Full wwPDB EM Validation Report (i)

May 13, 2023 – 01:13 PM EDT

PDB ID	:	8SI4
EMDB ID	:	EMD-40498
Title	:	Cryo-EM structure of TRPM7 N1098Q mutant in GDN detergent in open state
Authors	:	Nadezhdin, K.D.; Neuberger, A.; Sobolevsky, A.I.
Deposited on	:	2023-04-14
Resolution	:	2.46 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 (i) 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 (1)) were used in the production of this report:

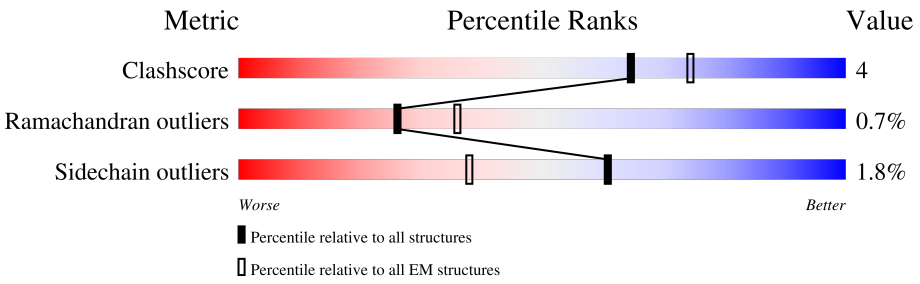
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.46 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	1279	40%, 75%, 11%, 14%
1	B	1279	40%, 75%, 11%, •, 14%
1	C	1279	40%, 75%, 11%, •, 14%
1	D	1279	40%, 76%, 10%, •, 14%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 79857 atoms, of which 40860 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 Transient receptor potential cation channel subfamily M member 7.

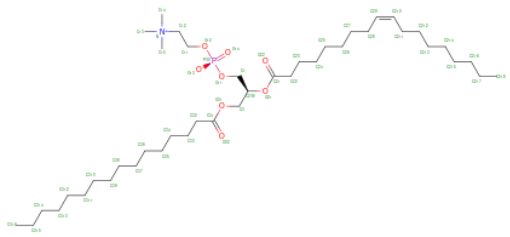
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1105	17966	5802	9037	1489	1578	60	0	0
1	B	1105	17966	5802	9037	1489	1578	60	0	0
1	C	1105	17966	5802	9037	1489	1578	60	0	0
1	D	1105	17966	5802	9037	1489	1578	60	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1098	GLN	ASN	engineered mutation	UNP Q923J1
B	1098	GLN	ASN	engineered mutation	UNP Q923J1
C	1098	GLN	ASN	engineered mutation	UNP Q923J1
D	1098	GLN	ASN	engineered mutation	UNP Q923J1

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

POV



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			79	25	44	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	B	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
2	B	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	B	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	B	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	B	1	79	25	44	1	8	1	0
			Total	C	H	N	O	P	
2	B	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	B	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	B	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	B	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	B	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	B	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	B	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	C	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	C	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	C	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	C	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	C	1	79	25	44	1	8	1	0
			Total	C	H	N	O	P	
2	C	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	C	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	C	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	C	1	134	42	82	1	8	1	0

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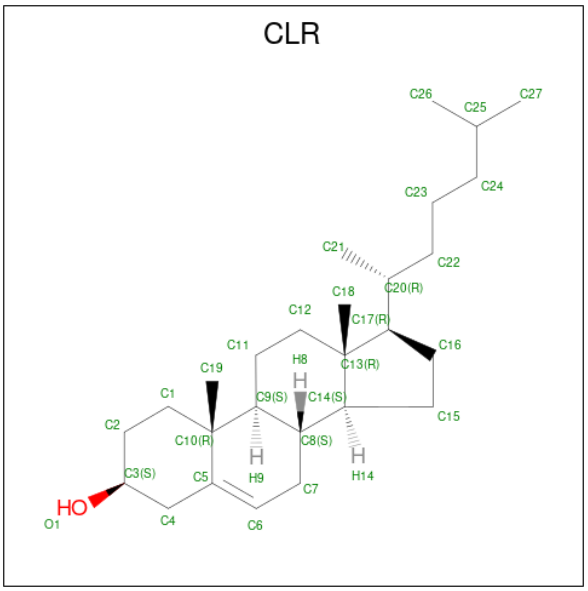
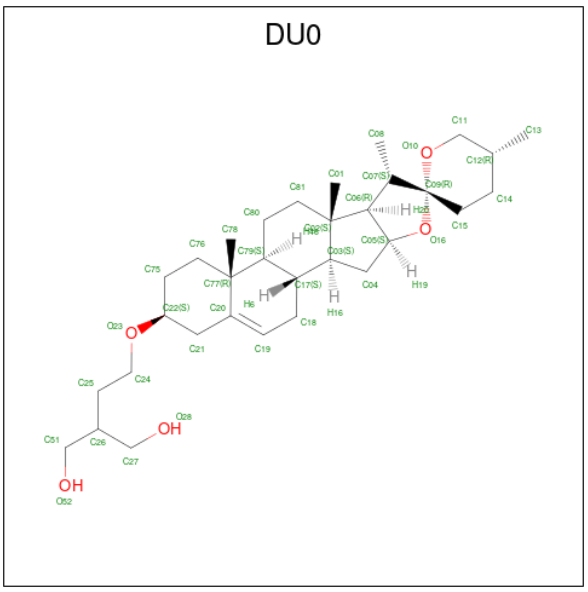
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
2	C	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	C	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	C	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	C	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	D	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	D	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	D	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	D	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	D	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	D	1	79	25	44	1	8	1	0
			Total	C	H	N	O	P	
2	D	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	D	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	D	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	D	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	D	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	D	1	134	42	82	1	8	1	0
			Total	C	H	N	O	P	
2	D	1	134	42	82	1	8	1	0

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
3	A	1	74	27	46	1	0
3	B	1	74	27	46	1	0
3	C	1	74	27	46	1	0
3	D	1	74	27	46	1	0

- Molecule 4 is 2-[2-[(1 {S},2 {S},4 {S},5' {R},6 {R},7 {S},8 {R},9 {S},12 {S},13 {R},16 {S})-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0^{2,9}.0^{4,8}.0^{13,18}]icos-18-ene-6 ,2'-oxane]-16-yl]oxyethyl]propane-1,3-diol (three-letter code: DU0) (formula: $C_{32}H_{52}O_5$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
4	A	1	89	32	52	5	0
4	A	1	89	32	52	5	0
4	B	1	89	32	52	5	0
4	B	1	89	32	52	5	0
4	B	1	89	32	52	5	0
4	C	1	89	32	52	5	0
4	D	1	89	32	52	5	0
4	D	1	89	32	52	5	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
5	A	1	1	1	0

- Molecule 6 is water.

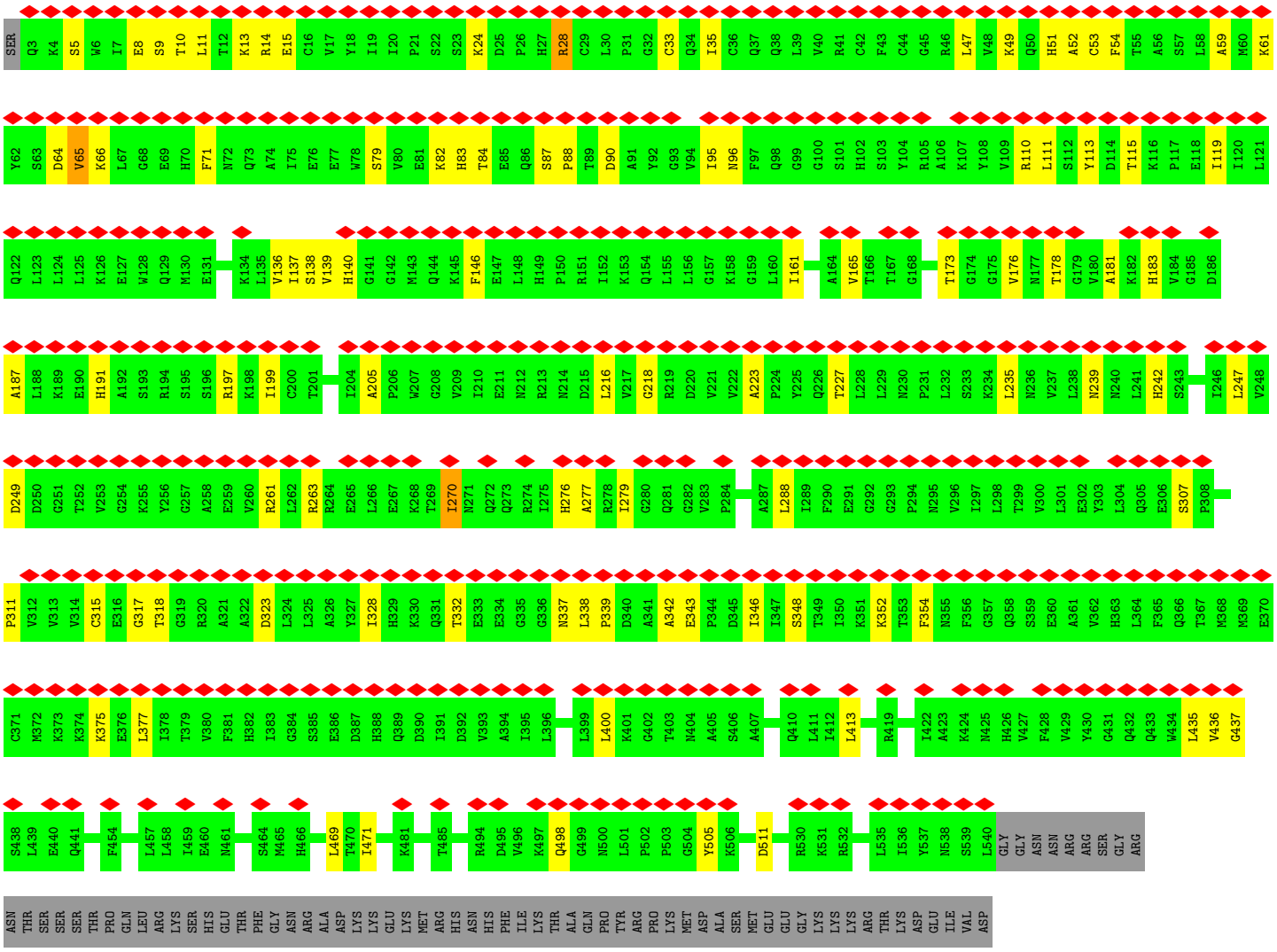
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
6	A	59	59	59	0
6	B	59	59	59	0
6	C	59	59	59	0
6	D	59	59	59	0

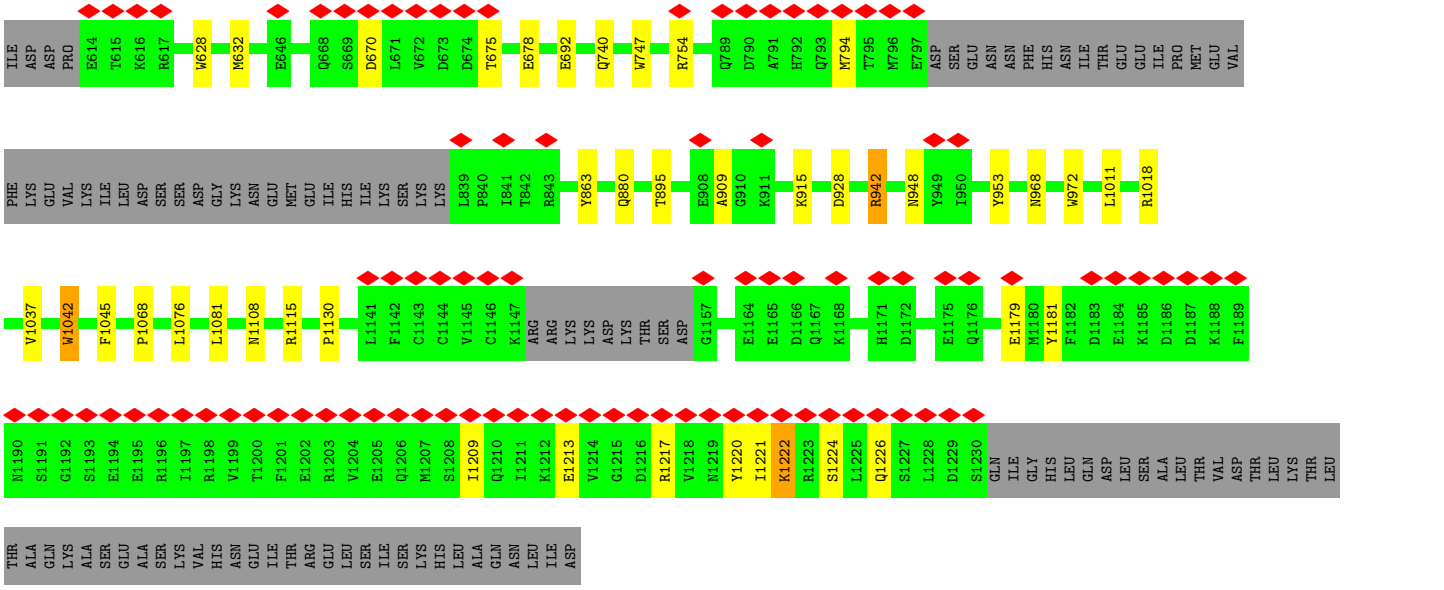
3 Residue-property plots (i)

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

- Molecule 1: Transient receptor potential cation channel subfamily M member 7

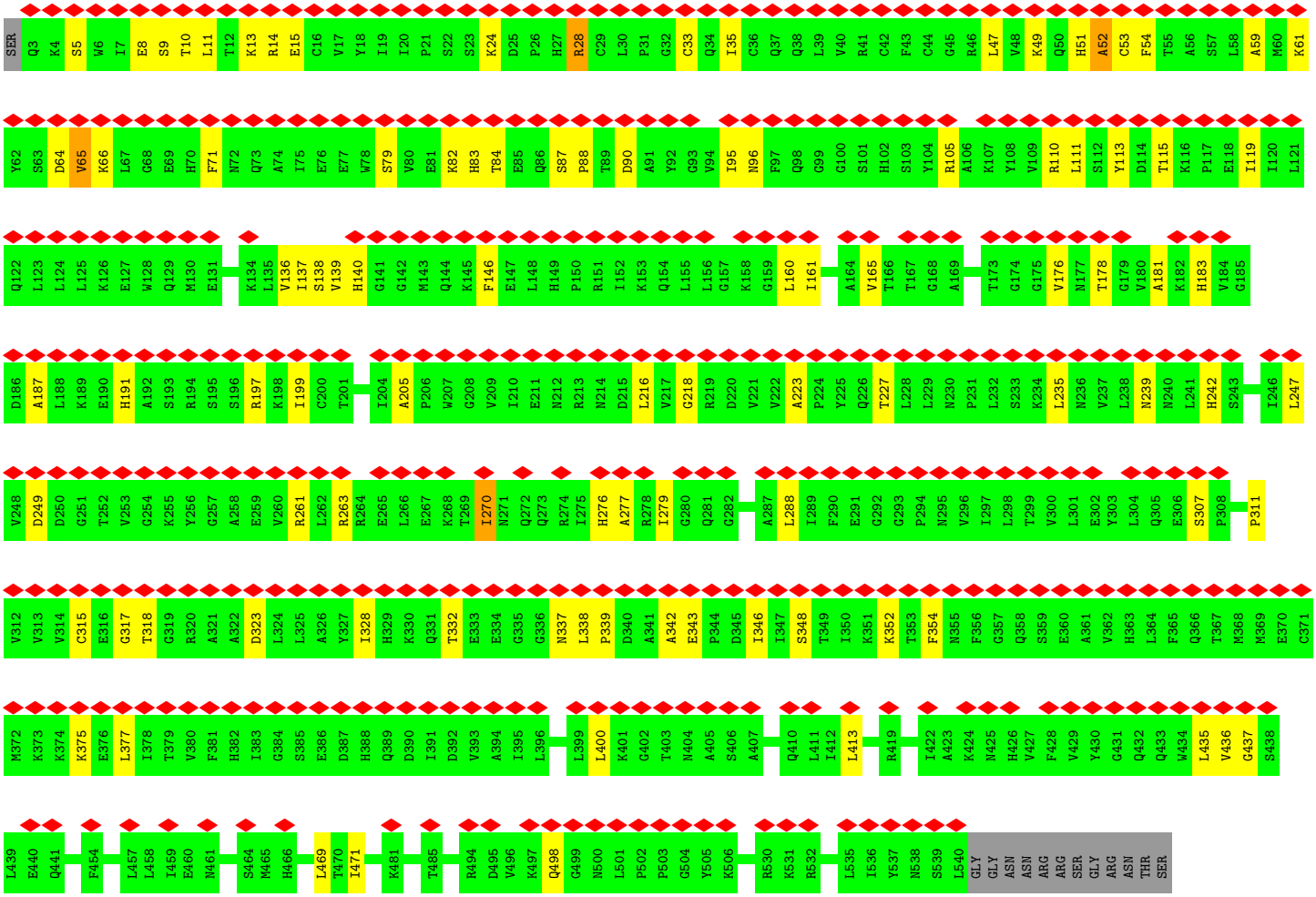
Chain A:

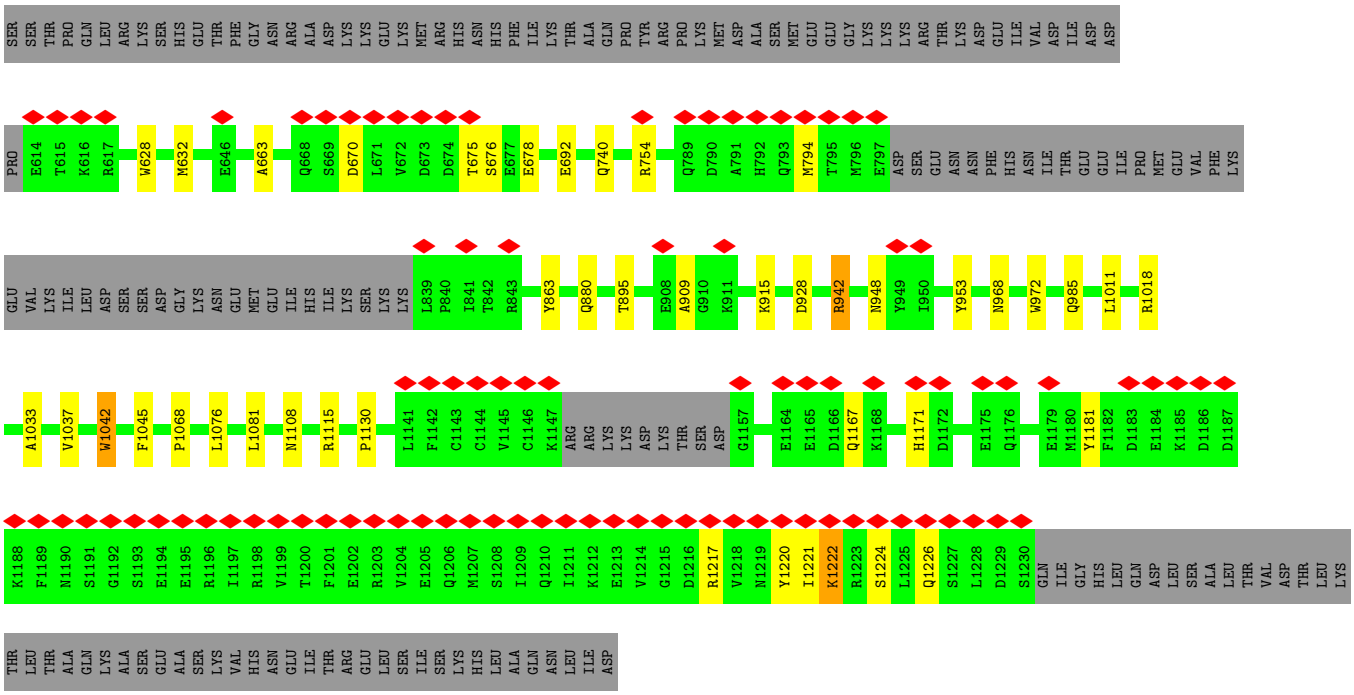




- Molecule 1: Transient receptor potential cation channel subfamily M member 7

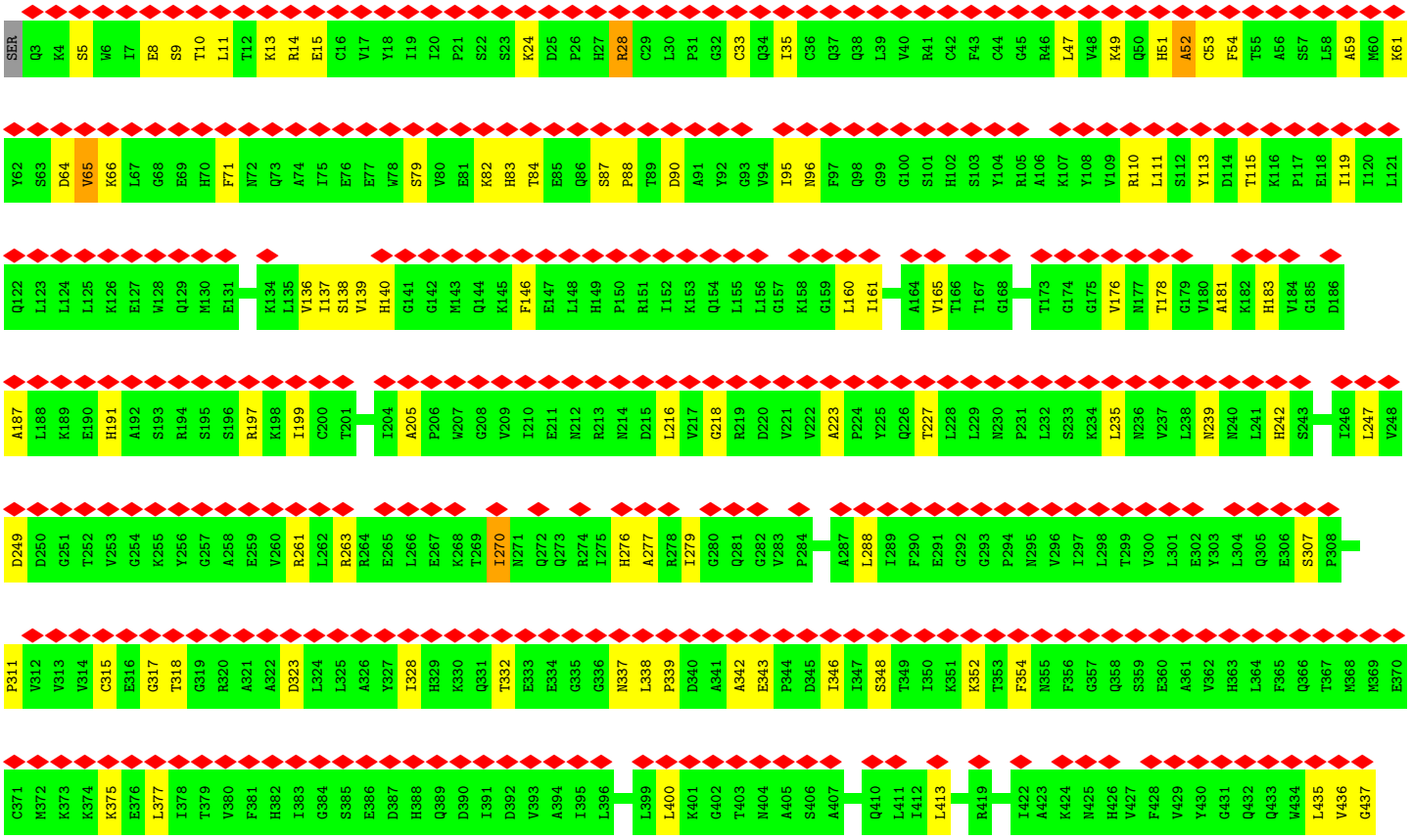
Chain B:

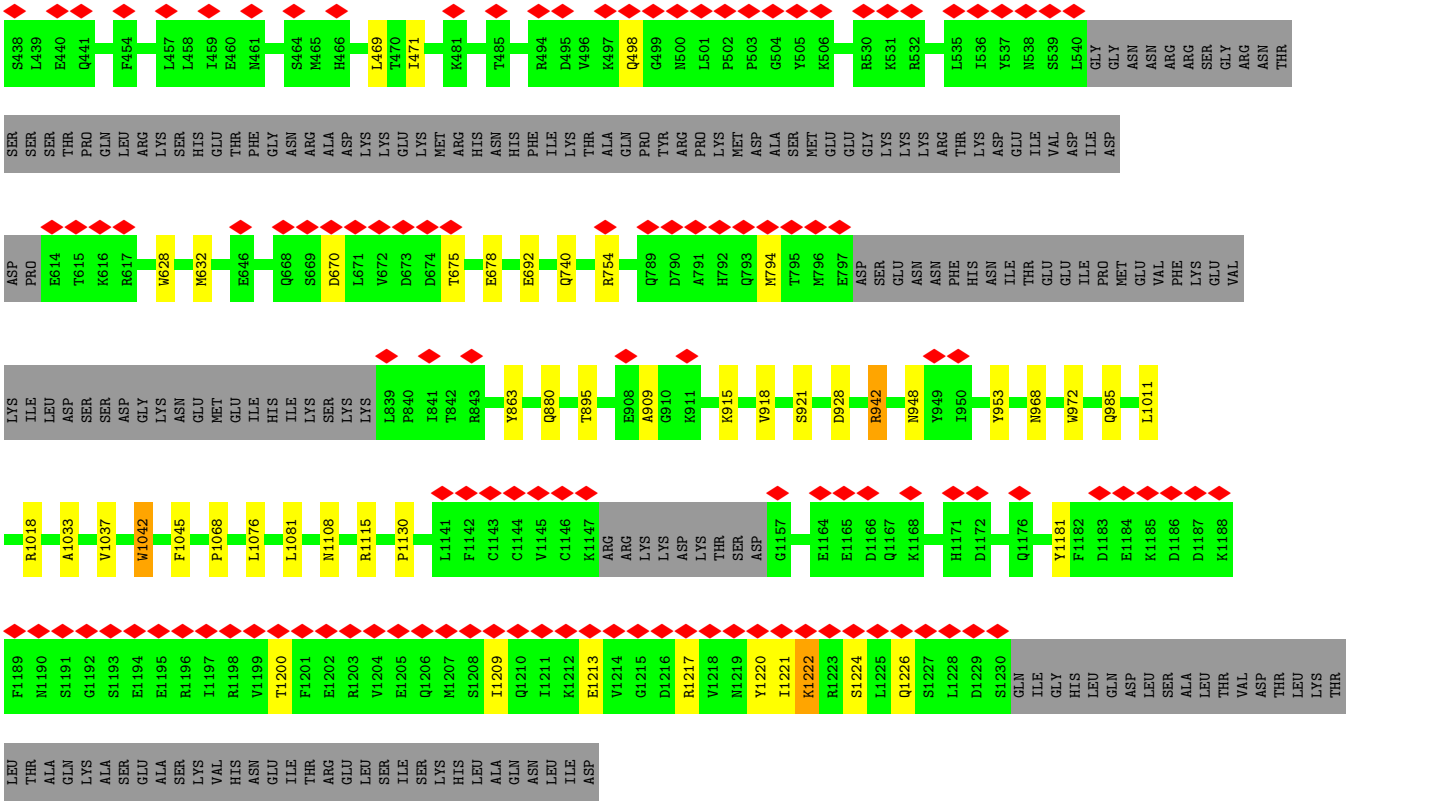




- Molecule 1: Transient receptor potential cation channel subfamily M member 7

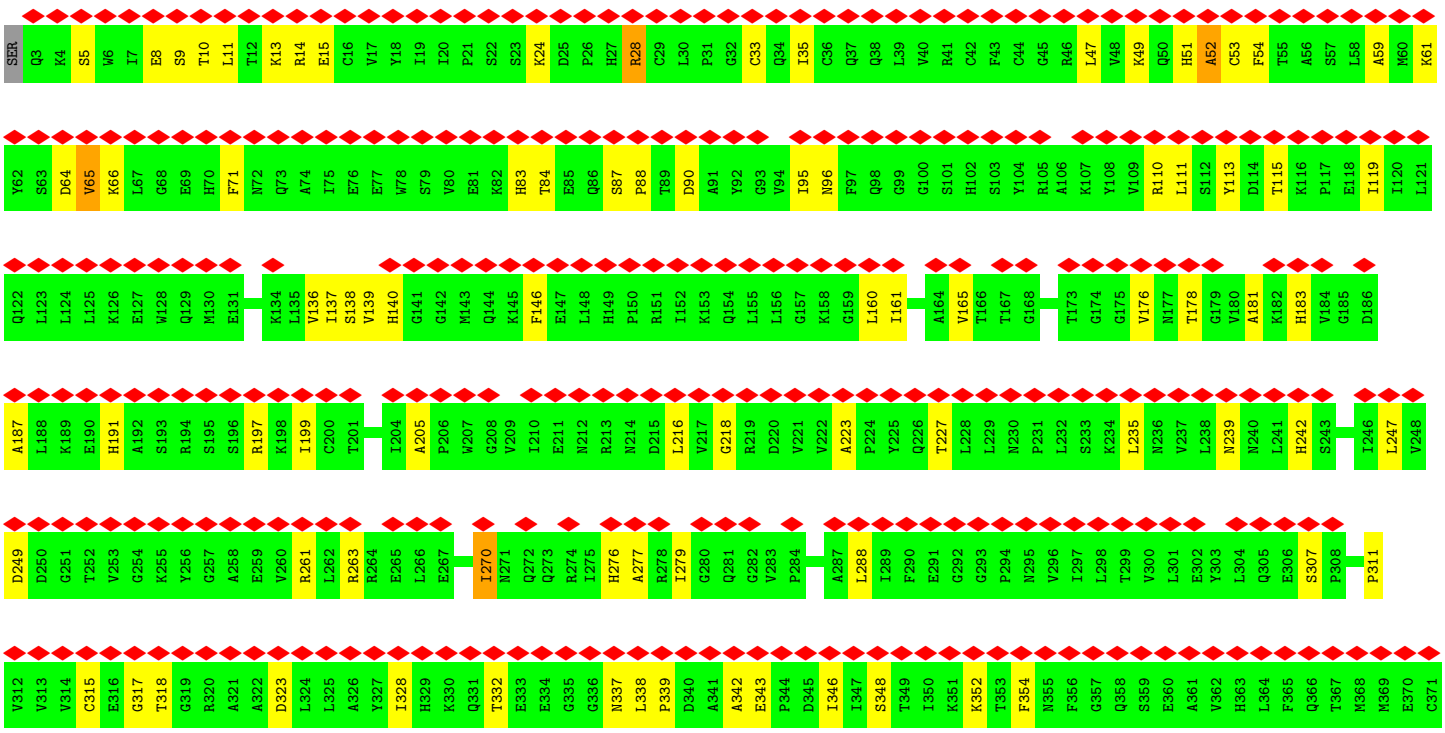
Chain C:

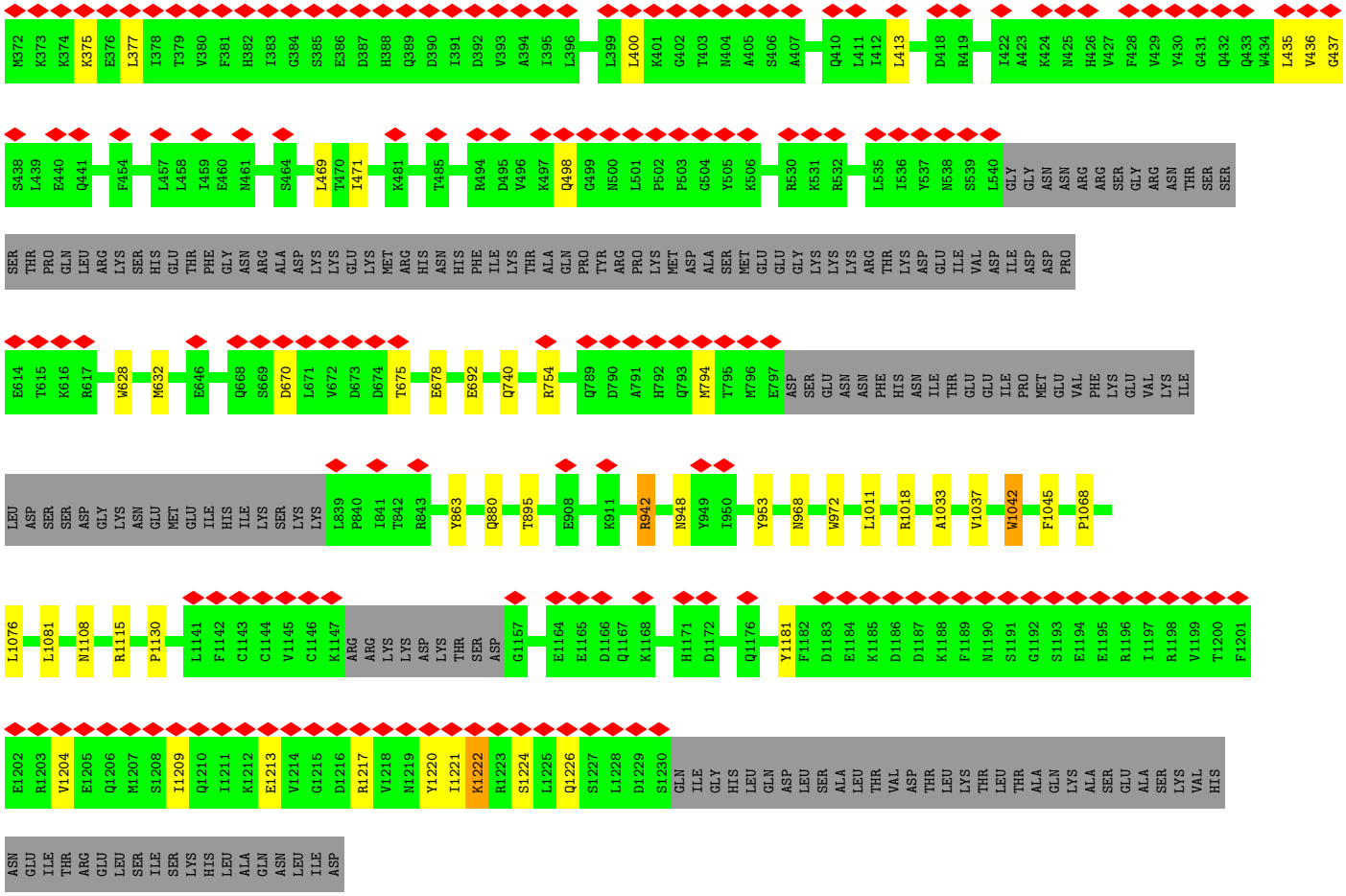




- Molecule 1: Transient receptor potential cation channel subfamily M member 7

Chain D:




M372 K373 K374 K375 E376 L377 I378 T379 V380 F381 H382 I383 G384 S385 E386 D387 H388 Q389 D390 I391 D392 V393 A394 I395 L396
L399 L400 K401 G402 T403 N404 A405 S406 A407
Q410 L411 I412 L413
D418 R419
I422 A423 K424 N425 H426 V427 F428 V429 Y430 G431 Q432 Q433 W434 L435 V436 G437
S438 L439 E440 Q441 F454 L457 L458 I459 E460 N461 S464 L469 T470 I471 K481 T485 R494 D495 V496 K497 Q498 G499 N500 L501 P502 P503 G504 Y505 K506 R530 K531 R532 L535 I536 Y537 N538 S539 L540 GLY GLY ASN ASN ARG ARG SER GLY ARG ASN THR SER SER
SER THR PRO GLN LEU ARG LYS SER HIS GLU THR PHE GLY ASN ARG ALA ASP LYS LYS GLU LYS MET ARG HIS ASN HIS PHE ILE LYS THR ALA GLN PRO TYR ARG PRO LYS MET ASP ALA SER MET GLU GLU GLY LYS LYS LYS ARG THR LYS ASP GLU ILE VAL ASP ILE ASP ASP PRO
E614 T615 K616 R617 W628 M632 E646 Q668 S669 D670 L671 V672 D673 D674 T675 E678 E692 Q740 R754 Q789 D790 A791 H792 Q793 M794 T795 M796 E797 ASP SER GLU ASN ASN PHE HIS ASN ILE THR GLU GLU ILE PRO MET GLU VAL PHE LYS GLU VAL LYS ILE
LEU ASP SER SER ASP GLY LYS ASN GLU MET GLU ILE HIS ILE LYS SER LYS LYS L839 P840 I841 T842 R843 Y863 Q880 T895 E908 K911 R942 N948 Y949 I950 Y953 N968 W972 L1011 R1018 A1033 V1037 W1042 F1045 P1068
L1076 L1081 N1108 R1115 P1130 L1141 F1142 C1143 C1144 V1145 C1146 K1147 ARG ARG LYS LYS ASP LYS THR SER ASP G1157 E1164 E1165 D1166 Q1167 K1168 H1171 D1172 Q1176 Y1181 F1182 D1183 E1184 K1185 D1186 D1187 K1188 F1189 N1190 S1191 G1192 S1193 E1194 E1195 R1196 I1197 R1198 V1199 T1200 F1201
E1202 R1203 V1204 E1205 Q1206 M1207 S1208 I1209 Q1210 I1211 K1212 E1213 V1214 G1215 D1216 R1217 V1218 N1219 Y1220 I1221 K1222 R1223 S1224 L1225 Q1226 S1227 L1228 D1229 S1230 GLN ILE GLY HIS LEU GLN ASP LEU SER ALA LEU THR VAL ASP THR LEU LYS THR LEU THR ALA GLN LYS ALA SER GLU ALA SER LYS VAL HIS
ASN GLU ILE THR ARG GLU LEU SER ILE SER LYS HIS LEU ALA GLN ASN LEU ILE ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157446	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.079	Depositor
Minimum map value	-1.403	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.218	Depositor
Map size (Å)	249.0, 249.0, 249.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, DU0, CLR, POV

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.58	1/9145 (0.0%)	0.66	0/12388
1	B	0.58	1/9145 (0.0%)	0.66	0/12388
1	C	0.58	1/9145 (0.0%)	0.66	0/12388
1	D	0.58	1/9145 (0.0%)	0.66	0/12388
All	All	0.58	4/36580 (0.0%)	0.66	0/49552

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
1	C	0	4
1	D	0	4
All	All	0	15

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1042	TRP	CE3-CZ3	-5.24	1.29	1.38
1	D	1042	TRP	CE3-CZ3	-5.23	1.29	1.38
1	C	1042	TRP	CE3-CZ3	-5.22	1.29	1.38
1	A	1042	TRP	CE3-CZ3	-5.17	1.29	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	235	LEU	Peptide
1	A	307	SER	Peptide
1	A	354	PHE	Peptide
1	B	235	LEU	Peptide
1	B	307	SER	Peptide
1	B	354	PHE	Peptide
1	B	52	ALA	Peptide
1	C	235	LEU	Peptide
1	C	307	SER	Peptide
1	C	354	PHE	Peptide
1	C	52	ALA	Peptide
1	D	235	LEU	Peptide
1	D	307	SER	Peptide
1	D	354	PHE	Peptide
1	D	52	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8929	9037	9033	76	0
1	B	8929	9037	9033	78	0
1	C	8929	9037	9033	77	0
1	D	8929	9037	9033	72	0
2	A	659	1028	1026	15	0
2	B	659	1028	1026	11	0
2	C	659	1028	1026	10	0
2	D	659	1028	1026	13	0
3	A	28	46	46	1	0
3	B	28	46	46	1	0
3	C	28	46	46	1	0
3	D	28	46	46	1	0
4	A	74	104	0	0	0
4	B	111	156	0	0	0
4	C	37	52	0	0	0
4	D	74	104	0	0	0
5	A	1	0	0	0	0
6	A	59	0	0	6	0
6	B	59	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	59	0	0	7	0
6	D	59	0	0	5	0
All	All	38997	40860	40420	333	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 4.

All (333) 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:111:LEU:O	1:A:249:ASP:N	2.19	0.76
1:A:187:ALA:O	1:A:191:HIS:ND1	2.19	0.75
1:D:111:LEU:O	1:D:249:ASP:N	2.19	0.75
1:C:111:LEU:O	1:C:249:ASP:N	2.19	0.75
1:B:111:LEU:O	1:B:249:ASP:N	2.19	0.75
2:D:1304:POV:O13	2:D:1305:POV:H15B	1.87	0.74
1:B:1018:ARG:NH2	6:B:1404:HOH:O	2.20	0.74
1:C:1018:ARG:NH2	6:C:1405:HOH:O	2.20	0.74
1:D:1018:ARG:NH2	6:D:1405:HOH:O	2.20	0.74
1:D:953:TYR:OH	6:D:1401:HOH:O	2.04	0.74
1:B:953:TYR:OH	6:B:1401:HOH:O	2.05	0.73
1:A:1045:PHE:O	6:A:1402:HOH:O	2.06	0.73
1:C:953:TYR:OH	6:C:1401:HOH:O	2.04	0.73
1:C:628:TRP:NE1	1:C:632:MET:SD	2.62	0.73
1:B:628:TRP:NE1	1:B:632:MET:SD	2.62	0.73
1:A:1018:ARG:NH2	6:A:1405:HOH:O	2.20	0.73
2:B:1302:POV:O13	2:B:1303:POV:H15B	1.88	0.73
1:D:1045:PHE:O	6:D:1402:HOH:O	2.06	0.73
1:B:187:ALA:O	1:B:191:HIS:ND1	2.19	0.73
1:C:1045:PHE:O	6:C:1402:HOH:O	2.06	0.72
1:A:628:TRP:NE1	1:A:632:MET:SD	2.62	0.72
1:B:1045:PHE:O	6:B:1402:HOH:O	2.07	0.72
1:D:628:TRP:NE1	1:D:632:MET:SD	2.62	0.72
1:D:692:GLU:OE1	1:D:1181:TYR:OH	2.07	0.72
1:C:692:GLU:OE1	1:C:1181:TYR:OH	2.07	0.72
1:B:692:GLU:OE1	1:B:1181:TYR:OH	2.07	0.72
1:D:187:ALA:O	1:D:191:HIS:ND1	2.19	0.71
2:A:1315:POV:O13	2:A:1316:POV:H15B	1.90	0.71
1:A:692:GLU:OE1	1:A:1181:TYR:OH	2.07	0.71
1:D:1221:ILE:O	1:D:1224:SER:OG	2.06	0.71
1:C:187:ALA:O	1:C:191:HIS:ND1	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1221:ILE:O	1:B:1224:SER:OG	2.06	0.69
1:C:895:THR:OG1	1:C:1130:PRO:O	2.04	0.69
1:A:1221:ILE:O	1:A:1224:SER:OG	2.06	0.69
1:A:895:THR:OG1	1:A:1130:PRO:O	2.04	0.69
1:C:328:ILE:O	1:C:332:THR:OG1	2.09	0.68
1:B:165:VAL:O	1:B:197:ARG:NH1	2.27	0.68
1:C:165:VAL:O	1:C:197:ARG:NH1	2.27	0.68
1:D:165:VAL:O	1:D:197:ARG:NH1	2.27	0.68
1:C:1221:ILE:O	1:C:1224:SER:OG	2.06	0.68
1:C:863:TYR:OH	1:C:972:TRP:O	2.12	0.68
1:D:895:THR:OG1	1:D:1130:PRO:O	2.04	0.68
1:A:165:VAL:O	1:A:197:ARG:NH1	2.27	0.68
1:B:863:TYR:OH	1:B:972:TRP:O	2.12	0.67
1:A:13:LYS:NZ	1:A:15:GLU:OE2	2.28	0.67
1:B:895:THR:OG1	1:B:1130:PRO:O	2.04	0.67
1:A:863:TYR:OH	1:A:972:TRP:O	2.12	0.67
1:B:13:LYS:NZ	1:B:15:GLU:OE2	2.28	0.66
1:D:863:TYR:OH	1:D:972:TRP:O	2.12	0.66
1:D:47:LEU:O	1:D:51:HIS:ND1	2.30	0.65
1:A:47:LEU:O	1:A:51:HIS:ND1	2.30	0.65
1:C:47:LEU:O	1:C:51:HIS:ND1	2.30	0.65
1:B:47:LEU:O	1:B:51:HIS:ND1	2.29	0.65
1:C:13:LYS:NZ	1:C:15:GLU:OE2	2.28	0.64
1:A:953:TYR:OH	6:A:1401:HOH:O	2.04	0.64
1:D:13:LYS:NZ	1:D:15:GLU:OE2	2.28	0.63
1:A:5:SER:O	1:A:8:GLU:N	2.33	0.62
1:B:5:SER:O	1:B:8:GLU:N	2.33	0.62
1:D:5:SER:O	1:D:8:GLU:N	2.33	0.62
1:C:5:SER:O	1:C:8:GLU:N	2.33	0.62
1:B:675:THR:OG1	1:B:678:GLU:OE1	2.19	0.61
1:C:205:ALA:HB3	1:C:247:LEU:CD2	2.31	0.61
1:A:14:ARG:N	1:A:249:ASP:OD2	2.34	0.61
1:A:205:ALA:HB3	1:A:247:LEU:CD2	2.31	0.61
1:A:675:THR:OG1	1:A:678:GLU:OE1	2.19	0.61
1:D:205:ALA:HB3	1:D:247:LEU:CD2	2.31	0.61
1:D:675:THR:OG1	1:D:678:GLU:OE1	2.19	0.61
2:C:1302:POV:O13	2:C:1303:POV:H15B	2.01	0.60
1:B:205:ALA:HB3	1:B:247:LEU:CD2	2.31	0.60
1:B:14:ARG:N	1:B:249:ASP:OD2	2.34	0.60
2:A:1312:POV:H210	2:A:1312:POV:H21D	1.84	0.59
1:C:675:THR:OG1	1:C:678:GLU:OE1	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1314:POV:H210	2:C:1314:POV:H21D	1.83	0.59
1:D:14:ARG:N	1:D:249:ASP:OD2	2.34	0.59
1:D:161:ILE:HG23	1:D:199:ILE:CD1	2.33	0.59
1:C:14:ARG:N	1:C:249:ASP:OD2	2.34	0.59
1:C:161:ILE:HG23	1:C:199:ILE:CD1	2.33	0.59
1:B:909:ALA:O	1:B:915:LYS:NZ	2.25	0.59
1:A:909:ALA:O	1:A:915:LYS:NZ	2.25	0.58
1:B:276:HIS:O	1:B:279:ILE:N	2.36	0.58
1:A:161:ILE:HG23	1:A:199:ILE:CD1	2.33	0.58
1:C:216:LEU:HD23	1:C:223:ALA:HB1	1.85	0.58
2:D:1301:POV:H21D	2:D:1301:POV:H210	1.84	0.58
1:B:317:GLY:N	1:B:323:ASP:OD1	2.37	0.58
1:C:139:VAL:O	1:C:263:ARG:NH2	2.37	0.58
1:C:317:GLY:N	1:C:323:ASP:OD1	2.37	0.58
1:A:216:LEU:HD23	1:A:223:ALA:HB1	1.85	0.58
1:B:161:ILE:HG23	1:B:199:ILE:CD1	2.33	0.58
1:B:176:VAL:O	1:B:181:ALA:HB3	2.04	0.58
1:B:216:LEU:HD23	1:B:223:ALA:HB1	1.85	0.58
1:A:317:GLY:N	1:A:323:ASP:OD1	2.37	0.57
1:C:176:VAL:O	1:C:181:ALA:HB3	2.04	0.57
1:B:139:VAL:O	1:B:263:ARG:NH2	2.37	0.57
1:D:139:VAL:O	1:D:263:ARG:NH2	2.37	0.57
1:A:176:VAL:O	1:A:181:ALA:HB3	2.04	0.57
2:B:1315:POV:H21D	2:B:1315:POV:H210	1.85	0.57
1:D:176:VAL:O	1:D:181:ALA:HB3	2.04	0.57
1:D:83:HIS:O	1:D:84:THR:OG1	2.22	0.57
1:C:276:HIS:O	1:C:279:ILE:N	2.36	0.57
1:C:332:THR:OG1	1:C:375:LYS:NZ	2.38	0.57
1:D:216:LEU:HD23	1:D:223:ALA:HB1	1.85	0.57
1:C:754:ARG:NH2	1:D:670:ASP:O	2.38	0.57
1:D:317:GLY:N	1:D:323:ASP:OD1	2.37	0.56
1:D:146:PHE:O	1:D:183:HIS:NE2	2.36	0.56
1:B:83:HIS:O	1:B:84:THR:OG1	2.22	0.56
1:A:139:VAL:O	1:A:263:ARG:NH2	2.37	0.56
1:D:332:THR:OG1	1:D:375:LYS:NZ	2.38	0.56
2:B:1304:POV:O14	2:B:1309:POV:H15B	2.06	0.56
1:C:181:ALA:O	1:C:239:ASN:ND2	2.39	0.56
1:B:181:ALA:O	1:B:239:ASN:ND2	2.39	0.56
1:D:276:HIS:O	1:D:279:ILE:N	2.36	0.56
1:B:332:THR:OG1	1:B:375:LYS:NZ	2.38	0.55
2:C:1304:POV:O14	2:C:1309:POV:H15B	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1306:POV:O14	2:D:1311:POV:H15B	2.06	0.55
1:A:332:THR:OG1	1:A:375:LYS:NZ	2.38	0.55
1:A:670:ASP:O	1:D:754:ARG:NH2	2.40	0.55
1:A:83:HIS:O	1:A:84:THR:OG1	2.22	0.55
1:A:181:ALA:O	1:A:239:ASN:ND2	2.39	0.55
1:A:146:PHE:O	1:A:183:HIS:NE2	2.36	0.54
1:D:181:ALA:O	1:D:239:ASN:ND2	2.39	0.54
1:A:754:ARG:NH2	1:B:670:ASP:O	2.39	0.54
1:B:754:ARG:NH2	1:C:670:ASP:O	2.39	0.54
1:C:1222:LYS:O	1:C:1226:GLN:NE2	2.41	0.54
1:D:1222:LYS:O	1:D:1226:GLN:NE2	2.40	0.54
1:A:276:HIS:O	1:A:279:ILE:N	2.36	0.54
1:A:1222:LYS:O	1:A:1226:GLN:NE2	2.40	0.54
1:A:52:ALA:O	1:A:54:PHE:N	2.41	0.54
1:B:1222:LYS:O	1:B:1226:GLN:NE2	2.41	0.54
1:B:138:SER:OG	1:B:140:HIS:NE2	2.40	0.54
1:D:52:ALA:O	1:D:54:PHE:N	2.41	0.54
1:C:52:ALA:O	1:C:54:PHE:N	2.41	0.54
1:C:83:HIS:O	1:C:84:THR:OG1	2.22	0.54
2:A:1301:POV:O14	2:A:1306:POV:H15B	2.08	0.53
1:B:146:PHE:O	1:B:183:HIS:NE2	2.36	0.53
1:B:52:ALA:O	1:B:54:PHE:N	2.41	0.53
1:B:740:GLN:OE1	1:B:1115:ARG:NH1	2.40	0.53
1:C:740:GLN:OE1	1:C:1115:ARG:NH1	2.40	0.53
1:D:138:SER:OG	1:D:140:HIS:NE2	2.40	0.53
1:A:138:SER:OG	1:A:140:HIS:NE2	2.40	0.53
1:C:205:ALA:HB3	1:C:247:LEU:HD23	1.90	0.53
1:A:205:ALA:HB3	1:A:247:LEU:HD23	1.90	0.53
1:A:1076:LEU:HD22	2:D:1306:POV:H218	1.89	0.53
2:A:1316:POV:H15A	2:A:1316:POV:O11	2.09	0.53
1:B:348:SER:O	1:B:352:LYS:N	2.42	0.53
1:C:348:SER:O	1:C:352:LYS:N	2.42	0.53
1:B:205:ALA:HB3	1:B:247:LEU:HD23	1.90	0.52
1:C:136:VAL:HG21	1:C:270:ILE:HG21	1.92	0.52
1:D:136:VAL:HG21	1:D:270:ILE:HG21	1.92	0.52
1:B:136:VAL:HG21	1:B:270:ILE:HG21	1.92	0.52
1:A:136:VAL:HG21	1:A:270:ILE:HG21	1.92	0.52
2:B:1312:POV:C23	2:B:1312:POV:H2	2.36	0.52
1:C:146:PHE:O	1:C:183:HIS:NE2	2.36	0.52
1:D:1217:ARG:O	1:D:1221:ILE:N	2.43	0.52
2:A:1301:POV:H218	1:B:1076:LEU:HD22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1305:POV:H312	2:D:1305:POV:H213	1.92	0.52
1:D:205:ALA:HB3	1:D:247:LEU:HD23	1.90	0.52
2:C:1314:POV:H218	2:D:1315:POV:H314	1.92	0.52
2:C:1304:POV:H218	1:D:1076:LEU:HD22	1.91	0.51
1:D:1018:ARG:NH2	6:D:1412:HOH:O	2.43	0.51
1:A:740:GLN:OE1	1:A:1115:ARG:NH1	2.40	0.51
1:A:1068:PRO:O	6:A:1404:HOH:O	2.19	0.51
2:B:1303:POV:H213	2:B:1303:POV:H312	1.93	0.51
1:D:90:ASP:O	1:D:218:GLY:N	2.44	0.51
1:A:328:ILE:O	1:A:332:THR:OG1	2.09	0.51
1:B:90:ASP:O	1:B:218:GLY:N	2.44	0.51
1:B:1217:ARG:O	1:B:1221:ILE:N	2.43	0.51
1:C:1217:ARG:O	1:C:1221:ILE:N	2.43	0.51
1:B:311:PRO:HA	1:B:377:LEU:HD23	1.93	0.51
1:C:311:PRO:HA	1:C:377:LEU:HD23	1.93	0.51
1:D:339:PRO:O	1:D:342:ALA:N	2.42	0.51
1:C:138:SER:OG	1:C:140:HIS:NE2	2.40	0.51
1:A:115:THR:HG23	1:A:119:ILE:HD11	1.93	0.50
1:D:318:THR:N	1:D:323:ASP:OD1	2.44	0.50
2:D:1305:POV:H15A	2:D:1305:POV:O11	2.11	0.50
1:A:1018:ARG:NH2	6:A:1411:HOH:O	2.44	0.50
1:B:318:THR:N	1:B:323:ASP:OD1	2.44	0.50
1:D:311:PRO:HA	1:D:377:LEU:HD23	1.93	0.50
1:A:90:ASP:O	1:A:218:GLY:N	2.44	0.50
1:A:348:SER:O	1:A:352:LYS:N	2.42	0.50
1:C:1018:ARG:NH2	6:C:1413:HOH:O	2.43	0.50
1:D:1068:PRO:O	6:D:1404:HOH:O	2.19	0.50
1:C:339:PRO:O	1:C:342:ALA:N	2.42	0.50
1:C:64:ASP:O	1:C:66:LYS:N	2.45	0.50
1:D:348:SER:O	1:D:352:LYS:N	2.42	0.50
1:D:740:GLN:OE1	1:D:1115:ARG:NH1	2.40	0.50
1:A:311:PRO:HA	1:A:377:LEU:HD23	1.93	0.50
1:A:318:THR:N	1:A:323:ASP:OD1	2.44	0.50
1:A:64:ASP:O	1:A:66:LYS:N	2.45	0.50
1:C:115:THR:HG23	1:C:119:ILE:HD11	1.93	0.50
1:C:909:ALA:O	1:C:915:LYS:NZ	2.25	0.50
1:B:115:THR:HG23	1:B:119:ILE:HD11	1.93	0.50
2:B:1303:POV:O11	2:B:1303:POV:H15A	2.12	0.49
1:C:90:ASP:O	1:C:218:GLY:N	2.44	0.49
1:D:115:THR:HG23	1:D:119:ILE:HD11	1.93	0.49
1:A:178:THR:HG23	1:A:178:THR:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:THR:N	1:C:323:ASP:OD1	2.44	0.49
1:D:178:THR:HG23	1:D:178:THR:O	2.13	0.49
1:A:1217:ARG:O	1:A:1221:ILE:N	2.43	0.49
1:B:178:THR:O	1:B:178:THR:HG23	2.13	0.49
1:B:1217:ARG:O	1:B:1220:TYR:N	2.46	0.49
1:D:64:ASP:O	1:D:66:LYS:N	2.45	0.49
1:A:1217:ARG:O	1:A:1220:TYR:N	2.46	0.49
1:A:880:GLN:O	1:A:942:ARG:NH2	2.46	0.49
1:C:1217:ARG:O	1:C:1220:TYR:N	2.46	0.48
1:C:1042:TRP:HZ3	1:D:1081:LEU:HD12	1.77	0.48
1:D:880:GLN:O	1:D:942:ARG:NH2	2.46	0.48
2:A:1316:POV:H312	2:A:1316:POV:H213	1.95	0.48
1:C:178:THR:HG23	1:C:178:THR:O	2.13	0.48
1:A:339:PRO:O	1:A:342:ALA:N	2.42	0.48
1:D:1217:ARG:O	1:D:1220:TYR:N	2.46	0.48
1:B:64:ASP:O	1:B:66:LYS:N	2.45	0.48
1:B:880:GLN:O	1:B:942:ARG:NH2	2.46	0.48
1:B:1018:ARG:NH2	6:B:1414:HOH:O	2.46	0.48
1:A:747:TRP:NE1	2:A:1312:POV:O14	2.47	0.48
1:C:161:ILE:HG23	1:C:199:ILE:HD11	1.96	0.48
1:A:505:TYR:OH	1:A:511:ASP:OD2	2.22	0.47
2:B:1304:POV:H218	1:C:1076:LEU:HD22	1.95	0.47
1:D:161:ILE:HG23	1:D:199:ILE:HD11	1.96	0.47
1:D:59:ALA:HB2	1:D:65:VAL:HG23	1.96	0.47
1:B:9:SER:OG	1:B:10:THR:N	2.48	0.47
1:B:59:ALA:HB2	1:B:65:VAL:HG23	1.96	0.47
1:D:328:ILE:O	1:D:332:THR:OG1	2.09	0.47
1:A:9:SER:OG	1:A:10:THR:N	2.48	0.47
1:A:59:ALA:HB2	1:A:65:VAL:HG23	1.96	0.47
1:A:1081:LEU:HD12	1:D:1042:TRP:HZ3	1.79	0.47
1:B:28:ARG:O	1:B:35:ILE:HG21	2.15	0.47
2:B:1315:POV:H218	2:C:1313:POV:H314	1.97	0.47
2:D:1310:POV:O12	2:D:1310:POV:H14B	2.14	0.47
1:A:28:ARG:O	1:A:35:ILE:HG21	2.15	0.47
1:D:28:ARG:O	1:D:35:ILE:HG21	2.15	0.47
1:A:161:ILE:HG23	1:A:199:ILE:HD11	1.96	0.47
1:B:328:ILE:O	1:B:332:THR:OG1	2.09	0.47
1:C:59:ALA:HB2	1:C:65:VAL:HG23	1.96	0.47
1:D:9:SER:OG	1:D:10:THR:N	2.48	0.47
1:C:9:SER:OG	1:C:10:THR:N	2.48	0.46
1:C:1068:PRO:O	6:C:1404:HOH:O	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1042:TRP:HZ3	1:C:1081:LEU:HD12	1.79	0.46
1:C:28:ARG:O	1:C:35:ILE:HG21	2.15	0.46
1:C:880:GLN:O	1:C:942:ARG:NH2	2.46	0.46
1:B:1068:PRO:O	6:B:1405:HOH:O	2.20	0.46
2:D:1314:POV:C23	2:D:1314:POV:H2	2.38	0.46
1:A:137:ILE:HG23	1:A:288:LEU:HD13	1.98	0.46
2:A:1316:POV:H216	1:D:1033:ALA:HB1	1.97	0.46
1:B:95:ILE:HA	1:B:223:ALA:HB3	1.99	0.45
1:C:928:ASP:OD1	6:C:1406:HOH:O	2.21	0.45
1:D:110:ARG:NH2	1:D:249:ASP:OD1	2.46	0.45
1:B:227:THR:O	1:B:227:THR:HG22	2.17	0.45
1:C:227:THR:HG22	1:C:227:THR:O	2.17	0.45
1:B:161:ILE:HG23	1:B:199:ILE:HD11	1.96	0.45
2:C:1302:POV:O13	2:C:1303:POV:H14A	2.16	0.45
1:A:95:ILE:HA	1:A:223:ALA:HB3	1.98	0.45
3:B:1307:CLR:H183	3:B:1307:CLR:H212	1.99	0.45
1:C:95:ILE:HA	1:C:223:ALA:HB3	1.99	0.45
1:B:339:PRO:O	1:B:342:ALA:N	2.42	0.45
1:C:918:VAL:O	1:C:921:SER:OG	2.28	0.45
1:D:95:ILE:HA	1:D:223:ALA:HB3	1.98	0.45
1:D:181:ALA:HB1	1:D:242:HIS:CE1	2.52	0.45
1:D:227:THR:O	1:D:227:THR:HG22	2.17	0.45
2:A:1309:POV:C23	2:A:1309:POV:H2	2.38	0.45
2:A:1309:POV:H2	2:A:1309:POV:H22A	1.67	0.45
1:B:137:ILE:HG23	1:B:288:LEU:HD13	1.98	0.45
1:B:181:ALA:HB1	1:B:242:HIS:CE1	2.52	0.45
1:A:1042:TRP:HZ3	1:B:1081:LEU:HD12	1.81	0.44
1:C:137:ILE:HG23	1:C:288:LEU:HD13	1.98	0.44
1:A:227:THR:HG22	1:A:227:THR:O	2.17	0.44
1:D:137:ILE:HG23	1:D:288:LEU:HD13	1.98	0.44
1:A:343:GLU:HA	1:A:346:ILE:HG22	1.99	0.44
2:A:1312:POV:H218	2:B:1313:POV:H314	1.98	0.44
1:C:79:SER:O	1:C:82:LYS:N	2.51	0.44
1:C:181:ALA:HB1	1:C:242:HIS:CE1	2.52	0.44
2:B:1312:POV:H2	2:B:1312:POV:H23	1.98	0.44
1:B:1033:ALA:HB1	2:C:1303:POV:H216	1.99	0.44
1:D:343:GLU:HA	1:D:346:ILE:HG22	1.99	0.44
2:A:1310:POV:H314	2:D:1301:POV:H218	1.99	0.44
1:A:181:ALA:HB1	1:A:242:HIS:CE1	2.52	0.44
3:A:1304:CLR:H212	3:A:1304:CLR:H183	1.99	0.44
1:B:343:GLU:HA	1:B:346:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1309:CLR:H183	3:D:1309:CLR:H212	1.99	0.43
1:B:400:LEU:HD21	1:B:413:LEU:HD23	2.00	0.43
1:B:928:ASP:OD1	6:B:1406:HOH:O	2.21	0.43
1:B:59:ALA:HB2	1:B:65:VAL:CG2	2.49	0.43
1:C:343:GLU:HA	1:C:346:ILE:HG22	1.99	0.43
1:C:400:LEU:HD21	1:C:413:LEU:HD23	2.00	0.43
1:C:1033:ALA:HB1	2:D:1305:POV:H216	2.01	0.43
1:C:59:ALA:HB2	1:C:65:VAL:CG2	2.49	0.43
1:A:928:ASP:OD1	6:A:1406:HOH:O	2.21	0.42
1:A:113:TYR:O	1:A:261:ARG:NH2	2.53	0.42
1:C:113:TYR:O	1:C:261:ARG:NH2	2.53	0.42
1:A:400:LEU:HD21	1:A:413:LEU:HD23	2.00	0.42
1:A:59:ALA:HB2	1:A:65:VAL:CG2	2.49	0.42
1:B:113:TYR:O	1:B:261:ARG:NH2	2.53	0.42
1:D:59:ALA:HB2	1:D:65:VAL:CG2	2.49	0.42
2:D:1303:POV:H15B	2:D:1305:POV:O13	2.20	0.42
1:A:110:ARG:NH2	1:A:249:ASP:OD1	2.46	0.42
2:A:1314:POV:H21J	2:D:1310:POV:H21D	2.01	0.42
2:B:1304:POV:O14	2:B:1309:POV:H14A	2.20	0.42
1:A:1209:ILE:O	1:A:1213:GLU:N	2.53	0.42
1:D:400:LEU:HD21	1:D:413:LEU:HD23	2.00	0.42
1:D:113:TYR:O	1:D:261:ARG:NH2	2.53	0.41
1:B:110:ARG:NH2	1:B:249:ASP:OD1	2.46	0.41
1:B:985:GLN:NE2	6:B:1420:HOH:O	2.51	0.41
1:A:79:SER:O	1:A:82:LYS:N	2.50	0.41
1:B:79:SER:O	1:B:82:LYS:N	2.51	0.41
1:B:1011:LEU:HD21	1:B:1037:VAL:HA	2.02	0.41
1:D:1011:LEU:HD21	1:D:1037:VAL:HA	2.02	0.41
1:A:173:THR:HG1	1:A:242:HIS:CD2	2.38	0.41
1:A:436:VAL:HG23	1:A:437:GLY:H	1.85	0.41
1:C:137:ILE:HG21	1:C:160:LEU:HD11	2.02	0.41
1:D:137:ILE:HG21	1:D:160:LEU:HD11	2.02	0.41
1:C:110:ARG:NH2	1:C:249:ASP:OD1	2.46	0.41
3:C:1307:CLR:H212	3:C:1307:CLR:H183	2.02	0.41
1:C:1011:LEU:HD21	1:C:1037:VAL:HA	2.02	0.41
1:D:436:VAL:HG23	1:D:437:GLY:H	1.85	0.41
1:C:985:GLN:NE2	6:C:1420:HOH:O	2.52	0.41
1:D:1209:ILE:O	1:D:1213:GLU:N	2.53	0.41
2:A:1312:POV:O13	2:A:1312:POV:H15B	2.20	0.41
1:C:11:LEU:HD21	1:C:110:ARG:O	2.21	0.41
1:C:436:VAL:HG23	1:C:437:GLY:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1200:THR:HG23	1:D:1204:VAL:HG21	2.03	0.41
1:B:137:ILE:HG21	1:B:160:LEU:HD11	2.02	0.41
1:B:216:LEU:CD2	1:B:223:ALA:HB1	2.51	0.41
1:B:663:ALA:O	1:B:676:SER:OG	2.37	0.41
2:C:1303:POV:H312	2:C:1303:POV:H213	2.03	0.41
1:A:11:LEU:HD21	1:A:110:ARG:O	2.21	0.40
1:A:1011:LEU:HD21	1:A:1037:VAL:HA	2.02	0.40
1:B:1167:GLN:O	1:B:1171:HIS:ND1	2.47	0.40
1:D:11:LEU:HD21	1:D:110:ARG:O	2.21	0.40
2:C:1303:POV:O11	2:C:1303:POV:H15A	2.21	0.40
1:B:11:LEU:HD21	1:B:110:ARG:O	2.21	0.40
1:B:436:VAL:HG23	1:B:437:GLY:H	1.85	0.40
1:C:1209:ILE:O	1:C:1213:GLU:N	2.53	0.40
1:A:1179:GLU:OE2	1:B:105:ARG:NH1	2.54	0.40
2:A:1316:POV:O12	2:A:1316:POV:H13B	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	1097/1279 (86%)	964 (88%)	125 (11%)	8 (1%)	22	25
1	B	1097/1279 (86%)	964 (88%)	125 (11%)	8 (1%)	22	25
1	C	1097/1279 (86%)	964 (88%)	125 (11%)	8 (1%)	22	25
1	D	1097/1279 (86%)	964 (88%)	125 (11%)	8 (1%)	22	25
All	All	4388/5116 (86%)	3856 (88%)	500 (11%)	32 (1%)	26	25

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	CYS
1	B	53	CYS
1	C	53	CYS
1	D	53	CYS
1	A	28	ARG
1	A	277	ALA
1	B	28	ARG
1	B	277	ALA
1	C	28	ARG
1	C	277	ALA
1	D	28	ARG
1	D	277	ALA
1	A	435	LEU
1	B	435	LEU
1	C	435	LEU
1	A	88	PRO
1	B	88	PRO
1	C	88	PRO
1	D	88	PRO
1	D	435	LEU
1	A	71	PHE
1	B	71	PHE
1	C	71	PHE
1	D	71	PHE
1	A	65	VAL
1	B	65	VAL
1	C	65	VAL
1	D	65	VAL
1	A	87	SER
1	B	87	SER
1	C	87	SER
1	D	87	SER

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	979/1138 (86%)	961 (98%)	18 (2%)	59	71
1	B	979/1138 (86%)	961 (98%)	18 (2%)	59	71
1	C	979/1138 (86%)	961 (98%)	18 (2%)	59	71
1	D	979/1138 (86%)	961 (98%)	18 (2%)	59	71
All	All	3916/4552 (86%)	3844 (98%)	72 (2%)	61	71

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	33	CYS
1	A	49	LYS
1	A	61	LYS
1	A	96	ASN
1	A	270	ILE
1	A	315	CYS
1	A	337	ASN
1	A	338	LEU
1	A	469	LEU
1	A	471	ILE
1	A	498	GLN
1	A	794	MET
1	A	942	ARG
1	A	948	ASN
1	A	968	ASN
1	A	1108	ASN
1	A	1222	LYS
1	B	24	LYS
1	B	33	CYS
1	B	49	LYS
1	B	61	LYS
1	B	96	ASN
1	B	270	ILE
1	B	315	CYS
1	B	337	ASN
1	B	338	LEU
1	B	469	LEU
1	B	471	ILE
1	B	498	GLN
1	B	794	MET
1	B	942	ARG
1	B	948	ASN

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Mol	Chain	Res	Type
1	B	968	ASN
1	B	1108	ASN
1	B	1222	LYS
1	C	24	LYS
1	C	33	CYS
1	C	49	LYS
1	C	61	LYS
1	C	96	ASN
1	C	270	ILE
1	C	315	CYS
1	C	337	ASN
1	C	338	LEU
1	C	469	LEU
1	C	471	ILE
1	C	498	GLN
1	C	794	MET
1	C	942	ARG
1	C	948	ASN
1	C	968	ASN
1	C	1108	ASN
1	C	1222	LYS
1	D	24	LYS
1	D	33	CYS
1	D	49	LYS
1	D	61	LYS
1	D	96	ASN
1	D	270	ILE
1	D	315	CYS
1	D	337	ASN
1	D	338	LEU
1	D	469	LEU
1	D	471	ILE
1	D	498	GLN
1	D	794	MET
1	D	942	ARG
1	D	948	ASN
1	D	968	ASN
1	D	1108	ASN
1	D	1222	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	98	GLN
1	A	129	GLN
1	A	226	GLN
1	A	281	GLN
1	A	329	HIS
1	A	337	ASN
1	A	789	GLN
1	A	956	HIS
1	A	1190	ASN
1	A	1210	GLN
1	A	1226	GLN
1	B	96	ASN
1	B	98	GLN
1	B	226	GLN
1	B	281	GLN
1	B	329	HIS
1	B	337	ASN
1	B	789	GLN
1	B	956	HIS
1	B	985	GLN
1	B	1108	ASN
1	B	1190	ASN
1	B	1210	GLN
1	B	1226	GLN
1	C	96	ASN
1	C	98	GLN
1	C	226	GLN
1	C	281	GLN
1	C	329	HIS
1	C	337	ASN
1	C	789	GLN
1	C	956	HIS
1	C	1108	ASN
1	C	1190	ASN
1	C	1210	GLN
1	C	1226	GLN
1	D	96	ASN
1	D	98	GLN
1	D	226	GLN
1	D	281	GLN
1	D	329	HIS
1	D	337	ASN

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Mol	Chain	Res	Type
1	D	789	GLN
1	D	1190	ASN
1	D	1210	GLN
1	D	1226	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 65 ligands modelled in this entry, 1 is monoatomic - leaving 64 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	$\#\|Z\| > 2$
2	POV	D	1303	-	51,51,51	0.35	0	57,59,59	0.59	1 (1%)
2	POV	A	1308	-	51,51,51	0.32	0	57,59,59	0.48	0
2	POV	C	1308	-	51,51,51	0.35	0	57,59,59	0.45	1 (1%)
2	POV	A	1315	-	51,51,51	0.31	0	57,59,59	0.39	0
2	POV	D	1307	-	34,34,51	0.42	0	39,42,59	0.57	0
2	POV	B	1303	-	51,51,51	0.36	0	57,59,59	0.58	1 (1%)
2	POV	A	1314	-	51,51,51	0.34	0	57,59,59	0.51	1 (1%)
2	POV	C	1306	-	51,51,51	0.35	0	57,59,59	0.51	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	POV	A	1301	-	51,51,51	0.49	0	57,59,59	0.61	1 (1%)
2	POV	B	1310	-	51,51,51	0.33	0	57,59,59	0.43	0
2	POV	C	1311	-	51,51,51	0.32	0	57,59,59	0.47	0
2	POV	A	1310	-	51,51,51	0.30	0	57,59,59	0.32	0
2	POV	A	1303	-	51,51,51	0.35	0	57,59,59	0.51	1 (1%)
2	POV	D	1310	-	51,51,51	0.38	0	57,59,59	0.71	2 (3%)
3	CLR	D	1309	-	31,31,31	0.26	0	48,48,48	0.39	0
2	POV	B	1304	-	51,51,51	0.48	0	57,59,59	0.61	1 (1%)
2	POV	D	1315	-	51,51,51	0.30	0	57,59,59	0.31	0
4	DU0	B	1314	-	42,42,42	0.21	0	66,66,66	0.55	1 (1%)
2	POV	C	1304	-	51,51,51	0.49	0	57,59,59	0.61	1 (1%)
2	POV	C	1310	-	51,51,51	0.33	0	57,59,59	0.43	0
2	POV	B	1311	-	51,51,51	0.32	0	57,59,59	0.48	0
2	POV	C	1303	-	51,51,51	0.36	0	57,59,59	0.56	1 (1%)
2	POV	C	1309	-	51,51,51	0.35	0	57,59,59	0.43	0
4	DU0	C	1315	-	42,42,42	0.23	0	66,66,66	0.57	1 (1%)
2	POV	C	1312	-	51,51,51	0.35	0	57,59,59	0.80	3 (5%)
4	DU0	D	1302	-	42,42,42	0.23	0	66,66,66	0.60	1 (1%)
3	CLR	C	1307	-	31,31,31	0.27	0	48,48,48	0.40	0
2	POV	B	1306	-	51,51,51	0.36	0	57,59,59	0.51	1 (1%)
2	POV	B	1309	-	51,51,51	0.33	0	57,59,59	0.41	0
2	POV	D	1306	-	51,51,51	0.48	0	57,59,59	0.60	1 (1%)
2	POV	C	1305	-	34,34,51	0.42	0	39,42,59	0.55	0
3	CLR	A	1304	-	31,31,31	0.27	0	48,48,48	0.40	0
3	CLR	B	1307	-	31,31,31	0.27	0	48,48,48	0.39	0
4	DU0	B	1317	-	42,42,42	0.21	0	66,66,66	0.58	1 (1%)
2	POV	A	1307	-	51,51,51	0.33	0	57,59,59	0.43	0
2	POV	A	1305	-	51,51,51	0.35	0	57,59,59	0.44	1 (1%)
2	POV	B	1308	-	51,51,51	0.34	0	57,59,59	0.44	0
2	POV	B	1312	-	51,51,51	0.35	0	57,59,59	0.80	3 (5%)
2	POV	D	1312	-	51,51,51	0.34	0	57,59,59	0.43	0
2	POV	D	1308	-	51,51,51	0.35	0	57,59,59	0.51	1 (1%)
2	POV	C	1313	-	51,51,51	0.30	0	57,59,59	0.31	0
2	POV	B	1305	-	34,34,51	0.42	0	39,42,59	0.54	0
2	POV	D	1305	-	51,51,51	0.36	0	57,59,59	0.57	1 (1%)
4	DU0	A	1313	-	42,42,42	0.24	0	66,66,66	0.63	1 (1%)
2	POV	C	1314	-	51,51,51	0.35	0	57,59,59	0.59	1 (1%)
2	POV	C	1302	-	51,51,51	0.31	0	57,59,59	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	POV	A	1306	-	51,51,51	0.34	0	57,59,59	0.44	0
2	POV	A	1309	-	51,51,51	0.35	0	57,59,59	0.80	3 (5%)
2	POV	D	1311	-	51,51,51	0.33	0	57,59,59	0.44	0
2	POV	B	1313	-	51,51,51	0.31	0	57,59,59	0.32	0
2	POV	D	1301	-	51,51,51	0.34	0	57,59,59	0.61	1 (1%)
2	POV	D	1313	-	51,51,51	0.33	0	57,59,59	0.47	0
4	DU0	D	1316	-	42,42,42	0.22	0	66,66,66	0.60	1 (1%)
2	POV	C	1301	-	51,51,51	0.34	0	57,59,59	0.57	1 (1%)
2	POV	D	1314	-	51,51,51	0.35	0	57,59,59	0.79	3 (5%)
2	POV	A	1302	-	34,34,51	0.42	0	39,42,59	0.57	0
2	POV	B	1315	-	51,51,51	0.34	0	57,59,59	0.60	1 (1%)
2	POV	D	1304	-	51,51,51	0.32	0	57,59,59	0.40	0
4	DU0	A	1311	-	42,42,42	0.22	0	66,66,66	0.56	1 (1%)
2	POV	A	1316	-	51,51,51	0.35	0	57,59,59	0.60	1 (1%)
2	POV	B	1301	-	51,51,51	0.35	0	57,59,59	0.58	1 (1%)
4	DU0	B	1316	-	42,42,42	0.22	0	66,66,66	0.52	1 (1%)
2	POV	B	1302	-	51,51,51	0.32	0	57,59,59	0.39	0
2	POV	A	1312	-	51,51,51	0.35	0	57,59,59	0.58	1 (1%)

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
2	POV	D	1303	-	-	25/55/55/55	-
2	POV	A	1308	-	-	26/55/55/55	-
2	POV	C	1308	-	-	19/55/55/55	-
2	POV	A	1315	-	-	24/55/55/55	-
2	POV	D	1307	-	-	13/38/38/55	-
2	POV	B	1303	-	-	26/55/55/55	-
2	POV	A	1314	-	-	27/55/55/55	-
2	POV	C	1306	-	-	19/55/55/55	-
2	POV	A	1301	-	-	31/55/55/55	-
2	POV	B	1310	-	-	24/55/55/55	-
2	POV	C	1311	-	-	25/55/55/55	-
2	POV	A	1310	-	-	17/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	A	1303	-	-	18/55/55/55	-
2	POV	D	1310	-	-	17/55/55/55	-
3	CLR	D	1309	-	-	4/10/68/68	0/4/4/4
2	POV	B	1304	-	-	29/55/55/55	-
2	POV	D	1315	-	-	18/55/55/55	-
4	DU0	B	1314	-	-	6/10/98/98	0/6/6/6
2	POV	C	1304	-	-	28/55/55/55	-
2	POV	C	1310	-	-	25/55/55/55	-
2	POV	B	1311	-	-	21/55/55/55	-
2	POV	C	1303	-	-	26/55/55/55	-
2	POV	C	1309	-	-	25/55/55/55	-
4	DU0	C	1315	-	-	0/10/98/98	0/6/6/6
2	POV	C	1312	-	-	23/55/55/55	-
4	DU0	D	1302	-	-	0/10/98/98	0/6/6/6
3	CLR	C	1307	-	-	4/10/68/68	0/4/4/4
2	POV	B	1306	-	-	17/55/55/55	-
2	POV	B	1309	-	-	23/55/55/55	-
2	POV	D	1306	-	-	27/55/55/55	-
2	POV	C	1305	-	-	13/38/38/55	-
3	CLR	A	1304	-	-	4/10/68/68	0/4/4/4
3	CLR	B	1307	-	-	4/10/68/68	0/4/4/4
4	DU0	B	1317	-	-	6/10/98/98	0/6/6/6
2	POV	A	1307	-	-	27/55/55/55	-
2	POV	A	1305	-	-	19/55/55/55	-
2	POV	B	1308	-	-	19/55/55/55	-
2	POV	B	1312	-	-	20/55/55/55	-
2	POV	D	1312	-	-	24/55/55/55	-
2	POV	D	1308	-	-	19/55/55/55	-
2	POV	C	1313	-	-	15/55/55/55	-
2	POV	B	1305	-	-	14/38/38/55	-
2	POV	D	1305	-	-	25/55/55/55	-
4	DU0	A	1313	-	-	1/10/98/98	0/6/6/6
2	POV	C	1314	-	-	24/55/55/55	-
2	POV	C	1302	-	-	22/55/55/55	-
2	POV	A	1306	-	-	24/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	A	1309	-	-	21/55/55/55	-
2	POV	D	1311	-	-	24/55/55/55	-
2	POV	B	1313	-	-	17/55/55/55	-
2	POV	D	1301	-	-	23/55/55/55	-
2	POV	D	1313	-	-	25/55/55/55	-
4	DU0	D	1316	-	-	6/10/98/98	0/6/6/6
2	POV	C	1301	-	-	29/55/55/55	-
2	POV	D	1314	-	-	18/55/55/55	-
2	POV	A	1302	-	-	16/38/38/55	-
2	POV	B	1315	-	-	23/55/55/55	-
2	POV	D	1304	-	-	26/55/55/55	-
4	DU0	A	1311	-	-	6/10/98/98	0/6/6/6
2	POV	A	1316	-	-	23/55/55/55	-
2	POV	B	1301	-	-	29/55/55/55	-
4	DU0	B	1316	-	-	0/10/98/98	0/6/6/6
2	POV	B	1302	-	-	26/55/55/55	-
2	POV	A	1312	-	-	23/55/55/55	-

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1313	DU0	C24-C25-C26	3.80	118.69	113.88
4	D	1316	DU0	C24-C25-C26	3.75	118.63	113.88
4	D	1302	DU0	C24-C25-C26	3.72	118.59	113.88
4	C	1315	DU0	C24-C25-C26	3.62	118.47	113.88
4	B	1317	DU0	C24-C25-C26	3.58	118.41	113.88
2	D	1310	POV	O21-C2-C1	3.36	120.58	108.40
4	B	1314	DU0	C24-C25-C26	3.35	118.12	113.88
4	A	1311	DU0	C24-C25-C26	3.34	118.10	113.88
4	B	1316	DU0	C24-C25-C26	3.29	118.04	113.88
2	C	1312	POV	C3-C2-C1	3.04	118.99	111.79
2	B	1312	POV	O21-C2-C3	3.02	119.32	108.40
2	C	1312	POV	O21-C2-C3	2.98	119.18	108.40
2	A	1309	POV	C3-C2-C1	2.97	118.80	111.79
2	D	1314	POV	C3-C2-C1	2.95	118.78	111.79
2	D	1314	POV	O21-C2-C3	2.95	119.07	108.40
2	A	1309	POV	O21-C2-C3	2.93	119.03	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1314	POV	C211-C210-C29	2.78	146.03	124.73
2	A	1309	POV	O21-C2-C1	2.77	118.44	108.40
2	D	1301	POV	C211-C210-C29	2.77	146.00	124.73
2	C	1304	POV	C2-O21-C21	2.77	124.61	117.79
2	B	1315	POV	C211-C210-C29	2.76	145.92	124.73
2	A	1301	POV	C2-O21-C21	2.76	124.58	117.79
2	A	1312	POV	C211-C210-C29	2.75	145.82	124.73
2	B	1304	POV	C2-O21-C21	2.73	124.52	117.79
2	B	1312	POV	O21-C2-C1	2.72	118.24	108.40
2	D	1306	POV	C2-O21-C21	2.72	124.48	117.79
2	D	1314	POV	O21-C2-C1	2.71	118.22	108.40
2	B	1312	POV	C3-C2-C1	2.71	118.19	111.79
2	C	1312	POV	O21-C2-C1	2.67	118.06	108.40
2	C	1301	POV	C2-O21-C21	2.56	124.09	117.79
2	D	1303	POV	C2-O21-C21	2.55	124.07	117.79
2	B	1301	POV	C2-O21-C21	2.55	124.06	117.79
2	C	1303	POV	O31-C3-C2	2.43	115.51	108.43
2	B	1303	POV	O31-C3-C2	2.37	115.34	108.43
2	D	1305	POV	O31-C3-C2	2.35	115.27	108.43
2	D	1310	POV	C2-O21-C21	2.33	123.53	117.79
2	A	1316	POV	O31-C3-C2	2.30	115.13	108.43
2	A	1303	POV	C2-O21-C21	2.23	123.28	117.79
2	C	1306	POV	C2-O21-C21	2.23	123.28	117.79
2	D	1308	POV	C2-O21-C21	2.23	123.27	117.79
2	B	1306	POV	C2-O21-C21	2.22	123.25	117.79
2	A	1314	POV	C2-O21-C21	2.16	123.10	117.79
2	C	1308	POV	O21-C2-C1	2.11	116.02	108.40
2	A	1305	POV	O21-C2-C1	2.07	115.88	108.40

There are no chirality outliers.

All (1202) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	POV	C1-O11-P-O14
2	A	1301	POV	C11-O12-P-O14
2	A	1301	POV	O12-C11-C12-N
2	A	1301	POV	C22-C21-O21-C2
2	A	1301	POV	O22-C21-O21-C2
2	A	1302	POV	C1-O11-P-O14
2	A	1302	POV	C11-O12-P-O14
2	A	1302	POV	C32-C31-O31-C3
2	A	1302	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
2	A	1303	POV	C11-O12-P-O11
2	A	1303	POV	C11-O12-P-O13
2	A	1303	POV	C11-O12-P-O14
2	A	1303	POV	C22-C21-O21-C2
2	A	1303	POV	O22-C21-O21-C2
2	A	1303	POV	C32-C31-O31-C3
2	A	1303	POV	O32-C31-O31-C3
2	A	1307	POV	C1-O11-P-O13
2	A	1307	POV	C11-O12-P-O13
2	A	1307	POV	O12-C11-C12-N
2	A	1307	POV	C32-C31-O31-C3
2	A	1307	POV	O32-C31-O31-C3
2	A	1308	POV	C1-O11-P-O12
2	A	1308	POV	C22-C21-O21-C2
2	A	1308	POV	O22-C21-O21-C2
2	A	1309	POV	C1-O11-P-O12
2	A	1309	POV	C11-O12-P-O14
2	A	1309	POV	O21-C2-C3-O31
2	A	1309	POV	O12-C11-C12-N
2	A	1309	POV	C22-C21-O21-C2
2	A	1309	POV	O22-C21-O21-C2
2	A	1310	POV	C1-O11-P-O13
2	A	1310	POV	C11-O12-P-O14
2	A	1310	POV	O21-C2-C3-O31
2	A	1312	POV	C12-C11-O12-P
2	A	1314	POV	C11-O12-P-O11
2	A	1314	POV	C11-O12-P-O13
2	A	1314	POV	C11-O12-P-O14
2	A	1314	POV	C22-C21-O21-C2
2	A	1314	POV	O22-C21-O21-C2
2	A	1315	POV	C11-O12-P-O13
2	A	1315	POV	O12-C11-C12-N
2	A	1316	POV	C1-O11-P-O14
2	A	1316	POV	C2-C1-O11-P
2	A	1316	POV	O21-C2-C3-O31
2	A	1316	POV	O12-C11-C12-N
2	B	1301	POV	C22-C21-O21-C2
2	B	1301	POV	O22-C21-O21-C2
2	B	1302	POV	C11-O12-P-O13
2	B	1302	POV	O12-C11-C12-N
2	B	1303	POV	C1-O11-P-O12
2	B	1303	POV	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
2	B	1303	POV	C1-O11-P-O14
2	B	1303	POV	C11-O12-P-O14
2	B	1303	POV	C2-C1-O11-P
2	B	1303	POV	O21-C2-C3-O31
2	B	1304	POV	C1-O11-P-O14
2	B	1304	POV	C11-O12-P-O14
2	B	1304	POV	O12-C11-C12-N
2	B	1304	POV	C22-C21-O21-C2
2	B	1304	POV	O22-C21-O21-C2
2	B	1305	POV	C11-O12-P-O14
2	B	1305	POV	C32-C31-O31-C3
2	B	1305	POV	O32-C31-O31-C3
2	B	1306	POV	C11-O12-P-O13
2	B	1306	POV	C22-C21-O21-C2
2	B	1306	POV	O22-C21-O21-C2
2	B	1306	POV	C32-C31-O31-C3
2	B	1306	POV	O32-C31-O31-C3
2	B	1310	POV	C1-O11-P-O13
2	B	1310	POV	C11-O12-P-O13
2	B	1310	POV	O12-C11-C12-N
2	B	1310	POV	C32-C31-O31-C3
2	B	1310	POV	O32-C31-O31-C3
2	B	1311	POV	C1-O11-P-O12
2	B	1311	POV	O11-C1-C2-O21
2	B	1311	POV	C22-C21-O21-C2
2	B	1311	POV	O22-C21-O21-C2
2	B	1312	POV	C22-C21-O21-C2
2	B	1312	POV	O22-C21-O21-C2
2	B	1313	POV	C1-O11-P-O13
2	B	1313	POV	C11-O12-P-O14
2	B	1313	POV	O21-C2-C3-O31
2	B	1315	POV	C12-C11-O12-P
2	C	1301	POV	C22-C21-O21-C2
2	C	1301	POV	O22-C21-O21-C2
2	C	1302	POV	C11-O12-P-O13
2	C	1302	POV	C2-C1-O11-P
2	C	1302	POV	O12-C11-C12-N
2	C	1303	POV	C1-O11-P-O13
2	C	1303	POV	C1-O11-P-O14
2	C	1303	POV	C2-C1-O11-P
2	C	1304	POV	C1-O11-P-O14
2	C	1304	POV	C11-O12-P-O14

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Mol	Chain	Res	Type	Atoms
2	C	1304	POV	O12-C11-C12-N
2	C	1304	POV	C22-C21-O21-C2
2	C	1304	POV	O22-C21-O21-C2
2	C	1305	POV	C11-O12-P-O11
2	C	1305	POV	C11-O12-P-O13
2	C	1305	POV	C11-O12-P-O14
2	C	1305	POV	C29-C210-C211-C212
2	C	1305	POV	C32-C31-O31-C3
2	C	1305	POV	O32-C31-O31-C3
2	C	1306	POV	C11-O12-P-O11
2	C	1306	POV	C11-O12-P-O13
2	C	1306	POV	C11-O12-P-O14
2	C	1306	POV	C22-C21-O21-C2
2	C	1306	POV	O22-C21-O21-C2
2	C	1306	POV	C32-C31-O31-C3
2	C	1306	POV	O32-C31-O31-C3
2	C	1310	POV	C1-O11-P-O13
2	C	1310	POV	C11-O12-P-O13
2	C	1310	POV	O12-C11-C12-N
2	C	1310	POV	C32-C31-O31-C3
2	C	1310	POV	O32-C31-O31-C3
2	C	1311	POV	C1-O11-P-O12
2	C	1311	POV	O11-C1-C2-O21
2	C	1311	POV	C22-C21-O21-C2
2	C	1311	POV	O22-C21-O21-C2
2	C	1312	POV	C1-O11-P-O13
2	C	1312	POV	C11-O12-P-O13
2	C	1312	POV	O21-C2-C3-O31
2	C	1312	POV	O12-C11-C12-N
2	C	1312	POV	C22-C21-O21-C2
2	C	1312	POV	O22-C21-O21-C2
2	C	1313	POV	C1-O11-P-O13
2	C	1313	POV	C11-O12-P-O14
2	C	1313	POV	O21-C2-C3-O31
2	C	1314	POV	C12-C11-O12-P
2	D	1301	POV	C12-C11-O12-P
2	D	1303	POV	C22-C21-O21-C2
2	D	1303	POV	O22-C21-O21-C2
2	D	1304	POV	C11-O12-P-O13
2	D	1304	POV	O12-C11-C12-N
2	D	1305	POV	C1-O11-P-O12
2	D	1305	POV	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
2	D	1305	POV	C1-O11-P-O14
2	D	1305	POV	C2-C1-O11-P
2	D	1305	POV	O21-C2-C3-O31
2	D	1306	POV	C1-O11-P-O14
2	D	1306	POV	C11-O12-P-O14
2	D	1306	POV	O12-C11-C12-N
2	D	1306	POV	C22-C21-O21-C2
2	D	1306	POV	O22-C21-O21-C2
2	D	1307	POV	C11-O12-P-O14
2	D	1307	POV	C29-C210-C211-C212
2	D	1307	POV	C32-C31-O31-C3
2	D	1307	POV	O32-C31-O31-C3
2	D	1308	POV	C11-O12-P-O11
2	D	1308	POV	C11-O12-P-O13
2	D	1308	POV	C11-O12-P-O14
2	D	1308	POV	C22-C21-O21-C2
2	D	1308	POV	O22-C21-O21-C2
2	D	1308	POV	C32-C31-O31-C3
2	D	1308	POV	O32-C31-O31-C3
2	D	1310	POV	C1-C2-O21-C21
2	D	1310	POV	O12-C11-C12-N
2	D	1312	POV	C1-O11-P-O13
2	D	1312	POV	C11-O12-P-O13
2	D	1312	POV	O12-C11-C12-N
2	D	1312	POV	C32-C31-O31-C3
2	D	1312	POV	O32-C31-O31-C3
2	D	1313	POV	C1-O11-P-O12
2	D	1313	POV	C22-C21-O21-C2
2	D	1313	POV	O22-C21-O21-C2
2	D	1314	POV	C22-C21-O21-C2
2	D	1314	POV	O22-C21-O21-C2
2	D	1315	POV	C1-O11-P-O13
2	D	1315	POV	C11-O12-P-O14
2	D	1315	POV	O21-C2-C3-O31
2	D	1304	POV	C214-C215-C216-C217
2	B	1306	POV	C214-C215-C216-C217
2	B	1302	POV	C2-C1-O11-P
2	D	1304	POV	C2-C1-O11-P
2	B	1315	POV	C11-C12-N-C14
2	C	1314	POV	C11-C12-N-C14
2	D	1301	POV	C11-C12-N-C14
2	D	1306	POV	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
2	A	1308	POV	C31-C32-C33-C34
2	C	1311	POV	C31-C32-C33-C34
2	D	1303	POV	C21-C22-C23-C24
3	A	1304	CLR	C17-C20-C22-C23
2	A	1308	POV	O11-C1-C2-O21
2	B	1301	POV	O11-C1-C2-O21
2	C	1301	POV	O11-C1-C2-O21
2	D	1303	POV	O11-C1-C2-O21
2	D	1313	POV	O11-C1-C2-O21
2	B	1301	POV	C21-C22-C23-C24
2	C	1301	POV	C21-C22-C23-C24
2	D	1313	POV	C31-C32-C33-C34
2	A	1312	POV	C31-C32-C33-C34
2	B	1311	POV	C31-C32-C33-C34
2	C	1313	POV	C21-C22-C23-C24
2	D	1315	POV	C31-C32-C33-C34
3	D	1309	CLR	C17-C20-C22-C23
2	A	1316	POV	C21-C22-C23-C24
2	C	1314	POV	C31-C32-C33-C34
2	D	1308	POV	C214-C215-C216-C217
2	A	1309	POV	C21-C22-C23-C24
2	A	1310	POV	C21-C22-C23-C24
2	B	1303	POV	C21-C22-C23-C24
2	B	1312	POV	C21-C22-C23-C24
2	B	1313	POV	C21-C22-C23-C24
2	B	1315	POV	C31-C32-C33-C34
2	C	1303	POV	C21-C22-C23-C24
2	C	1312	POV	C21-C22-C23-C24
2	D	1301	POV	C31-C32-C33-C34
2	D	1305	POV	C21-C22-C23-C24
2	D	1314	POV	C21-C22-C23-C24
3	B	1307	CLR	C17-C20-C22-C23
3	C	1307	CLR	C17-C20-C22-C23
3	A	1304	CLR	C21-C20-C22-C23
3	B	1307	CLR	C21-C20-C22-C23
3	C	1307	CLR	C21-C20-C22-C23
3	D	1309	CLR	C21-C20-C22-C23
2	D	1312	POV	C2-C1-O11-P
2	A	1312	POV	C11-C12-N-C14
2	C	1313	POV	C31-C32-C33-C34
2	D	1310	POV	C24-C25-C26-C27
2	A	1303	POV	C214-C215-C216-C217

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Mol	Chain	Res	Type	Atoms
2	B	1313	POV	C31-C32-C33-C34
2	A	1305	POV	C24-C25-C26-C27
2	C	1308	POV	C24-C25-C26-C27
2	C	1306	POV	C214-C215-C216-C217
2	D	1306	POV	C312-C313-C314-C315
2	A	1302	POV	C11-O12-P-O11
2	A	1307	POV	C1-O11-P-O12
2	A	1307	POV	C11-O12-P-O11
2	A	1309	POV	C11-O12-P-O11
2	A	1316	POV	C11-O12-P-O11
2	B	1301	POV	C11-O12-P-O11
2	B	1304	POV	C1-O11-P-O12
2	B	1306	POV	C11-O12-P-O11
2	B	1310	POV	C1-O11-P-O12
2	B	1310	POV	C11-O12-P-O11
2	C	1301	POV	C11-O12-P-O11
2	C	1303	POV	C1-O11-P-O12
2	C	1303	POV	C11-O12-P-O11
2	C	1310	POV	C1-O11-P-O12
2	C	1310	POV	C11-O12-P-O11
2	C	1312	POV	C1-O11-P-O12
2	C	1312	POV	C11-O12-P-O11
2	D	1303	POV	C11-O12-P-O11
2	D	1305	POV	C11-O12-P-O11
2	D	1307	POV	C11-O12-P-O11
2	D	1312	POV	C1-O11-P-O12
2	D	1312	POV	C11-O12-P-O11
2	D	1315	POV	C21-C22-C23-C24
2	B	1301	POV	C215-C216-C217-C218
2	C	1314	POV	C21-C22-C23-C24
2	B	1304	POV	C312-C313-C314-C315
2	A	1301	POV	C11-C12-N-C13
2	A	1301	POV	C11-C12-N-C15
2	A	1312	POV	C11-C12-N-C13
2	A	1312	POV	C11-C12-N-C15
2	B	1304	POV	C11-C12-N-C13
2	B	1304	POV	C11-C12-N-C15
2	C	1304	POV	C11-C12-N-C13
2	C	1304	POV	C11-C12-N-C15
2	C	1314	POV	C11-C12-N-C15
2	D	1306	POV	C11-C12-N-C15
3	C	1307	CLR	C23-C24-C25-C27

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Mol	Chain	Res	Type	Atoms
2	A	1310	POV	C31-C32-C33-C34
2	D	1310	POV	C26-C27-C28-C29
2	A	1305	POV	C36-C37-C38-C39
2	A	1315	POV	C213-C214-C215-C216
2	B	1304	POV	C34-C35-C36-C37
2	B	1310	POV	C213-C214-C215-C216
2	A	1312	POV	C25-C26-C27-C28
2	A	1316	POV	C34-C35-C36-C37
2	B	1301	POV	C213-C214-C215-C216
2	B	1308	POV	C211-C212-C213-C214
2	C	1308	POV	C36-C37-C38-C39
2	C	1310	POV	C213-C214-C215-C216
2	D	1303	POV	C213-C214-C215-C216
2	D	1305	POV	C34-C35-C36-C37
2	D	1306	POV	C34-C35-C36-C37
2	D	1312	POV	C213-C214-C215-C216
2	A	1301	POV	C32-C33-C34-C35
2	A	1307	POV	C213-C214-C215-C216
2	A	1316	POV	C25-C26-C27-C28
2	B	1303	POV	C34-C35-C36-C37
2	C	1304	POV	C32-C33-C34-C35
2	D	1310	POV	C211-C212-C213-C214
2	D	1311	POV	C312-C313-C314-C315
2	A	1302	POV	C23-C24-C25-C26
2	B	1302	POV	C214-C215-C216-C217
2	B	1303	POV	C25-C26-C27-C28
2	B	1304	POV	C32-C33-C34-C35
2	C	1314	POV	C25-C26-C27-C28
2	A	1307	POV	C2-C1-O11-P
2	A	1315	POV	C2-C1-O11-P
2	B	1310	POV	C2-C1-O11-P
2	C	1310	POV	C2-C1-O11-P
2	A	1306	POV	C37-C38-C39-C310
2	A	1316	POV	C310-C311-C312-C313
2	C	1305	POV	C23-C24-C25-C26
2	D	1305	POV	C25-C26-C27-C28
2	D	1311	POV	C211-C212-C213-C214
2	B	1301	POV	C36-C37-C38-C39
2	C	1303	POV	C25-C26-C27-C28
2	C	1303	POV	C34-C35-C36-C37
2	C	1304	POV	C34-C35-C36-C37
2	D	1306	POV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
2	D	1310	POV	C34-C35-C36-C37
2	A	1301	POV	C34-C35-C36-C37
2	B	1309	POV	C24-C25-C26-C27
2	C	1302	POV	C212-C213-C214-C215
2	D	1307	POV	C23-C24-C25-C26
2	D	1311	POV	C24-C25-C26-C27
3	A	1304	CLR	C23-C24-C25-C27
3	B	1307	CLR	C23-C24-C25-C27
2	A	1306	POV	C24-C25-C26-C27
2	B	1315	POV	C25-C26-C27-C28
2	C	1302	POV	C39-C310-C311-C312
2	C	1309	POV	C24-C25-C26-C27
2	D	1306	POV	C310-C311-C312-C313
2	A	1301	POV	C310-C311-C312-C313
2	B	1309	POV	C311-C312-C313-C314
2	C	1309	POV	C211-C212-C213-C214
4	A	1311	DU0	C75-C22-O23-C24
4	B	1314	DU0	C75-C22-O23-C24
4	B	1317	DU0	C75-C22-O23-C24
4	D	1316	DU0	C75-C22-O23-C24
2	A	1306	POV	C312-C313-C314-C315
2	B	1304	POV	C214-C215-C216-C217
2	B	1305	POV	C23-C24-C25-C26
2	B	1308	POV	C24-C25-C26-C27
2	C	1301	POV	C312-C313-C314-C315
2	C	1309	POV	C37-C38-C39-C310
2	D	1311	POV	C311-C312-C313-C314
4	A	1311	DU0	C25-C24-O23-C22
4	B	1314	DU0	C25-C24-O23-C22
4	B	1317	DU0	C25-C24-O23-C22
4	D	1316	DU0	C25-C24-O23-C22
2	B	1311	POV	C35-C36-C37-C38
2	C	1304	POV	C310-C311-C312-C313
2	D	1303	POV	C36-C37-C38-C39
2	A	1305	POV	C26-C27-C28-C29
2	B	1311	POV	C26-C27-C28-C29
2	C	1301	POV	C210-C211-C212-C213
2	C	1308	POV	C26-C27-C28-C29
2	D	1303	POV	C26-C27-C28-C29
2	A	1306	POV	C211-C212-C213-C214
2	A	1316	POV	C213-C214-C215-C216
2	B	1303	POV	C213-C214-C215-C216

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Mol	Chain	Res	Type	Atoms
2	B	1304	POV	C213-C214-C215-C216
2	B	1309	POV	C211-C212-C213-C214
2	B	1313	POV	C310-C311-C312-C313
2	C	1303	POV	C213-C214-C215-C216
2	C	1309	POV	C312-C313-C314-C315
2	C	1310	POV	C211-C212-C213-C214
2	D	1301	POV	C25-C26-C27-C28
2	D	1305	POV	C213-C214-C215-C216
2	D	1311	POV	C37-C38-C39-C310
2	A	1301	POV	C11-C12-N-C14
2	B	1304	POV	C11-C12-N-C14
2	B	1315	POV	C11-C12-N-C13
2	C	1304	POV	C11-C12-N-C14
2	C	1314	POV	C11-C12-N-C13
2	D	1301	POV	C11-C12-N-C13
2	D	1306	POV	C11-C12-N-C14
3	D	1309	CLR	C23-C24-C25-C27
2	A	1307	POV	C211-C212-C213-C214
2	C	1301	POV	C34-C35-C36-C37
2	C	1304	POV	C312-C313-C314-C315
2	D	1312	POV	C37-C38-C39-C310
2	B	1304	POV	C310-C311-C312-C313
2	B	1308	POV	C36-C37-C38-C39
2	B	1309	POV	C37-C38-C39-C310
2	C	1301	POV	C213-C214-C215-C216
2	D	1310	POV	C36-C37-C38-C39
2	D	1315	POV	C310-C311-C312-C313
2	A	1314	POV	C21-C22-C23-C24
2	B	1304	POV	C31-C32-C33-C34
2	A	1301	POV	C214-C215-C216-C217
2	A	1310	POV	C310-C311-C312-C313
2	A	1312	POV	C213-C214-C215-C216
2	A	1315	POV	C24-C25-C26-C27
2	B	1301	POV	C39-C310-C311-C312
2	C	1313	POV	C310-C311-C312-C313
2	D	1303	POV	C215-C216-C217-C218
2	A	1314	POV	C213-C214-C215-C216
2	D	1314	POV	C311-C312-C313-C314
2	A	1302	POV	C22-C23-C24-C25
2	A	1306	POV	C32-C33-C34-C35
2	B	1312	POV	C311-C312-C313-C314
2	D	1305	POV	C310-C311-C312-C313

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Mol	Chain	Res	Type	Atoms
2	D	1310	POV	C35-C36-C37-C38
2	B	1315	POV	C21-C22-C23-C24
2	A	1301	POV	C312-C313-C314-C315
2	A	1309	POV	C311-C312-C313-C314
2	A	1314	POV	C36-C37-C38-C39
2	B	1303	POV	C310-C311-C312-C313
2	B	1310	POV	C32-C33-C34-C35
2	B	1313	POV	C37-C38-C39-C310
2	C	1312	POV	C311-C312-C313-C314
2	D	1315	POV	C37-C38-C39-C310
2	C	1314	POV	C213-C214-C215-C216
2	A	1306	POV	C311-C312-C313-C314
2	D	1311	POV	C32-C33-C34-C35
2	B	1302	POV	C212-C213-C214-C215
2	B	1309	POV	C32-C33-C34-C35
2	B	1310	POV	C211-C212-C213-C214
2	B	1312	POV	C32-C33-C34-C35
2	C	1301	POV	C36-C37-C38-C39
2	C	1309	POV	C32-C33-C34-C35
2	A	1303	POV	C26-C27-C28-C29
2	B	1301	POV	C26-C27-C28-C29
2	B	1306	POV	C210-C211-C212-C213
2	C	1301	POV	C26-C27-C28-C29
2	D	1310	POV	C210-C211-C212-C213
2	B	1311	POV	C213-C214-C215-C216
2	C	1314	POV	C311-C310-C39-C38
2	A	1315	POV	C39-C310-C311-C312
2	C	1303	POV	C214-C215-C216-C217
2	D	1303	POV	C39-C310-C311-C312
2	A	1312	POV	C21-C22-C23-C24
2	A	1306	POV	C33-C34-C35-C36
2	B	1302	POV	C39-C310-C311-C312
2	C	1304	POV	C214-C215-C216-C217
2	D	1306	POV	C214-C215-C216-C217
2	C	1313	POV	C37-C38-C39-C310
2	B	1315	POV	C213-C214-C215-C216
2	C	1309	POV	C311-C312-C313-C314
2	D	1301	POV	C213-C214-C215-C216
2	B	1315	POV	C11-C12-N-C15
2	D	1301	POV	C11-C12-N-C15
2	D	1306	POV	C31-C32-C33-C34
2	B	1303	POV	C211-C212-C213-C214

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Mol	Chain	Res	Type	Atoms
2	C	1303	POV	C310-C311-C312-C313
2	C	1310	POV	C32-C33-C34-C35
2	D	1304	POV	C39-C310-C311-C312
2	D	1305	POV	C211-C212-C213-C214
2	C	1311	POV	C35-C36-C37-C38
2	A	1305	POV	C34-C35-C36-C37
2	A	1308	POV	C35-C36-C37-C38
2	A	1314	POV	C312-C313-C314-C315
2	A	1315	POV	C310-C311-C312-C313
2	D	1313	POV	C311-C312-C313-C314
3	B	1307	CLR	C23-C24-C25-C26
2	A	1306	POV	C26-C27-C28-C29
2	B	1301	POV	C210-C211-C212-C213
2	B	1302	POV	C26-C27-C28-C29
2	B	1308	POV	C26-C27-C28-C29
2	D	1303	POV	C210-C211-C212-C213
2	D	1314	POV	C32-C33-C34-C35
2	A	1312	POV	C311-C310-C39-C38
2	A	1314	POV	C215-C216-C217-C218
2	A	1316	POV	C211-C212-C213-C214
2	A	1316	POV	C214-C215-C216-C217
2	D	1304	POV	C212-C213-C214-C215
2	D	1313	POV	C35-C36-C37-C38
2	A	1306	POV	C21-C22-C23-C24
2	B	1310	POV	C31-C32-C33-C34
2	D	1308	POV	C21-C22-C23-C24
2	D	1311	POV	C21-C22-C23-C24
2	A	1307	POV	C32-C33-C34-C35
2	A	1312	POV	C211-C212-C213-C214
2	C	1303	POV	C211-C212-C213-C214
2	D	1303	POV	C312-C313-C314-C315
2	D	1313	POV	C36-C37-C38-C39
2	C	1305	POV	C22-C23-C24-C25
2	D	1304	POV	C310-C311-C312-C313
2	A	1301	POV	C31-C32-C33-C34
2	A	1303	POV	C21-C22-C23-C24
2	B	1306	POV	C21-C22-C23-C24
2	C	1304	POV	C31-C32-C33-C34
2	C	1306	POV	C21-C22-C23-C24
2	A	1315	POV	O11-C1-C2-O21
2	B	1304	POV	C311-C310-C39-C38
2	C	1311	POV	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
2	A	1308	POV	C36-C37-C38-C39
2	C	1308	POV	C34-C35-C36-C37
2	B	1315	POV	C211-C212-C213-C214
2	C	1314	POV	C211-C212-C213-C214
2	C	1303	POV	O21-C2-C3-O31
2	D	1314	POV	O21-C2-C3-O31
2	B	1301	POV	C23-C24-C25-C26
2	C	1311	POV	C213-C214-C215-C216
2	A	1314	POV	C210-C211-C212-C213
2	A	1314	POV	C26-C27-C28-C29
2	B	1309	POV	C26-C27-C28-C29
2	C	1306	POV	C26-C27-C28-C29
2	C	1309	POV	C26-C27-C28-C29
2	D	1304	POV	C26-C27-C28-C29
2	D	1308	POV	C26-C27-C28-C29
2	D	1311	POV	C26-C27-C28-C29
2	B	1302	POV	C310-C311-C312-C313
2	B	1310	POV	C34-C35-C36-C37
2	D	1301	POV	C211-C212-C213-C214
2	A	1307	POV	C37-C38-C39-C310
2	B	1303	POV	C311-C312-C313-C314
2	B	1305	POV	C22-C23-C24-C25
2	B	1315	POV	C311-C310-C39-C38
2	D	1301	POV	C311-C310-C39-C38
2	D	1312	POV	C211-C212-C213-C214
2	D	1313	POV	C213-C214-C215-C216
3	C	1307	CLR	C23-C24-C25-C26
3	D	1309	CLR	C23-C24-C25-C26
2	B	1309	POV	C22-C23-C24-C25
2	D	1303	POV	C34-C35-C36-C37
2	A	1301	POV	C1-O11-P-O12
2	A	1301	POV	C11-O12-P-O11
2	B	1302	POV	C11-O12-P-O11
2	B	1303	POV	C11-O12-P-O11
2	B	1304	POV	C11-O12-P-O11
2	B	1313	POV	C1-O11-P-O12
2	C	1302	POV	C11-O12-P-O11
2	C	1304	POV	C1-O11-P-O12
2	C	1304	POV	C11-O12-P-O11
2	C	1313	POV	C1-O11-P-O12
2	D	1304	POV	C11-O12-P-O11
2	D	1306	POV	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
2	D	1306	POV	C11-O12-P-O11
2	A	1309	POV	C32-C33-C34-C35
2	B	1301	POV	C312-C313-C314-C315
2	D	1311	POV	C33-C34-C35-C36
2	B	1309	POV	C21-C22-C23-C24
2	A	1308	POV	C213-C214-C215-C216
2	D	1307	POV	C22-C23-C24-C25
2	A	1308	POV	O11-C1-C2-C3
2	B	1301	POV	O11-C1-C2-C3
2	B	1311	POV	O11-C1-C2-C3
2	C	1301	POV	O11-C1-C2-C3
2	C	1303	POV	O11-C1-C2-C3
2	C	1312	POV	O11-C1-C2-C3
2	D	1303	POV	O11-C1-C2-C3
2	D	1313	POV	O11-C1-C2-C3
2	D	1314	POV	O11-C1-C2-C3
2	B	1311	POV	C39-C310-C311-C312
2	C	1309	POV	C22-C23-C24-C25
2	A	1308	POV	C311-C312-C313-C314
2	C	1301	POV	C215-C216-C217-C218
3	A	1304	CLR	C23-C24-C25-C26
2	A	1308	POV	C310-C311-C312-C313
2	D	1313	POV	C310-C311-C312-C313
2	C	1302	POV	C26-C27-C28-C29
2	A	1301	POV	C311-C310-C39-C38
2	C	1310	POV	C37-C38-C39-C310
2	C	1311	POV	C310-C311-C312-C313
2	D	1306	POV	C311-C310-C39-C38
2	C	1312	POV	C32-C33-C34-C35
2	A	1310	POV	C37-C38-C39-C310
2	B	1311	POV	C310-C311-C312-C313
2	D	1314	POV	C25-C26-C27-C28
2	C	1309	POV	C21-C22-C23-C24
2	A	1315	POV	C211-C212-C213-C214
2	C	1303	POV	C311-C312-C313-C314
2	A	1302	POV	C1-C2-C3-O31
2	A	1306	POV	C215-C216-C217-C218
2	A	1314	POV	C1-C2-C3-O31
2	B	1301	POV	C1-C2-C3-O31
2	B	1303	POV	C1-C2-C3-O31
2	B	1305	POV	C1-C2-C3-O31
2	C	1301	POV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
2	C	1303	POV	C1-C2-C3-O31
2	C	1305	POV	C1-C2-C3-O31
2	C	1311	POV	C311-C312-C313-C314
2	D	1303	POV	C1-C2-C3-O31
2	D	1305	POV	C1-C2-C3-O31
2	D	1305	POV	C311-C312-C313-C314
2	D	1307	POV	C1-C2-C3-O31
2	B	1311	POV	C36-C37-C38-C39
2	C	1304	POV	C311-C310-C39-C38
2	B	1311	POV	C21-C22-C23-C24
2	C	1310	POV	C31-C32-C33-C34
4	A	1311	DU0	O23-C24-C25-C26
4	B	1314	DU0	O23-C24-C25-C26
4	B	1317	DU0	O23-C24-C25-C26
4	D	1316	DU0	O23-C24-C25-C26
2	C	1301	POV	C39-C310-C311-C312
2	C	1310	POV	C34-C35-C36-C37
2	D	1312	POV	C32-C33-C34-C35
2	B	1309	POV	C215-C216-C217-C218
2	C	1309	POV	C215-C216-C217-C218
2	C	1309	POV	C33-C34-C35-C36
2	D	1303	POV	C23-C24-C25-C26
2	C	1309	POV	C310-C311-C312-C313
2	C	1311	POV	C39-C310-C311-C312
2	D	1310	POV	C37-C38-C39-C310
2	D	1311	POV	C215-C216-C217-C218
2	C	1314	POV	C313-C314-C315-C316
2	B	1308	POV	C210-C211-C212-C213
2	D	1304	POV	C210-C211-C212-C213
2	D	1308	POV	C210-C211-C212-C213
2	A	1308	POV	C39-C310-C311-C312
2	A	1312	POV	C313-C314-C315-C316
2	B	1310	POV	C37-C38-C39-C310
2	B	1309	POV	C313-C314-C315-C316
2	B	1312	POV	C25-C26-C27-C28
2	D	1311	POV	C22-C23-C24-C25
2	A	1316	POV	C39-C310-C311-C312
2	B	1308	POV	C313-C314-C315-C316
2	D	1312	POV	C36-C37-C38-C39
2	A	1306	POV	C22-C23-C24-C25
2	B	1309	POV	C312-C313-C314-C315
2	B	1302	POV	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
2	B	1308	POV	O11-C1-C2-O21
2	D	1304	POV	O11-C1-C2-O21
2	D	1311	POV	O11-C1-C2-O21
2	D	1301	POV	C23-C24-C25-C26
2	D	1313	POV	C39-C310-C311-C312
2	D	1301	POV	C313-C314-C315-C316
2	C	1303	POV	C2-C3-O31-C31
2	A	1306	POV	O21-C2-C3-O31
2	B	1309	POV	O21-C2-C3-O31
2	B	1312	POV	O21-C2-C3-O31
2	C	1309	POV	O21-C2-C3-O31
2	D	1311	POV	O21-C2-C3-O31
2	A	1307	POV	C34-C35-C36-C37
2	B	1315	POV	C313-C314-C315-C316
2	A	1307	POV	C31-C32-C33-C34
2	B	1309	POV	C33-C34-C35-C36
4	A	1311	DU0	C21-C22-O23-C24
4	D	1316	DU0	C21-C22-O23-C24
2	A	1303	POV	C24-C25-C26-C27
2	C	1306	POV	C33-C34-C35-C36
2	C	1302	POV	C215-C216-C217-C218
2	A	1301	POV	C213-C214-C215-C216
2	B	1313	POV	C212-C213-C214-C215
2	A	1309	POV	C25-C26-C27-C28
2	A	1303	POV	C33-C34-C35-C36
2	B	1308	POV	C212-C213-C214-C215
2	A	1306	POV	O11-C1-C2-C3
2	B	1303	POV	O11-C1-C2-C3
2	C	1309	POV	O11-C1-C2-C3
2	C	1311	POV	O11-C1-C2-C3
2	D	1305	POV	O11-C1-C2-C3
2	D	1311	POV	O11-C1-C2-C3
2	D	1310	POV	C212-C213-C214-C215
4	A	1311	DU0	C51-C26-C27-O28
4	B	1314	DU0	C51-C26-C27-O28
4	B	1317	DU0	C51-C26-C27-O28
4	D	1316	DU0	C51-C26-C27-O28
2	C	1306	POV	C24-C25-C26-C27
2	C	1311	POV	C22-C23-C24-C25
2	D	1310	POV	C312-C313-C314-C315
2	A	1308	POV	C22-C23-C24-C25
2	B	1306	POV	C312-C313-C314-C315

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Mol	Chain	Res	Type	Atoms
2	C	1312	POV	C25-C26-C27-C28
2	C	1303	POV	C311-C310-C39-C38
2	A	1308	POV	C2-C1-O11-P
2	B	1311	POV	C2-C1-O11-P
2	C	1311	POV	C2-C1-O11-P
2	D	1313	POV	C2-C1-O11-P
2	B	1311	POV	C311-C312-C313-C314
2	A	1314	POV	C310-C311-C312-C313
2	D	1315	POV	C212-C213-C214-C215
2	A	1306	POV	C1-C2-C3-O31
2	A	1308	POV	C1-C2-C3-O31
2	B	1309	POV	C1-C2-C3-O31
2	B	1311	POV	C1-C2-C3-O31
2	B	1313	POV	C1-C2-C3-O31
2	C	1301	POV	C1-C2-C3-O31
2	D	1311	POV	C1-C2-C3-O31
2	D	1313	POV	C1-C2-C3-O31
2	D	1315	POV	C1-C2-C3-O31
2	C	1302	POV	C34-C35-C36-C37
2	C	1312	POV	C310-C311-C312-C313
2	D	1308	POV	C24-C25-C26-C27
2	D	1311	POV	C313-C314-C315-C316
2	D	1313	POV	C214-C215-C216-C217
2	A	1310	POV	C1-O11-P-O12
2	D	1315	POV	C1-O11-P-O12
4	A	1311	DU0	C25-C26-C27-O28
4	B	1314	DU0	C25-C26-C27-O28
4	B	1317	DU0	C25-C26-C27-O28
4	D	1316	DU0	C25-C26-C27-O28
2	D	1313	POV	C22-C23-C24-C25
2	A	1308	POV	C214-C215-C216-C217
2	C	1313	POV	C212-C213-C214-C215
2	A	1306	POV	O11-C1-C2-O21
2	B	1309	POV	O11-C1-C2-O21
2	B	1315	POV	O11-C1-C2-O21
2	C	1302	POV	O11-C1-C2-O21
2	C	1308	POV	O11-C1-C2-O21
2	C	1309	POV	O11-C1-C2-O21
2	A	1315	POV	C210-C211-C212-C213
2	B	1313	POV	C25-C26-C27-C28
2	B	1308	POV	C34-C35-C36-C37
2	A	1314	POV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
2	A	1302	POV	O21-C2-C3-O31
2	A	1314	POV	O21-C2-C3-O31
2	B	1311	POV	O21-C2-C3-O31
2	A	1314	POV	C32-C33-C34-C35
2	A	1306	POV	C310-C311-C312-C313
2	D	1310	POV	C23-C24-C25-C26
2	A	1309	POV	C2-C1-O11-P
2	B	1308	POV	C2-C1-O11-P
2	D	1311	POV	C2-C1-O11-P
2	D	1308	POV	C33-C34-C35-C36
2	A	1309	POV	C310-C311-C312-C313
2	A	1315	POV	C311-C310-C39-C38
2	B	1304	POV	C212-C213-C214-C215
2	A	1302	POV	C29-C210-C211-C212
2	B	1305	POV	C29-C210-C211-C212
2	C	1308	POV	C35-C36-C37-C38
2	C	1302	POV	C313-C314-C315-C316
2	C	1304	POV	C25-C26-C27-C28
2	A	1309	POV	O11-C1-C2-C3
2	A	1315	POV	O11-C1-C2-C3
2	B	1302	POV	O11-C1-C2-C3
2	B	1309	POV	O11-C1-C2-C3
2	B	1312	POV	O11-C1-C2-C3
2	D	1304	POV	O11-C1-C2-C3
2	A	1305	POV	C35-C36-C37-C38
2	D	1305	POV	C39-C310-C311-C312
2	B	1315	POV	C312-C313-C314-C315
2	D	1306	POV	C25-C26-C27-C28
2	A	1301	POV	C25-C26-C27-C28
2	B	1313	POV	C215-C216-C217-C218
2	B	1308	POV	C37-C38-C39-C310
2	A	1312	POV	C33-C34-C35-C36
2	D	1315	POV	C215-C216-C217-C218
2	B	1311	POV	C24-C25-C26-C27
2	C	1313	POV	C25-C26-C27-C28
2	A	1310	POV	C212-C213-C214-C215
2	B	1304	POV	C25-C26-C27-C28
2	B	1302	POV	C210-C211-C212-C213
2	A	1310	POV	C1-C2-C3-O31
2	A	1316	POV	C1-C2-C3-O31
2	B	1309	POV	C2-C1-O11-P
2	C	1311	POV	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
2	C	1313	POV	C1-C2-C3-O31
2	C	1304	POV	C213-C214-C215-C216
2	A	1305	POV	O11-C1-C2-O21
2	A	1312	POV	O11-C1-C2-O21
2	D	1301	POV	O11-C1-C2-O21
2	D	1305	POV	O11-C1-C2-O21
2	B	1301	POV	C34-C35-C36-C37
2	C	1308	POV	C213-C214-C215-C216
2	C	1302	POV	C310-C311-C312-C313
2	B	1303	POV	C39-C310-C311-C312
2	C	1313	POV	C215-C216-C217-C218
2	A	1310	POV	C25-C26-C27-C28
2	D	1301	POV	C312-C313-C314-C315
2	B	1301	POV	O21-C2-C3-O31
2	D	1312	POV	O21-C2-C3-O31
2	C	1301	POV	C35-C36-C37-C38
2	D	1305	POV	C214-C215-C216-C217
2	A	1316	POV	C23-C24-C25-C26
2	C	1311	POV	C214-C215-C216-C217
2	A	1303	POV	C210-C211-C212-C213
2	B	1315	POV	C215-C216-C217-C218
4	B	1314	DU0	C21-C22-O23-C24
4	B	1317	DU0	C21-C22-O23-C24
2	D	1301	POV	C215-C216-C217-C218
2	C	1314	POV	C310-C311-C312-C313
2	A	1315	POV	C11-O12-P-O11
2	C	1314	POV	C11-O12-P-O11
2	D	1315	POV	C11-O12-P-O11
2	B	1309	POV	C23-C24-C25-C26
2	D	1308	POV	C312-C313-C314-C315
2	A	1306	POV	C2-C1-O11-P
2	A	1314	POV	C2-C1-O11-P
2	B	1301	POV	C2-C1-O11-P
2	B	1312	POV	C2-C1-O11-P
2	C	1312	POV	C2-C1-O11-P
2	D	1303	POV	C2-C1-O11-P
2	D	1314	POV	C2-C1-O11-P
2	A	1301	POV	C1-O11-P-O13
2	A	1301	POV	C11-O12-P-O13
2	A	1302	POV	C11-O12-P-O13
2	A	1308	POV	C1-O11-P-O13
2	A	1309	POV	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
2	A	1309	POV	C11-O12-P-O13
2	A	1310	POV	C1-O11-P-O14
2	A	1315	POV	C11-C12-N-C14
2	A	1316	POV	C11-O12-P-O13
2	A	1316	POV	C11-O12-P-O14
2	B	1301	POV	C11-O12-P-O14
2	B	1302	POV	C11-O12-P-O14
2	B	1303	POV	C11-O12-P-O13
2	B	1304	POV	C1-O11-P-O13
2	B	1304	POV	C11-O12-P-O13
2	B	1305	POV	C11-O12-P-O13
2	B	1311	POV	C1-O11-P-O13
2	B	1313	POV	C1-O11-P-O14
2	C	1301	POV	C11-O12-P-O14
2	C	1302	POV	C11-O12-P-O14
2	C	1303	POV	C11-O12-P-O13
2	C	1303	POV	C11-O12-P-O14
2	C	1304	POV	C1-O11-P-O13
2	C	1304	POV	C11-O12-P-O13
2	C	1311	POV	C1-O11-P-O13
2	C	1313	POV	C1-O11-P-O14
2	D	1303	POV	C11-O12-P-O14
2	D	1304	POV	C1-O11-P-O14
2	D	1304	POV	C11-O12-P-O14
2	D	1305	POV	C11-O12-P-O13
2	D	1305	POV	C11-O12-P-O14
2	D	1306	POV	C1-O11-P-O13
2	D	1306	POV	C11-O12-P-O13
2	D	1307	POV	C11-O12-P-O13
2	D	1313	POV	C1-O11-P-O13
2	D	1315	POV	C11-O12-P-O13
2	A	1305	POV	O11-C1-C2-C3
2	A	1312	POV	O11-C1-C2-C3
2	B	1310	POV	O11-C1-C2-C3
2	C	1308	POV	O11-C1-C2-C3
2	C	1314	POV	O11-C1-C2-C3
2	D	1301	POV	O11-C1-C2-C3
2	A	1314	POV	C34-C35-C36-C37
2	A	1316	POV	O31-C31-C32-C33
2	A	1314	POV	C23-C24-C25-C26
2	D	1306	POV	C213-C214-C215-C216
2	A	1305	POV	C213-C214-C215-C216

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Mol	Chain	Res	Type	Atoms
2	B	1308	POV	C23-C24-C25-C26
2	A	1315	POV	C12-C11-O12-P
2	A	1305	POV	C210-C211-C212-C213
2	B	1306	POV	C26-C27-C28-C29
2	C	1306	POV	C210-C211-C212-C213
2	C	1308	POV	C210-C211-C212-C213
2	A	1301	POV	C212-C213-C214-C215
2	A	1307	POV	C311-C312-C313-C314
2	A	1312	POV	C310-C311-C312-C313
2	B	1315	POV	C23-C24-C25-C26
2	A	1307	POV	O11-C1-C2-O21
2	B	1303	POV	O11-C1-C2-O21
2	B	1310	POV	O11-C1-C2-O21
2	C	1303	POV	O11-C1-C2-O21
2	C	1310	POV	O11-C1-C2-O21
2	C	1314	POV	O11-C1-C2-O21
2	D	1312	POV	O11-C1-C2-O21
2	D	1301	POV	C310-C311-C312-C313
2	C	1301	POV	C214-C215-C216-C217
2	C	1308	POV	C37-C38-C39-C310
2	C	1310	POV	C212-C213-C214-C215
2	C	1314	POV	C312-C313-C314-C315
2	D	1311	POV	C23-C24-C25-C26
2	D	1314	POV	C310-C311-C312-C313
2	B	1312	POV	C11-C12-N-C15
2	D	1304	POV	C11-C12-N-C14
2	A	1306	POV	C23-C24-C25-C26
2	B	1310	POV	C311-C312-C313-C314
2	A	1306	POV	O12-C11-C12-N
2	A	1308	POV	O12-C11-C12-N
2	B	1309	POV	O12-C11-C12-N
2	B	1311	POV	O12-C11-C12-N
2	C	1309	POV	C1-C2-C3-O31
2	C	1309	POV	O12-C11-C12-N
2	C	1311	POV	O12-C11-C12-N
2	D	1311	POV	O12-C11-C12-N
2	D	1313	POV	O12-C11-C12-N
2	A	1308	POV	O21-C2-C3-O31
2	B	1305	POV	O21-C2-C3-O31
2	C	1301	POV	O21-C2-C3-O31
2	C	1311	POV	O21-C2-C3-O31
2	D	1303	POV	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
2	D	1307	POV	O21-C2-C3-O31
2	D	1313	POV	O21-C2-C3-O31
2	C	1310	POV	C311-C312-C313-C314
2	D	1304	POV	C311-C310-C39-C38
2	D	1311	POV	C210-C211-C212-C213
2	D	1304	POV	C211-C212-C213-C214
2	A	1310	POV	C215-C216-C217-C218
2	D	1304	POV	C313-C314-C315-C316
2	A	1312	POV	C23-C24-C25-C26
2	A	1305	POV	C2-C1-O11-P
2	C	1301	POV	C2-C1-O11-P
2	C	1308	POV	C2-C1-O11-P
2	C	1309	POV	C2-C1-O11-P
2	C	1314	POV	C215-C216-C217-C218
2	B	1310	POV	C212-C213-C214-C215
2	C	1304	POV	C211-C212-C213-C214
2	C	1304	POV	C311-C312-C313-C314
2	A	1301	POV	C311-C312-C313-C314
2	A	1307	POV	C212-C213-C214-C215
2	D	1306	POV	C215-C216-C217-C218
2	D	1312	POV	C311-C312-C313-C314
2	A	1305	POV	C313-C314-C315-C316
2	A	1312	POV	C312-C313-C314-C315
2	B	1304	POV	C210-C211-C212-C213
2	C	1308	POV	C313-C314-C315-C316
2	D	1306	POV	C211-C212-C213-C214
2	A	1315	POV	C11-C12-N-C13
2	B	1302	POV	C11-C12-N-C14
2	D	1312	POV	C212-C213-C214-C215
2	A	1316	POV	C311-C312-C313-C314
2	C	1309	POV	C23-C24-C25-C26
2	D	1301	POV	C29-C210-C211-C212
2	A	1305	POV	C37-C38-C39-C310
2	A	1316	POV	C33-C34-C35-C36
2	B	1301	POV	C313-C314-C315-C316
2	B	1302	POV	C313-C314-C315-C316
2	D	1312	POV	C31-C32-C33-C34
2	A	1306	POV	C313-C314-C315-C316
2	A	1307	POV	O11-C1-C2-C3
2	B	1308	POV	O11-C1-C2-C3
2	B	1315	POV	O11-C1-C2-C3
2	C	1310	POV	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	D	1312	POV	O11-C1-C2-C3
2	A	1307	POV	C36-C37-C38-C39
2	D	1301	POV	C21-C22-C23-C24
2	A	1303	POV	C29-C210-C211-C212
2	B	1315	POV	C29-C210-C211-C212
2	C	1306	POV	C29-C210-C211-C212
2	C	1303	POV	C33-C34-C35-C36
2	D	1306	POV	C311-C312-C313-C314
2	B	1303	POV	O31-C31-C32-C33
2	D	1305	POV	O31-C31-C32-C33
2	B	1312	POV	C11-C12-N-C14
2	A	1305	POV	C23-C24-C25-C26
2	A	1309	POV	C36-C37-C38-C39
2	B	1302	POV	C311-C310-C39-C38
2	C	1314	POV	C29-C210-C211-C212
2	A	1307	POV	O21-C2-C3-O31
2	C	1305	POV	O21-C2-C3-O31
2	C	1310	POV	O21-C2-C3-O31
2	B	1312	POV	C36-C37-C38-C39
2	C	1304	POV	C215-C216-C217-C218
2	D	1303	POV	C313-C314-C315-C316
2	A	1302	POV	C1-O11-P-O12
2	A	1312	POV	C11-O12-P-O11
2	A	1316	POV	C1-O11-P-O12
2	B	1305	POV	C1-O11-P-O12
2	B	1312	POV	C1-O11-P-O12
2	B	1315	POV	C11-O12-P-O11
2	C	1305	POV	C1-O11-P-O12
2	D	1301	POV	C11-O12-P-O11
2	D	1307	POV	C1-O11-P-O12
2	D	1314	POV	C1-O11-P-O12
2	A	1315	POV	C34-C35-C36-C37
2	C	1312	POV	C39-C310-C311-C312
2	B	1303	POV	C214-C215-C216-C217
2	B	1312	POV	C310-C311-C312-C313
2	B	1302	POV	C211-C212-C213-C214
2	D	1310	POV	C1-C2-C3-O31
2	D	1308	POV	C29-C210-C211-C212
2	C	1303	POV	O31-C31-C32-C33
2	C	1308	POV	C23-C24-C25-C26
2	B	1315	POV	C310-C311-C312-C313
2	C	1302	POV	C210-C211-C212-C213

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Mol	Chain	Res	Type	Atoms
2	C	1312	POV	C36-C37-C38-C39
2	D	1314	POV	C36-C37-C38-C39
2	D	1312	POV	C34-C35-C36-C37
4	A	1313	DU0	C21-C22-O23-C24
2	D	1313	POV	C215-C216-C217-C218
2	A	1312	POV	C215-C216-C217-C218
2	C	1306	POV	C212-C213-C214-C215
2	A	1312	POV	C29-C210-C211-C212
2	B	1305	POV	C27-C28-C29-C210
2	A	1308	POV	C215-C216-C217-C218
2	C	1314	POV	C23-C24-C25-C26
2	B	1309	POV	C210-C211-C212-C213
2	A	1309	POV	C39-C310-C311-C312
2	D	1315	POV	C25-C26-C27-C28
2	D	1304	POV	C11-C12-N-C13
2	A	1314	POV	C22-C23-C24-C25
2	D	1313	POV	C24-C25-C26-C27
2	C	1308	POV	C312-C313-C314-C315
2	B	1303	POV	C311-C310-C39-C38
2	A	1301	POV	C211-C212-C213-C214
2	B	1304	POV	C311-C312-C313-C314
2	D	1313	POV	C21-C22-C23-C24
2	D	1310	POV	C313-C314-C315-C316
2	A	1303	POV	C212-C213-C214-C215
2	D	1310	POV	O21-C2-C3-O31
2	D	1308	POV	C212-C213-C214-C215
2	A	1315	POV	C11-C12-N-C15
2	A	1305	POV	C312-C313-C314-C315
2	B	1306	POV	C310-C311-C312-C313
2	C	1304	POV	C212-C213-C214-C215
2	C	1304	POV	C24-C25-C26-C27
2	A	1315	POV	C313-C314-C315-C316
2	C	1309	POV	C313-C314-C315-C316
2	C	1310	POV	C36-C37-C38-C39
2	A	1301	POV	C24-C25-C26-C27
2	B	1313	POV	C211-C212-C213-C214
2	B	1306	POV	C33-C34-C35-C36
2	D	1314	POV	C39-C310-C311-C312
2	A	1314	POV	C311-C312-C313-C314
2	A	1310	POV	C33-C34-C35-C36
2	A	1305	POV	C1-C2-O21-C21
2	B	1301	POV	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
2	B	1308	POV	C1-C2-O21-C21
2	C	1301	POV	C3-C2-O21-C21
2	C	1308	POV	C1-C2-O21-C21
2	D	1303	POV	C3-C2-O21-C21
2	B	1312	POV	C11-C12-N-C13
2	D	1304	POV	C11-C12-N-C15
2	D	1303	POV	C27-C28-C29-C210
2	D	1303	POV	C22-C23-C24-C25
2	B	1305	POV	C11-O12-P-O11
2	D	1304	POV	C1-O11-P-O12
2	A	1307	POV	C312-C313-C314-C315
2	C	1304	POV	C33-C34-C35-C36
2	C	1302	POV	O11-C1-C2-C3
2	A	1302	POV	C27-C28-C29-C210
2	C	1311	POV	C21-C22-C23-C24
2	A	1308	POV	C21-C22-C23-C24
2	A	1301	POV	C215-C216-C217-C218
2	B	1310	POV	O21-C2-C3-O31
2	D	1312	POV	C312-C313-C314-C315
2	B	1312	POV	C39-C310-C311-C312
2	C	1309	POV	C210-C211-C212-C213
2	C	1306	POV	C39-C310-C311-C312
2	B	1304	POV	C24-C25-C26-C27
2	C	1303	POV	C39-C310-C311-C312
2	C	1310	POV	C310-C311-C312-C313
2	D	1306	POV	C212-C213-C214-C215
2	D	1306	POV	C24-C25-C26-C27
2	B	1310	POV	C310-C311-C312-C313
2	C	1311	POV	C215-C216-C217-C218
2	B	1304	POV	C39-C310-C311-C312
2	B	1306	POV	C2-C1-O11-P
2	B	1308	POV	C312-C313-C314-C315
2	B	1310	POV	C312-C313-C314-C315
2	A	1315	POV	C32-C33-C34-C35
2	C	1310	POV	C312-C313-C314-C315
2	B	1301	POV	C32-C33-C34-C35
2	A	1301	POV	C33-C34-C35-C36
2	A	1308	POV	C24-C25-C26-C27
2	D	1305	POV	C311-C310-C39-C38
2	A	1309	POV	C27-C28-C29-C210
2	A	1312	POV	C27-C28-C29-C210
2	C	1312	POV	C27-C28-C29-C210

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Mol	Chain	Res	Type	Atoms
2	C	1314	POV	C27-C28-C29-C210
2	D	1311	POV	C29-C210-C211-C212
2	B	1310	POV	C36-C37-C38-C39
2	A	1314	POV	C313-C314-C315-C316
2	B	1306	POV	C24-C25-C26-C27
2	C	1311	POV	C24-C25-C26-C27
2	D	1315	POV	C312-C313-C314-C315
2	D	1308	POV	C2-C1-O11-P
2	A	1314	POV	C214-C215-C216-C217
2	A	1306	POV	C29-C210-C211-C212
2	A	1310	POV	C27-C28-C29-C210
2	D	1301	POV	O21-C21-C22-C23
2	D	1301	POV	C33-C34-C35-C36
2	B	1302	POV	C1-O11-P-O12
2	C	1302	POV	C1-O11-P-O12
2	C	1302	POV	C311-C310-C39-C38
2	B	1308	POV	O21-C21-C22-C23
2	B	1301	POV	C25-C26-C27-C28
2	B	1315	POV	C33-C34-C35-C36
2	A	1316	POV	C26-C27-C28-C29
2	B	1303	POV	C312-C313-C314-C315
2	B	1304	POV	C27-C28-C29-C210
2	B	1309	POV	C29-C210-C211-C212
2	C	1301	POV	C29-C210-C211-C212
2	C	1309	POV	C29-C210-C211-C212
2	A	1315	POV	C1-C2-O21-C21
2	B	1301	POV	C1-C2-O21-C21
2	B	1302	POV	C1-C2-O21-C21
2	C	1301	POV	C1-C2-O21-C21
2	C	1302	POV	C1-C2-O21-C21
2	D	1303	POV	C1-C2-O21-C21
2	D	1304	POV	C1-C2-O21-C21
2	A	1306	POV	C34-C35-C36-C37
2	C	1301	POV	C25-C26-C27-C28
2	A	1307	POV	C310-C311-C312-C313
2	A	1305	POV	O21-C21-C22-C23
2	C	1308	POV	O21-C21-C22-C23
2	D	1305	POV	C33-C34-C35-C36
2	A	1306	POV	C25-C26-C27-C28
2	B	1315	POV	O21-C21-C22-C23
2	B	1301	POV	C27-C28-C29-C210
2	B	1313	POV	C27-C28-C29-C210

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Mol	Chain	Res	Type	Atoms
2	B	1315	POV	C27-C28-C29-C210
2	C	1313	POV	C27-C28-C29-C210
2	D	1301	POV	C27-C28-C29-C210
2	D	1307	POV	C27-C28-C29-C210
2	A	1303	POV	C1-C2-C3-O31
2	D	1308	POV	C1-C2-C3-O31
2	A	1302	POV	C11-C12-N-C13
2	B	1302	POV	C11-C12-N-C15
2	C	1302	POV	C11-C12-N-C14
2	D	1311	POV	C310-C311-C312-C313
2	B	1301	POV	C22-C23-C24-C25
2	B	1303	POV	C33-C34-C35-C36
2	D	1305	POV	C312-C313-C314-C315
2	C	1314	POV	C33-C34-C35-C36
2	A	1301	POV	C27-C28-C29-C210
2	C	1301	POV	C27-C28-C29-C210
2	C	1304	POV	C27-C28-C29-C210
2	B	1308	POV	C214-C215-C216-C217
2	B	1313	POV	C312-C313-C314-C315
2	B	1306	POV	C29-C210-C211-C212
2	D	1306	POV	C27-C28-C29-C210
2	C	1314	POV	O21-C21-C22-C23
2	B	1302	POV	C11-C12-N-C13
2	A	1308	POV	C26-C27-C28-C29
2	A	1309	POV	C213-C214-C215-C216
2	A	1307	POV	C27-C28-C29-C210
2	A	1314	POV	C27-C28-C29-C210
2	B	1310	POV	C27-C28-C29-C210
2	D	1314	POV	C215-C216-C217-C218
2	B	1303	POV	C2-C3-O31-C31
2	D	1305	POV	C2-C3-O31-C31
2	A	1310	POV	C32-C33-C34-C35
2	B	1309	POV	C25-C26-C27-C28
2	D	1308	POV	C39-C310-C311-C312
2	D	1304	POV	C32-C33-C34-C35
2	C	1312	POV	C213-C214-C215-C216
2	C	1310	POV	C29-C210-C211-C212
2	C	1310	POV	C27-C28-C29-C210
2	C	1311	POV	C26-C27-C28-C29
2	C	1311	POV	C313-C314-C315-C316
2	C	1308	POV	C11-C12-N-C13
2	A	1305	POV	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
2	B	1312	POV	C215-C216-C217-C218
2	B	1315	POV	O22-C21-C22-C23
2	B	1304	POV	C215-C216-C217-C218
2	B	1308	POV	O22-C21-C22-C23
2	C	1303	POV	C312-C313-C314-C315
2	A	1307	POV	C29-C210-C211-C212
2	A	1314	POV	C29-C210-C211-C212
2	B	1301	POV	C29-C210-C211-C212
2	C	1305	POV	C27-C28-C29-C210
2	D	1312	POV	C27-C28-C29-C210
2	C	1308	POV	O22-C21-C22-C23
2	D	1301	POV	O22-C21-C22-C23
2	A	1307	POV	C1-C2-C3-O31
2	C	1306	POV	C1-C2-C3-O31
2	D	1312	POV	C1-C2-C3-O31
2	C	1301	POV	C311-C312-C313-C314
2	D	1311	POV	C25-C26-C27-C28
2	C	1314	POV	O22-C21-C22-C23
2	A	1308	POV	C313-C314-C315-C316
2	C	1306	POV	C2-C1-O11-P
2	A	1301	POV	C313-C314-C315-C316
2	A	1303	POV	C39-C310-C311-C312
2	C	1309	POV	C34-C35-C36-C37
2	A	1305	POV	C11-C12-N-C13
2	A	1315	POV	C1-O11-P-O14
2	A	1315	POV	C11-O12-P-O14
2	B	1302	POV	C1-O11-P-O14
2	C	1302	POV	C1-O11-P-O14
2	C	1305	POV	C1-O11-P-O14
2	D	1307	POV	C1-O11-P-O14
2	D	1315	POV	C1-O11-P-O14
2	D	1313	POV	C313-C314-C315-C316
2	B	1303	POV	C23-C24-C25-C26
2	C	1314	POV	C37-C38-C39-C310
2	A	1312	POV	O21-C21-C22-C23
2	D	1310	POV	O21-C21-C22-C23
2	C	1309	POV	O21-C21-C22-C23
2	C	1310	POV	O31-C31-C32-C33
2	C	1312	POV	C215-C216-C217-C218
2	A	1302	POV	C12-C11-O12-P
2	A	1305	POV	C3-C2-O21-C21
2	A	1308	POV	C12-C11-O12-P

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Mol	Chain	Res	Type	Atoms
2	A	1310	POV	C12-C11-O12-P
2	A	1315	POV	C3-C2-O21-C21
2	B	1302	POV	C3-C2-O21-C21
2	B	1302	POV	C12-C11-O12-P
2	B	1305	POV	C12-C11-O12-P
2	B	1311	POV	C12-C11-O12-P
2	B	1313	POV	C12-C11-O12-P
2	C	1302	POV	C3-C2-O21-C21
2	C	1302	POV	C12-C11-O12-P
2	C	1308	POV	C3-C2-O21-C21
2	C	1311	POV	C12-C11-O12-P
2	C	1312	POV	C12-C11-O12-P
2	C	1313	POV	C12-C11-O12-P
2	D	1304	POV	C3-C2-O21-C21
2	D	1304	POV	C12-C11-O12-P
2	D	1313	POV	C12-C11-O12-P
2	D	1315	POV	C12-C11-O12-P
2	A	1316	POV	O32-C31-C32-C33
2	A	1301	POV	C39-C310-C311-C312
2	A	1314	POV	C35-C36-C37-C38
2	B	1312	POV	C213-C214-C215-C216
2	A	1312	POV	O22-C21-C22-C23
2	A	1302	POV	C11-C12-N-C15
2	B	1305	POV	O21-C21-C22-C23
2	C	1301	POV	O21-C21-C22-C23
2	D	1312	POV	O31-C31-C32-C33
2	D	1314	POV	O31-C31-C32-C33
2	C	1301	POV	C310-C311-C312-C313
2	C	1303	POV	C23-C24-C25-C26
2	B	1301	POV	C311-C312-C313-C314
2	D	1304	POV	C33-C34-C35-C36
2	A	1307	POV	O31-C31-C32-C33
2	B	1309	POV	O21-C21-C22-C23
2	C	1312	POV	O31-C31-C32-C33
2	D	1311	POV	O21-C21-C22-C23
2	C	1309	POV	C25-C26-C27-C28
2	B	1312	POV	O32-C31-C32-C33
2	B	1312	POV	O31-C31-C32-C33
2	D	1314	POV	C27-C28-C29-C210
2	D	1315	POV	C27-C28-C29-C210
2	B	1302	POV	C32-C33-C34-C35
2	D	1313	POV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
2	D	1314	POV	C213-C214-C215-C216
2	C	1312	POV	O32-C31-C32-C33
2	A	1309	POV	O31-C31-C32-C33
2	B	1304	POV	C211-C212-C213-C214
2	A	1301	POV	C210-C211-C212-C213
2	B	1302	POV	C33-C34-C35-C36
2	B	1306	POV	C39-C310-C311-C312
2	A	1303	POV	C32-C33-C34-C35
2	A	1307	POV	C22-C23-C24-C25
2	D	1314	POV	O32-C31-C32-C33
2	B	1308	POV	C11-C12-N-C13
2	A	1308	POV	C25-C26-C27-C28
2	C	1306	POV	C32-C33-C34-C35
2	B	1310	POV	C29-C210-C211-C212
2	D	1303	POV	C29-C210-C211-C212
2	A	1306	POV	O21-C21-C22-C23
2	B	1301	POV	O21-C21-C22-C23

There are no ring outliers.

34 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1303	POV	1	0
2	A	1315	POV	1	0
2	B	1303	POV	3	0
2	A	1314	POV	1	0
2	A	1301	POV	2	0
2	A	1310	POV	1	0
2	D	1310	POV	2	0
3	D	1309	CLR	1	0
2	B	1304	POV	3	0
2	D	1315	POV	1	0
2	C	1304	POV	2	0
2	C	1303	POV	5	0
2	C	1309	POV	1	0
3	C	1307	CLR	1	0
2	B	1309	POV	2	0
2	D	1306	POV	2	0
3	A	1304	CLR	1	0
3	B	1307	CLR	1	0
2	B	1312	POV	2	0
2	C	1313	POV	1	0

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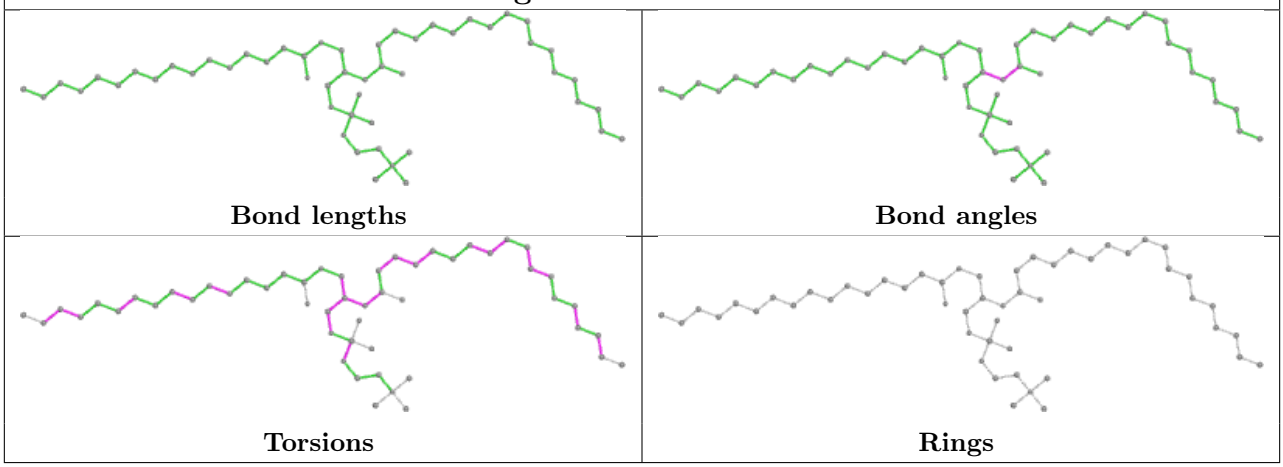
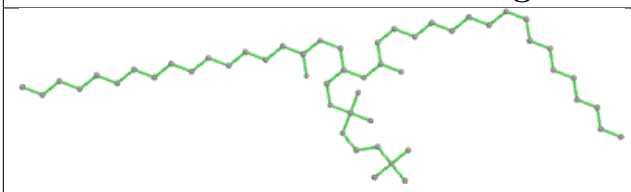
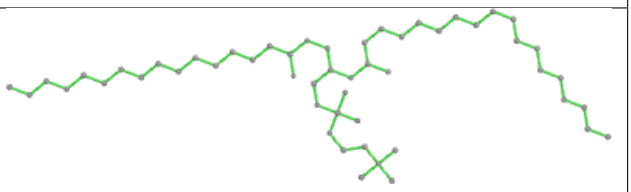
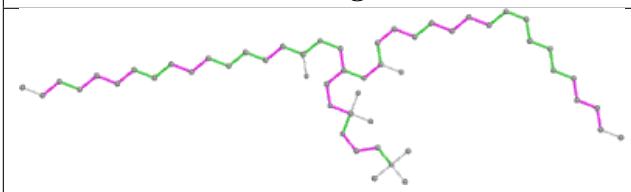
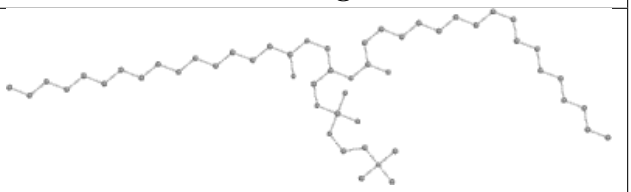
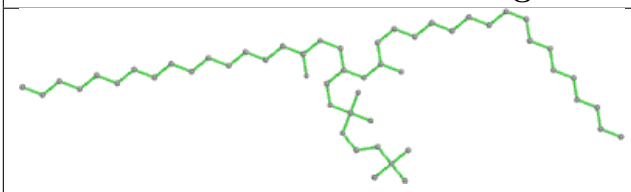
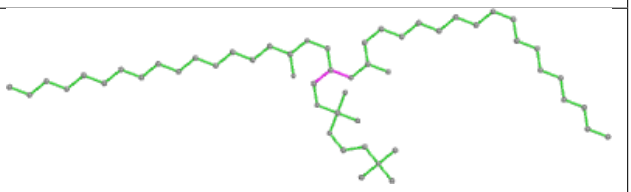
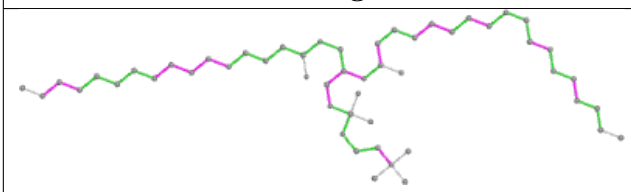
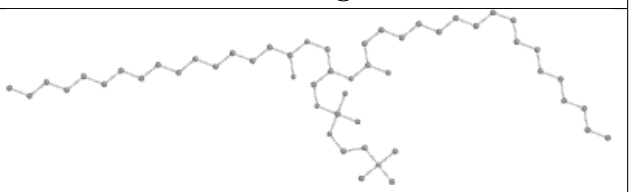
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1305	POV	5	0
2	C	1314	POV	2	0
2	C	1302	POV	2	0
2	A	1306	POV	1	0
2	A	1309	POV	2	0
2	D	1311	POV	1	0
2	B	1313	POV	1	0
2	D	1301	POV	2	0
2	D	1314	POV	1	0
2	B	1315	POV	2	0
2	D	1304	POV	1	0
2	A	1316	POV	5	0
2	B	1302	POV	1	0
2	A	1312	POV	4	0

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

Ligand POV D 1303



Ligand POV A 1308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV C 1308	
 Bond lengths	 Bond angles
 Torsions	 Rings

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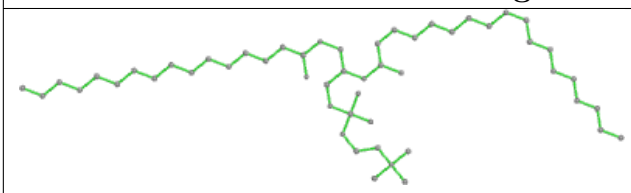
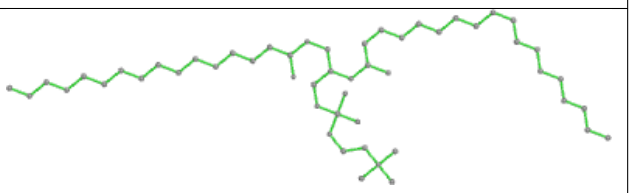
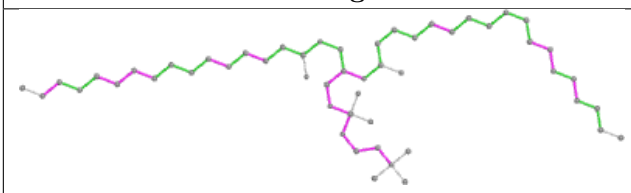
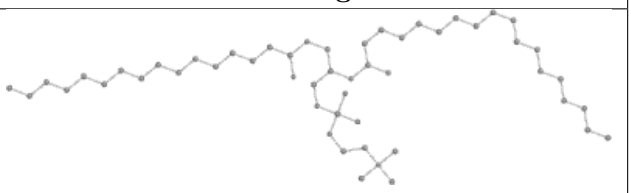
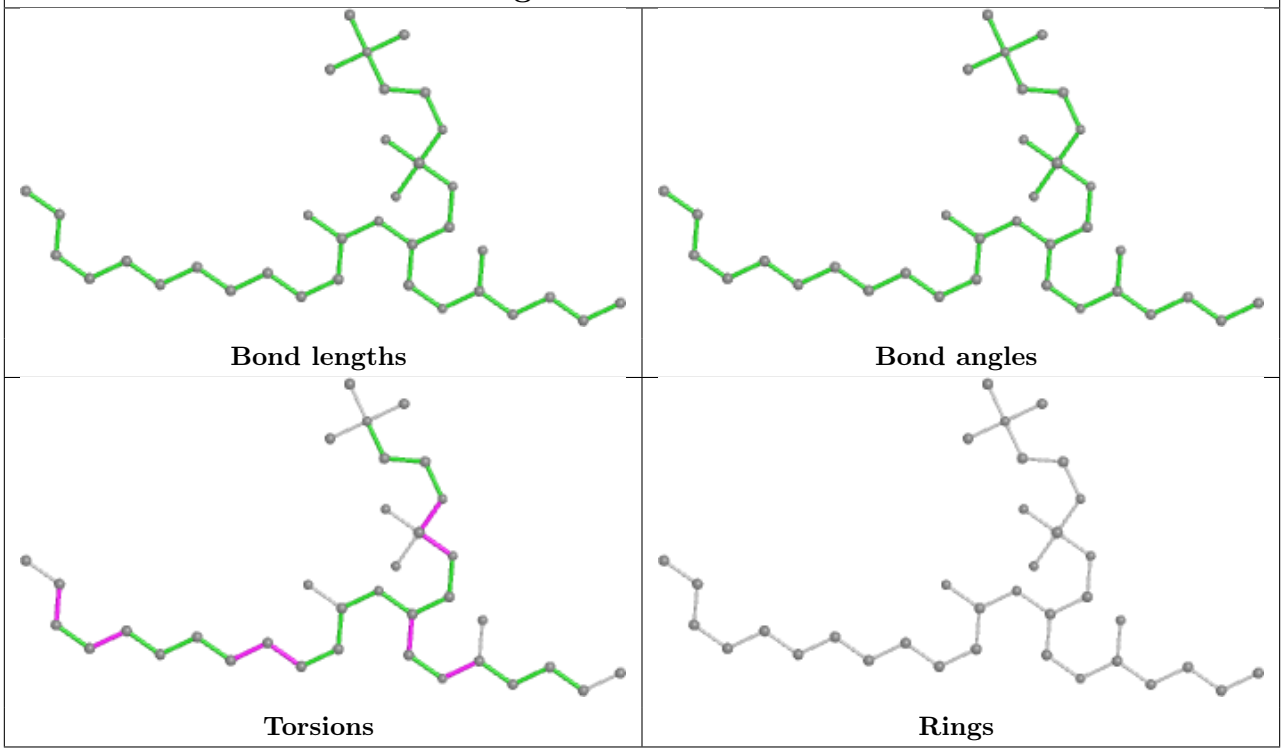
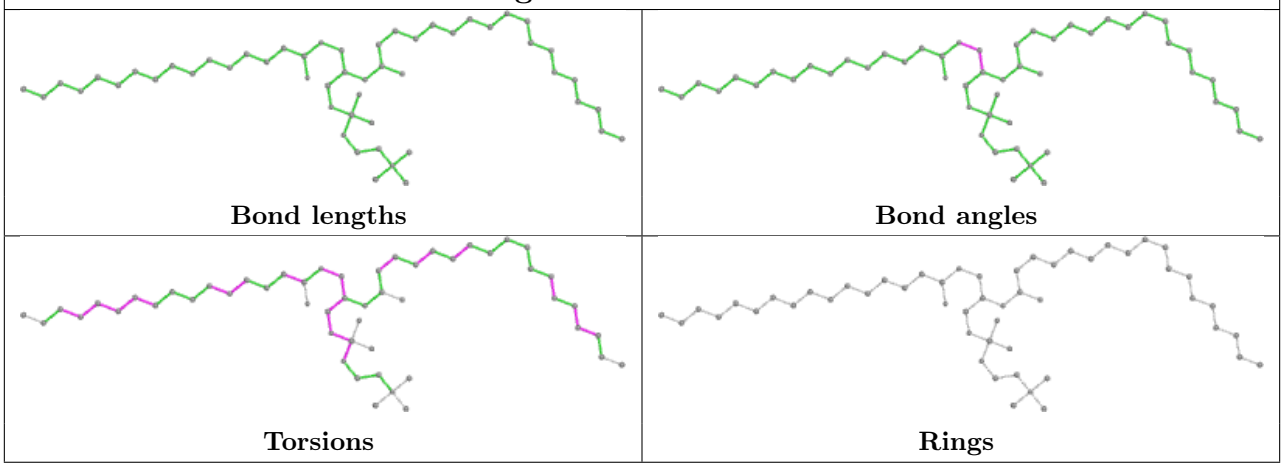
 Bond lengths	 Bond angles
 Torsions	 Rings

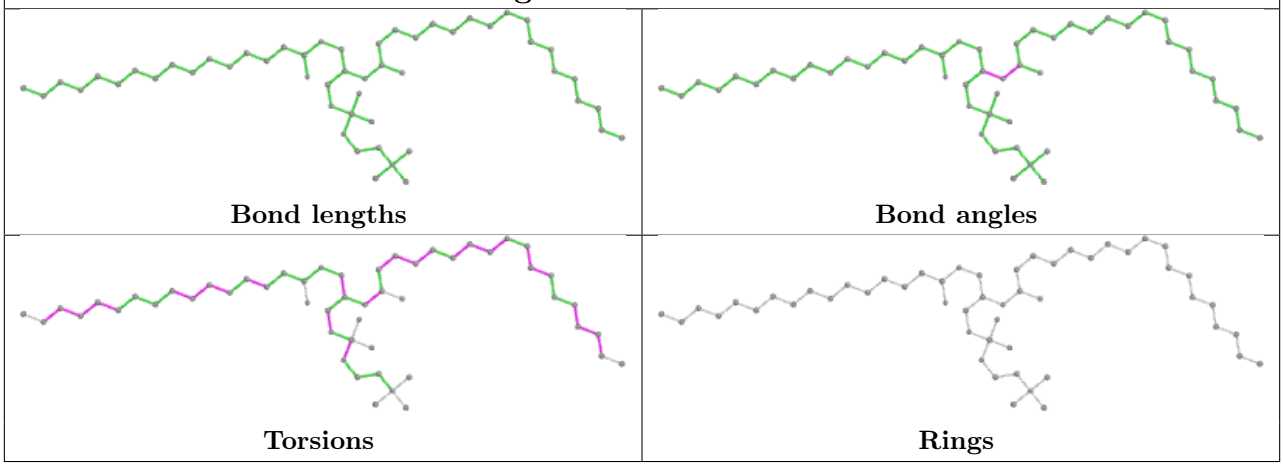
Ligand POV D 1307



Ligand POV B 1303



Ligand POV A 1314



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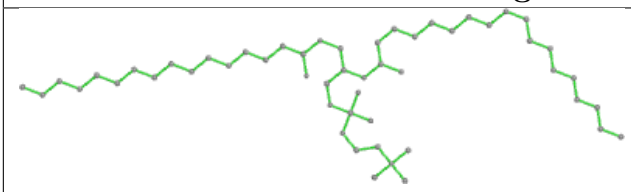
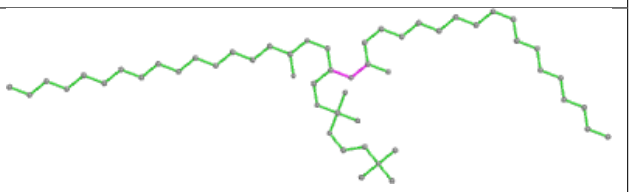
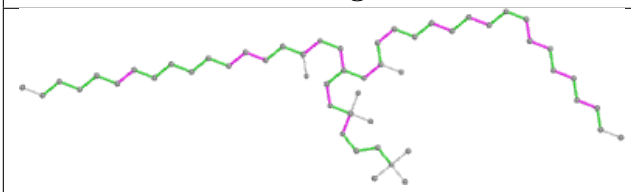
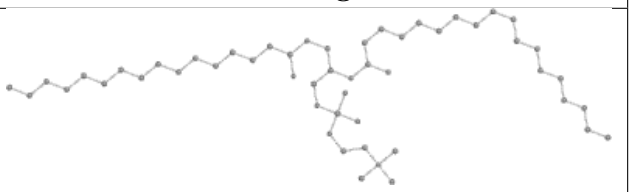
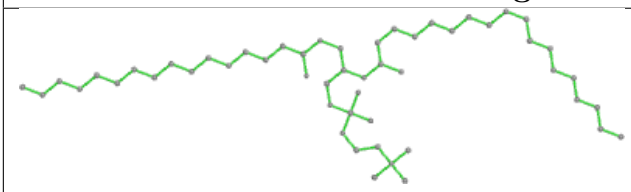
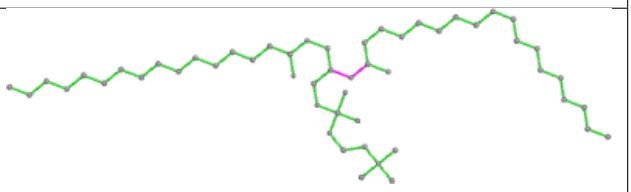
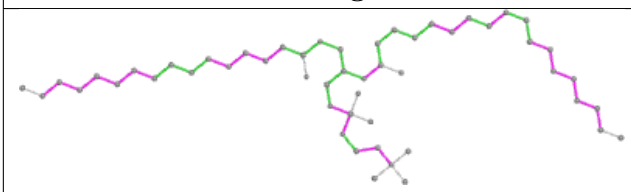
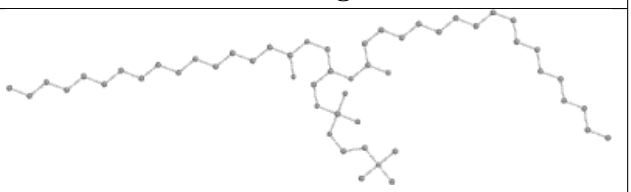
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV A 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

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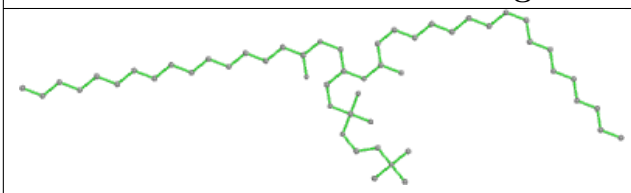
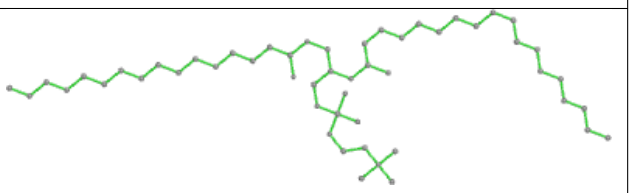
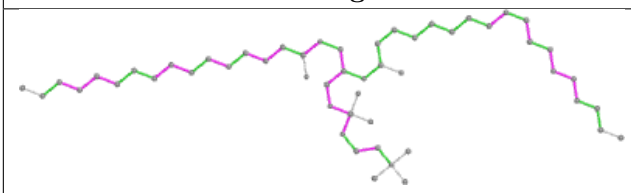
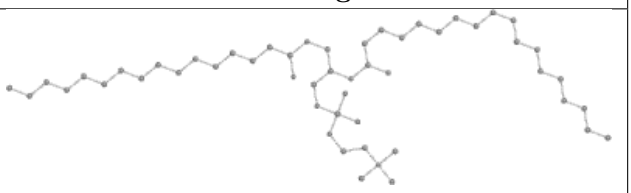
 Bond lengths	 Bond angles
 Torsions	 Rings

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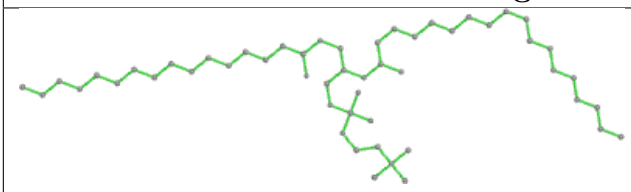
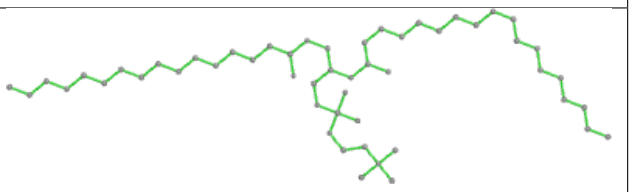
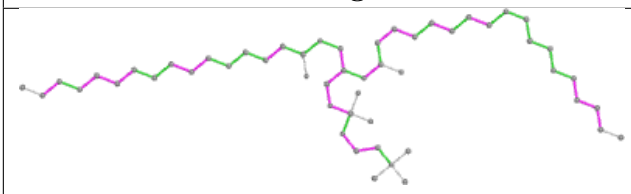
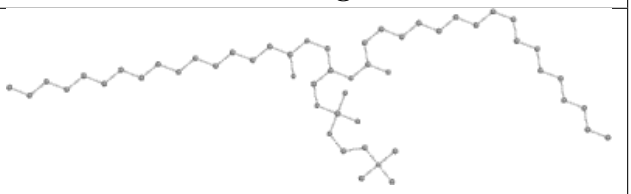
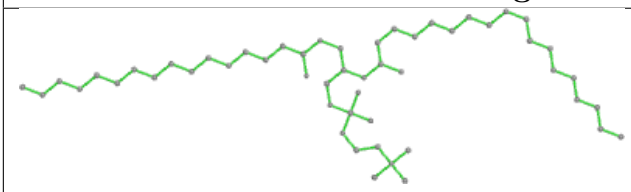
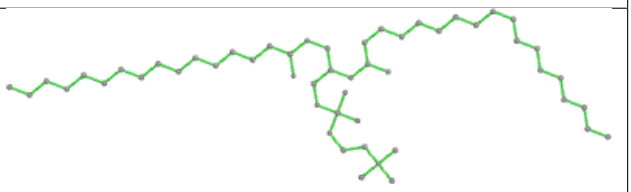
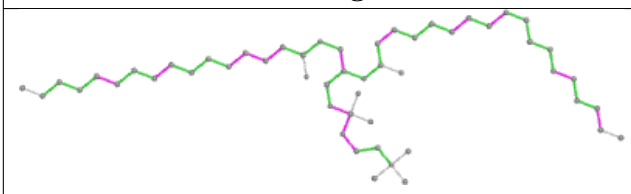
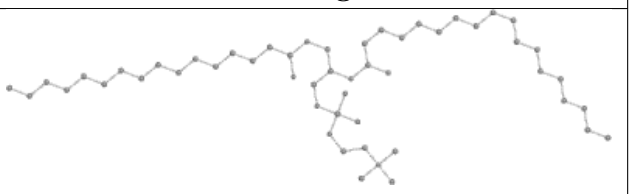
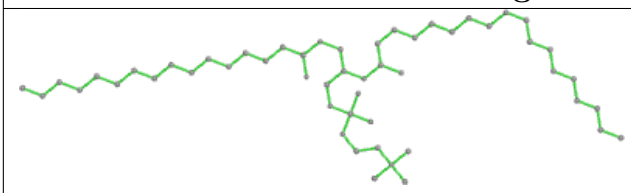
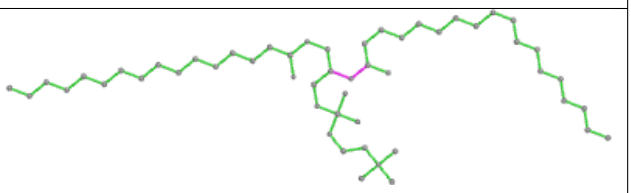
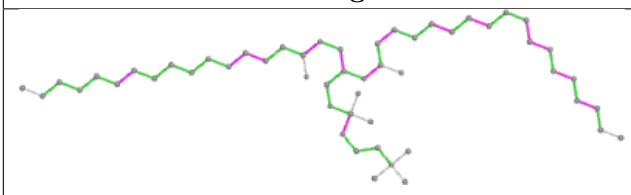
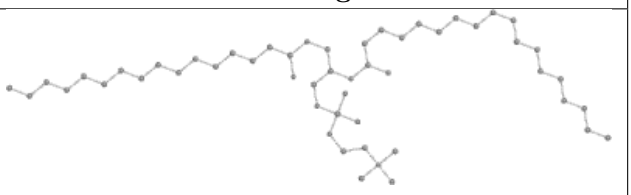
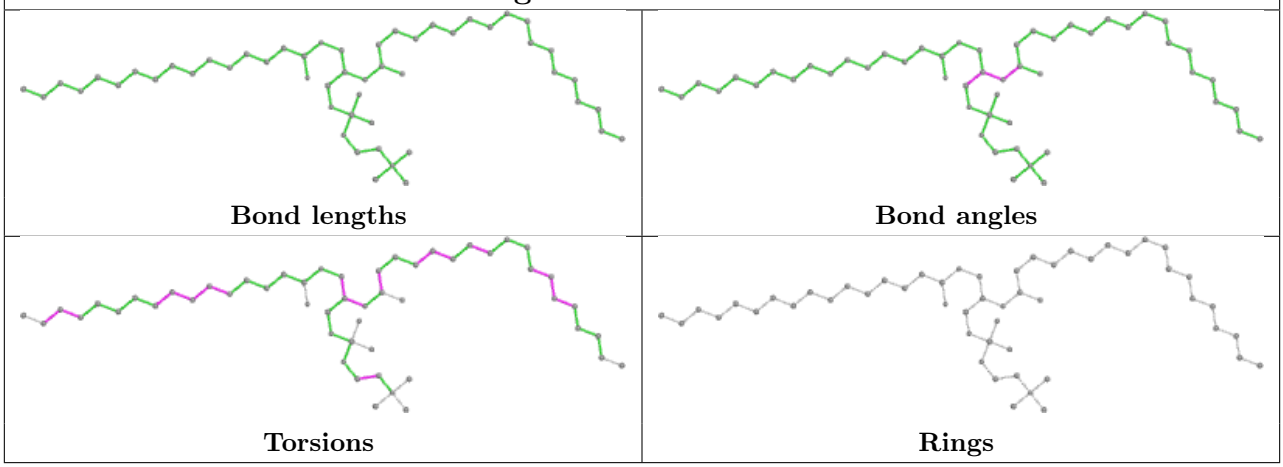
 Bond lengths	 Bond angles
 Torsions	 Rings

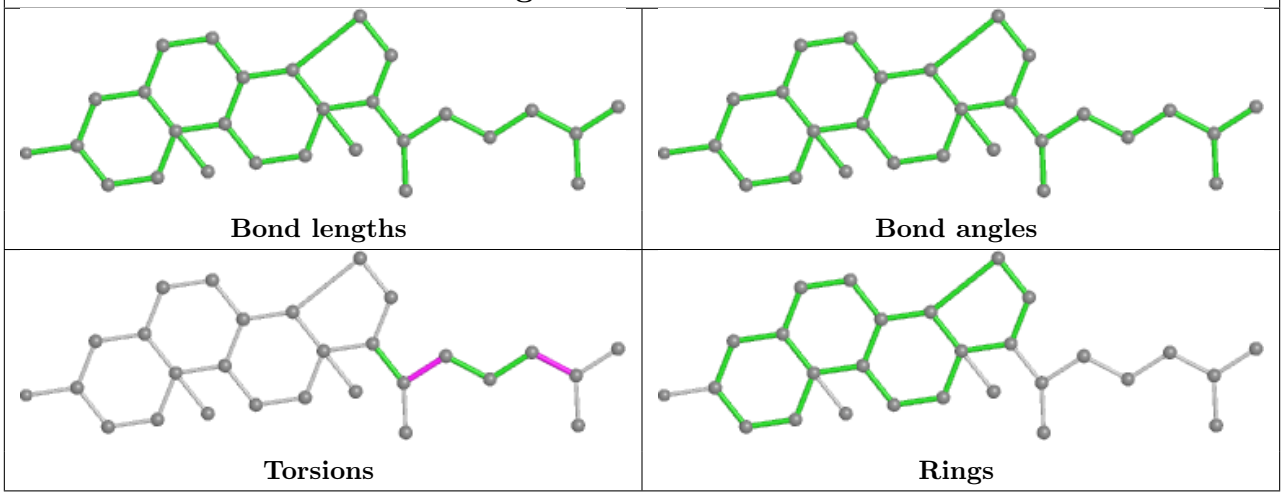
Ligand POV A 1310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV A 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

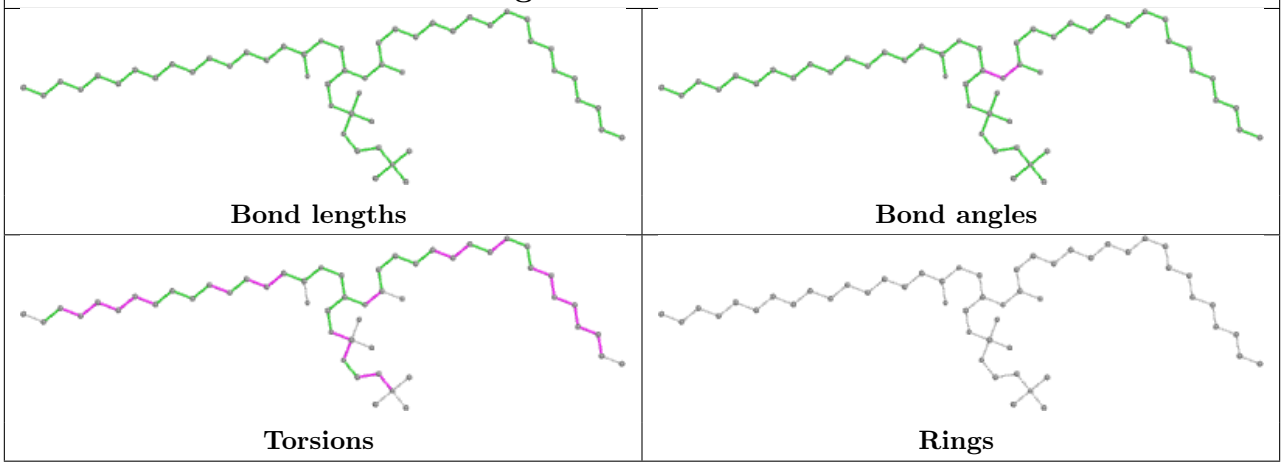
Ligand POV D 1310



Ligand CLR D 1309



Ligand POV B 1304



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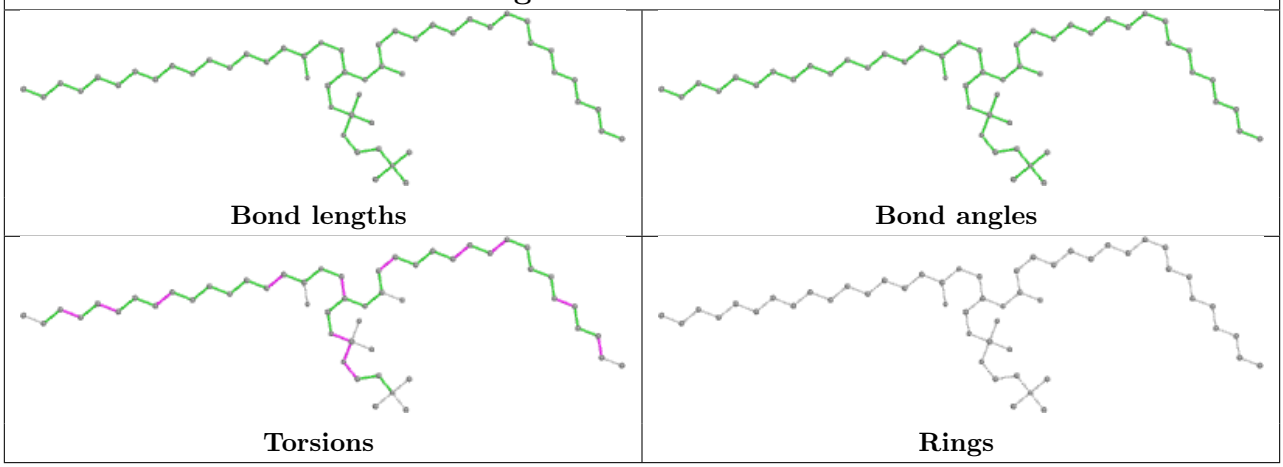
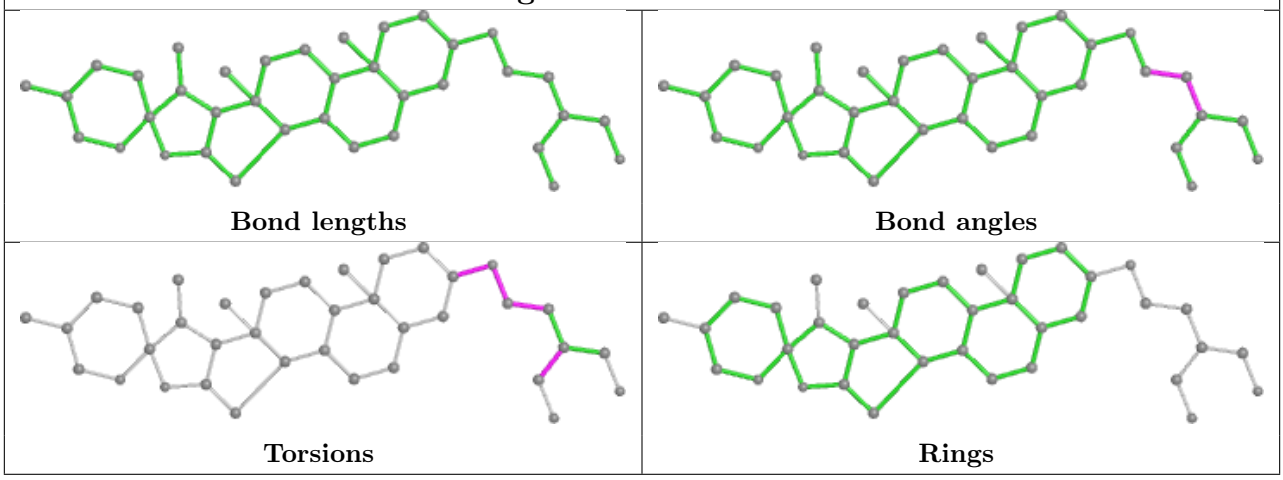
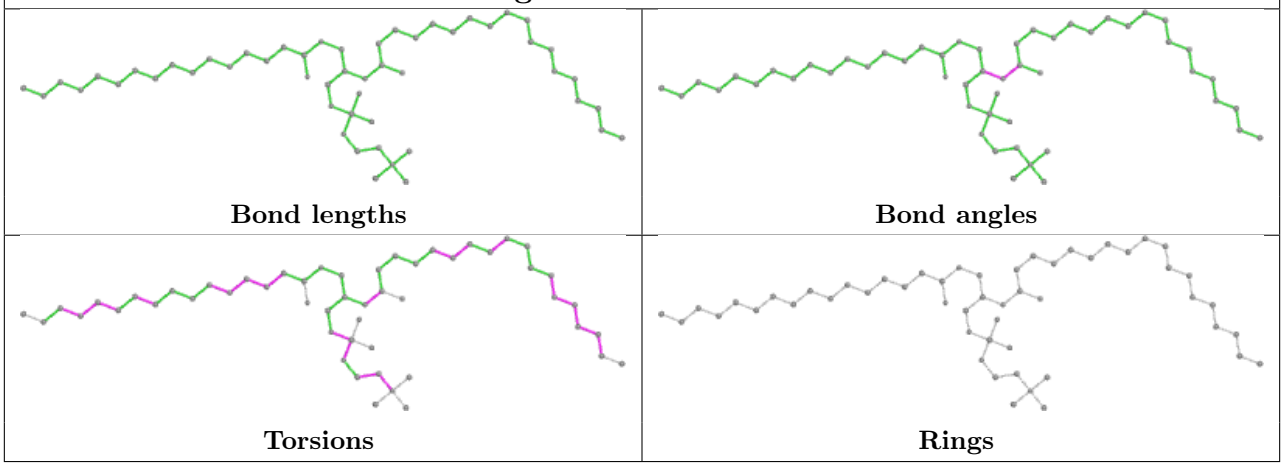


Ligand DU0 B 1314



Ligand POV C 1304



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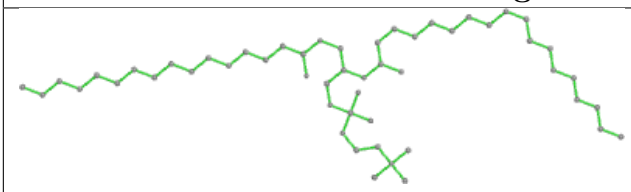
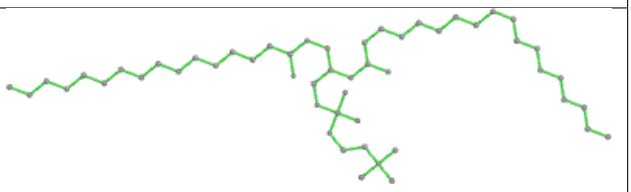
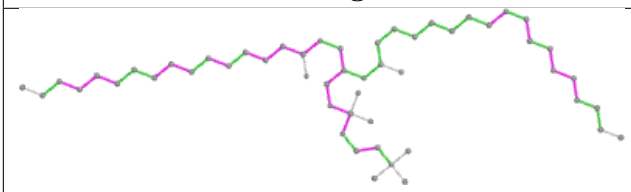


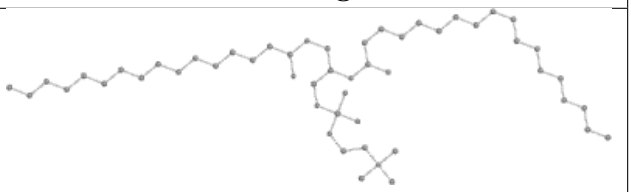
Bond lengths



Bond angles

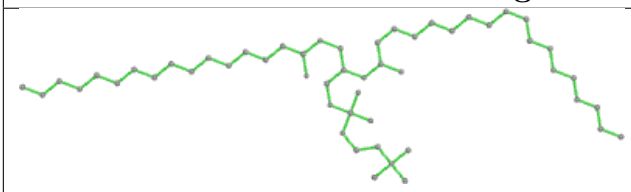


Torsions



Rings

Ligand POV B 1311



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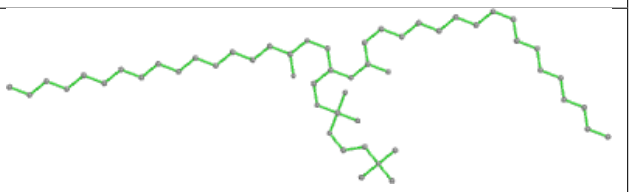
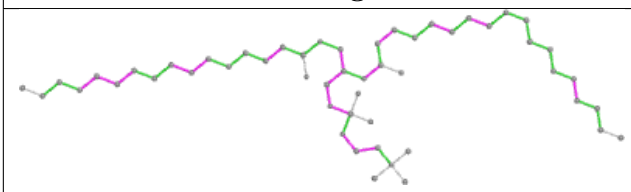
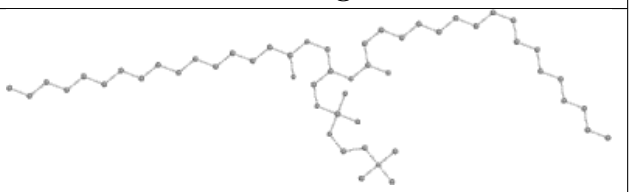


Bond angles

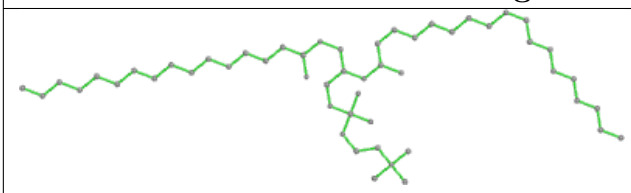


Torsions

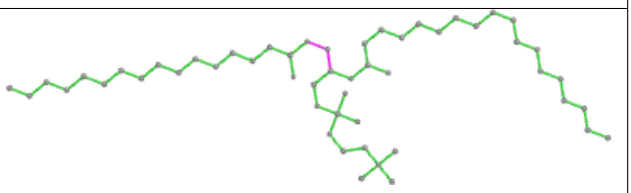


Rings

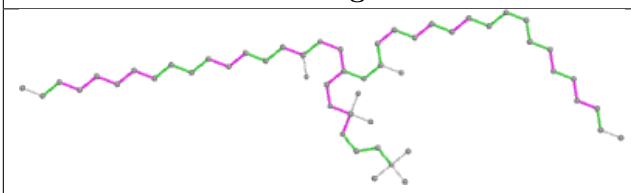
Ligand POV C 1303



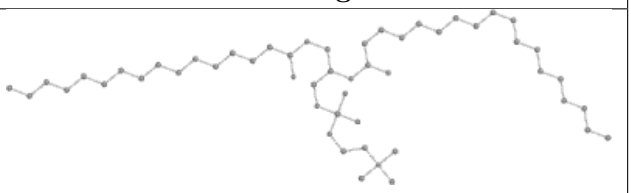
Bond lengths



Bond angles

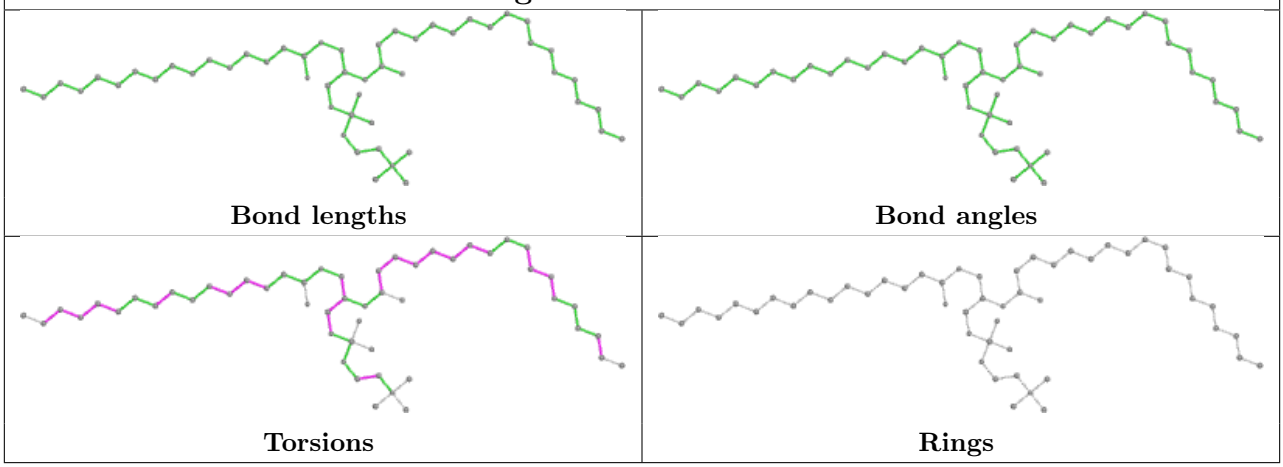


Torsions

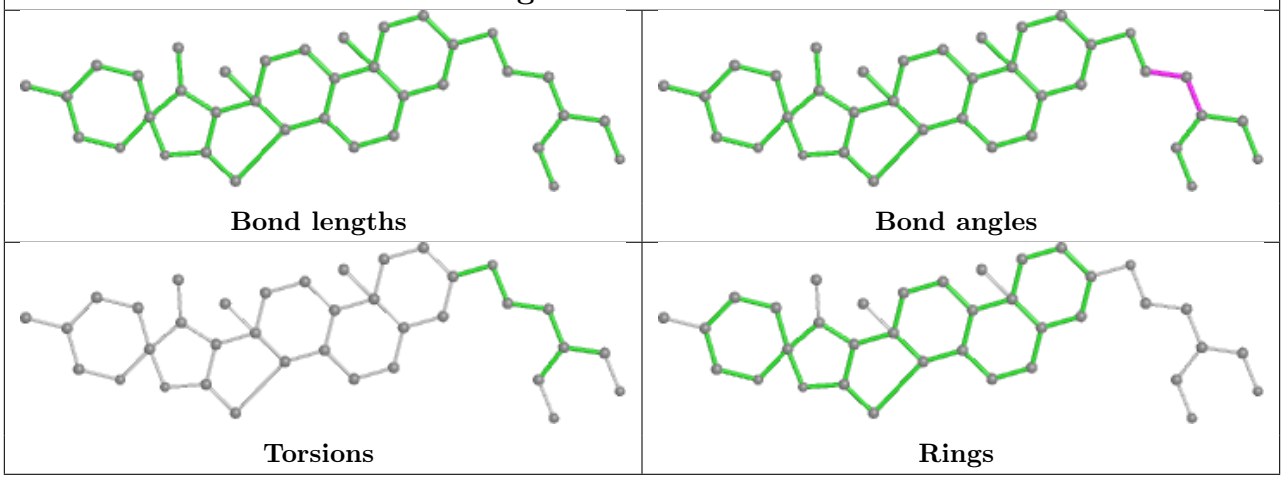


Rings

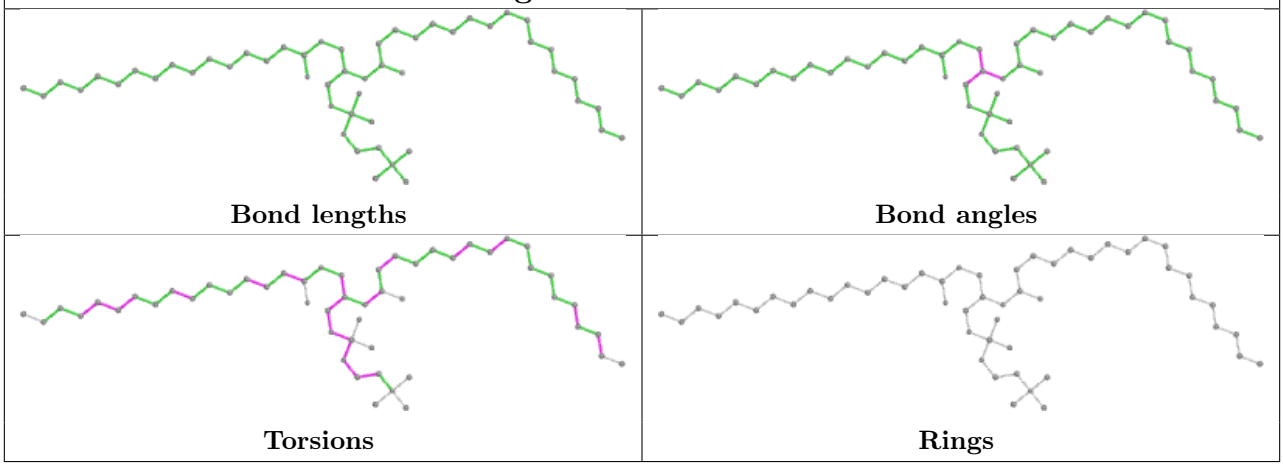
Ligand POV C 1309



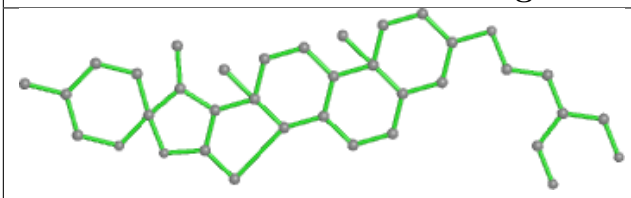
Ligand DU0 C 1315



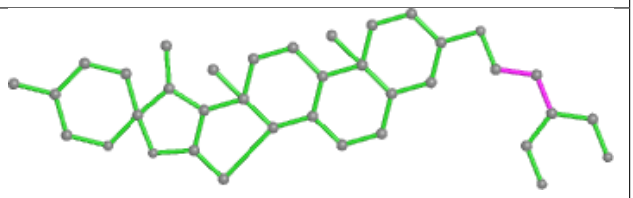
Ligand POV C 1312



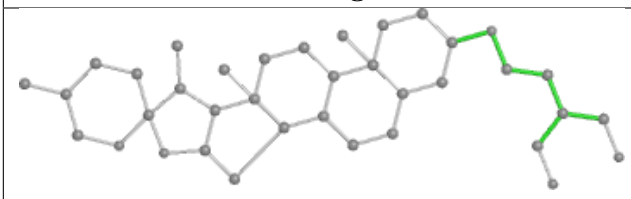
Ligand DU0 D 1302



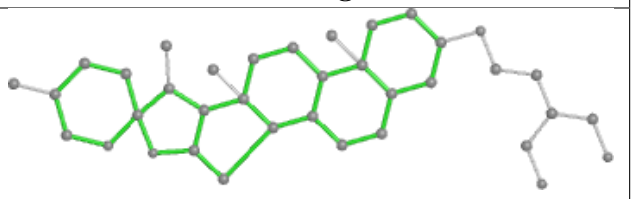
Bond lengths



Bond angles

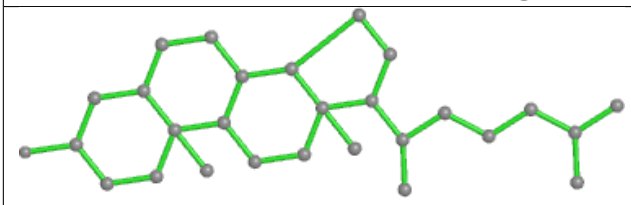


Torsions

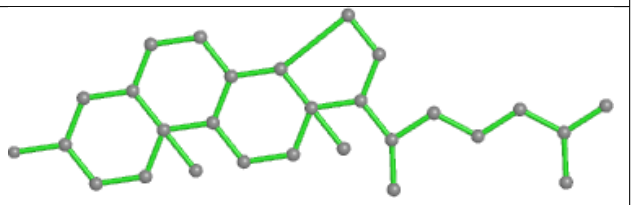


Rings

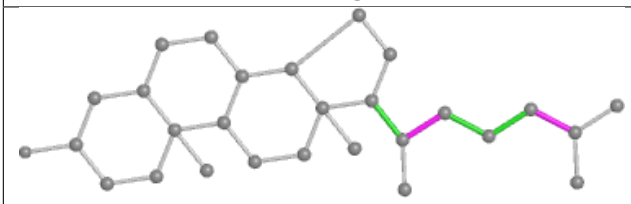
Ligand CLR C 1307



Bond lengths



Bond angles



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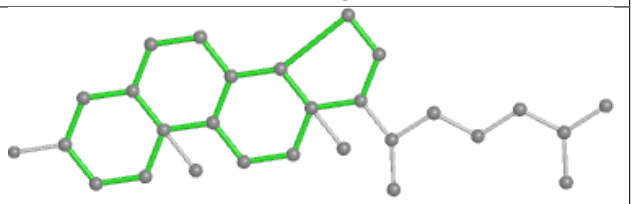
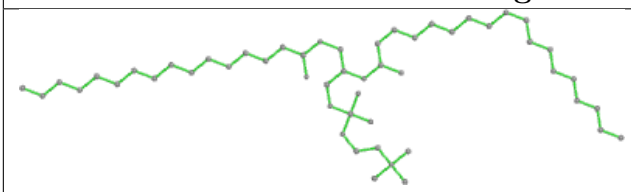


Rings

Ligand POV B 1306



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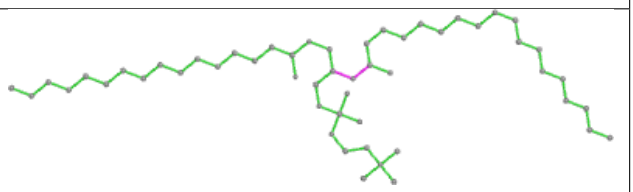
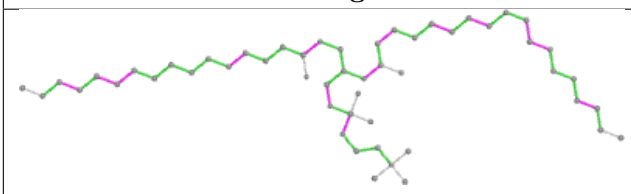


Bond angles



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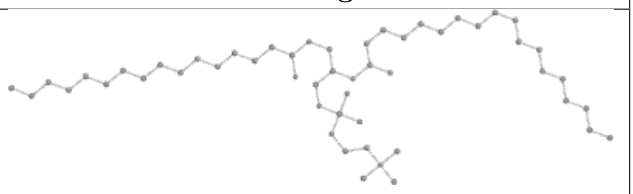
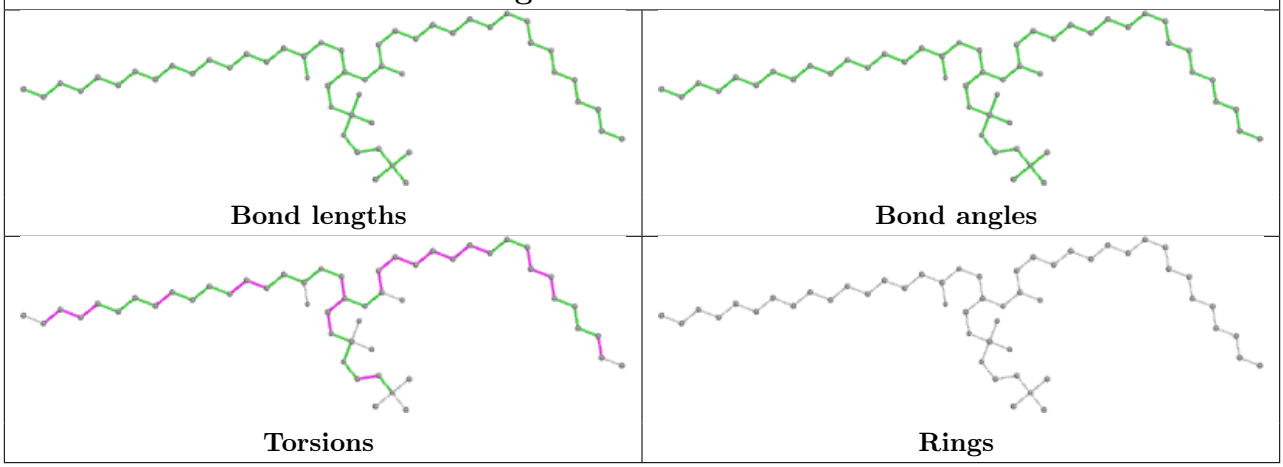
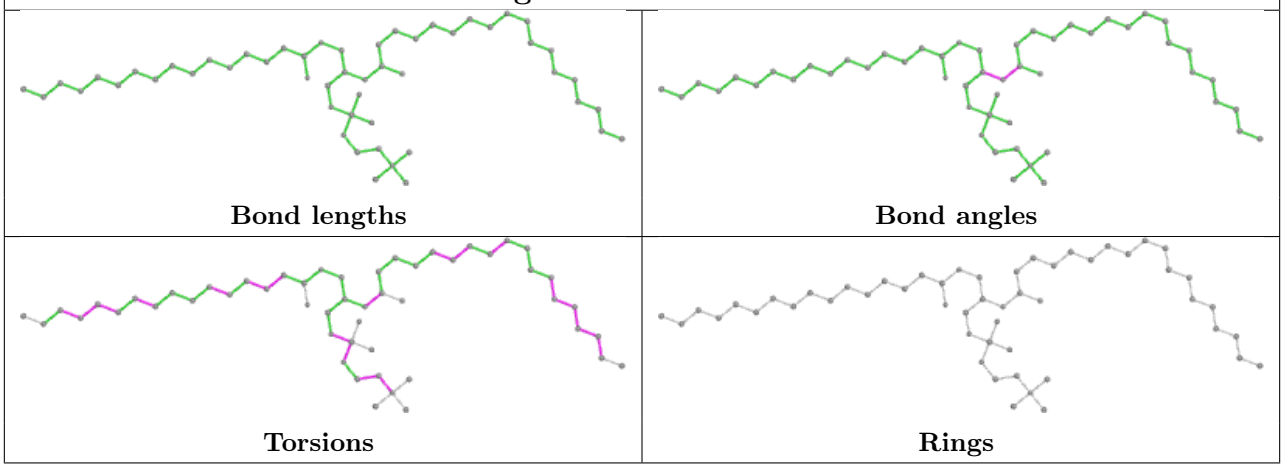


Rings

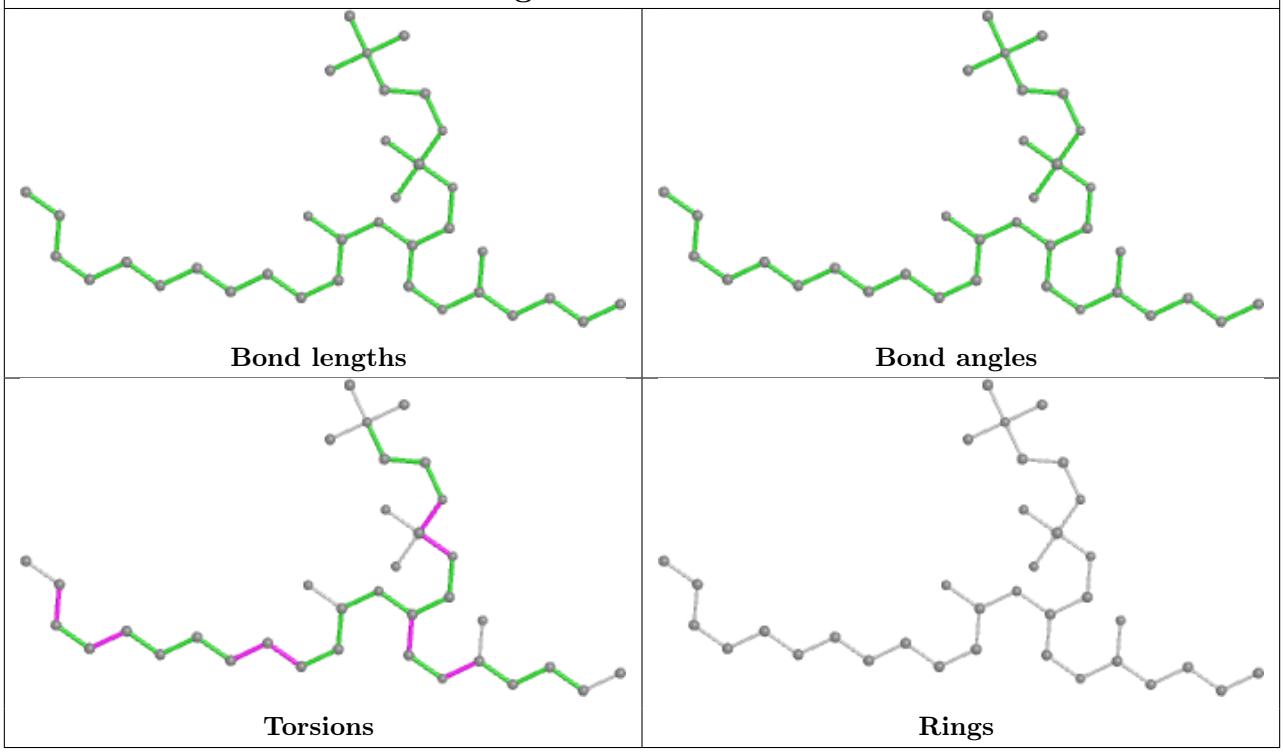
Ligand POV B 1309



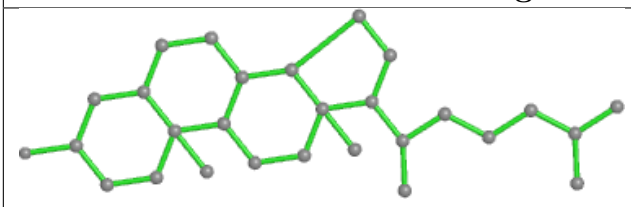
Ligand POV D 1306



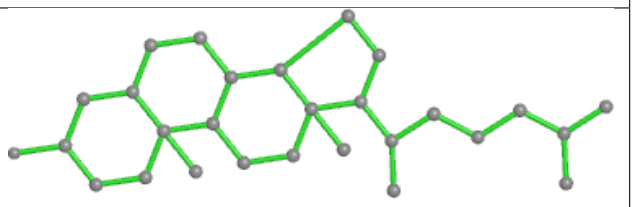
Ligand POV C 1305



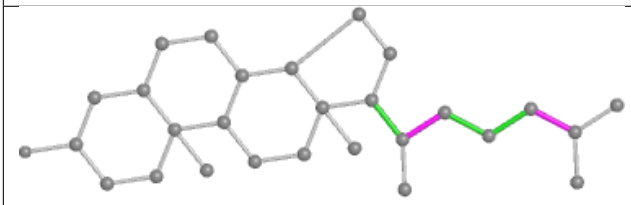
Ligand CLR A 1304



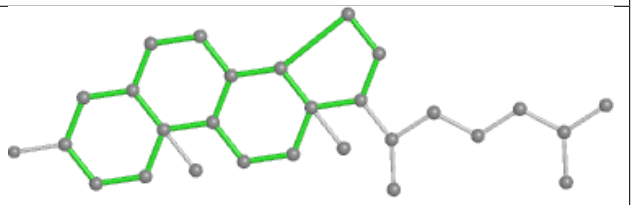
Bond lengths



Bond angles

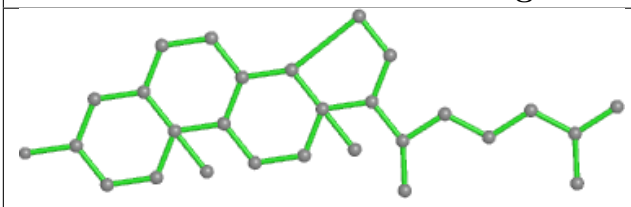


Torsions



Rings

Ligand CLR B 1307



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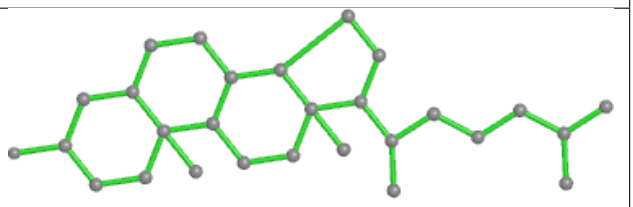
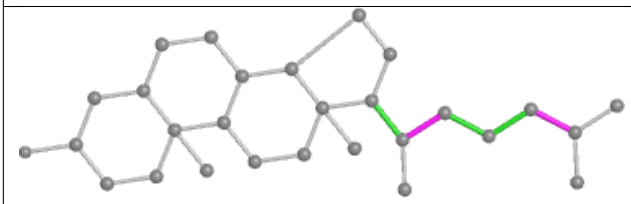
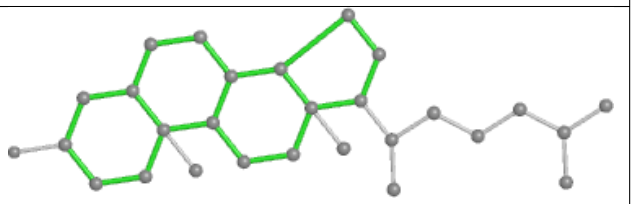


Bond angles

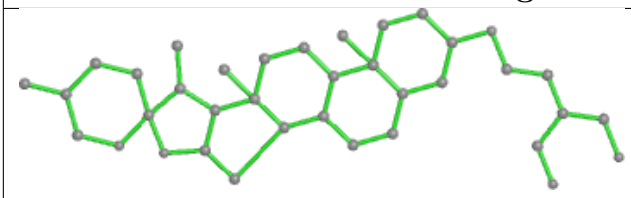


Torsions



Rings

Ligand DU0 B 1317



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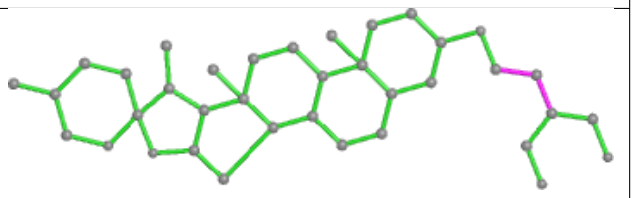
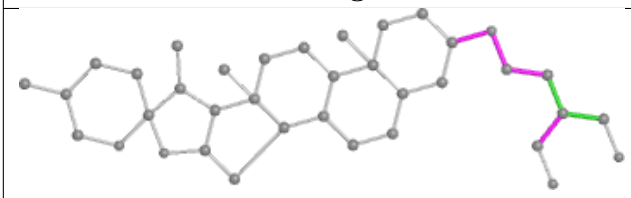


Bond angles



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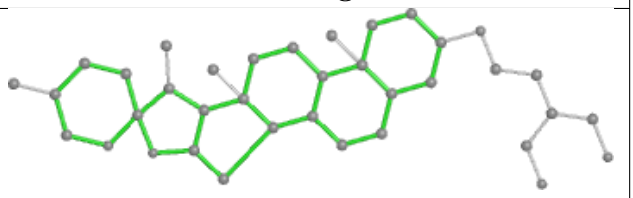
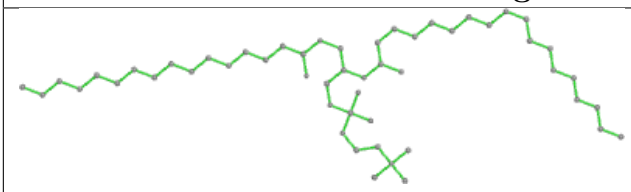
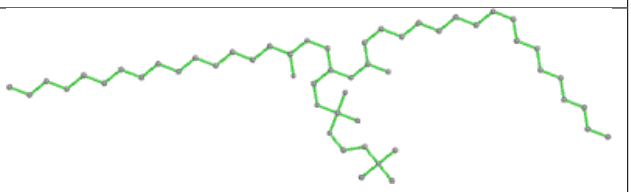
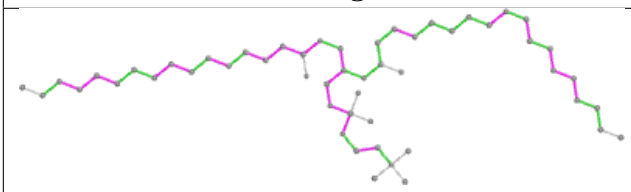
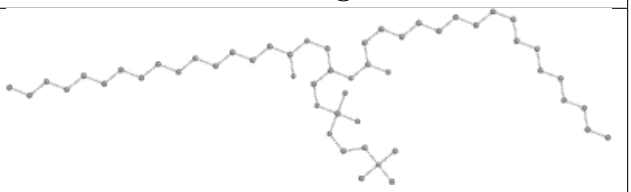
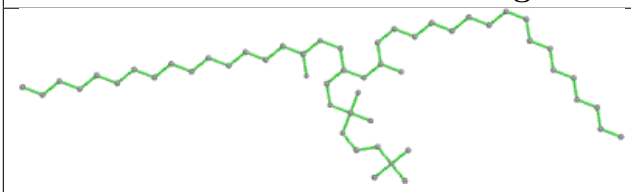
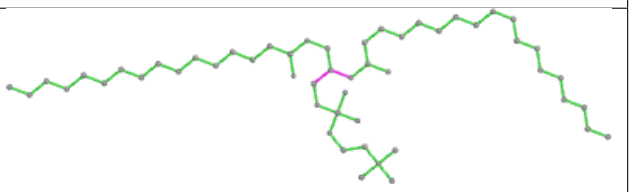
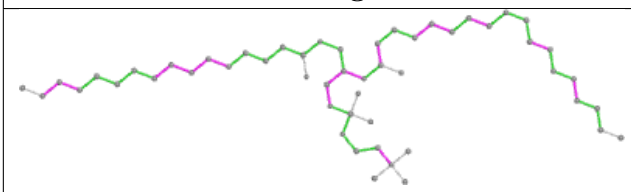
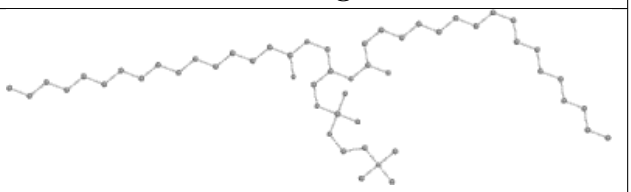
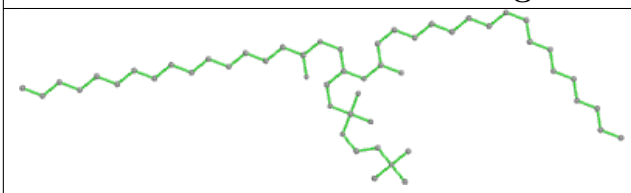
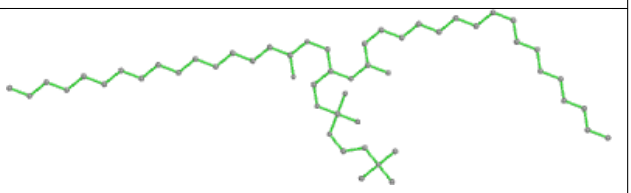
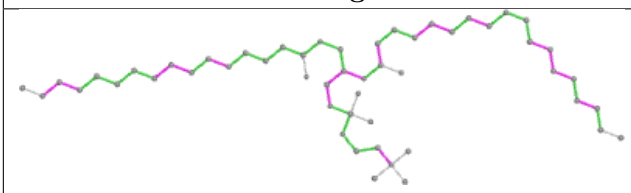
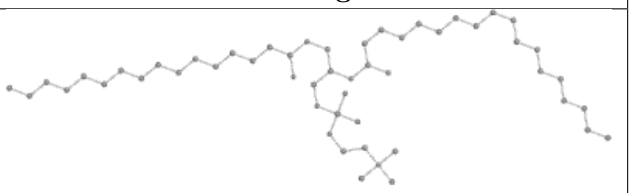
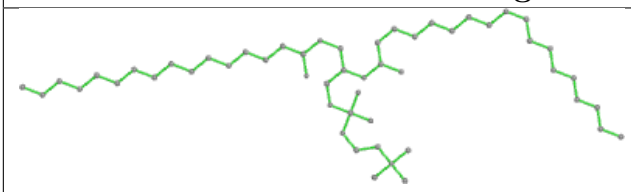
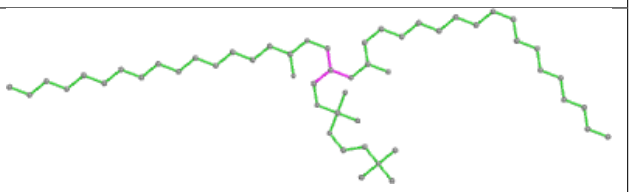
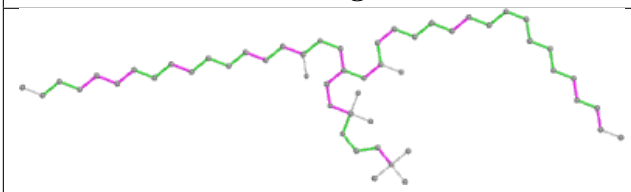
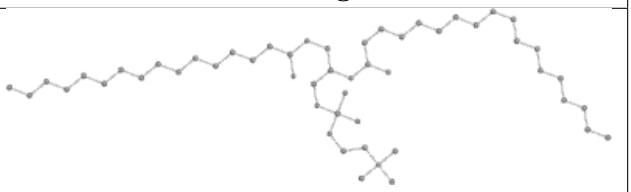


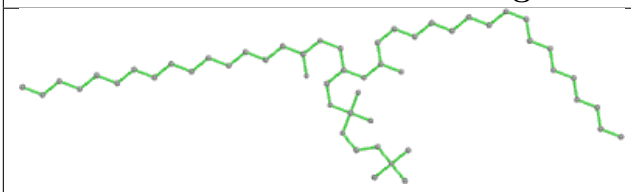
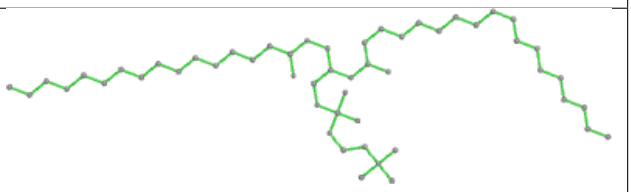
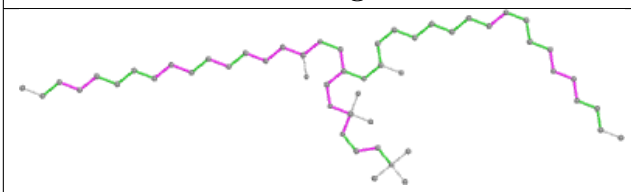
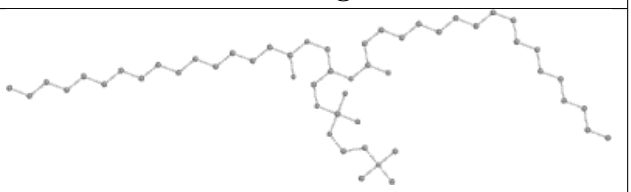
Rings

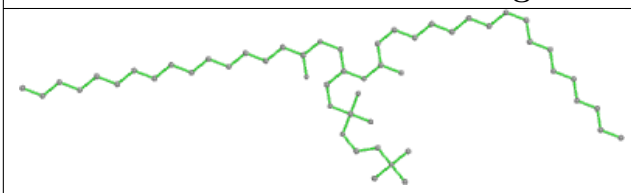
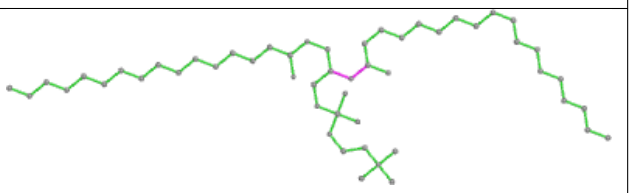
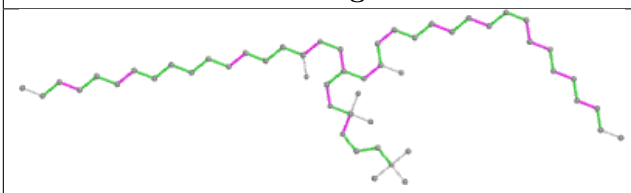
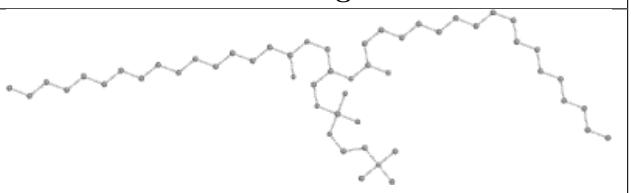
Ligand POV A 1307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV A 1305	
 Bond lengths	 Bond angles
 Torsions	 Rings

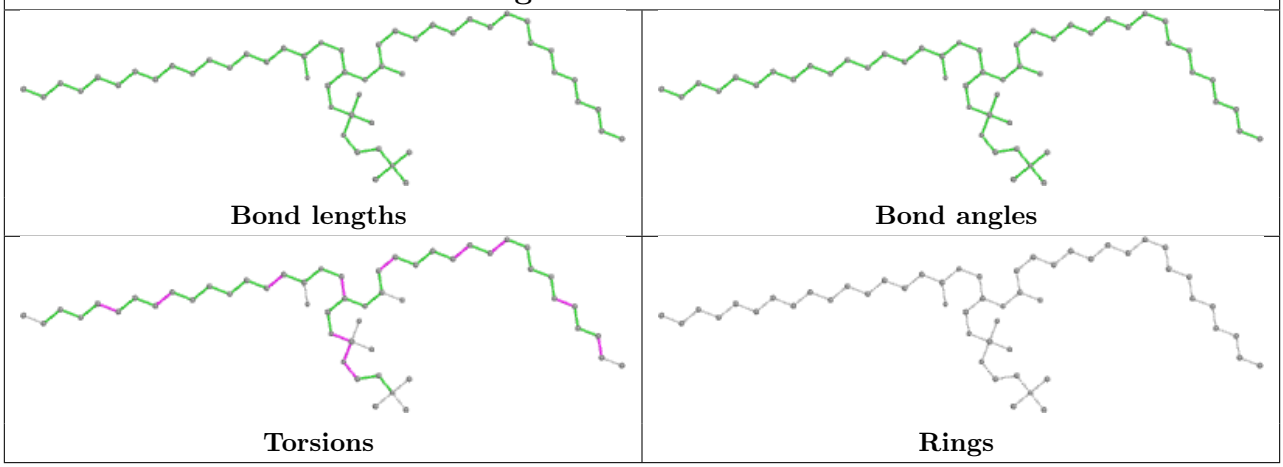
Ligand POV B 1308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV B 1312	
 Bond lengths	 Bond angles
 Torsions	 Rings

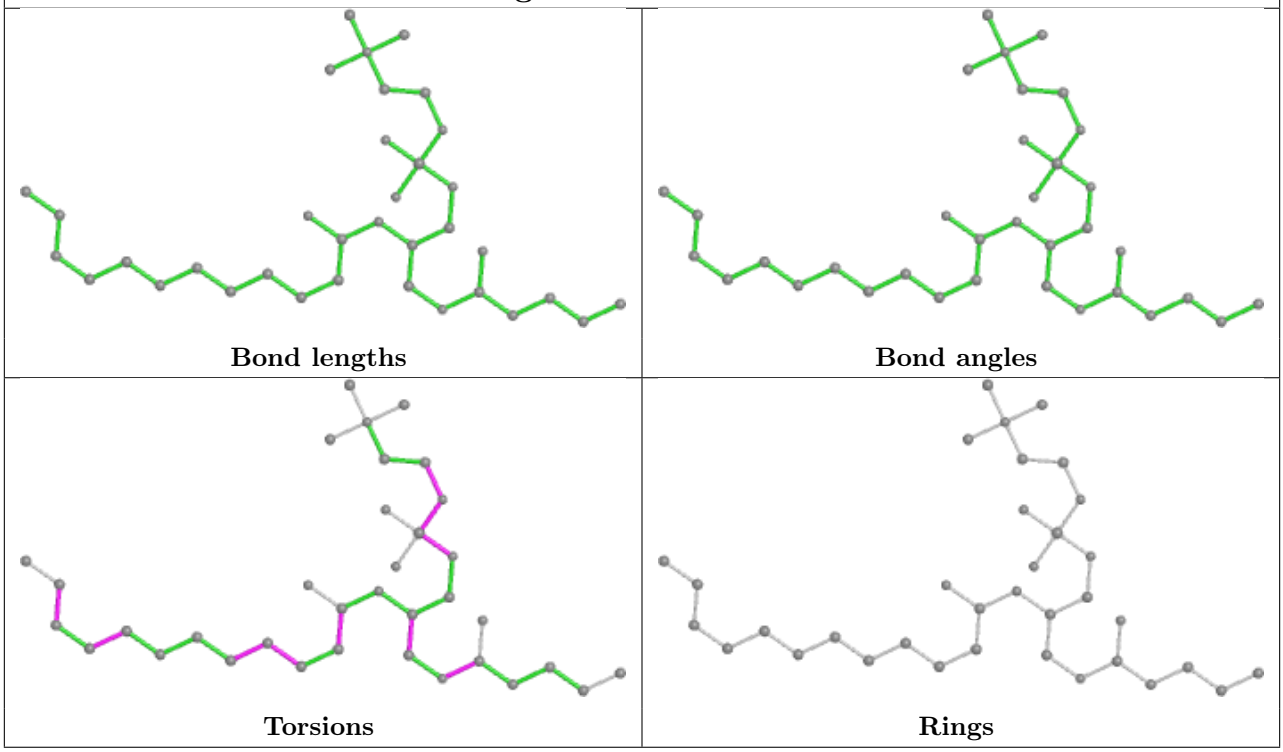
Ligand POV D 1312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV D 1308	
 Bond lengths	 Bond angles
 Torsions	 Rings

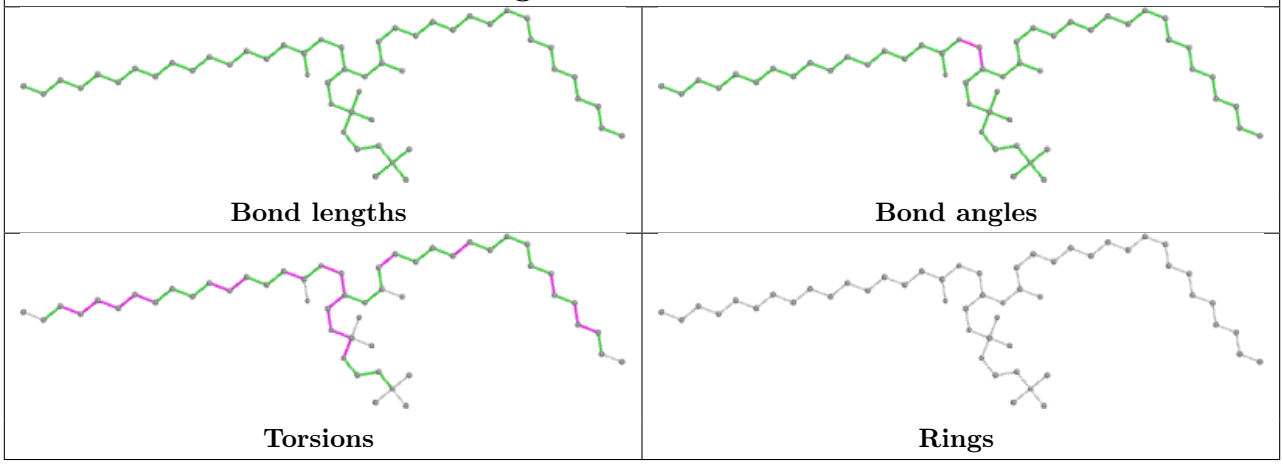
Ligand POV C 1313

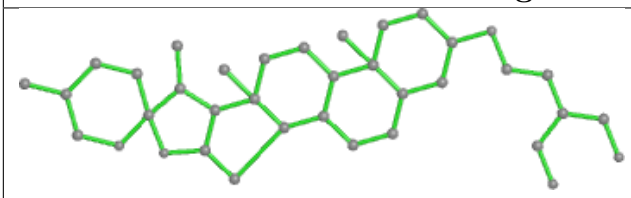
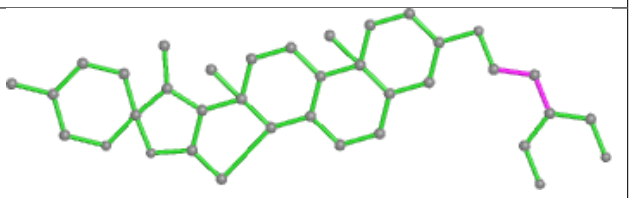
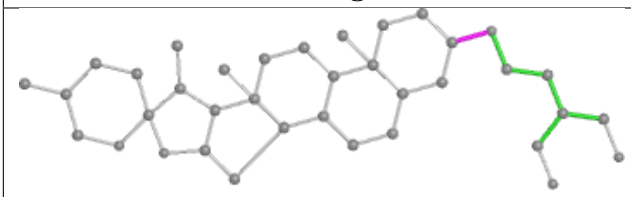
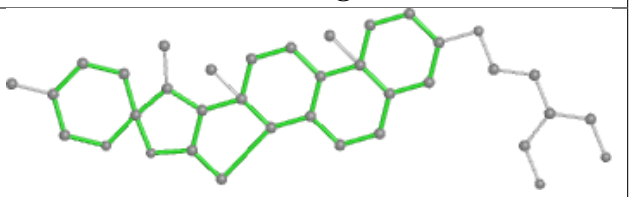


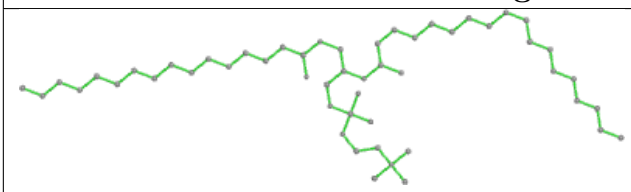
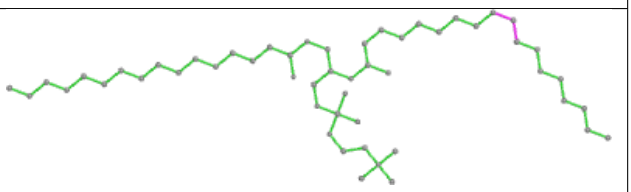
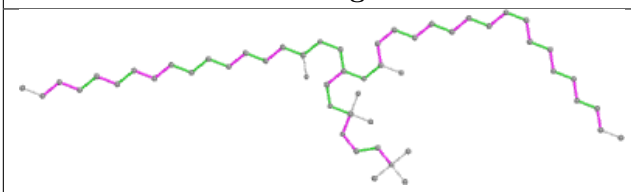
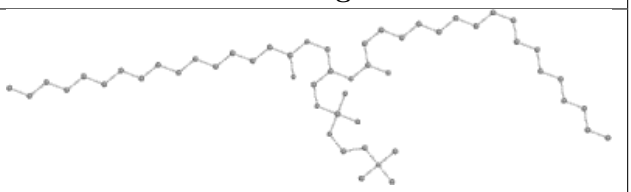
Ligand POV B 1305

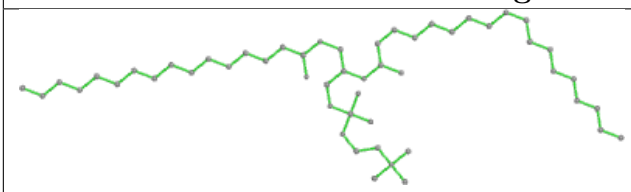
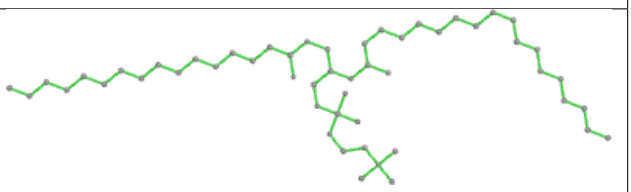
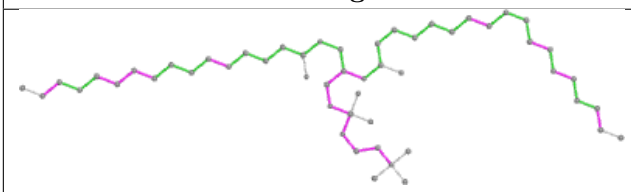
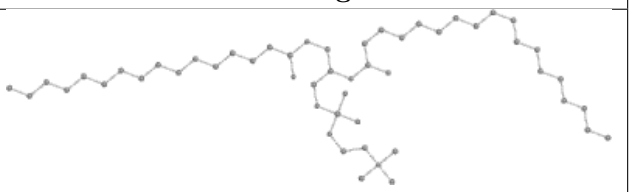


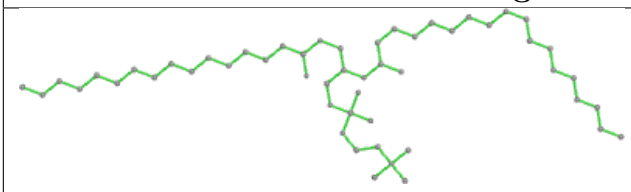
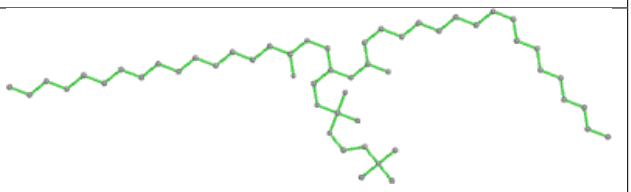
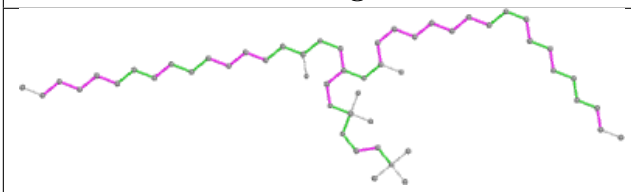
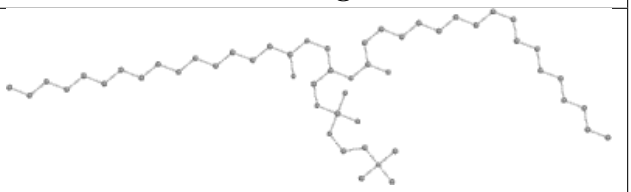
Ligand POV D 1305



Ligand DU0 A 1313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV C 1314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV C 1302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV A 1306	
 Bond lengths	 Bond angles
 Torsions	 Rings

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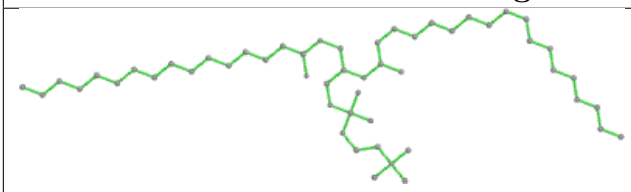
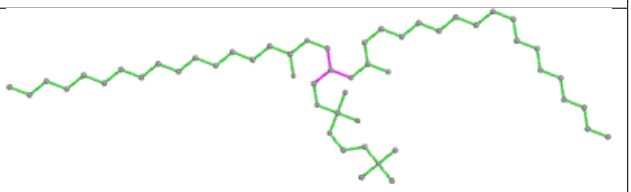
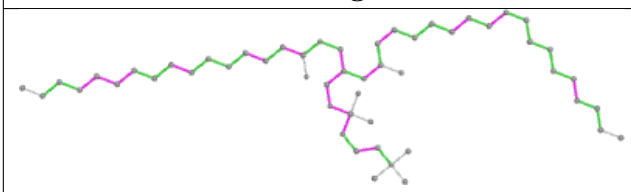
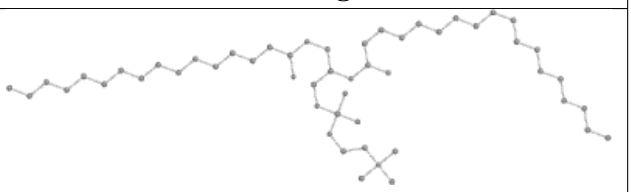
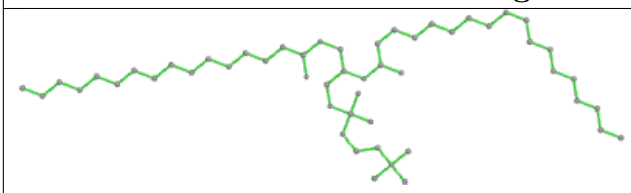
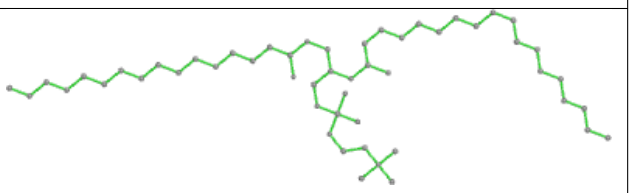
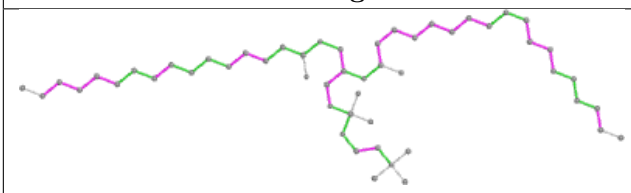
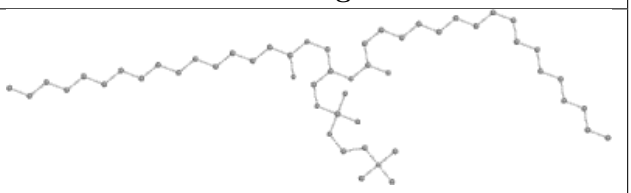
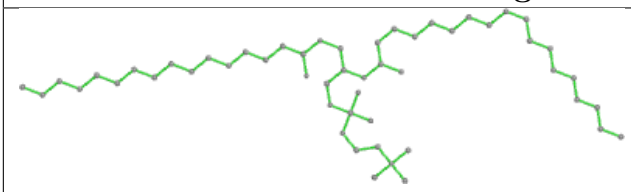
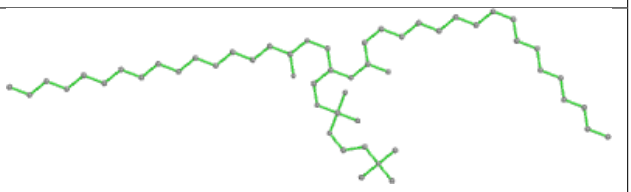
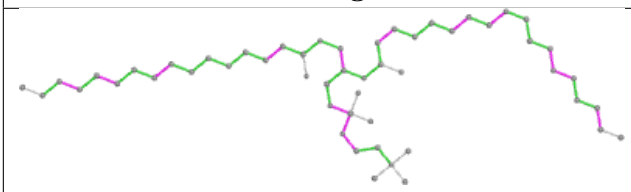
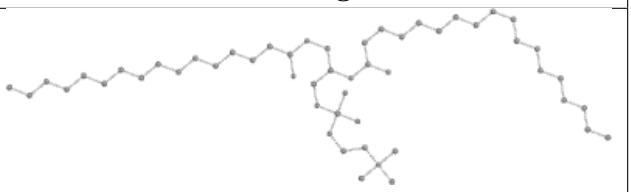
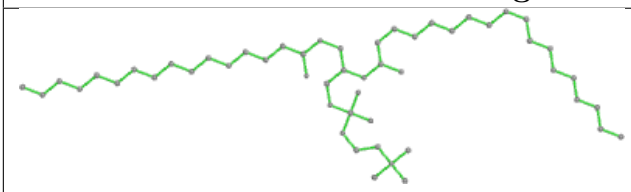
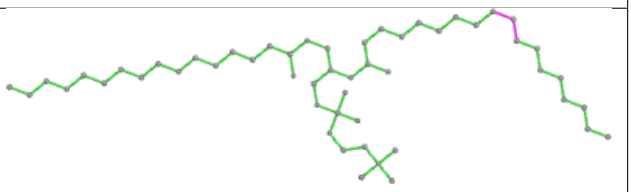
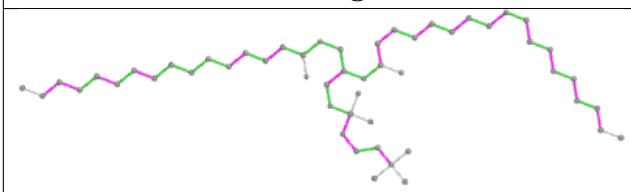
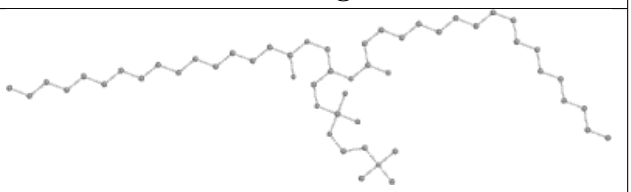
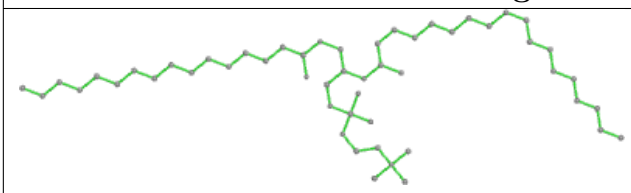
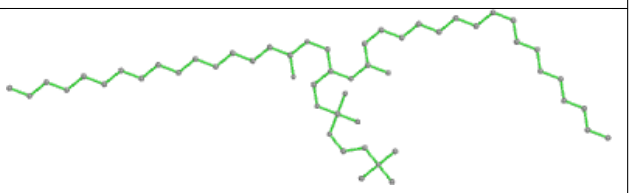
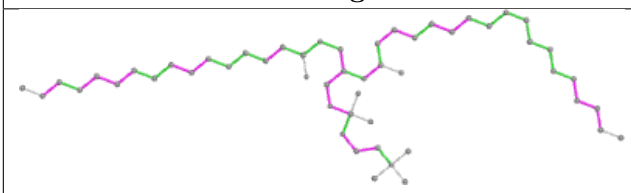
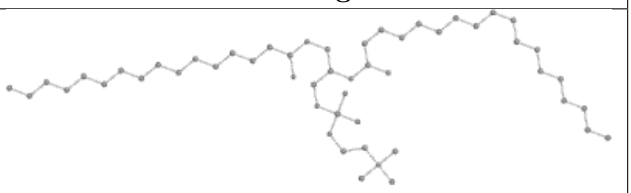
 Bond lengths	 Bond angles
 Torsions	 Rings

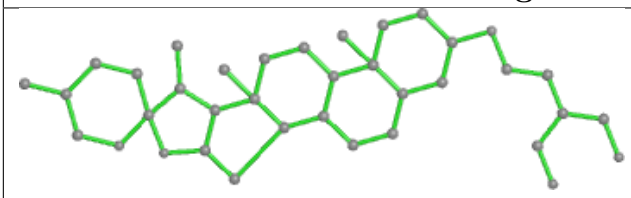
Ligand POV D 1311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV B 1313	
 Bond lengths	 Bond angles
 Torsions	 Rings

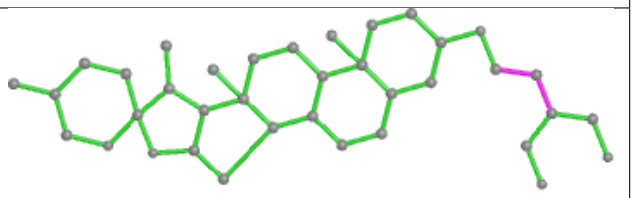
Ligand POV D 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV D 1313	
 Bond lengths	 Bond angles
 Torsions	 Rings

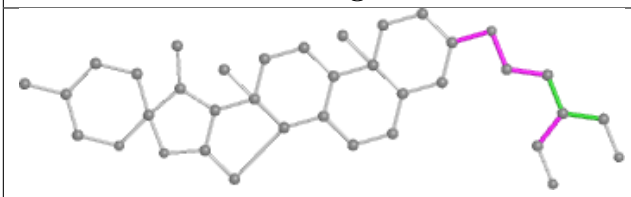
Ligand DU0 D 1316



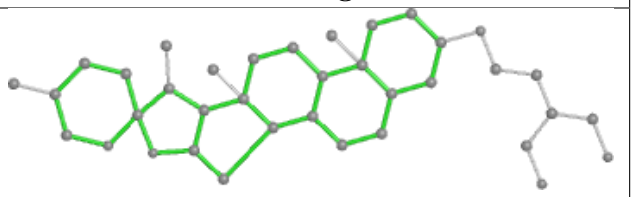
Bond lengths



Bond angles

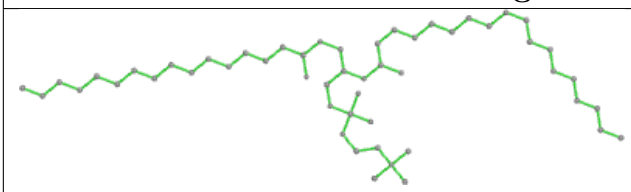


Torsions

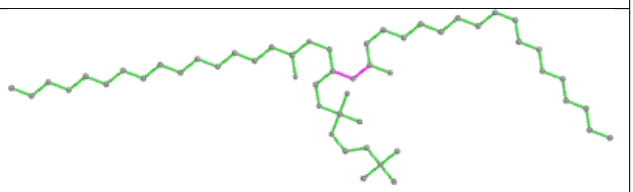


Rings

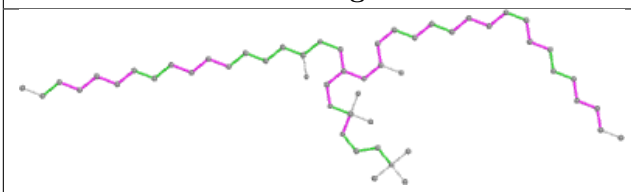
Ligand POV C 1301



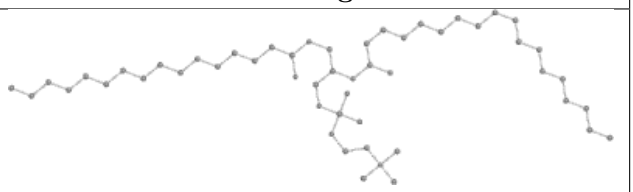
Bond lengths



Bond angles

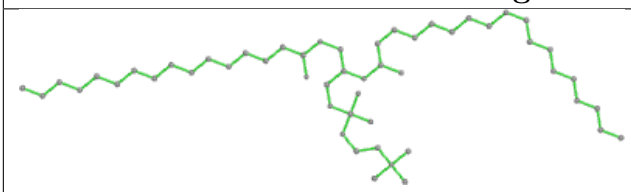


Torsions

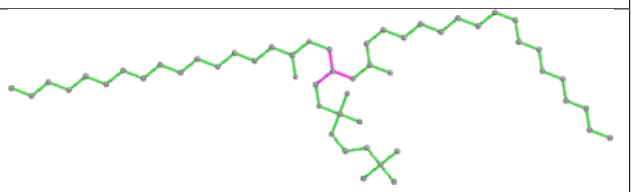


Rings

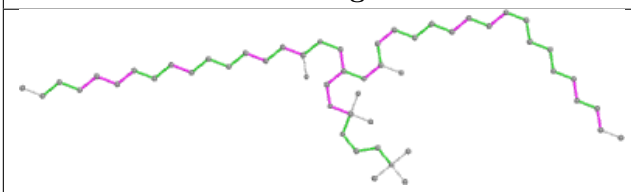
Ligand POV D 1314



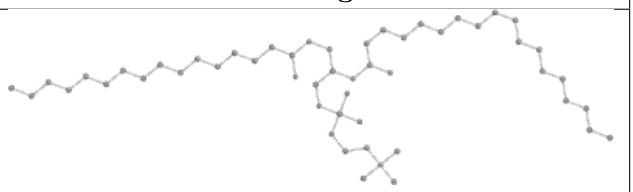
Bond lengths



Bond angles

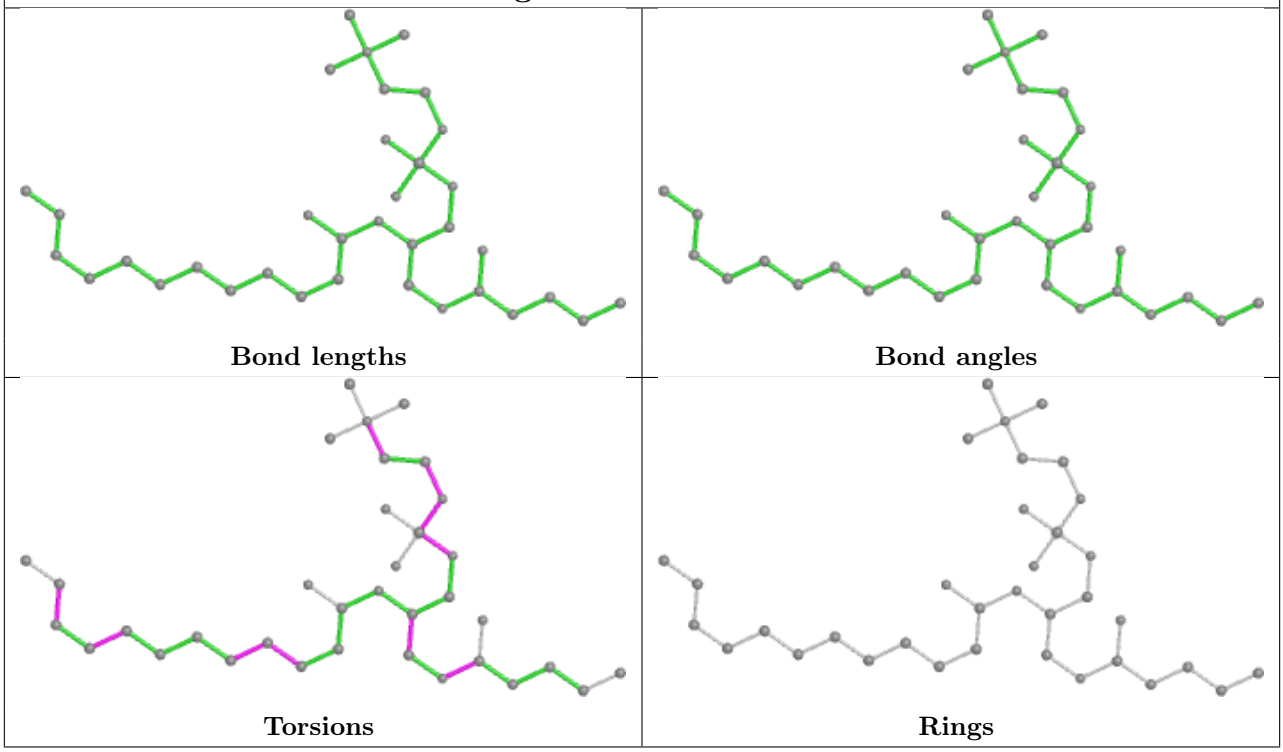


Torsions

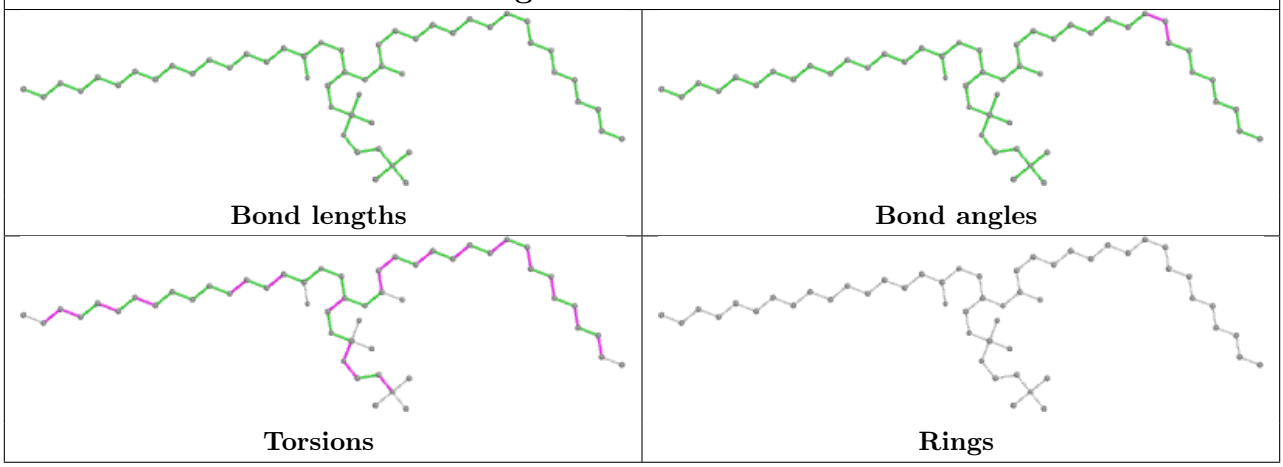


Rings

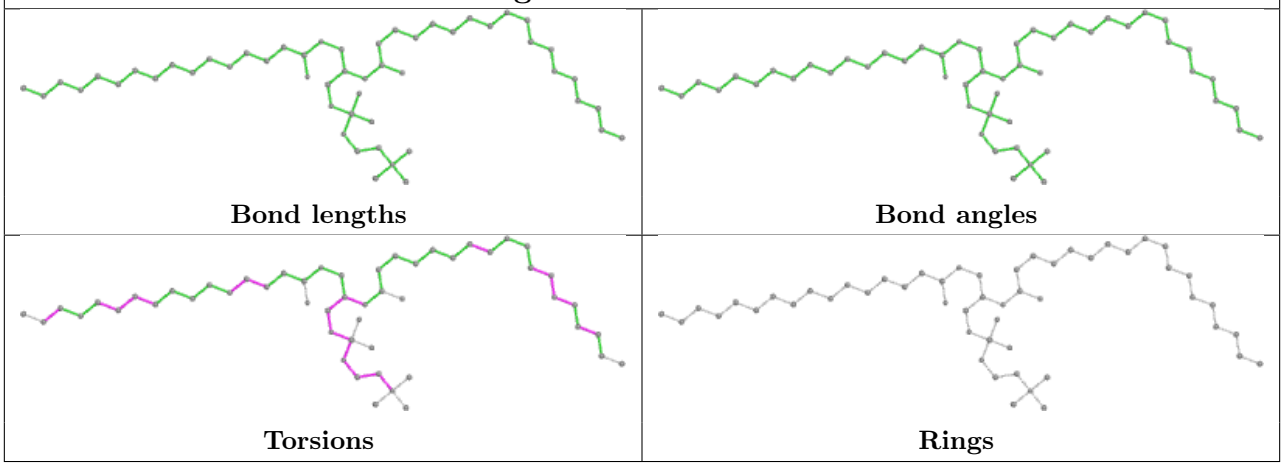
Ligand POV A 1302



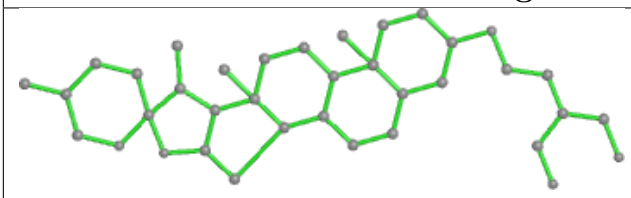
Ligand POV B 1315



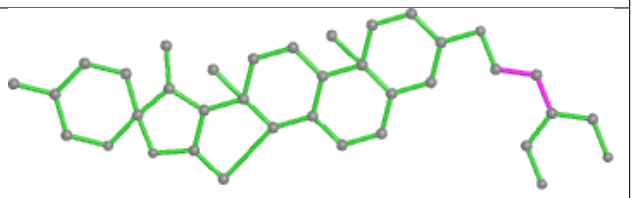
Ligand POV D 1304



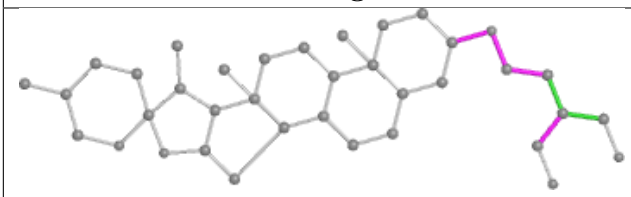
Ligand DU0 A 1311



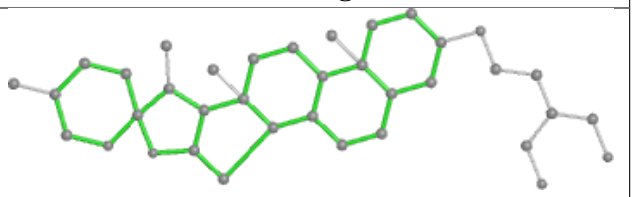
Bond lengths



Bond angles

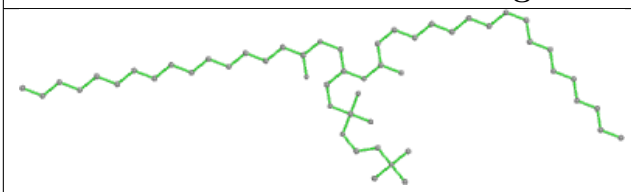


Torsions

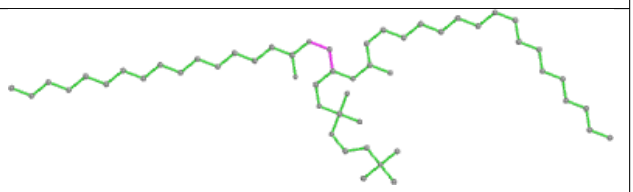


Rings

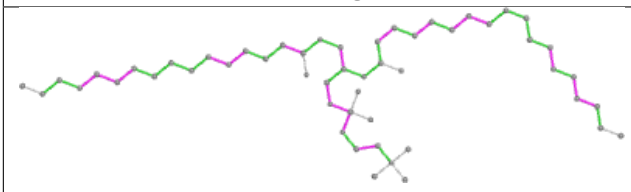
Ligand POV A 1316



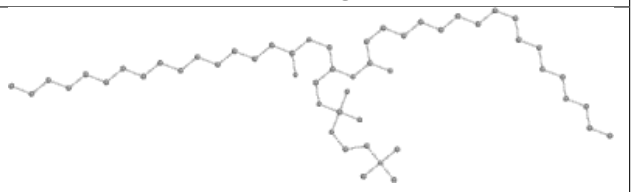
Bond lengths



Bond angles

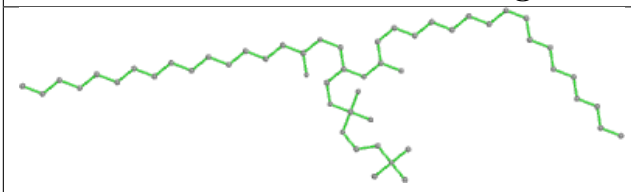


Torsions

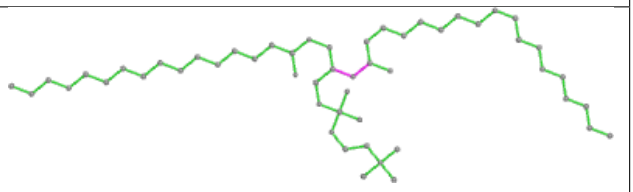


Rings

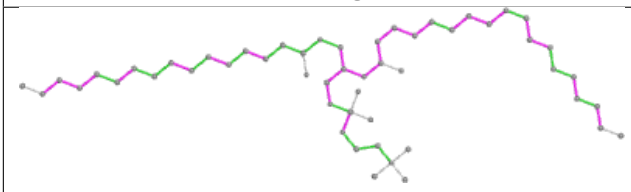
Ligand POV B 1301



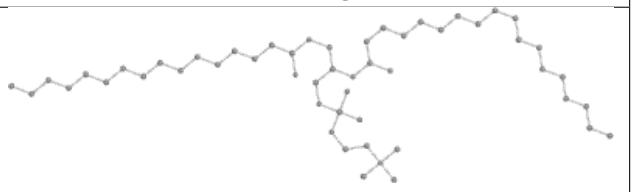
Bond lengths



Bond angles

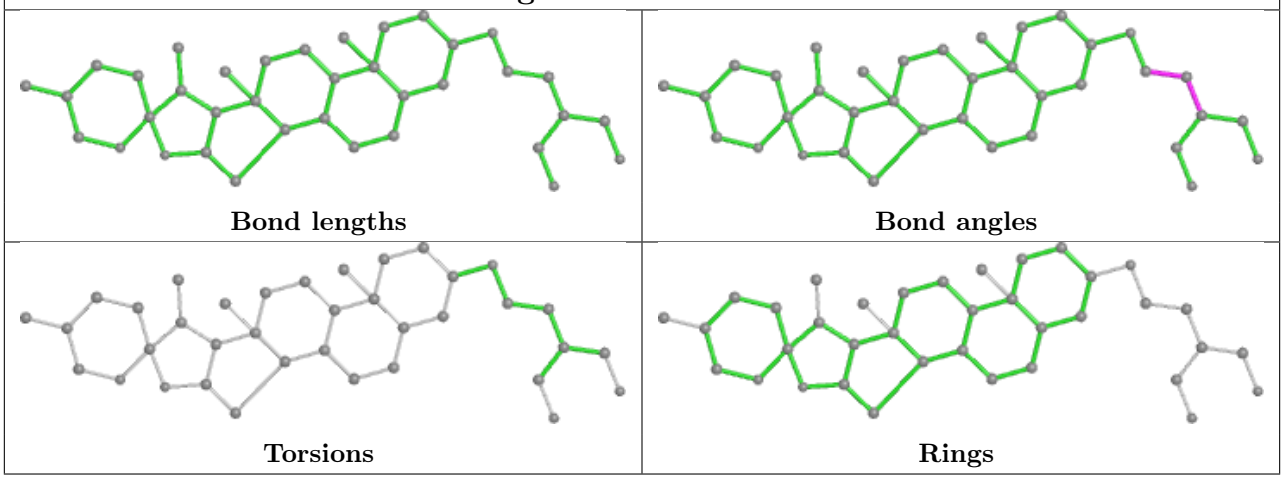


Torsions

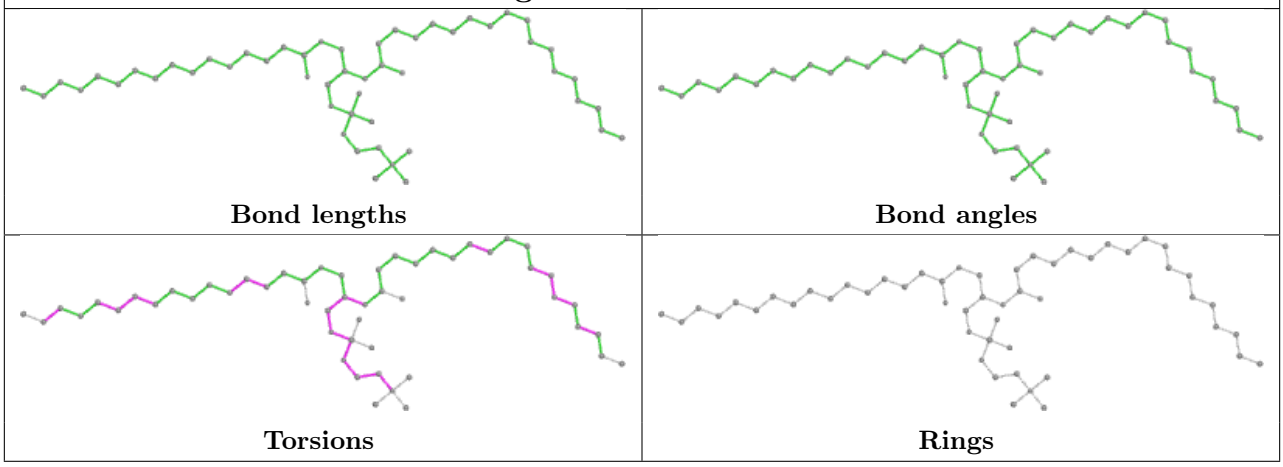


Rings

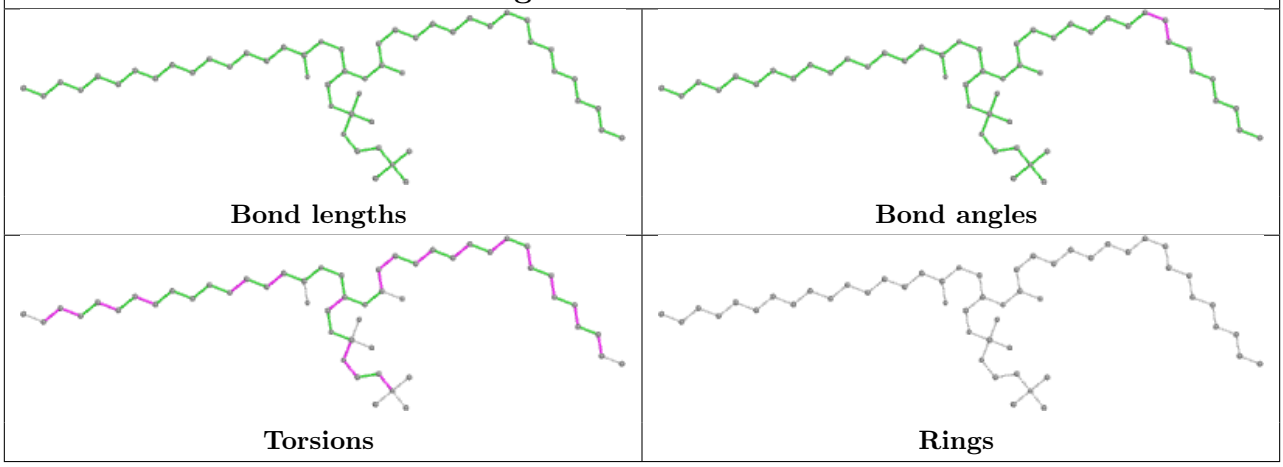
Ligand DU0 B 1316



Ligand POV B 1302



Ligand POV A 1312



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

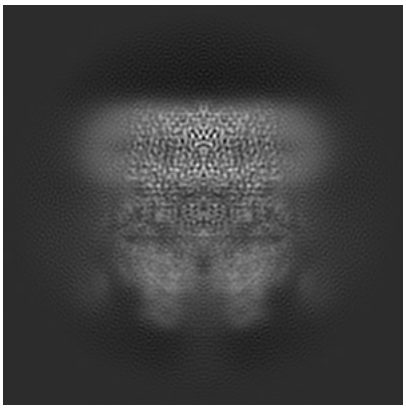
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-40498. These allow visual inspection of the internal detail of the map and identification of artifacts.

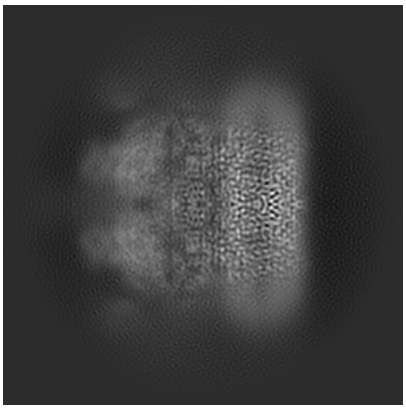
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

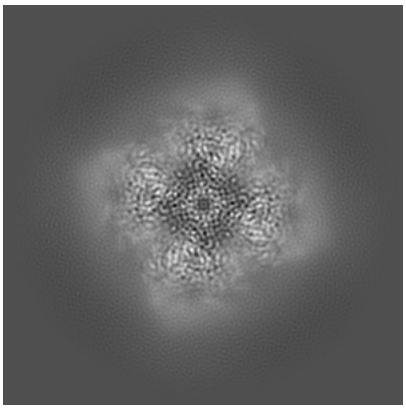
6.1.1 Primary map



X

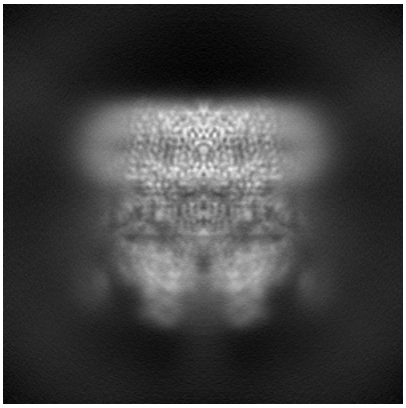


Y

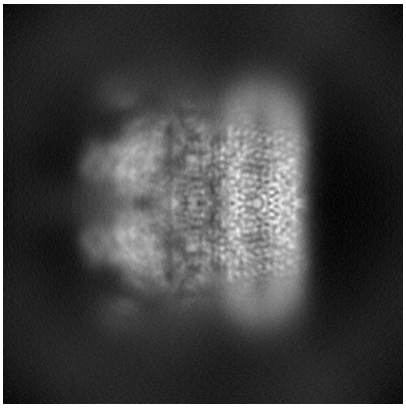


Z

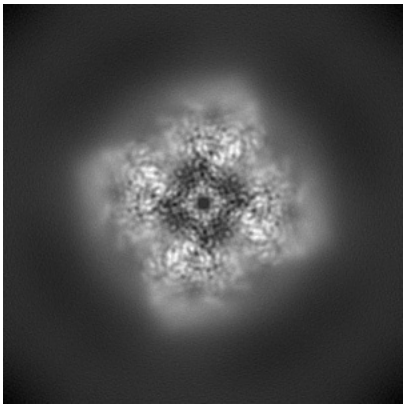
6.1.2 Raw map



X



Y

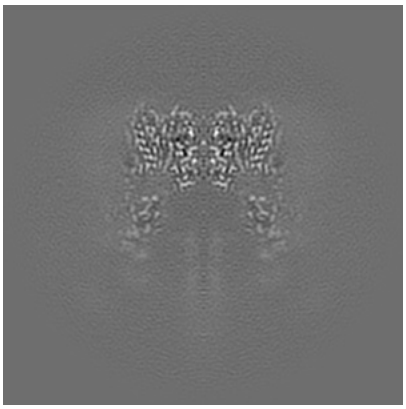


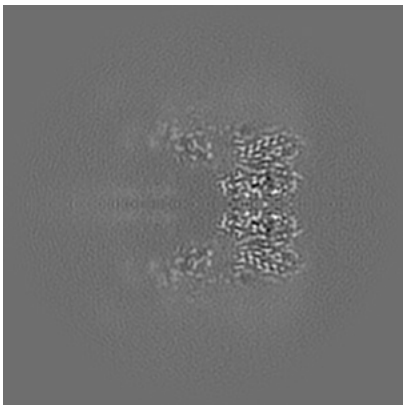
Z

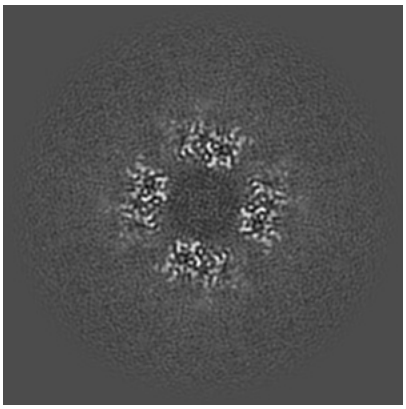
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

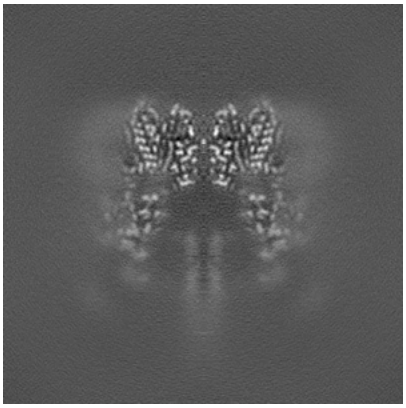
6.2.1 Primary map

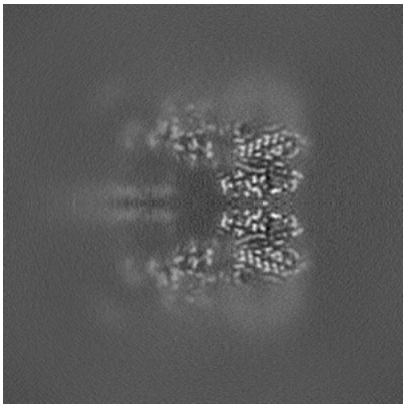

X Index: 150

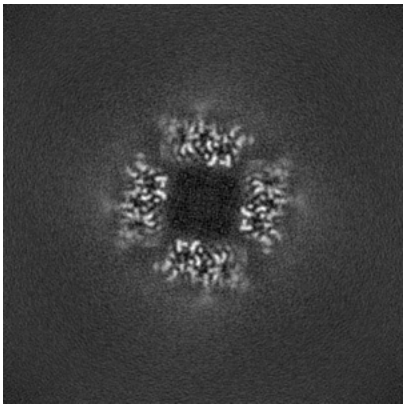

Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150

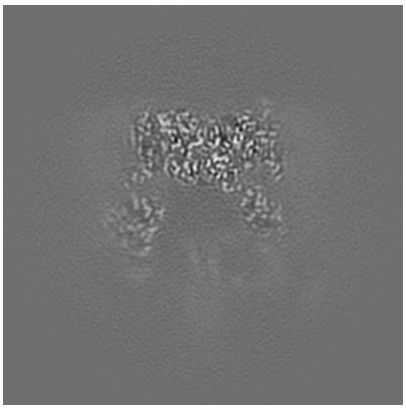

Y Index: 150

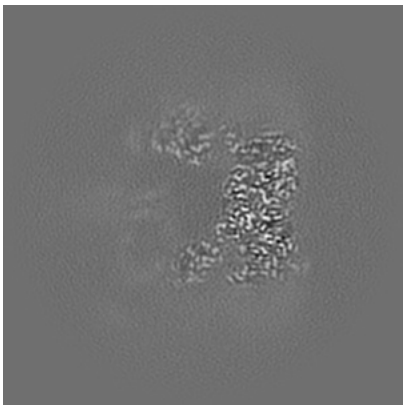

Z Index: 150

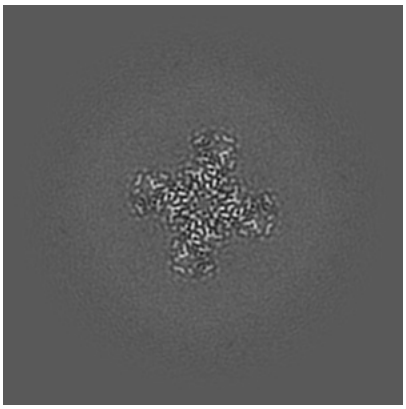
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

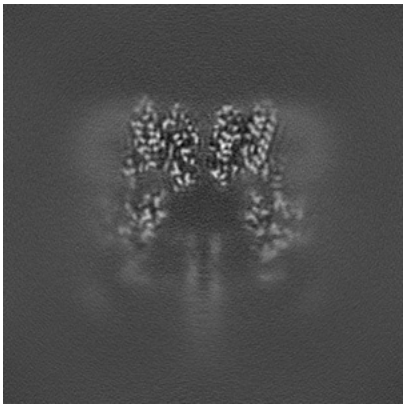
6.3.1 Primary map

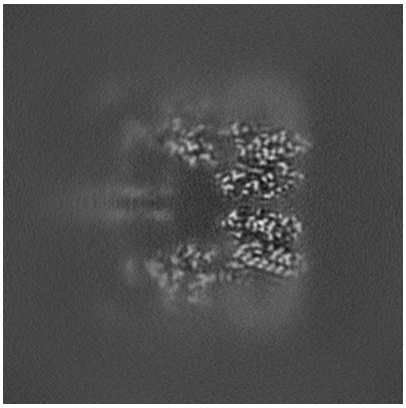

X Index: 155

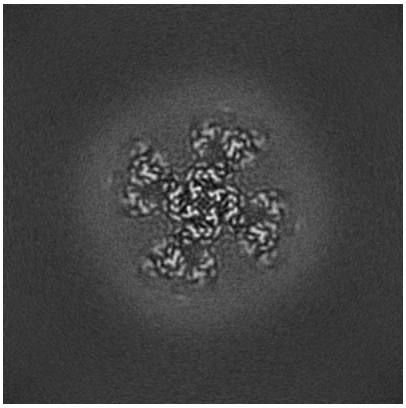

Y Index: 155


Z Index: 200

6.3.2 Raw map


X Index: 148

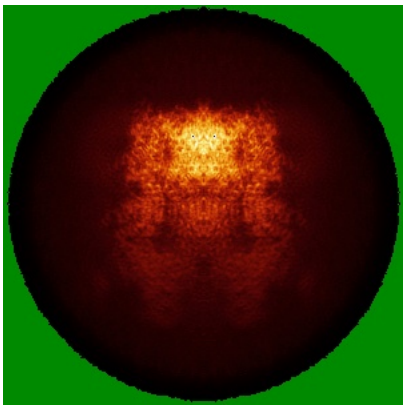

Y Index: 148

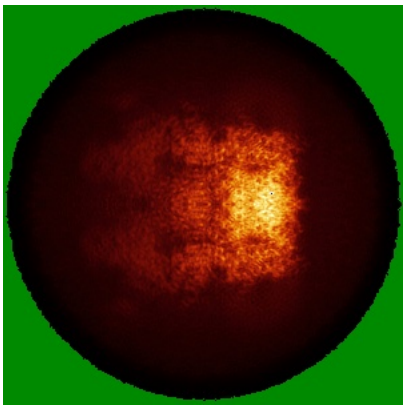

Z Index: 175

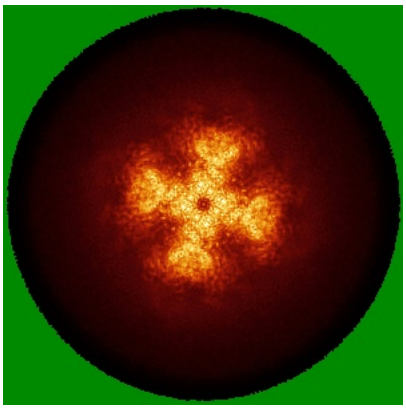
The images above show the largest variance slices of the map in three orthogonal directions.

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

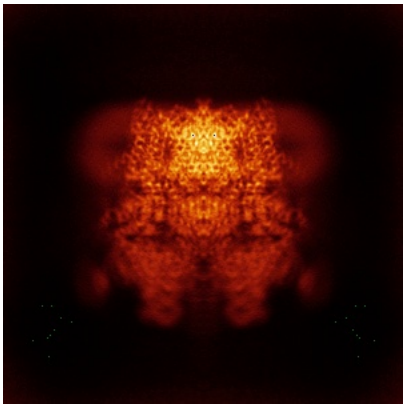
6.4.1 Primary map

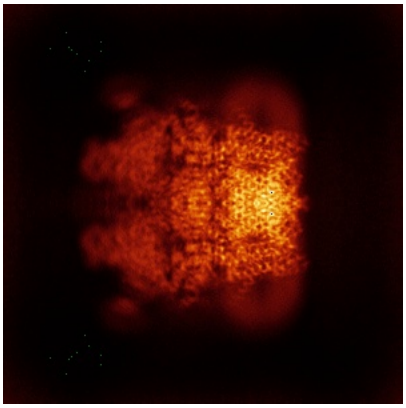

X

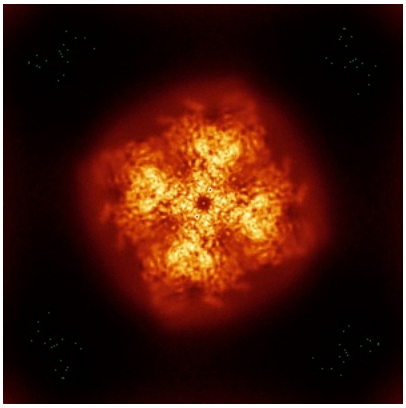

Y


Z

6.4.2 Raw 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.

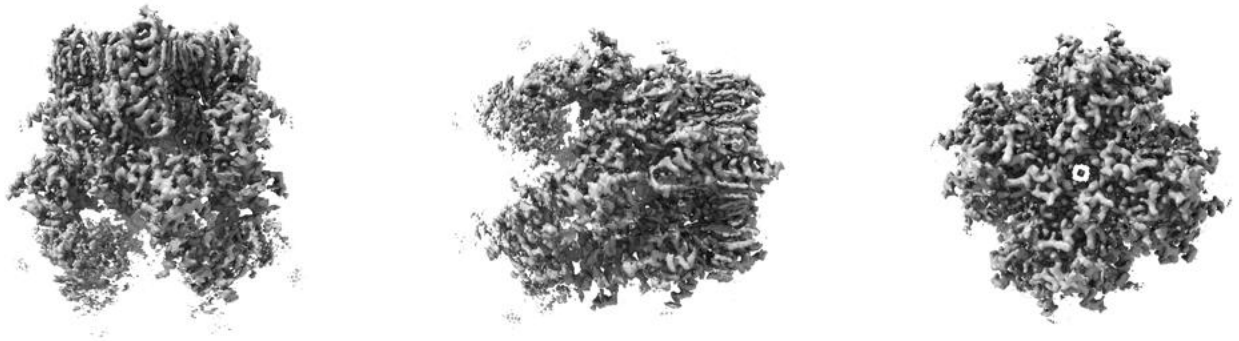
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.218. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

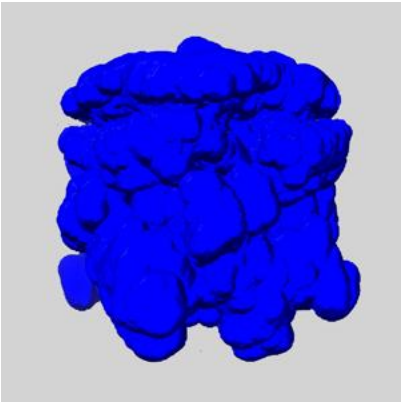
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

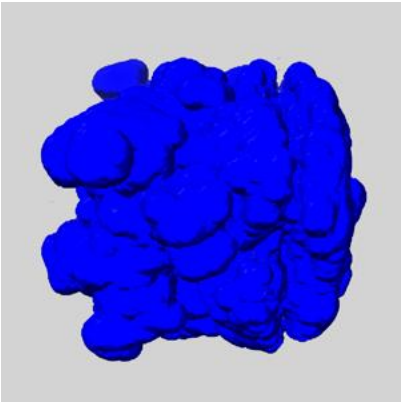
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

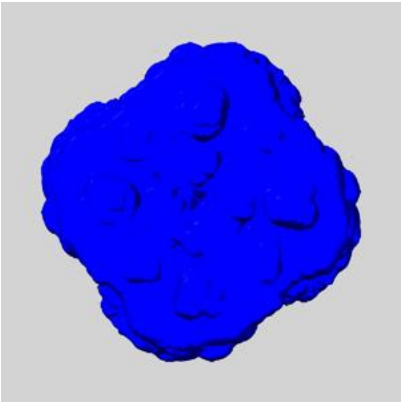
6.6.1 emd_40498_msk_1.map (i)



X



Y

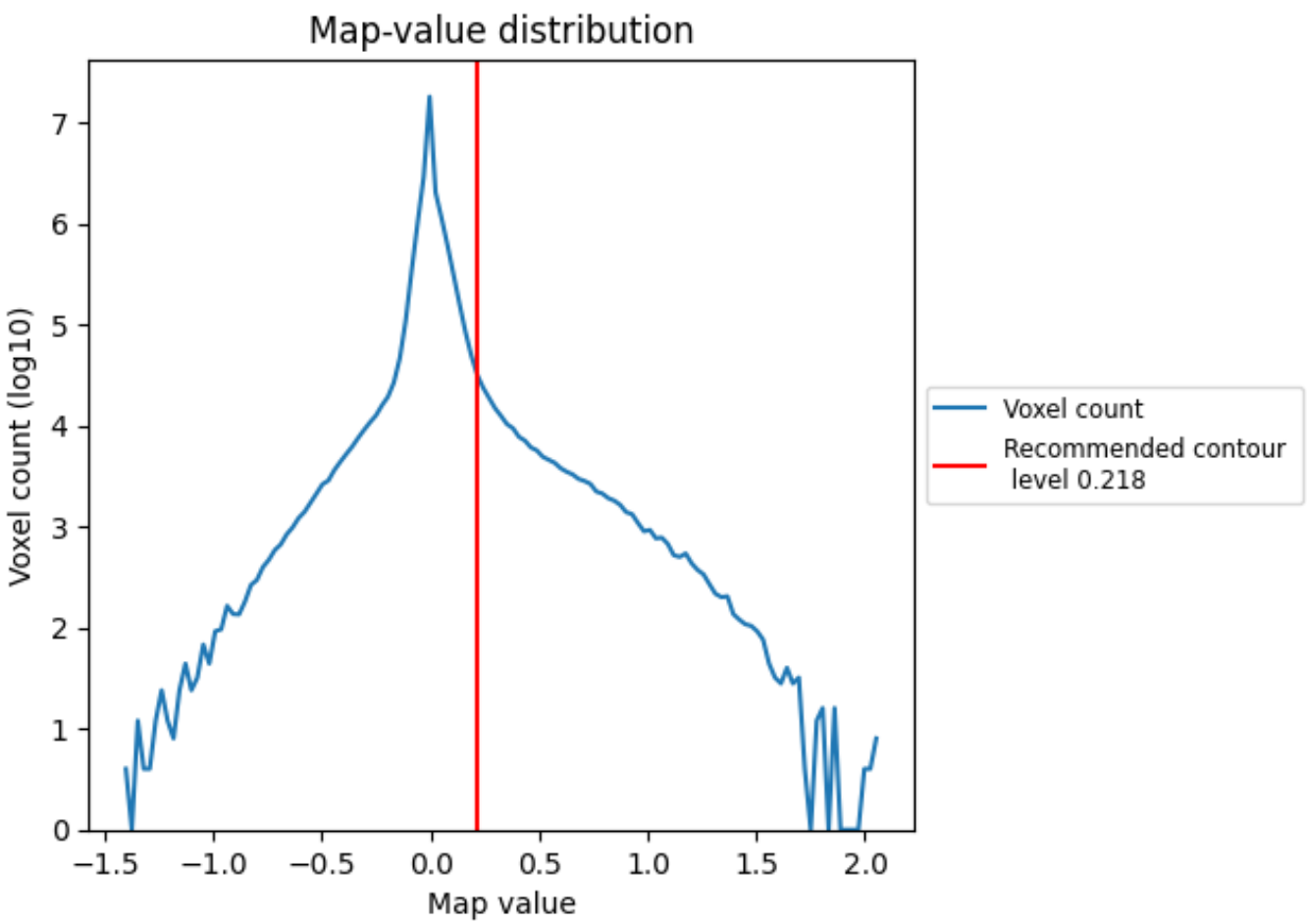


Z

7 Map analysis (i)

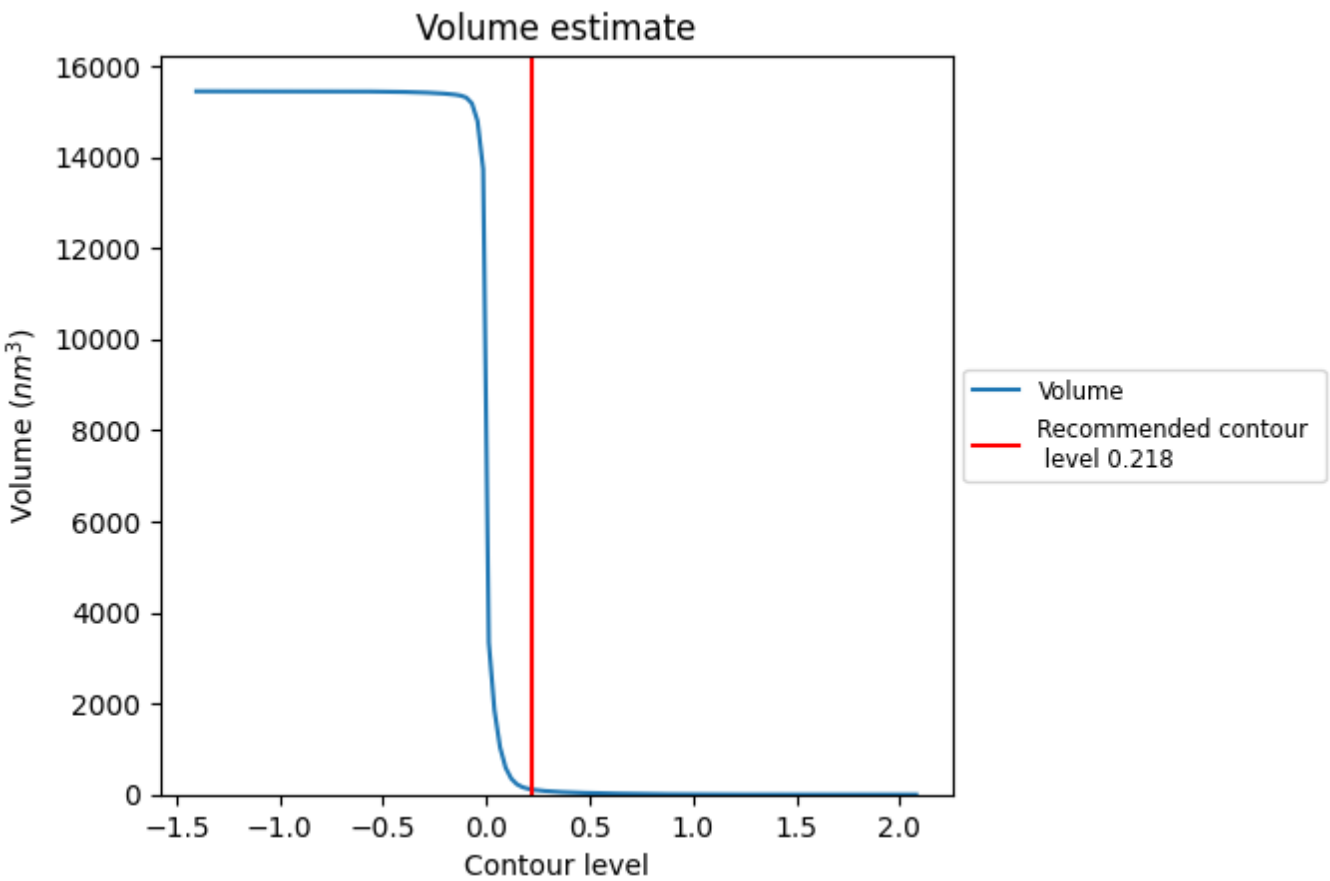
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

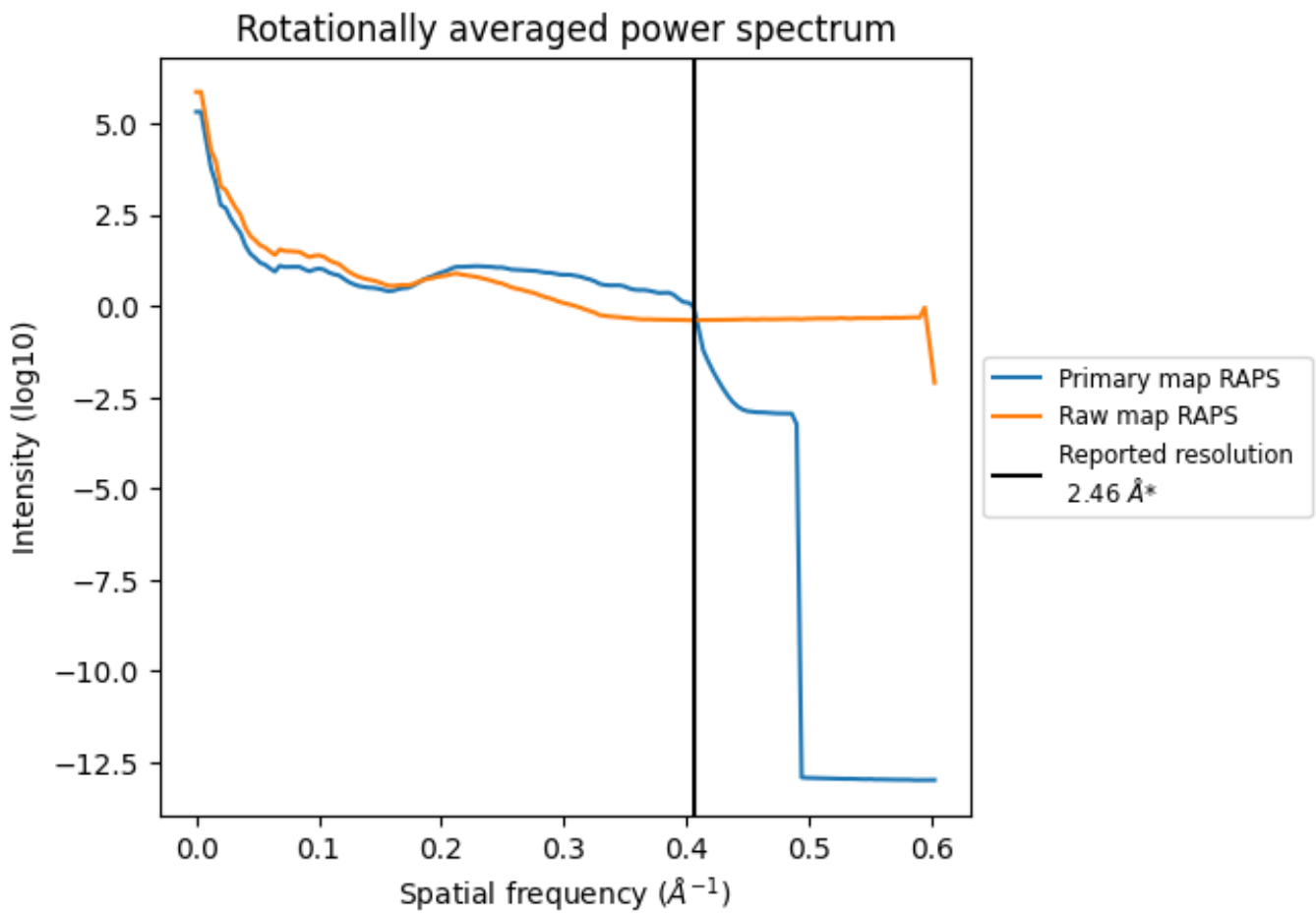
7.2 Volume estimate (i)



The volume at the recommended contour level is 114 nm^3; this corresponds to an approximate mass of 103 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)

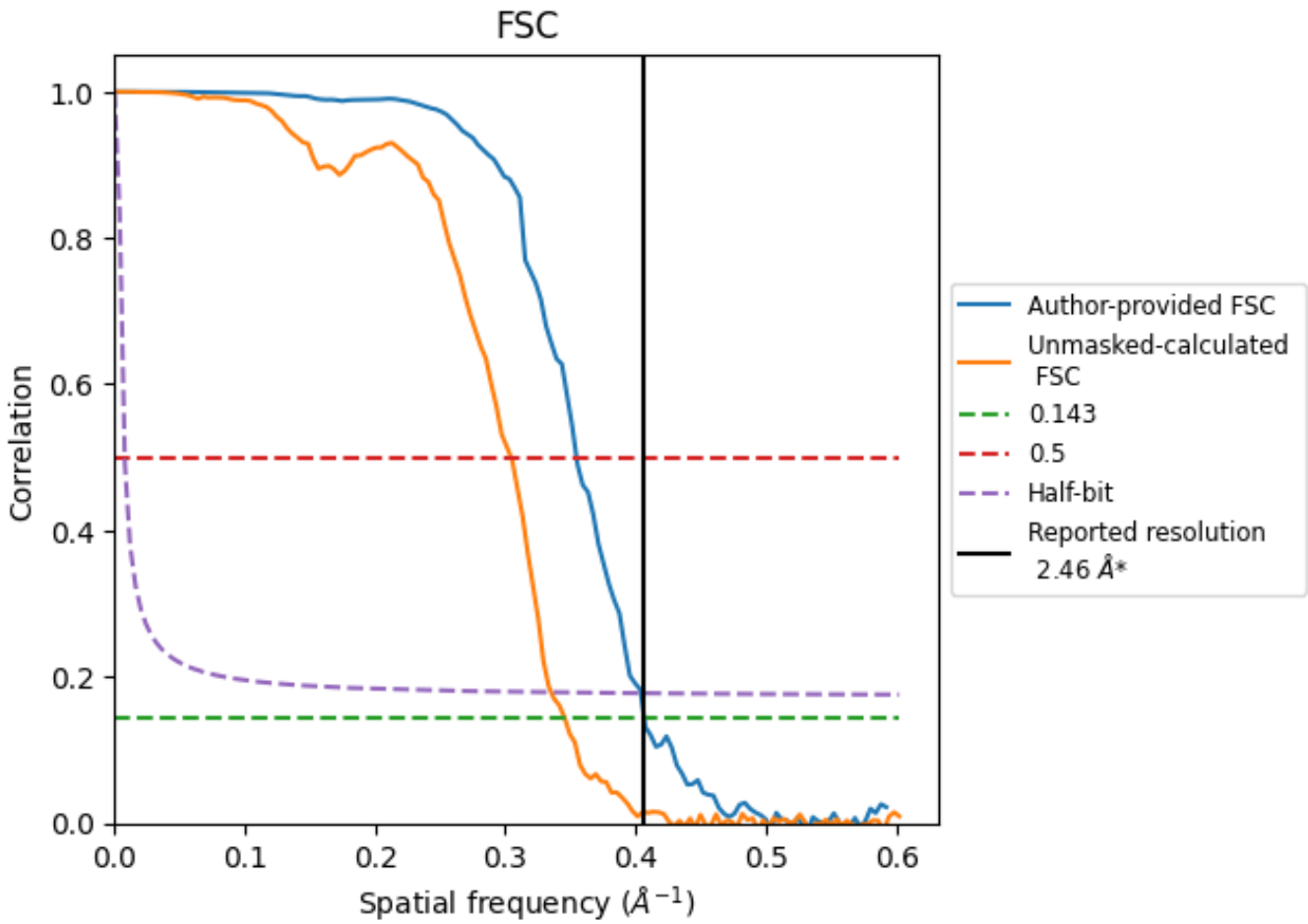


*Reported resolution corresponds to spatial frequency of 0.407 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.407 Å^{-1}

8.2 Resolution estimates (i)

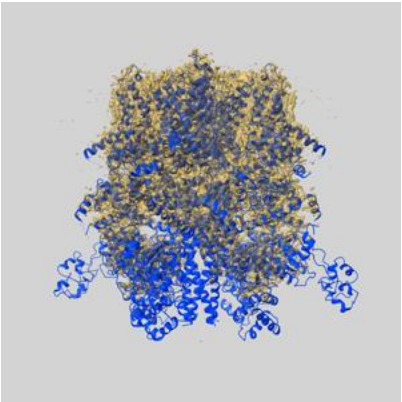
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.46	-	-
Author-provided FSC curve	2.46	2.82	2.48
Unmasked-calculated*	2.89	3.28	2.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.89 differs from the reported value 2.46 by more than 10 %

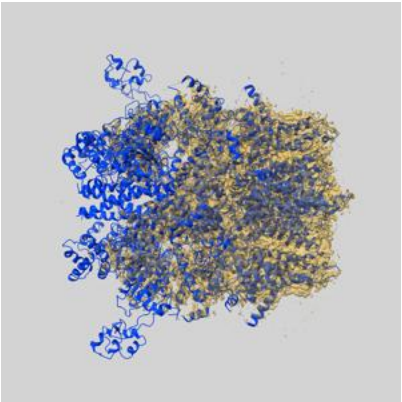
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-40498 and PDB model 8SI4. Per-residue inclusion information can be found in section 3 on page 9.

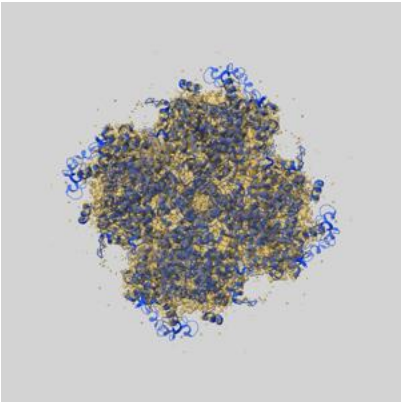
9.1 Map-model overlay (i)



X



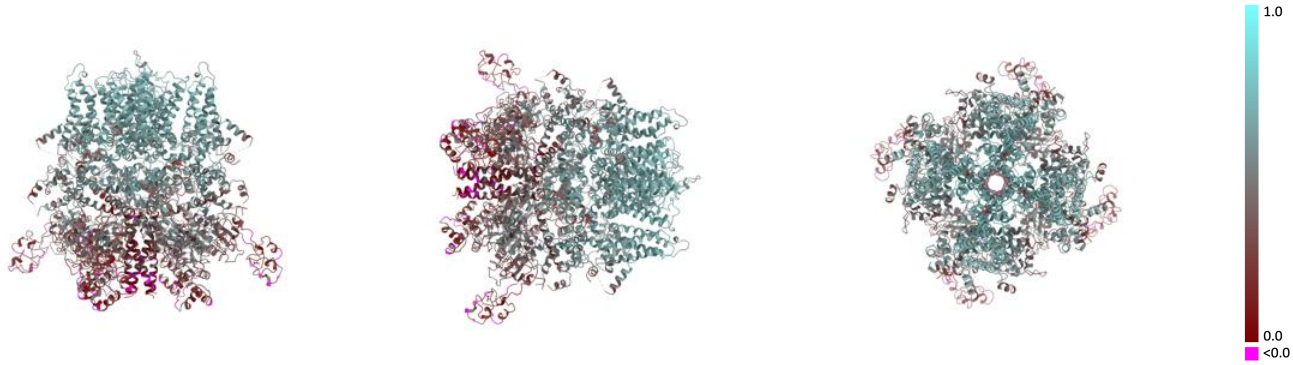
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.218 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

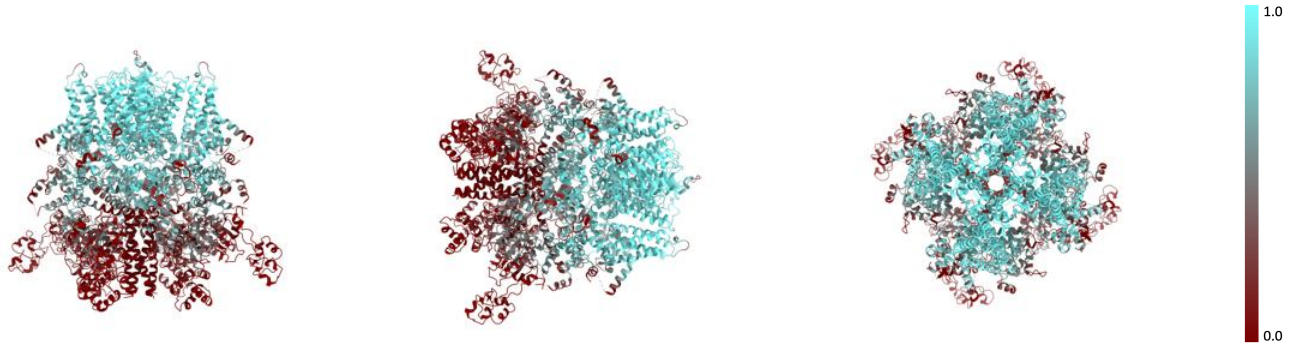
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

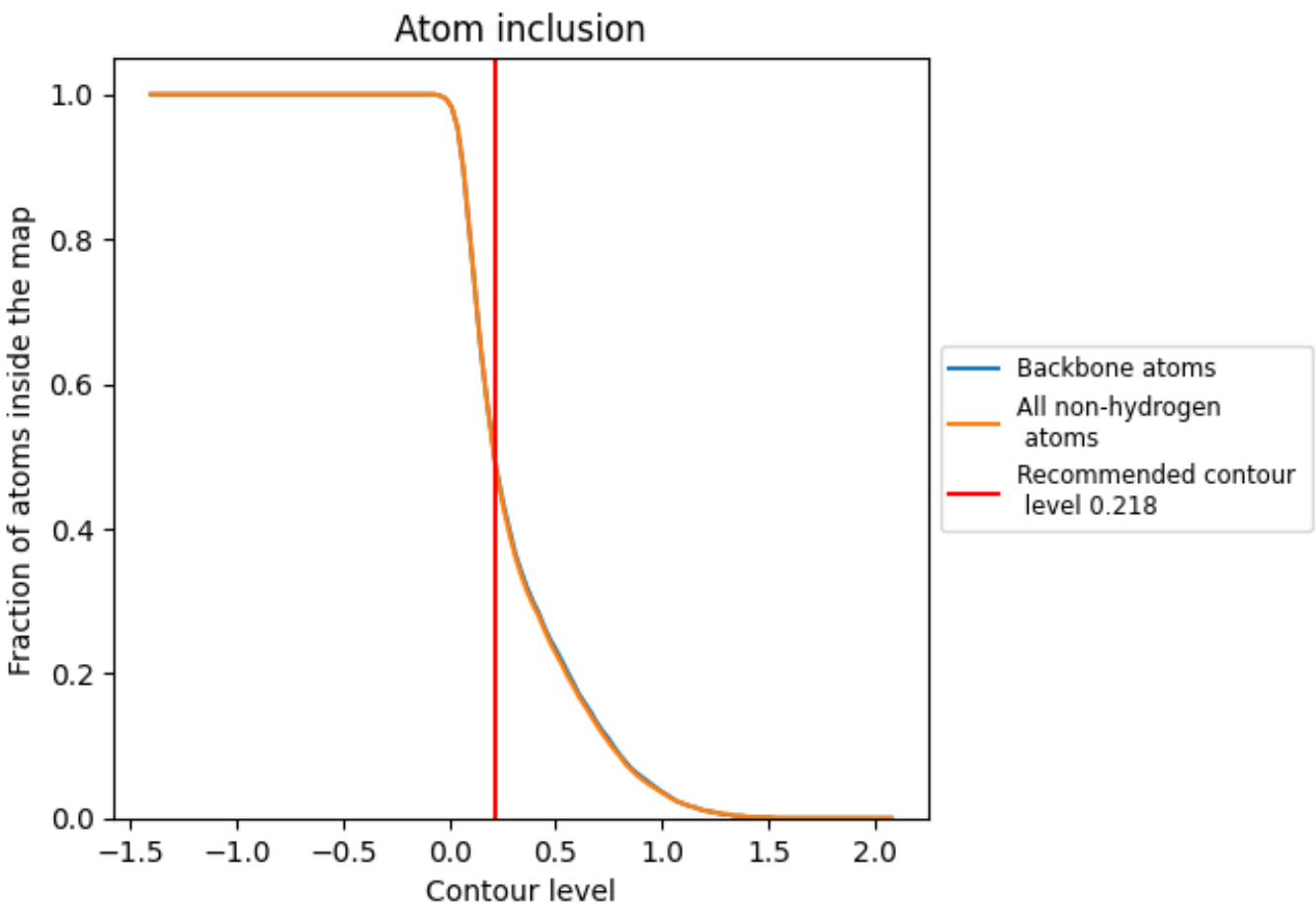
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.218).

9.4 Atom inclusion (i)



At the recommended contour level, 49% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.218) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4850	0.4620
A	0.4890	0.4620
B	0.4910	0.4630
C	0.4880	0.4610
D	0.4890	0.4620