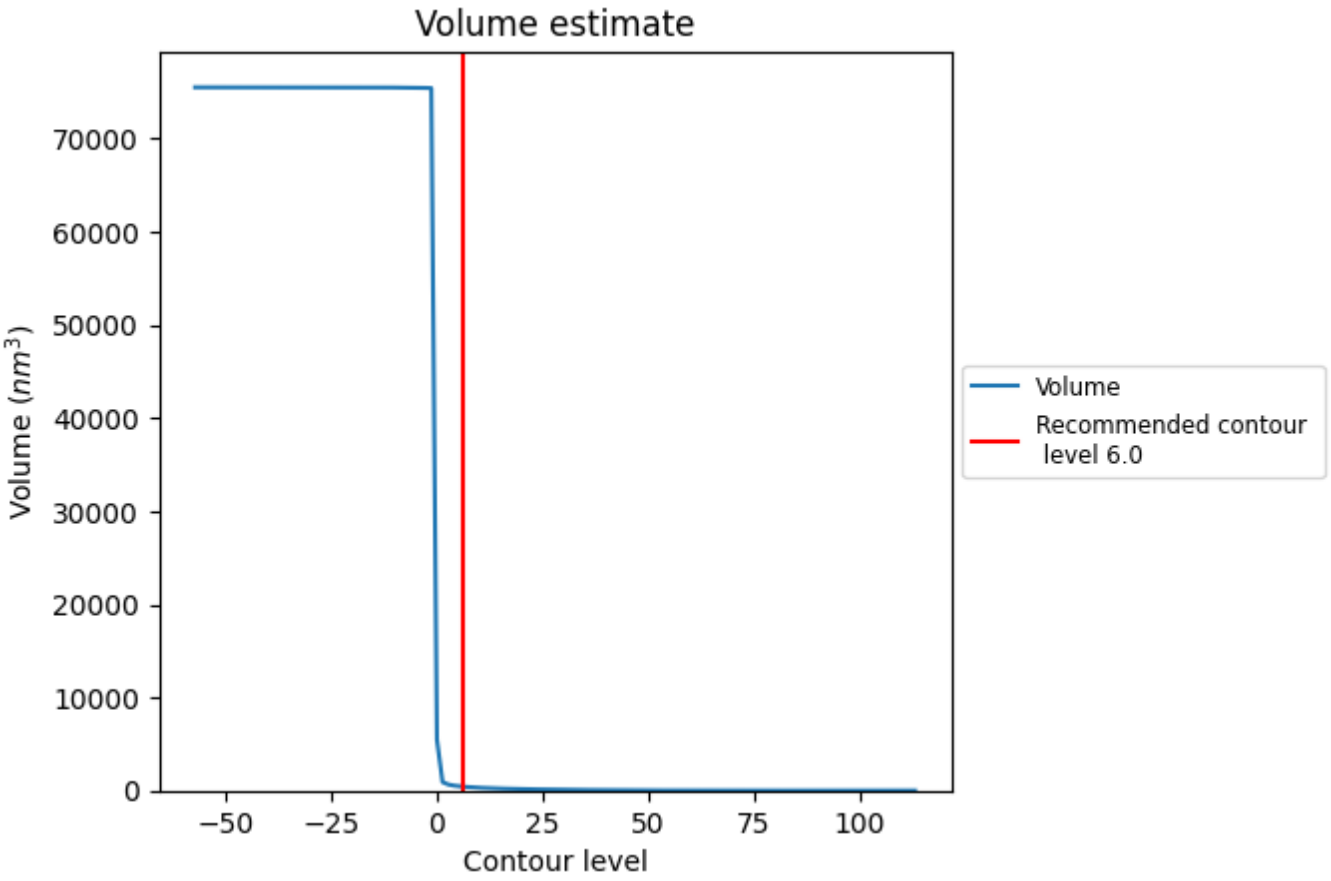
This section contains the results of statistical analysis of the map.

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.

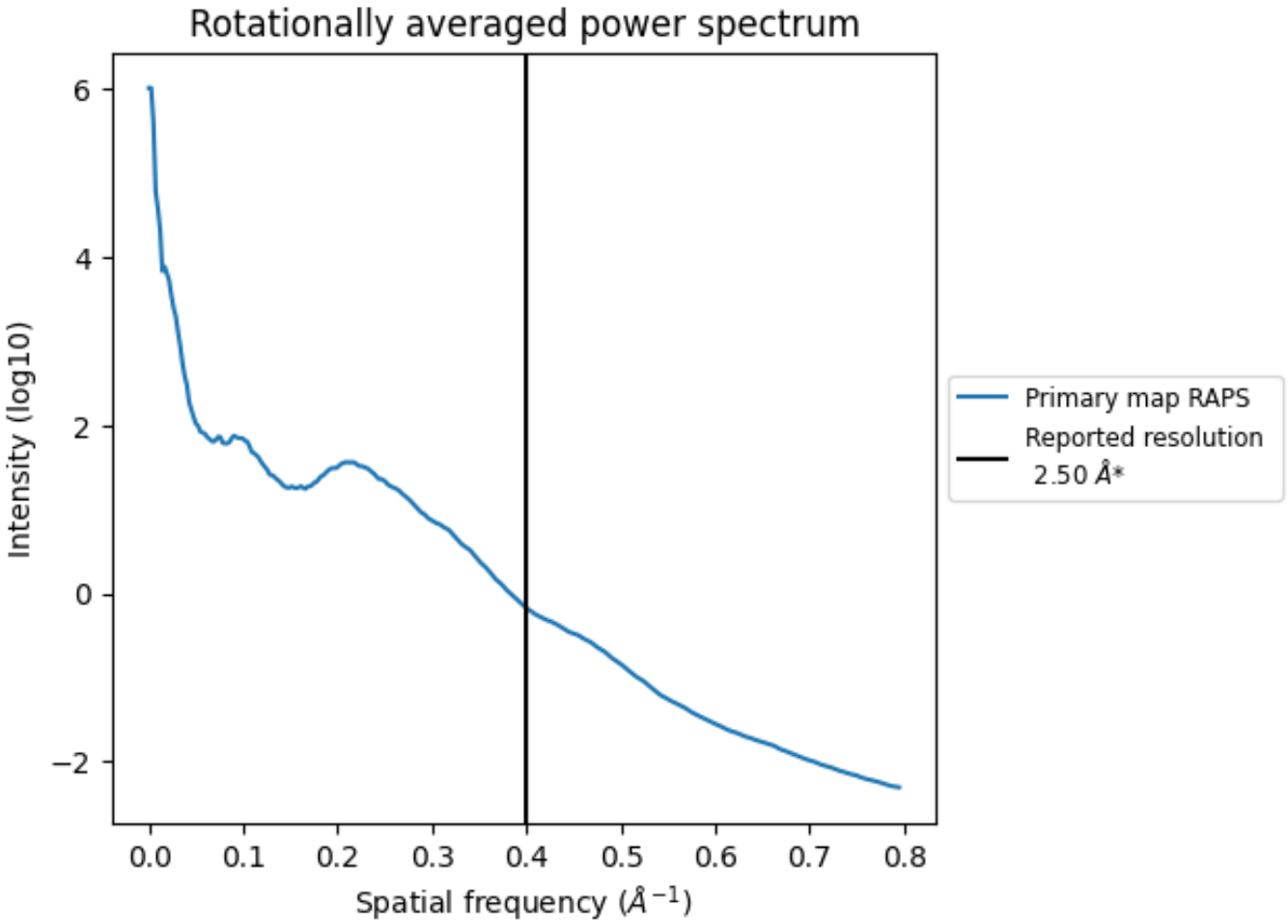
7.2 Volume estimate



The volume at the recommended contour level is 428 nm^3; this corresponds to an approximate mass of 387 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 0.400 $Å^{-1}$

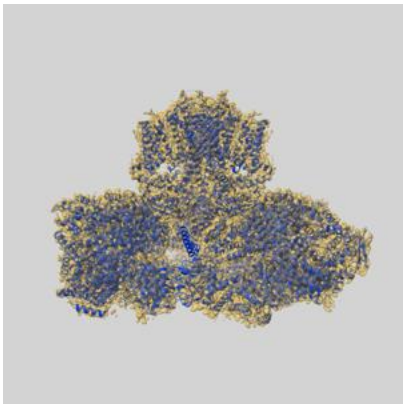
8 Fourier-Shell correlation (i)

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

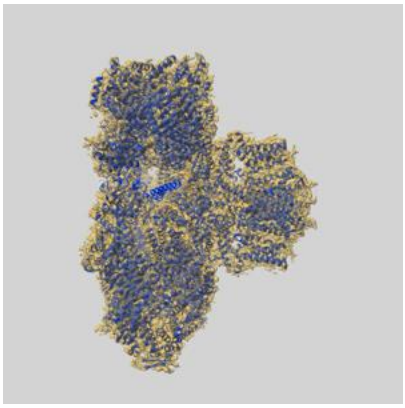
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41350 and PDB model 8TKG. Per-residue inclusion information can be found in section 3 on page 8.

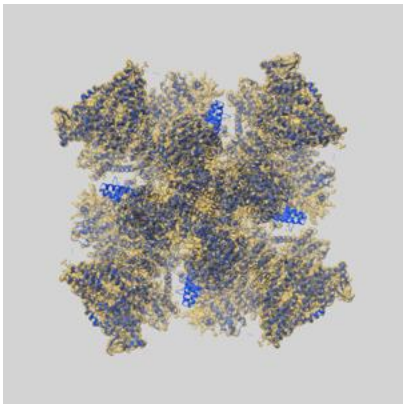
9.1 Map-model overlay



X



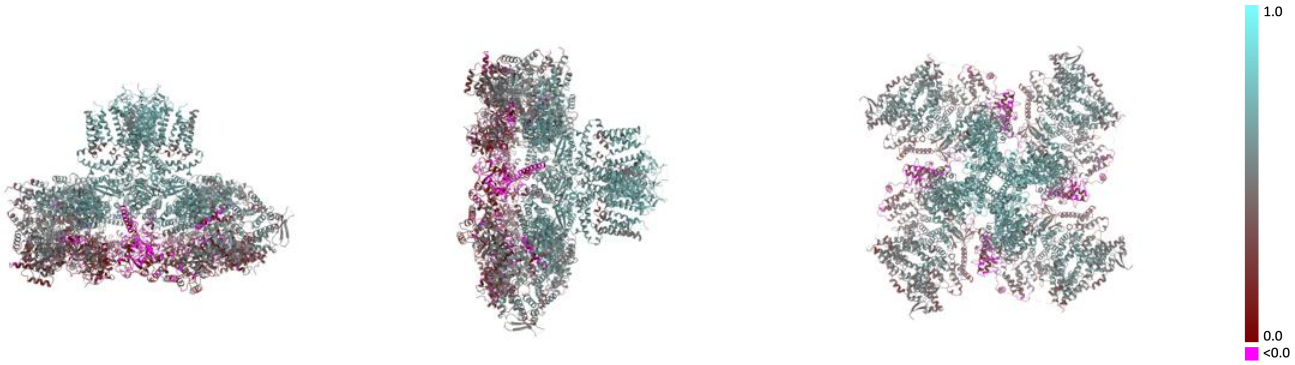
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

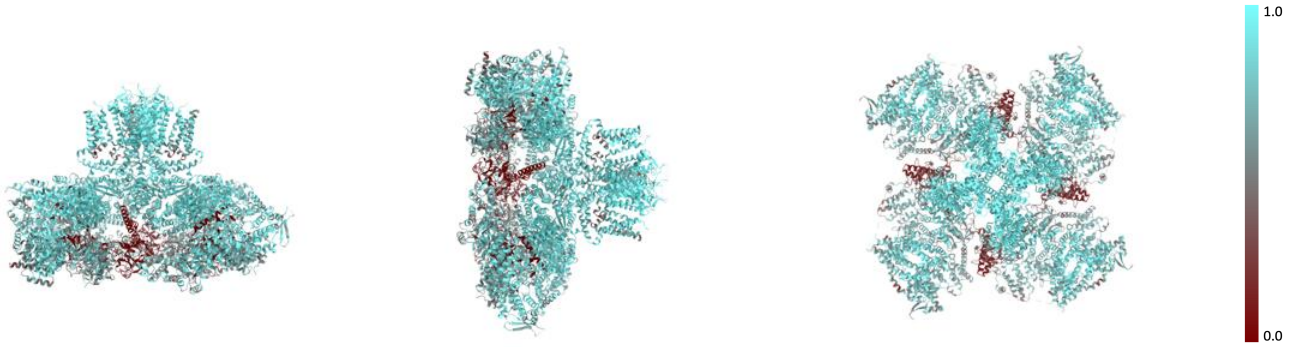
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

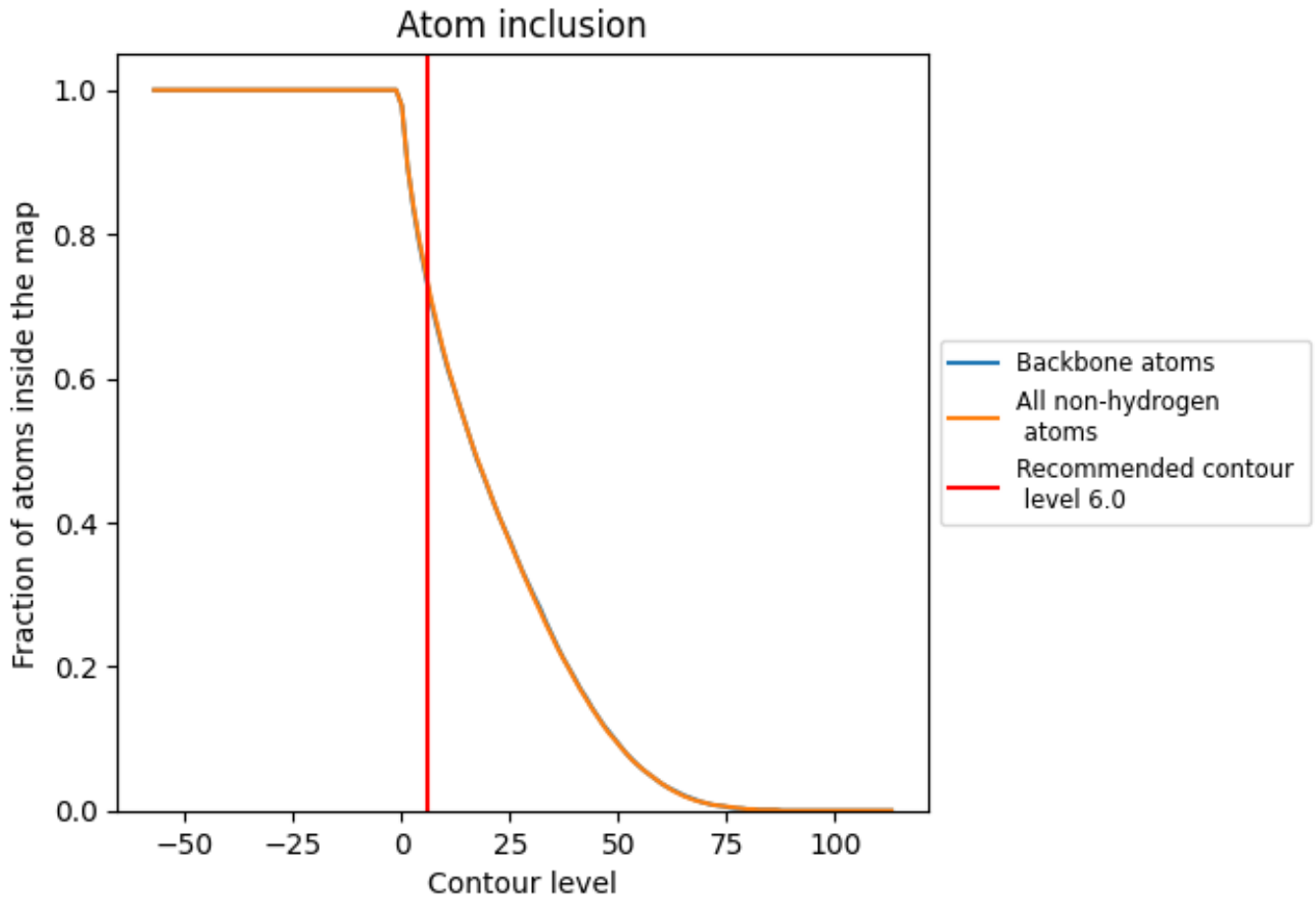
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.0).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 73% 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 (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7320	0.4410
A	0.7480	0.4520
B	0.7380	0.4430
C	0.7250	0.4260
D	0.7420	0.4450