Full wwPDB EM Validation Report ⓘ

Nov 4, 2026 – 02:51 PM JST

PDB ID	:	27MX / pdb_000027mx
EMDB ID	:	EMD-81270
Title	:	Cryo-EM structure of the ATOM complex from Trypanosoma brucei
Authors	:	Wang, S.S.; Cai, H.J.; Li, L.
Deposited on	:	2026-06-05
Resolution	:	2.82 Å(reported)

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

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

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

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

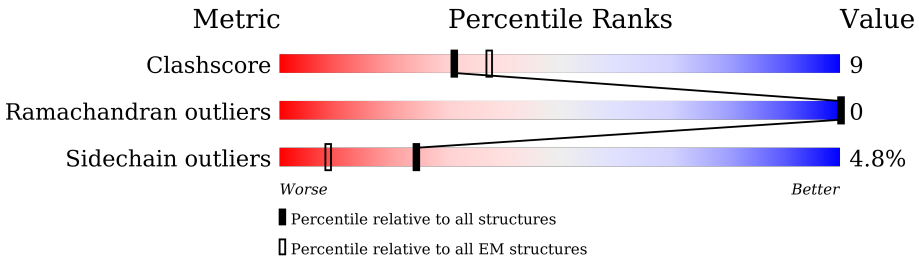
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

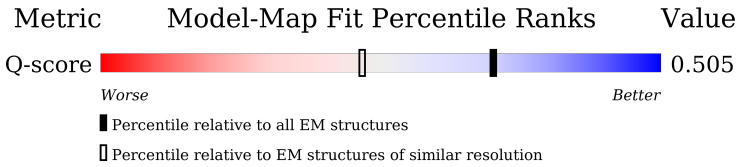
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.82 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.





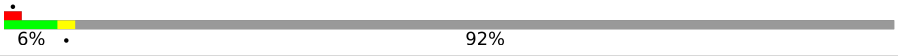
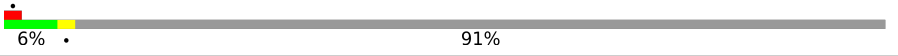
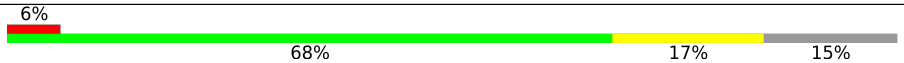
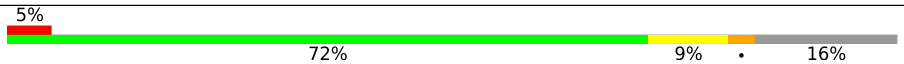
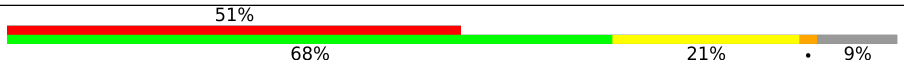
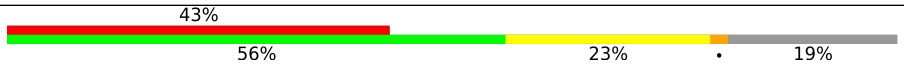
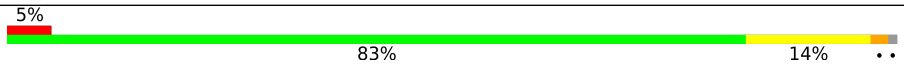
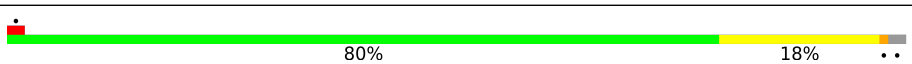
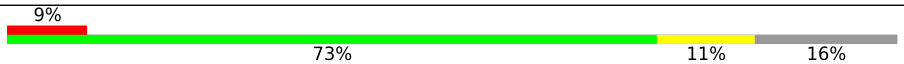
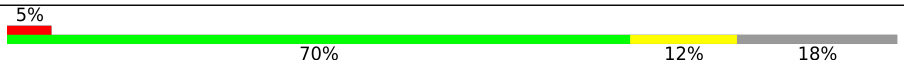
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11795 (2.32 - 3.32)

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	119	14% 71% 19% 10%
1	B	119	12% 71% 17% • 11%
2	C	405	8% 63% 18% • 18%
2	D	405	8% 66% 15% • 18%

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Mol	Chain	Length	Quality of chain
3	E	100	
3	F	100	
4	G	623	
4	H	623	
5	I	105	
5	J	105	
6	K	419	
6	L	419	
7	M	168	
7	N	168	
8	O	56	
8	P	56	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 20790 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Archaic Translocase of outer membrane 14 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	107	Total	C	N	O	S	0	0
			857	536	157	161	3		
1	B	106	Total	C	N	O	S	0	0
			853	534	156	160	3		

- Molecule 2 is a protein called Archaic translocase outer mitochondrial membrane 40.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	332	Total	C	N	O	S	0	0
			2542	1604	441	479	18		
2	D	332	Total	C	N	O	S	0	0
			2542	1604	441	479	18		

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	352	SER	-	expression tag	UNP Q38E31
C	353	ARG	-	expression tag	UNP Q38E31
C	354	GLY	-	expression tag	UNP Q38E31
C	355	GLY	-	expression tag	UNP Q38E31
C	356	SER	-	expression tag	UNP Q38E31
C	357	LEU	-	expression tag	UNP Q38E31
C	358	GLU	-	expression tag	UNP Q38E31
C	359	VAL	-	expression tag	UNP Q38E31
C	360	LEU	-	expression tag	UNP Q38E31
C	361	PHE	-	expression tag	UNP Q38E31
C	362	GLN	-	expression tag	UNP Q38E31
C	363	GLY	-	expression tag	UNP Q38E31
C	364	PRO	-	expression tag	UNP Q38E31
C	365	TRP	-	expression tag	UNP Q38E31
C	366	SER	-	expression tag	UNP Q38E31
C	367	HIS	-	expression tag	UNP Q38E31
C	368	PRO	-	expression tag	UNP Q38E31

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Chain	Residue	Modelled	Actual	Comment	Reference
C	369	GLN	-	expression tag	UNP Q38E31
C	370	PHE	-	expression tag	UNP Q38E31
C	371	GLU	-	expression tag	UNP Q38E31
C	372	LYS	-	expression tag	UNP Q38E31
C	373	GLY	-	expression tag	UNP Q38E31
C	374	GLY	-	expression tag	UNP Q38E31
C	375	GLY	-	expression tag	UNP Q38E31
C	376	SER	-	expression tag	UNP Q38E31
C	377	GLY	-	expression tag	UNP Q38E31
C	378	GLY	-	expression tag	UNP Q38E31
C	379	GLY	-	expression tag	UNP Q38E31
C	380	SER	-	expression tag	UNP Q38E31
C	381	GLY	-	expression tag	UNP Q38E31
C	382	GLY	-	expression tag	UNP Q38E31
C	383	GLY	-	expression tag	UNP Q38E31
C	384	SER	-	expression tag	UNP Q38E31
C	385	TRP	-	expression tag	UNP Q38E31
C	386	SER	-	expression tag	UNP Q38E31
C	387	HIS	-	expression tag	UNP Q38E31
C	388	PRO	-	expression tag	UNP Q38E31
C	389	GLN	-	expression tag	UNP Q38E31
C	390	PHE	-	expression tag	UNP Q38E31
C	391	GLU	-	expression tag	UNP Q38E31
C	392	LYS	-	expression tag	UNP Q38E31
C	393	GLY	-	expression tag	UNP Q38E31
C	394	GLY	-	expression tag	UNP Q38E31
C	395	SER	-	expression tag	UNP Q38E31
C	396	HIS	-	expression tag	UNP Q38E31
C	397	HIS	-	expression tag	UNP Q38E31
C	398	HIS	-	expression tag	UNP Q38E31
C	399	HIS	-	expression tag	UNP Q38E31
C	400	HIS	-	expression tag	UNP Q38E31
C	401	HIS	-	expression tag	UNP Q38E31
C	402	HIS	-	expression tag	UNP Q38E31
C	403	HIS	-	expression tag	UNP Q38E31
C	404	HIS	-	expression tag	UNP Q38E31
C	405	HIS	-	expression tag	UNP Q38E31
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D	353	ARG	-	expression tag	UNP Q38E31
D	354	GLY	-	expression tag	UNP Q38E31
D	355	GLY	-	expression tag	UNP Q38E31
D	356	SER	-	expression tag	UNP Q38E31

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Chain	Residue	Modelled	Actual	Comment	Reference
D	357	LEU	-	expression tag	UNP Q38E31
D	358	GLU	-	expression tag	UNP Q38E31
D	359	VAL	-	expression tag	UNP Q38E31
D	360	LEU	-	expression tag	UNP Q38E31
D	361	PHE	-	expression tag	UNP Q38E31
D	362	GLN	-	expression tag	UNP Q38E31
D	363	GLY	-	expression tag	UNP Q38E31
D	364	PRO	-	expression tag	UNP Q38E31
D	365	TRP	-	expression tag	UNP Q38E31
D	366	SER	-	expression tag	UNP Q38E31
D	367	HIS	-	expression tag	UNP Q38E31
D	368	PRO	-	expression tag	UNP Q38E31
D	369	GLN	-	expression tag	UNP Q38E31
D	370	PHE	-	expression tag	UNP Q38E31
D	371	GLU	-	expression tag	UNP Q38E31
D	372	LYS	-	expression tag	UNP Q38E31
D	373	GLY	-	expression tag	UNP Q38E31
D	374	GLY	-	expression tag	UNP Q38E31
D	375	GLY	-	expression tag	UNP Q38E31
D	376	SER	-	expression tag	UNP Q38E31
D	377	GLY	-	expression tag	UNP Q38E31
D	378	GLY	-	expression tag	UNP Q38E31
D	379	GLY	-	expression tag	UNP Q38E31
D	380	SER	-	expression tag	UNP Q38E31
D	381	GLY	-	expression tag	UNP Q38E31
D	382	GLY	-	expression tag	UNP Q38E31
D	383	GLY	-	expression tag	UNP Q38E31
D	384	SER	-	expression tag	UNP Q38E31
D	385	TRP	-	expression tag	UNP Q38E31
D	386	SER	-	expression tag	UNP Q38E31
D	387	HIS	-	expression tag	UNP Q38E31
D	388	PRO	-	expression tag	UNP Q38E31
D	389	GLN	-	expression tag	UNP Q38E31
D	390	PHE	-	expression tag	UNP Q38E31
D	391	GLU	-	expression tag	UNP Q38E31
D	392	LYS	-	expression tag	UNP Q38E31
D	393	GLY	-	expression tag	UNP Q38E31
D	394	GLY	-	expression tag	UNP Q38E31
D	395	SER	-	expression tag	UNP Q38E31
D	396	HIS	-	expression tag	UNP Q38E31
D	397	HIS	-	expression tag	UNP Q38E31
D	398	HIS	-	expression tag	UNP Q38E31

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Chain	Residue	Modelled	Actual	Comment	Reference
D	399	HIS	-	expression tag	UNP Q38E31
D	400	HIS	-	expression tag	UNP Q38E31
D	401	HIS	-	expression tag	UNP Q38E31
D	402	HIS	-	expression tag	UNP Q38E31
D	403	HIS	-	expression tag	UNP Q38E31
D	404	HIS	-	expression tag	UNP Q38E31
D	405	HIS	-	expression tag	UNP Q38E31

- Molecule 3 is a protein called Archaic translocase of outer membrane 11 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	78	Total	C	N	O	S	0	0
			617	412	99	103	3		
3	F	77	Total	C	N	O	S	0	0
			610	407	98	102	3		

- Molecule 4 is a protein called CS domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	51	Total	C	N	O	0	0
			401	271	64	66		
4	H	53	Total	C	N	O	0	0
			418	280	69	69		

- Molecule 5 is a protein called Archaic translocase of outer membrane 12 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	89	Total	C	N	O	S	0	0
			717	456	128	131	2		
5	J	88	Total	C	N	O	S	0	0
			708	451	127	128	2		

- Molecule 6 is a protein called ATOM46.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	381	Total	C	N	O	S	0	0
			2979	1876	533	552	18		
6	L	340	Total	C	N	O	S	0	0
			2685	1702	479	487	17		

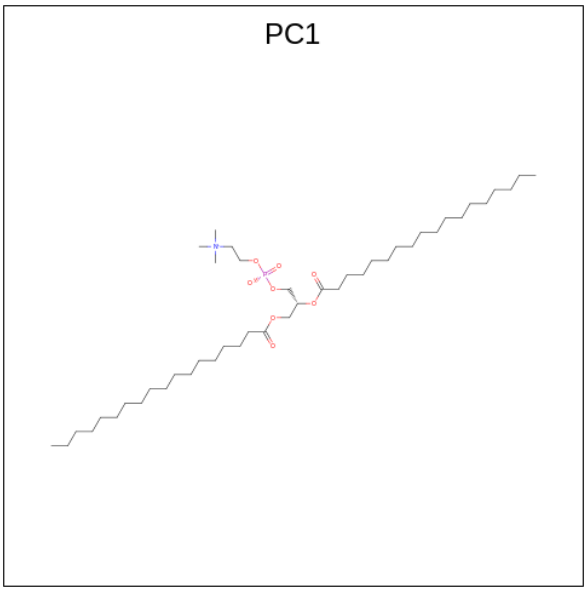
- Molecule 7 is a protein called ATOM19.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	166	Total	C	N	O	S	0	0
			1328	837	247	239	5		
7	N	165	Total	C	N	O	S	0	0
			1321	833	246	237	5		

- Molecule 8 is a protein called ATOM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	47	Total	C	N	O	S	0	0
			370	238	64	66	2		
8	P	46	Total	C	N	O	S	0	0
			366	236	63	65	2		

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			22	13	1	7	1	
9	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
9	A	1	Total	C	N	O	P	0
			17	9	1	6	1	
9	B	1	Total	C	N	O	P	0
			34	24	1	8	1	
9	B	1	Total	C	N	O	P	0
			25	16	1	7	1	

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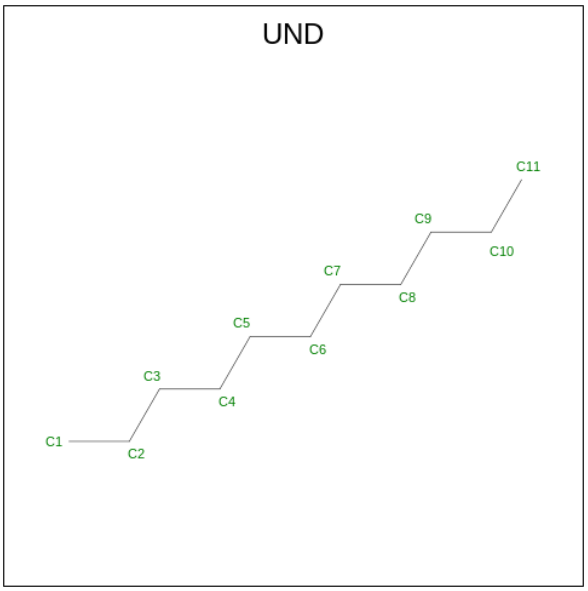
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9	C	1	Total C N O P 31 21 1 8 1	0
9	C	1	Total C N O P 27 18 1 7 1	0
9	C	1	Total C N O P 19 10 1 7 1	0
9	C	1	Total C O 19 15 4	0
9	C	1	Total C N O P 26 17 1 7 1	0
9	D	1	Total C O P 24 15 8 1	0
9	D	1	Total C N O P 21 12 1 7 1	0
9	D	1	Total C N O P 24 15 1 7 1	0
9	D	1	Total C N O P 28 18 1 8 1	0
9	D	1	Total C O 21 17 4	0
9	D	1	Total C N O P 29 19 1 8 1	0
9	D	1	Total C O P 27 18 8 1	0
9	E	1	Total C N O P 31 21 1 8 1	0
9	E	1	Total C N O P 29 19 1 8 1	0
9	E	1	Total C N O P 22 13 1 7 1	0
9	E	1	Total C N O P 25 16 1 7 1	0
9	F	1	Total C N O P 29 19 1 8 1	0
9	F	1	Total C N O P 30 20 1 8 1	0
9	F	1	Total C N O P 28 19 1 7 1	0
9	F	1	Total C N O P 23 14 1 7 1	0

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Mol	Chain	Residues	Atoms					AltConf
9	F	1	Total	C	N	O	P	0
			29	20	1	7	1	
9	H	1	Total	C	N	O	P	0
			20	11	1	7	1	
9	H	1	Total	C	N	O	P	0
			19	10	1	7	1	
9	I	1	Total	C	N	O	P	0
			21	12	1	7	1	
9	I	1	Total	C	N	O	P	0
			29	20	1	7	1	
9	I	1	Total	C	N	O	P	0
			19	10	1	7	1	
9	J	1	Total	C	N	O	P	0
			16	8	1	6	1	
9	J	1	Total	C	O			0
			32	28	4			
9	K	1	Total	C	N	O	P	0
			24	15	1	7	1	
9	K	1	Total	C	N	O	P	0
			24	15	1	7	1	
9	L	1	Total	C	N	O	P	0
			21	12	1	7	1	
9	L	1	Total	C	N	O	P	0
			17	9	1	6	1	
9	M	1	Total	C	N	O	P	0
			29	19	1	8	1	
9	M	1	Total	C	N	O	P	0
			26	17	1	7	1	
9	M	1	Total	C	N	O	P	0
			29	20	1	7	1	
9	M	1	Total	C	N	O	P	0
			16	8	1	6	1	
9	N	1	Total	C	N	O	P	0
			28	18	1	8	1	
9	N	1	Total	C	N	O	P	0
			21	12	1	7	1	
9	N	1	Total	C	N	O	P	0
			27	18	1	7	1	
9	N	1	Total	C	N	O	P	0
			25	16	1	7	1	

- Molecule 10 is UNDECANE (CCD ID: UND) (formula: $C_{11}H_{24}$).



Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C 9 9	0
10	A	1	Total C 10 10	0
10	B	1	Total C 11 11	0
10	B	1	Total C 10 10	0
10	C	1	Total C 8 8	0
10	C	1	Total C 10 10	0
10	C	1	Total C 9 9	0
10	D	1	Total C 9 9	0
10	E	1	Total C 11 11	0
10	E	1	Total C 8 8	0
10	F	1	Total C 7 7	0
10	F	1	Total C 11 11	0
10	G	1	Total C 9 9	0
10	G	1	Total C 9 9	0

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Mol	Chain	Residues	Atoms	AltConf
10	G	1	Total C 9 9	0
10	G	1	Total C 9 9	0
10	H	1	Total C 9 9	0
10	H	1	Total C 11 11	0
10	H	1	Total C 10 10	0
10	I	1	Total C 9 9	0
10	J	1	Total C 10 10	0
10	J	1	Total C 8 8	0
10	K	1	Total C 11 11	0
10	K	1	Total C 7 7	0
10	K	1	Total C 11 11	0
10	K	1	Total C 7 7	0
10	L	1	Total C 7 7	0
10	M	1	Total C 10 10	0
10	M	1	Total C 11 11	0
10	M	1	Total C 8 8	0
10	M	1	Total C 8 8	0
10	M	1	Total C 11 11	0
10	M	1	Total C 11 11	0
10	O	1	Total C 11 11	0
10	O	1	Total C 11 11	0

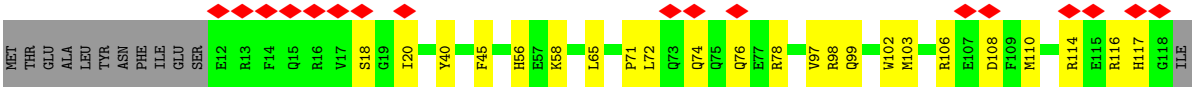
3 Residue-property plots (i)

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: Archaic Translocase of outer membrane 14 kDa subunit

Chain A:

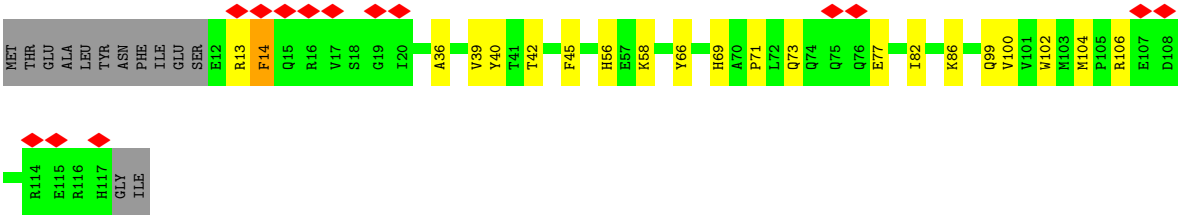




• Molecule 1: Archaic Translocase of outer membrane 14 kDa subunit

Chain B:

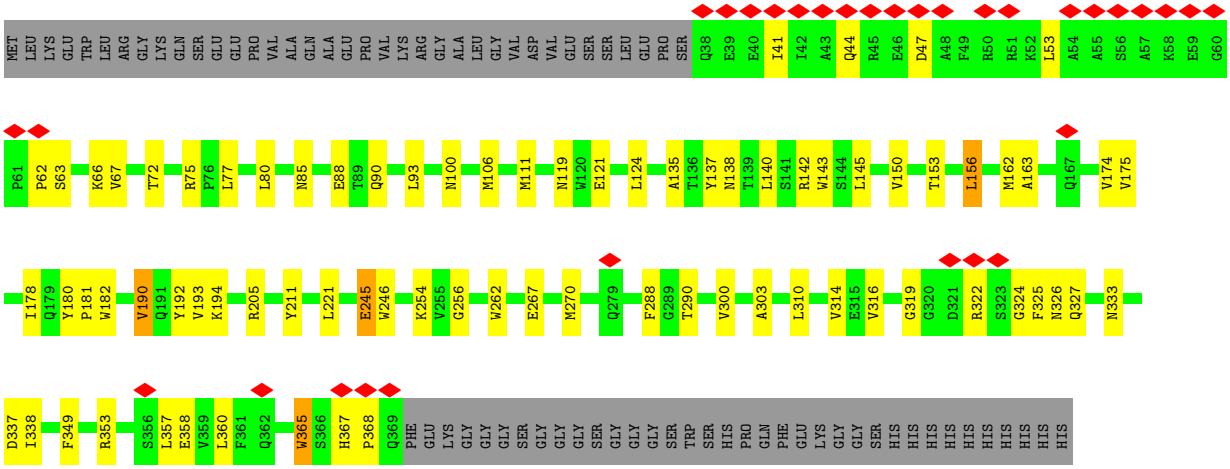




• Molecule 2: Archaic translocase outer mitochondrial membrane 40

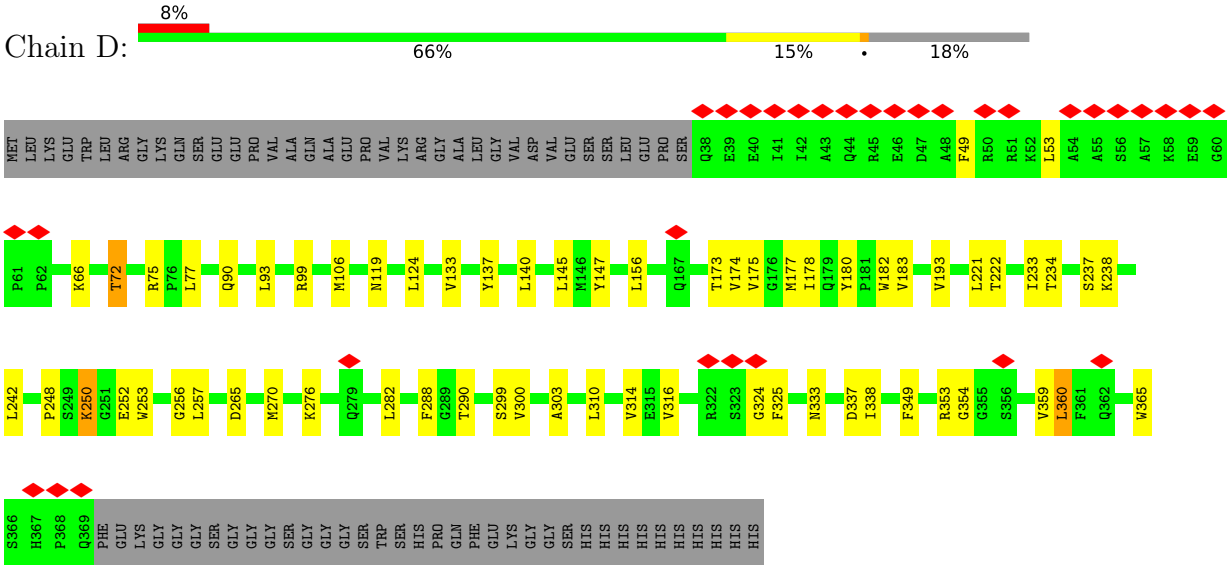
Chain C:





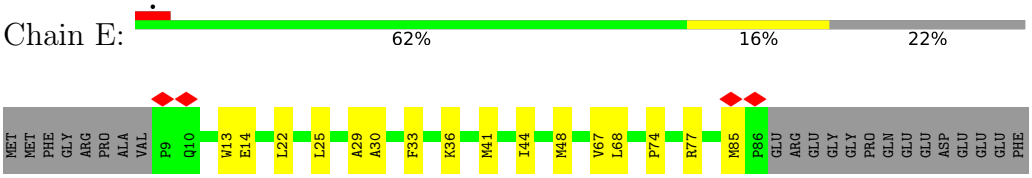
• Molecule 2: Archaic translocase outer mitochondrial membrane 40

Chain D:



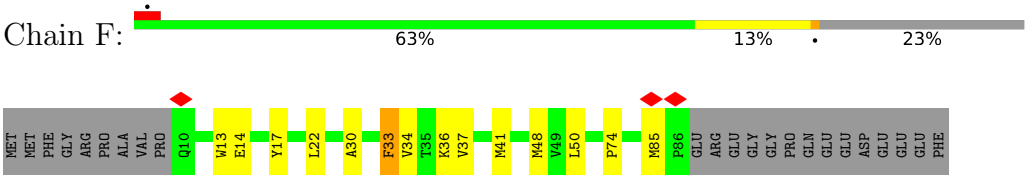
• Molecule 3: Archaic translocase of outer membrane 11 kDa subunit

Chain E:



• Molecule 3: Archaic translocase of outer membrane 11 kDa subunit

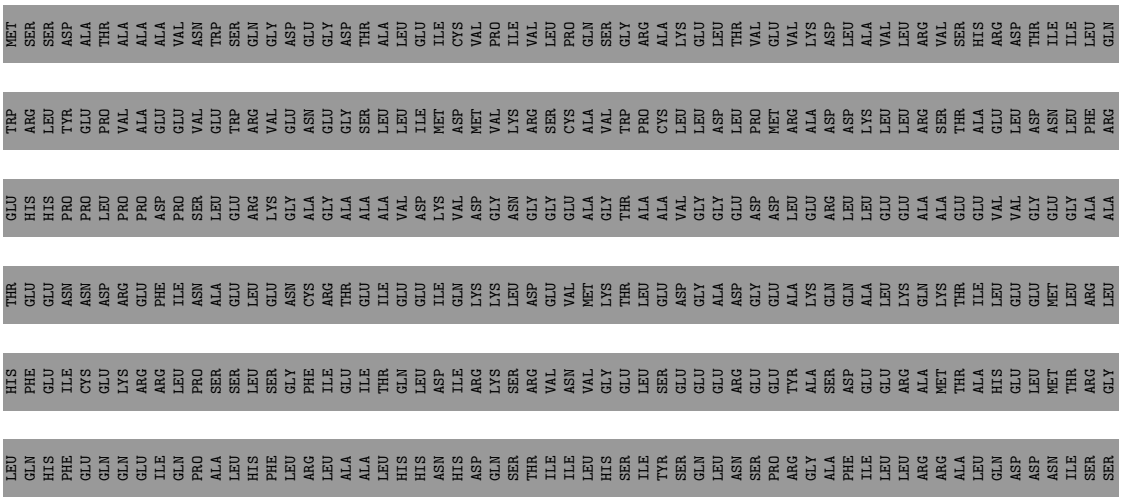
Chain F:

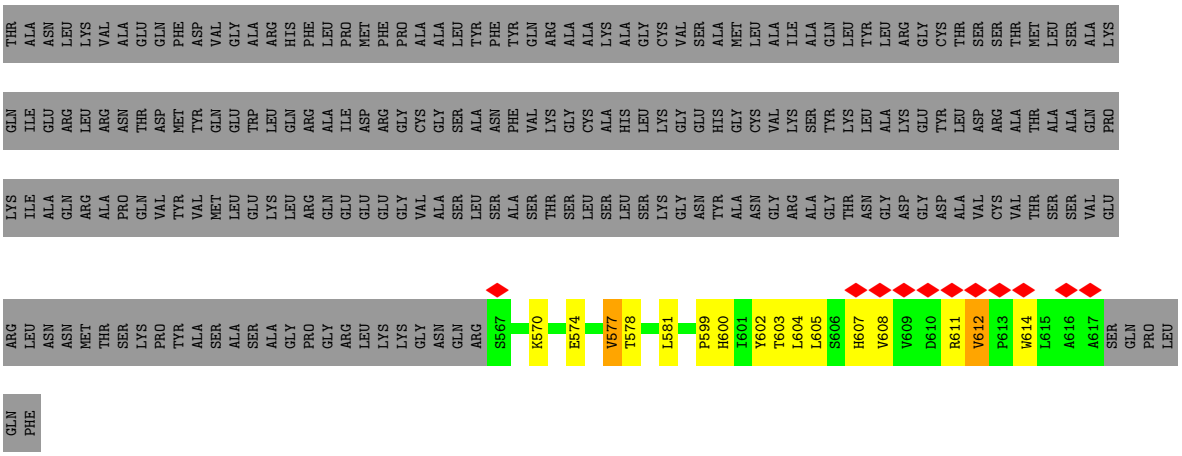


• Molecule 4: CS domain-containing protein

Chain G:

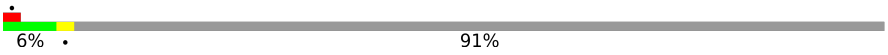


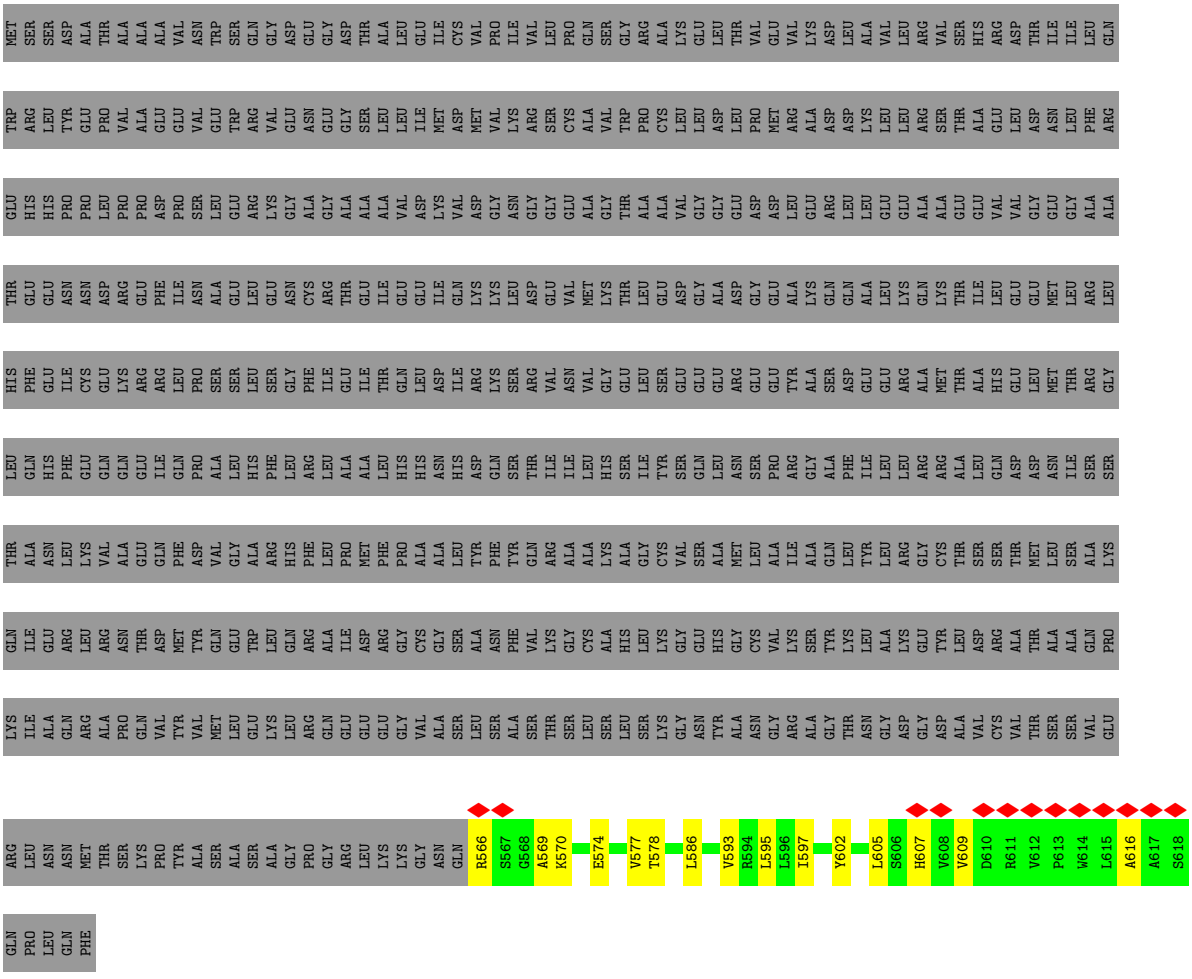




• Molecule 4: CS domain-containing protein

Chain H:





• Molecule 5: Archaic translocase of outer membrane 12 kDa subunit

Chain I:

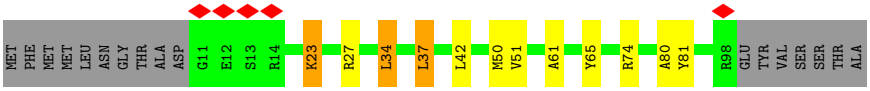




• Molecule 5: Archaic translocase of outer membrane 12 kDa subunit

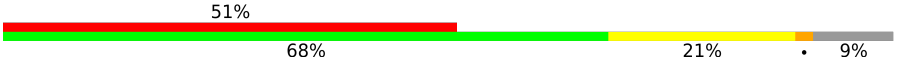
Chain J:

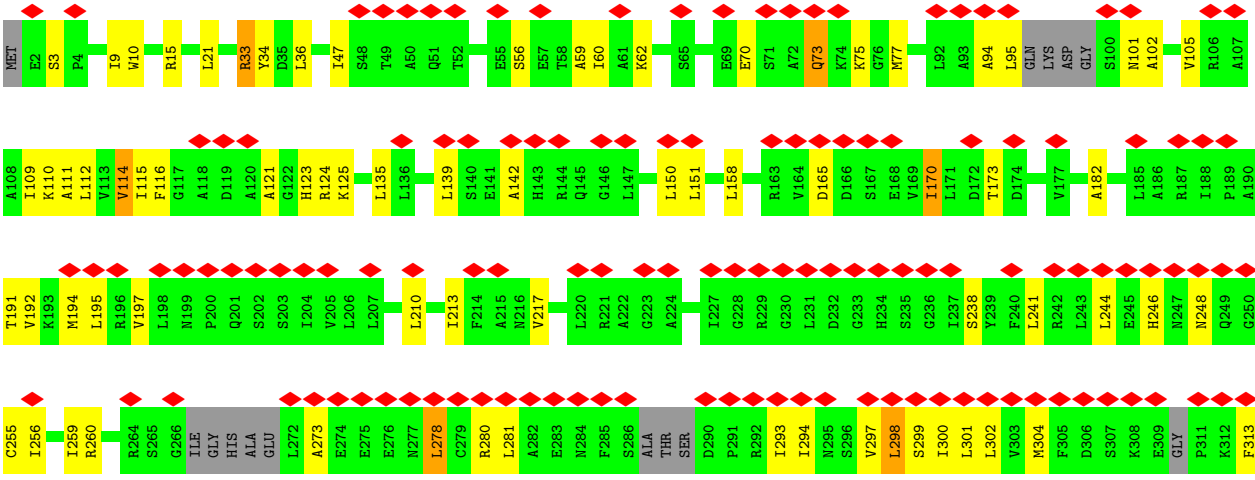




• Molecule 6: ATOM46

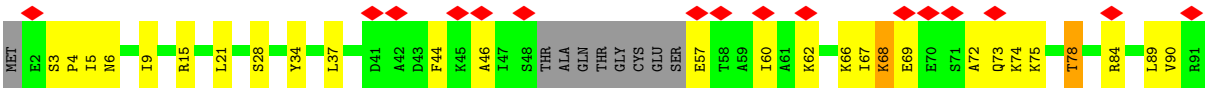
Chain K:

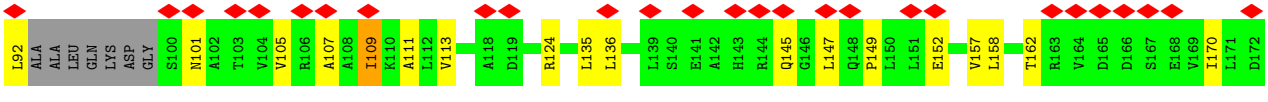


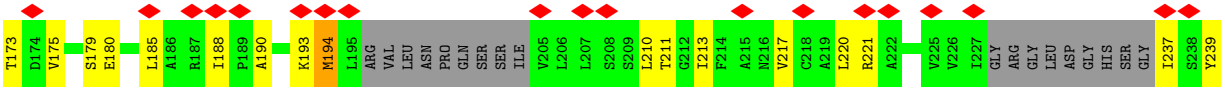


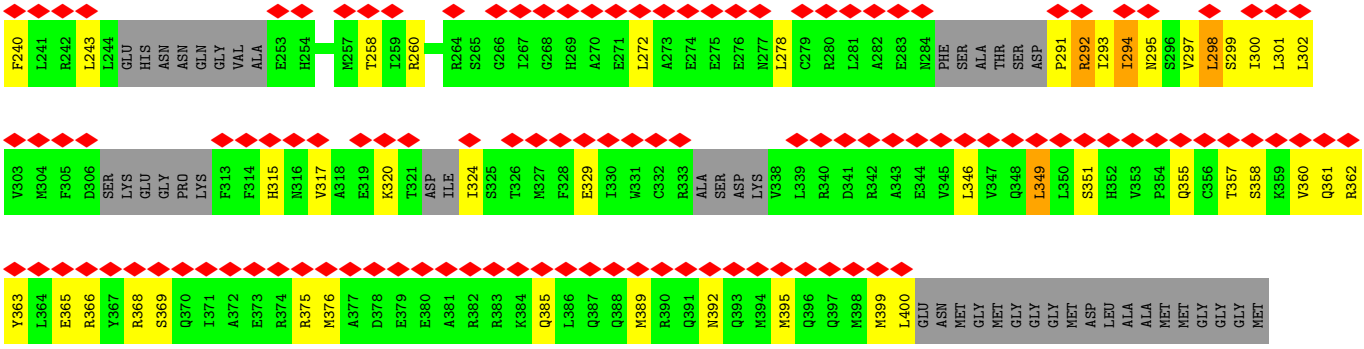
• Molecule 6: ATOM46

Chain L:





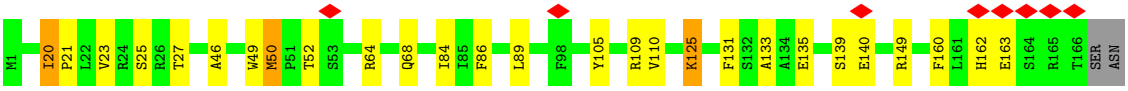




• Molecule 7: ATOM19

Chain M:

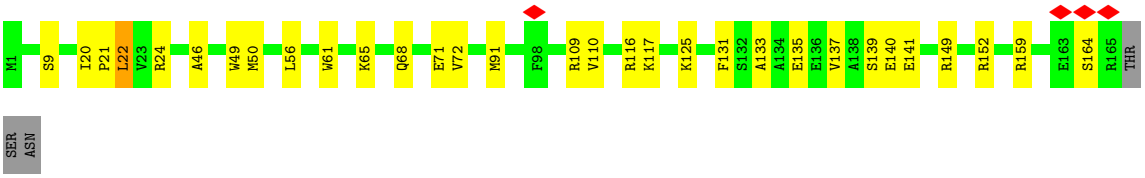




• Molecule 7: ATOM19

Chain N:





• Molecule 8: ATOM6

Chain O:

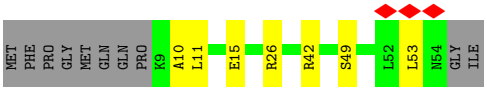




• Molecule 8: ATOM6

Chain P:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73458	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.427	Depositor
Minimum map value	-0.777	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UND, PC1

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	0.17	0/875	0.30	0/1180
1	B	0.17	0/871	0.33	0/1175
2	C	0.20	0/2596	0.34	0/3508
2	D	0.19	0/2596	0.29	0/3508
3	E	0.16	0/642	0.32	0/880
3	F	0.17	0/634	0.35	0/869
4	G	0.14	0/414	0.30	0/570
4	H	0.13	0/431	0.30	0/592
5	I	0.14	0/737	0.27	0/999
5	J	0.13	0/728	0.22	0/987
6	K	0.11	0/3018	0.32	0/4064
6	L	0.11	0/2716	0.29	0/3649
7	M	0.14	0/1360	0.29	0/1843
7	N	0.12	0/1353	0.23	0/1833
8	O	0.15	0/378	0.25	0/512
8	P	0.14	0/374	0.23	0/507
All	All	0.15	0/19723	0.30	0/26676

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	857	0	829	18	0
1	B	853	0	826	21	0
2	C	2542	0	2510	54	0
2	D	2542	0	2510	44	0
3	E	617	0	606	18	0
3	F	610	0	598	14	0
4	G	401	0	414	9	0
4	H	418	0	432	12	0
5	I	717	0	684	11	0
5	J	708	0	680	10	0
6	K	2979	0	3042	63	0
6	L	2685	0	2764	74	0
7	M	1328	0	1314	21	0
7	N	1321	0	1307	22	0
8	O	370	0	369	3	0
8	P	366	0	366	4	0
9	A	72	0	82	4	0
9	B	89	0	106	4	0
9	C	122	0	139	2	0
9	D	174	0	184	8	0
9	E	107	0	122	4	0
9	F	139	0	163	6	0
9	H	39	0	38	2	0
9	I	69	0	74	1	0
9	J	48	0	64	3	0
9	K	48	0	56	0	0
9	L	38	0	40	1	0
9	M	100	0	120	5	0
9	N	101	0	116	4	0
10	A	19	0	36	0	0
10	B	21	0	43	2	0
10	C	27	0	51	0	0
10	D	9	0	17	0	0
10	E	19	0	39	0	0
10	F	18	0	37	1	0
10	G	36	0	68	1	0
10	H	30	0	60	0	0
10	I	9	0	17	0	0
10	J	18	0	34	2	0
10	K	36	0	72	2	0
10	L	7	0	10	0	0
10	M	59	0	118	3	0
10	O	22	0	48	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20790	0	21205	369	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 9.

All (369) 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)
2:C:77:LEU:HD11	2:C:256:GLY:HA3	1.55	0.87
2:C:325:PHE:HA	2:C:353:ARG:HA	1.57	0.84
2:D:77:LEU:HD11	2:D:256:GLY:HA3	1.62	0.81
1:B:13:ARG:HE	1:B:13:ARG:HA	1.47	0.77
2:C:90:GLN:H	2:C:333:ASN:HD21	1.36	0.73
2:D:324:GLY:HA2	3:F:85:MET:HE1	1.69	0.72
2:D:99:ARG:HD3	2:D:353:ARG:HB3	1.71	0.72
7:N:20:ILE:HD12	7:N:21:PRO:HD2	1.73	0.70
2:D:325:PHE:HD1	2:D:353:ARG:HG3	1.57	0.69
1:B:82:ILE:HD11	7:M:133:ALA:HB1	1.73	0.69
6:K:121:ALA:O	6:K:124:ARG:HB2	1.93	0.69
2:C:175:VAL:HG22	2:C:193:VAL:HG13	1.75	0.68
2:D:72:THR:HA	2:D:75:ARG:HB2	1.75	0.68
7:M:135:GLU:O	7:M:139:SER:HB2	1.94	0.68
1:A:102:TRP:HA	7:N:159:ARG:HD2	1.76	0.67
6:K:327:MET:HE3	6:K:327:MET:H	1.59	0.67
6:K:355:GLN:HE21	6:K:356:CYS:H	1.43	0.67
2:D:53:LEU:HB3	8:P:49:SER:HB2	1.76	0.66
1:B:66:TYR:HA	1:B:69:HIS:HB2	1.78	0.66
6:L:302:LEU:HD12	6:L:349:LEU:HD22	1.78	0.66
6:K:301:LEU:HD13	6:K:346:LEU:HD11	1.77	0.66
1:A:110:MET:HA	1:A:110:MET:HE3	1.77	0.66
6:L:57:GLU:HA	6:L:60:ILE:HD12	1.77	0.65
2:D:137:TYR:HB3	3:F:41:MET:HE2	1.79	0.65
6:L:109:ILE:HG23	6:L:157:VAL:HG21	1.79	0.65
6:L:365:GLU:HA	6:L:368:ARG:HG2	1.79	0.64
2:D:175:VAL:HG22	2:D:193:VAL:HG13	1.80	0.64
2:C:53:LEU:HB3	8:O:49:SER:HB2	1.80	0.64
2:D:290:THR:HB	5:J:50:MET:HE2	1.81	0.63
6:L:237:ILE:HG23	6:L:239:TYR:H	1.63	0.63
1:B:42:THR:HG21	5:J:42:LEU:HD23	1.80	0.63
4:H:574:GLU:O	4:H:578:THR:HG23	1.99	0.62
2:C:106:MET:HE3	3:E:67:VAL:HG12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:325:PHE:HB2	2:D:353:ARG:HA	1.82	0.62
1:A:110:MET:HB3	1:A:114:ARG:NH2	2.14	0.61
6:L:351:SER:HB2	6:L:357:THR:HG23	1.81	0.61
2:D:90:GLN:H	2:D:333:ASN:HD21	1.48	0.61
6:K:396:GLN:HA	6:K:400:LEU:HB3	1.82	0.61
4:G:574:GLU:O	4:G:578:THR:HG23	2.01	0.60
2:C:143:TRP:HB2	2:C:163:ALA:HB3	1.83	0.60
5:I:17:LYS:HD3	5:I:17:LYS:C	2.26	0.60
6:K:102:ALA:HA	6:K:105:VAL:HB	1.83	0.60
2:C:111:MET:HE2	2:C:119:ASN:HD21	1.67	0.59
2:C:290:THR:HB	5:I:50:MET:HE2	1.84	0.59
6:K:298:LEU:O	6:K:302:LEU:HD22	2.01	0.59
2:D:174:VAL:HG21	3:F:30:ALA:HB1	1.84	0.59
6:L:294:ILE:HD12	6:L:295:ASN:H	1.67	0.59
6:L:113:VAL:HG21	6:L:157:VAL:HG22	1.85	0.59
7:N:135:GLU:O	7:N:139:SER:HB2	2.03	0.59
2:C:322:ARG:HE	3:E:85:MET:HG2	1.68	0.58
6:K:304:MET:HE3	6:K:304:MET:HA	1.83	0.58
3:F:13:TRP:HB2	4:H:570:LYS:HB2	1.84	0.58
2:C:135:ALA:HB2	3:E:44:ILE:HD12	1.84	0.58
6:K:255:CYS:O	6:K:259:ILE:HG12	2.03	0.58
6:L:392:ASN:HA	6:L:395:MET:SD	2.44	0.57
6:K:260:ARG:HD2	6:K:299:SER:HB2	1.87	0.57
10:B:204:UND:H81	5:J:34:LEU:HD11	1.87	0.57
2:D:276:LYS:HD2	2:D:282:LEU:HG	1.86	0.57
3:F:36:LYS:HD2	9:F:205:PC1:H12	1.86	0.57
6:K:73:GLN:NE2	6:K:75:LYS:HB3	2.19	0.57
2:C:90:GLN:H	2:C:333:ASN:ND2	2.02	0.56
6:L:294:ILE:HA	6:L:297:VAL:HG22	1.87	0.56
6:L:37:LEU:HD13	6:L:84:ARG:HD3	1.87	0.56
3:F:34:VAL:O	3:F:37:VAL:HG23	2.06	0.56
3:E:44:ILE:O	3:E:48:MET:HG3	2.06	0.55
6:K:324:ILE:HB	6:K:359:LYS:HZ2	1.71	0.55
1:B:71:PRO:HA	1:B:77:GLU:HB3	1.86	0.55
6:L:375:ARG:HB3	6:L:376:MET:HE3	1.89	0.55
1:B:58:LYS:HG2	7:M:131:PHE:HE1	1.70	0.55
2:C:365:TRP:H	2:C:365:TRP:CD1	2.22	0.55
6:L:68:LYS:HE2	6:L:78:THR:HB	1.89	0.55
1:A:40:TYR:HA	3:F:74:PRO:HB3	1.89	0.55
1:A:58:LYS:HG2	7:N:131:PHE:HE1	1.72	0.55
6:L:136:LEU:HD23	6:L:185:LEU:HD22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:145:LEU:HD22	3:F:33:PHE:HE2	1.70	0.55
6:K:73:GLN:HE21	6:K:75:LYS:HB3	1.72	0.54
2:D:90:GLN:H	2:D:333:ASN:ND2	2.04	0.54
3:E:36:LYS:HD2	9:E:204:PC1:H11	1.91	0.54
5:I:65:TYR:CZ	5:I:74:ARG:HD3	2.43	0.54
6:K:246:HIS:CD2	6:K:251:VAL:HG21	2.43	0.54
4:G:602:TYR:HE2	6:K:3:SER:HA	1.74	0.53
6:K:353:VAL:HB	6:K:355:GLN:HE22	1.72	0.53
2:C:67:VAL:HG11	2:C:181:PRO:HG3	1.91	0.53
6:L:351:SER:HB3	6:L:360:VAL:HG11	1.89	0.53
2:C:62:PRO:HG2	2:C:67:VAL:HG12	1.91	0.53
6:K:302:LEU:HD13	6:K:346:LEU:HD23	1.91	0.53
2:D:359:VAL:HG23	2:D:360:LEU:H	1.74	0.52
6:L:210:LEU:HA	6:L:213:ILE:HD12	1.91	0.52
6:L:315:HIS:HA	6:L:355:GLN:NE2	2.24	0.52
2:C:72:THR:HA	2:C:75:ARG:HB2	1.91	0.52
6:K:294:ILE:HA	6:K:297:VAL:HG22	1.90	0.52
2:C:137:TYR:HB3	3:E:41:MET:HE2	1.90	0.52
4:H:566:ARG:HD3	4:H:569:ALA:HB2	1.91	0.52
7:N:22:LEU:HD21	9:N:204:PC1:H2	1.92	0.52
6:L:292:ARG:HA	6:L:295:ASN:ND2	2.24	0.52
6:L:294:ILE:HD12	6:L:295:ASN:N	2.24	0.52
2:C:93:LEU:HD11	2:C:349:PHE:HE2	1.74	0.52
5:J:80:ALA:HA	7:N:109:ARG:HB3	1.92	0.52
7:M:46:ALA:O	7:M:50:MET:HB3	2.09	0.52
3:F:22:LEU:HD11	6:L:21:LEU:HD22	1.91	0.52
1:A:99:GLN:O	1:A:103:MET:HB2	2.10	0.51
2:C:300:VAL:HG22	2:C:314:VAL:HG13	1.92	0.51
2:D:119:ASN:HB3	2:D:140:LEU:HG	1.92	0.51
6:L:170:ILE:HD13	7:N:68:GLN:HB2	1.91	0.51
6:L:5:ILE:HD12	6:L:5:ILE:H	1.75	0.51
6:K:182:ALA:HB1	6:K:217:VAL:HA	1.93	0.51
6:K:170:ILE:HD12	7:M:64:ARG:HG3	1.93	0.51
3:E:22:LEU:HD11	6:K:21:LEU:HD22	1.93	0.50
5:J:65:TYR:CZ	5:J:74:ARG:HD3	2.46	0.50
6:L:329:GLU:HG3	6:L:363:TYR:HB3	1.94	0.50
6:L:90:VAL:O	6:L:92:LEU:HD12	2.12	0.50
6:L:240:PHE:HA	6:L:243:LEU:HD12	1.94	0.50
2:D:124:LEU:HB3	3:F:48:MET:SD	2.52	0.49
2:D:300:VAL:HG22	2:D:314:VAL:HG13	1.94	0.49
2:D:265:ASP:OD2	7:N:116:ARG:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:66:LYS:HD2	2:C:66:LYS:O	2.12	0.49
1:A:98:ARG:HG3	1:A:98:ARG:HH11	1.78	0.49
6:K:194:MET:HE2	6:K:194:MET:N	2.27	0.49
6:L:278:LEU:HD21	6:L:317:VAL:HG13	1.95	0.49
2:C:270:MET:HG2	7:M:86:PHE:CD1	2.47	0.49
9:F:201:PC1:H322	9:F:201:PC1:H221	1.94	0.49
2:C:138:ASN:HB2	2:C:142:ARG:HB2	1.95	0.48
2:D:325:PHE:H	2:D:325:PHE:HD2	1.60	0.48
1:A:106:ARG:HB3	1:A:106:ARG:NH1	2.28	0.48
2:D:93:LEU:HD11	2:D:349:PHE:HE2	1.78	0.48
2:C:93:LEU:HD11	2:C:349:PHE:CE2	2.48	0.48
2:C:150:VAL:HG22	2:C:156:LEU:HD12	1.94	0.48
6:K:241:LEU:HA	6:K:244:LEU:HB2	1.96	0.48
3:E:13:TRP:HB2	4:G:570:LYS:HB2	1.96	0.48
9:M:202:PC1:H341	9:M:202:PC1:H371	1.64	0.48
1:B:36:ALA:HA	10:B:205:UND:H72	1.95	0.48
2:C:182:TRP:H	2:C:182:TRP:CD1	2.32	0.48
3:E:14:GLU:OE2	3:E:14:GLU:HA	2.13	0.48
5:I:80:ALA:HA	7:M:109:ARG:HB3	1.96	0.48
2:C:310:LEU:HB2	2:C:338:ILE:HD11	1.95	0.47
6:L:295:ASN:HA	6:L:298:LEU:CD2	2.43	0.47
1:A:116:ARG:NH2	7:N:149:ARG:HD3	2.29	0.47
1:B:45:PHE:CD2	2:D:310:LEU:HD23	2.49	0.47
6:K:10:TRP:HE1	10:K:503:UND:H51	1.79	0.47
9:E:202:PC1:H153	9:E:202:PC1:H112	1.64	0.47
6:K:238:SER:HA	6:K:241:LEU:HD23	1.95	0.47
6:K:253:GLU:O	6:K:256:ILE:HG22	2.15	0.47
6:L:145:GLN:HB3	6:L:147:LEU:HD12	1.96	0.47
4:G:600:HIS:O	4:G:604:LEU:HD13	2.13	0.47
6:L:6:ASN:O	6:L:9:ILE:HG22	2.14	0.47
6:L:101:ASN:HA	6:L:105:VAL:HG21	1.96	0.47
2:C:106:MET:HE1	3:E:68:LEU:HG	1.97	0.47
2:C:119:ASN:HB3	2:C:140:LEU:HG	1.97	0.47
2:D:234:THR:HG21	2:D:238:LYS:HD2	1.96	0.47
2:D:253:TRP:CD1	9:D:501:PC1:H221	2.48	0.47
6:K:60:ILE:HG23	6:K:111:ALA:HB2	1.96	0.47
6:L:179:SER:HB2	6:L:220:LEU:HD11	1.95	0.47
1:B:40:TYR:HA	3:E:74:PRO:HB3	1.97	0.47
2:C:174:VAL:HG21	3:E:30:ALA:HB1	1.95	0.47
2:C:180:TYR:OH	6:K:15:ARG:HG2	2.15	0.47
6:L:188:ILE:HD12	6:L:190:ALA:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:60:ILE:HG23	6:L:107:ALA:HB2	1.97	0.47
6:L:73:GLN:H	6:L:75:LYS:HZ2	1.63	0.47
2:C:205:ARG:HB2	2:C:211:TYR:CE2	2.49	0.46
6:L:124:ARG:HD3	6:L:180:GLU:HG2	1.96	0.46
8:P:11:LEU:HD23	8:P:15:GLU:HG3	1.96	0.46
9:A:201:PC1:H321	9:F:203:PC1:H111	1.97	0.46
5:I:40:ALA:HA	10:M:207:UND:H41	1.98	0.46
6:K:192:VAL:O	6:K:195:LEU:HB2	2.15	0.46
7:N:46:ALA:O	7:N:50:MET:HG2	2.14	0.46
6:L:315:HIS:HA	6:L:355:GLN:HE22	1.81	0.46
1:A:45:PHE:CD2	2:C:310:LEU:HD23	2.50	0.46
1:B:86:LYS:HD3	7:M:140:GLU:HB3	1.98	0.46
9:C:502:PC1:H111	9:C:502:PC1:H142	1.64	0.46
6:K:341:ASP:HA	6:K:344:GLU:HG3	1.97	0.46
1:B:56:HIS:CD2	2:D:316:VAL:HG13	2.51	0.46
9:B:203:PC1:H152	3:E:77:ARG:HG3	1.97	0.46
4:G:599:PRO:O	4:G:603:THR:HG23	2.15	0.46
7:N:24:ARG:HH11	7:N:24:ARG:HB3	1.81	0.46
2:C:80:LEU:HD21	2:C:267:GLU:HB2	1.97	0.46
9:E:203:PC1:H112	9:E:203:PC1:H143	1.65	0.46
7:M:125:LYS:HB2	7:M:125:LYS:HE3	1.63	0.46
2:D:233:ILE:HD13	9:D:506:PC1:H142	1.97	0.46
6:K:244:LEU:HD23	6:K:280:ARG:HB3	1.98	0.46
1:A:56:HIS:CD2	2:C:316:VAL:HG13	2.50	0.46
9:J:202:PC1:H3D2	9:J:202:PC1:H3A1	1.76	0.45
6:L:385:GLN:O	6:L:389:MET:HG2	2.16	0.45
2:C:145:LEU:HD23	3:E:33:PHE:HE2	1.80	0.45
2:D:156:LEU:HD23	2:D:177:MET:HE1	1.97	0.45
6:K:293:ILE:O	6:K:297:VAL:HG13	2.16	0.45
6:K:299:SER:HA	6:K:302:LEU:HD23	1.97	0.45
6:L:362:ARG:O	6:L:366:ARG:HG2	2.16	0.45
9:L:502:PC1:H112	9:L:502:PC1:H143	1.73	0.45
2:D:66:LYS:HA	2:D:66:LYS:HD2	1.75	0.45
5:I:17:LYS:HE2	9:I:203:PC1:H132	1.98	0.45
2:D:182:TRP:H	2:D:182:TRP:CD1	2.35	0.45
6:K:273:ALA:HA	6:K:313:PHE:HE1	1.81	0.45
6:L:68:LYS:H	6:L:68:LYS:HD2	1.81	0.45
7:M:89:LEU:HD21	10:M:207:UND:H32	1.98	0.45
9:B:201:PC1:H132	9:B:201:PC1:H111	1.63	0.45
2:C:75:ARG:HD2	2:C:75:ARG:HA	1.67	0.45
5:J:37:LEU:HD23	5:J:37:LEU:HA	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:260:ARG:HD2	6:L:299:SER:HB2	1.98	0.45
3:F:14:GLU:HA	3:F:14:GLU:OE2	2.15	0.45
3:F:50:LEU:HD11	10:F:207:UND:H31	1.99	0.45
4:H:574:GLU:O	4:H:577:VAL:HG12	2.16	0.45
4:G:611:ARG:HG3	4:G:612:VAL:HG12	1.99	0.45
6:L:67:ILE:HD11	6:L:111:ALA:HA	1.99	0.45
6:L:272:LEU:HD23	6:L:272:LEU:H	1.82	0.45
2:C:319:GLY:HA3	2:C:327:GLN:HA	1.98	0.45
2:C:288:PHE:O	2:C:303:ALA:HA	2.17	0.45
10:J:203:UND:H42	10:J:203:UND:H72	1.82	0.45
6:L:298:LEU:HA	6:L:301:LEU:HG	1.98	0.45
3:E:29:ALA:HB1	4:G:581:LEU:HD22	1.99	0.44
5:J:23:LYS:HD2	9:J:201:PC1:H153	1.98	0.44
6:K:125:LYS:HE2	6:K:125:LYS:HB2	1.79	0.44
6:K:248:ASN:HB3	6:K:251:VAL:HG22	2.00	0.44
6:L:292:ARG:HA	6:L:295:ASN:HD21	1.81	0.44
2:D:180:TYR:OH	6:L:15:ARG:HG2	2.16	0.44
9:M:203:PC1:H361	9:M:203:PC1:H392	1.71	0.44
1:B:99:GLN:HG2	5:J:81:TYR:CZ	2.53	0.44
1:B:106:ARG:NH1	1:B:106:ARG:HB3	2.32	0.44
2:C:262:TRP:NE1	5:I:82:GLU:HG2	2.32	0.44
9:D:503:PC1:H112	9:D:503:PC1:H153	1.68	0.44
4:H:570:LYS:O	4:H:574:GLU:HG3	2.18	0.44
6:K:278:LEU:HD12	6:K:321:THR:HG23	2.00	0.44
6:L:194:MET:HE3	6:L:194:MET:HB3	1.90	0.44
1:B:69:HIS:O	1:B:73:GLN:HG2	2.16	0.44
5:I:61:ALA:HB1	7:M:110:VAL:HB	1.98	0.44
6:K:135:LEU:HD23	6:K:135:LEU:HA	1.79	0.44
6:L:44:PHE:HE2	6:L:66:LYS:HG3	1.83	0.44
6:L:297:VAL:O	6:L:300:ILE:HG22	2.17	0.44
1:A:71:PRO:HA	1:A:78:ARG:HB2	1.99	0.44
2:D:93:LEU:HD11	2:D:349:PHE:CE2	2.52	0.44
2:D:310:LEU:HB2	2:D:338:ILE:HD11	2.00	0.44
2:D:359:VAL:HG23	2:D:360:LEU:N	2.33	0.44
6:K:278:LEU:H	6:K:278:LEU:HD23	1.82	0.44
6:K:364:LEU:HD13	6:K:368:ARG:HE	1.81	0.44
9:M:203:PC1:H372	9:M:203:PC1:H341	1.58	0.44
2:C:44:GLN:HA	2:C:47:ASP:OD2	2.18	0.44
2:C:324:GLY:C	2:C:326:ASN:H	2.26	0.44
9:D:501:PC1:H32	7:N:61:TRP:HH2	1.83	0.44
6:K:115:ILE:HG13	6:K:116:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:324:ILE:HD12	6:L:324:ILE:HA	1.90	0.44
6:L:368:ARG:HD2	6:L:368:ARG:HA	1.84	0.44
2:C:245:GLU:HB3	2:C:254:LYS:HB3	2.00	0.44
9:F:203:PC1:H342	9:F:203:PC1:H372	1.63	0.44
6:K:142:ALA:HB1	6:K:151:LEU:HB2	1.99	0.44
7:N:133:ALA:O	7:N:137:VAL:HG13	2.18	0.44
1:A:97:VAL:HG22	7:M:105:TYR:CZ	2.53	0.43
2:C:124:LEU:HB3	3:E:48:MET:SD	2.58	0.43
2:D:250:LYS:HB2	2:D:252:GLU:HG3	1.99	0.43
2:D:288:PHE:O	2:D:303:ALA:HA	2.17	0.43
8:P:49:SER:O	8:P:53:LEU:HB2	2.19	0.43
1:B:58:LYS:HG2	7:M:131:PHE:CE1	2.51	0.43
5:I:34:LEU:HD23	5:I:34:LEU:HA	1.85	0.43
5:J:34:LEU:HD23	5:J:34:LEU:HA	1.84	0.43
6:L:66:LYS:HD2	6:L:66:LYS:HA	1.78	0.43
9:F:205:PC1:H331	9:F:205:PC1:H362	1.79	0.43
6:L:188:ILE:HD12	6:L:190:ALA:N	2.33	0.43
7:M:20:ILE:HD12	7:M:21:PRO:HD2	2.00	0.43
1:B:13:ARG:HA	1:B:13:ARG:NE	2.25	0.43
9:D:506:PC1:H152	9:D:506:PC1:H112	1.74	0.43
9:H:702:PC1:H112	9:H:702:PC1:H153	1.71	0.43
5:J:61:ALA:HB1	7:N:110:VAL:HB	2.00	0.43
9:J:202:PC1:H221	9:J:202:PC1:H251	1.67	0.43
4:H:602:TYR:CD1	6:L:4:PRO:HD2	2.53	0.43
9:F:202:PC1:H143	9:F:202:PC1:H111	1.84	0.43
4:H:593:VAL:O	4:H:597:ILE:HG23	2.18	0.43
9:E:204:PC1:H153	9:E:204:PC1:H111	1.76	0.43
7:M:84:ILE:HG13	10:M:209:UND:H41	2.01	0.43
2:C:41:ILE:O	2:C:44:GLN:HG2	2.19	0.43
6:K:36:LEU:HD22	6:K:77:MET:HG3	2.00	0.43
6:L:149:PRO:O	6:L:152:GLU:HG3	2.19	0.43
2:D:353:ARG:HG3	2:D:354:GLY:H	1.82	0.43
6:L:221:ARG:HD3	6:L:221:ARG:HA	1.93	0.43
3:F:17:TYR:HB3	6:L:28:SER:HB2	2.01	0.42
1:A:98:ARG:HG3	1:A:98:ARG:NH1	2.34	0.42
7:M:160:PHE:HA	7:M:163:GLU:HG3	2.00	0.42
9:M:202:PC1:H111	9:M:202:PC1:H133	1.78	0.42
2:D:310:LEU:HD22	2:D:338:ILE:HD11	2.01	0.42
10:J:204:UND:H13	10:J:204:UND:H42	1.84	0.42
6:L:237:ILE:HD12	6:L:237:ILE:HA	1.87	0.42
6:L:317:VAL:HA	6:L:320:LYS:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ARG:NH2	7:N:152:ARG:HB3	2.34	0.42
6:K:124:ARG:HA	6:K:124:ARG:HD2	1.60	0.42
6:L:46:ALA:HB3	6:L:62:LYS:HD2	2.02	0.42
6:L:376:MET:HE3	6:L:376:MET:N	2.34	0.42
7:M:23:VAL:HG12	7:M:27:THR:HB	2.00	0.42
7:N:46:ALA:HA	7:N:49:TRP:NE1	2.33	0.42
8:O:11:LEU:HD23	8:O:15:GLU:HG3	2.01	0.42
9:A:202:PC1:H111	9:A:202:PC1:H142	1.70	0.42
4:H:602:TYR:CE1	6:L:3:SER:HA	2.54	0.42
2:C:192:TYR:CZ	2:C:194:LYS:HA	2.54	0.42
2:C:246:TRP:CZ3	9:C:503:PC1:H12	2.55	0.42
9:D:502:PC1:H142	9:D:502:PC1:H111	1.72	0.42
6:K:34:TYR:CD1	6:K:34:TYR:C	2.98	0.42
6:K:297:VAL:HA	6:K:300:ILE:HG22	2.01	0.42
9:N:202:PC1:H112	9:N:202:PC1:H153	1.66	0.42
1:A:20:ILE:HD13	1:A:20:ILE:HA	1.91	0.42
9:H:701:PC1:H153	9:H:701:PC1:H112	1.79	0.42
6:K:56:SER:O	6:K:60:ILE:HD13	2.18	0.42
6:L:185:LEU:HD12	6:L:217:VAL:HG22	2.01	0.42
6:L:346:LEU:HA	6:L:349:LEU:HD23	2.01	0.42
9:B:203:PC1:H111	9:B:203:PC1:H143	1.68	0.42
6:K:300:ILE:O	6:K:304:MET:HB2	2.20	0.42
1:B:100:VAL:O	1:B:104:MET:HG3	2.19	0.42
4:H:595:LEU:HD23	4:H:595:LEU:HA	1.86	0.42
6:L:72:ALA:C	6:L:74:LYS:H	2.28	0.42
6:L:358:SER:O	6:L:361:GLN:HG3	2.19	0.42
7:N:65:LYS:HB3	7:N:72:VAL:HG11	2.02	0.42
2:D:133:VAL:HB	2:D:147:TYR:HD1	1.85	0.41
2:D:270:MET:HE3	2:D:270:MET:HB3	1.84	0.41
3:F:13:TRP:CB	4:H:570:LYS:HB2	2.49	0.41
1:B:14:PHE:HD1	1:B:14:PHE:HA	1.74	0.41
6:K:135:LEU:HD13	6:K:158:LEU:HG	2.02	0.41
6:K:377:ALA:O	6:K:380:GLU:HG3	2.20	0.41
6:L:34:TYR:CD1	6:L:34:TYR:C	2.97	0.41
7:M:46:ALA:HA	7:M:49:TRP:NE1	2.35	0.41
1:B:102:TRP:HH2	7:M:162:HIS:CG	2.38	0.41
2:C:100:ASN:ND2	2:C:357:LEU:HD22	2.36	0.41
2:D:49:PHE:HZ	7:N:9:SER:HB3	1.84	0.41
9:D:504:PC1:H31	9:D:504:PC1:H241	2.02	0.41
10:K:503:UND:H72	10:K:503:UND:H42	1.86	0.41
6:L:193:LYS:HD3	6:L:193:LYS:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:91:MET:HE1	9:N:204:PC1:H32	2.01	0.41
6:K:94:ALA:HB3	6:K:101:ASN:HD21	1.85	0.41
1:B:82:ILE:HD11	7:M:133:ALA:CB	2.48	0.41
9:B:202:PC1:H143	9:B:202:PC1:H111	1.73	0.41
2:D:222:THR:HA	8:P:10:ALA:HA	2.02	0.41
9:M:201:PC1:H31	9:M:201:PC1:H321	1.83	0.41
6:L:68:LYS:HD2	6:L:69:GLU:H	1.85	0.41
6:L:135:LEU:HG	6:L:158:LEU:HD21	2.02	0.41
2:C:85:ASN:HB2	2:C:367:HIS:ND1	2.36	0.41
2:D:248:PRO:HB2	9:D:502:PC1:H122	2.02	0.41
6:L:297:VAL:O	6:L:301:LEU:HG	2.21	0.41
7:N:71:GLU:HG2	7:N:72:VAL:N	2.34	0.41
10:O:101:UND:H32	10:O:101:UND:H61	1.92	0.41
2:C:121:GLU:HA	2:C:137:TYR:O	2.21	0.41
2:C:145:LEU:HD23	3:E:33:PHE:CE2	2.56	0.41
4:G:574:GLU:O	4:G:577:VAL:HG12	2.21	0.41
6:K:353:VAL:HG12	6:K:354:PRO:HD2	2.03	0.41
1:A:74:GLN:HG3	1:A:76:GLN:H	1.86	0.41
9:A:203:PC1:H152	9:A:203:PC1:H112	1.79	0.41
1:B:39:VAL:O	1:B:42:THR:HG22	2.21	0.41
2:C:162:MET:HE1	2:C:368:PRO:HB3	2.01	0.41
4:G:602:TYR:CE2	6:K:3:SER:HA	2.55	0.41
10:G:702:UND:H51	10:G:702:UND:H82	1.83	0.41
6:K:110:LYS:O	6:K:114:VAL:HG23	2.20	0.41
6:K:191:THR:O	6:K:194:MET:HB2	2.20	0.41
6:L:89:LEU:HD12	6:L:89:LEU:HA	1.90	0.41
9:N:201:PC1:H143	9:N:201:PC1:H111	1.87	0.41
6:L:291:PRO:HD2	6:L:293:ILE:HG22	2.03	0.41
3:E:25:LEU:HD23	3:E:25:LEU:HA	1.93	0.40
4:H:602:TYR:CE1	6:L:4:PRO:HD2	2.56	0.40
7:N:117:LYS:HZ2	7:N:117:LYS:HG2	1.80	0.40
4:H:609:VAL:HG21	4:H:616:ALA:HB2	2.03	0.40
6:K:315:HIS:HB3	6:K:355:GLN:HG3	2.03	0.40
7:N:140:GLU:HG3	7:N:141:GLU:HG2	2.03	0.40
2:D:242:LEU:HD12	2:D:257:LEU:HG	2.03	0.40
6:K:33:ARG:HB2	8:O:21:TRP:CZ2	2.56	0.40
6:K:281:LEU:HD21	6:K:297:VAL:HG12	2.02	0.40
2:C:63:SER:O	2:C:67:VAL:HG13	2.21	0.40
6:K:59:ALA:O	6:K:62:LYS:HE2	2.22	0.40
6:K:102:ALA:HB1	6:K:150:LEU:HD13	2.04	0.40
6:K:332:CYS:C	6:K:374:ARG:HD3	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:158:LEU:O	6:L:162:THR:HG22	2.21	0.40
1:A:65:LEU:HD13	5:I:64:HIS:HB2	2.04	0.40
9:A:201:PC1:H111	9:A:201:PC1:H132	1.78	0.40
2:C:178:ILE:CG2	2:C:190:VAL:HG22	2.51	0.40
2:C:270:MET:HG2	7:M:86:PHE:HD1	1.87	0.40
5:I:38:THR:HB	5:I:39:PRO:HD3	2.04	0.40
6:K:62:LYS:HE2	6:K:62:LYS:HB3	1.87	0.40
6:K:210:LEU:HA	6:K:213:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/119 (88%)	104 (99%)	1 (1%)	0	100	100
1	B	104/119 (87%)	103 (99%)	1 (1%)	0	100	100
2	C	330/405 (82%)	318 (96%)	12 (4%)	0	100	100
2	D	330/405 (82%)	314 (95%)	16 (5%)	0	100	100
3	E	76/100 (76%)	73 (96%)	3 (4%)	0	100	100
3	F	75/100 (75%)	73 (97%)	2 (3%)	0	100	100
4	G	49/623 (8%)	48 (98%)	1 (2%)	0	100	100
4	H	51/623 (8%)	49 (96%)	2 (4%)	0	100	100
5	I	87/105 (83%)	85 (98%)	2 (2%)	0	100	100
5	J	86/105 (82%)	85 (99%)	1 (1%)	0	100	100
6	K	369/419 (88%)	357 (97%)	12 (3%)	0	100	100
6	L	320/419 (76%)	310 (97%)	10 (3%)	0	100	100
7	M	164/168 (98%)	159 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	N	163/168 (97%)	159 (98%)	4 (2%)	0	100	100
8	O	45/56 (80%)	45 (100%)	0	0	100	100
8	P	44/56 (79%)	44 (100%)	0	0	100	100
All	All	2398/3990 (60%)	2326 (97%)	72 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	89/100 (89%)	85 (96%)	4 (4%)	24	57
1	B	89/100 (89%)	88 (99%)	1 (1%)	65	86
2	C	272/328 (83%)	262 (96%)	10 (4%)	30	63
2	D	272/328 (83%)	260 (96%)	12 (4%)	25	58
3	E	65/83 (78%)	65 (100%)	0	100	100
3	F	64/83 (77%)	63 (98%)	1 (2%)	55	82
4	G	42/514 (8%)	36 (86%)	6 (14%)	3	10
4	H	44/514 (9%)	41 (93%)	3 (7%)	14	40
5	I	70/83 (84%)	64 (91%)	6 (9%)	10	29
5	J	69/83 (83%)	64 (93%)	5 (7%)	13	37
6	K	323/346 (93%)	303 (94%)	20 (6%)	16	44
6	L	290/346 (84%)	275 (95%)	15 (5%)	21	51
7	M	142/144 (99%)	135 (95%)	7 (5%)	22	53
7	N	141/144 (98%)	137 (97%)	4 (3%)	38	71
8	O	40/48 (83%)	38 (95%)	2 (5%)	22	53
8	P	40/48 (83%)	38 (95%)	2 (5%)	22	53
All	All	2052/3292 (62%)	1954 (95%)	98 (5%)	24	54

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	72	LEU
1	A	108	ASP
1	A	117	HIS
1	B	14	PHE
2	C	88	GLU
2	C	153	THR
2	C	156	LEU
2	C	190	VAL
2	C	221	LEU
2	C	245	GLU
2	C	337	ASP
2	C	358	GLU
2	C	360	LEU
2	C	365	TRP
2	D	72	THR
2	D	106	MET
2	D	173	THR
2	D	178	ILE
2	D	183	VAL
2	D	221	LEU
2	D	237	SER
2	D	250	LYS
2	D	299	SER
2	D	337	ASP
2	D	360	LEU
2	D	365	TRP
3	F	33	PHE
4	G	577	VAL
4	G	605	LEU
4	G	607	HIS
4	G	608	VAL
4	G	612	VAL
4	G	614	TRP
4	H	586	LEU
4	H	605	LEU
4	H	607	HIS
5	I	22	THR
5	I	23	LYS
5	I	37	LEU
5	I	51	VAL
5	I	53	GLN

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Mol	Chain	Res	Type
5	I	72	GLU
5	J	23	LYS
5	J	27	ARG
5	J	34	LEU
5	J	37	LEU
5	J	51	VAL
6	K	9	ILE
6	K	33	ARG
6	K	47	ILE
6	K	70	GLU
6	K	73	GLN
6	K	95	LEU
6	K	109	ILE
6	K	112	LEU
6	K	114	VAL
6	K	123	HIS
6	K	139	LEU
6	K	165	ASP
6	K	170	ILE
6	K	173	THR
6	K	197	VAL
6	K	278	LEU
6	K	298	LEU
6	K	315	HIS
6	K	349	LEU
6	K	353	VAL
6	L	68	LYS
6	L	78	THR
6	L	109	ILE
6	L	173	THR
6	L	175	VAL
6	L	194	MET
6	L	211	THR
6	L	258	THR
6	L	292	ARG
6	L	294	ILE
6	L	298	LEU
6	L	349	LEU
6	L	369	SER
6	L	399	MET
6	L	400	LEU
7	M	20	ILE

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Mol	Chain	Res	Type
7	M	25	SER
7	M	50	MET
7	M	52	THR
7	M	68	GLN
7	M	125	LYS
7	M	149	ARG
7	N	22	LEU
7	N	56	LEU
7	N	125	LYS
7	N	164	SER
8	O	26	ARG
8	O	42	ARG
8	P	26	ARG
8	P	42	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	B	75	GLN
2	C	179	GLN
2	C	189	GLN
2	C	333	ASN
2	C	339	HIS
2	C	369	GLN
2	D	44	GLN
2	D	179	GLN
2	D	339	HIS
5	I	76	GLN
5	J	16	ASN
5	J	20	GLN
6	K	249	GLN
6	K	355	GLN
6	K	387	GLN
6	L	397	GLN
7	N	43	HIS
7	N	150	GLN

5.3.3 RNA

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

81 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	PC1	N	202	-	20,20,53	1.27	2 (10%)	25,27,61	0.85	1 (4%)
10	UND	C	506	-	7,7,10	0.29	0	6,6,9	0.71	0
10	UND	K	503	-	10,10,10	0.28	0	9,9,9	0.84	0
10	UND	C	508	-	8,8,10	0.29	0	7,7,9	0.77	0
9	PC1	D	504	-	27,27,53	1.31	4 (14%)	33,35,61	3.89	9 (27%)
9	PC1	A	202	-	32,32,53	1.21	4 (12%)	38,40,61	1.11	2 (5%)
9	PC1	J	201	-	15,15,53	1.14	0	19,21,61	0.46	0
10	UND	M	210	-	10,10,10	0.30	0	9,9,9	0.80	0
10	UND	A	204	-	8,8,10	0.28	0	7,7,9	0.80	0
10	UND	G	703	-	8,8,10	0.29	0	7,7,9	0.77	0
9	PC1	F	201	-	28,28,53	1.28	4 (14%)	34,36,61	1.14	2 (5%)
9	PC1	E	203	-	21,21,53	1.23	2 (9%)	26,28,61	0.82	1 (3%)
9	PC1	H	701	-	19,19,53	1.29	2 (10%)	24,26,61	0.91	1 (4%)
9	PC1	N	203	-	26,26,53	1.11	2 (7%)	31,33,61	0.86	1 (3%)
9	PC1	I	201	-	20,20,53	1.27	2 (10%)	25,27,61	0.88	1 (4%)
10	UND	F	206	-	6,6,10	0.30	0	5,5,9	0.65	0
9	PC1	C	504	-	18,18,53	1.43	4 (22%)	20,20,61	1.57	3 (15%)
9	PC1	N	201	-	27,27,53	1.30	4 (14%)	33,35,61	1.14	2 (6%)
10	UND	M	207	-	7,7,10	0.29	0	6,6,9	0.73	0
9	PC1	B	203	-	29,29,53	1.26	4 (13%)	35,37,61	1.16	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	PC1	F	202	-	29,29,53	1.25	4 (13%)	35,37,61	1.13	2 (5%)
9	PC1	E	201	-	30,30,53	1.23	4 (13%)	36,38,61	1.07	2 (5%)
9	PC1	M	201	-	28,28,53	1.26	4 (14%)	34,36,61	1.11	2 (5%)
9	PC1	D	505	-	20,20,53	1.08	2 (10%)	21,21,61	1.20	2 (9%)
10	UND	J	204	-	7,7,10	0.29	0	6,6,9	0.72	0
9	PC1	I	203	-	18,18,53	1.23	1 (5%)	23,25,61	0.70	0
9	PC1	D	503	-	23,23,53	1.19	2 (8%)	28,30,61	0.85	1 (3%)
10	UND	K	506	-	6,6,10	0.30	0	5,5,9	0.67	0
10	UND	K	505	-	10,10,10	0.30	0	9,9,9	0.80	0
9	PC1	M	204	-	15,15,53	1.15	0	19,21,61	0.49	0
10	UND	M	208	-	7,7,10	0.28	0	6,6,9	0.73	0
9	PC1	E	202	-	28,28,53	1.28	4 (14%)	34,36,61	1.11	2 (5%)
9	PC1	F	205	-	28,28,53	1.07	2 (7%)	33,35,61	0.86	1 (3%)
10	UND	I	204	-	8,8,10	0.29	0	7,7,9	0.76	0
10	UND	M	209	-	10,10,10	0.29	0	9,9,9	0.79	0
9	PC1	B	202	-	24,24,53	1.16	2 (8%)	29,31,61	0.85	1 (3%)
10	UND	E	206	-	7,7,10	0.30	0	6,6,9	0.70	0
9	PC1	N	204	-	24,24,53	1.16	2 (8%)	29,31,61	0.87	1 (3%)
10	UND	L	503	-	6,6,10	0.30	0	5,5,9	0.67	0
10	UND	G	702	-	8,8,10	0.30	0	7,7,9	0.77	0
10	UND	O	102	-	10,10,10	0.29	0	9,9,9	0.82	0
9	PC1	A	201	-	21,21,53	1.23	2 (9%)	26,28,61	0.85	1 (3%)
10	UND	C	507	-	9,9,10	0.29	0	8,8,9	0.76	0
10	UND	B	205	-	9,9,10	0.28	0	8,8,9	0.79	0
9	PC1	C	505	-	25,25,53	1.14	2 (8%)	30,32,61	0.86	1 (3%)
10	UND	O	101	-	10,10,10	0.29	0	9,9,9	0.82	0
9	PC1	I	202	-	28,28,53	1.08	2 (7%)	33,35,61	0.85	1 (3%)
9	PC1	K	501	-	23,23,53	1.18	2 (8%)	28,30,61	0.84	1 (3%)
10	UND	E	205	-	10,10,10	0.29	0	9,9,9	0.81	0
10	UND	H	704	-	10,10,10	0.29	0	9,9,9	0.81	0
9	PC1	F	204	-	22,22,53	1.21	2 (9%)	27,29,61	0.85	1 (3%)
9	PC1	J	202	-	31,31,53	0.88	2 (6%)	32,32,61	1.14	2 (6%)
9	PC1	C	501	-	30,30,53	1.23	4 (13%)	36,38,61	1.01	2 (5%)
10	UND	F	207	-	10,10,10	0.29	0	9,9,9	0.81	0
9	PC1	D	502	-	20,20,53	1.26	2 (10%)	25,27,61	0.82	1 (4%)
10	UND	M	206	-	10,10,10	0.29	0	9,9,9	0.81	0
9	PC1	D	501	-	23,23,53	1.31	5 (21%)	27,28,61	1.25	2 (7%)
9	PC1	D	507	-	26,26,53	1.23	5 (19%)	30,31,61	1.21	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	UND	K	504	-	6,6,10	0.29	0	5,5,9	0.71	0
10	UND	M	205	-	9,9,10	0.28	0	8,8,9	0.79	0
9	PC1	H	702	-	18,18,53	1.23	1 (5%)	23,25,61	0.73	0
9	PC1	A	203	-	16,16,53	1.10	0	20,22,61	0.53	0
10	UND	A	205	-	9,9,10	0.28	0	8,8,9	0.80	0
10	UND	J	203	-	9,9,10	0.29	0	8,8,9	0.79	0
9	PC1	D	506	-	28,28,53	1.26	4 (14%)	34,36,61	1.07	2 (5%)
9	PC1	C	503	-	18,18,53	1.24	1 (5%)	23,25,61	0.76	0
10	UND	H	703	-	8,8,10	0.29	0	7,7,9	0.76	0
10	UND	G	704	-	8,8,10	0.30	0	7,7,9	0.76	0
9	PC1	L	502	-	16,16,53	1.10	0	20,22,61	0.52	0
9	PC1	M	203	-	28,28,53	1.07	2 (7%)	33,35,61	0.87	1 (3%)
10	UND	B	204	-	10,10,10	0.28	0	9,9,9	0.80	0
9	PC1	K	502	-	23,23,53	1.18	2 (8%)	28,30,61	0.83	1 (3%)
9	PC1	L	501	-	20,20,53	1.27	2 (10%)	25,27,61	0.85	1 (4%)
9	PC1	B	201	-	33,33,53	1.19	4 (12%)	39,41,61	1.09	2 (5%)
10	UND	D	508	-	8,8,10	0.28	0	7,7,9	0.76	0
10	UND	G	701	-	8,8,10	0.29	0	7,7,9	0.76	0
9	PC1	F	203	-	27,27,53	1.10	2 (7%)	32,34,61	0.84	1 (3%)
10	UND	H	705	-	9,9,10	0.29	0	8,8,9	0.79	0
9	PC1	E	204	-	24,24,53	1.16	2 (8%)	29,31,61	0.84	1 (3%)
9	PC1	M	202	-	25,25,53	1.14	2 (8%)	30,32,61	0.85	1 (3%)
9	PC1	C	502	-	26,26,53	1.11	2 (7%)	31,33,61	0.85	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PC1	N	202	-	-	6/22/22/57	-
10	UND	C	506	-	-	1/5/5/8	-
10	UND	K	503	-	-	0/8/8/8	-
10	UND	C	508	-	-	0/6/6/8	-
9	PC1	D	504	-	-	18/31/31/57	-
9	PC1	A	202	-	-	15/36/36/57	-
9	PC1	J	201	-	-	5/16/16/57	-
10	UND	M	210	-	-	0/8/8/8	-
10	UND	A	204	-	-	0/6/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	UND	G	703	-	-	0/6/6/8	-
9	PC1	F	201	-	-	11/32/32/57	-
9	PC1	E	203	-	-	11/23/23/57	-
9	PC1	H	701	-	-	14/21/21/57	-
9	PC1	N	203	-	-	15/28/28/57	-
9	PC1	I	201	-	-	7/22/22/57	-
10	UND	F	206	-	-	0/4/4/8	-
9	PC1	C	504	-	-	5/19/19/57	-
9	PC1	N	201	-	-	15/31/31/57	-
10	UND	M	207	-	-	1/5/5/8	-
9	PC1	B	203	-	-	16/33/33/57	-
9	PC1	F	202	-	-	14/33/33/57	-
9	PC1	E	201	-	-	14/34/34/57	-
9	PC1	M	201	-	-	16/32/32/57	-
9	PC1	D	505	-	-	13/20/20/57	-
10	UND	J	204	-	-	0/5/5/8	-
9	PC1	I	203	-	-	12/19/19/57	-
9	PC1	D	503	-	-	13/25/25/57	-
10	UND	K	506	-	-	0/4/4/8	-
10	UND	K	505	-	-	2/8/8/8	-
9	PC1	M	204	-	-	10/16/16/57	-
10	UND	M	208	-	-	0/5/5/8	-
9	PC1	E	202	-	-	15/32/32/57	-
9	PC1	F	205	-	-	15/30/30/57	-
10	UND	I	204	-	-	1/6/6/8	-
10	UND	M	209	-	-	2/8/8/8	-
9	PC1	B	202	-	-	13/26/26/57	-
10	UND	E	206	-	-	1/5/5/8	-
9	PC1	N	204	-	-	18/26/26/57	-
10	UND	L	503	-	-	0/4/4/8	-
10	UND	G	702	-	-	0/6/6/8	-
10	UND	O	102	-	-	1/8/8/8	-
9	PC1	A	201	-	-	7/23/23/57	-
10	UND	C	507	-	-	2/7/7/8	-
10	UND	B	205	-	-	4/7/7/8	-
9	PC1	C	505	-	-	15/27/27/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	UND	O	101	-	-	0/8/8/8	-
9	PC1	I	202	-	-	14/30/30/57	-
9	PC1	K	501	-	-	14/25/25/57	-
10	UND	E	205	-	-	0/8/8/8	-
10	UND	H	704	-	-	0/8/8/8	-
9	PC1	F	204	-	-	10/24/24/57	-
9	PC1	J	202	-	-	18/31/31/57	-
9	PC1	C	501	-	-	18/34/34/57	-
10	UND	F	207	-	-	2/8/8/8	-
9	PC1	D	502	-	-	9/22/22/57	-
10	UND	M	206	-	-	3/8/8/8	-
9	PC1	D	501	-	-	16/25/25/57	-
9	PC1	D	507	-	-	14/28/28/57	-
10	UND	K	504	-	-	0/4/4/8	-
10	UND	M	205	-	-	0/7/7/8	-
9	PC1	H	702	-	-	9/19/19/57	-
9	PC1	A	203	-	-	7/17/17/57	-
10	UND	A	205	-	-	4/7/7/8	-
10	UND	J	203	-	-	2/7/7/8	-
9	PC1	D	506	-	-	17/32/32/57	-
9	PC1	C	503	-	-	7/19/19/57	-
10	UND	H	703	-	-	0/6/6/8	-
10	UND	G	704	-	-	0/6/6/8	-
9	PC1	L	502	-	-	11/17/17/57	-
9	PC1	M	203	-	-	15/30/30/57	-
10	UND	B	204	-	-	3/8/8/8	-
9	PC1	K	502	-	-	12/25/25/57	-
9	PC1	L	501	-	-	12/22/22/57	-
9	PC1	B	201	-	-	16/37/37/57	-
10	UND	D	508	-	-	1/6/6/8	-
10	UND	G	701	-	-	0/6/6/8	-
9	PC1	F	203	-	-	16/29/29/57	-
10	UND	H	705	-	-	0/7/7/8	-
9	PC1	E	204	-	-	12/26/26/57	-
9	PC1	M	202	-	-	15/27/27/57	-
9	PC1	C	502	-	-	16/28/28/57	-

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	504	PC1	O21-C2	-3.92	1.40	1.47
9	D	501	PC1	P-O13	2.69	1.65	1.54
9	D	507	PC1	P-O13	2.66	1.65	1.54
9	N	201	PC1	O21-C2	-2.63	1.40	1.46
9	B	203	PC1	O21-C2	-2.58	1.40	1.46
9	E	202	PC1	O21-C2	-2.56	1.40	1.46
9	A	202	PC1	O21-C2	-2.55	1.40	1.46
9	F	201	PC1	O21-C2	-2.54	1.40	1.46
9	D	504	PC1	O21-C2	-2.53	1.40	1.46
9	D	501	PC1	O21-C2	-2.53	1.40	1.46
9	D	507	PC1	O21-C2	-2.49	1.40	1.46
9	B	201	PC1	O21-C2	-2.49	1.40	1.46
9	F	202	PC1	O21-C2	-2.49	1.40	1.46
9	M	201	PC1	O21-C2	-2.48	1.40	1.46
9	J	202	PC1	O21-C21	2.40	1.40	1.33
9	C	501	PC1	O21-C21	2.39	1.41	1.34
9	L	501	PC1	O31-C31	2.38	1.40	1.33
9	F	201	PC1	O31-C31	2.38	1.40	1.33
9	B	201	PC1	O31-C31	2.38	1.40	1.33
9	F	202	PC1	O31-C31	2.37	1.40	1.33
9	K	502	PC1	O31-C31	2.37	1.40	1.33
9	N	201	PC1	O31-C31	2.37	1.40	1.33
9	D	507	PC1	O31-C31	2.36	1.40	1.33
9	I	201	PC1	O31-C31	2.36	1.40	1.33
9	B	203	PC1	O31-C31	2.36	1.40	1.33
9	D	505	PC1	O21-C21	2.36	1.40	1.33
9	C	501	PC1	O31-C31	2.36	1.40	1.33
9	N	202	PC1	O31-C31	2.35	1.40	1.33
9	I	202	PC1	O31-C31	2.35	1.40	1.33
9	D	501	PC1	O31-C31	2.35	1.40	1.33
9	M	201	PC1	O31-C31	2.35	1.40	1.33
9	E	203	PC1	O31-C31	2.34	1.40	1.33
9	D	503	PC1	O31-C31	2.34	1.40	1.33
9	D	502	PC1	O31-C31	2.34	1.40	1.33
9	E	201	PC1	O31-C31	2.34	1.40	1.33
9	H	701	PC1	O31-C31	2.34	1.40	1.33
9	D	506	PC1	O31-C31	2.33	1.40	1.33
9	E	204	PC1	O31-C31	2.33	1.40	1.33
9	B	202	PC1	O31-C31	2.33	1.40	1.33
9	N	203	PC1	O31-C31	2.33	1.40	1.33
9	F	204	PC1	O31-C31	2.33	1.40	1.33
9	F	205	PC1	O31-C31	2.33	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	201	PC1	O31-C31	2.32	1.40	1.33
9	D	505	PC1	O31-C31	2.32	1.40	1.33
9	M	202	PC1	O31-C31	2.32	1.40	1.33
9	K	501	PC1	O31-C31	2.32	1.40	1.33
9	C	504	PC1	O31-C31	2.31	1.40	1.33
9	C	505	PC1	O31-C31	2.31	1.40	1.33
9	E	202	PC1	O31-C31	2.31	1.40	1.33
9	M	203	PC1	O31-C31	2.30	1.40	1.33
9	J	202	PC1	O31-C31	2.30	1.40	1.33
9	F	203	PC1	O31-C31	2.30	1.40	1.33
9	D	504	PC1	O31-C31	2.29	1.40	1.33
9	D	504	PC1	O31-C3	-2.29	1.39	1.45
9	C	502	PC1	O31-C31	2.28	1.40	1.33
9	N	204	PC1	O31-C31	2.28	1.40	1.33
9	E	201	PC1	O21-C2	-2.27	1.40	1.46
9	N	204	PC1	O31-C3	-2.27	1.40	1.45
9	E	201	PC1	O21-C21	2.26	1.40	1.34
9	A	202	PC1	O31-C3	-2.26	1.40	1.45
9	E	202	PC1	O31-C3	-2.24	1.40	1.45
9	A	202	PC1	O31-C31	2.24	1.39	1.33
9	C	502	PC1	O31-C3	-2.23	1.40	1.45
9	M	202	PC1	O31-C3	-2.22	1.40	1.45
9	D	506	PC1	O21-C2	-2.21	1.41	1.46
9	D	503	PC1	O31-C3	-2.21	1.40	1.45
9	K	501	PC1	O31-C3	-2.21	1.40	1.45
9	F	203	PC1	O31-C3	-2.21	1.40	1.45
9	F	204	PC1	O31-C3	-2.21	1.40	1.45
9	F	205	PC1	O31-C3	-2.21	1.40	1.45
9	B	202	PC1	O31-C3	-2.20	1.40	1.45
9	C	503	PC1	O31-C3	-2.20	1.40	1.45
9	C	505	PC1	O31-C3	-2.19	1.40	1.45
9	F	201	PC1	O31-C3	-2.19	1.40	1.45
9	D	506	PC1	O21-C21	2.19	1.40	1.34
9	D	501	PC1	O31-C3	-2.19	1.40	1.45
9	H	701	PC1	O31-C3	-2.19	1.40	1.45
9	C	501	PC1	O31-C3	-2.19	1.40	1.45
9	M	203	PC1	O31-C3	-2.19	1.40	1.45
9	B	201	PC1	O31-C3	-2.19	1.40	1.45
9	E	203	PC1	O31-C3	-2.19	1.40	1.45
9	N	203	PC1	O31-C3	-2.18	1.40	1.45
9	D	506	PC1	O31-C3	-2.18	1.40	1.45
9	C	504	PC1	O31-C3	-2.18	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	202	PC1	O31-C3	-2.18	1.40	1.45
9	I	201	PC1	O31-C3	-2.18	1.40	1.45
9	D	502	PC1	O31-C3	-2.18	1.40	1.45
9	I	203	PC1	O31-C3	-2.17	1.40	1.45
9	A	201	PC1	O31-C3	-2.17	1.40	1.45
9	E	204	PC1	O31-C3	-2.17	1.40	1.45
9	D	507	PC1	O31-C3	-2.17	1.40	1.45
9	E	201	PC1	O31-C3	-2.17	1.40	1.45
9	I	202	PC1	O31-C3	-2.17	1.40	1.45
9	F	202	PC1	O21-C21	2.17	1.40	1.34
9	D	507	PC1	O21-C21	2.16	1.40	1.34
9	B	203	PC1	O31-C3	-2.16	1.40	1.45
9	N	201	PC1	O31-C3	-2.16	1.40	1.45
9	F	201	PC1	O21-C21	2.16	1.40	1.34
9	F	202	PC1	O31-C3	-2.16	1.40	1.45
9	M	201	PC1	O21-C21	2.15	1.40	1.34
9	H	702	PC1	O31-C3	-2.15	1.40	1.45
9	L	501	PC1	O31-C3	-2.15	1.40	1.45
9	K	502	PC1	O31-C3	-2.15	1.40	1.45
9	A	202	PC1	O21-C21	2.14	1.40	1.34
9	M	201	PC1	O31-C3	-2.14	1.40	1.45
9	D	501	PC1	O21-C21	2.13	1.40	1.34
9	D	504	PC1	O21-C21	2.12	1.40	1.34
9	C	501	PC1	O21-C2	-2.11	1.41	1.46
9	B	201	PC1	O21-C21	2.11	1.40	1.34
9	C	504	PC1	O21-C21	2.11	1.40	1.34
9	B	203	PC1	O21-C21	2.09	1.40	1.34
9	E	202	PC1	O21-C21	2.08	1.40	1.34
9	N	201	PC1	O21-C21	2.03	1.40	1.34

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	504	PC1	C15-N-C13	-11.28	79.97	108.97
9	D	504	PC1	C15-N-C14	-11.04	80.59	108.97
9	D	504	PC1	C14-N-C13	8.50	130.83	108.97
9	D	504	PC1	C14-N-C12	-7.41	79.59	109.92
9	D	504	PC1	C13-N-C12	-7.14	80.71	109.92
9	D	504	PC1	C15-N-C12	5.34	131.78	109.92
9	B	203	PC1	O21-C21-C22	4.16	120.47	111.50
9	F	201	PC1	O21-C21-C22	4.10	120.35	111.50
9	N	201	PC1	O21-C21-C22	4.04	120.22	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	201	PC1	O21-C21-C22	4.04	120.20	111.50
9	C	504	PC1	O21-C21-C22	3.99	120.10	111.50
9	M	201	PC1	O21-C21-C22	3.98	120.07	111.50
9	D	506	PC1	O21-C21-C22	3.96	120.04	111.50
9	F	202	PC1	O21-C21-C22	3.94	120.00	111.50
9	A	202	PC1	O21-C21-C22	3.94	120.00	111.50
9	E	202	PC1	O21-C21-C22	3.93	119.96	111.50
9	D	504	PC1	O21-C21-C22	3.93	119.96	111.50
9	E	201	PC1	O21-C21-C22	3.88	119.87	111.50
9	D	501	PC1	O21-C21-C22	3.87	119.83	111.50
9	D	507	PC1	O21-C21-C22	3.83	119.76	111.50
9	C	501	PC1	O21-C21-C22	3.63	119.33	111.50
9	H	701	PC1	O31-C31-C32	3.23	119.86	111.38
9	C	504	PC1	C2-O21-C21	-3.06	113.94	117.88
9	M	201	PC1	O31-C31-C32	2.86	120.87	111.91
9	F	202	PC1	O31-C31-C32	2.83	120.78	111.91
9	F	201	PC1	O31-C31-C32	2.72	120.45	111.91
9	E	202	PC1	O31-C31-C32	2.70	120.38	111.91
9	I	201	PC1	O31-C31-C32	2.69	120.35	111.91
9	E	201	PC1	O31-C31-C32	2.68	120.32	111.91
9	N	202	PC1	O31-C31-C32	2.66	120.24	111.91
9	D	506	PC1	O31-C31-C32	2.65	120.23	111.91
9	D	503	PC1	O31-C31-C32	2.65	120.22	111.91
9	C	505	PC1	O31-C31-C32	2.64	120.19	111.91
9	F	204	PC1	O31-C31-C32	2.64	120.18	111.91
9	K	502	PC1	O31-C31-C32	2.63	120.17	111.91
9	F	205	PC1	O31-C31-C32	2.62	120.14	111.91
9	D	501	PC1	O31-C31-C32	2.62	120.14	111.91
9	N	201	PC1	O31-C31-C32	2.61	120.11	111.91
9	D	507	PC1	O31-C31-C32	2.61	120.10	111.91
9	I	202	PC1	O31-C31-C32	2.61	120.10	111.91
9	N	204	PC1	O31-C31-C32	2.60	120.06	111.91
9	D	505	PC1	O21-C21-C22	2.60	120.06	111.91
9	L	501	PC1	O31-C31-C32	2.59	120.03	111.91
9	J	202	PC1	O21-C21-C22	2.58	120.01	111.91
9	A	201	PC1	O31-C31-C32	2.58	120.01	111.91
9	K	501	PC1	O31-C31-C32	2.58	120.00	111.91
9	D	505	PC1	O31-C31-C32	2.58	119.99	111.91
9	B	203	PC1	O31-C31-C32	2.58	119.99	111.91
9	E	203	PC1	O31-C31-C32	2.57	119.99	111.91
9	N	203	PC1	O31-C31-C32	2.57	119.97	111.91
9	M	203	PC1	O31-C31-C32	2.57	119.97	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	202	PC1	O31-C31-C32	2.57	119.97	111.91
9	M	202	PC1	O31-C31-C32	2.56	119.95	111.91
9	E	204	PC1	O31-C31-C32	2.56	119.94	111.91
9	D	502	PC1	O31-C31-C32	2.56	119.94	111.91
9	D	504	PC1	O31-C31-C32	2.55	119.91	111.91
9	C	502	PC1	O31-C31-C32	2.55	119.90	111.91
9	B	201	PC1	O31-C31-C32	2.54	119.89	111.91
9	B	202	PC1	O31-C31-C32	2.54	119.88	111.91
9	C	504	PC1	O31-C31-C32	2.54	119.88	111.91
9	A	202	PC1	O31-C31-C32	2.52	119.80	111.91
9	F	203	PC1	O31-C31-C32	2.52	119.80	111.91
9	C	501	PC1	O31-C31-C32	2.43	119.53	111.91
9	D	504	PC1	C11-C12-N	-2.02	109.05	115.78

There are no chirality outliers.

All (621) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	201	PC1	C1-O11-P-O12
9	A	202	PC1	C11-O13-P-O14
9	A	202	PC1	C11-O13-P-O11
9	A	202	PC1	C22-C21-O21-C2
9	A	203	PC1	O13-C11-C12-N
9	A	203	PC1	C1-C2-C3-O31
9	B	201	PC1	C11-O13-P-O12
9	B	201	PC1	C1-O11-P-O12
9	B	201	PC1	C1-O11-P-O14
9	B	201	PC1	C1-O11-P-O13
9	B	202	PC1	C1-O11-P-O12
9	B	202	PC1	C1-O11-P-O14
9	B	202	PC1	O13-C11-C12-N
9	B	202	PC1	O21-C2-C3-O31
9	B	203	PC1	C11-O13-P-O11
9	B	203	PC1	O13-C11-C12-N
9	B	203	PC1	C22-C21-O21-C2
9	B	203	PC1	C32-C31-O31-C3
9	C	501	PC1	C11-O13-P-O14
9	C	501	PC1	C1-O11-P-O12
9	C	501	PC1	C1-O11-P-O14
9	C	502	PC1	C11-O13-P-O11
9	C	502	PC1	C1-O11-P-O12
9	C	502	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
9	C	502	PC1	O11-C1-C2-O21
9	C	502	PC1	C1-C2-C3-O31
9	C	503	PC1	C1-O11-P-O12
9	C	503	PC1	C1-C2-C3-O31
9	C	505	PC1	C11-O13-P-O12
9	C	505	PC1	O13-C11-C12-N
9	C	505	PC1	C1-C2-C3-O31
9	D	501	PC1	C1-O11-P-O12
9	D	501	PC1	C1-O11-P-O14
9	D	501	PC1	C1-O11-P-O13
9	D	502	PC1	C1-O11-P-O12
9	D	502	PC1	C1-O11-P-O14
9	D	502	PC1	C1-O11-P-O13
9	D	503	PC1	O11-C1-C2-O21
9	D	503	PC1	C1-C2-C3-O31
9	D	503	PC1	O21-C2-C3-O31
9	D	504	PC1	C11-O13-P-O12
9	D	504	PC1	C1-O11-P-O12
9	D	504	PC1	C1-O11-P-O14
9	D	504	PC1	C1-O11-P-O13
9	D	504	PC1	O13-C11-C12-N
9	D	506	PC1	C22-C21-O21-C2
9	E	201	PC1	C12-C11-O13-P
9	E	201	PC1	O13-C11-C12-N
9	E	202	PC1	C11-O13-P-O12
9	E	202	PC1	C11-O13-P-O14
9	E	202	PC1	C11-O13-P-O11
9	E	203	PC1	C1-O11-P-O12
9	E	203	PC1	C1-O11-P-O14
9	E	203	PC1	C12-C11-O13-P
9	E	203	PC1	O21-C2-C3-O31
9	E	204	PC1	O13-C11-C12-N
9	E	204	PC1	O11-C1-C2-O21
9	F	201	PC1	C12-C11-O13-P
9	F	201	PC1	O13-C11-C12-N
9	F	201	PC1	O22-C21-O21-C2
9	F	201	PC1	C22-C21-O21-C2
9	F	202	PC1	C11-O13-P-O11
9	F	202	PC1	O21-C2-C3-O31
9	F	202	PC1	C22-C21-O21-C2
9	F	203	PC1	O13-C11-C12-N
9	F	203	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
9	F	204	PC1	C11-O13-P-O11
9	F	204	PC1	C1-O11-P-O12
9	F	205	PC1	C12-C11-O13-P
9	H	701	PC1	C11-O13-P-O12
9	H	701	PC1	C11-O13-P-O14
9	H	701	PC1	C1-O11-P-O12
9	H	701	PC1	C1-O11-P-O14
9	H	701	PC1	C1-O11-P-O13
9	H	701	PC1	C1-C2-C3-O31
9	H	702	PC1	C11-O13-P-O14
9	H	702	PC1	C1-O11-P-O12
9	H	702	PC1	C1-C2-C3-O31
9	H	702	PC1	O21-C2-C3-O31
9	I	202	PC1	C1-O11-P-O12
9	I	202	PC1	C1-C2-C3-O31
9	I	203	PC1	C11-O13-P-O12
9	I	203	PC1	O13-C11-C12-N
9	I	203	PC1	O11-C1-C2-O21
9	I	203	PC1	C1-C2-C3-O31
9	J	201	PC1	O13-C11-C12-N
9	J	201	PC1	C1-C2-C3-O31
9	K	501	PC1	C2-C1-O11-P
9	K	501	PC1	C1-C2-C3-O31
9	K	502	PC1	C11-O13-P-O14
9	K	502	PC1	C1-C2-C3-O31
9	K	502	PC1	O21-C2-C3-O31
9	L	501	PC1	C11-O13-P-O11
9	L	501	PC1	C1-O11-P-O12
9	L	501	PC1	C1-O11-P-O14
9	L	501	PC1	O21-C2-C3-O31
9	L	502	PC1	C1-O11-P-O12
9	L	502	PC1	C1-O11-P-O14
9	L	502	PC1	C1-O11-P-O13
9	M	201	PC1	C11-O13-P-O11
9	M	201	PC1	C22-C21-O21-C2
9	M	202	PC1	C11-O13-P-O14
9	M	202	PC1	C11-O13-P-O11
9	M	202	PC1	C1-O11-P-O14
9	M	202	PC1	C2-C1-O11-P
9	M	202	PC1	O11-C1-C2-C3
9	M	202	PC1	C1-C2-C3-O31
9	M	203	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
9	M	203	PC1	C1-O11-P-O12
9	M	203	PC1	C1-O11-P-O14
9	M	203	PC1	C1-O11-P-O13
9	M	203	PC1	C1-C2-C3-O31
9	M	204	PC1	C1-O11-P-O12
9	M	204	PC1	C1-O11-P-O14
9	M	204	PC1	O13-C11-C12-N
9	M	204	PC1	C1-C2-C3-O31
9	M	204	PC1	O21-C2-C3-O31
9	N	201	PC1	C1-O11-P-O14
9	N	201	PC1	C1-O11-P-O13
9	N	201	PC1	O13-C11-C12-N
9	N	201	PC1	O22-C21-O21-C2
9	N	202	PC1	C11-O13-P-O11
9	N	202	PC1	C1-O11-P-O12
9	N	202	PC1	C1-O11-P-O14
9	N	202	PC1	C1-O11-P-O13
9	N	203	PC1	C11-O13-P-O11
9	N	203	PC1	C1-C2-C3-O31
9	N	203	PC1	O21-C2-C3-O31
9	N	204	PC1	C11-O13-P-O14
9	N	204	PC1	C11-O13-P-O11
9	N	204	PC1	O13-C11-C12-N
9	N	204	PC1	O21-C2-C3-O31
9	I	203	PC1	C32-C31-O31-C3
9	B	202	PC1	O32-C31-O31-C3
9	B	203	PC1	O32-C31-O31-C3
9	I	202	PC1	O32-C31-O31-C3
9	J	202	PC1	O32-C31-O31-C3
9	K	501	PC1	O32-C31-O31-C3
9	M	201	PC1	O32-C31-O31-C3
9	N	202	PC1	O32-C31-O31-C3
9	J	202	PC1	C32-C31-O31-C3
9	K	501	PC1	C32-C31-O31-C3
9	M	201	PC1	C32-C31-O31-C3
9	N	202	PC1	C32-C31-O31-C3
9	C	504	PC1	O32-C31-O31-C3
9	C	505	PC1	O32-C31-O31-C3
9	D	501	PC1	O32-C31-O31-C3
9	D	503	PC1	O32-C31-O31-C3
9	D	504	PC1	O32-C31-O31-C3
9	D	505	PC1	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
9	E	201	PC1	O32-C31-O31-C3
9	F	201	PC1	O32-C31-O31-C3
9	F	202	PC1	O32-C31-O31-C3
9	F	203	PC1	O32-C31-O31-C3
9	F	204	PC1	O32-C31-O31-C3
9	I	201	PC1	O32-C31-O31-C3
9	J	202	PC1	O22-C21-O21-C2
9	A	202	PC1	O22-C21-O21-C2
9	B	203	PC1	O22-C21-O21-C2
9	D	506	PC1	O22-C21-O21-C2
9	E	201	PC1	O22-C21-O21-C2
9	F	202	PC1	O22-C21-O21-C2
9	M	201	PC1	O22-C21-O21-C2
9	B	202	PC1	C32-C31-O31-C3
9	C	504	PC1	C32-C31-O31-C3
9	C	505	PC1	C32-C31-O31-C3
9	D	503	PC1	C32-C31-O31-C3
9	D	504	PC1	C32-C31-O31-C3
9	D	505	PC1	C32-C31-O31-C3
9	E	201	PC1	C32-C31-O31-C3
9	F	201	PC1	C32-C31-O31-C3
9	F	202	PC1	C32-C31-O31-C3
9	F	203	PC1	C32-C31-O31-C3
9	F	204	PC1	C32-C31-O31-C3
9	I	201	PC1	C32-C31-O31-C3
9	I	202	PC1	C32-C31-O31-C3
9	N	203	PC1	C32-C31-O31-C3
9	E	201	PC1	C22-C21-O21-C2
9	N	201	PC1	C22-C21-O21-C2
9	I	203	PC1	O32-C31-O31-C3
9	E	202	PC1	O32-C31-O31-C3
9	D	501	PC1	C32-C31-O31-C3
9	J	202	PC1	C22-C21-O21-C2
9	N	203	PC1	O32-C31-O31-C3
9	F	205	PC1	O11-C1-C2-O21
9	M	202	PC1	O11-C1-C2-O21
9	D	507	PC1	C32-C31-O31-C3
9	A	203	PC1	O21-C2-C3-O31
9	C	503	PC1	O21-C2-C3-O31
9	C	505	PC1	O21-C2-C3-O31
9	H	701	PC1	O21-C2-C3-O31
9	I	202	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
9	I	203	PC1	O21-C2-C3-O31
9	B	201	PC1	C22-C21-O21-C2
9	D	504	PC1	C22-C21-O21-C2
9	E	202	PC1	C32-C31-O31-C3
9	B	201	PC1	O22-C21-O21-C2
9	F	202	PC1	C2-C1-O11-P
9	D	507	PC1	O32-C31-O31-C3
9	N	204	PC1	C32-C31-O31-C3
9	D	505	PC1	O21-C2-C3-O31
9	N	204	PC1	O11-C1-C2-C3
9	D	504	PC1	O22-C21-O21-C2
9	I	201	PC1	C1-C2-C3-O31
9	L	502	PC1	C1-C2-C3-O31
9	K	502	PC1	O11-C1-C2-O21
9	D	505	PC1	C21-C22-C23-C24
9	C	502	PC1	O21-C2-C3-O31
9	F	202	PC1	C21-C22-C23-C24
9	B	203	PC1	C31-C32-C33-C34
9	C	501	PC1	C31-C32-C33-C34
9	D	506	PC1	C21-C22-C23-C24
9	E	201	PC1	C21-C22-C23-C24
9	M	201	PC1	C31-C32-C33-C34
9	M	202	PC1	C34-C35-C36-C37
9	D	506	PC1	C31-C32-C33-C34
9	L	502	PC1	O11-C1-C2-O21
9	N	204	PC1	O11-C1-C2-O21
9	N	204	PC1	O32-C31-O31-C3
9	F	201	PC1	C21-C22-C23-C24
9	D	502	PC1	O21-C2-C3-O31
9	F	205	PC1	O21-C2-C3-O31
9	I	201	PC1	O21-C2-C3-O31
9	L	502	PC1	O21-C2-C3-O31
9	M	202	PC1	O21-C2-C3-O31
9	M	203	PC1	O21-C2-C3-O31
9	A	201	PC1	C1-O11-P-O13
9	A	202	PC1	C1-O11-P-O13
9	A	203	PC1	C11-O13-P-O11
9	B	201	PC1	C11-O13-P-O11
9	B	202	PC1	C1-O11-P-O13
9	B	203	PC1	C1-O11-P-O13
9	C	501	PC1	C1-O11-P-O13
9	C	502	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
9	C	505	PC1	C11-O13-P-O11
9	D	504	PC1	C11-O13-P-O11
9	E	201	PC1	C11-O13-P-O11
9	E	203	PC1	C11-O13-P-O11
9	E	203	PC1	C1-O11-P-O13
9	E	204	PC1	C1-O11-P-O13
9	F	201	PC1	C11-O13-P-O11
9	F	204	PC1	C1-O11-P-O13
9	F	205	PC1	C11-O13-P-O11
9	F	205	PC1	C1-O11-P-O13
9	H	701	PC1	C11-O13-P-O11
9	I	202	PC1	C1-O11-P-O13
9	I	203	PC1	C11-O13-P-O11
9	I	203	PC1	C1-O11-P-O13
9	K	501	PC1	C11-O13-P-O11
9	K	501	PC1	C1-O11-P-O13
9	K	502	PC1	C11-O13-P-O11
9	L	501	PC1	C1-O11-P-O13
9	M	201	PC1	C1-O11-P-O13
9	M	204	PC1	C1-O11-P-O13
9	N	201	PC1	C11-O13-P-O11
9	N	204	PC1	C1-O11-P-O13
9	C	502	PC1	O11-C1-C2-C3
9	D	503	PC1	O11-C1-C2-C3
9	E	204	PC1	O11-C1-C2-C3
9	F	205	PC1	O11-C1-C2-C3
9	I	203	PC1	O11-C1-C2-C3
9	L	502	PC1	O11-C1-C2-C3
9	L	502	PC1	C2-C3-O31-C31
9	D	504	PC1	C11-C12-N-C13
9	H	701	PC1	C32-C31-O31-C3
9	B	202	PC1	C32-C33-C34-C35
9	I	202	PC1	C34-C35-C36-C37
9	J	202	PC1	C25-C26-C27-C28
9	M	201	PC1	C32-C33-C34-C35
10	B	204	UND	C2-C3-C4-C5
9	D	502	PC1	C1-C2-C3-O31
9	E	203	PC1	C1-C2-C3-O31
9	F	205	PC1	C1-C2-C3-O31
9	L	501	PC1	C1-C2-C3-O31
9	N	204	PC1	C1-C2-C3-O31
9	B	203	PC1	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
9	C	505	PC1	C34-C35-C36-C37
9	F	203	PC1	C35-C36-C37-C38
10	C	506	UND	C4-C5-C6-C7
9	D	507	PC1	C24-C25-C26-C27
9	J	202	PC1	C26-C27-C28-C29
9	J	202	PC1	C34-C35-C36-C37
9	E	203	PC1	C2-C1-O11-P
9	F	203	PC1	C36-C37-C38-C39
9	K	501	PC1	O11-C1-C2-O21
9	B	201	PC1	C31-C32-C33-C34
9	M	202	PC1	C35-C36-C37-C38
9	K	501	PC1	C32-C33-C34-C35
9	A	202	PC1	C24-C25-C26-C27
9	F	204	PC1	C32-C33-C34-C35
9	M	202	PC1	C32-C33-C34-C35
9	N	204	PC1	C33-C34-C35-C36
9	N	204	PC1	C34-C35-C36-C37
9	A	202	PC1	C23-C24-C25-C26
9	B	201	PC1	C34-C35-C36-C37
9	K	502	PC1	C32-C33-C34-C35
10	C	507	UND	C2-C3-C4-C5
9	C	504	PC1	C22-C21-O21-C2
9	F	205	PC1	C31-C32-C33-C34
9	N	204	PC1	C31-C32-C33-C34
9	B	201	PC1	C32-C33-C34-C35
9	C	502	PC1	C34-C35-C36-C37
9	D	504	PC1	C11-C12-N-C14
9	N	203	PC1	C34-C35-C36-C37
9	B	201	PC1	C33-C34-C35-C36
9	F	203	PC1	C32-C33-C34-C35
9	I	202	PC1	C35-C36-C37-C38
9	J	202	PC1	C35-C36-C37-C38
9	B	202	PC1	C31-C32-C33-C34
9	J	202	PC1	C21-C22-C23-C24
9	M	203	PC1	C31-C32-C33-C34
9	A	201	PC1	C32-C31-O31-C3
9	C	502	PC1	C32-C31-O31-C3
9	B	203	PC1	C32-C33-C34-C35
9	N	203	PC1	C33-C34-C35-C36
10	A	205	UND	C4-C5-C6-C7
9	D	501	PC1	C31-C32-C33-C34
9	D	501	PC1	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
9	J	201	PC1	O21-C2-C3-O31
9	D	503	PC1	C32-C33-C34-C35
9	I	202	PC1	C38-C39-C3A-C3B
9	J	202	PC1	C24-C25-C26-C27
9	H	701	PC1	O32-C31-O31-C3
9	M	201	PC1	C21-C22-C23-C24
9	C	501	PC1	C22-C23-C24-C25
9	C	504	PC1	O22-C21-O21-C2
9	D	501	PC1	O22-C21-O21-C2
10	O	102	UND	C6-C7-C8-C9
9	B	201	PC1	C35-C36-C37-C38
9	C	502	PC1	C33-C34-C35-C36
9	C	504	PC1	C22-C23-C24-C25
9	K	501	PC1	O21-C2-C3-O31
9	I	202	PC1	C37-C38-C39-C3A
9	F	203	PC1	C33-C34-C35-C36
9	A	201	PC1	O32-C31-O31-C3
9	C	502	PC1	O32-C31-O31-C3
9	J	202	PC1	C33-C34-C35-C36
9	F	203	PC1	C34-C35-C36-C37
9	F	203	PC1	C31-C32-C33-C34
9	F	204	PC1	C31-C32-C33-C34
9	F	203	PC1	C1-C2-C3-O31
9	E	202	PC1	C32-C33-C34-C35
10	F	207	UND	C5-C6-C7-C8
9	N	203	PC1	C35-C36-C37-C38
9	E	203	PC1	C31-C32-C33-C34
9	E	202	PC1	C22-C21-O21-C2
10	M	206	UND	C5-C6-C7-C8
9	D	502	PC1	O11-C1-C2-O21
9	F	202	PC1	C24-C25-C26-C27
9	D	507	PC1	O21-C2-C3-O31
9	N	201	PC1	O21-C2-C3-O31
9	E	204	PC1	C32-C33-C34-C35
9	D	507	PC1	C22-C21-O21-C2
9	C	503	PC1	C1-O11-P-O13
9	H	702	PC1	C1-O11-P-O13
9	I	201	PC1	C11-O13-P-O11
9	M	202	PC1	C1-O11-P-O13
9	M	203	PC1	C11-O13-P-O11
9	M	202	PC1	C31-C32-C33-C34
9	D	506	PC1	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
9	C	505	PC1	C32-C33-C34-C35
10	F	207	UND	C2-C3-C4-C5
10	M	209	UND	C2-C3-C4-C5
9	D	501	PC1	C1-C2-C3-O31
9	D	505	PC1	C32-C33-C34-C35
9	E	201	PC1	C1-C2-C3-O31
9	B	203	PC1	C35-C36-C37-C38
9	N	204	PC1	C35-C36-C37-C38
9	D	505	PC1	C26-C27-C28-C29
9	A	202	PC1	O31-C31-C32-C33
9	B	202	PC1	C34-C35-C36-C37
9	E	203	PC1	C32-C33-C34-C35
9	A	202	PC1	C32-C33-C34-C35
9	B	201	PC1	C24-C25-C26-C27
9	B	202	PC1	C35-C36-C37-C38
9	B	202	PC1	C1-C2-C3-O31
9	D	506	PC1	C3-C2-O21-C21
9	E	201	PC1	C3-C2-O21-C21
9	E	202	PC1	O22-C21-O21-C2
9	D	505	PC1	C24-C25-C26-C27
9	L	501	PC1	C32-C31-O31-C3
9	D	501	PC1	C32-C33-C34-C35
9	E	201	PC1	C34-C35-C36-C37
9	K	502	PC1	C34-C35-C36-C37
10	B	204	UND	C6-C7-C8-C9
9	A	202	PC1	C21-C22-C23-C24
9	D	501	PC1	O21-C2-C3-O31
9	D	504	PC1	O21-C2-C3-O31
9	A	201	PC1	C32-C33-C34-C35
10	M	206	UND	C4-C5-C6-C7
9	D	501	PC1	C22-C23-C24-C25
9	B	201	PC1	C22-C23-C24-C25
9	D	505	PC1	C25-C26-C27-C28
9	E	202	PC1	C33-C34-C35-C36
9	F	205	PC1	C34-C35-C36-C37
9	D	507	PC1	O11-C1-C2-C3
9	E	202	PC1	O11-C1-C2-C3
9	M	203	PC1	C35-C36-C37-C38
9	A	202	PC1	C33-C34-C35-C36
10	K	505	UND	C4-C5-C6-C7
9	D	507	PC1	O22-C21-O21-C2
9	I	201	PC1	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
9	I	202	PC1	C2-C1-O11-P
9	D	505	PC1	C22-C21-O21-C2
9	D	507	PC1	C25-C26-C27-C28
9	D	507	PC1	C1-C2-C3-O31
9	N	201	PC1	C1-C2-C3-O31
9	D	505	PC1	C23-C24-C25-C26
9	E	204	PC1	O21-C2-C3-O31
10	M	207	UND	C4-C5-C6-C7
9	K	502	PC1	C1-O11-P-O13
9	D	507	PC1	O11-C1-C2-O21
9	N	201	PC1	O11-C1-C2-O21
9	N	204	PC1	C32-C33-C34-C35
10	B	205	UND	C3-C4-C5-C6
9	E	202	PC1	C22-C23-C24-C25
9	L	501	PC1	O32-C31-O31-C3
9	D	503	PC1	C34-C35-C36-C37
9	B	203	PC1	O21-C2-C3-O31
9	A	202	PC1	C26-C27-C28-C29
9	C	505	PC1	O11-C1-C2-C3
9	K	502	PC1	O11-C1-C2-C3
9	A	201	PC1	C2-C1-O11-P
9	D	506	PC1	C2-C1-O11-P
9	I	203	PC1	C2-C1-O11-P
9	L	501	PC1	C2-C1-O11-P
9	L	502	PC1	C2-C1-O11-P
9	N	204	PC1	C2-C1-O11-P
9	I	202	PC1	C32-C33-C34-C35
9	E	202	PC1	C21-C22-C23-C24
9	N	201	PC1	C21-C22-C23-C24
9	C	501	PC1	O11-C1-C2-C3
9	F	202	PC1	C23-C24-C25-C26
10	B	205	UND	C4-C5-C6-C7
9	J	202	PC1	C28-C29-C2A-C2B
9	C	502	PC1	C2-C1-O11-P
9	D	504	PC1	C1-C2-C3-O31
9	F	202	PC1	C1-C2-C3-O31
9	H	701	PC1	C2-C1-O11-P
9	H	702	PC1	C2-C1-O11-P
9	M	204	PC1	C2-C1-O11-P
9	D	501	PC1	O11-C1-C2-O21
9	E	202	PC1	O11-C1-C2-O21
9	C	501	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
9	D	505	PC1	O22-C21-O21-C2
9	D	504	PC1	C31-C32-C33-C34
9	N	201	PC1	C31-C32-C33-C34
9	D	504	PC1	C22-C23-C24-C25
9	C	505	PC1	C35-C36-C37-C38
9	K	501	PC1	C34-C35-C36-C37
9	C	501	PC1	C11-O13-P-O11
9	L	502	PC1	C11-O13-P-O11
9	E	204	PC1	C35-C36-C37-C38
9	F	204	PC1	C2-C1-O11-P
9	F	205	PC1	C2-C1-O11-P
9	N	203	PC1	C2-C1-O11-P
9	A	202	PC1	C1-O11-P-O14
9	A	203	PC1	C11-O13-P-O14
9	B	203	PC1	C1-O11-P-O12
9	C	503	PC1	C1-O11-P-O14
9	D	504	PC1	C11-O13-P-O14
9	E	201	PC1	C11-O13-P-O12
9	E	203	PC1	C11-O13-P-O12
9	E	204	PC1	C1-O11-P-O12
9	F	201	PC1	C11-O13-P-O14
9	F	205	PC1	C11-O13-P-O12
9	F	205	PC1	C1-O11-P-O12
9	H	702	PC1	C1-O11-P-O14
9	I	203	PC1	C1-O11-P-O12
9	K	501	PC1	C11-O13-P-O14
9	K	501	PC1	C1-O11-P-O12
9	M	201	PC1	C1-O11-P-O12
9	M	201	PC1	C1-O11-P-O14
9	M	202	PC1	C1-O11-P-O12
9	N	201	PC1	C11-O13-P-O12
9	N	204	PC1	C1-O11-P-O12
9	D	501	PC1	O11-C1-C2-C3
9	A	203	PC1	C12-C11-O13-P
9	C	501	PC1	C12-C11-O13-P
9	C	505	PC1	C12-C11-O13-P
9	K	501	PC1	C12-C11-O13-P
9	K	502	PC1	C12-C11-O13-P
9	L	501	PC1	C12-C11-O13-P
9	N	201	PC1	C12-C11-O13-P
9	N	204	PC1	C12-C11-O13-P
9	C	501	PC1	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
9	D	506	PC1	O11-C1-C2-O21
9	C	501	PC1	C22-C21-O21-C2
9	M	201	PC1	C11-C12-N-C14
9	B	203	PC1	C1-C2-C3-O31
9	C	503	PC1	O13-C11-C12-N
9	D	503	PC1	O13-C11-C12-N
9	F	202	PC1	O13-C11-C12-N
9	F	204	PC1	O13-C11-C12-N
9	H	701	PC1	O13-C11-C12-N
9	H	702	PC1	O13-C11-C12-N
9	I	201	PC1	O13-C11-C12-N
9	L	501	PC1	O13-C11-C12-N
9	L	502	PC1	O13-C11-C12-N
9	M	202	PC1	O13-C11-C12-N
9	M	203	PC1	O13-C11-C12-N
9	N	203	PC1	O13-C11-C12-N
9	E	201	PC1	O21-C2-C3-O31
9	D	506	PC1	C32-C33-C34-C35
10	A	205	UND	C6-C7-C8-C9
9	D	507	PC1	C26-C27-C28-C29
9	E	204	PC1	C33-C34-C35-C36
9	M	201	PC1	C22-C23-C24-C25
9	D	507	PC1	C22-C23-C24-C25
9	C	501	PC1	C1-C2-O21-C21
9	D	502	PC1	C2-C1-O11-P
9	M	203	PC1	C34-C35-C36-C37
9	M	203	PC1	C38-C39-C3A-C3B
9	E	201	PC1	O11-C1-C2-O21
9	M	201	PC1	C11-C12-N-C15
9	J	202	PC1	C38-C39-C3A-C3B
9	A	201	PC1	C11-O13-P-O11
9	B	202	PC1	C11-O13-P-O11
9	C	503	PC1	C11-O13-P-O11
9	D	502	PC1	C11-O13-P-O11
9	D	503	PC1	C11-O13-P-O11
9	D	506	PC1	C11-O13-P-O11
9	E	204	PC1	C11-O13-P-O11
9	F	203	PC1	C11-O13-P-O11
9	I	202	PC1	C11-O13-P-O11
9	J	201	PC1	C11-O13-P-O11
9	M	204	PC1	C11-O13-P-O11
9	N	203	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
9	A	202	PC1	O32-C31-C32-C33
9	D	503	PC1	C2-C1-O11-P
9	K	502	PC1	C2-C1-O11-P
9	C	505	PC1	C31-C32-C33-C34
9	J	201	PC1	O11-C1-C2-C3
10	J	203	UND	C5-C6-C7-C8
9	L	501	PC1	C31-C32-C33-C34
9	D	507	PC1	C23-C24-C25-C26
9	A	203	PC1	C2-C3-O31-C31
9	B	201	PC1	C23-C24-C25-C26
9	I	202	PC1	C33-C34-C35-C36
9	K	502	PC1	O31-C31-C32-C33
9	J	202	PC1	C36-C37-C38-C39
9	C	501	PC1	C2-C1-O11-P
9	N	201	PC1	C2-C1-O11-P
9	B	201	PC1	C21-C22-C23-C24
9	D	504	PC1	C23-C24-C25-C26
9	M	201	PC1	C11-C12-N-C13
9	H	701	PC1	O31-C31-C32-C33
9	F	201	PC1	C23-C24-C25-C26
10	E	206	UND	C6-C7-C8-C9
10	M	206	UND	C2-C3-C4-C5
9	K	501	PC1	O11-C1-C2-C3
9	M	203	PC1	O11-C1-C2-C3
9	N	203	PC1	O11-C1-C2-C3
9	J	202	PC1	C29-C2A-C2B-C2C
9	D	501	PC1	C24-C25-C26-C27
9	C	501	PC1	C23-C24-C25-C26
9	J	202	PC1	C32-C33-C34-C35
9	C	501	PC1	C21-C22-C23-C24
9	F	203	PC1	C38-C39-C3A-C3B
10	B	205	UND	C6-C7-C8-C9
9	F	205	PC1	C33-C34-C35-C36
10	M	209	UND	C3-C4-C5-C6
9	N	201	PC1	O11-C1-C2-C3
9	F	201	PC1	C24-C25-C26-C27
10	A	205	UND	C3-C4-C5-C6
9	D	507	PC1	C1-O11-P-O13
9	C	502	PC1	O31-C31-C32-C33
9	D	506	PC1	O31-C31-C32-C33
9	D	506	PC1	O21-C21-C22-C23
9	D	505	PC1	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
9	F	205	PC1	C38-C39-C3A-C3B
9	J	202	PC1	C39-C3A-C3B-C3C
9	C	502	PC1	C37-C38-C39-C3A
9	J	202	PC1	C22-C23-C24-C25
9	A	202	PC1	C25-C26-C27-C28
9	H	701	PC1	O32-C31-C32-C33
10	B	205	UND	C11-C10-C9-C8
9	N	203	PC1	O31-C31-C32-C33
9	D	502	PC1	C11-C12-N-C14
9	D	505	PC1	O21-C21-C22-C23
9	M	203	PC1	C33-C34-C35-C36
9	C	501	PC1	O21-C21-C22-C23
9	C	505	PC1	O11-C1-C2-O21
10	J	203	UND	C2-C3-C4-C5
10	K	505	UND	C6-C7-C8-C9
9	C	502	PC1	O32-C31-C32-C33
9	B	203	PC1	C1-O11-P-O14
9	C	505	PC1	C1-O11-P-O14
9	D	506	PC1	C11-O13-P-O14
9	E	202	PC1	C1-O11-P-O14
9	E	204	PC1	C11-O13-P-O14
9	E	204	PC1	C1-O11-P-O14
9	F	202	PC1	C1-O11-P-O14
9	F	203	PC1	C11-O13-P-O14
9	F	203	PC1	C1-O11-P-O14
9	F	204	PC1	C11-O13-P-O12
9	F	205	PC1	C1-O11-P-O14
9	M	204	PC1	C11-O13-P-O14
9	D	506	PC1	O22-C21-C22-C23
9	C	501	PC1	O22-C21-C22-C23
10	A	205	UND	C1-C2-C3-C4
9	B	203	PC1	C12-C11-O13-P
9	D	503	PC1	C12-C11-O13-P
9	E	202	PC1	C12-C11-O13-P
9	H	702	PC1	C12-C11-O13-P
9	M	201	PC1	C12-C11-O13-P
9	M	203	PC1	C12-C11-O13-P
9	M	204	PC1	C12-C11-O13-P
9	D	506	PC1	O32-C31-C32-C33
9	D	503	PC1	C33-C34-C35-C36
10	D	508	UND	C7-C8-C9-C10
9	F	202	PC1	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
10	B	204	UND	C5-C6-C7-C8
9	N	203	PC1	O32-C31-C32-C33
9	D	506	PC1	C23-C24-C25-C26
10	C	507	UND	C5-C6-C7-C8
10	I	204	UND	C6-C7-C8-C9
9	N	203	PC1	O11-C1-C2-O21
9	D	501	PC1	O31-C31-C32-C33
9	F	203	PC1	O31-C31-C32-C33
9	D	506	PC1	C11-C12-N-C15

There are no ring outliers.

42 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	N	202	PC1	1	0
10	K	503	UND	2	0
9	D	504	PC1	1	0
9	A	202	PC1	1	0
9	J	201	PC1	1	0
9	F	201	PC1	1	0
9	E	203	PC1	1	0
9	H	701	PC1	1	0
9	N	201	PC1	1	0
10	M	207	UND	2	0
9	B	203	PC1	2	0
9	F	202	PC1	1	0
9	M	201	PC1	1	0
10	J	204	UND	1	0
9	I	203	PC1	1	0
9	D	503	PC1	1	0
9	E	202	PC1	1	0
9	F	205	PC1	2	0
10	M	209	UND	1	0
9	B	202	PC1	1	0
9	N	204	PC1	2	0
10	G	702	UND	1	0
9	A	201	PC1	2	0
10	B	205	UND	1	0
10	O	101	UND	1	0
9	J	202	PC1	2	0
10	F	207	UND	1	0
9	D	502	PC1	2	0

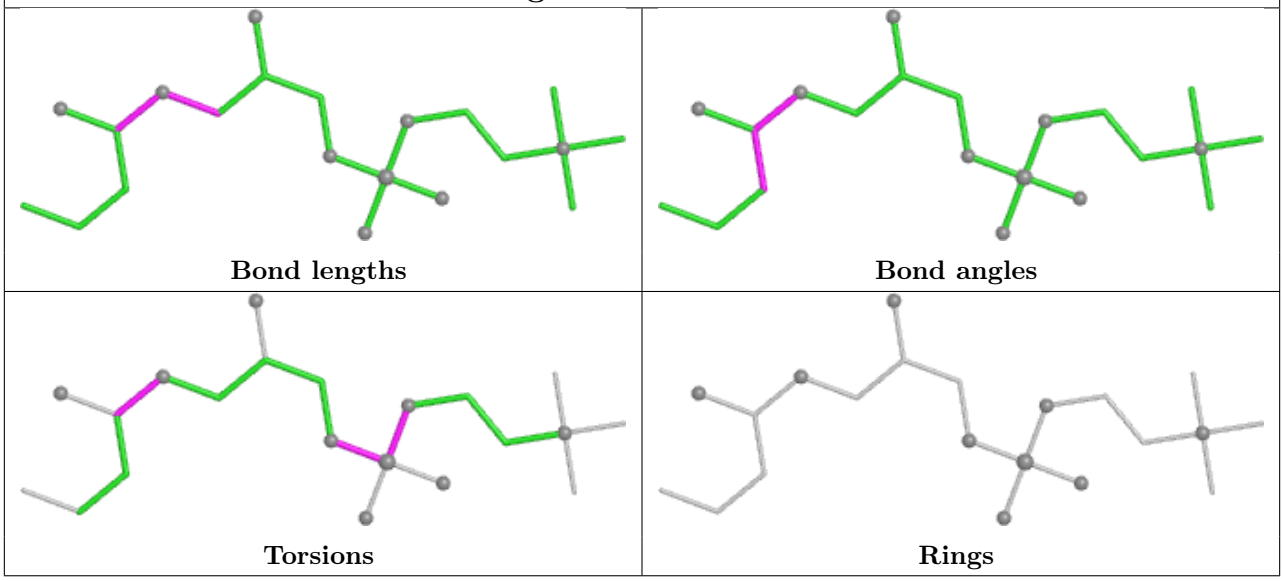
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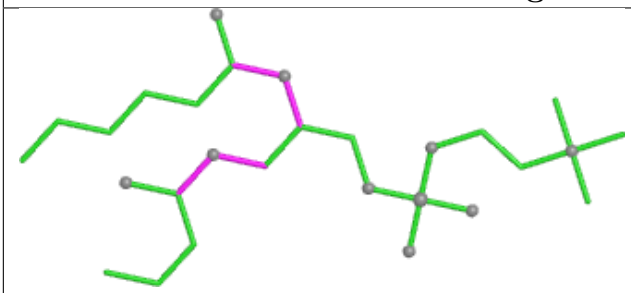
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	PC1	2	0
9	H	702	PC1	1	0
9	A	203	PC1	1	0
10	J	203	UND	1	0
9	D	506	PC1	2	0
9	C	503	PC1	1	0
9	L	502	PC1	1	0
9	M	203	PC1	2	0
10	B	204	UND	1	0
9	B	201	PC1	1	0
9	F	203	PC1	2	0
9	E	204	PC1	2	0
9	M	202	PC1	2	0
9	C	502	PC1	1	0

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

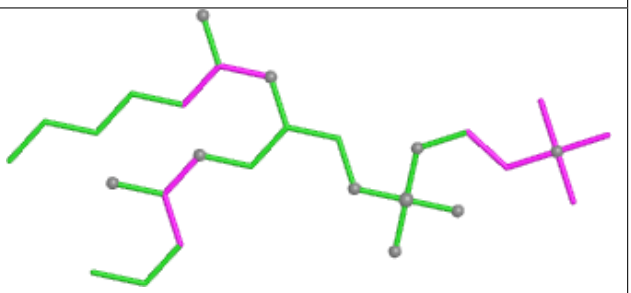
Ligand PC1 N 202



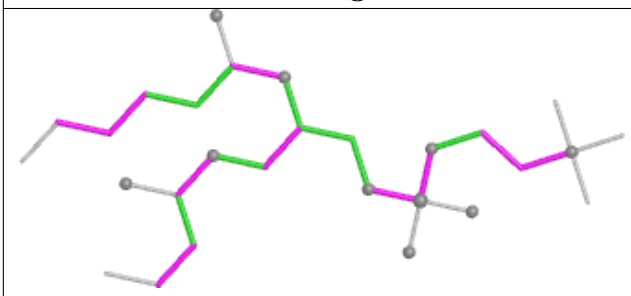
Ligand PC1 D 504



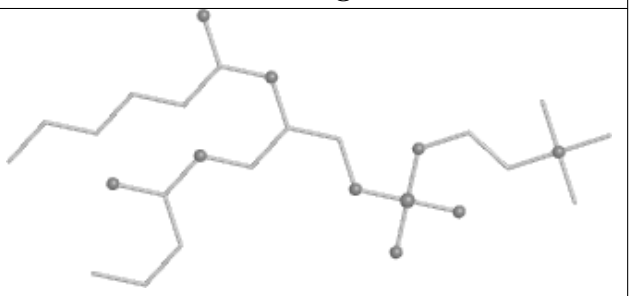
Bond lengths



Bond angles

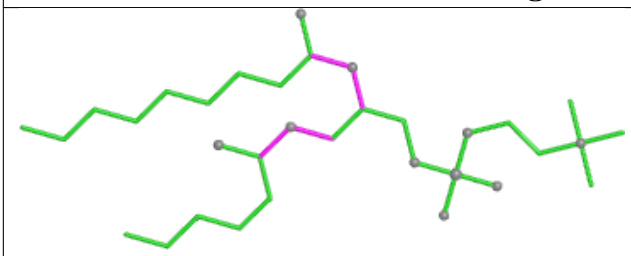


Torsions

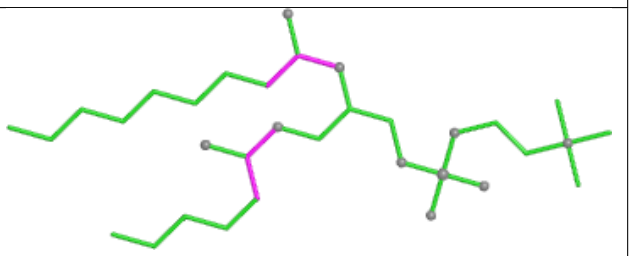


Rings

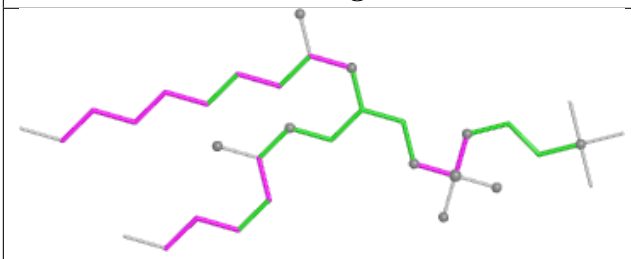
Ligand PC1 A 202



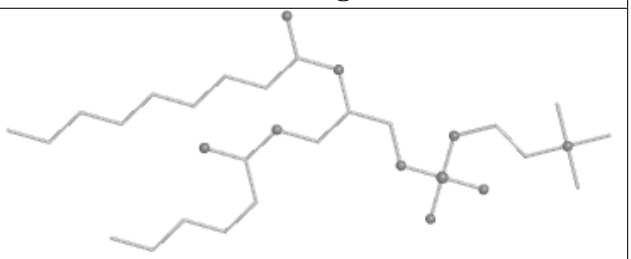
Bond lengths



Bond angles

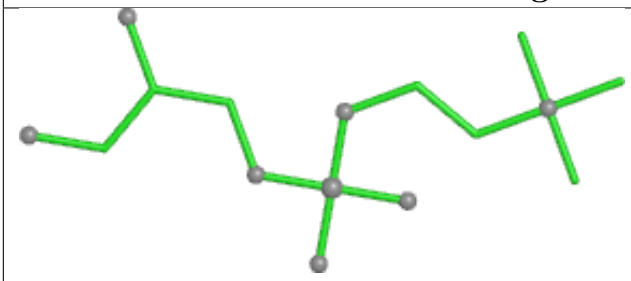


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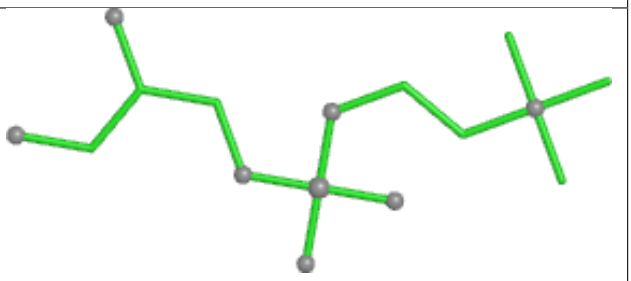


Rings

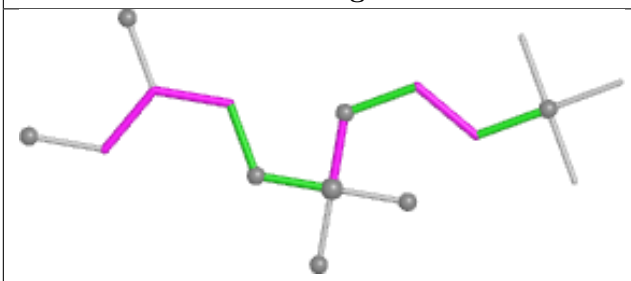
Ligand PC1 J 201



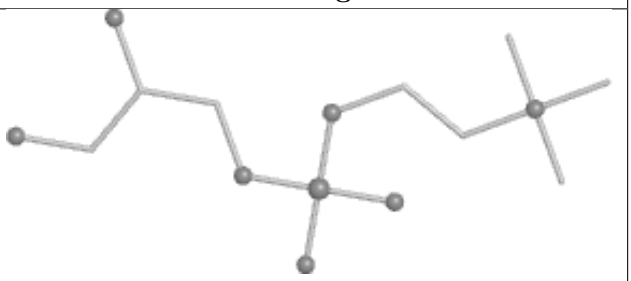
Bond lengths



Bond angles

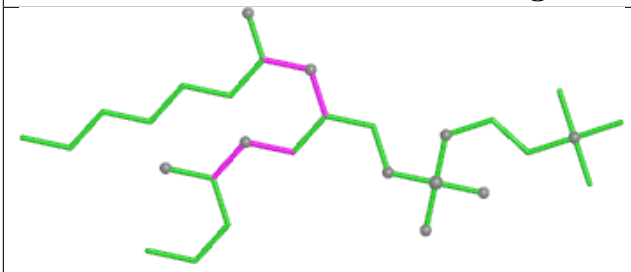


Torsions

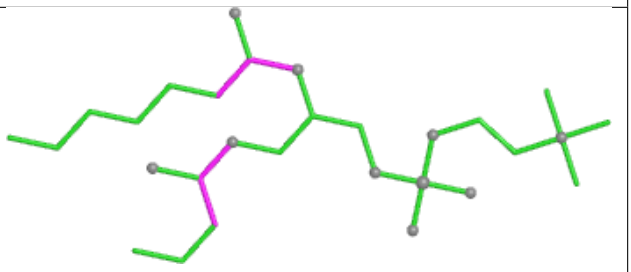


Rings

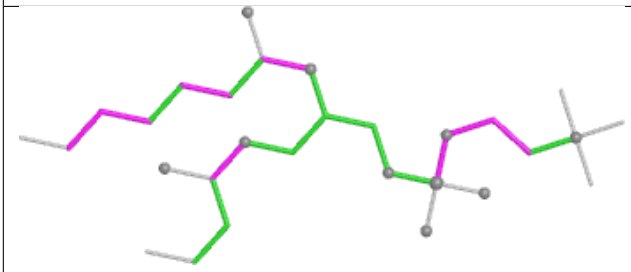
Ligand PC1 F 201



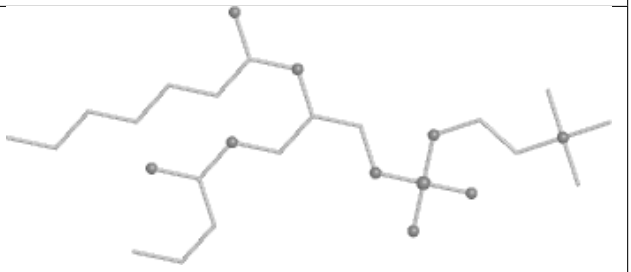
Bond lengths



Bond angles

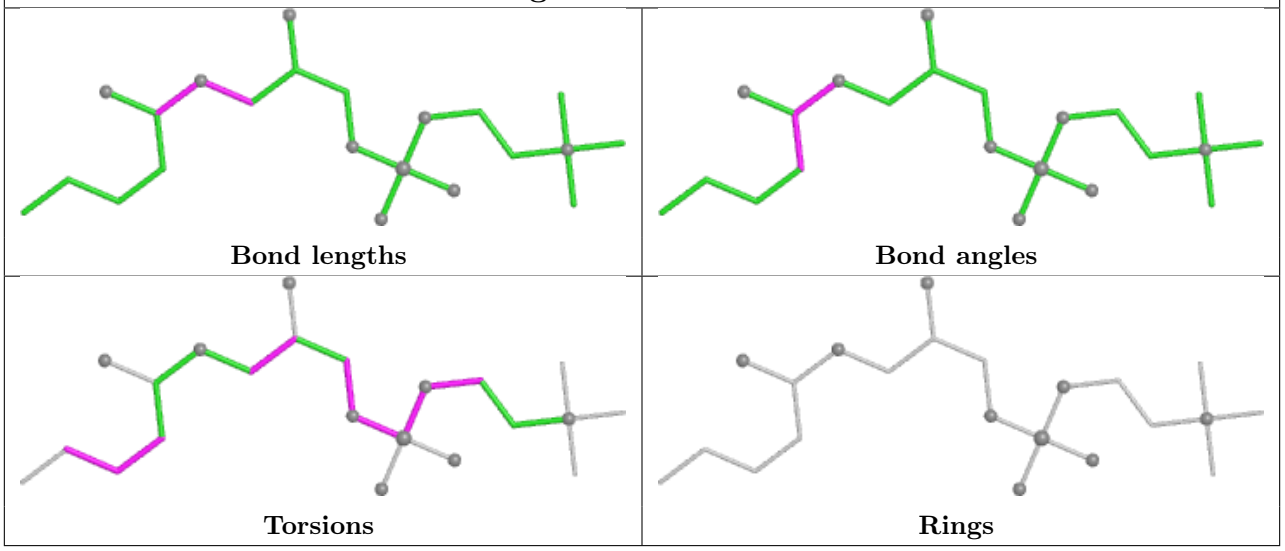


Torsions

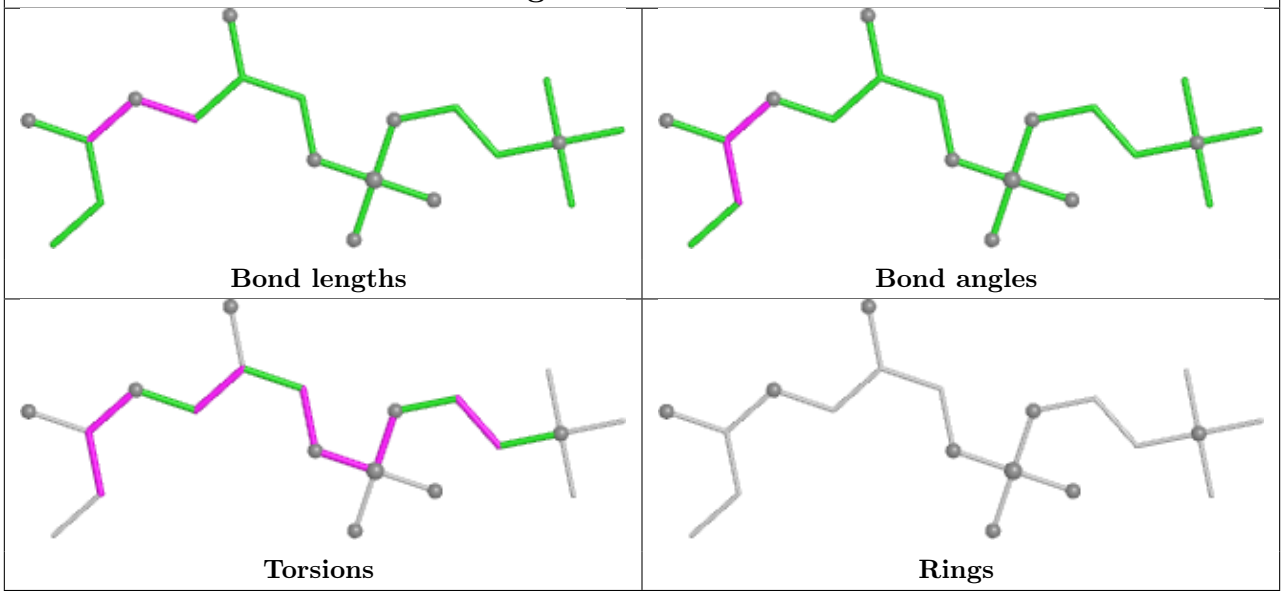


Rings

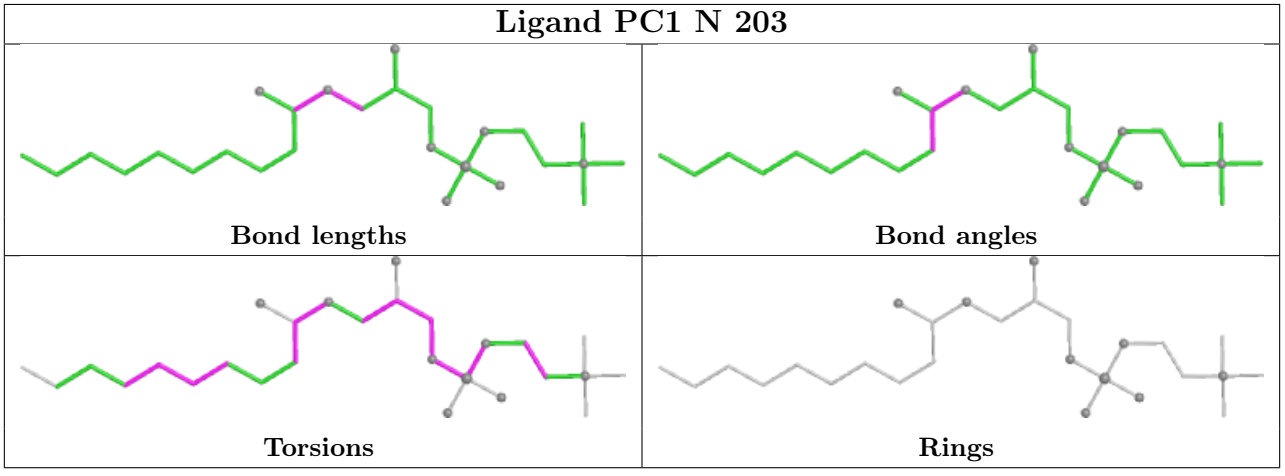
Ligand PC1 E 203



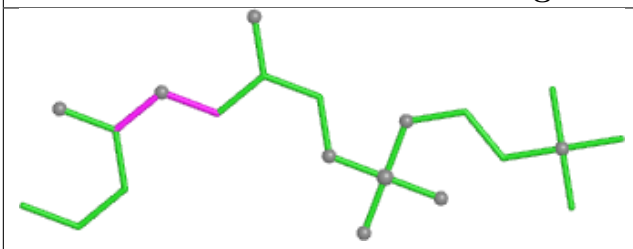
Ligand PC1 H 701



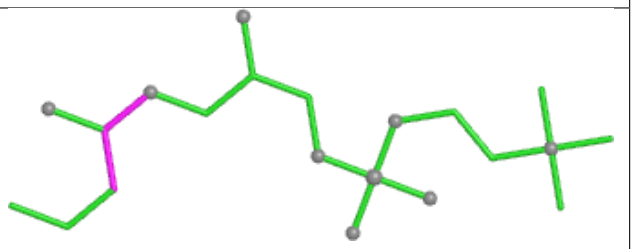
Ligand PC1 N 203



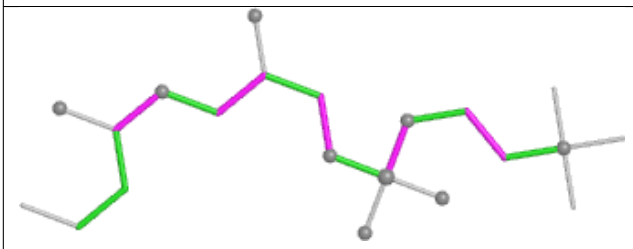
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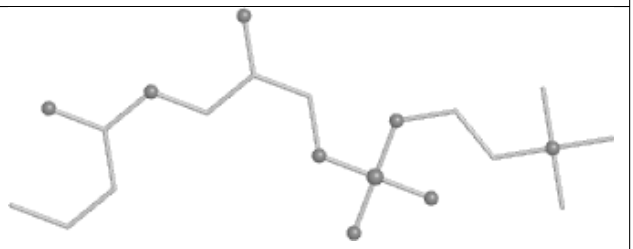
Bond lengths



Bond angles

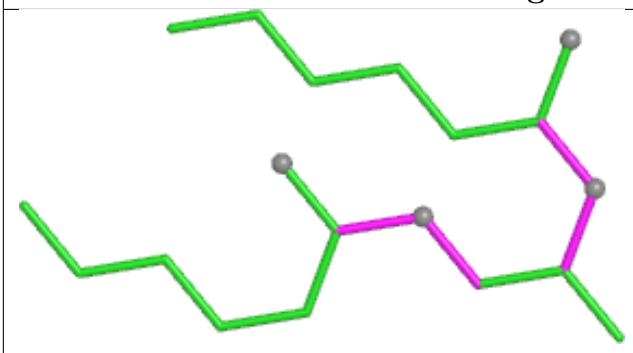


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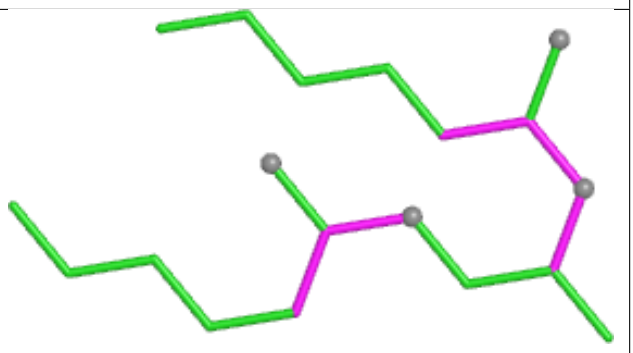


Rings

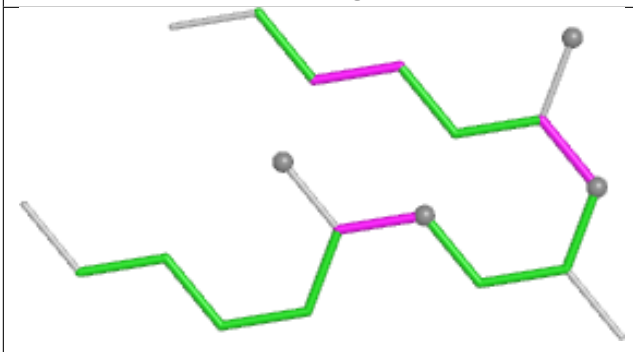
Ligand PC1 C 504



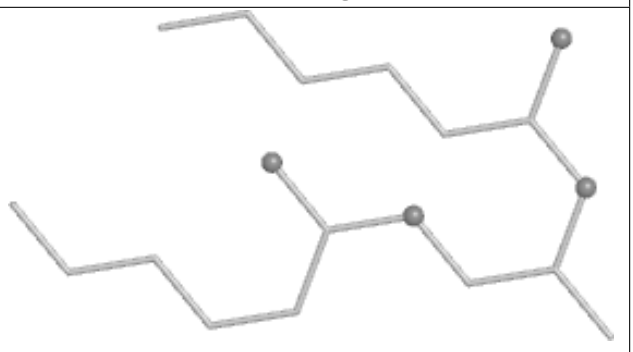
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Bond angles

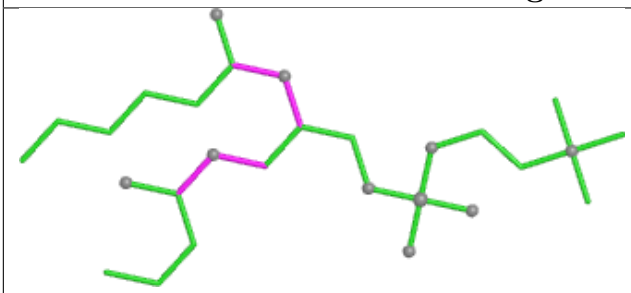


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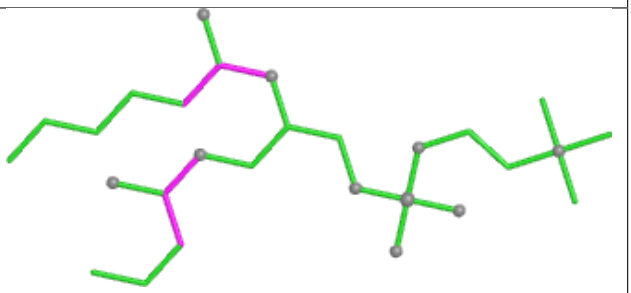


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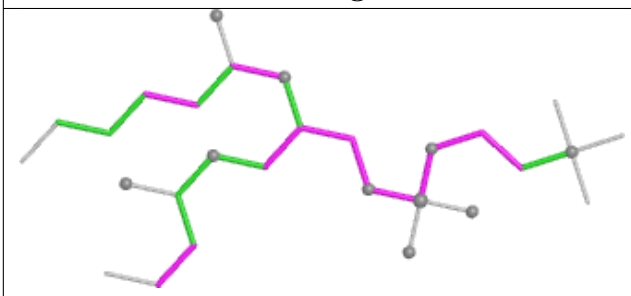
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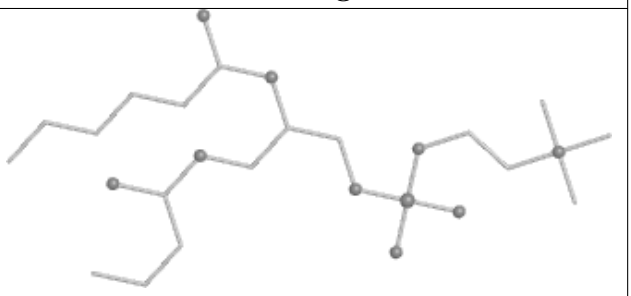
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Bond angles

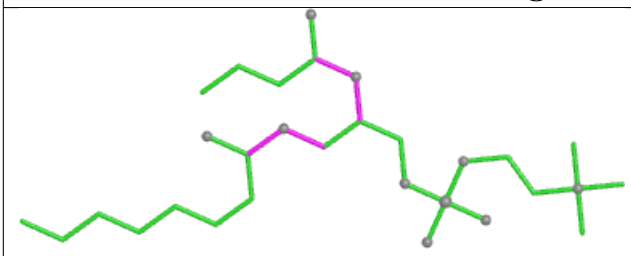


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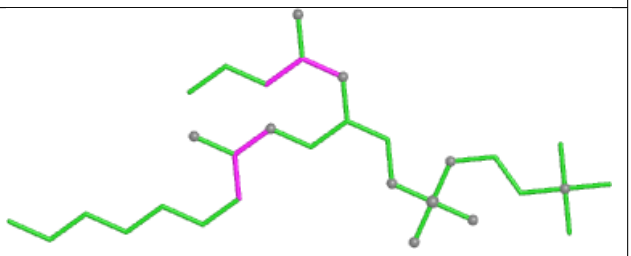


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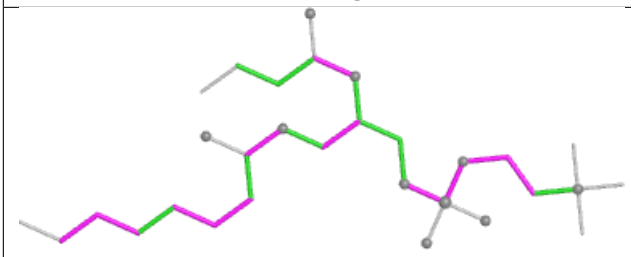
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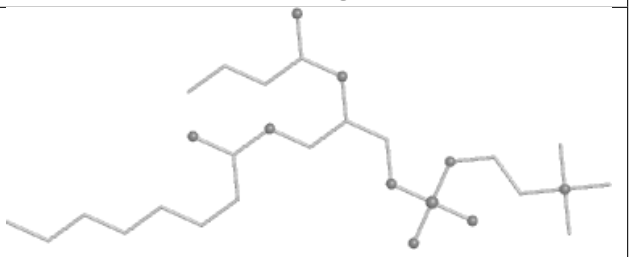
Bond lengths



Bond angles

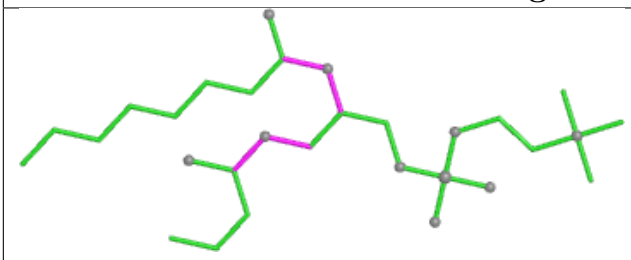


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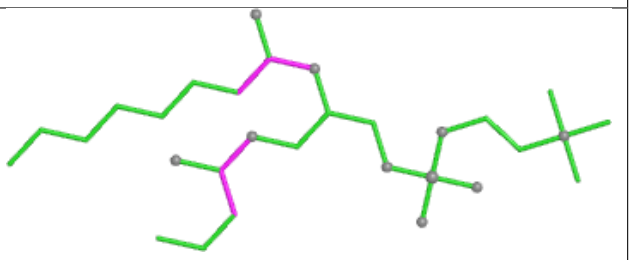


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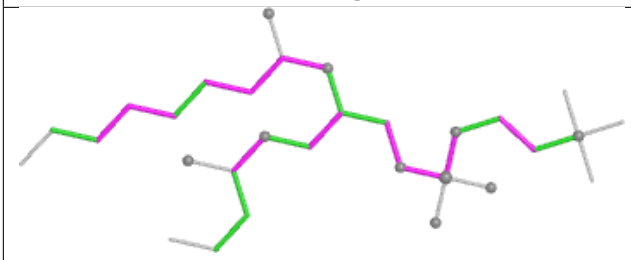
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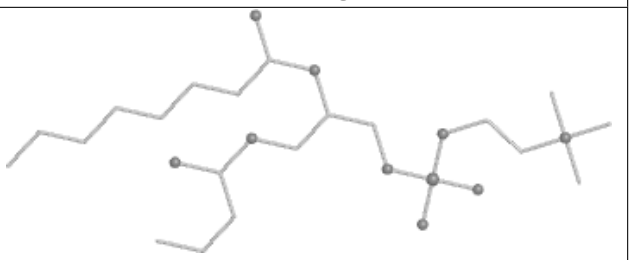
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Bond angles

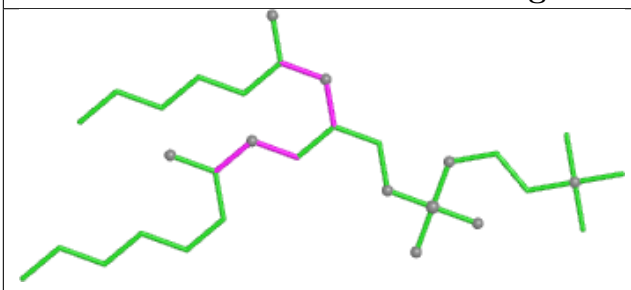


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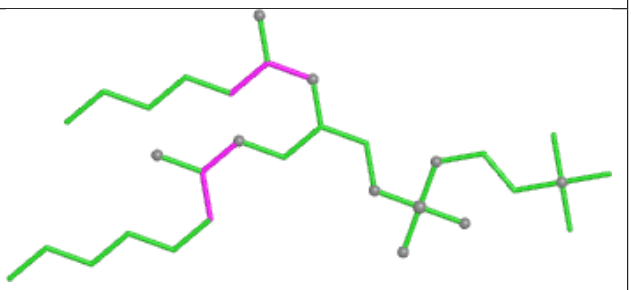


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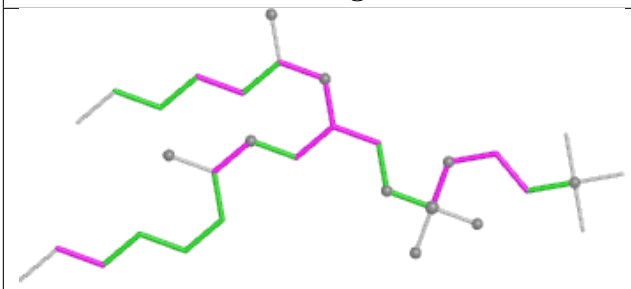
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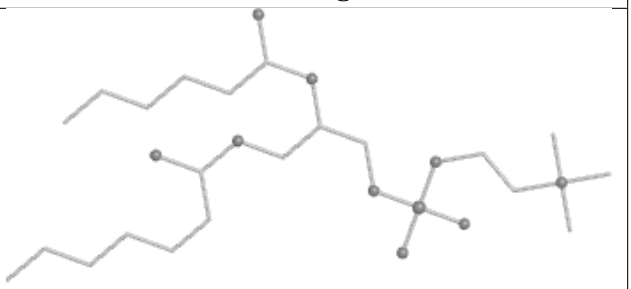
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Bond angles

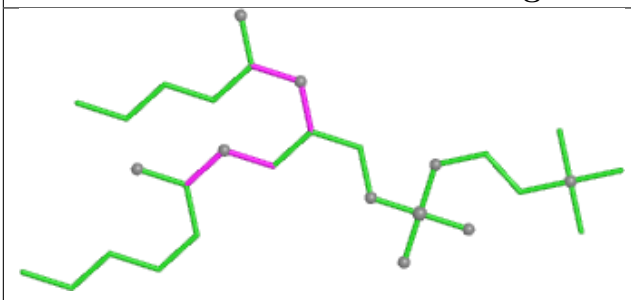


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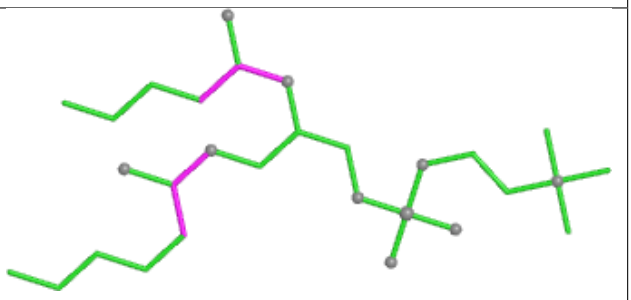


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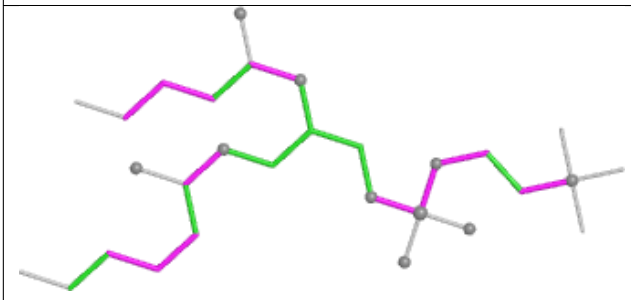
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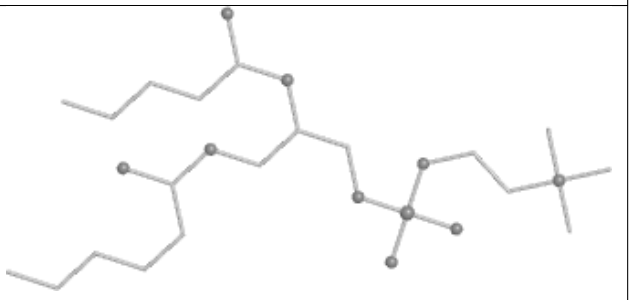
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Bond angles

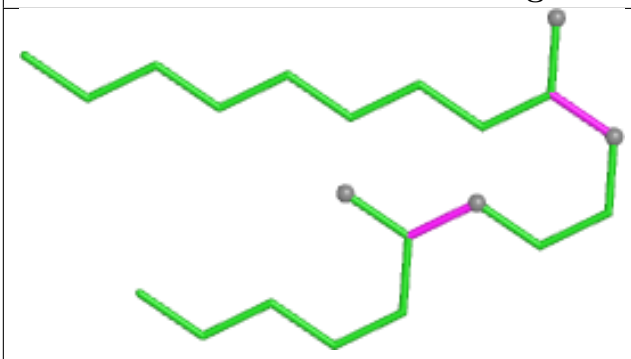


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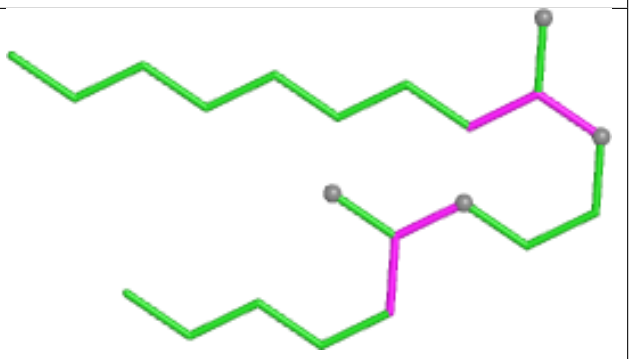


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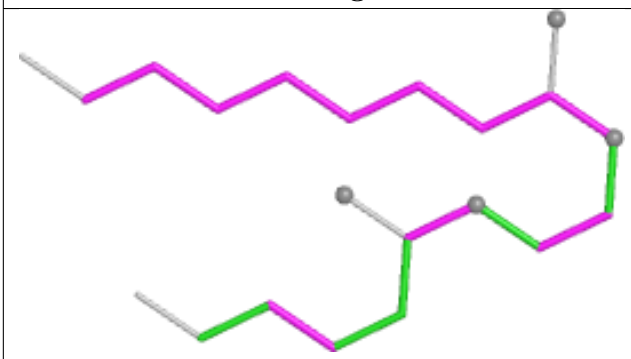
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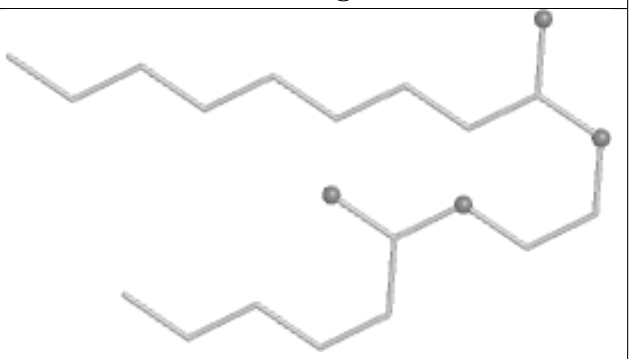
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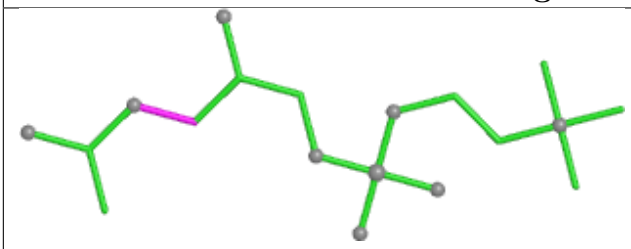


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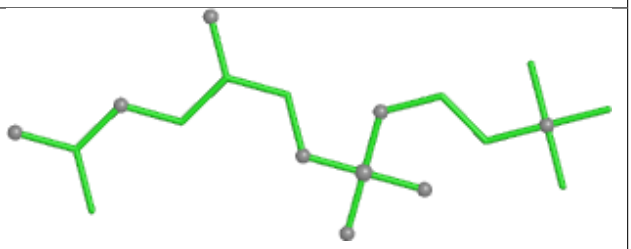


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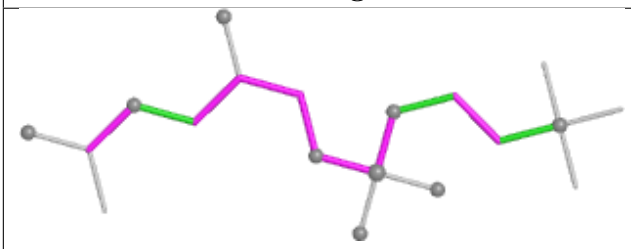
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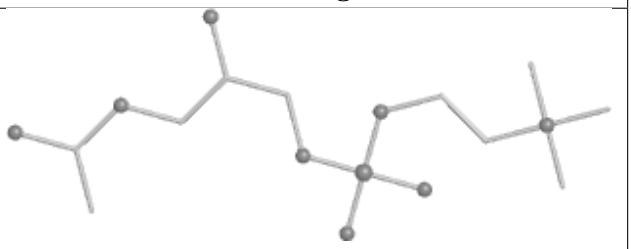
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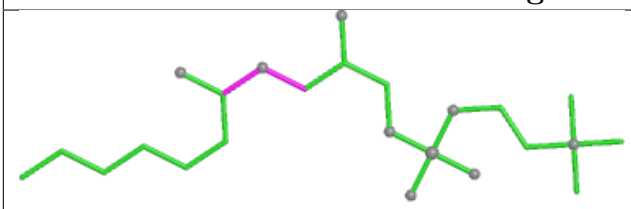


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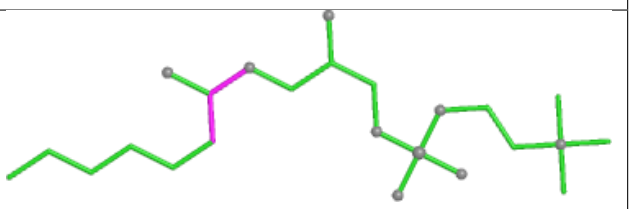


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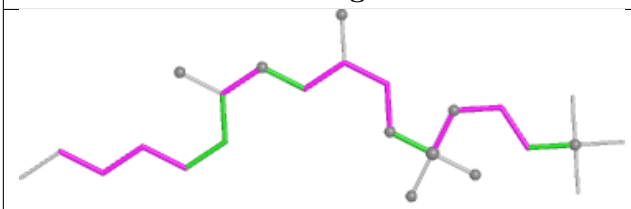
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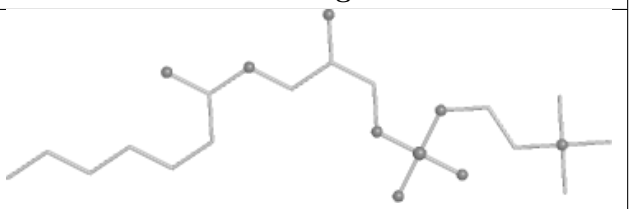
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Bond angles

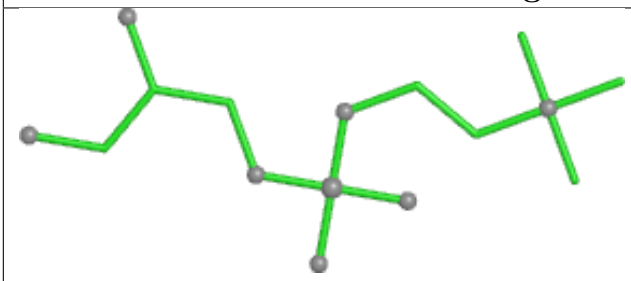


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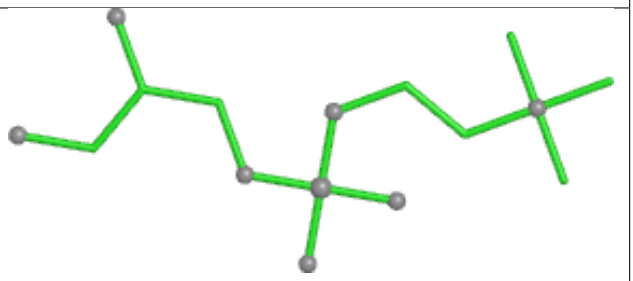


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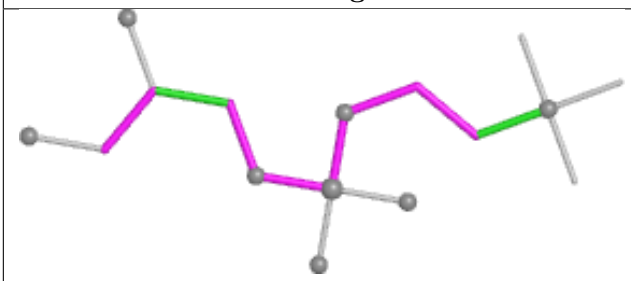
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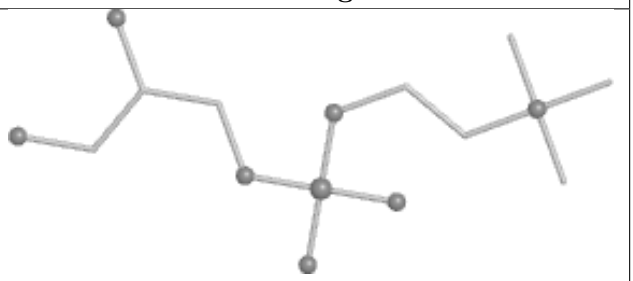
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Bond angles

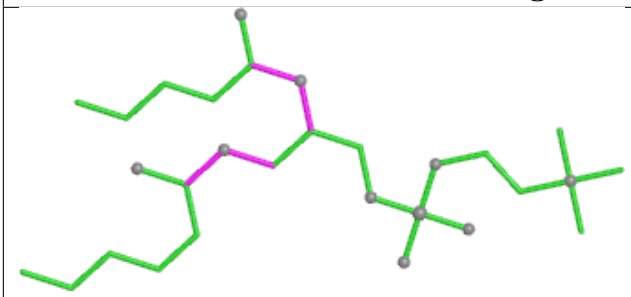


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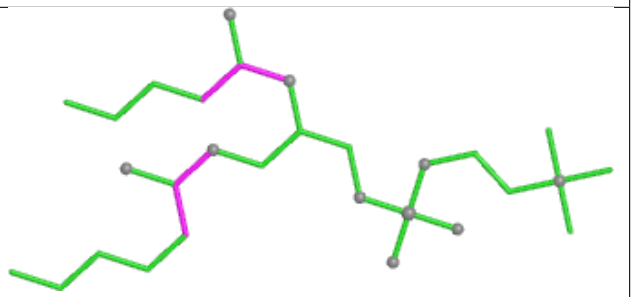


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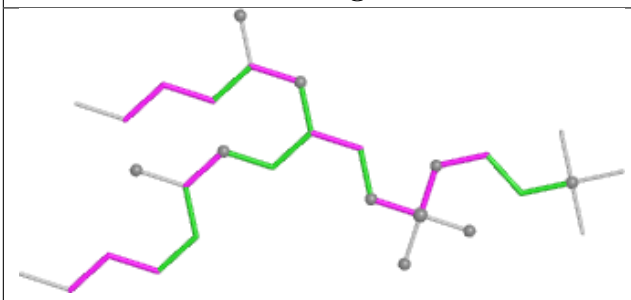
Ligand PC1 E 202



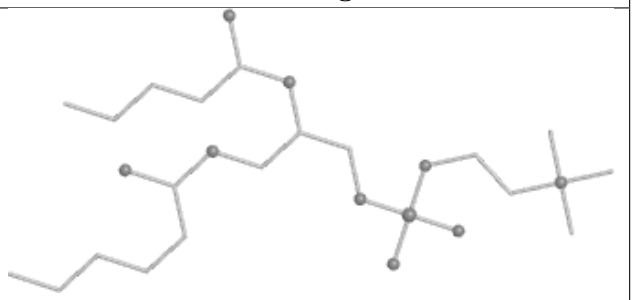
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Bond angles

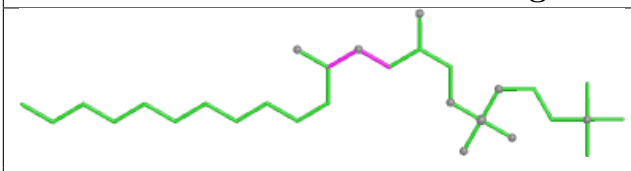


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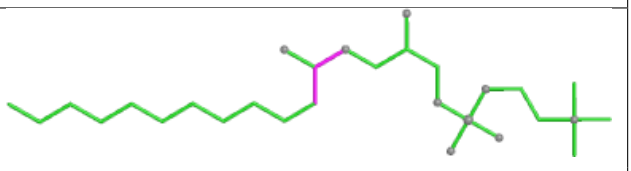


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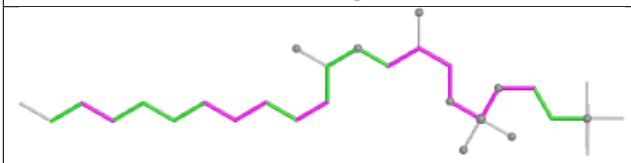
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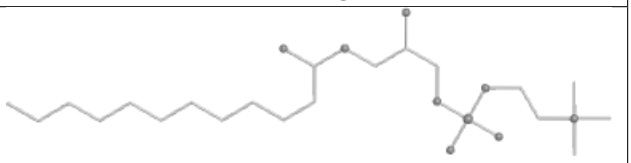
Bond lengths



Bond angles

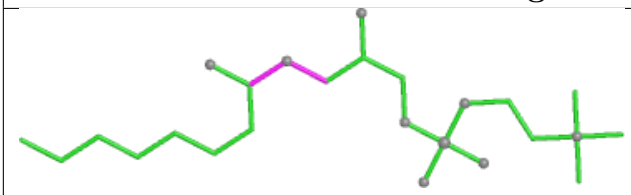


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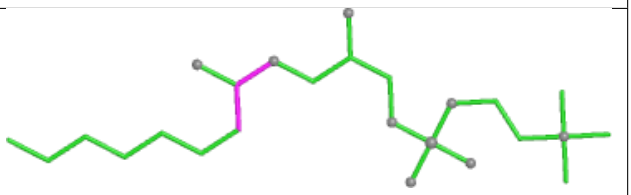


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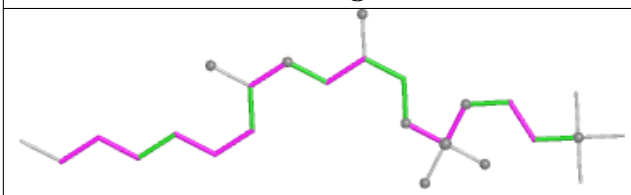
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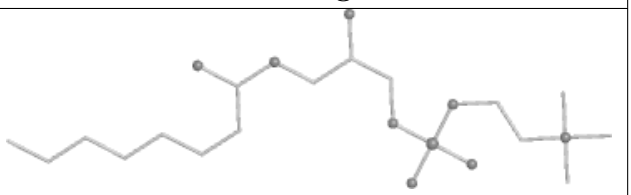
Bond lengths



Bond angles

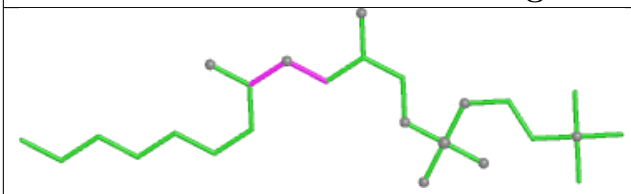


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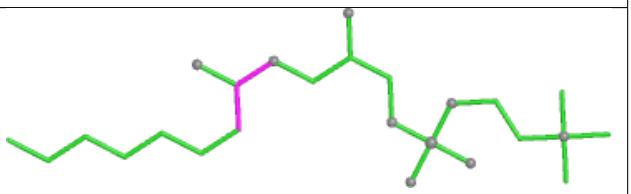


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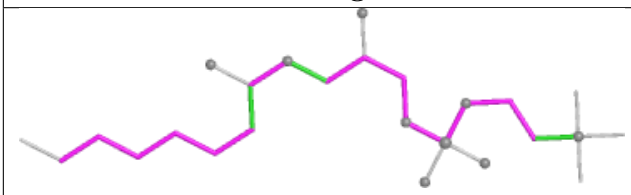
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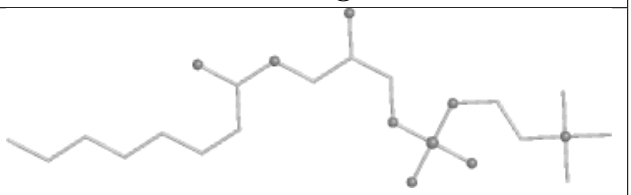
Bond lengths



Bond angles

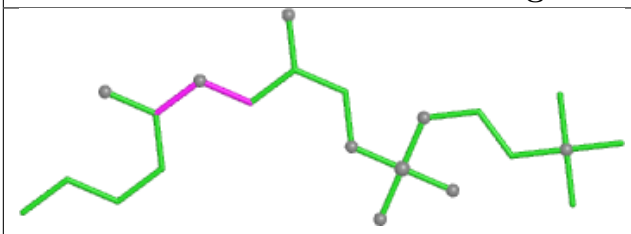


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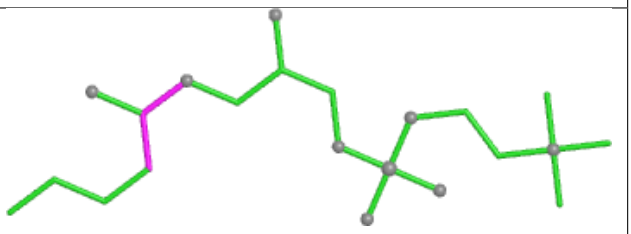


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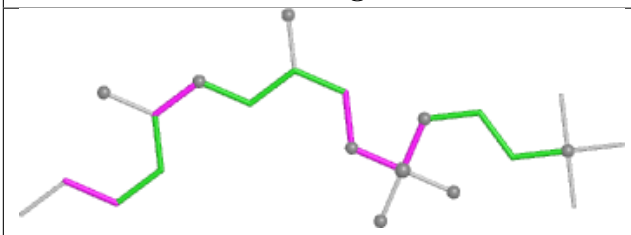
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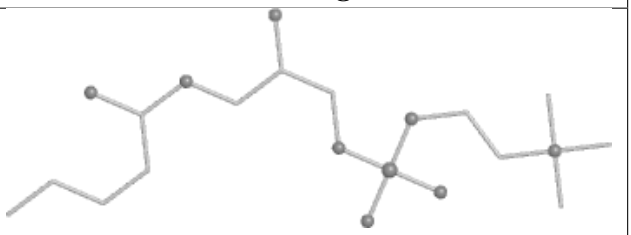
Bond lengths



Bond angles

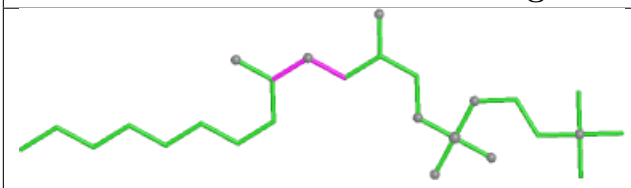


Torsions

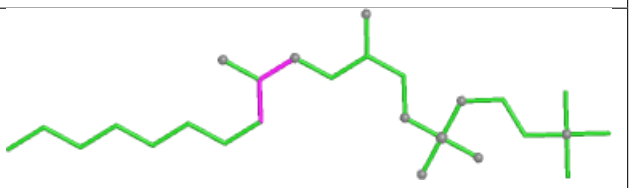


Rings

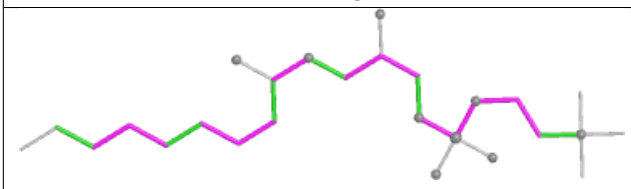
Ligand PC1 C 505



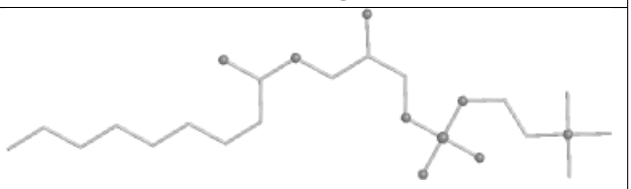
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Bond angles

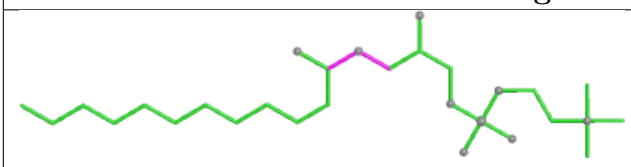


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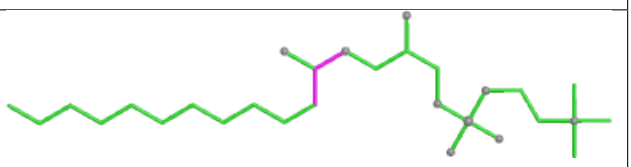


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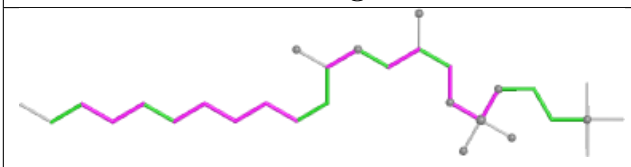
Ligand PC1 I 202



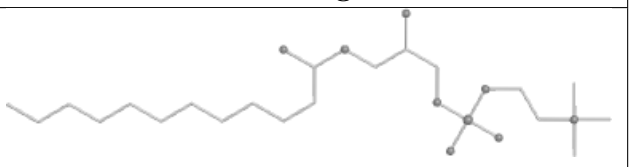
Bond lengths



Bond angles

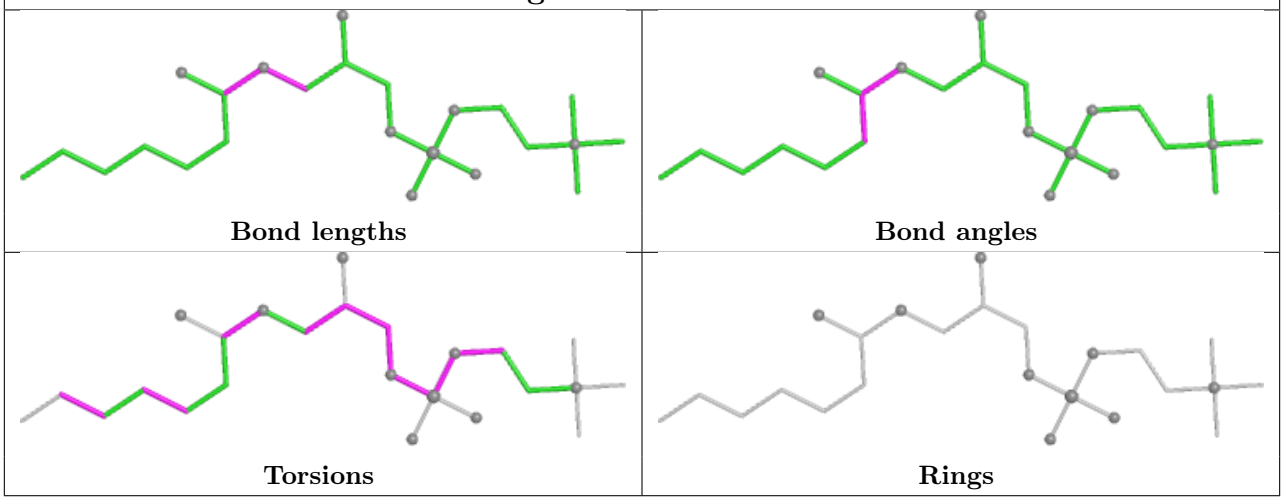


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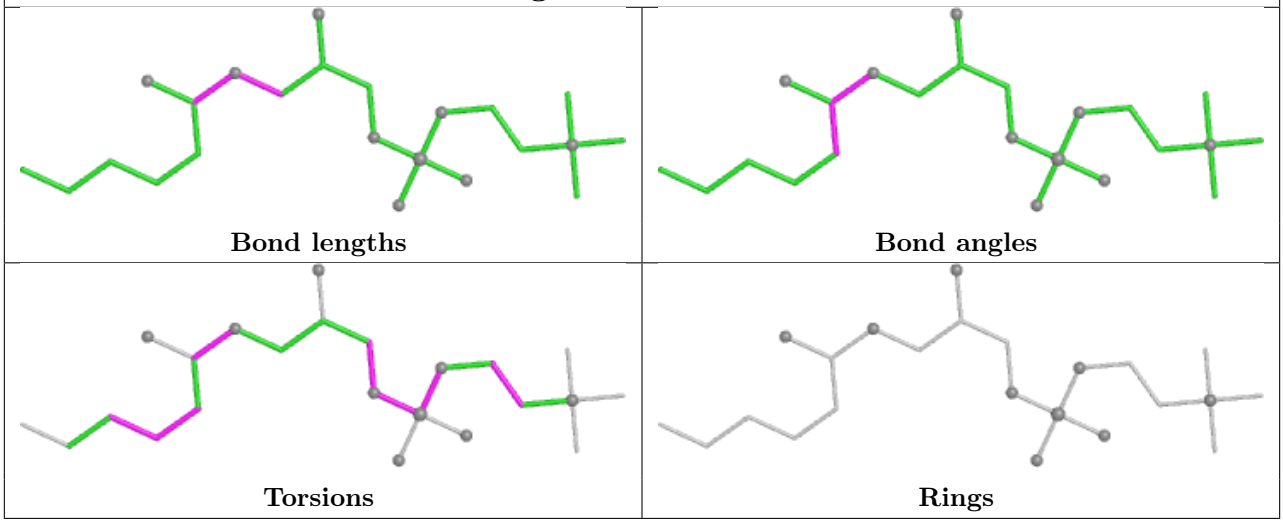


Rings

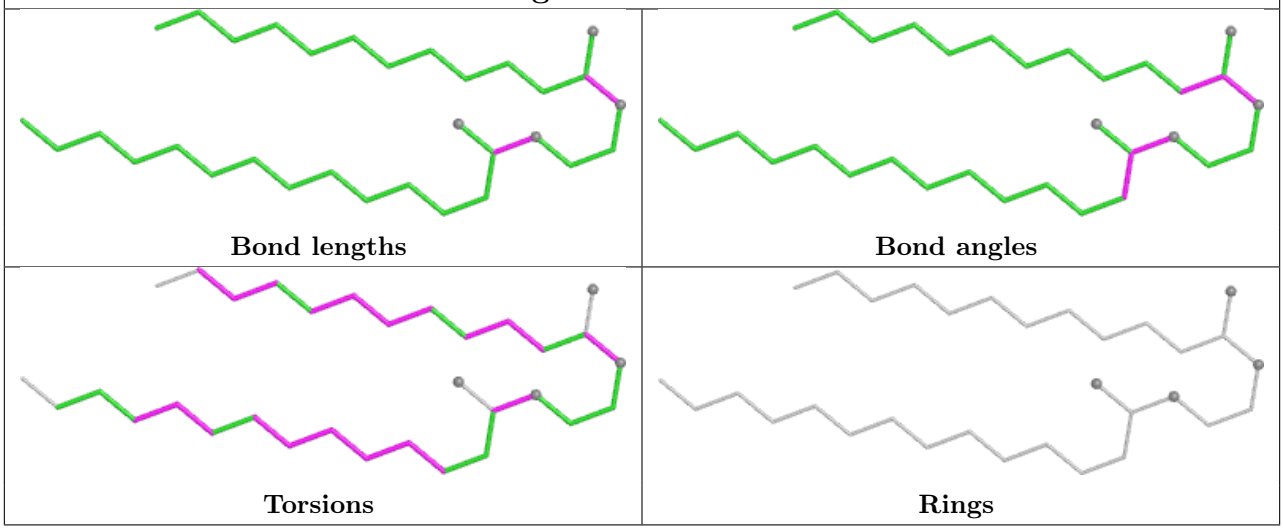
Ligand PC1 K 501



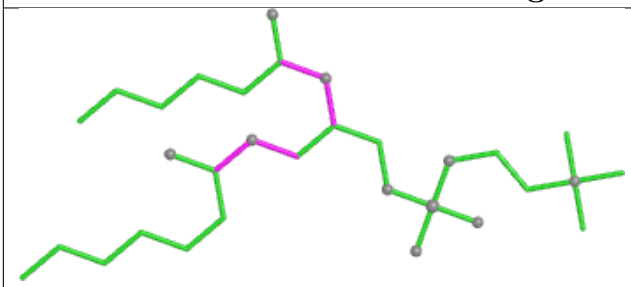
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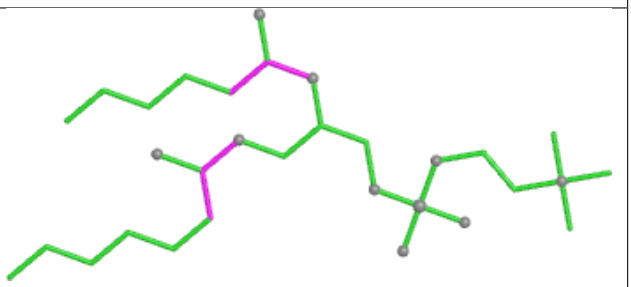
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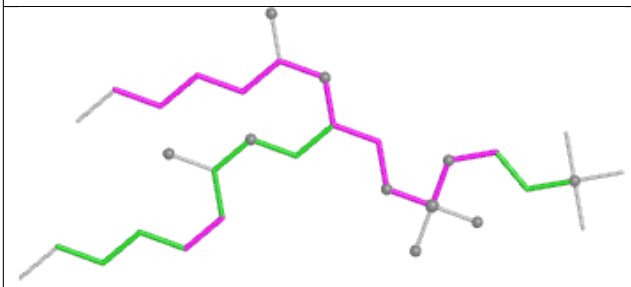
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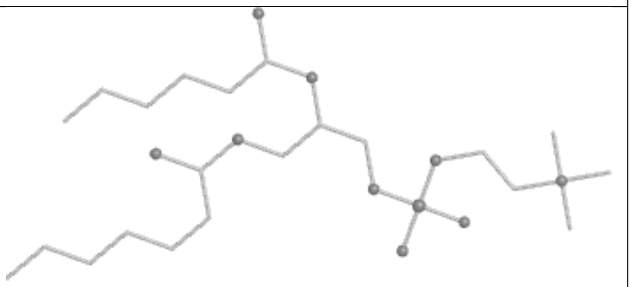
Bond lengths



Bond angles

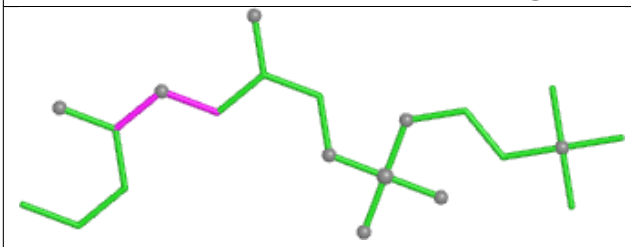


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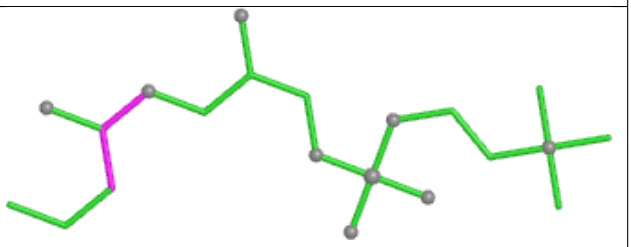


Rings

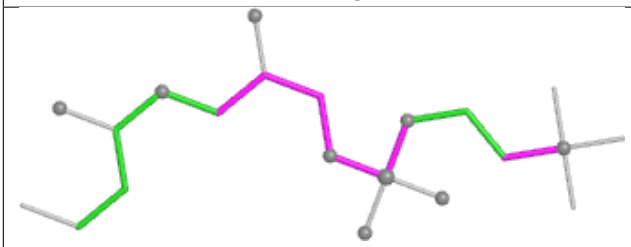
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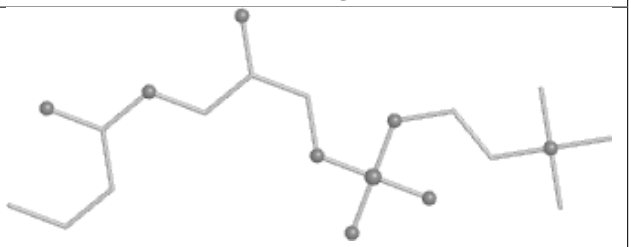
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Bond angles

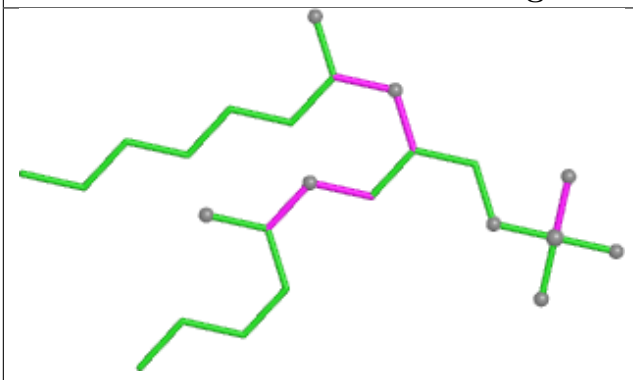


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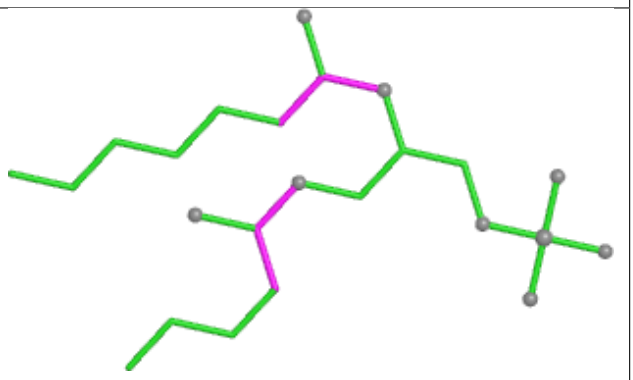


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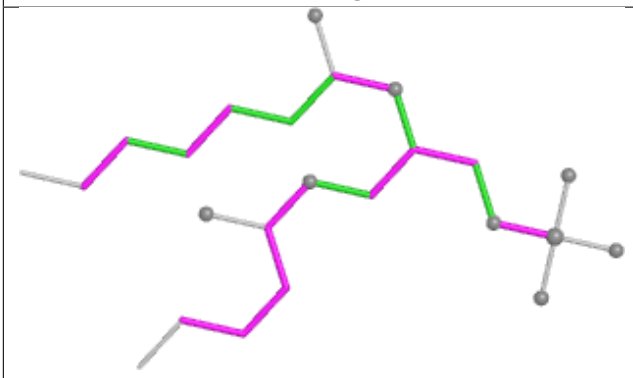
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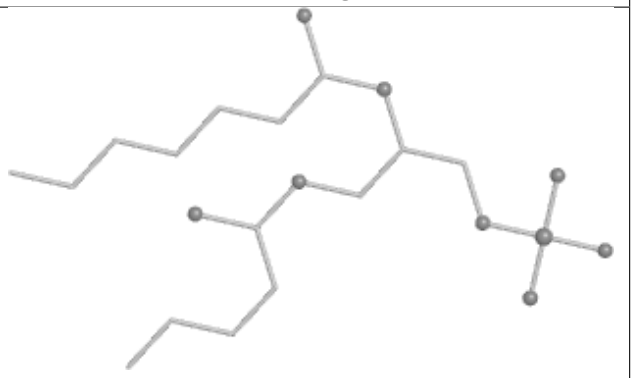
Bond lengths



Bond angles

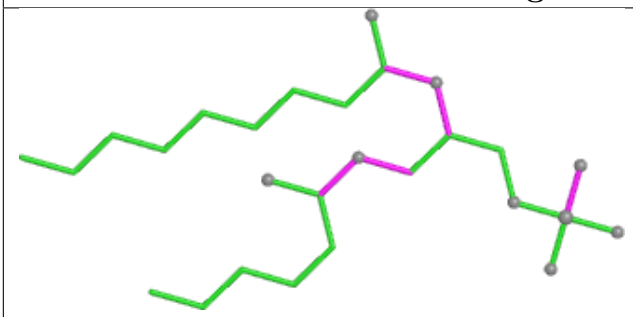


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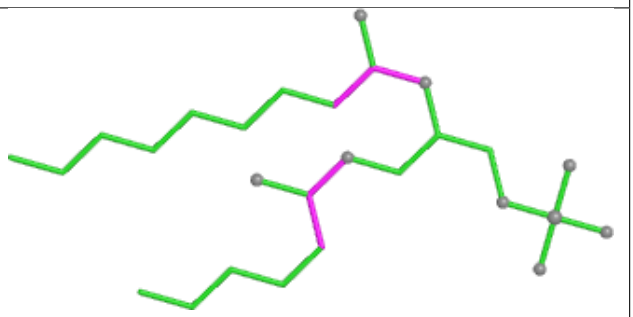


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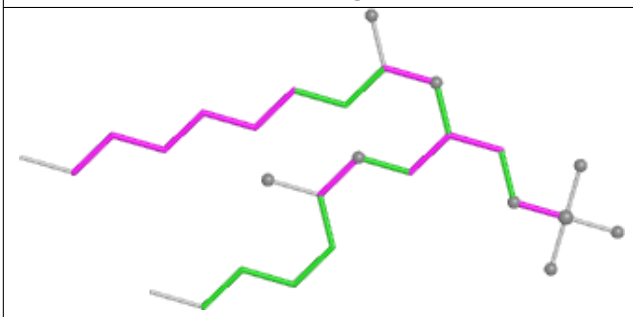
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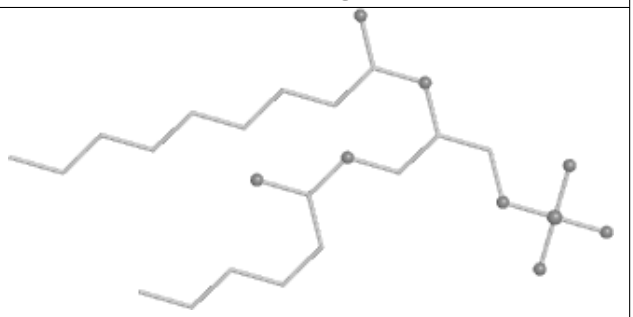
Bond lengths



Bond angles

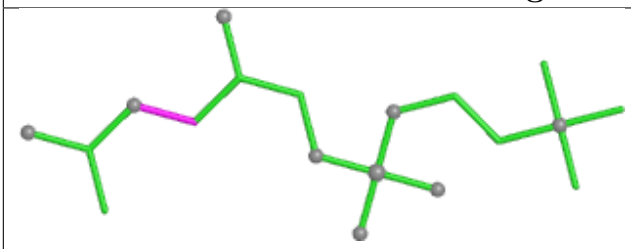


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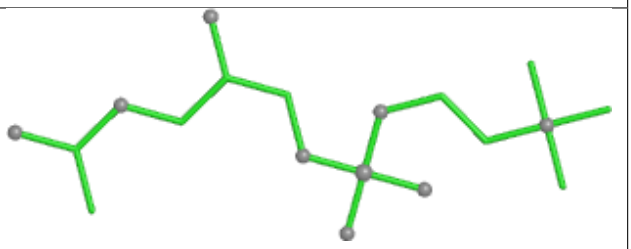


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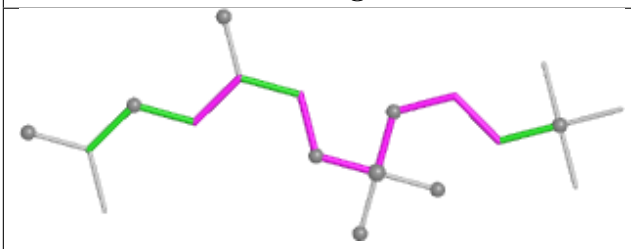
Ligand PC1 H 702



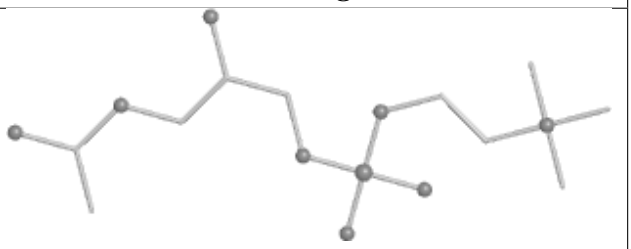
Bond lengths



Bond angles

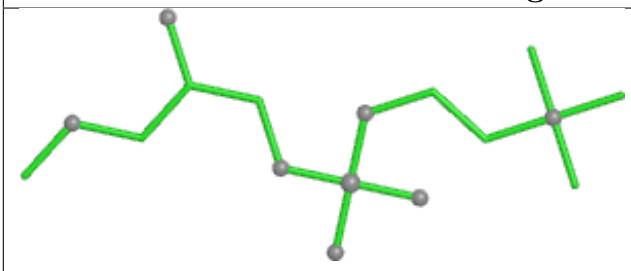


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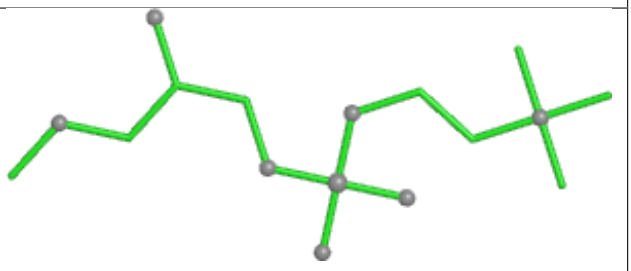


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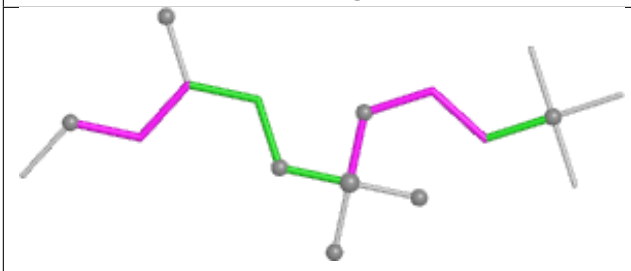
Ligand PC1 A 203



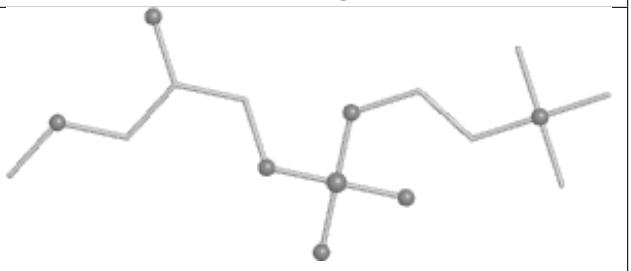
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Bond angles

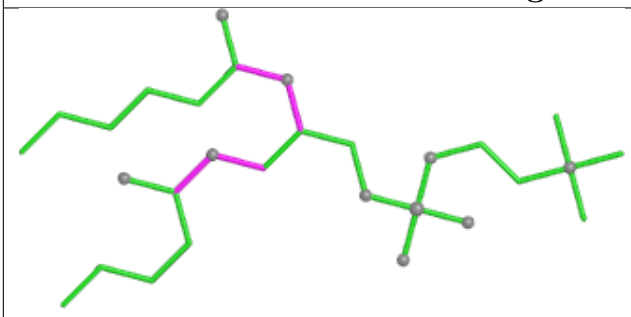


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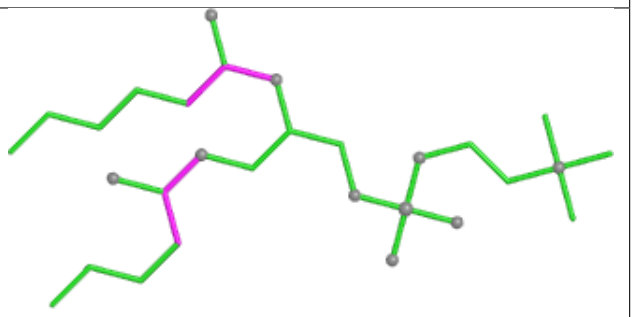


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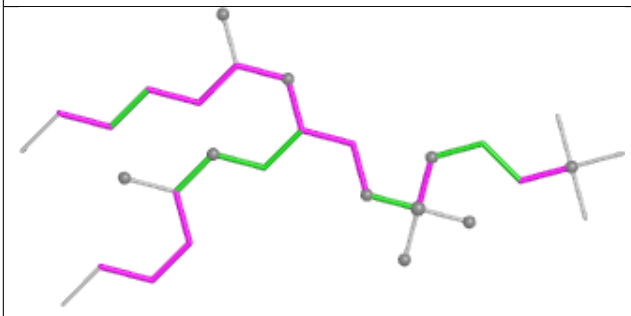
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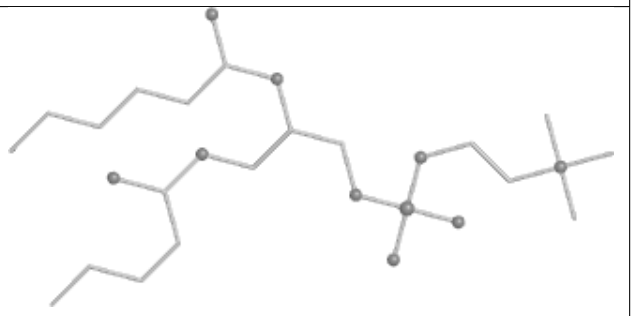
Bond lengths



Bond angles

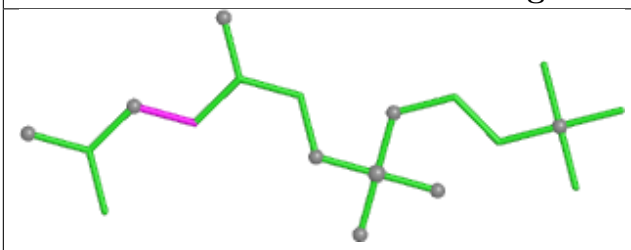


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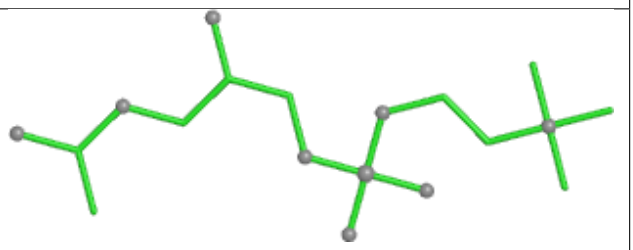


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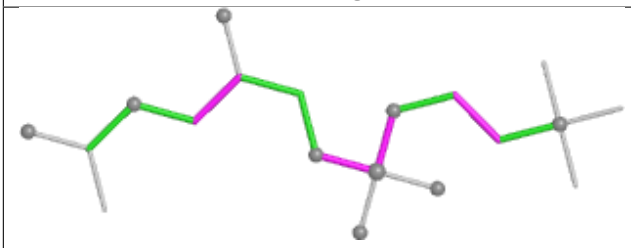
Ligand PC1 C 503



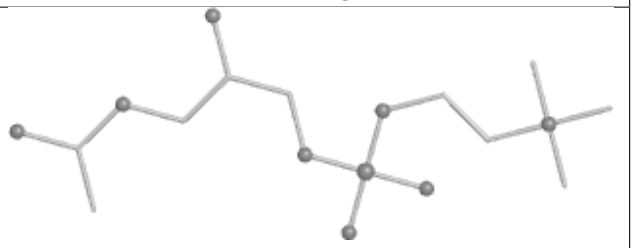
Bond lengths



Bond angles

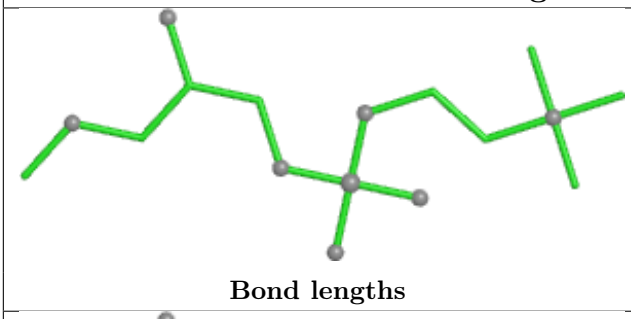


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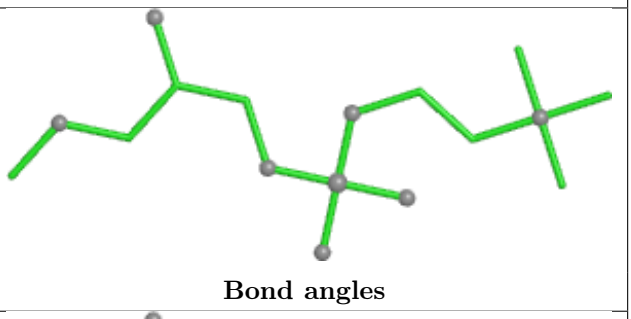


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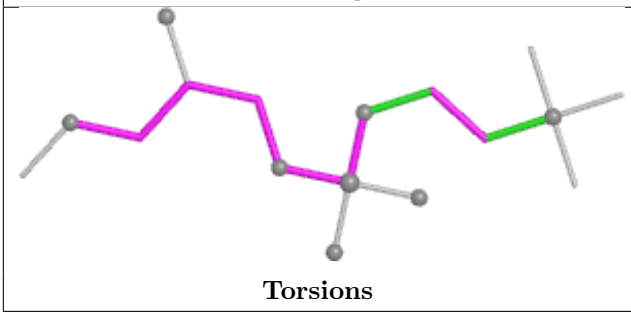
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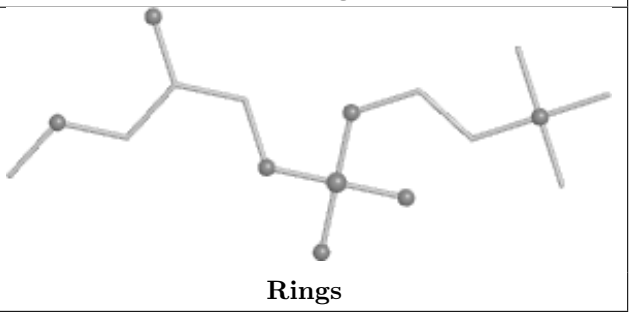
Bond lengths



Bond angles

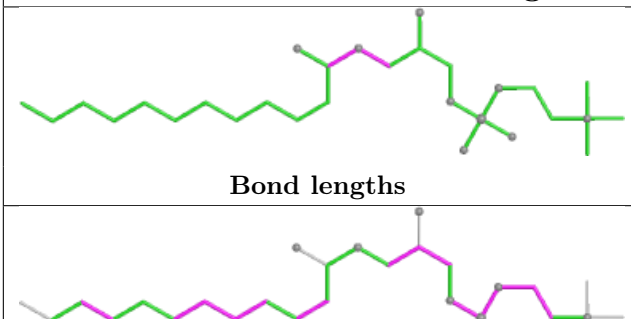


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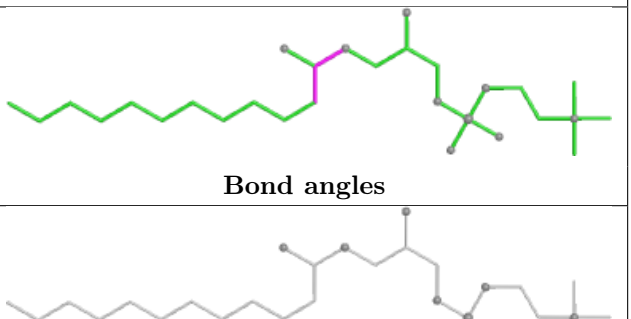


Rings

Ligand PC1 M 203



Bond lengths

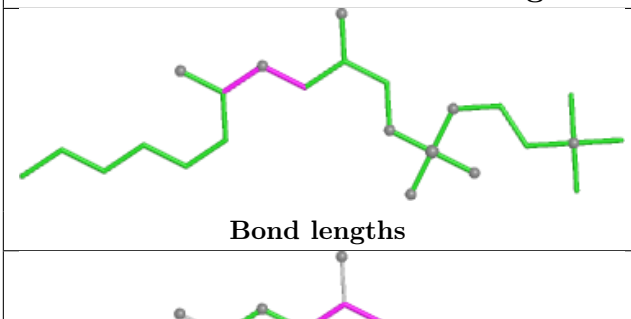


Bond angles

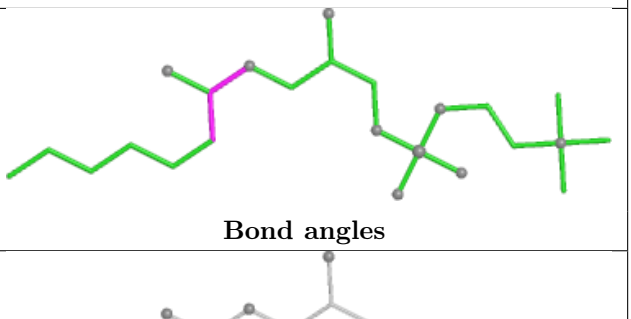
Torsions

Rings

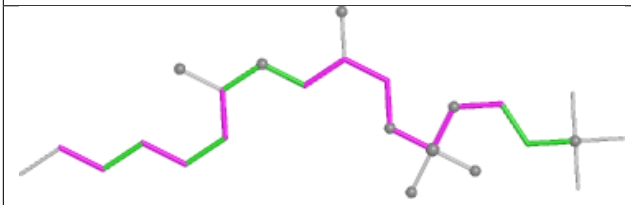
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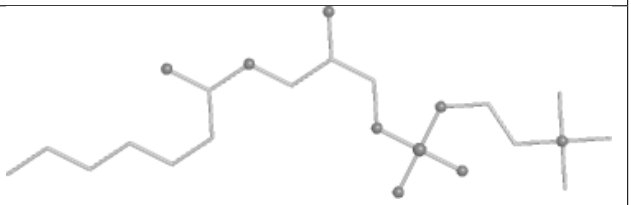
Bond lengths



Bond angles

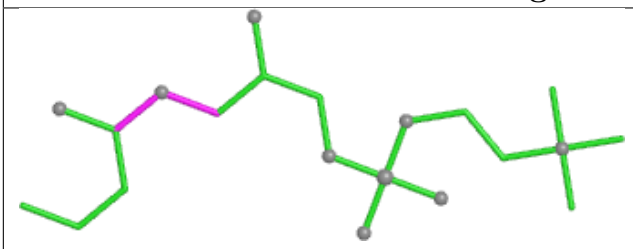


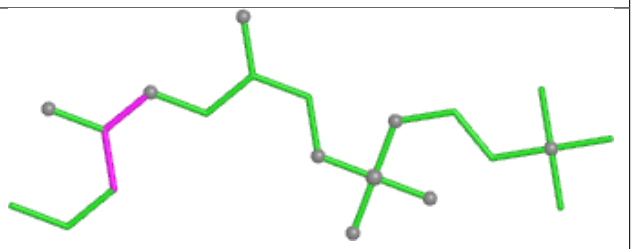
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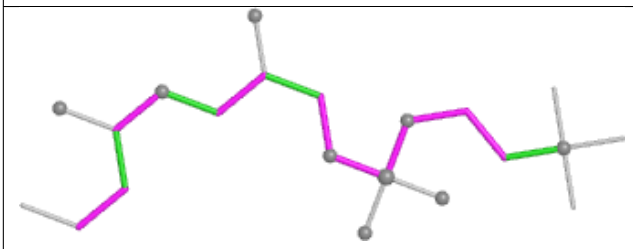


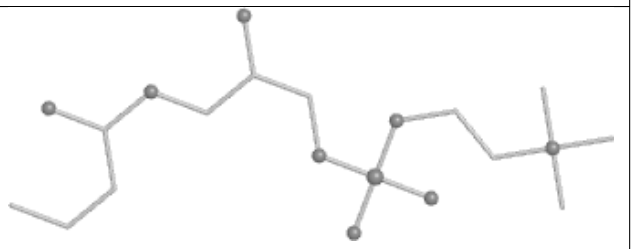
Rings

Ligand PC1 L 501

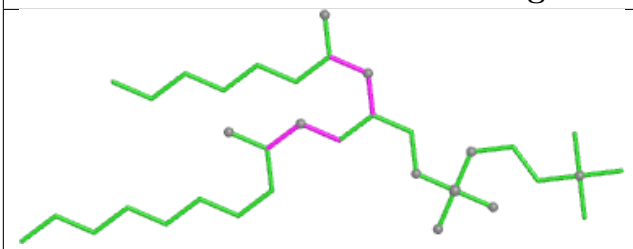

Bond lengths

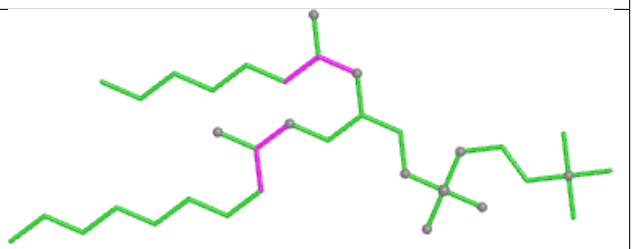

Bond angles

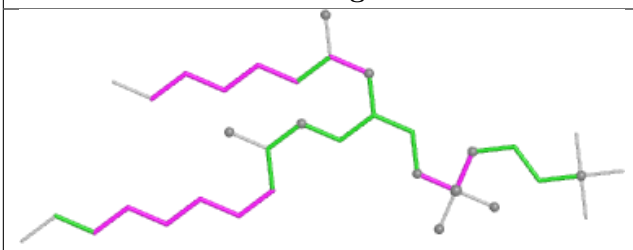

Torsions

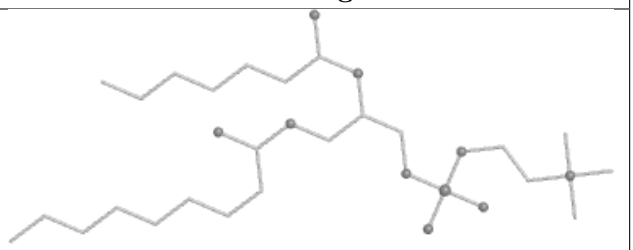

Rings

Ligand PC1 B 201

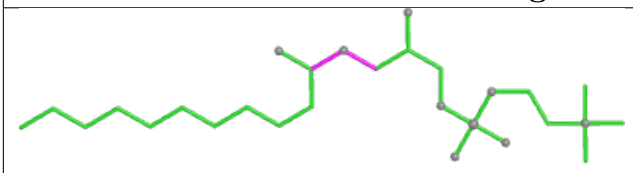

Bond lengths

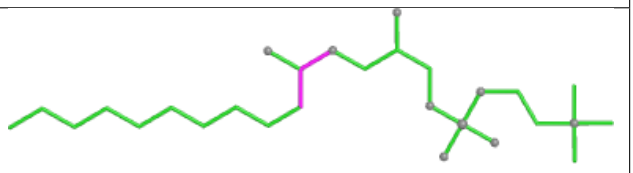

Bond angles

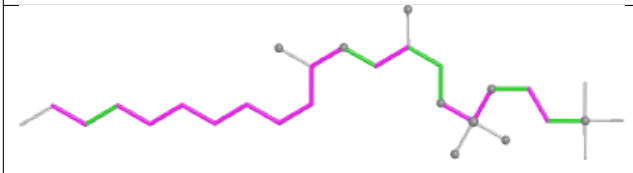

Torsions

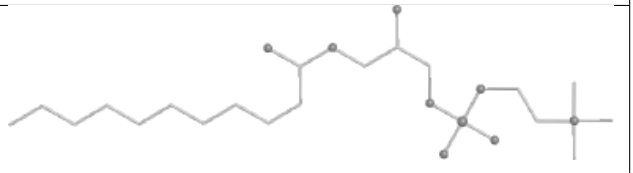

Rings

Ligand PC1 F 203

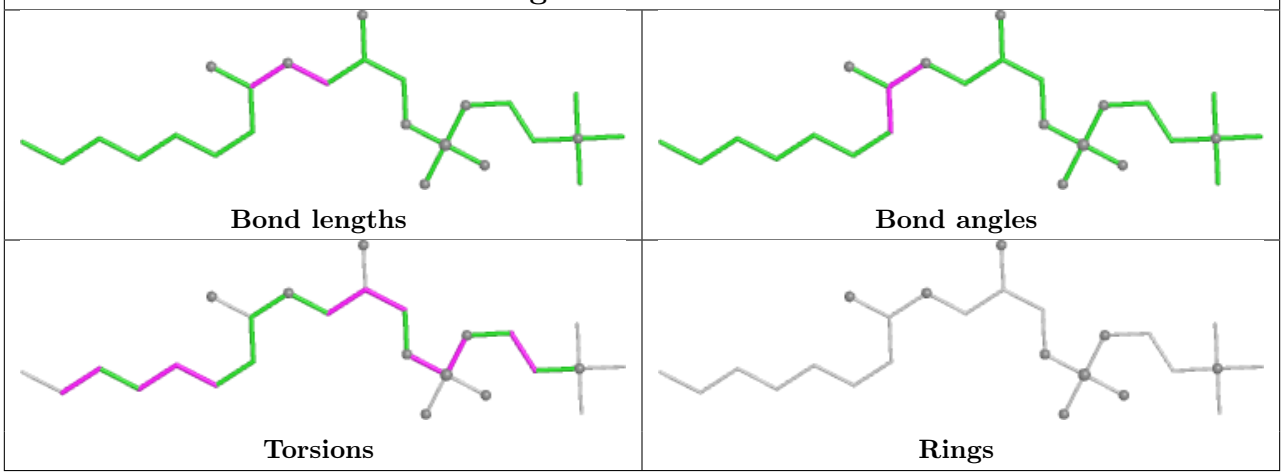

Bond lengths


Bond angles

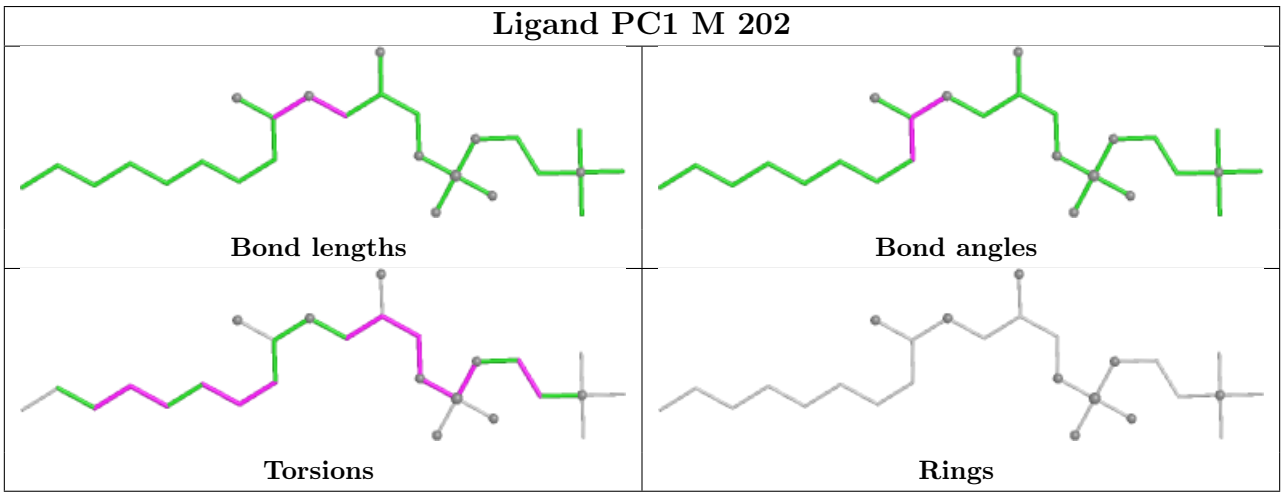

Torsions


Rings

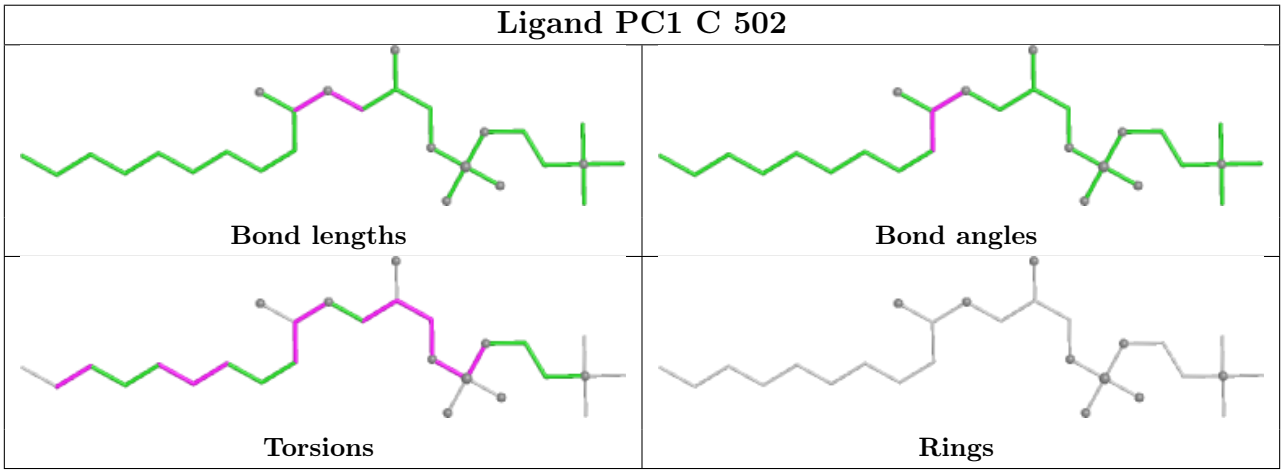
Ligand PC1 E 204



Ligand PC1 M 202



Ligand PC1 C 502



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

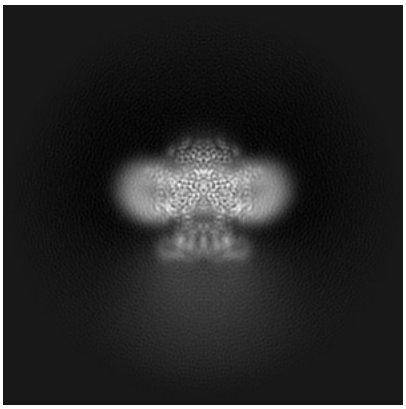
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-81270. These allow visual inspection of the internal detail of the map and identification of artifacts.

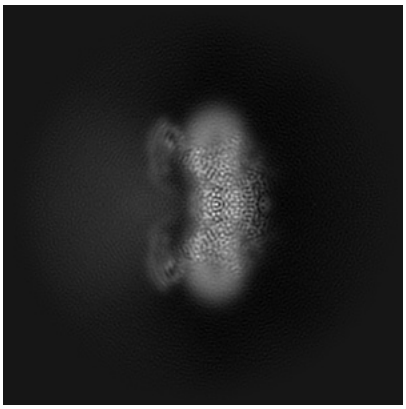
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

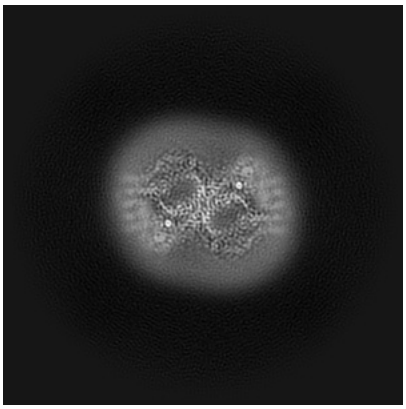
6.1.1 Primary map



X

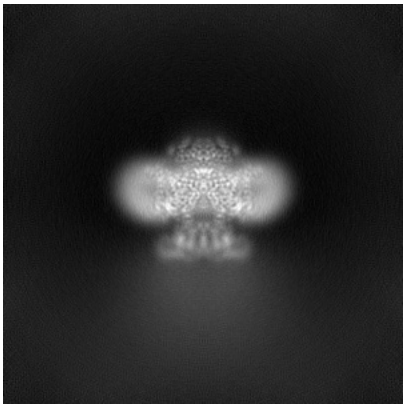


Y

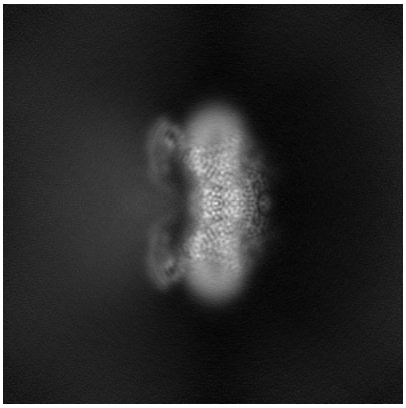


Z

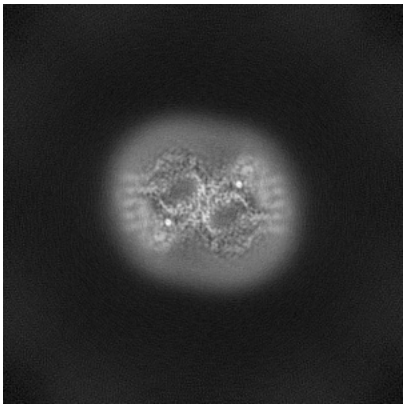
6.1.2 Raw map



X



Y

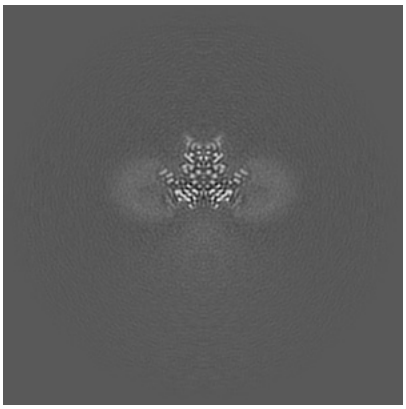


Z

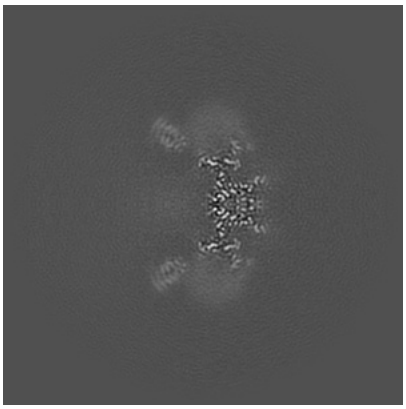
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

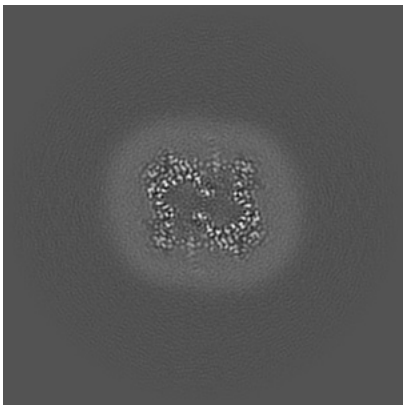
6.2.1 Primary map



X Index: 160

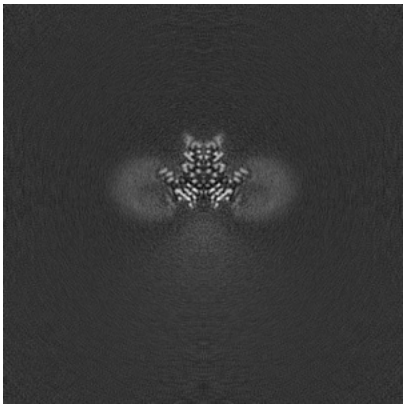


Y Index: 160

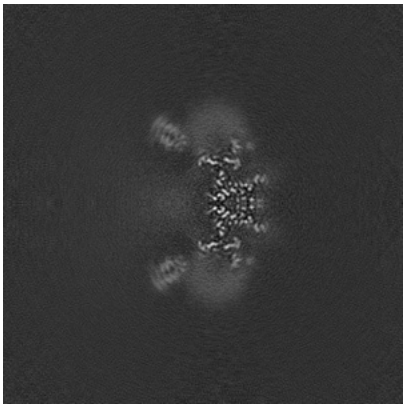


Z Index: 160

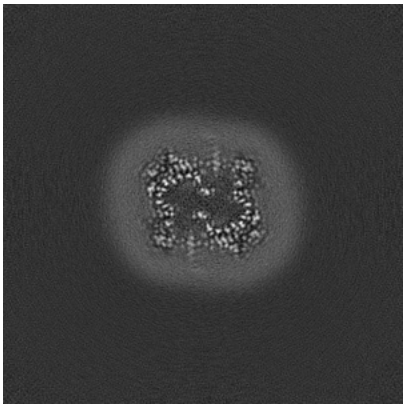
6.2.2 Raw map



X Index: 160



Y Index: 160

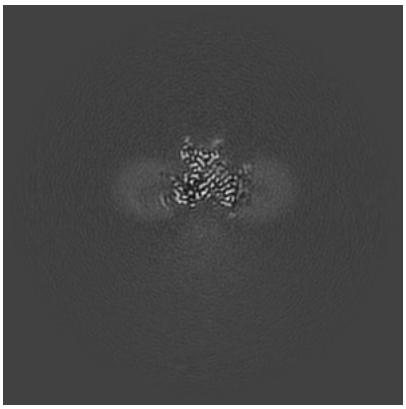


Z Index: 160

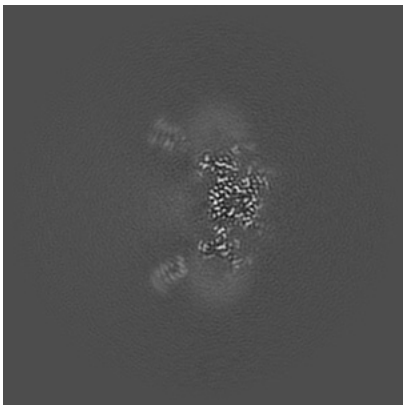
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

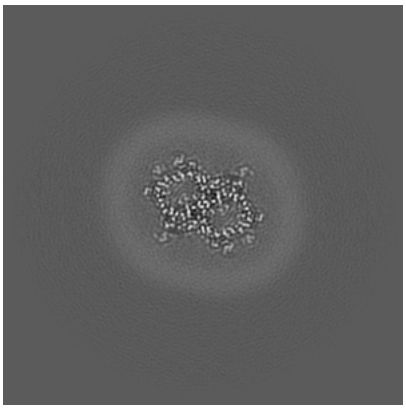
6.3.1 Primary map



X Index: 156

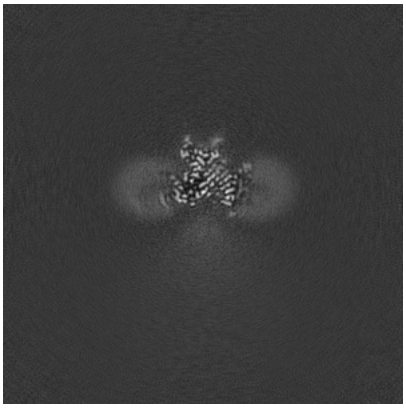


Y Index: 162

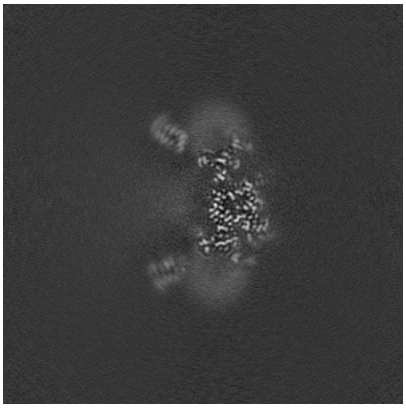


Z Index: 170

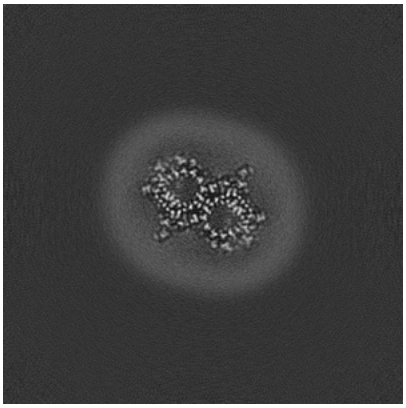
6.3.2 Raw map



X Index: 156



Y Index: 158

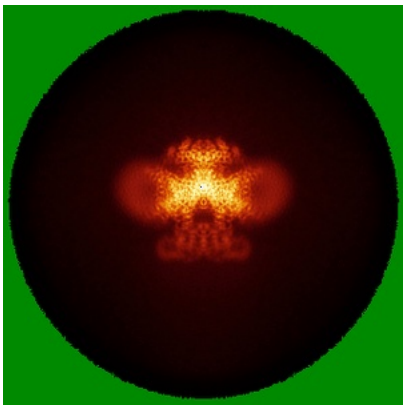


Z Index: 174

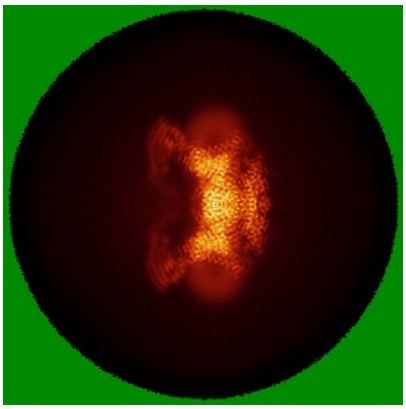
The images above show the largest variance slices of the map in three orthogonal directions.

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

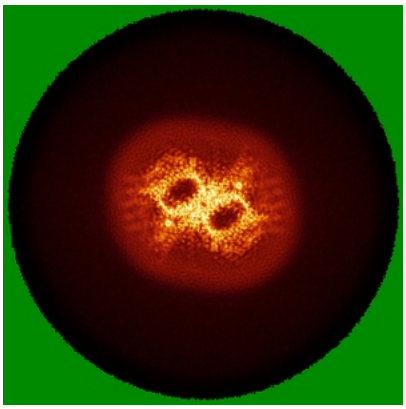
6.4.1 Primary map



X

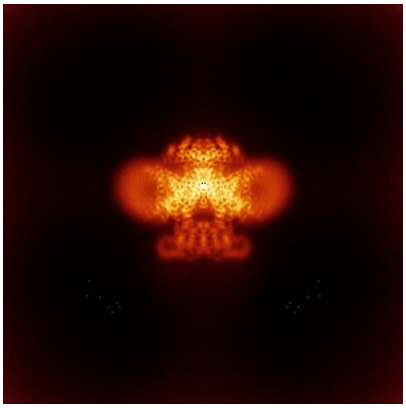


Y

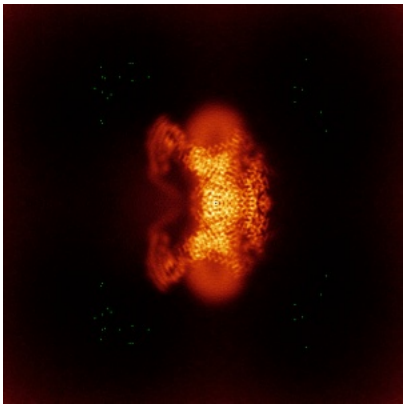


Z

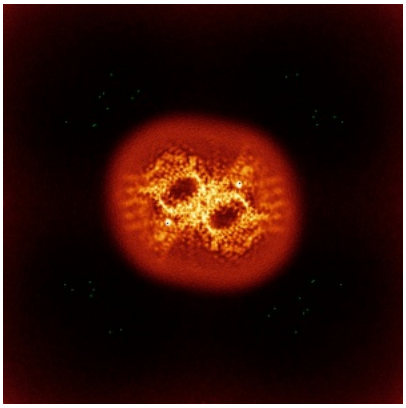
6.4.2 Raw map



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 0.19. 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.

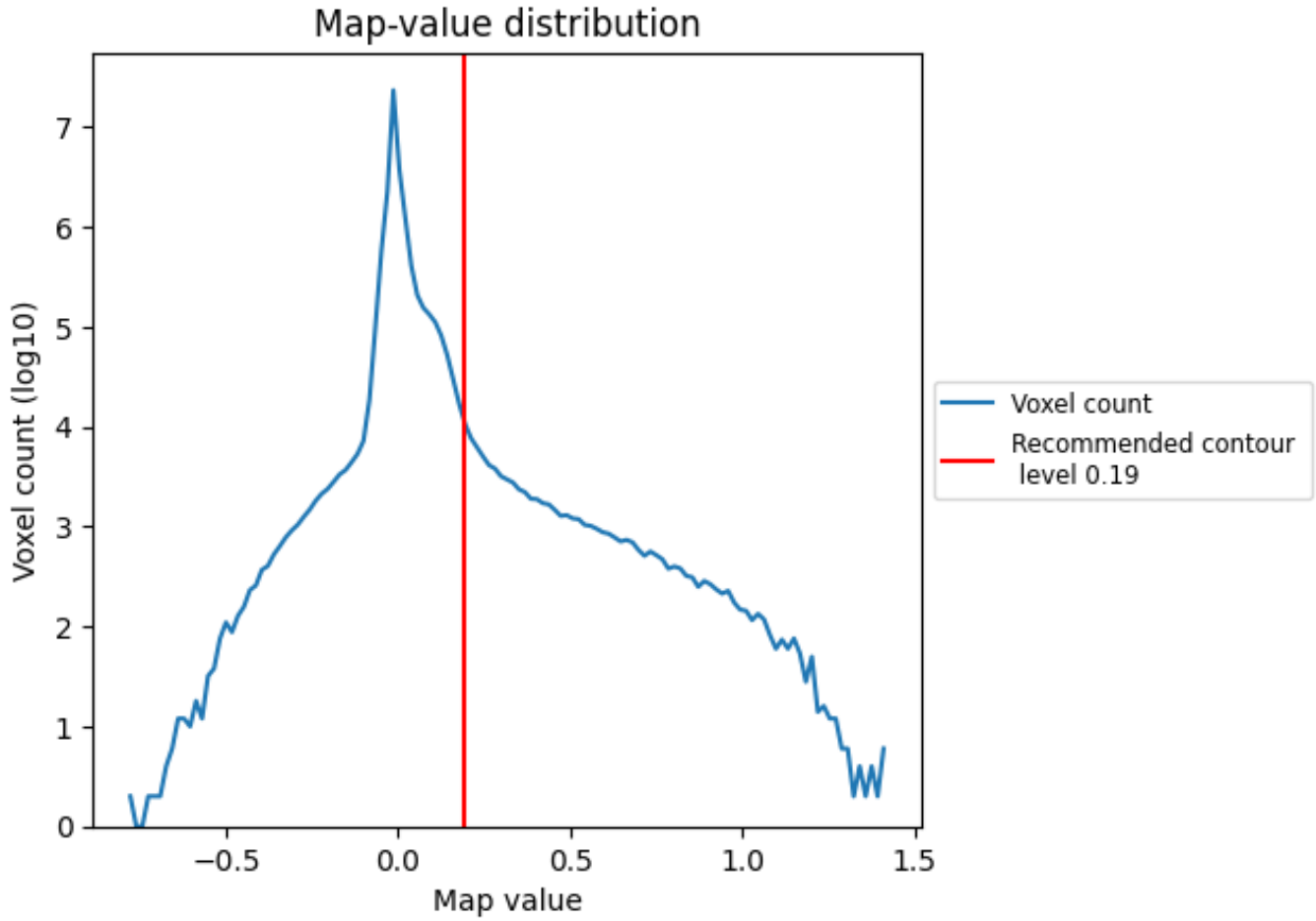
6.6 Mask visualisation (i)

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

7 Map analysis

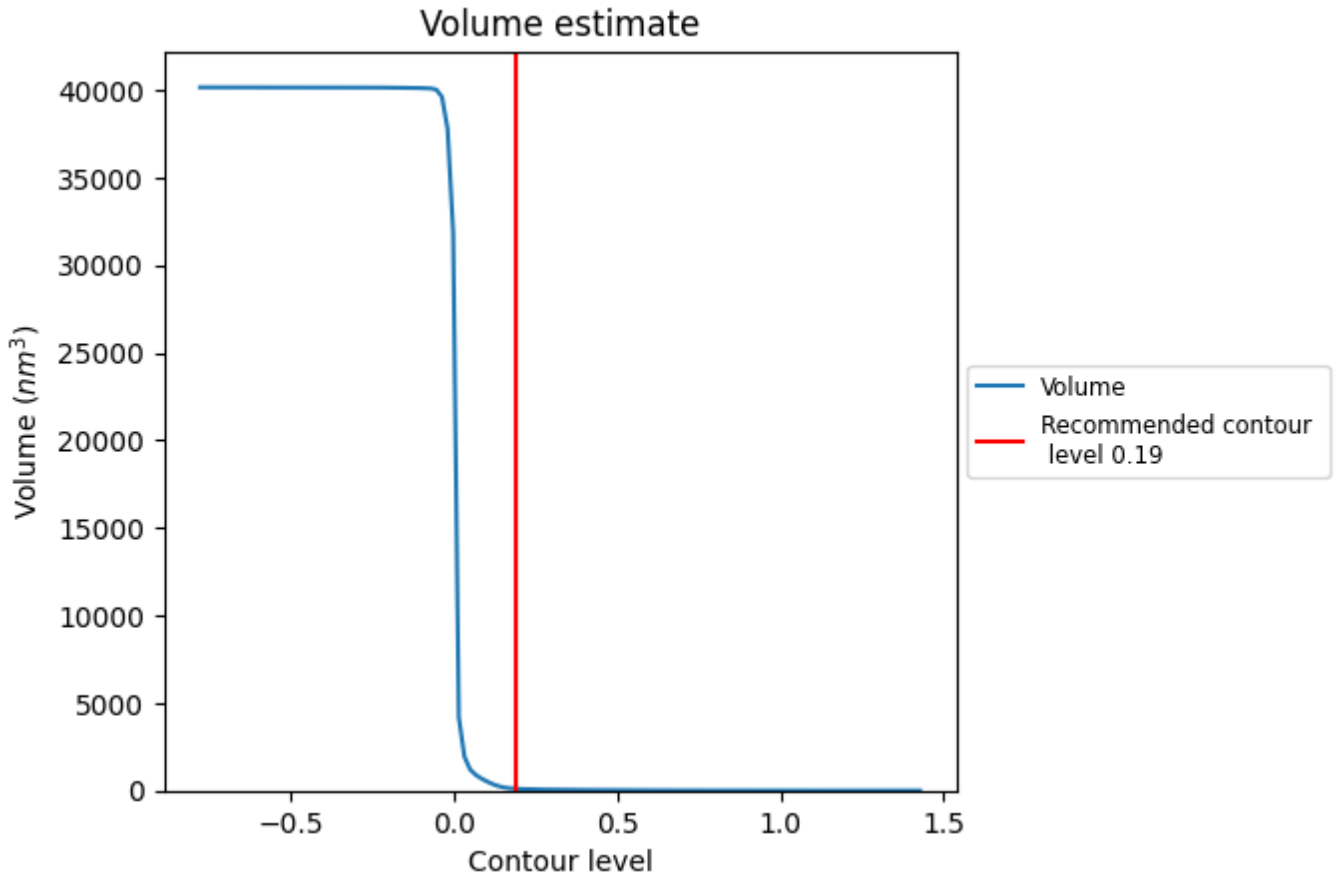
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

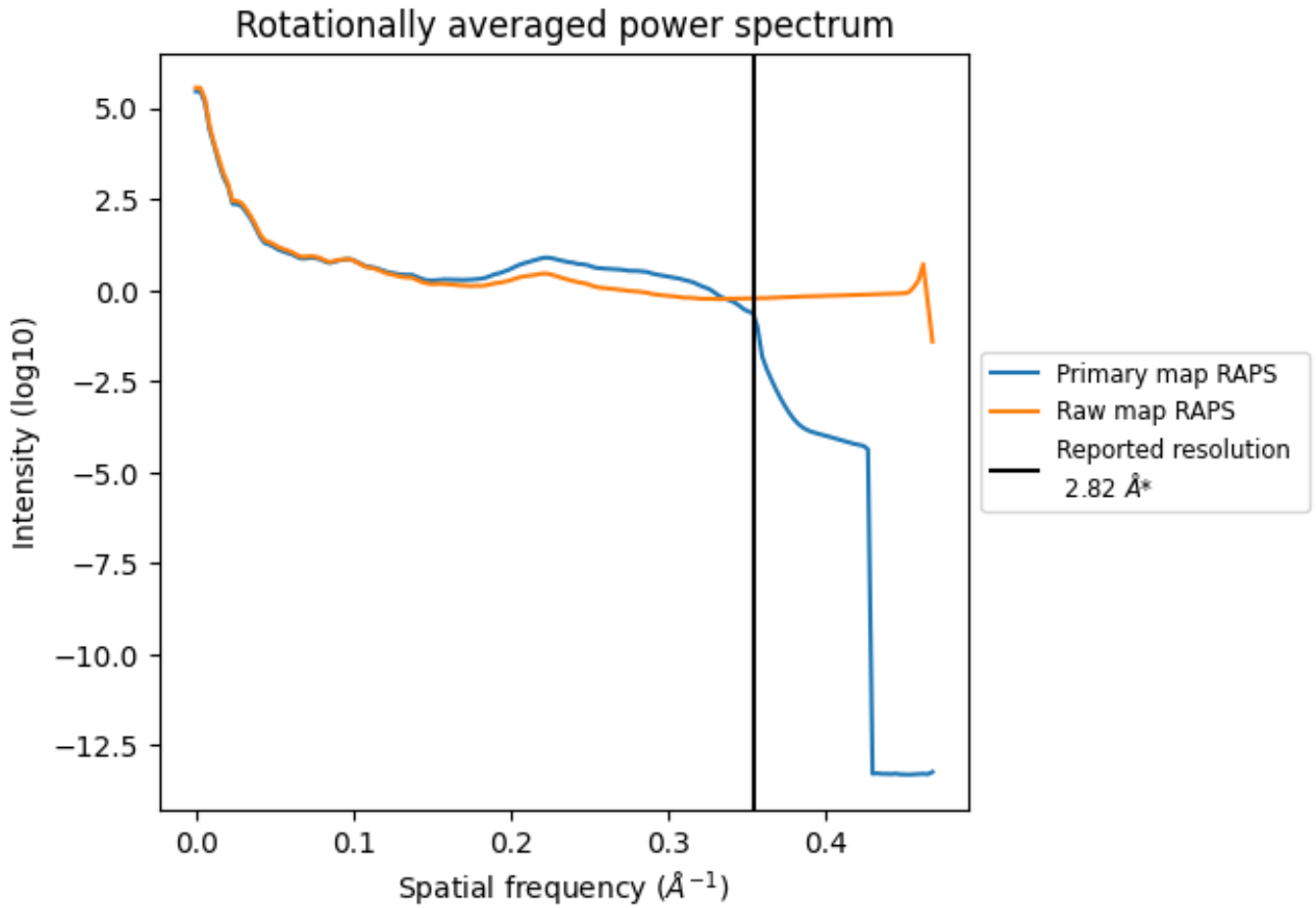
7.2 Volume estimate



The volume at the recommended contour level is 103 nm^3; this corresponds to an approximate mass of 93 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)

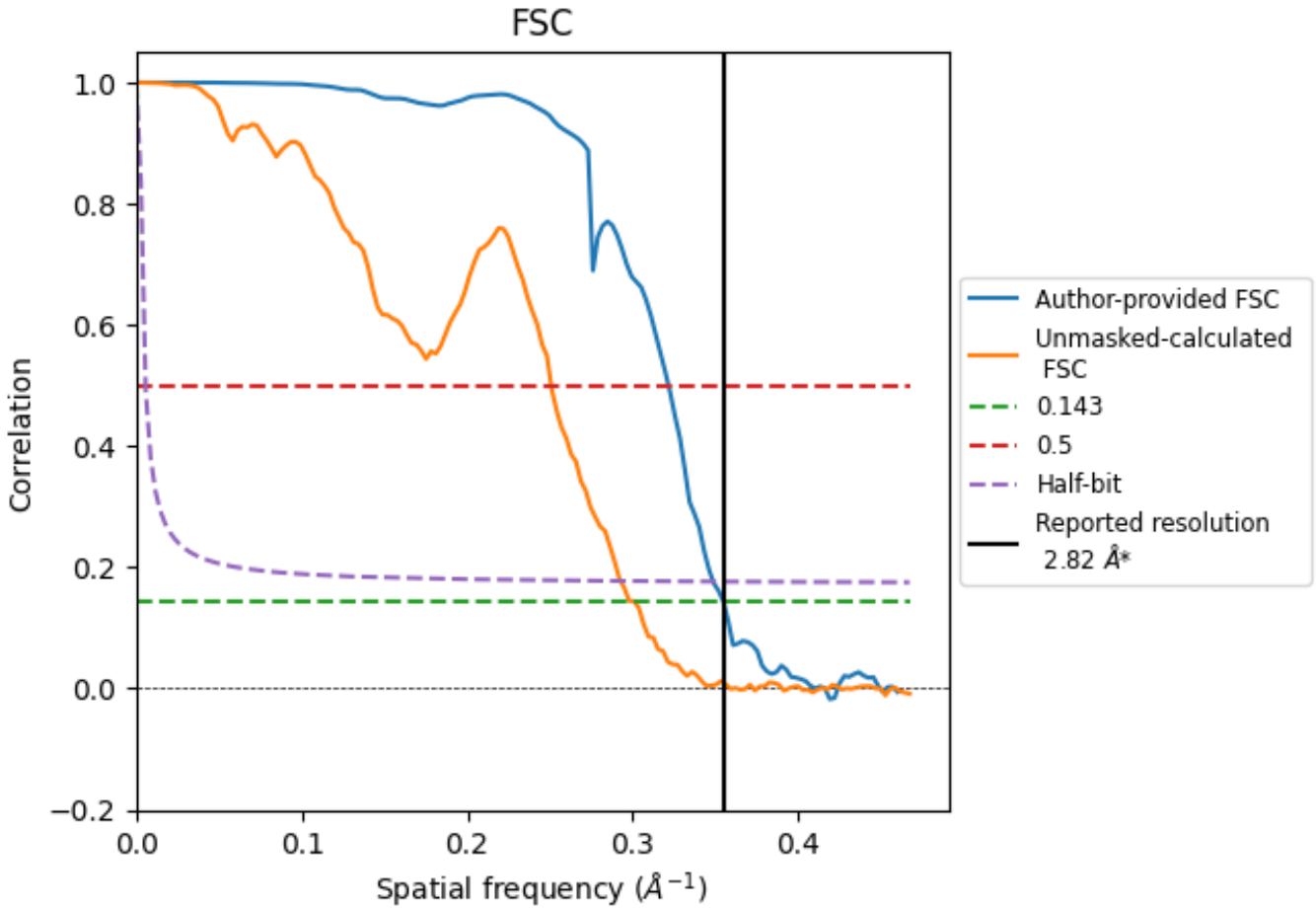


*Reported resolution corresponds to spatial frequency of 0.355 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.355 Å^{-1}

8.2 Resolution estimates (i)

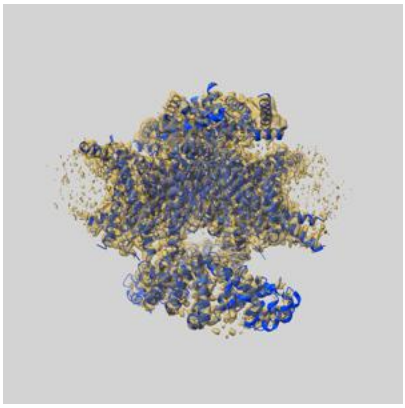
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.82	-	-
Author-provided FSC curve	2.82	3.11	2.87
Unmasked-calculated*	3.32	3.99	3.42

*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 3.32 differs from the reported value 2.82 by more than 10 %

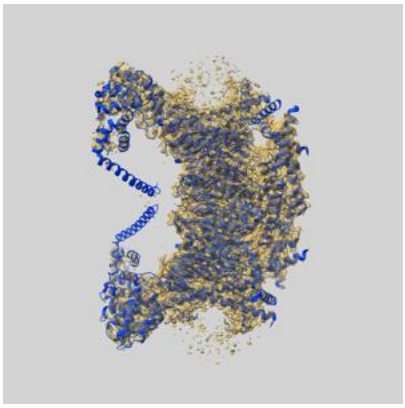
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-81270 and PDB model 27MX. Per-residue inclusion information can be found in section 3 on page 13.

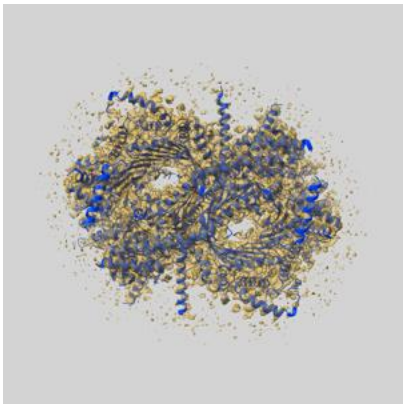
9.1 Map-model overlay



X



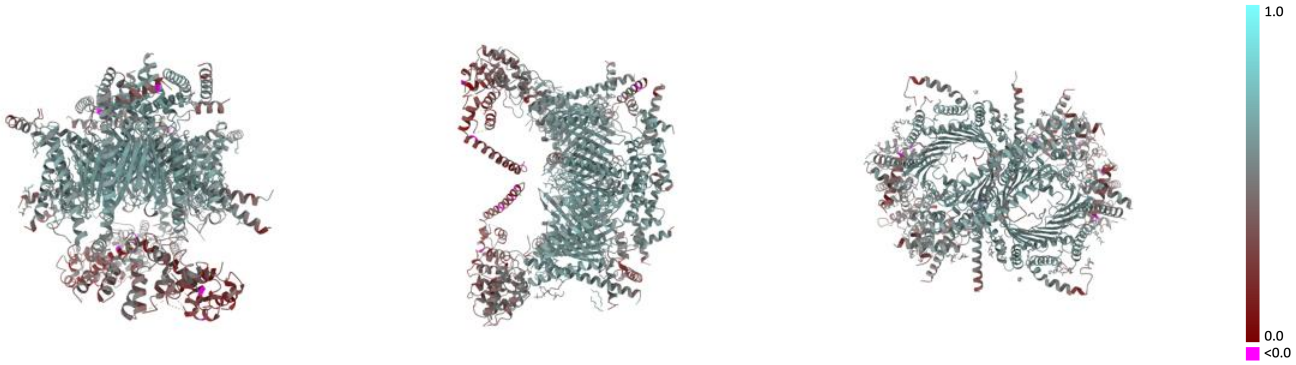
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.19 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.

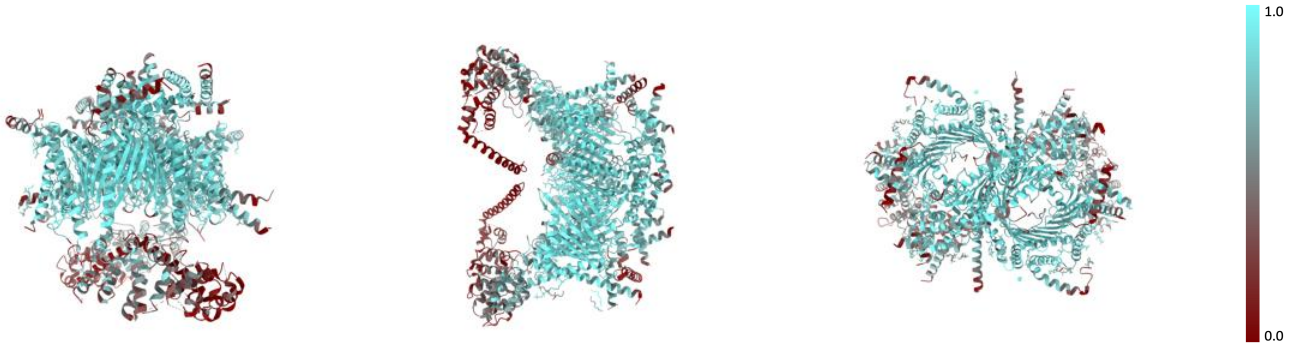
9.2 Q-score mapped to coordinate model (i)



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.

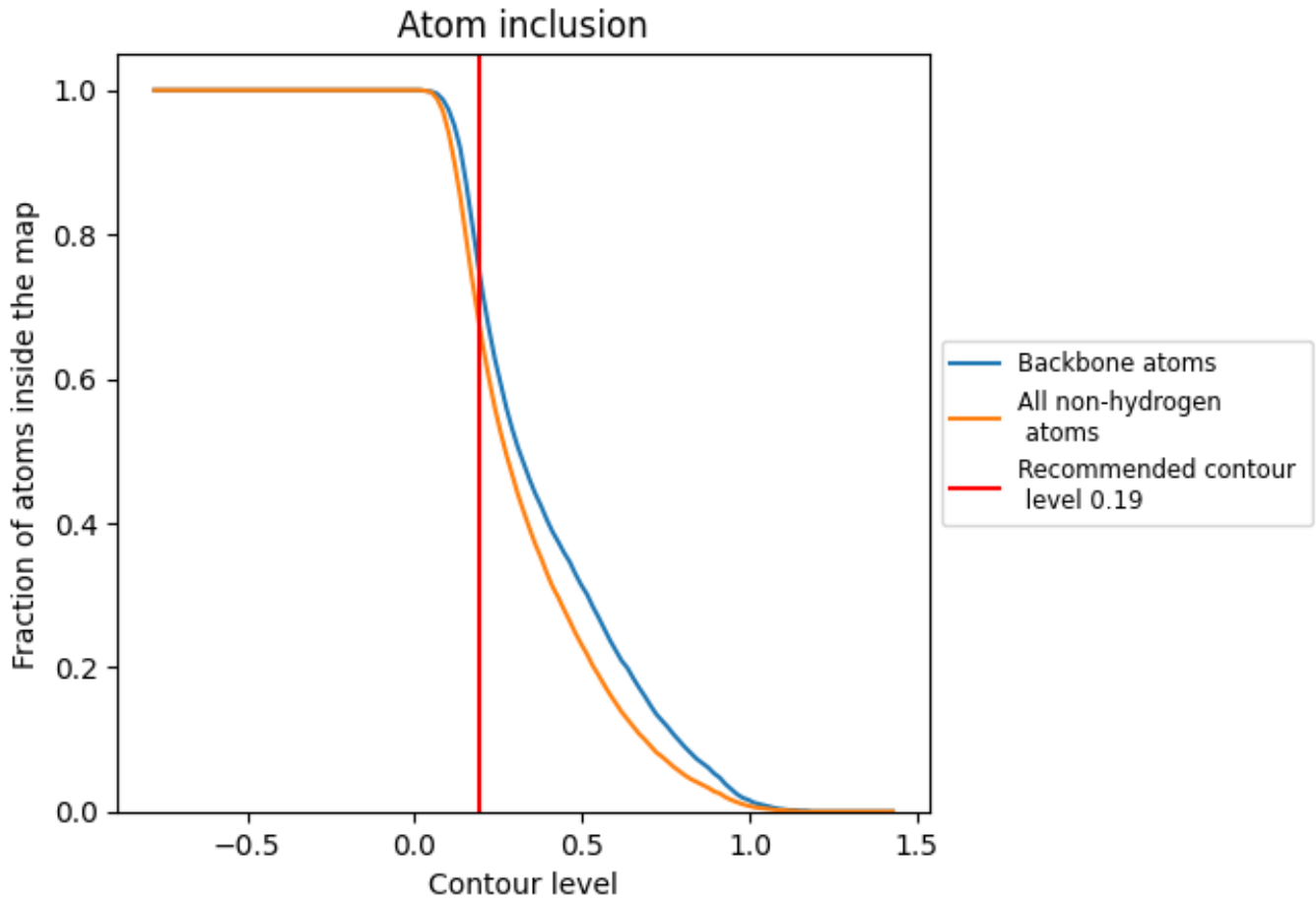
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.19).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6840	0.5050
A	0.7510	0.5320
B	0.7640	0.5420
C	0.8480	0.5770
D	0.8410	0.5800
E	0.8560	0.5850
F	0.8520	0.5770
G	0.7010	0.5100
H	0.6720	0.5020
I	0.7740	0.5480
J	0.7960	0.5630
K	0.3600	0.3570
L	0.3820	0.3680
M	0.7870	0.5490
N	0.7860	0.5480
O	0.8120	0.5570
P	0.8070	0.5700

