wwPDB EM Validation Summary Report (i)

Aug 6, 2026 – 04:49 PM JST

PDB ID	:	7YLY / pdb_00007yly
EMDB ID	:	EMD-33921
Title	:	yeast TRiC-plp2 complex at S5 closed TRiC state
Authors	:	Han, W.Y.
Deposited on	:	2022-07-27
Resolution	:	3.05 Å(reported)

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

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

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

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

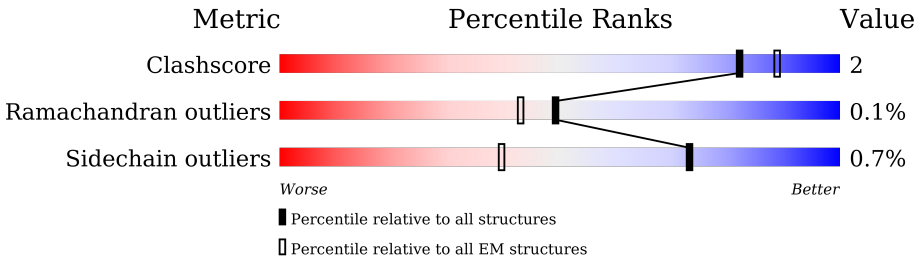
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.50

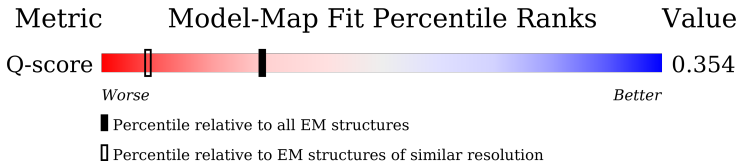
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.05 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	13971 (2.55 - 3.55)

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	559	91% 7%
1	a	559	92% 5%
2	B	527	93% 6%
2	b	527	90% 7%

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Mol	Chain	Length	Quality of chain
3	D	528	91% 7%
3	d	528	94% 5%
4	E	562	88% 7% 5%
4	e	562	87% 7% 5%
5	G	594	78% 9% 12%
5	g	594	84% 12%
6	H	550	89% 5% 5%
6	h	550	89% 6%
7	P	286	17% 61% 6% 33%
7	p	286	18% 60% 6% 33%
8	Q	568	5% 89% 6%
8	q	568	90% 5% 5%
9	Z	546	91% 7%
9	z	546	94%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	AF3	B	603	-	-	X	-
12	AF3	D	603	-	-	X	-
12	AF3	E	603	-	-	X	-
12	AF3	G	603	-	-	X	-
12	AF3	d	603	-	-	X	-
12	AF3	e	603	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 68656 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 T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	550	Total	C	N	O	S	0	0
			4158	2599	725	813	21		
1	a	546	Total	C	N	O	S	0	0
			4129	2582	721	806	20		

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	518	Total	C	N	O	S	0	0
			3937	2461	680	782	14		
2	b	518	Total	C	N	O	S	0	0
			3937	2461	680	782	14		

- Molecule 3 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	523	Total	C	N	O	S	0	0
			3998	2492	711	778	17		
3	d	524	Total	C	N	O	S	0	0
			4005	2497	712	779	17		

- Molecule 4 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	536	Total	C	N	O	S	0	0
			4133	2595	710	806	22		
4	e	535	Total	C	N	O	S	0	0
			4124	2590	709	803	22		

- Molecule 5 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	520	Total	C	N	O	S	0	0
			4004	2510	703	764	27		
5	g	520	Total	C	N	O	S	0	0
			4003	2511	703	762	27		

There are 122 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	375	LEU	-	see sequence details	UNP P39077
G	376	GLU	-	see sequence details	UNP P39077
G	377	GLY	-	see sequence details	UNP P39077
G	378	SER	-	see sequence details	UNP P39077
G	379	GLY	-	see sequence details	UNP P39077
G	380	SER	-	see sequence details	UNP P39077
G	381	GLY	-	see sequence details	UNP P39077
G	382	TRP	-	see sequence details	UNP P39077
G	383	SER	-	see sequence details	UNP P39077
G	384	HIS	-	see sequence details	UNP P39077
G	385	PRO	-	see sequence details	UNP P39077
G	386	GLN	-	see sequence details	UNP P39077
G	387	PHE	-	see sequence details	UNP P39077
G	388	GLU	-	see sequence details	UNP P39077
G	389	LYS	-	see sequence details	UNP P39077
G	390	GLY	-	see sequence details	UNP P39077
G	391	SER	-	see sequence details	UNP P39077
G	392	GLY	-	see sequence details	UNP P39077
G	393	LYS	-	see sequence details	UNP P39077
G	394	ARG	-	see sequence details	UNP P39077
G	395	ARG	-	see sequence details	UNP P39077
G	396	TRP	-	see sequence details	UNP P39077
G	397	LYS	-	see sequence details	UNP P39077
G	398	LYS	-	see sequence details	UNP P39077
G	399	ASN	-	see sequence details	UNP P39077
G	400	PHE	-	see sequence details	UNP P39077
G	401	ILE	-	see sequence details	UNP P39077
G	402	ALA	-	see sequence details	UNP P39077
G	403	VAL	-	see sequence details	UNP P39077
G	404	SER	-	see sequence details	UNP P39077
G	405	ALA	-	see sequence details	UNP P39077
G	406	ALA	-	see sequence details	UNP P39077
G	407	ASN	-	see sequence details	UNP P39077
G	408	ARG	-	see sequence details	UNP P39077
G	409	PHE	-	see sequence details	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
G	410	LYS	-	see sequence details	UNP P39077
G	411	LYS	-	see sequence details	UNP P39077
G	412	ILE	-	see sequence details	UNP P39077
G	413	SER	-	see sequence details	UNP P39077
G	414	SER	-	see sequence details	UNP P39077
G	415	SER	-	see sequence details	UNP P39077
G	416	GLY	-	see sequence details	UNP P39077
G	417	ALA	-	see sequence details	UNP P39077
G	418	LEU	-	see sequence details	UNP P39077
G	419	GLY	-	see sequence details	UNP P39077
G	420	SER	-	see sequence details	UNP P39077
G	421	GLY	-	see sequence details	UNP P39077
G	422	HIS	-	see sequence details	UNP P39077
G	423	HIS	-	see sequence details	UNP P39077
G	424	HIS	-	see sequence details	UNP P39077
G	425	HIS	-	see sequence details	UNP P39077
G	426	HIS	-	see sequence details	UNP P39077
G	427	HIS	-	see sequence details	UNP P39077
G	428	HIS	-	see sequence details	UNP P39077
G	429	HIS	-	see sequence details	UNP P39077
G	430	GLY	-	see sequence details	UNP P39077
G	431	SER	-	see sequence details	UNP P39077
G	432	GLY	-	see sequence details	UNP P39077
G	433	LEU	-	see sequence details	UNP P39077
G	434	GLN	-	see sequence details	UNP P39077
G	435	LYS	-	see sequence details	UNP P39077
g	375	LEU	-	see sequence details	UNP P39077
g	376	GLU	-	see sequence details	UNP P39077
g	377	GLY	-	see sequence details	UNP P39077
g	378	SER	-	see sequence details	UNP P39077
g	379	GLY	-	see sequence details	UNP P39077
g	380	SER	-	see sequence details	UNP P39077
g	381	GLY	-	see sequence details	UNP P39077
g	382	TRP	-	see sequence details	UNP P39077
g	383	SER	-	see sequence details	UNP P39077
g	384	HIS	-	see sequence details	UNP P39077
g	385	PRO	-	see sequence details	UNP P39077
g	386	GLN	-	see sequence details	UNP P39077
g	387	PHE	-	see sequence details	UNP P39077
g	388	GLU	-	see sequence details	UNP P39077
g	389	LYS	-	see sequence details	UNP P39077
g	390	GLY	-	see sequence details	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
g	391	SER	-	see sequence details	UNP P39077
g	392	GLY	-	see sequence details	UNP P39077
g	393	LYS	-	see sequence details	UNP P39077
g	394	ARG	-	see sequence details	UNP P39077
g	395	ARG	-	see sequence details	UNP P39077
g	396	TRP	-	see sequence details	UNP P39077
g	397	LYS	-	see sequence details	UNP P39077
g	398	LYS	-	see sequence details	UNP P39077
g	399	ASN	-	see sequence details	UNP P39077
g	400	PHE	-	see sequence details	UNP P39077
g	401	ILE	-	see sequence details	UNP P39077
g	402	ALA	-	see sequence details	UNP P39077
g	403	VAL	-	see sequence details	UNP P39077
g	404	SER	-	see sequence details	UNP P39077
g	405	ALA	-	see sequence details	UNP P39077
g	406	ALA	-	see sequence details	UNP P39077
g	407	ASN	-	see sequence details	UNP P39077
g	408	ARG	-	see sequence details	UNP P39077
g	409	PHE	-	see sequence details	UNP P39077
g	410	LYS	-	see sequence details	UNP P39077
g	411	LYS	-	see sequence details	UNP P39077
g	412	ILE	-	see sequence details	UNP P39077
g	413	SER	-	see sequence details	UNP P39077
g	414	SER	-	see sequence details	UNP P39077
g	415	SER	-	see sequence details	UNP P39077
g	416	GLY	-	see sequence details	UNP P39077
g	417	ALA	-	see sequence details	UNP P39077
g	418	LEU	-	see sequence details	UNP P39077
g	419	GLY	-	see sequence details	UNP P39077
g	420	SER	-	see sequence details	UNP P39077
g	421	GLY	-	see sequence details	UNP P39077
g	422	HIS	-	see sequence details	UNP P39077
g	423	HIS	-	see sequence details	UNP P39077
g	424	HIS	-	see sequence details	UNP P39077
g	425	HIS	-	see sequence details	UNP P39077
g	426	HIS	-	see sequence details	UNP P39077
g	427	HIS	-	see sequence details	UNP P39077
g	428	HIS	-	see sequence details	UNP P39077
g	429	HIS	-	see sequence details	UNP P39077
g	430	GLY	-	see sequence details	UNP P39077
g	431	SER	-	see sequence details	UNP P39077
g	432	GLY	-	see sequence details	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
g	433	LEU	-	see sequence details	UNP P39077
g	434	GLN	-	see sequence details	UNP P39077
g	435	LYS	-	see sequence details	UNP P39077

- Molecule 6 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	520	Total	C	N	O	S	0	0
			3980	2510	678	773	19		
6	h	527	Total	C	N	O	S	0	0
			4032	2540	688	784	20		

- Molecule 7 is a protein called Phosducin-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	191	Total	C	N	O	S	0	0
			1571	983	272	310	6		
7	p	191	Total	C	N	O	S	0	0
			1571	983	272	310	6		

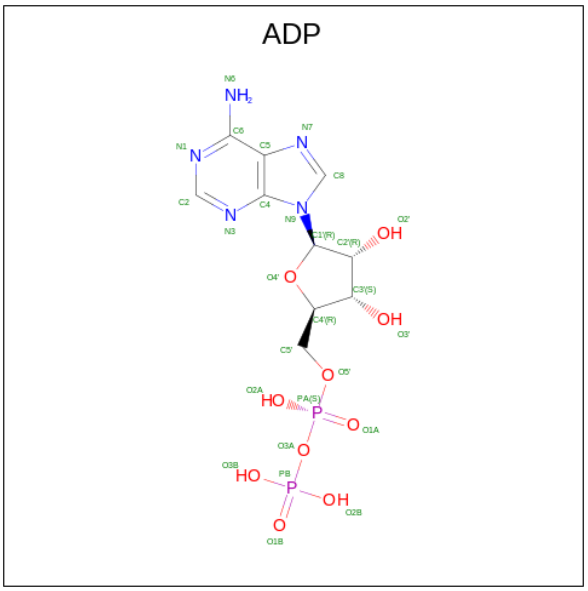
- Molecule 8 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	548	Total	C	N	O	S	0	0
			4163	2622	711	804	26		
8	q	541	Total	C	N	O	S	0	0
			4115	2592	703	794	26		

- Molecule 9 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	538	Total	C	N	O	S	0	0
			4139	2599	717	806	17		
9	z	538	Total	C	N	O	S	0	0
			4139	2599	717	806	17		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	Q	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	Z	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	a	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	b	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	d	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	e	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	g	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	h	1	Total	C	N	O	P	0
			27	10	5	10	2	

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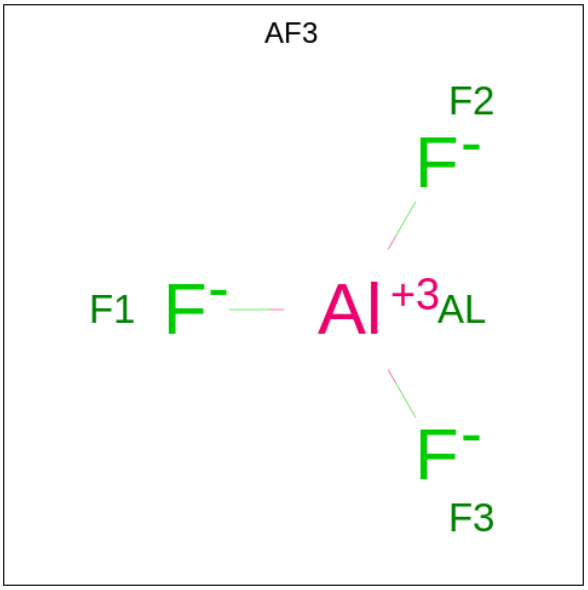
Mol	Chain	Residues	Atoms					AltConf
10	q	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	z	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Mg	0
			1	1	
11	B	1	Total	Mg	0
			1	1	
11	D	1	Total	Mg	0
			1	1	
11	E	1	Total	Mg	0
			1	1	
11	G	1	Total	Mg	0
			1	1	
11	H	1	Total	Mg	0
			1	1	
11	Q	1	Total	Mg	0
			1	1	
11	Z	1	Total	Mg	0
			1	1	
11	a	1	Total	Mg	0
			1	1	
11	b	1	Total	Mg	0
			1	1	
11	d	1	Total	Mg	0
			1	1	
11	e	1	Total	Mg	0
			1	1	
11	g	1	Total	Mg	0
			1	1	
11	h	1	Total	Mg	0
			1	1	
11	q	1	Total	Mg	0
			1	1	
11	z	1	Total	Mg	0
			1	1	

- Molecule 12 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3) (labeled as "Lig-

and of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total Al F 4 1 3	0
12	B	1	Total Al F 4 1 3	0
12	D	1	Total Al F 4 1 3	0
12	E	1	Total Al F 4 1 3	0
12	G	1	Total Al F 4 1 3	0
12	H	1	Total Al F 4 1 3	0
12	Z	1	Total Al F 4 1 3	0
12	a	1	Total Al F 4 1 3	0
12	b	1	Total Al F 4 1 3	0
12	d	1	Total Al F 4 1 3	0
12	e	1	Total Al F 4 1 3	0
12	g	1	Total Al F 4 1 3	0
12	h	1	Total Al F 4 1 3	0

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Mol	Chain	Residues	Atoms	AltConf
12	z	1	Total Al F 4 1 3	0

- Molecule 13 is water.

Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total O 1 1	0
13	B	1	Total O 1 1	0
13	D	1	Total O 1 1	0
13	E	1	Total O 1 1	0
13	G	1	Total O 1 1	0
13	H	1	Total O 1 1	0
13	Z	1	Total O 1 1	0
13	a	1	Total O 1 1	0
13	b	1	Total O 1 1	0
13	d	1	Total O 1 1	0
13	e	1	Total O 1 1	0
13	g	1	Total O 1 1	0
13	h	1	Total O 1 1	0
13	z	1	Total O 1 1	0

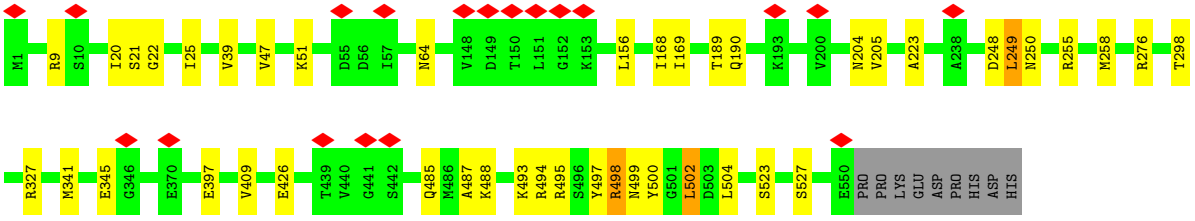
3 Residue-property plots (i)

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: T-complex protein 1 subunit alpha

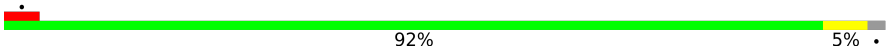
Chain A:

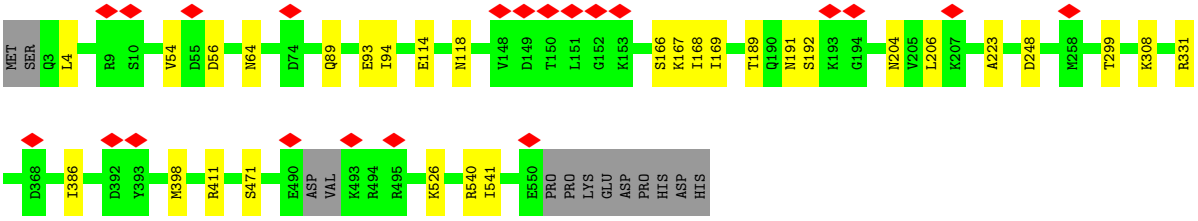




• Molecule 1: T-complex protein 1 subunit alpha

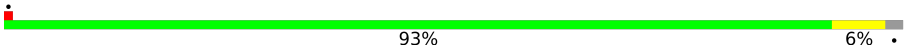
Chain a:





• Molecule 2: T-complex protein 1 subunit beta

Chain B:

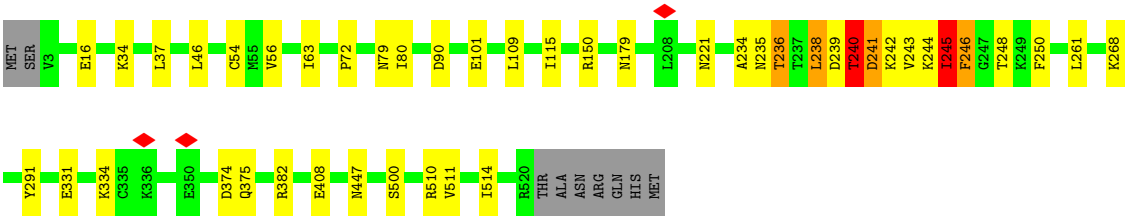


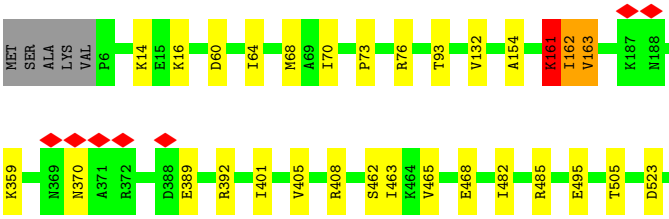


• Molecule 2: T-complex protein 1 subunit beta

Chain b:

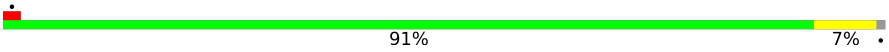






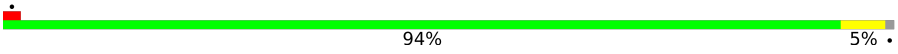
• Molecule 3: T-complex protein 1 subunit delta

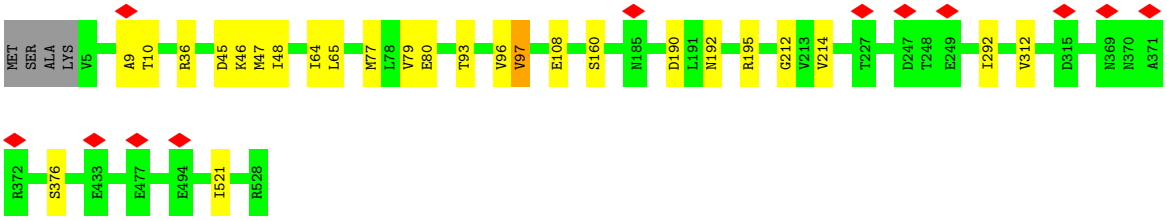
Chain D:



• Molecule 3: T-complex protein 1 subunit delta

Chain d:

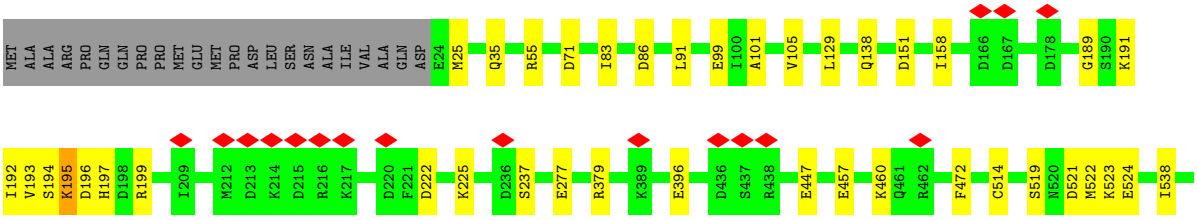


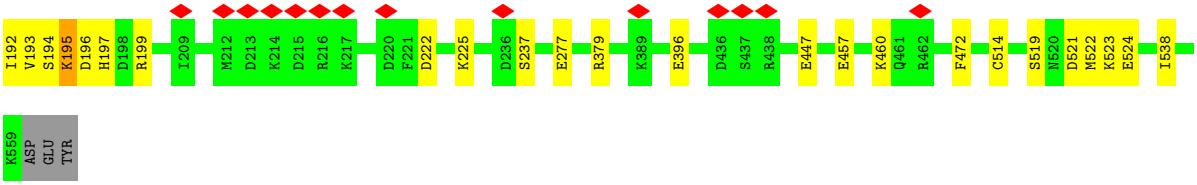


• Molecule 4: T-complex protein 1 subunit epsilon

Chain E:



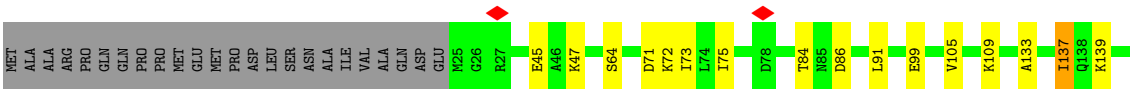


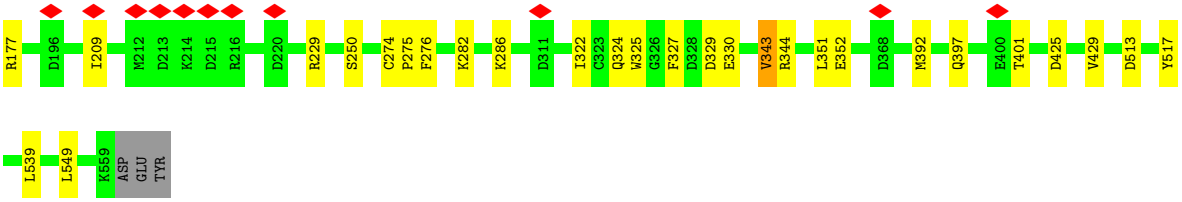


• Molecule 4: T-complex protein 1 subunit epsilon

Chain e:



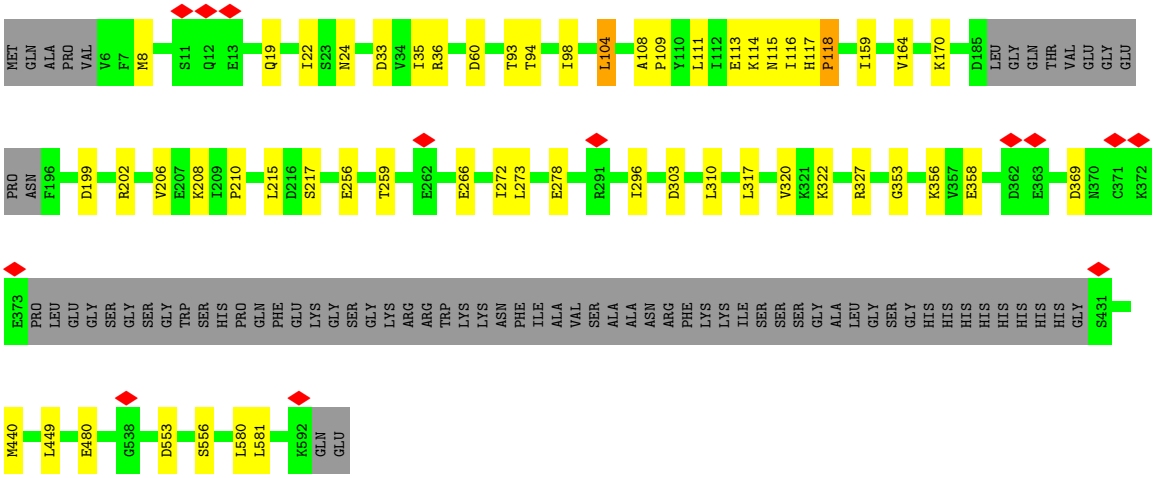




• Molecule 5: T-complex protein 1 subunit gamma

Chain G:

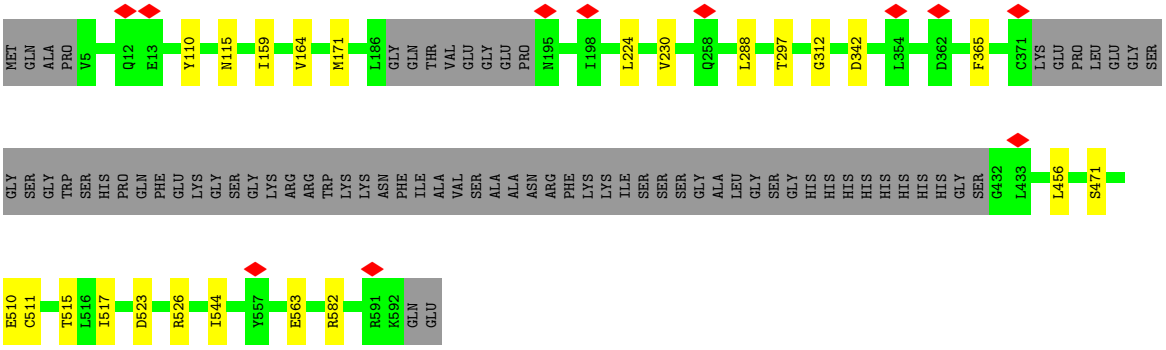




• Molecule 5: T-complex protein 1 subunit gamma

Chain g:



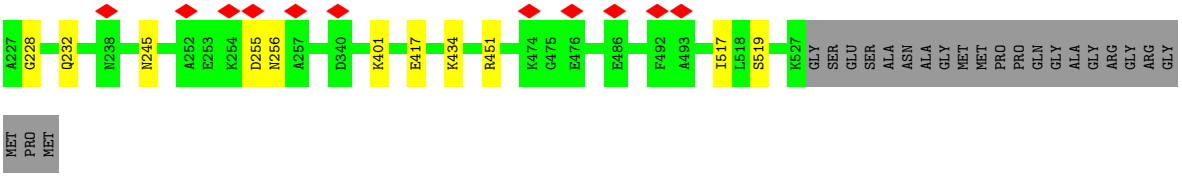


• Molecule 6: T-complex protein 1 subunit eta

Chain H:



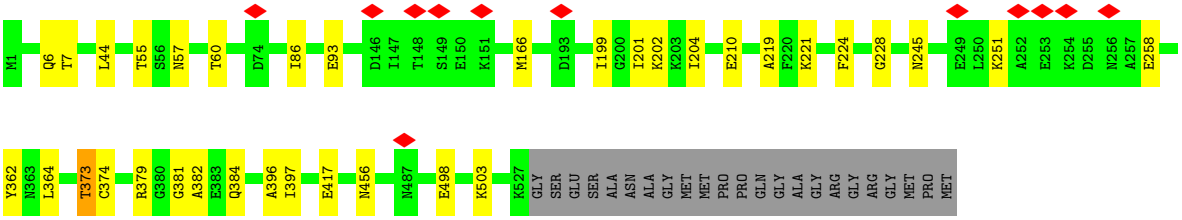




• Molecule 6: T-complex protein 1 subunit eta

Chain h:

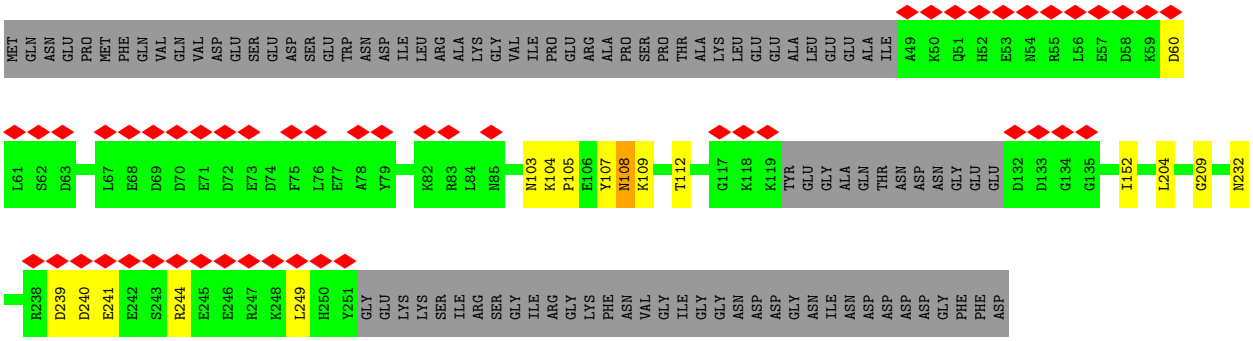




• Molecule 7: Phosducin-like protein 2

Chain P:

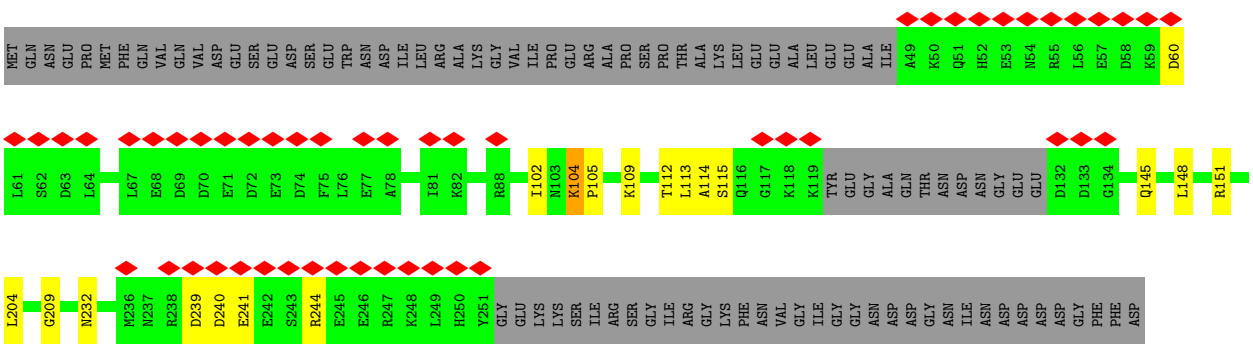




• Molecule 7: Phosducin-like protein 2

Chain p:

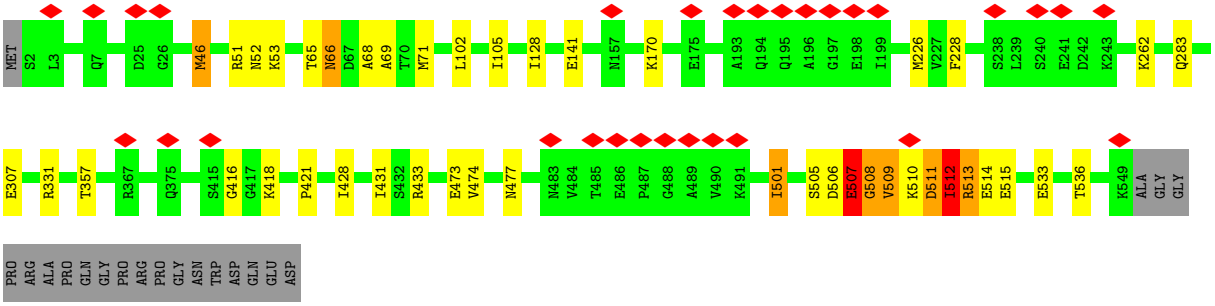




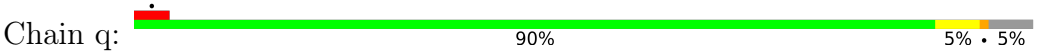
• Molecule 8: T-complex protein 1 subunit theta

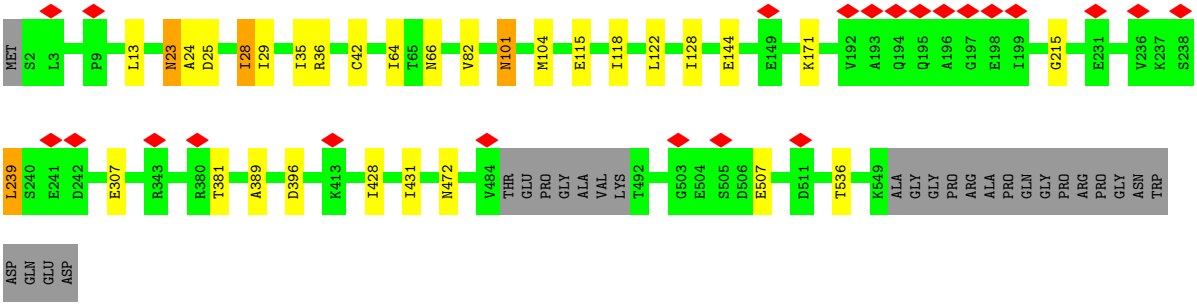
Chain Q:



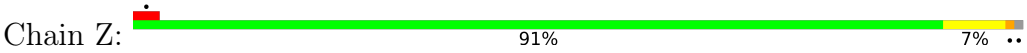


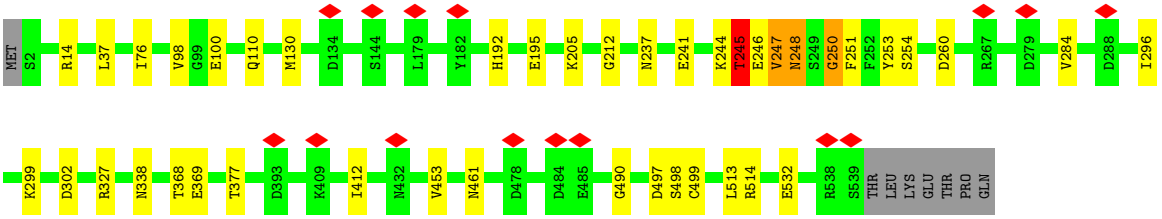
• Molecule 8: T-complex protein 1 subunit theta



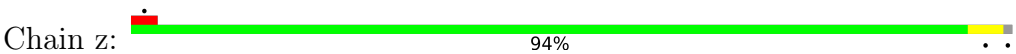


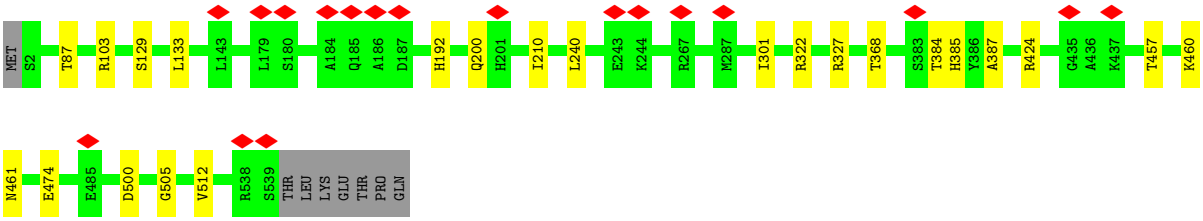
• Molecule 9: T-complex protein 1 subunit zeta





• Molecule 9: T-complex protein 1 subunit zeta





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	178976	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.922	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	337.408, 337.408, 337.408	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.318, 1.318, 1.318	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AF3, ADP

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	0.37	2/4196 (0.0%)	0.56	8/5661 (0.1%)
1	a	0.23	0/4166	0.44	0/5619
2	B	0.32	0/3976	0.45	3/5358 (0.1%)
2	b	0.38	2/3976 (0.1%)	0.54	9/5358 (0.2%)
3	D	0.35	1/4036 (0.0%)	0.49	4/5440 (0.1%)
3	d	0.25	0/4043	0.44	1/5451 (0.0%)
4	E	0.40	1/4184 (0.0%)	0.55	6/5629 (0.1%)
4	e	0.39	0/4175	0.53	3/5617 (0.1%)
5	G	0.38	0/4048	0.52	7/5459 (0.1%)
5	g	0.30	0/4047	0.47	0/5460
6	H	0.32	0/4030	0.49	2/5440 (0.0%)
6	h	0.38	1/4083 (0.0%)	0.49	2/5511 (0.0%)
7	P	0.44	3/1594 (0.2%)	0.52	3/2134 (0.1%)
7	p	0.45	0/1594	0.57	4/2134 (0.2%)
8	Q	0.48	5/4214 (0.1%)	0.60	5/5689 (0.1%)
8	q	0.41	1/4164 (0.0%)	0.53	5/5619 (0.1%)
9	Z	0.32	2/4191 (0.0%)	0.51	4/5663 (0.1%)
9	z	0.30	0/4191	0.46	4/5663 (0.1%)
All	All	0.36	18/68908 (0.0%)	0.51	70/92905 (0.1%)

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Q	46	MET	CA-C	-6.97	1.44	1.52
8	Q	511	ASP	CA-C	-6.93	1.43	1.52
8	Q	509	VAL	CA-C	-6.78	1.44	1.52
1	A	498	ARG	CA-C	-6.70	1.43	1.52
3	D	462	SER	CA-C	-6.66	1.44	1.52

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	Q	512	ILE	N-CA-C	-14.47	98.68	112.29
2	b	235	ASN	N-CA-C	-11.12	101.18	112.97
2	b	238	LEU	N-CA-C	-9.18	101.63	112.92
8	Q	65	THR	N-CA-C	9.09	122.88	109.07
9	Z	250	GLY	N-CA-C	8.75	123.44	111.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4158	0	4322	24	0
1	a	4129	0	4291	19	0
2	B	3937	0	4043	17	0
2	b	3937	0	4043	29	0
3	D	3998	0	4170	28	0
3	d	4005	0	4178	15	0
4	E	4133	0	4237	27	0
4	e	4124	0	4231	27	0
5	G	4004	0	4152	38	0
5	g	4003	0	4154	13	0
6	H	3980	0	4060	20	0
6	h	4032	0	4116	21	0
7	P	1571	0	1537	10	0
7	p	1571	0	1537	9	0
8	Q	4163	0	4300	36	0
8	q	4115	0	4249	18	0
9	Z	4139	0	4233	25	0
9	z	4139	0	4233	13	0
10	A	27	0	12	1	0
10	B	27	0	12	1	0
10	D	27	0	12	3	0
10	E	27	0	12	0	0
10	G	27	0	12	1	0
10	H	27	0	12	0	0
10	Q	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	Z	27	0	12	1	0
10	a	27	0	12	1	0
10	b	27	0	12	0	0
10	d	27	0	12	1	0
10	e	27	0	12	1	0
10	g	27	0	12	0	0
10	h	27	0	12	1	0
10	q	27	0	12	0	0
10	z	27	0	12	1	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	D	1	0	0	0	0
11	E	1	0	0	0	0
11	G	1	0	0	0	0
11	H	1	0	0	0	0
11	Q	1	0	0	0	0
11	Z	1	0	0	0	0
11	a	1	0	0	0	0
11	b	1	0	0	0	0
11	d	1	0	0	0	0
11	e	1	0	0	0	0
11	g	1	0	0	0	0
11	h	1	0	0	0	0
11	q	1	0	0	0	0
11	z	1	0	0	0	0
12	A	4	0	0	1	0
12	B	4	0	0	3	0
12	D	4	0	0	3	0
12	E	4	0	0	4	0
12	G	4	0	0	2	0
12	H	4	0	0	1	0
12	Z	4	0	0	1	0
12	a	4	0	0	1	0
12	b	4	0	0	1	0
12	d	4	0	0	2	0
12	e	4	0	0	2	0
12	g	4	0	0	0	0
12	h	4	0	0	1	0
12	z	4	0	0	1	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
13	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	E	1	0	0	0	0
13	G	1	0	0	0	0
13	H	1	0	0	0	0
13	Z	1	0	0	0	0
13	a	1	0	0	0	0
13	b	1	0	0	0	0
13	d	1	0	0	0	0
13	e	1	0	0	0	0
13	g	1	0	0	0	0
13	h	1	0	0	0	0
13	z	1	0	0	0	0
All	All	68656	0	70278	347	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 2.

The worst 5 of 347 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)
4:E:191:LYS:CE	12:E:603:AF3:F1	1.83	1.17
4:E:191:LYS:HE2	12:E:603:AF3:F1	0.97	1.03
8:Q:477:ASN:HD21	8:Q:506:ASP:HB3	1.36	0.88
2:b:240:THR:H	2:b:291:TYR:HE2	1.18	0.86
9:Z:241:GLU:HA	9:Z:302:ASP:HB2	1.56	0.86

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	548/559 (98%)	523 (95%)	25 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	542/559 (97%)	516 (95%)	26 (5%)	0	100	100
2	B	516/527 (98%)	499 (97%)	17 (3%)	0	100	100
2	b	516/527 (98%)	501 (97%)	15 (3%)	0	100	100
3	D	521/528 (99%)	506 (97%)	14 (3%)	1 (0%)	43	70
3	d	522/528 (99%)	508 (97%)	14 (3%)	0	100	100
4	E	534/562 (95%)	508 (95%)	23 (4%)	3 (1%)	21	48
4	e	533/562 (95%)	515 (97%)	18 (3%)	0	100	100
5	G	514/594 (86%)	489 (95%)	25 (5%)	0	100	100
5	g	514/594 (86%)	494 (96%)	20 (4%)	0	100	100
6	H	516/550 (94%)	496 (96%)	20 (4%)	0	100	100
6	h	525/550 (96%)	510 (97%)	14 (3%)	1 (0%)	43	70
7	P	187/286 (65%)	176 (94%)	11 (6%)	0	100	100
7	p	187/286 (65%)	177 (95%)	10 (5%)	0	100	100
8	Q	546/568 (96%)	518 (95%)	25 (5%)	3 (0%)	24	52
8	q	537/568 (94%)	501 (93%)	36 (7%)	0	100	100
9	Z	536/546 (98%)	518 (97%)	17 (3%)	1 (0%)	43	70
9	z	536/546 (98%)	522 (97%)	14 (3%)	0	100	100
All	All	8830/9440 (94%)	8477 (96%)	344 (4%)	9 (0%)	49	75

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	196	ASP
8	Q	513	ARG
8	Q	514	GLU
9	Z	247	VAL
3	D	468	GLU

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	462/471 (98%)	455 (98%)	7 (2%)	57 73
1	a	458/471 (97%)	457 (100%)	1 (0%)	87 87
2	B	433/441 (98%)	431 (100%)	2 (0%)	81 82
2	b	433/441 (98%)	427 (99%)	6 (1%)	59 73
3	D	449/453 (99%)	446 (99%)	3 (1%)	76 80
3	d	450/453 (99%)	446 (99%)	4 (1%)	70 78
4	E	461/483 (95%)	459 (100%)	2 (0%)	84 84
4	e	460/483 (95%)	458 (100%)	2 (0%)	84 84
5	G	443/501 (88%)	440 (99%)	3 (1%)	76 80
5	g	443/501 (88%)	441 (100%)	2 (0%)	81 82
6	H	434/454 (96%)	433 (100%)	1 (0%)	87 87
6	h	440/454 (97%)	437 (99%)	3 (1%)	76 80
7	P	173/251 (69%)	172 (99%)	1 (1%)	78 81
7	p	173/251 (69%)	173 (100%)	0	100 100
8	Q	458/473 (97%)	452 (99%)	6 (1%)	61 74
8	q	453/473 (96%)	447 (99%)	6 (1%)	61 74
9	Z	455/463 (98%)	450 (99%)	5 (1%)	65 76
9	z	455/463 (98%)	455 (100%)	0	100 100
All	All	7533/7980 (94%)	7479 (99%)	54 (1%)	73 80

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	Z	284	VAL
2	b	245	ILE
8	q	29	ILE
9	Z	296	ILE
2	b	221	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
8	q	8	ASN
8	q	52	ASN
8	q	472	ASN
6	H	245	ASN

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Mol	Chain	Res	Type
6	H	231	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 46 ligands modelled in this entry, 16 are monoatomic - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	ADP	d	601	11,12	27,29,29	1.35	4 (14%)	42,45,45	2.00	11 (26%)
10	ADP	E	601	11,12	27,29,29	1.34	4 (14%)	42,45,45	1.98	11 (26%)
10	ADP	a	601	11	27,29,29	1.35	4 (14%)	42,45,45	2.03	11 (26%)
12	AF3	d	603	10,3	0,3,3	-	-	-		
12	AF3	a	603	-	0,3,3	-	-	-		
12	AF3	E	603	10,4	0,3,3	-	-	-		
10	ADP	g	601	11	27,29,29	1.34	4 (14%)	42,45,45	2.03	11 (26%)
10	ADP	b	601	11,12	27,29,29	1.34	4 (14%)	42,45,45	2.04	11 (26%)
10	ADP	A	601	11,12	27,29,29	1.35	4 (14%)	42,45,45	1.98	11 (26%)
10	ADP	D	601	11,12	27,29,29	1.35	4 (14%)	42,45,45	2.03	11 (26%)
12	AF3	b	603	10	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	ADP	q	601	11	27,29,29	1.35	4 (14%)	42,45,45	2.02	11 (26%)
10	ADP	e	601	11,12	27,29,29	1.35	4 (14%)	42,45,45	2.06	11 (26%)
12	AF3	G	603	10	0,3,3	-	-	-		
10	ADP	Z	601	11,12	27,29,29	1.35	4 (14%)	42,45,45	2.00	11 (26%)
10	ADP	G	601	11,12	27,29,29	1.35	4 (14%)	42,45,45	1.96	11 (26%)
10	ADP	B	601	11	27,29,29	1.35	4 (14%)	42,45,45	2.05	11 (26%)
12	AF3	H	603	10,6	0,3,3	-	-	-		
12	AF3	Z	603	10	0,3,3	-	-	-		
12	AF3	B	603	2	0,3,3	-	-	-		
12	AF3	g	603	5	0,3,3	-	-	-		
10	ADP	H	601	11,12	27,29,29	1.35	4 (14%)	42,45,45	1.95	10 (23%)
12	AF3	A	603	10	0,3,3	-	-	-		
12	AF3	e	603	10	0,3,3	-	-	-		
10	ADP	z	601	11	27,29,29	1.35	4 (14%)	42,45,45	2.02	12 (28%)
10	ADP	h	601	11,12	27,29,29	1.35	4 (14%)	42,45,45	1.98	11 (26%)
12	AF3	D	603	10	0,3,3	-	-	-		
10	ADP	Q	602	11	27,29,29	1.35	4 (14%)	42,45,45	2.00	11 (26%)
12	AF3	z	603	-	0,3,3	-	-	-		
12	AF3	h	603	10	0,3,3	-	-	-		

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
10	ADP	q	601	11	-	3/16/32/32	0/3/3/3
10	ADP	Z	601	11,12	-	5/16/32/32	0/3/3/3
10	ADP	A	601	11,12	-	2/16/32/32	0/3/3/3
10	ADP	G	601	11,12	-	2/16/32/32	0/3/3/3
10	ADP	B	601	11	-	3/16/32/32	0/3/3/3
10	ADP	D	601	11,12	-	1/16/32/32	0/3/3/3
10	ADP	d	601	11,12	-	0/16/32/32	0/3/3/3
10	ADP	z	601	11	-	2/16/32/32	0/3/3/3
10	ADP	E	601	11,12	-	3/16/32/32	0/3/3/3
10	ADP	a	601	11	-	5/16/32/32	0/3/3/3
10	ADP	H	601	11,12	-	0/16/32/32	0/3/3/3
10	ADP	h	601	11,12	-	4/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ADP	e	601	11,12	-	4/16/32/32	0/3/3/3
10	ADP	Q	602	11	-	4/16/32/32	0/3/3/3
10	ADP	g	601	11	-	5/16/32/32	0/3/3/3
10	ADP	b	601	11,12	-	0/16/32/32	0/3/3/3

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	601	ADP	C5-C4	4.49	1.47	1.39
10	e	601	ADP	C5-C4	4.49	1.47	1.39
10	D	601	ADP	C5-C4	4.48	1.47	1.39
10	A	601	ADP	C5-C4	4.46	1.47	1.39
10	Q	602	ADP	C5-C4	4.46	1.47	1.39

The worst 5 of 176 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	e	601	ADP	C5-C4-N3	-6.31	118.52	126.75
10	D	601	ADP	C5-C4-N3	-6.30	118.53	126.75
10	b	601	ADP	C5-C4-N3	-6.27	118.57	126.75
10	q	601	ADP	C5-C4-N3	-6.25	118.59	126.75
10	a	601	ADP	C5-C4-N3	-6.24	118.60	126.75

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	E	601	ADP	C5'-O5'-PA-O1A
10	E	601	ADP	C5'-O5'-PA-O2A
10	Q	602	ADP	C5'-O5'-PA-O1A
10	Q	602	ADP	C5'-O5'-PA-O2A
10	Z	601	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

24 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	d	601	ADP	1	0
10	a	601	ADP	1	0
12	d	603	AF3	2	0

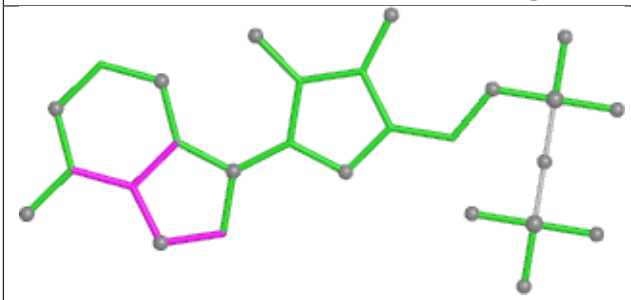
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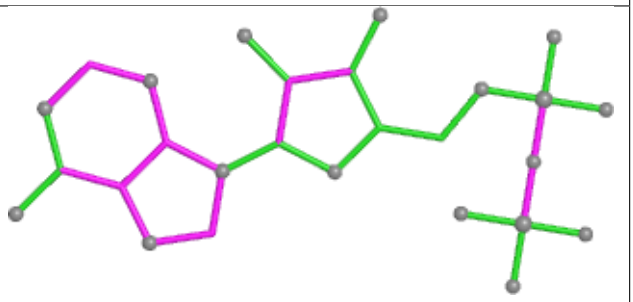
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	a	603	AF3	1	0
12	E	603	AF3	4	0
10	A	601	ADP	1	0
10	D	601	ADP	3	0
12	b	603	AF3	1	0
10	e	601	ADP	1	0
12	G	603	AF3	2	0
10	Z	601	ADP	1	0
10	G	601	ADP	1	0
10	B	601	ADP	1	0
12	H	603	AF3	1	0
12	Z	603	AF3	1	0
12	B	603	AF3	3	0
12	A	603	AF3	1	0
12	e	603	AF3	2	0
10	z	601	ADP	1	0
10	h	601	ADP	1	0
12	D	603	AF3	3	0
10	Q	602	ADP	1	0
12	z	603	AF3	1	0
12	h	603	AF3	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.

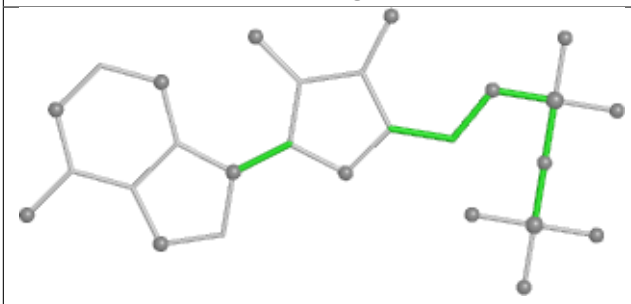
Ligand ADP d 601



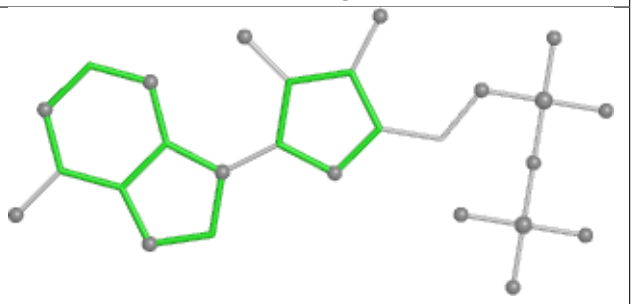
Bond lengths



Bond angles

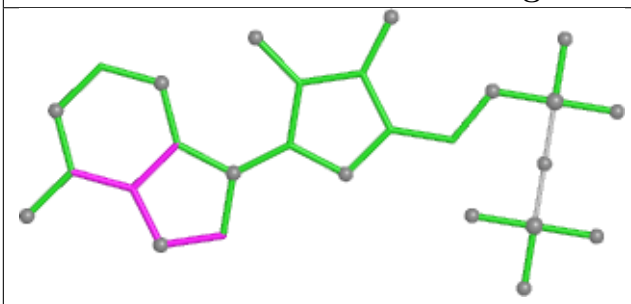


Torsions

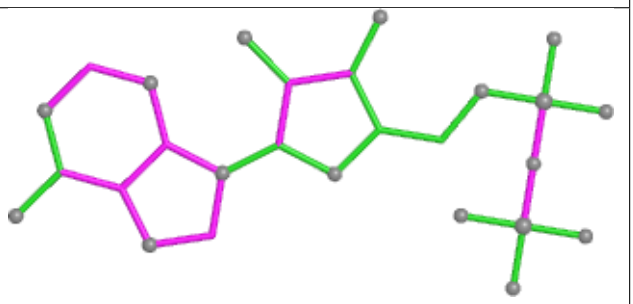


Rings

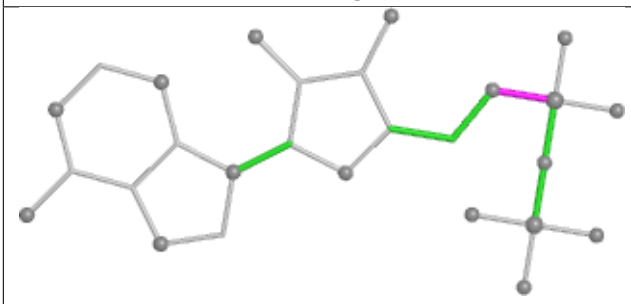
Ligand ADP E 601



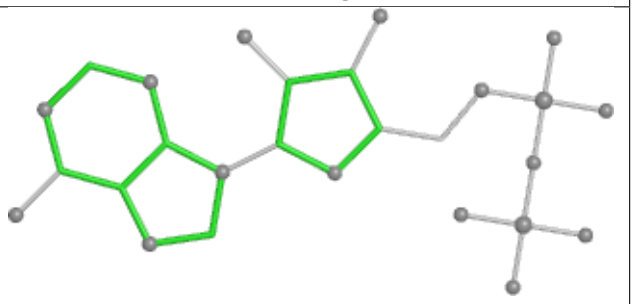
Bond lengths



Bond angles

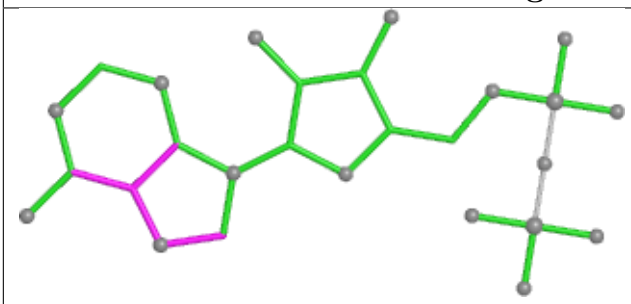


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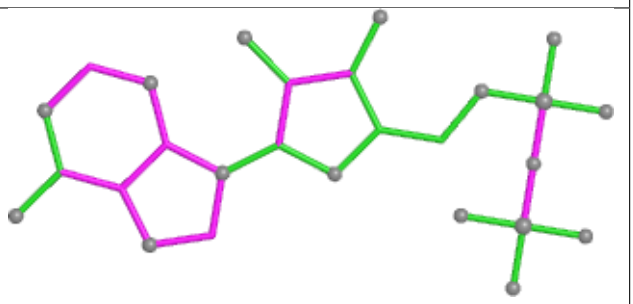


Rings

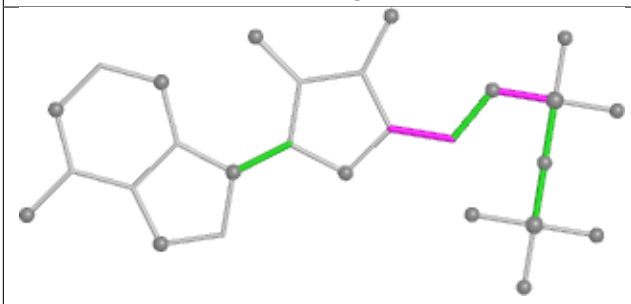
Ligand ADP a 601



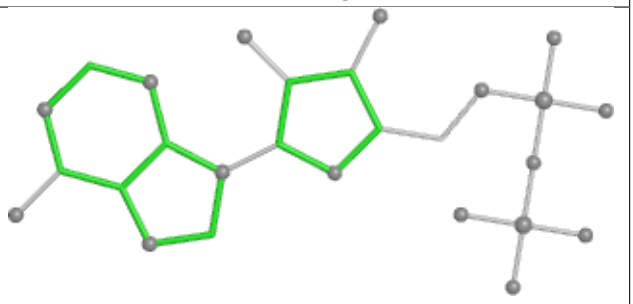
Bond lengths



Bond angles

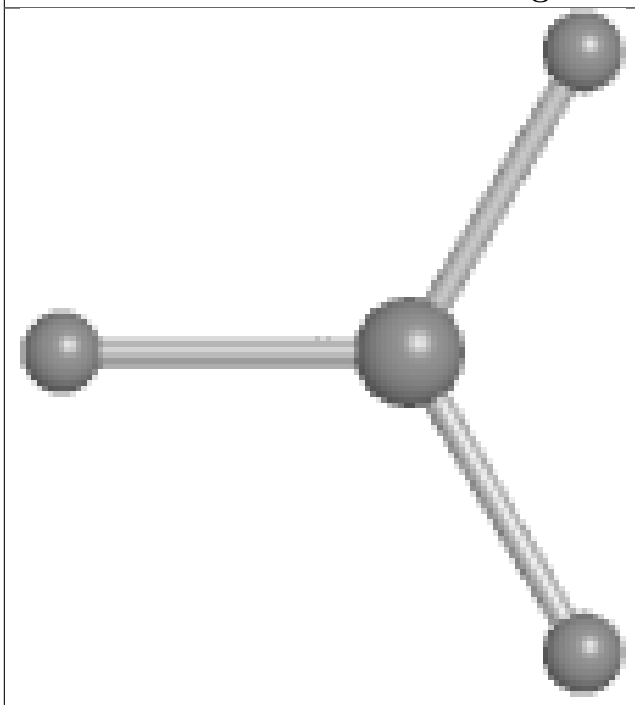


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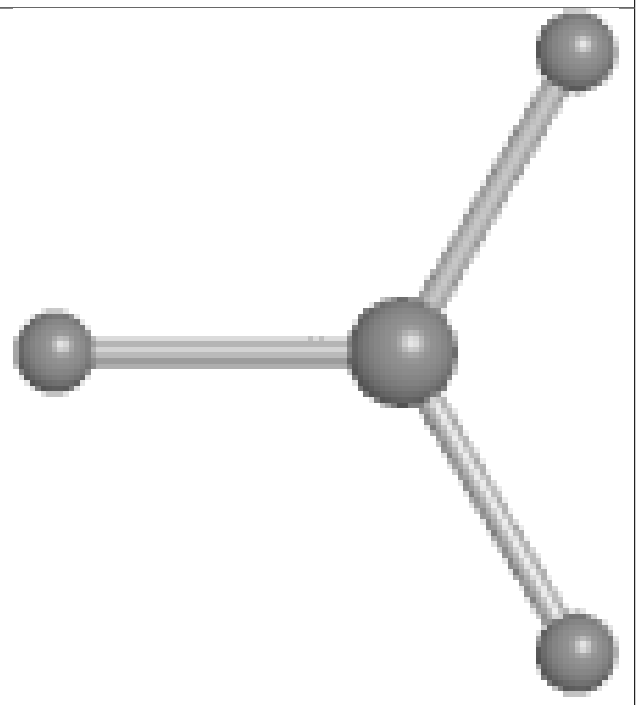


Rings

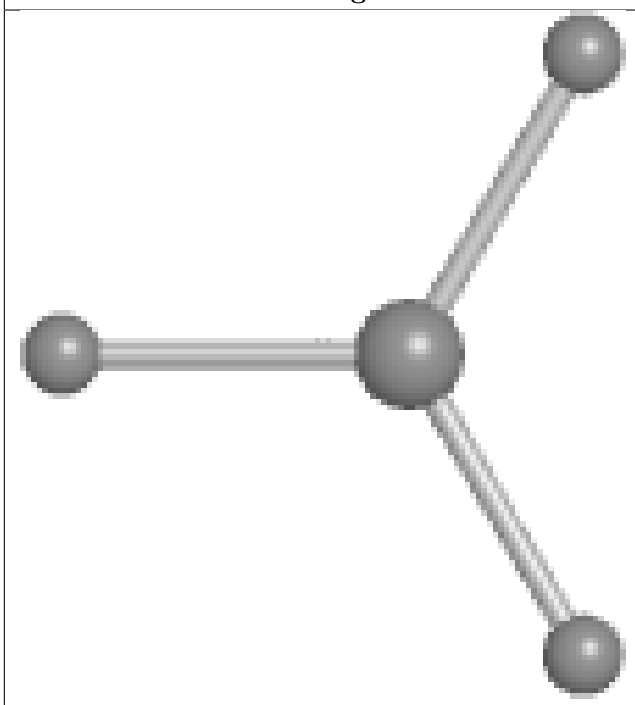
Ligand AF3 d 603



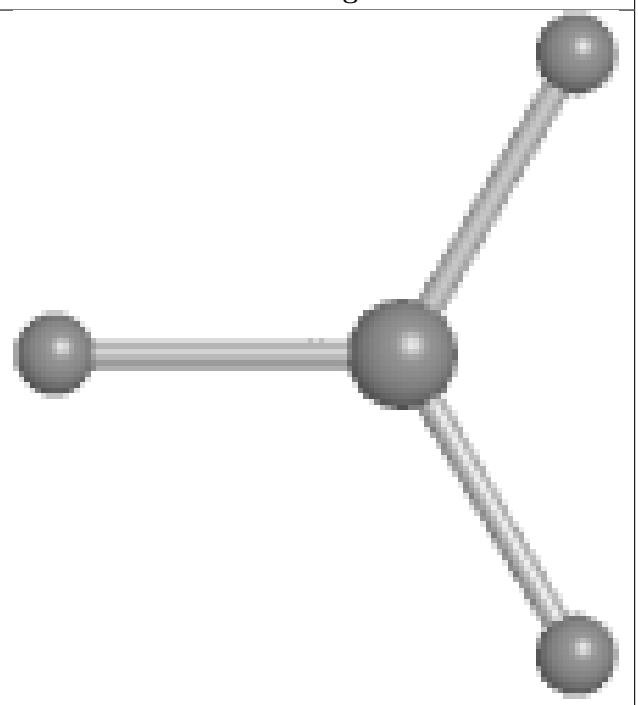
Bond lengths



Bond angles

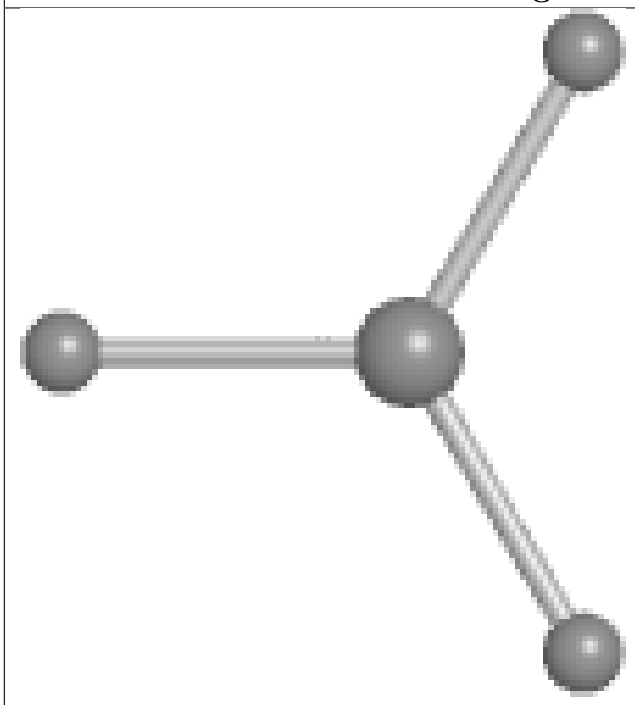


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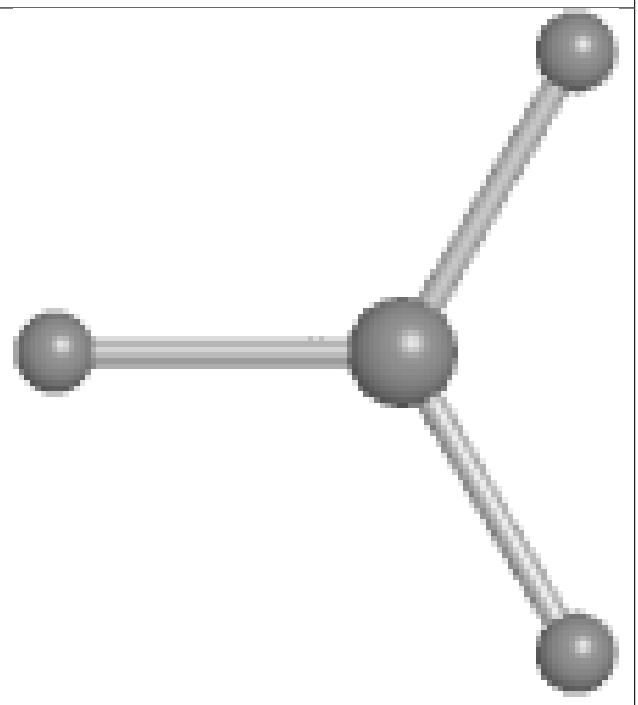


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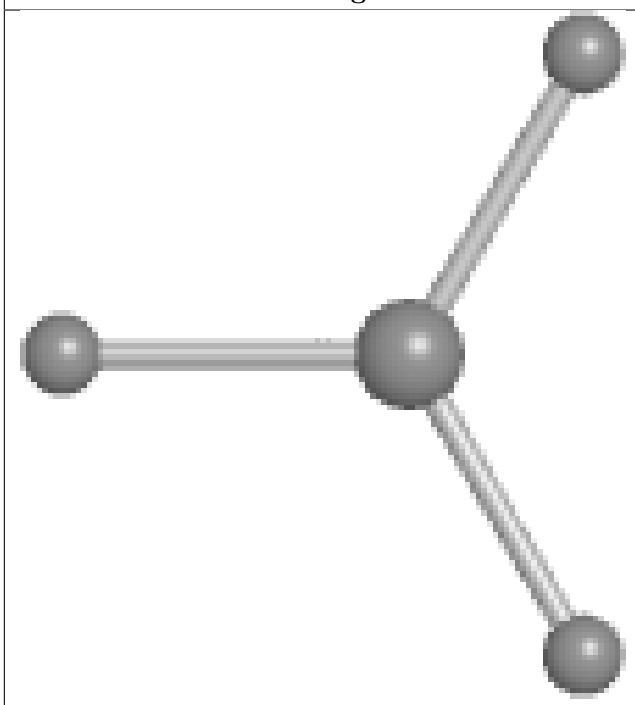
Ligand AF3 a 603



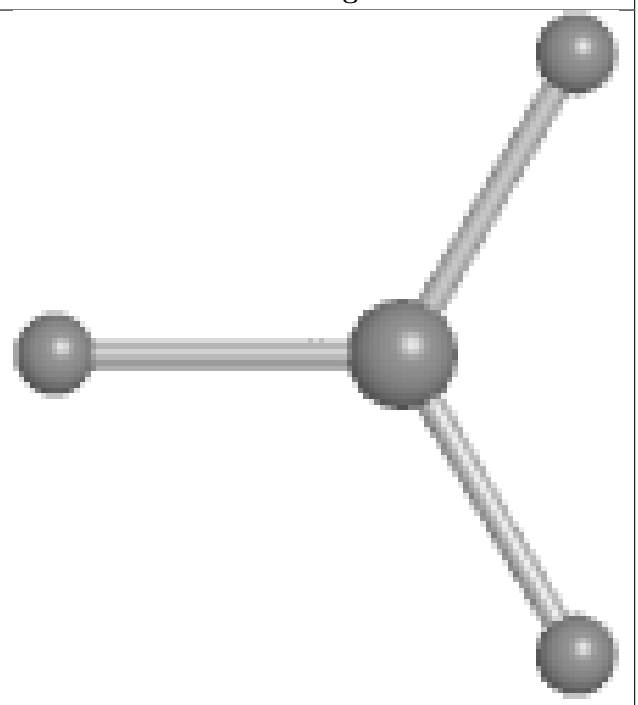
Bond lengths



Bond angles

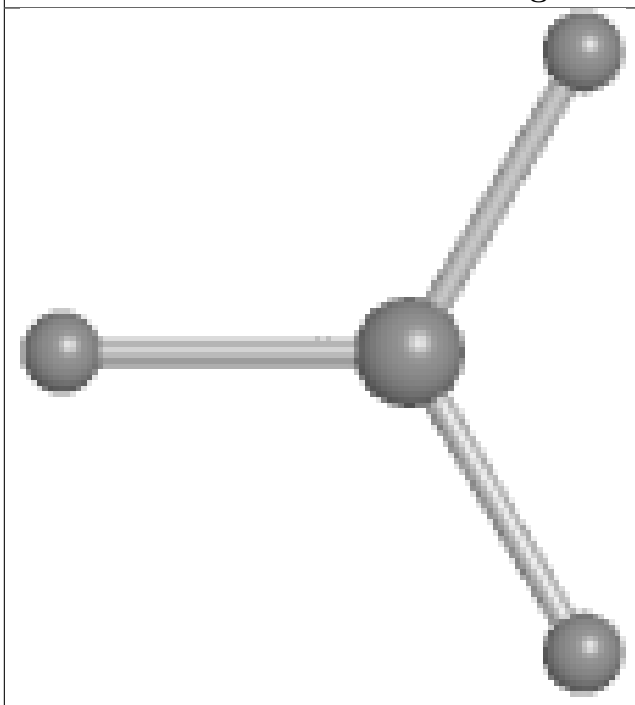


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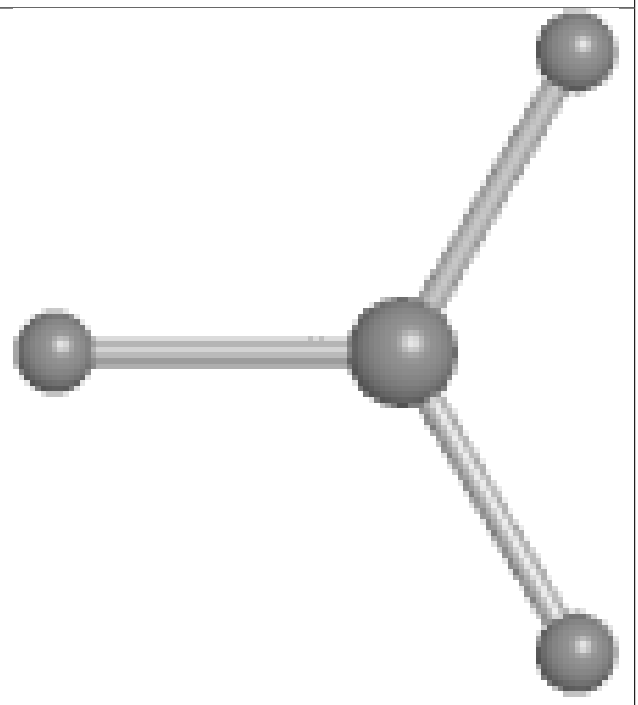


Rings

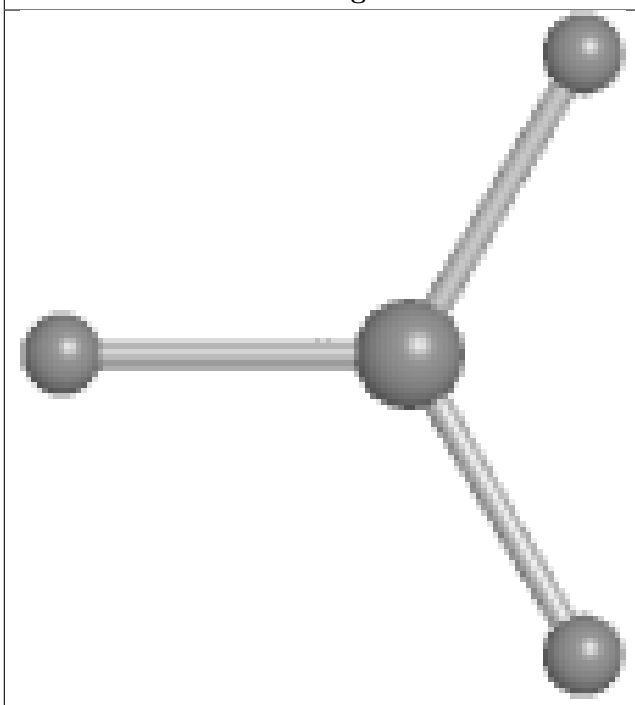
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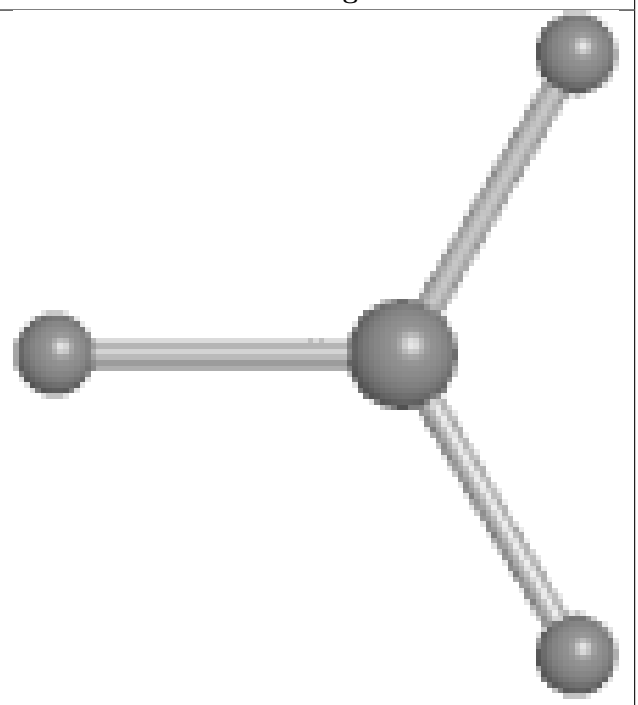
Bond lengths



Bond angles

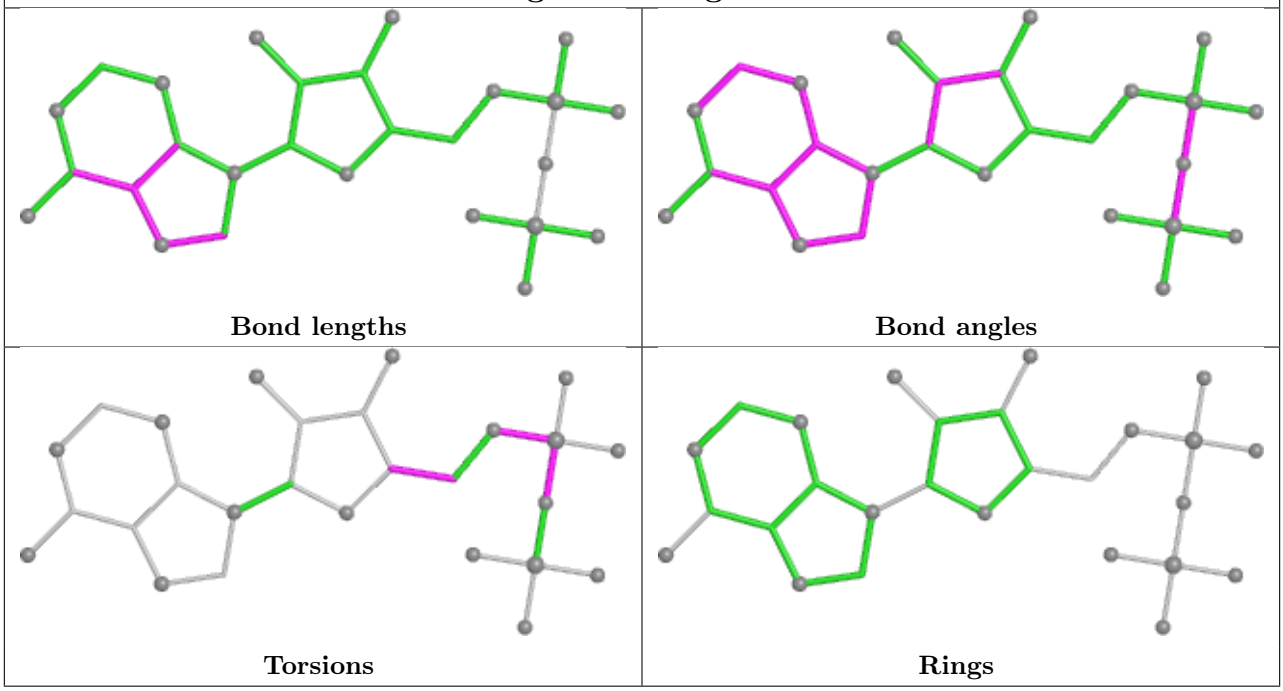


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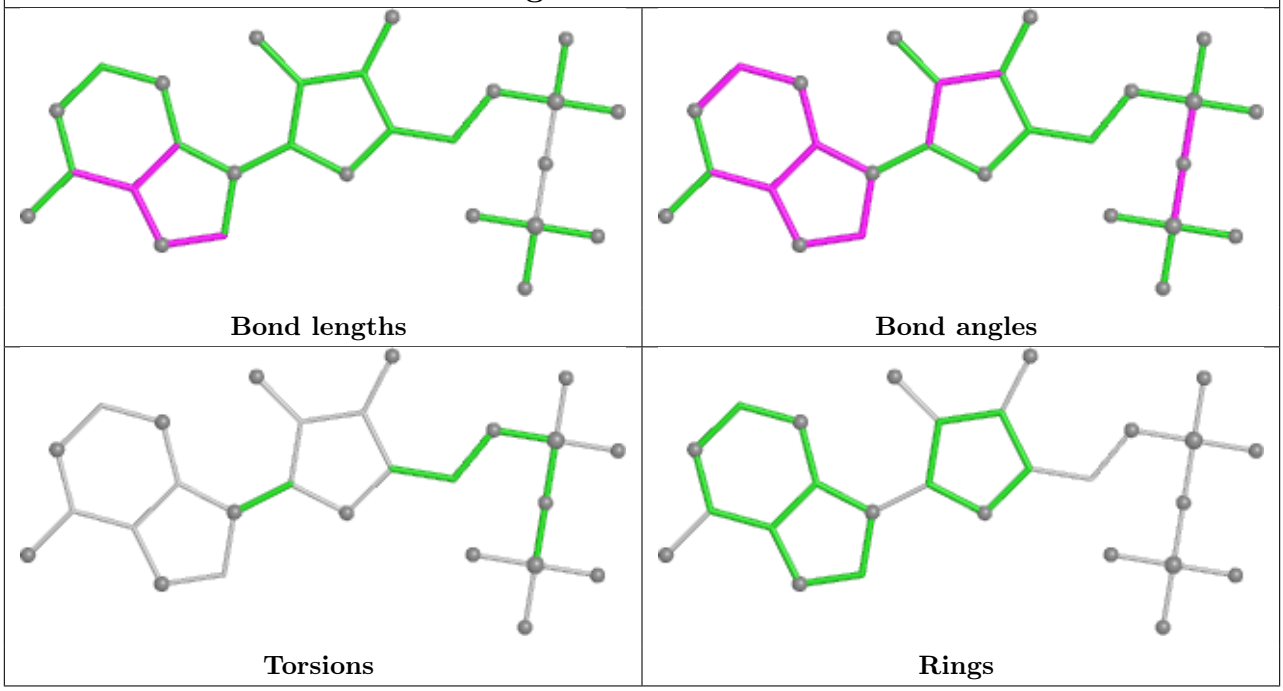


Rings

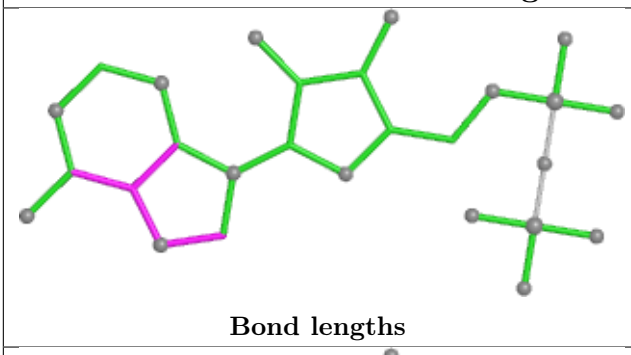
Ligand ADP g 601



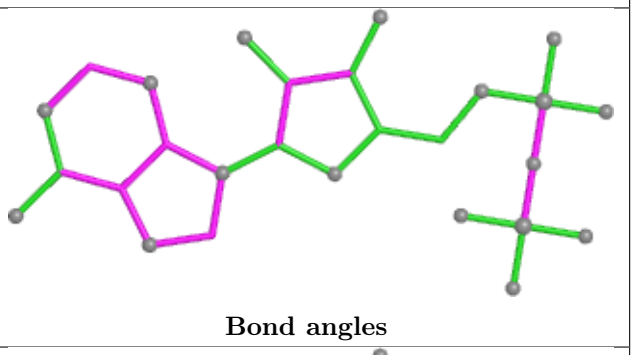
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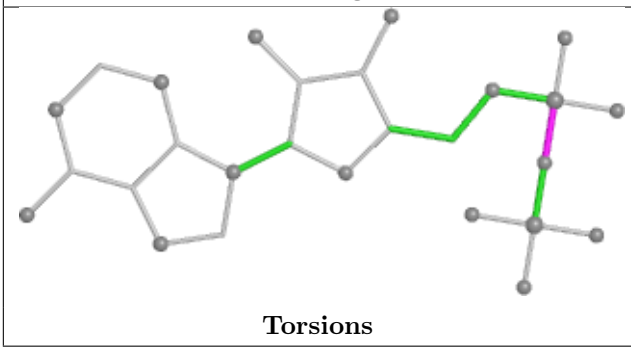
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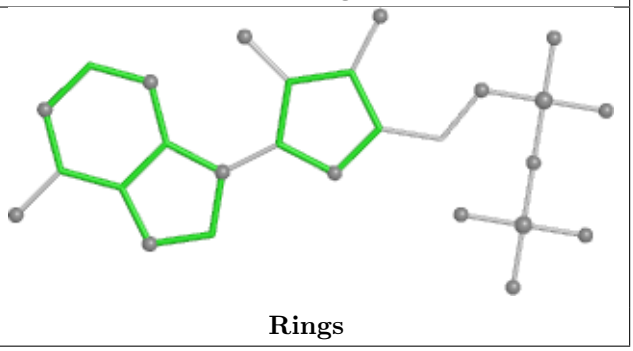
Bond lengths



Bond angles

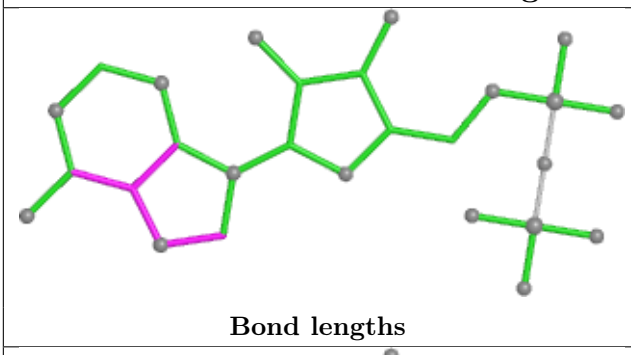


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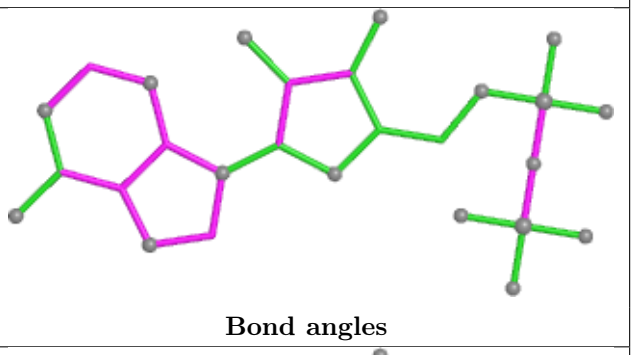


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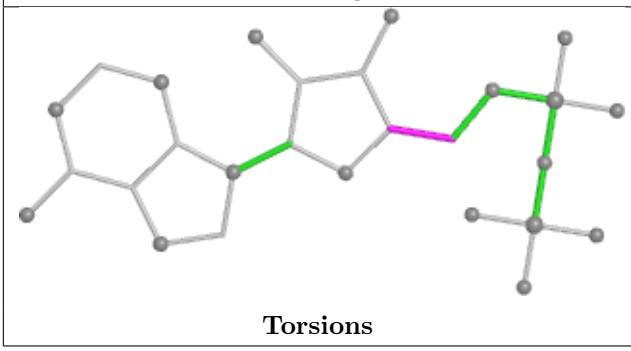
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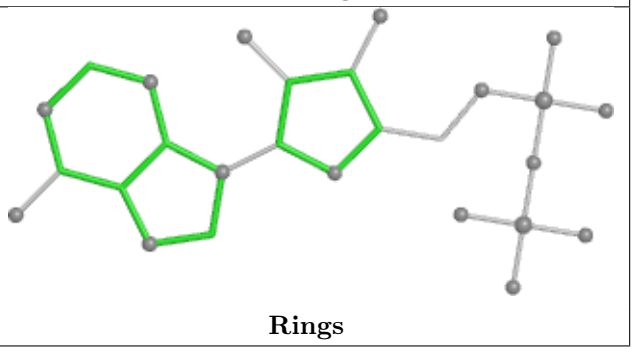
Bond lengths



Bond angles

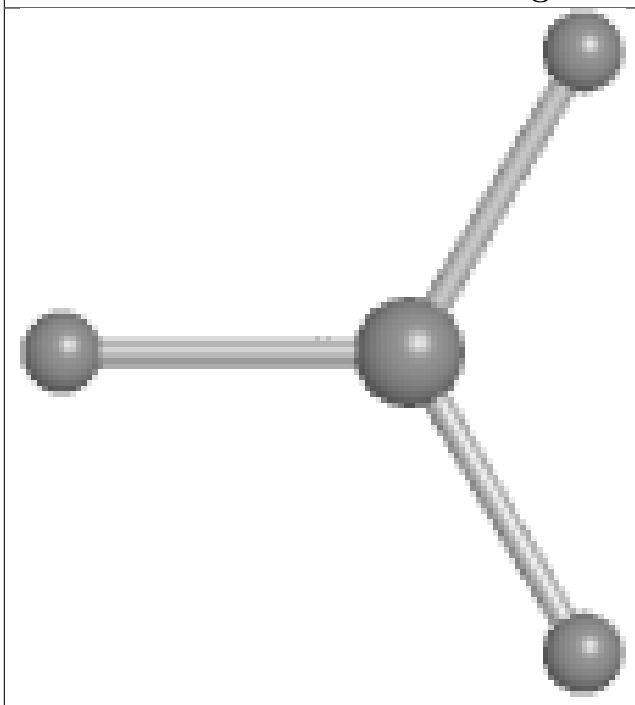


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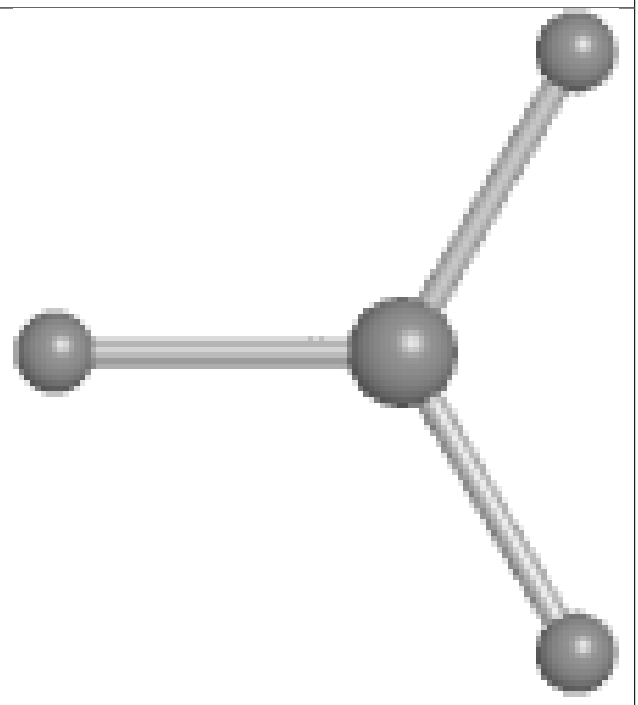


Rings

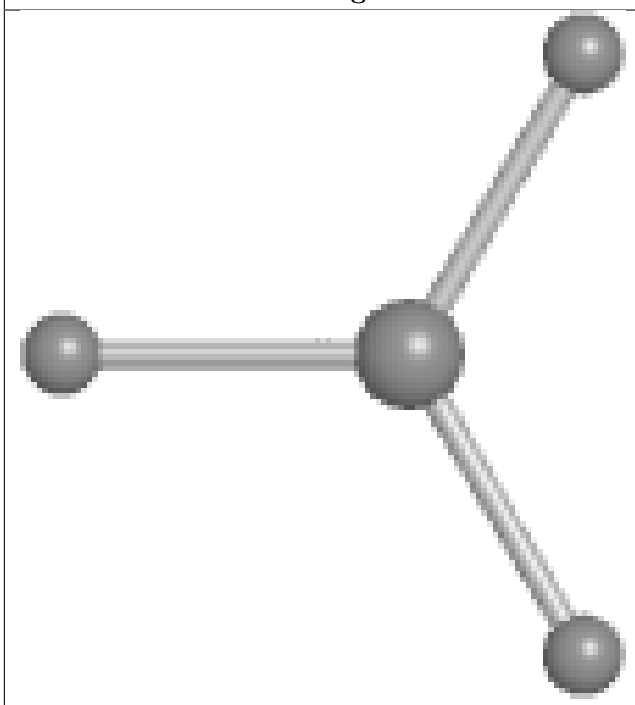
Ligand AF3 b 603



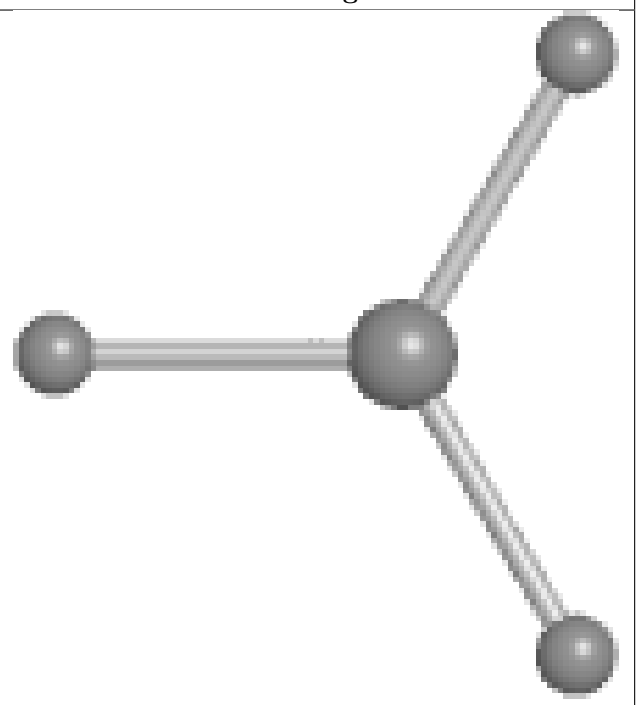
Bond lengths



Bond angles

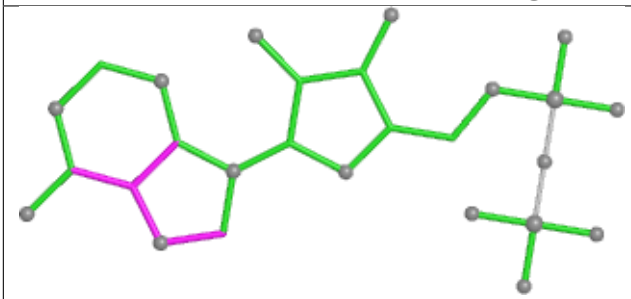


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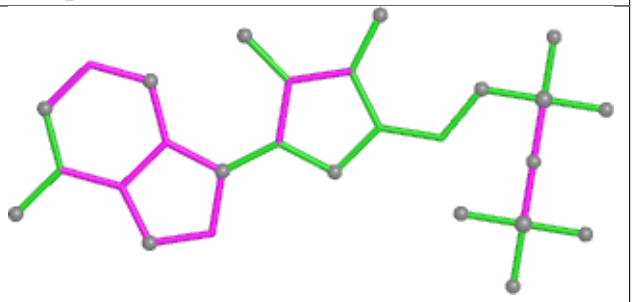


Rings

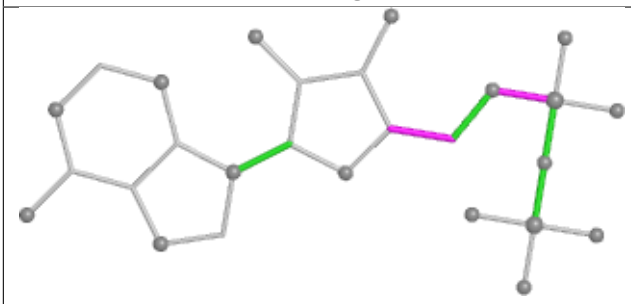
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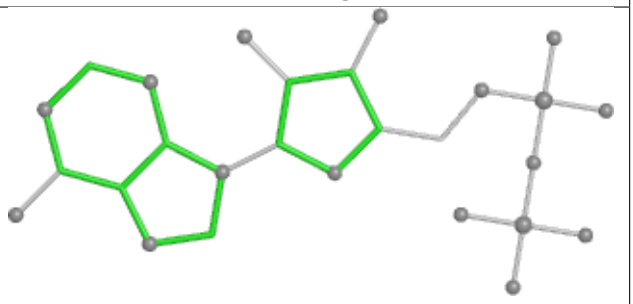
Bond lengths



Bond angles

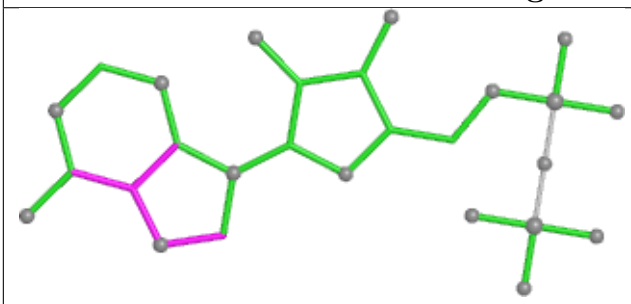


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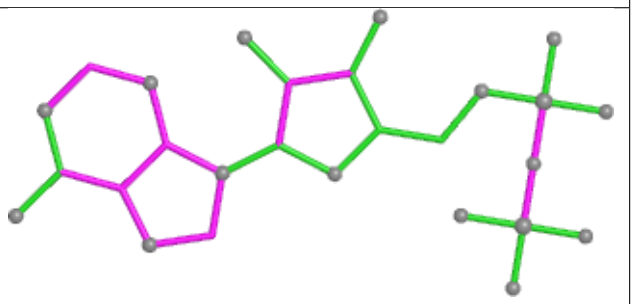


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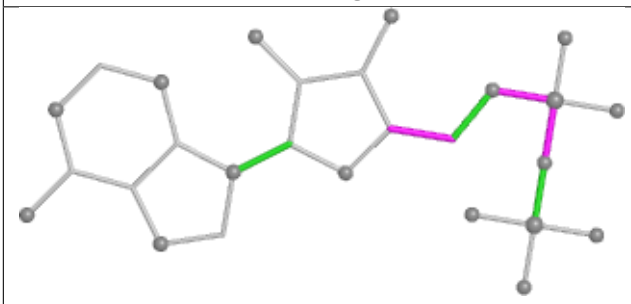
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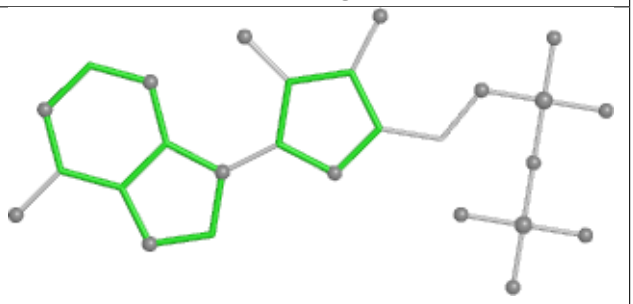
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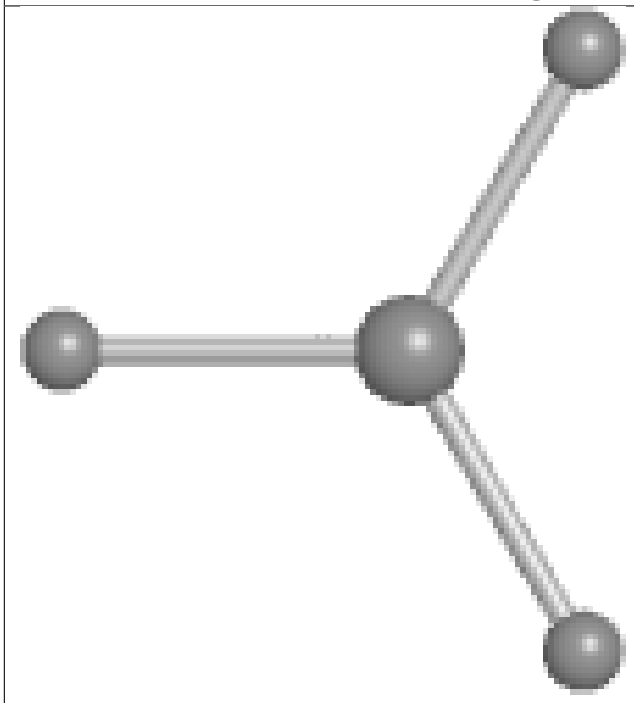


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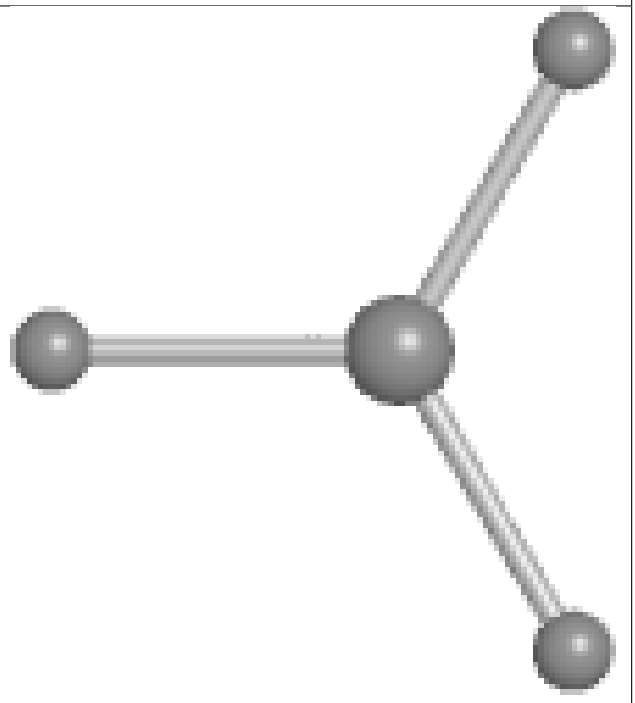


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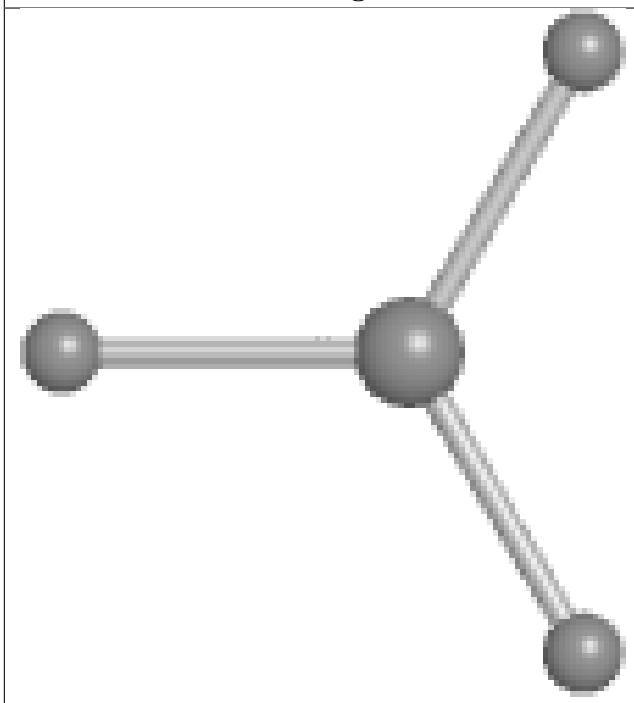
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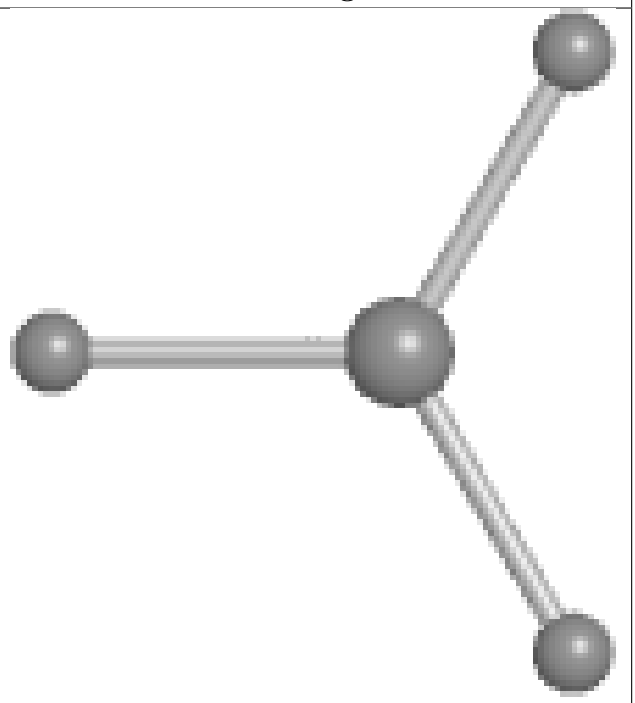
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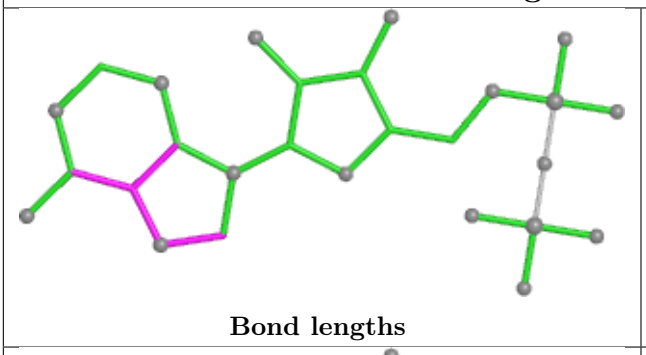


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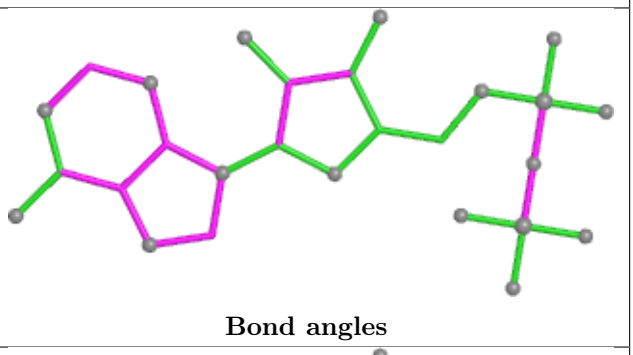


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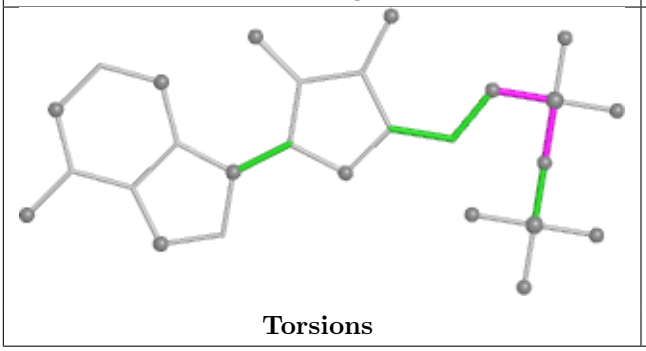
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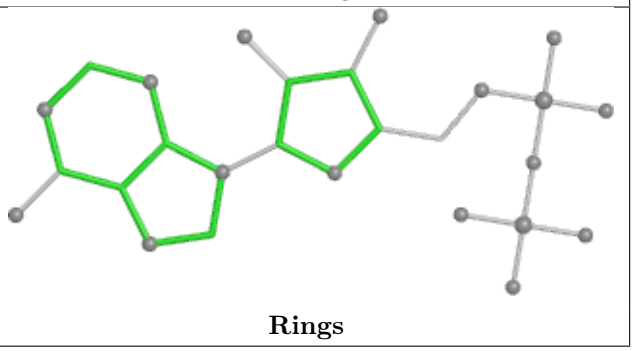
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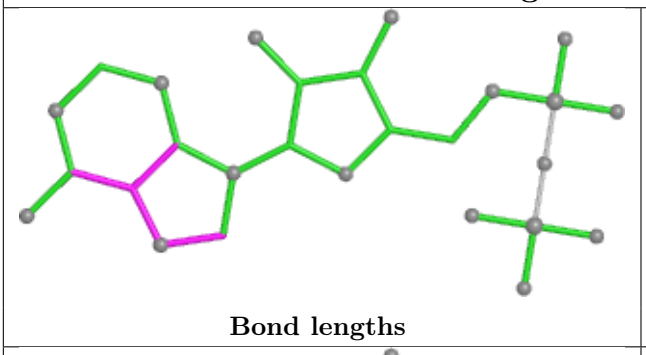


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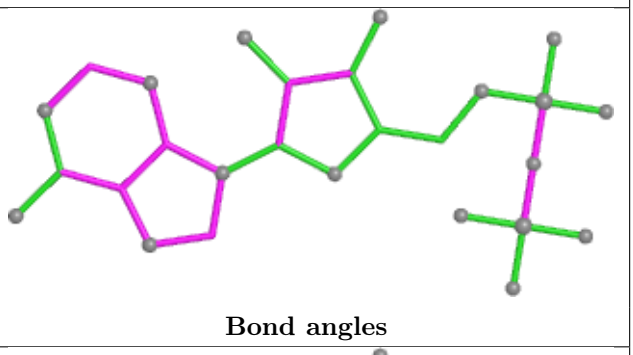


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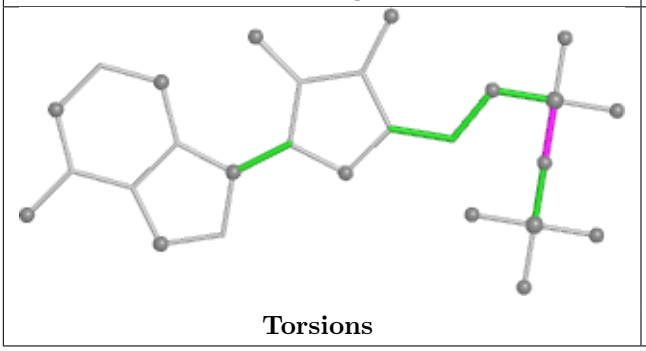
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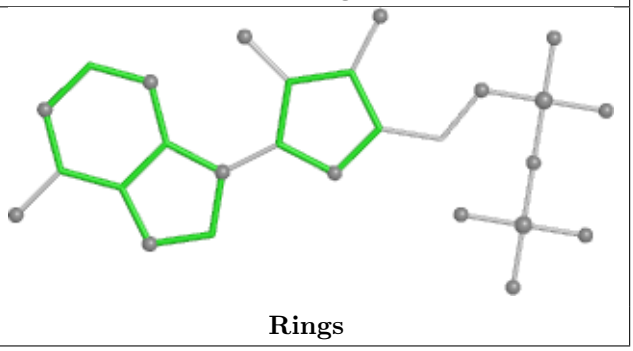
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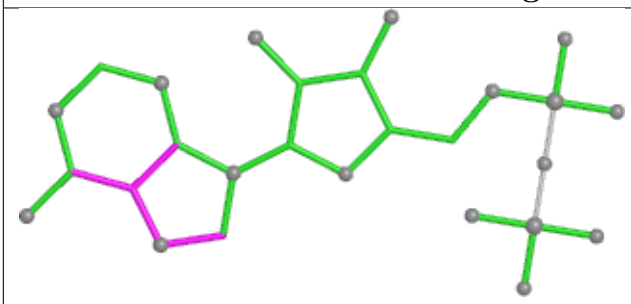


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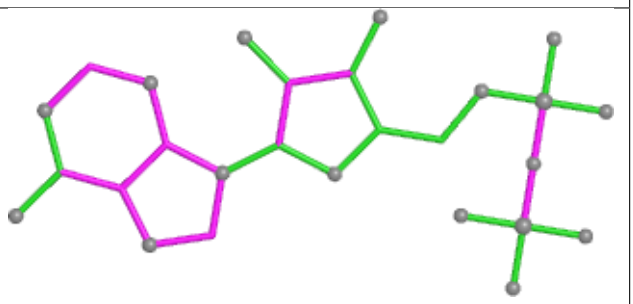


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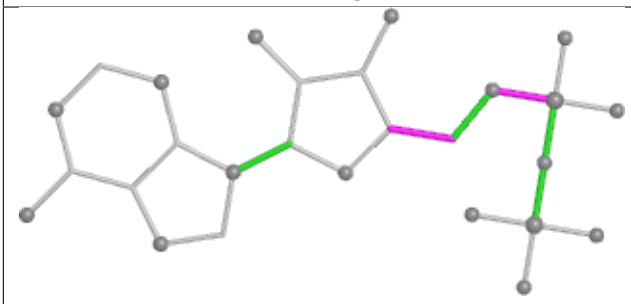
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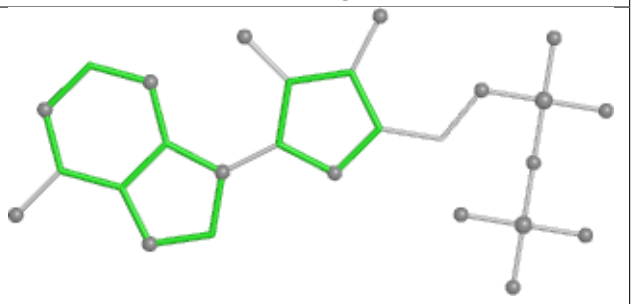
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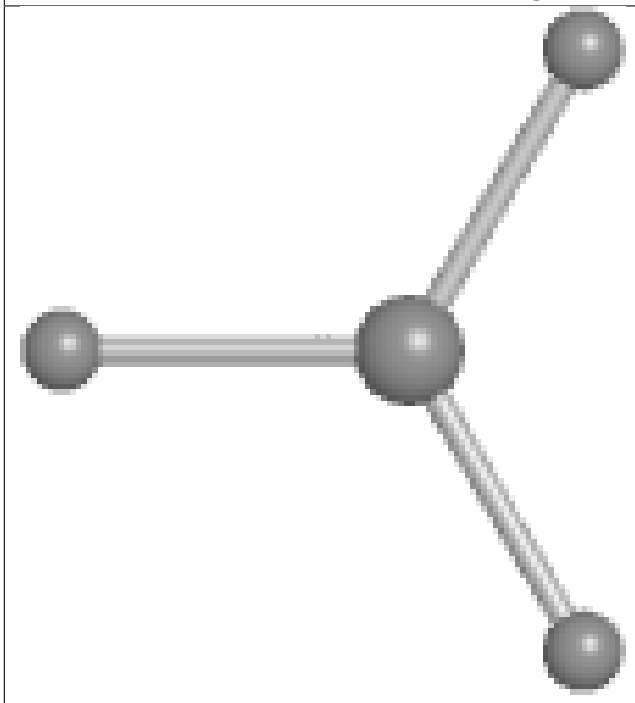


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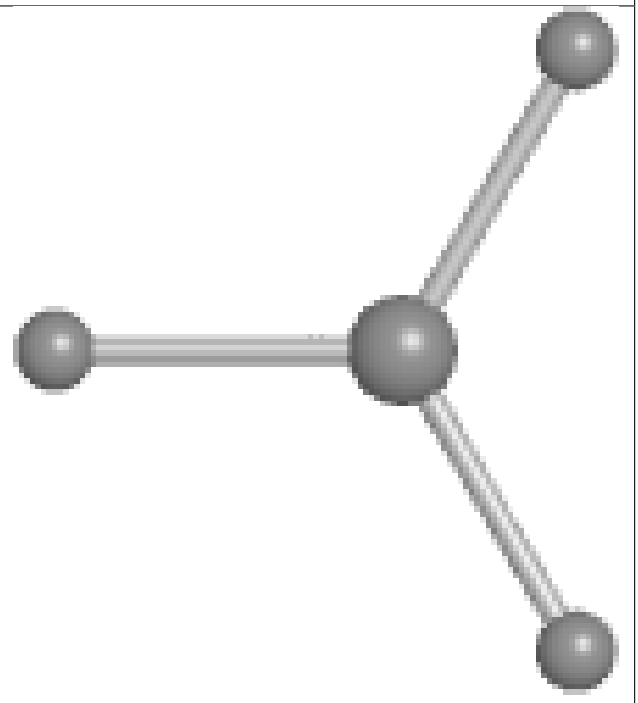


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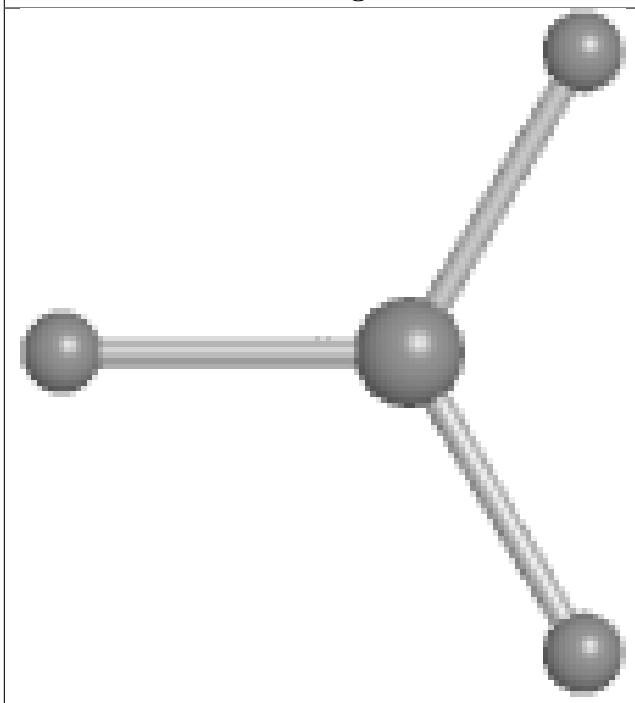
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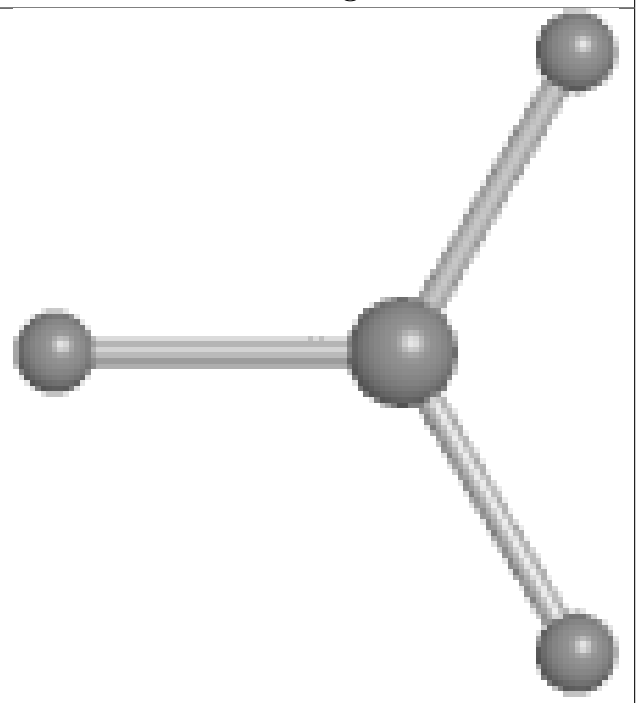
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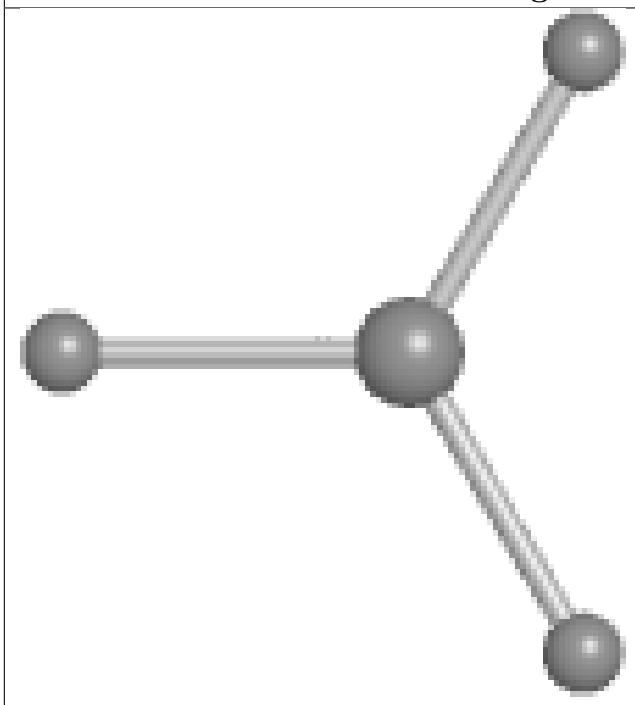


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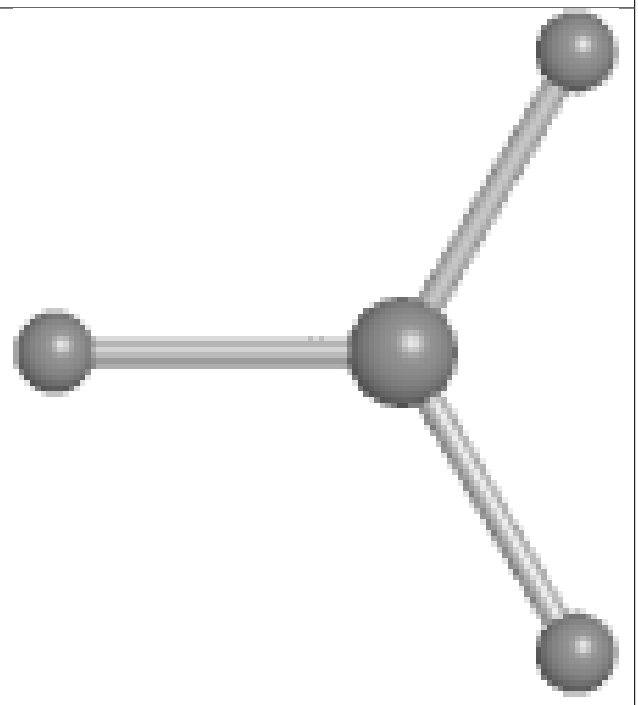


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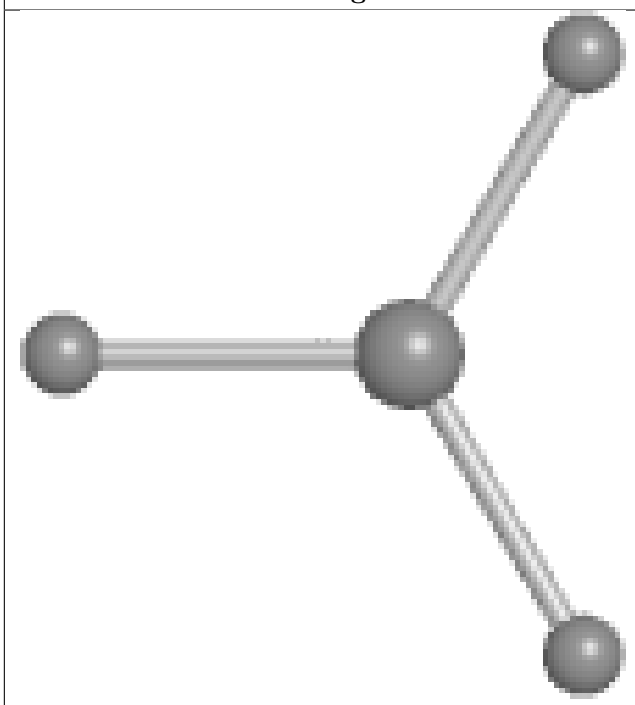
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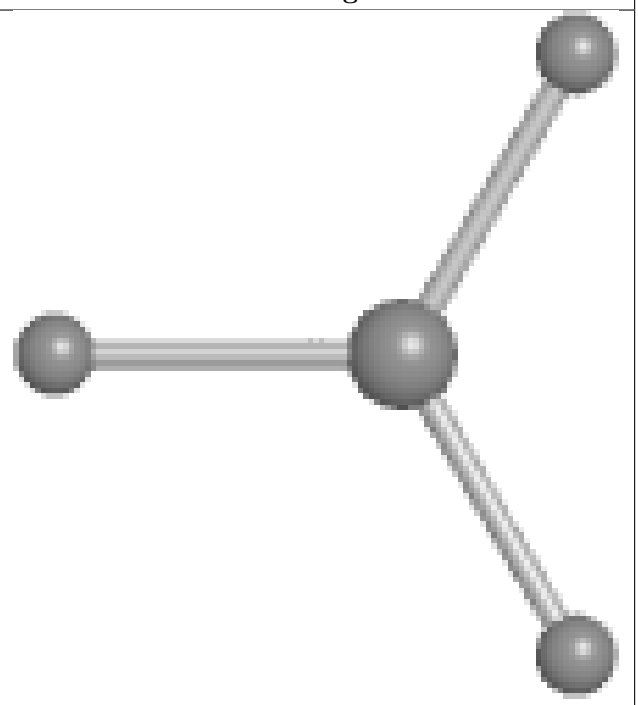
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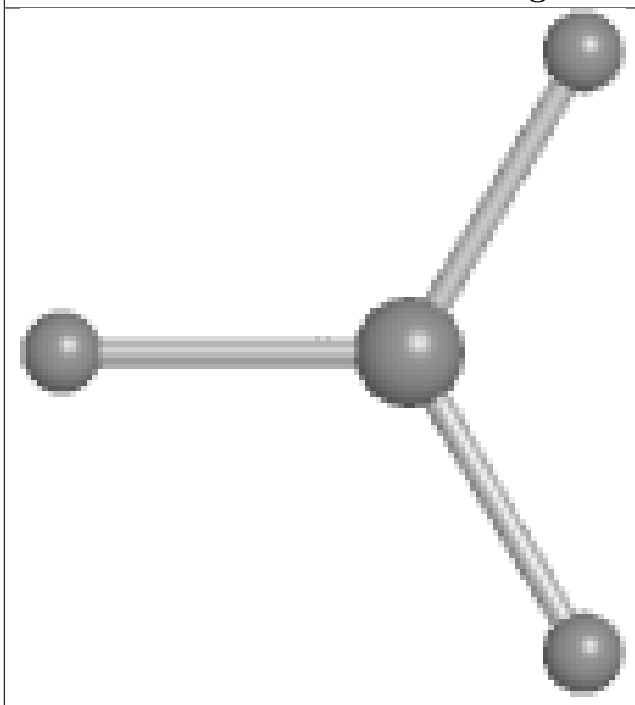


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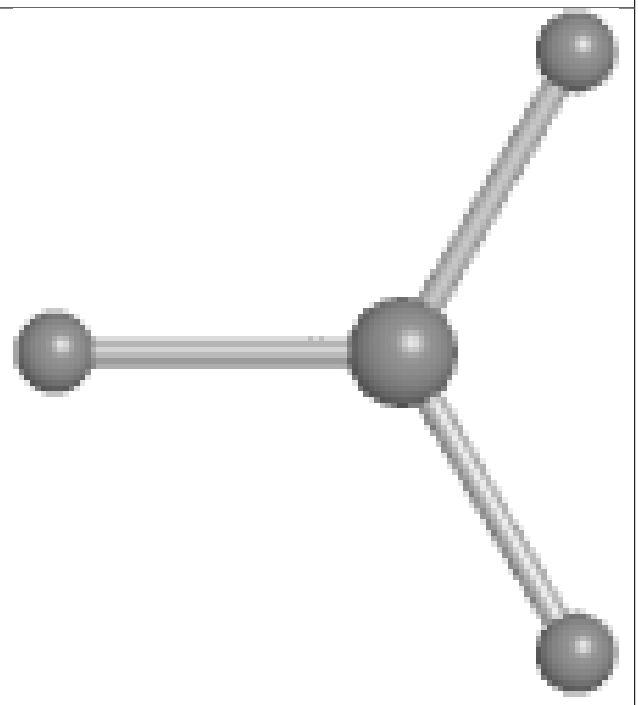


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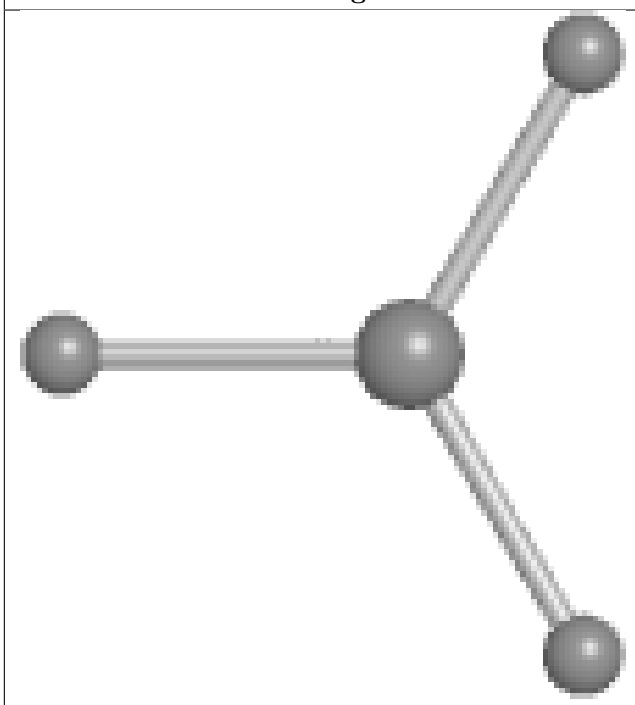
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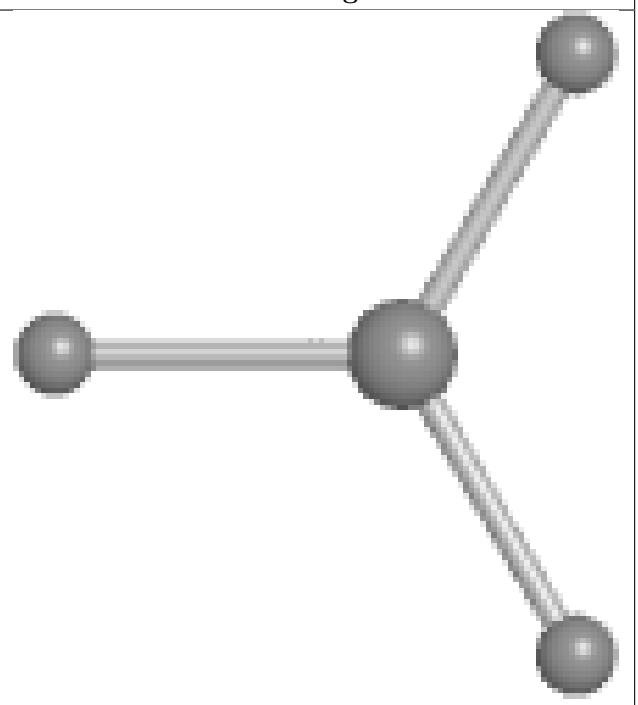
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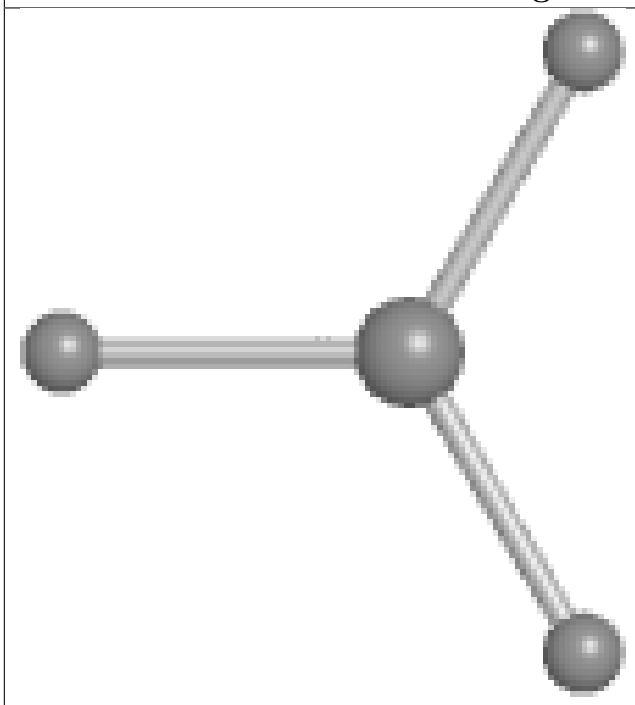


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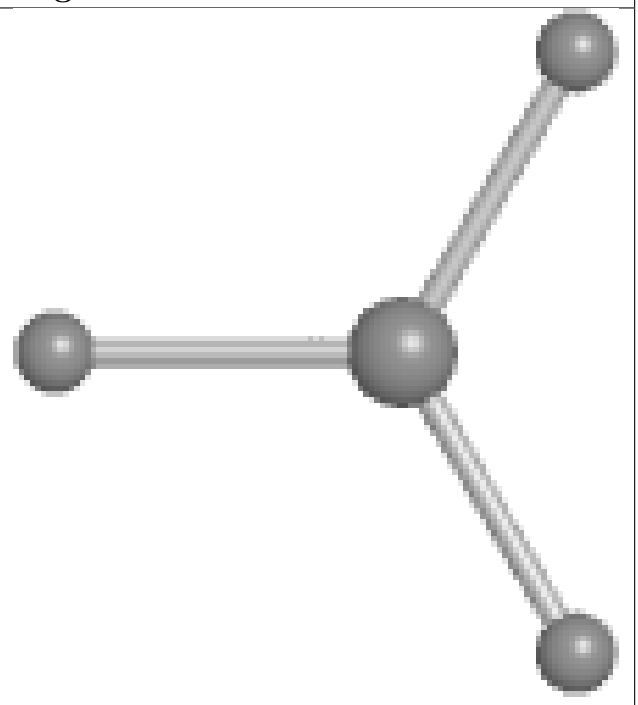


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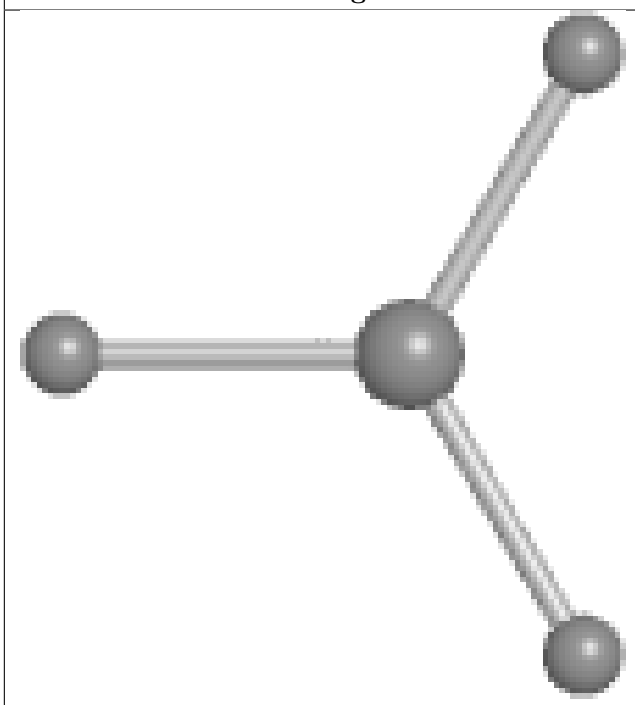
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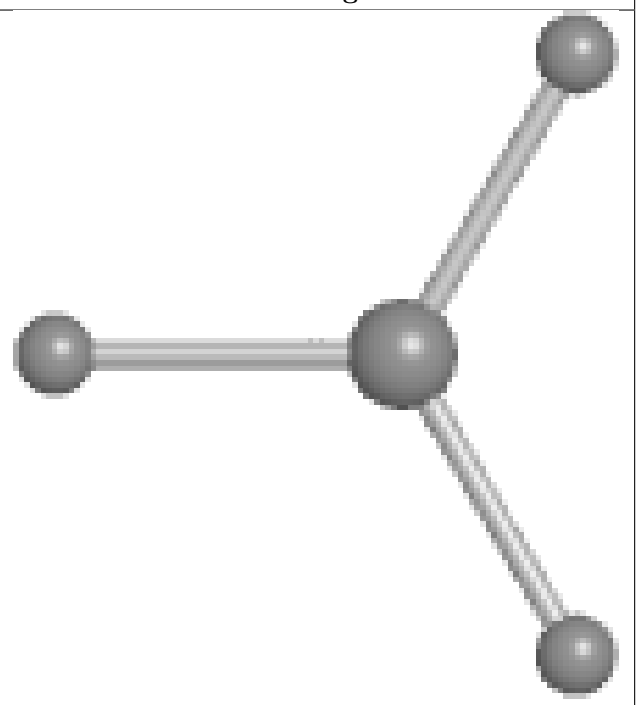
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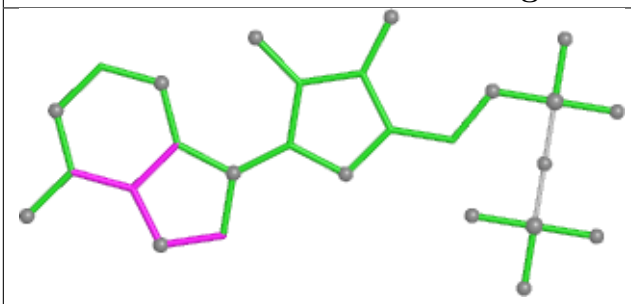


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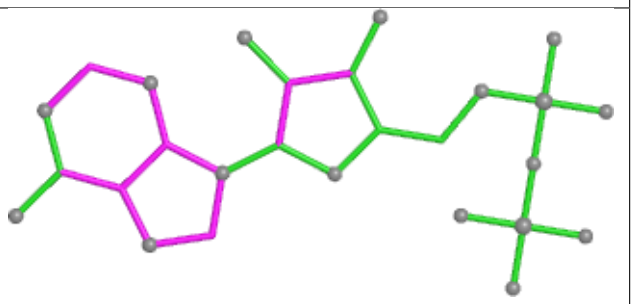


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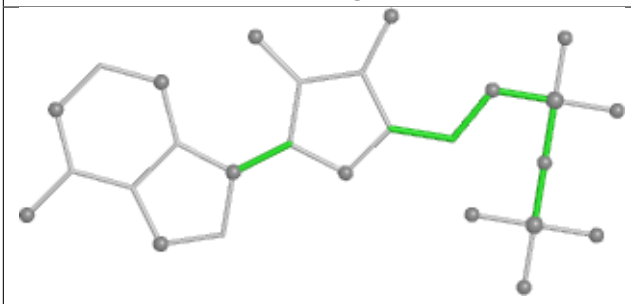
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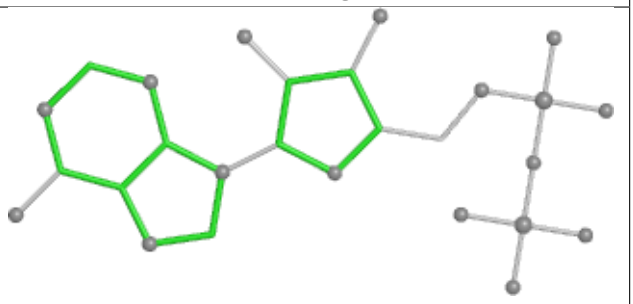
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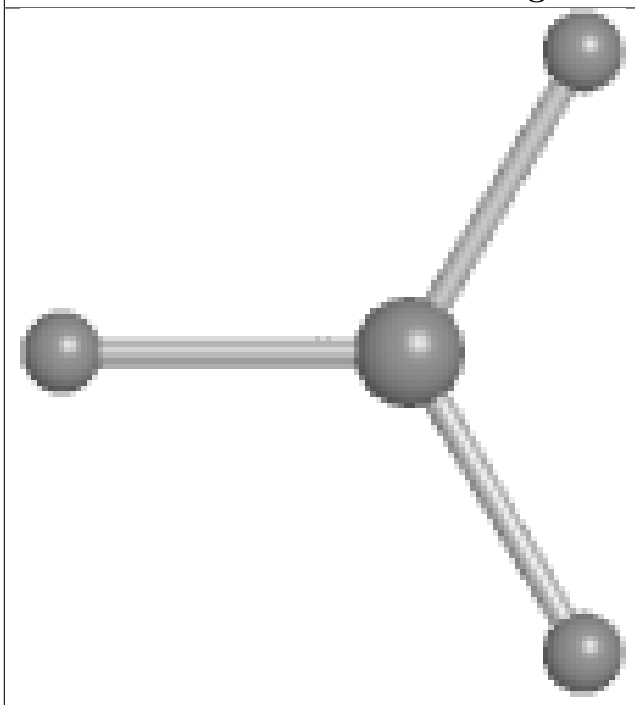


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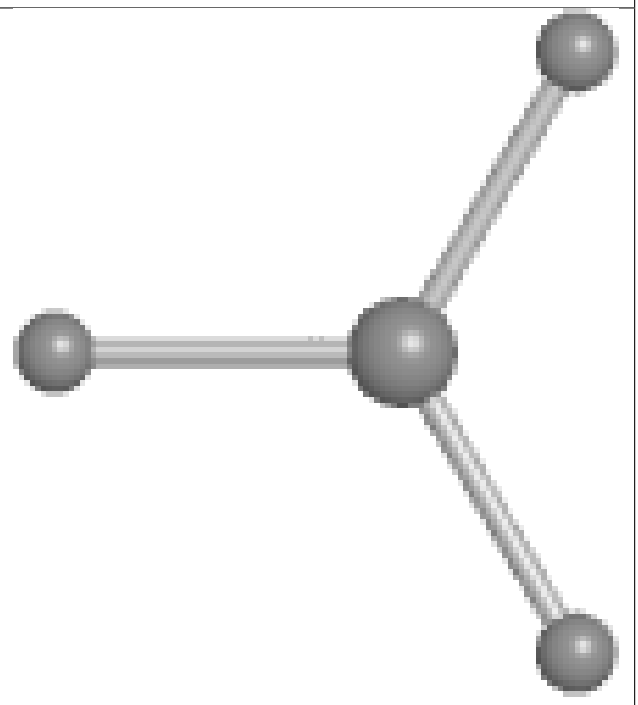


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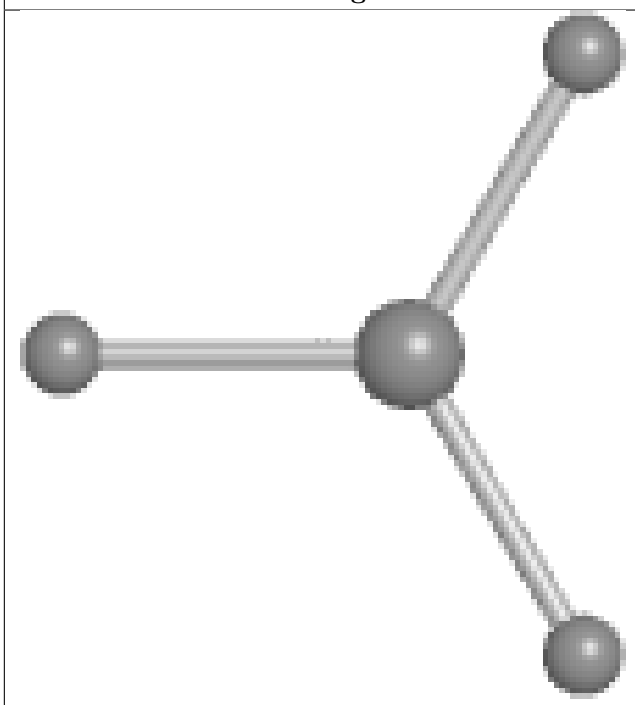
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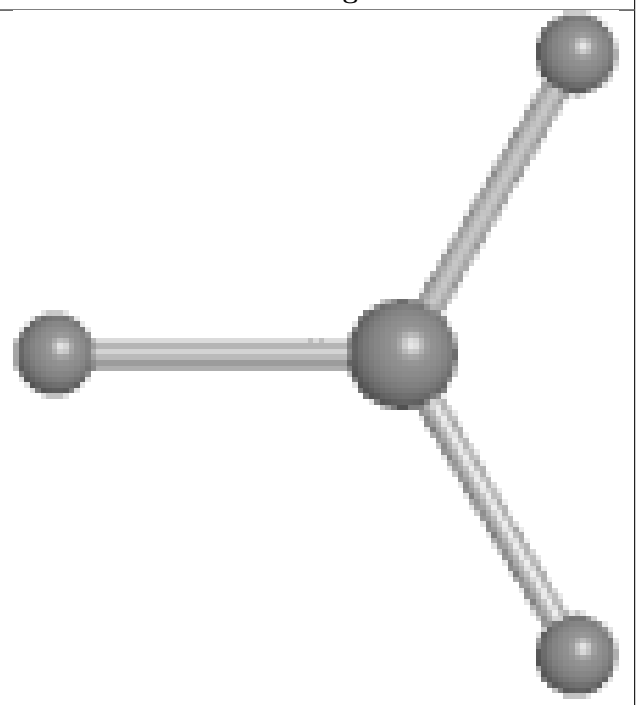
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Bond angles

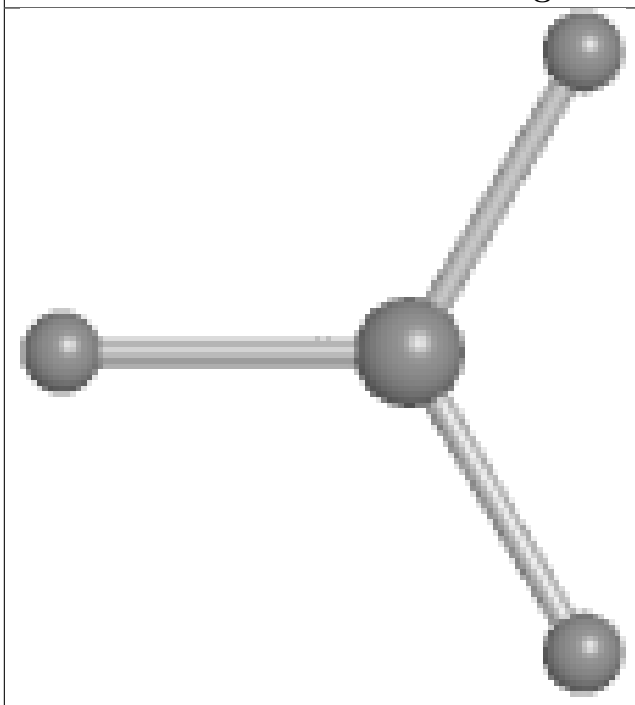


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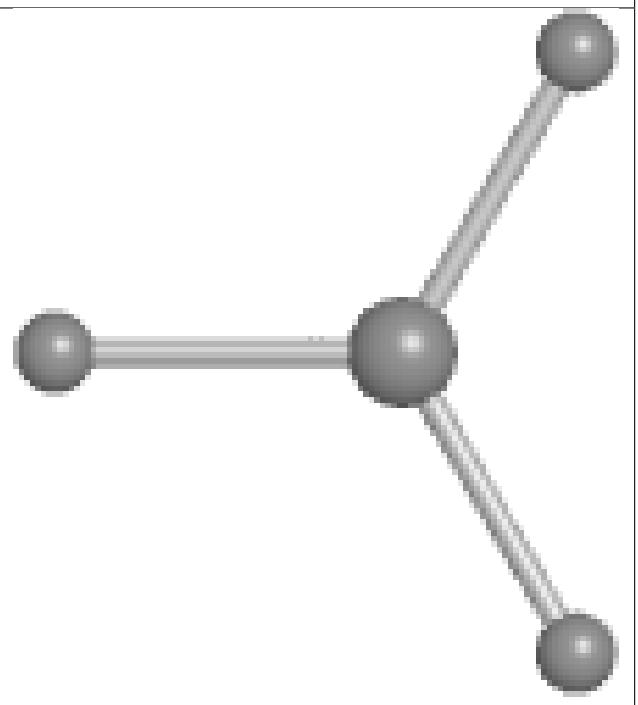


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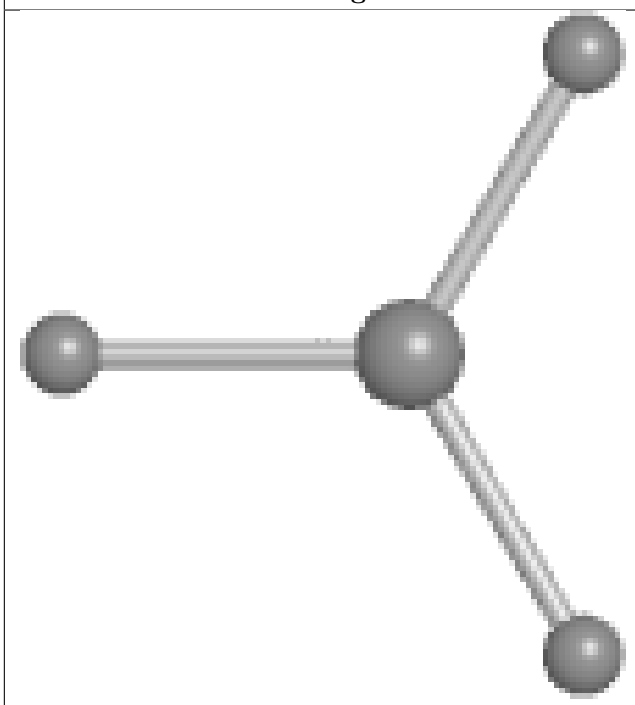
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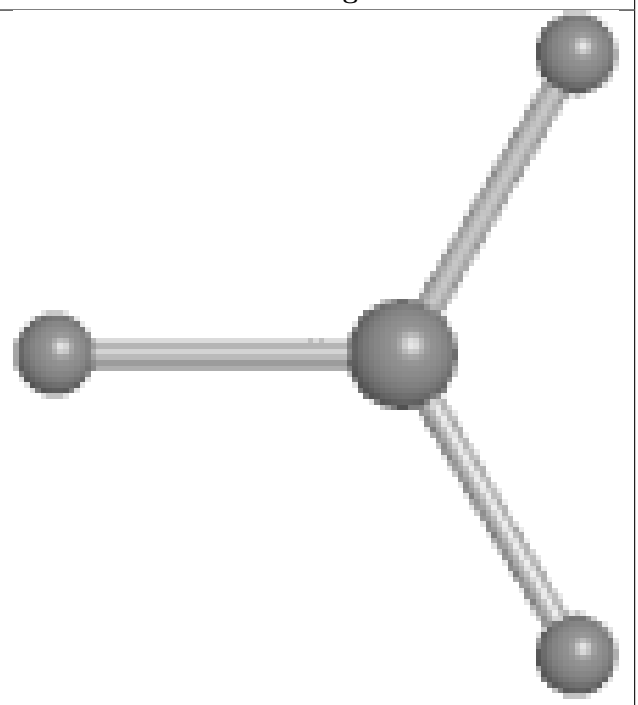
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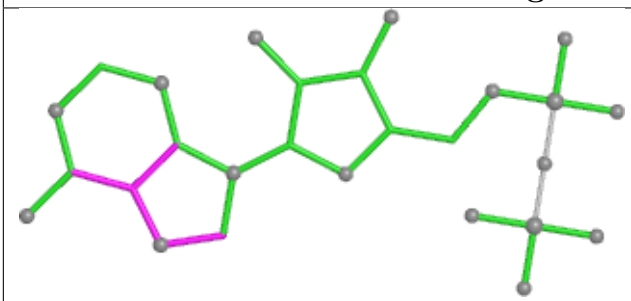


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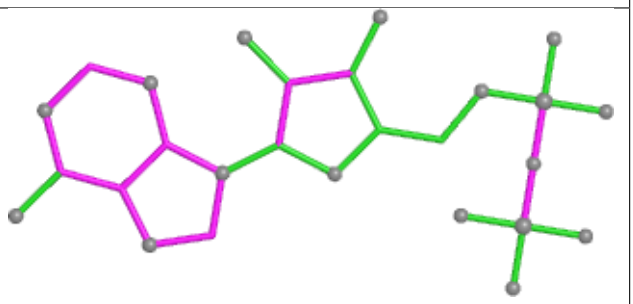


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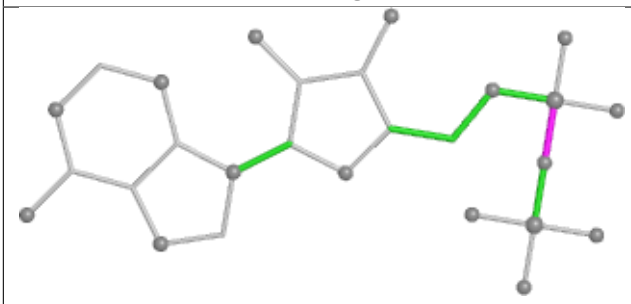
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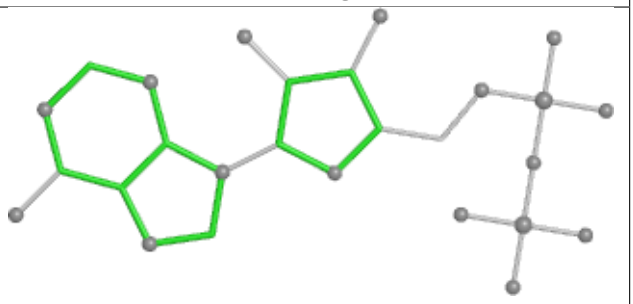
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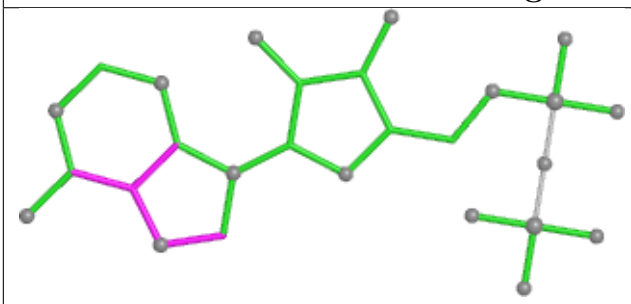


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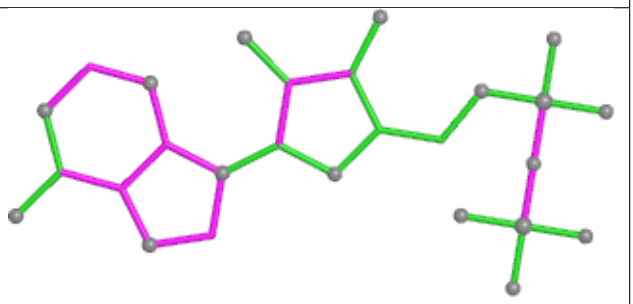


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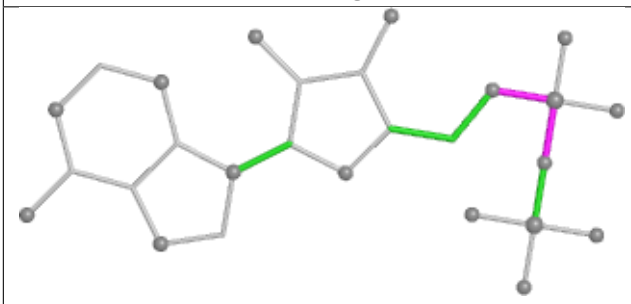
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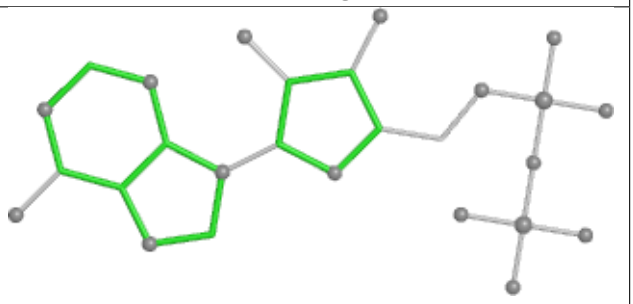
Bond lengths



Bond angles

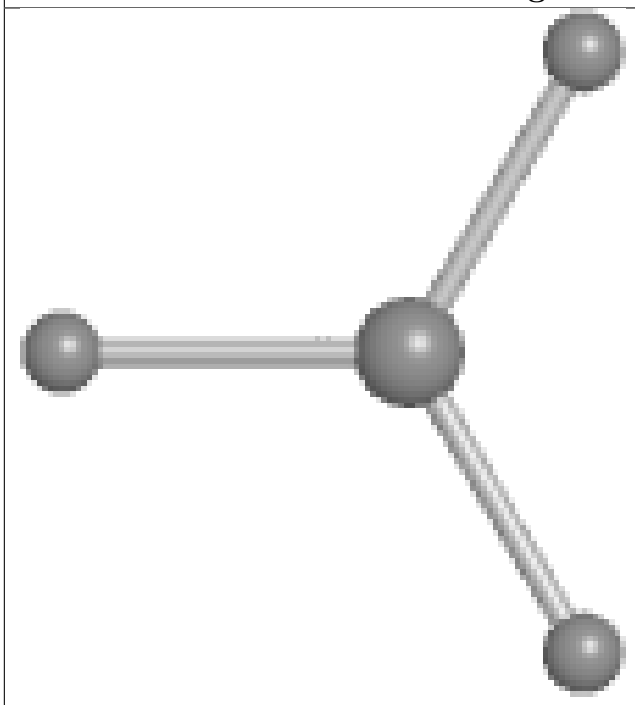


Torsions

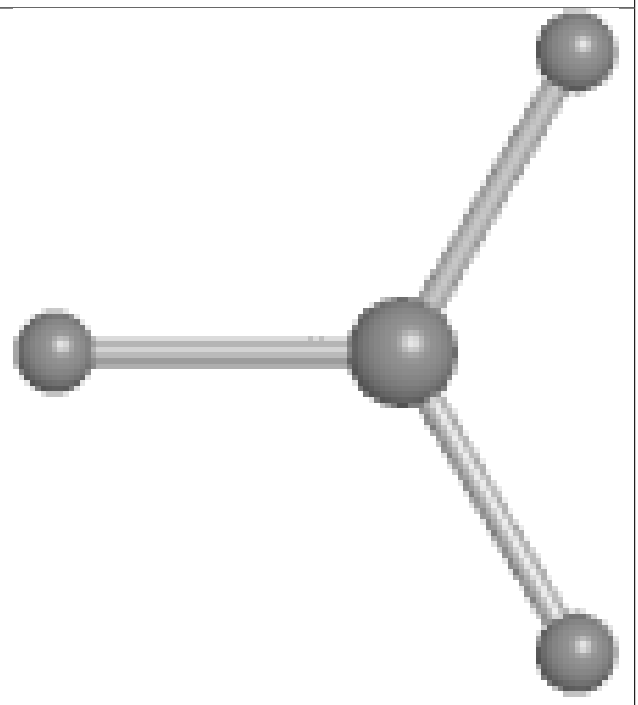


Rings

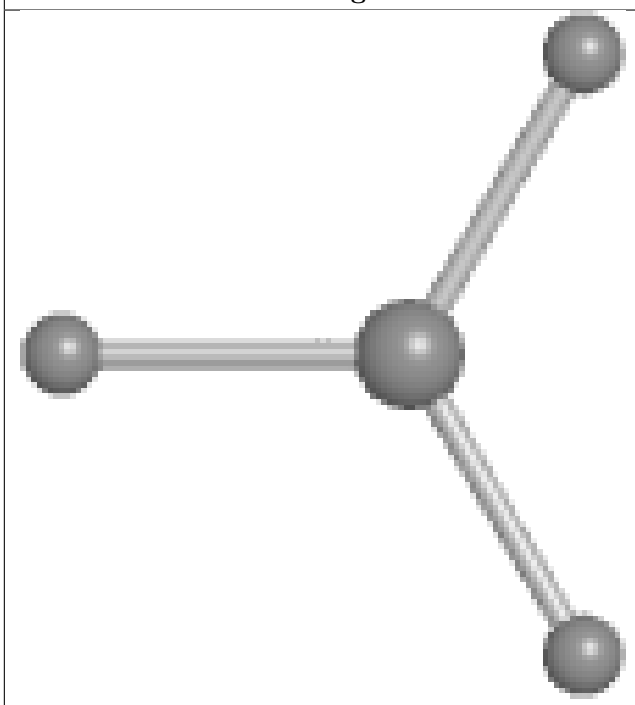
Ligand AF3 D 603



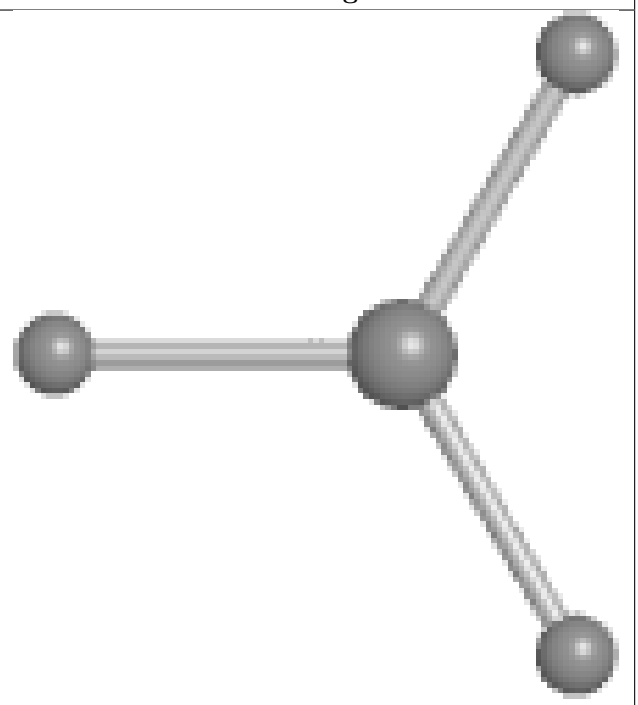
Bond lengths



Bond angles

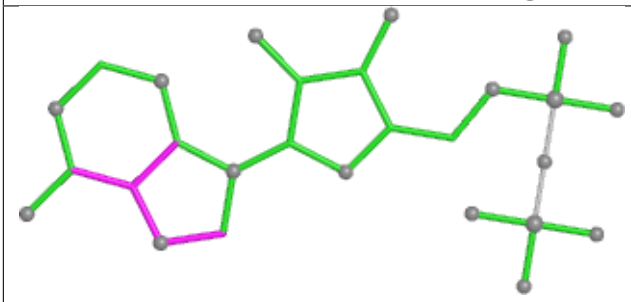


Torsions

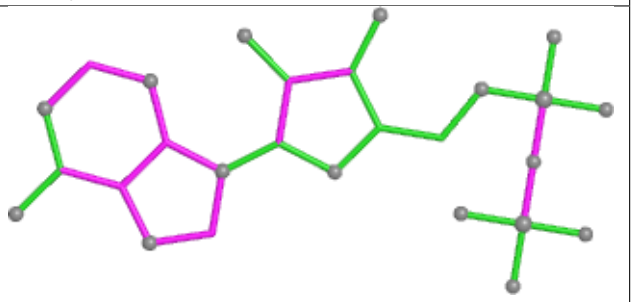


Rings

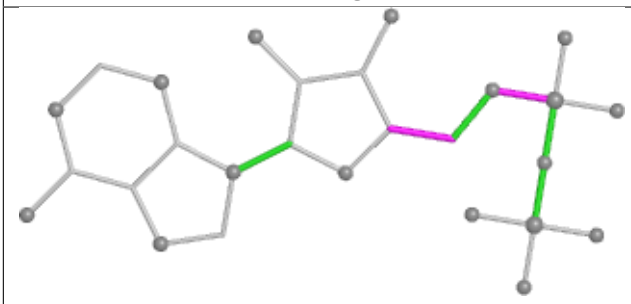
Ligand ADP Q 602



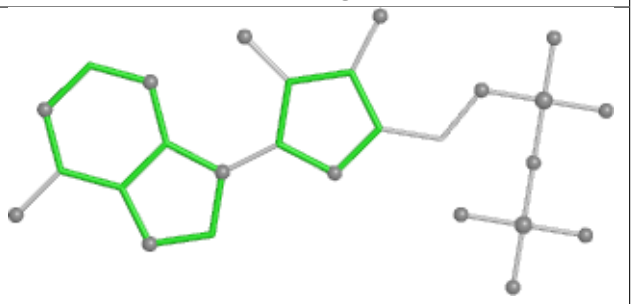
Bond lengths



Bond angles

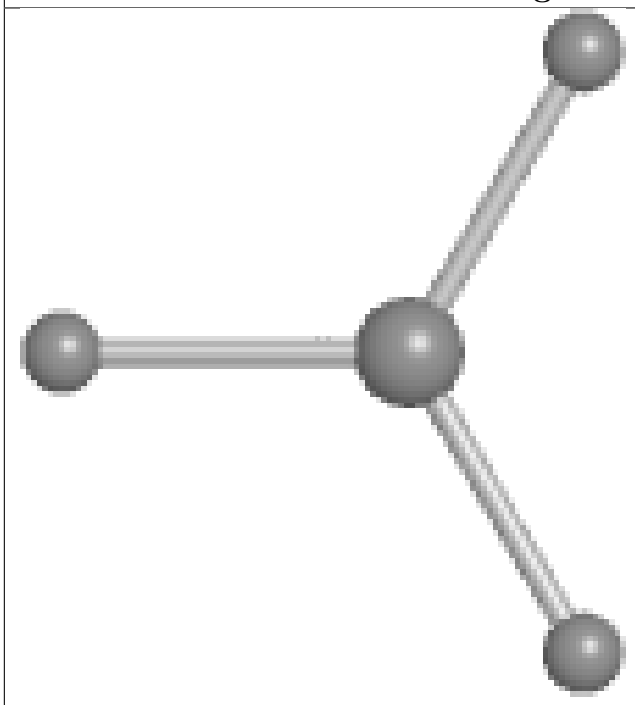


Torsions

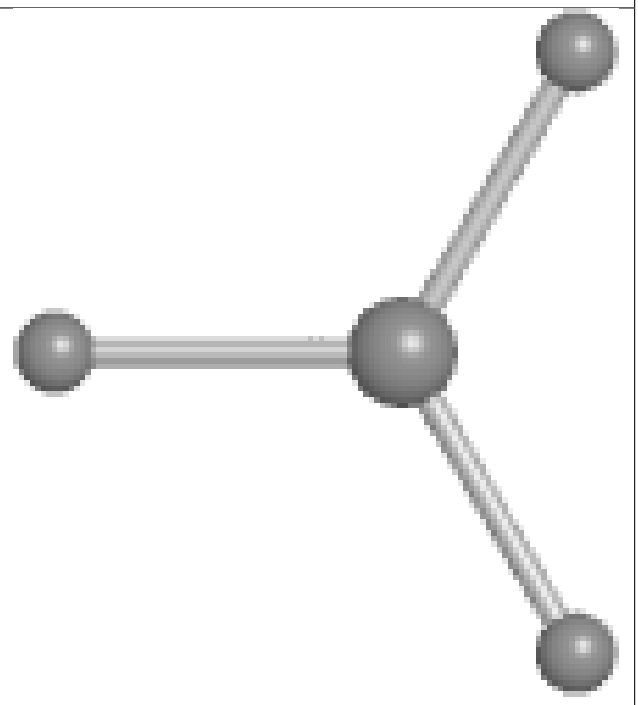


Rings

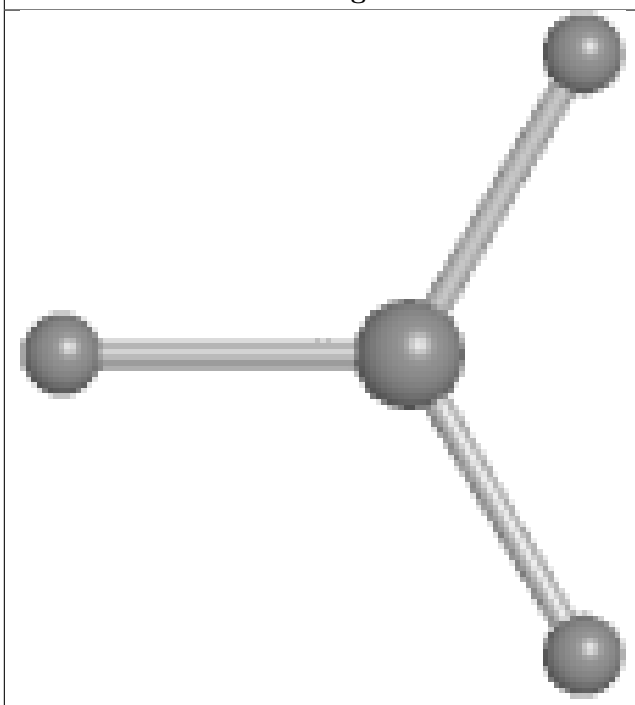
Ligand AF3 z 603



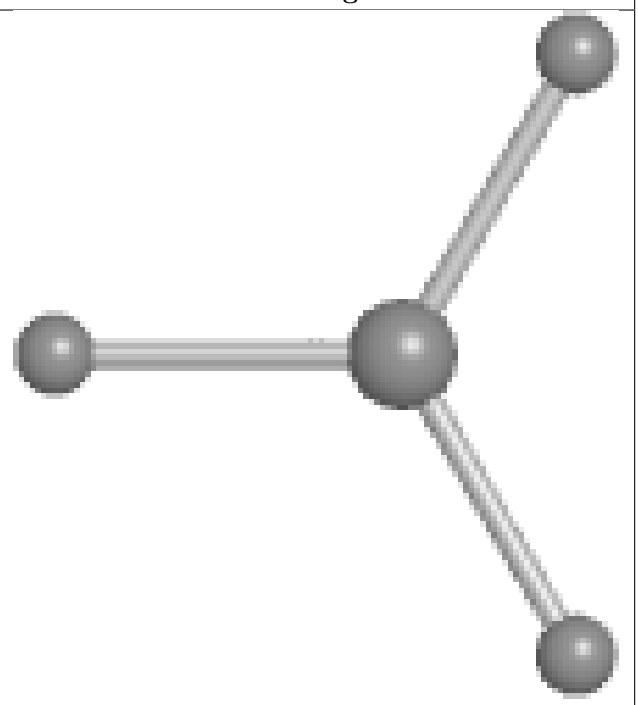
Bond lengths



Bond angles

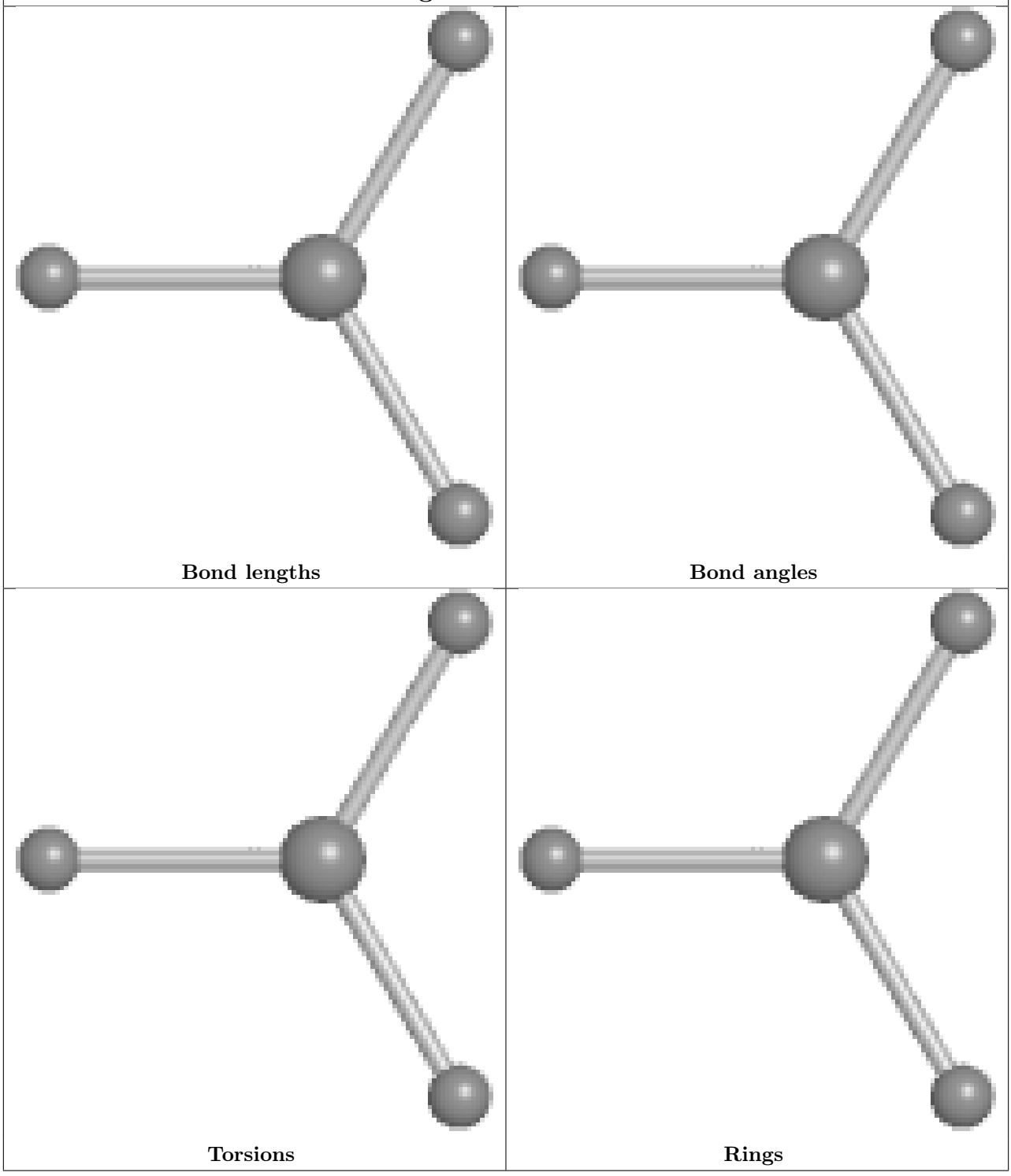


Torsions



Rings

Ligand AF3 h 603



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

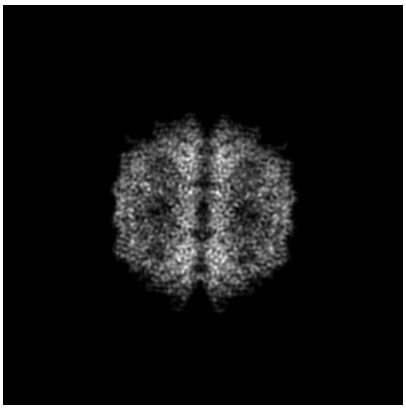
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33921. These allow visual inspection of the internal detail of the map and identification of artifacts.

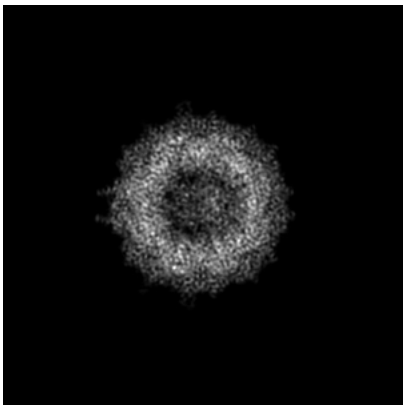
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

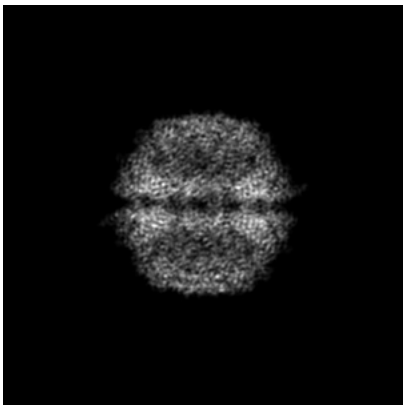
6.1.1 Primary map



X

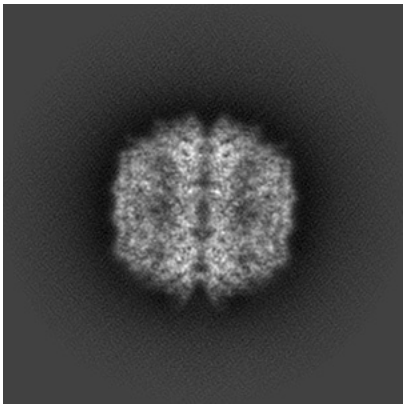


Y

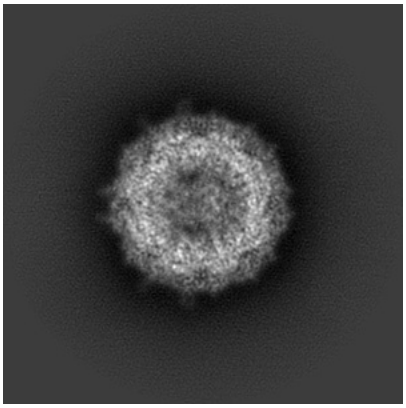


Z

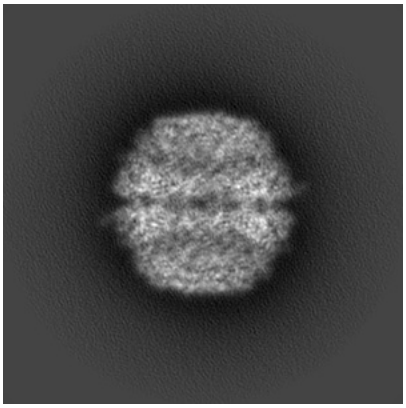
6.1.2 Raw map



X



Y



Z

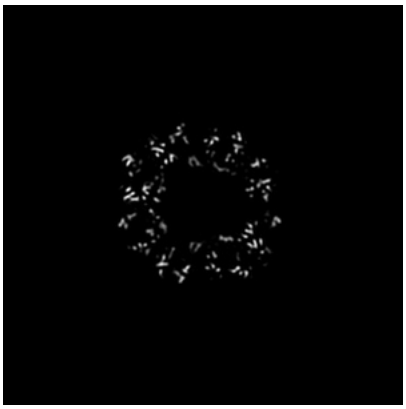
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 128

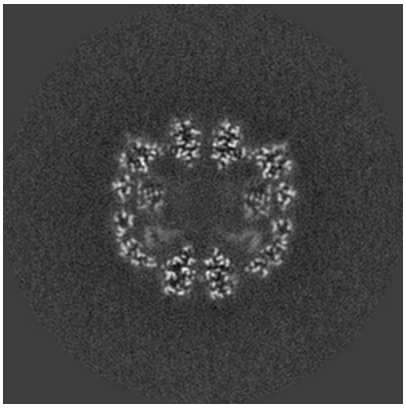


Y Index: 128

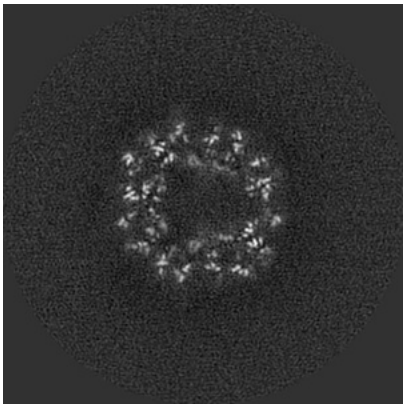


Z Index: 128

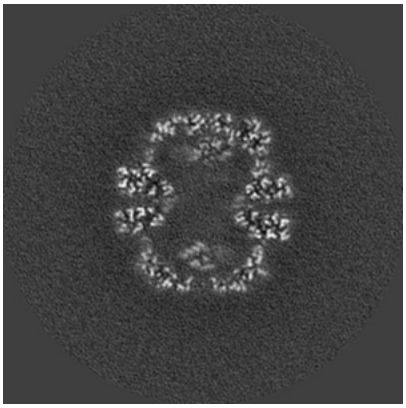
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

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

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 154

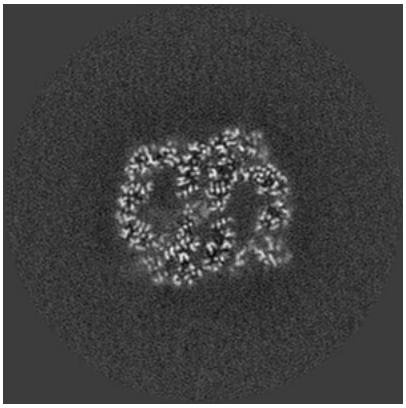


Y Index: 118

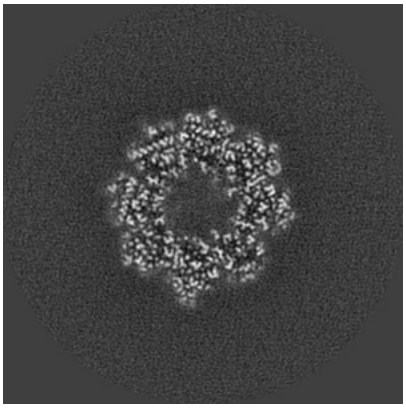


Z Index: 100

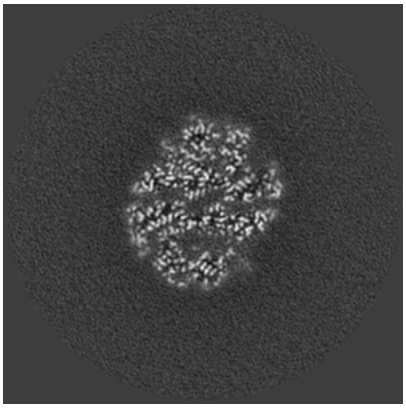
6.3.2 Raw map



X Index: 103



Y Index: 118

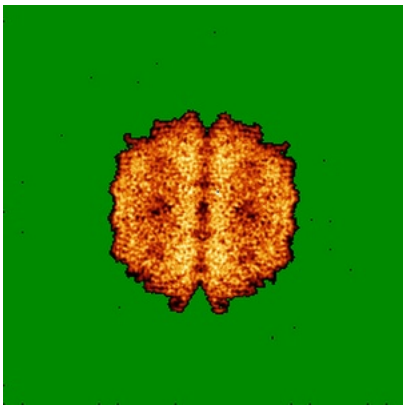


Z Index: 157

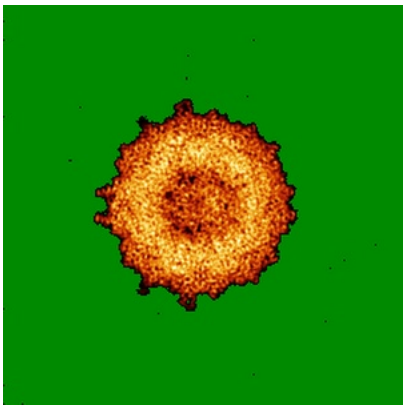
The images above show the largest variance slices of the map in three orthogonal directions.

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

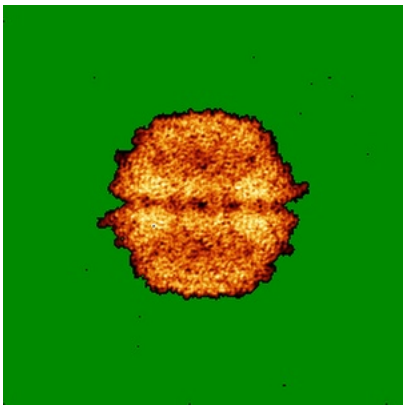
6.4.1 Primary map



X

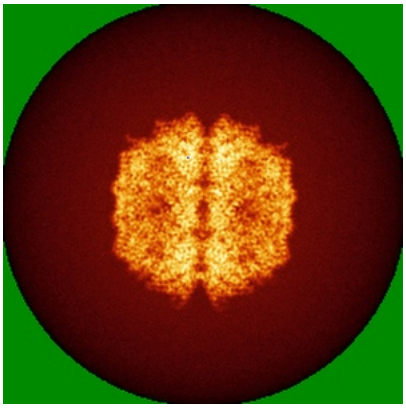


Y

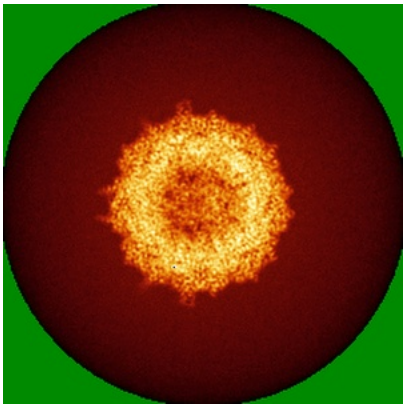


Z

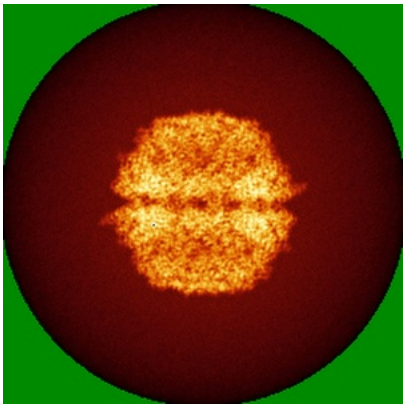
6.4.2 Raw map



X



Y

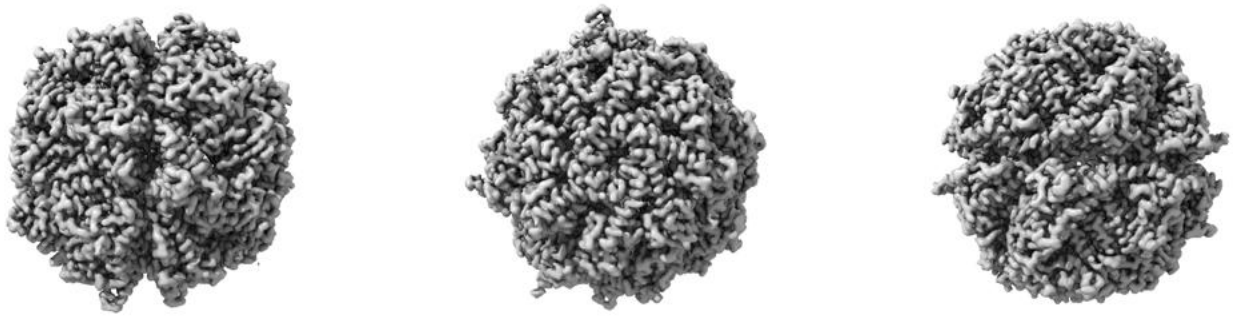


Z

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)

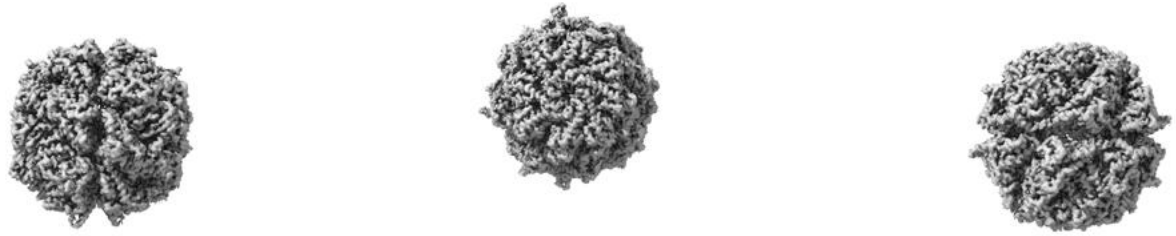
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

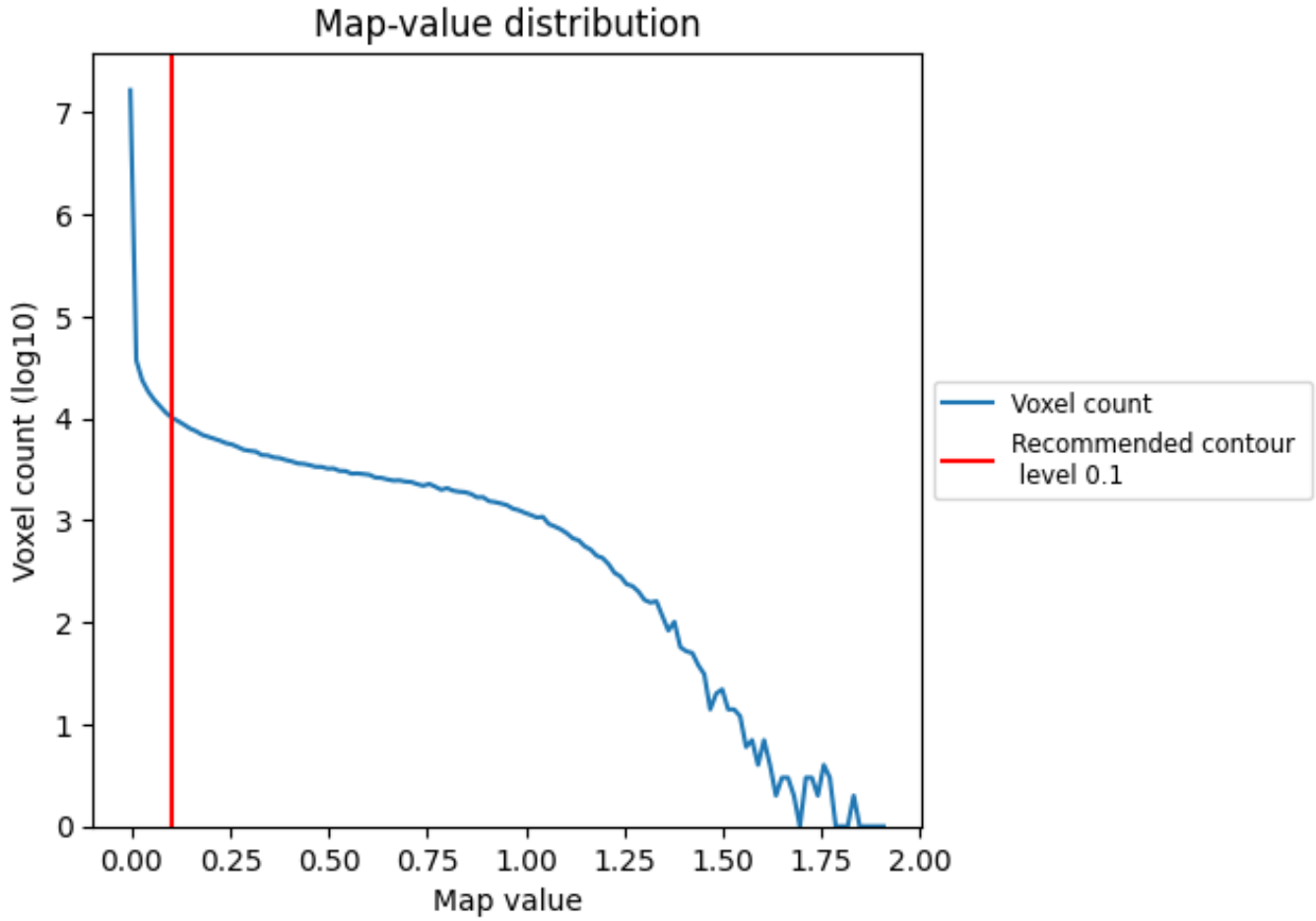
6.6 Mask visualisation (i)

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

7 Map analysis

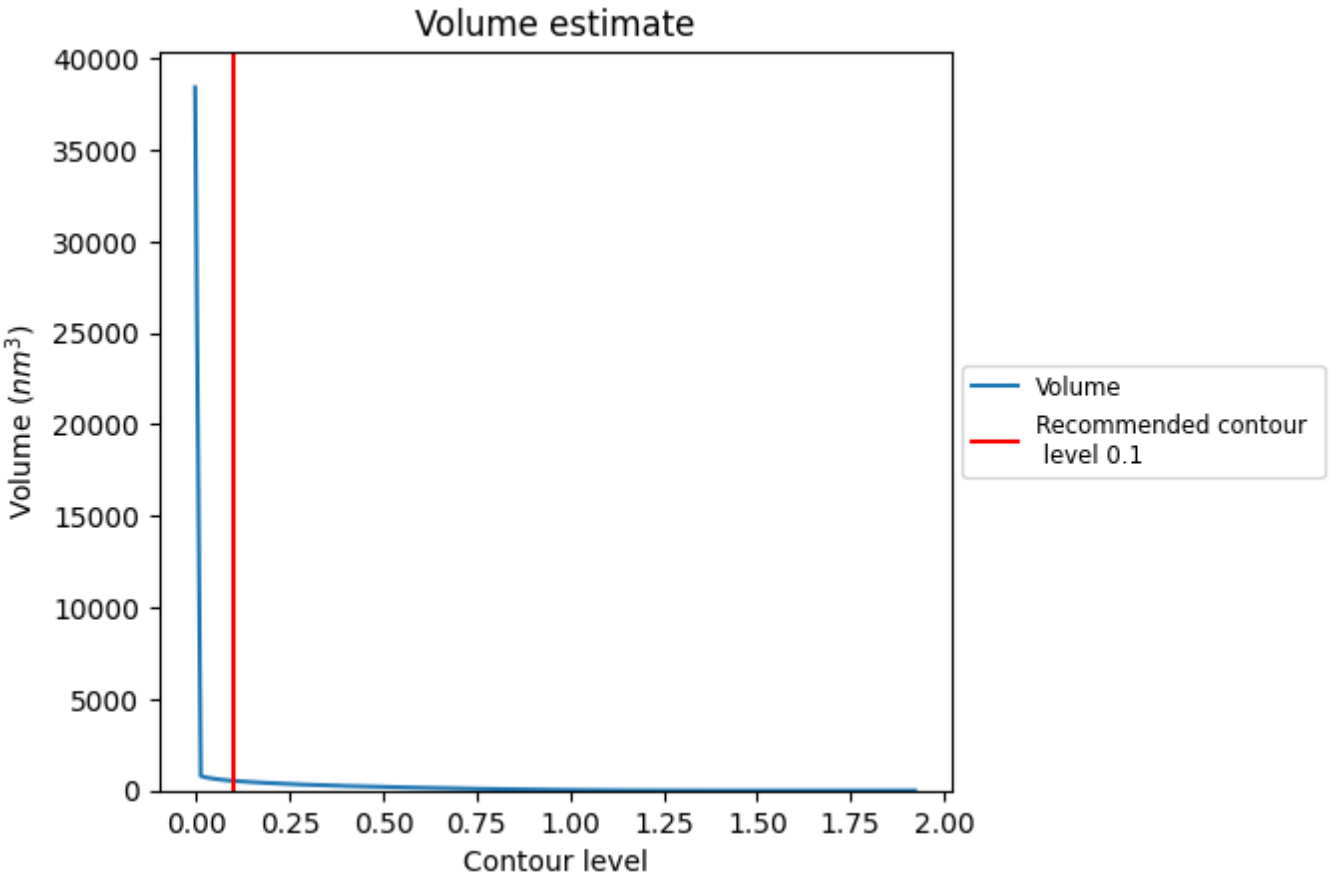
This section contains the results of statistical analysis of the map.

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.

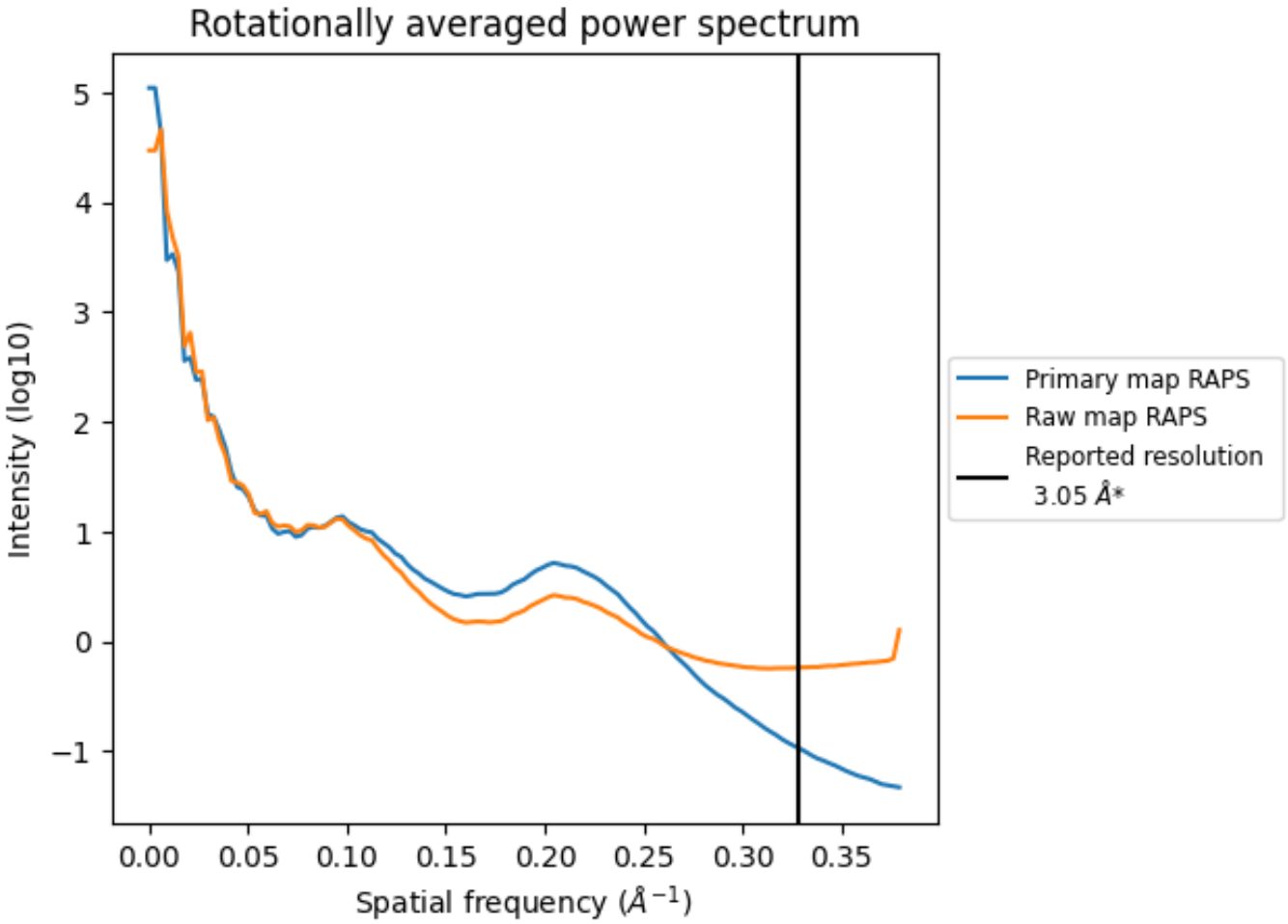
7.2 Volume estimate (i)



The volume at the recommended contour level is 530 nm^3; this corresponds to an approximate mass of 479 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)

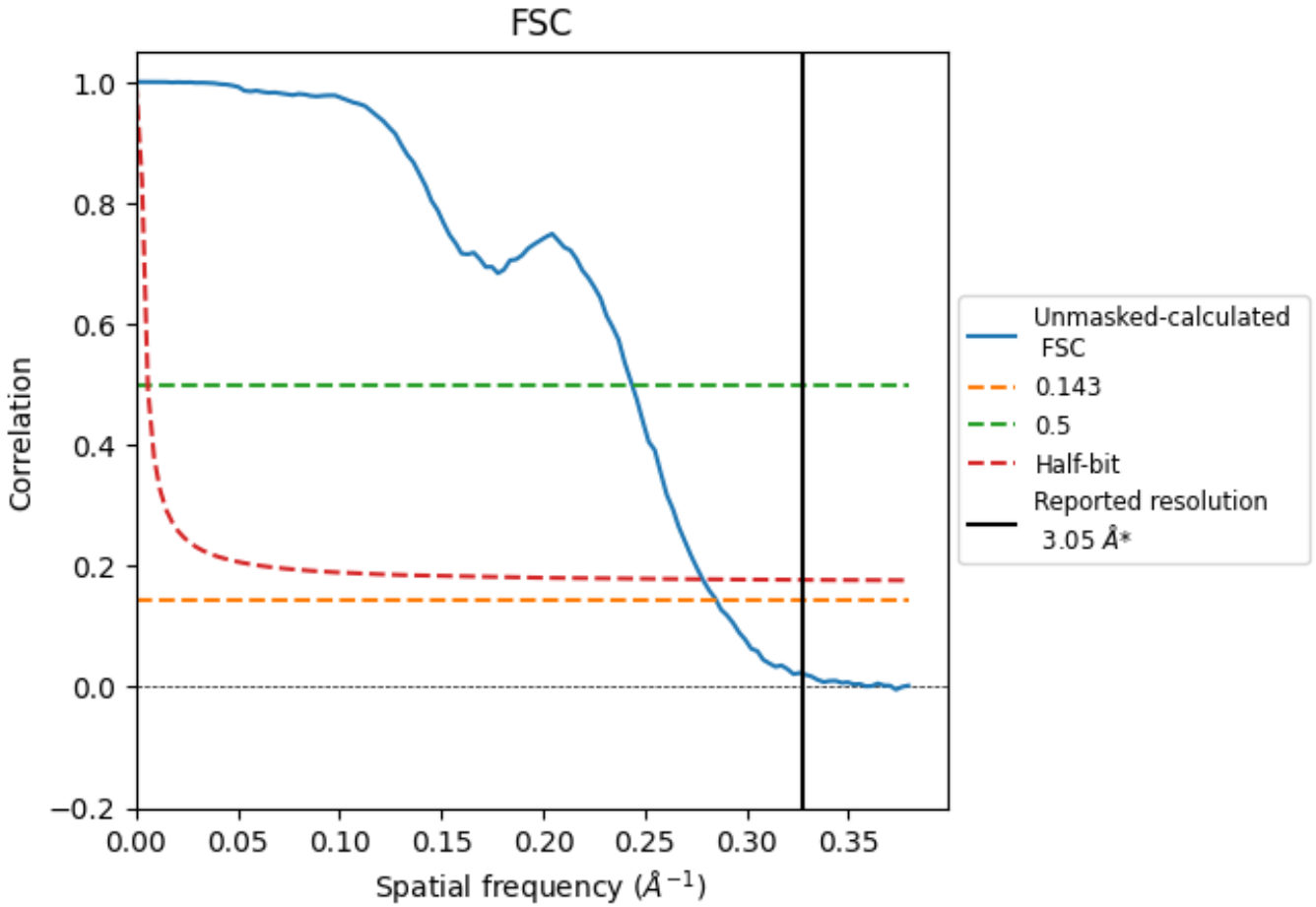


*Reported resolution corresponds to spatial frequency of 0.328 Å^{-1}

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 0.328 Å^{-1}

8.2 Resolution estimates (i)

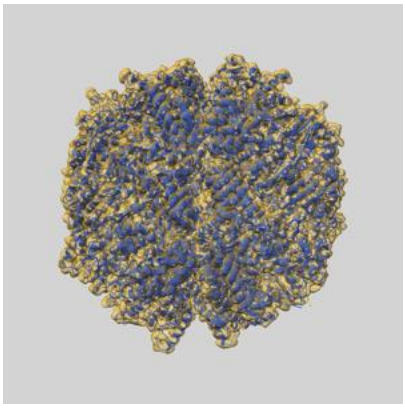
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.51	4.10	3.59

*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 3.51 differs from the reported value 3.05 by more than 10 %

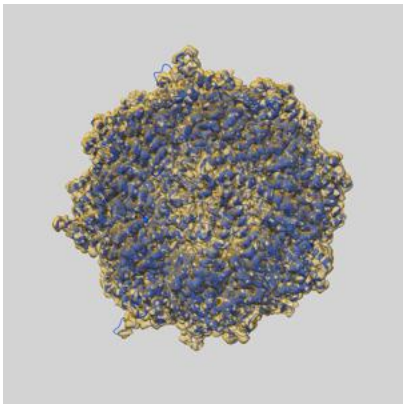
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33921 and PDB model 7YLY. Per-residue inclusion information can be found in section 3 on page 13.

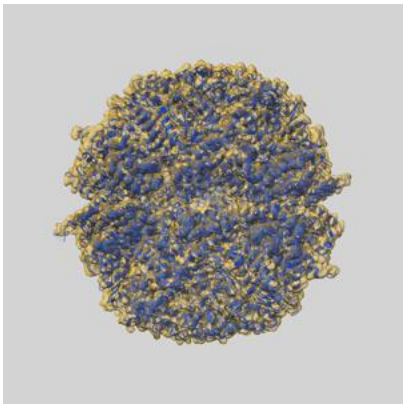
9.1 Map-model overlay



X



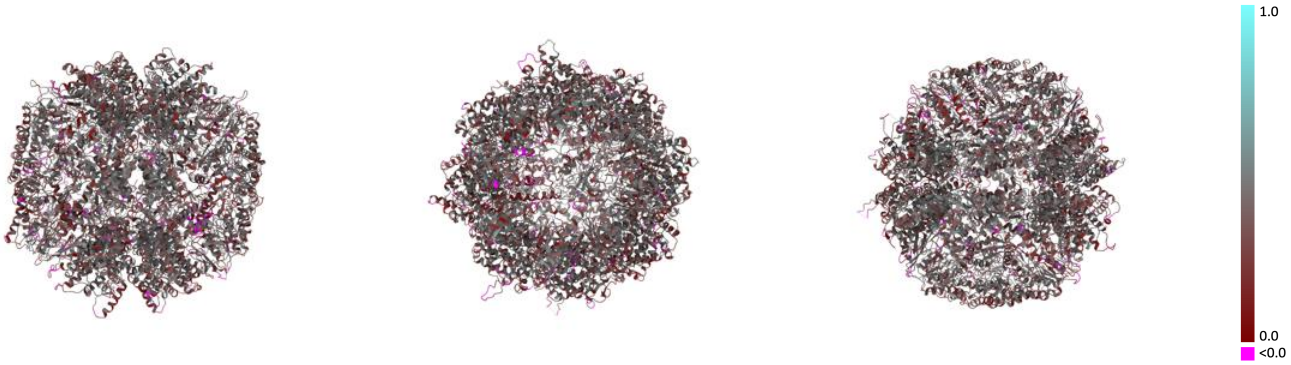
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

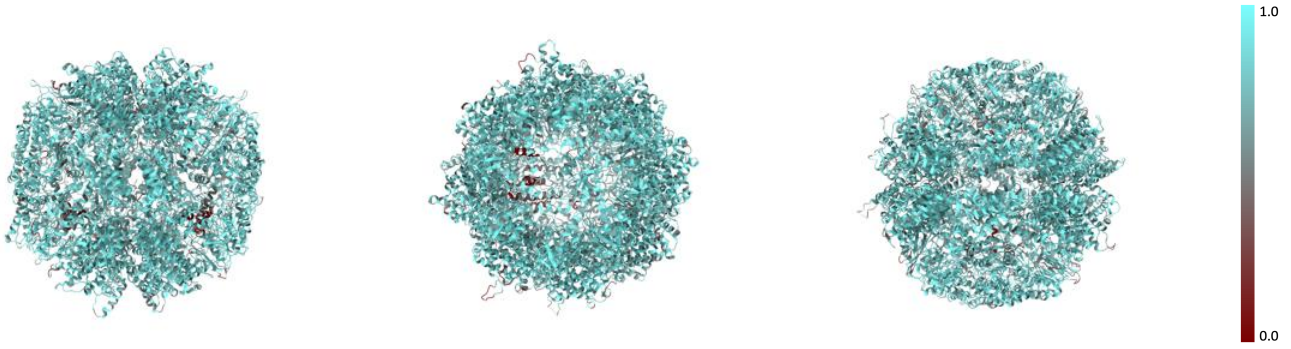
9.2 Q-score mapped to coordinate model



X Y Z

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

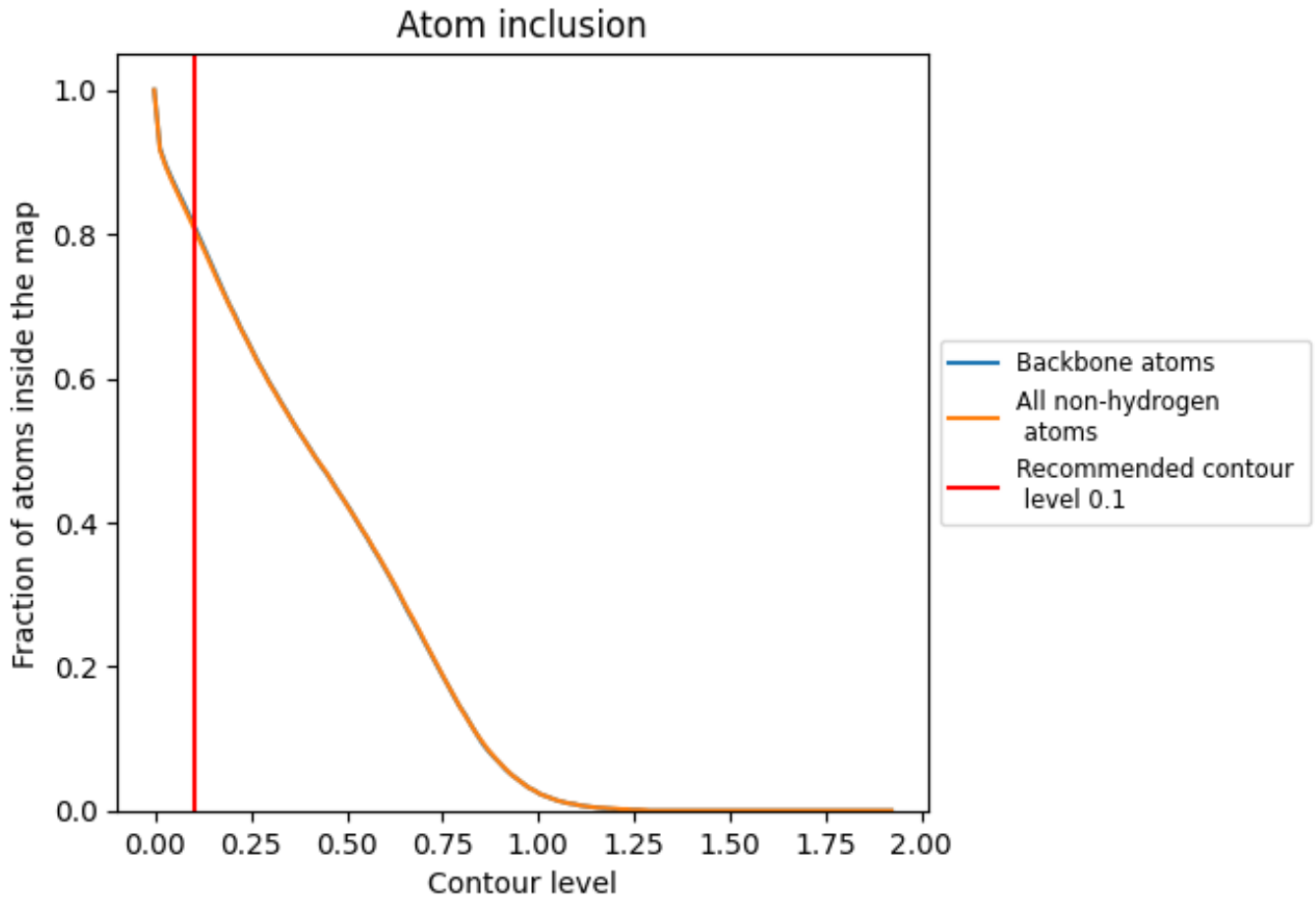
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.3540
A	0.8240	0.3460
B	0.8420	0.3800
D	0.8330	0.3670
E	0.8110	0.3520
G	0.8260	0.3570
H	0.8280	0.3520
P	0.5750	0.2710
Q	0.8080	0.3470
Z	0.8250	0.3490
a	0.8170	0.3470
b	0.8500	0.3890
d	0.8260	0.3590
e	0.8200	0.3530
g	0.8340	0.3590
h	0.8330	0.3650
p	0.5850	0.2720
q	0.8120	0.3480
z	0.8330	0.3580

