Full wwPDB EM Validation Report (i)

Mar 20, 2024 – 02:25 AM JST

PDB ID	:	6KS6
EMDB ID	:	EMD-0758
Title	:	TRiC at 0.2 mM ADP-AlFx, Conformation 1, 0.2-C1
Authors	:	Jin, M.; Cong, Y.
Deposited on	:	2019-08-23
Resolution	:	2.99 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

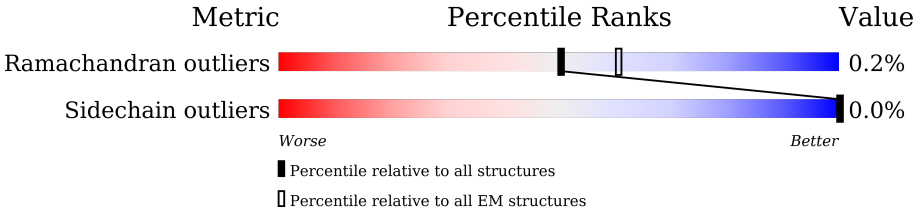
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.99 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	559	12% 98% .
1	a	559	11% 98% .
2	B	527	6% 98% .
2	b	527	6% 98% .
3	D	528	7% 99% .
3	d	528	9% 99% .
4	E	562	7% 95% 5%
4	e	562	6% 95% 5%
5	G	594	7% 88% 12%

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Mol	Chain	Length	Quality of chain
5	g	594	5% 87% 12%
6	H	550	7% 94% 5%
6	h	550	7% 96%
7	Q	568	12% 96%
7	q	568	11% 95% 5%
8	Z	546	12% 98%
8	z	546	11% 99%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 65514 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
			Total	C	N	O	S		
1	a	546	4129	2582	721	806	20	0	0
1	A	550	4158	2599	725	813	21	0	0

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

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

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

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

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

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

- Molecule 5 is a protein called fusion protein of T-complex protein 1 subunit gamma,rep-His-CBP and T-complex protein 1 subunit gamma.

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

There are 120 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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
G	433	LEU	-	see sequence details	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
G	434	GLN	-	see sequence details	UNP P39077

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

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

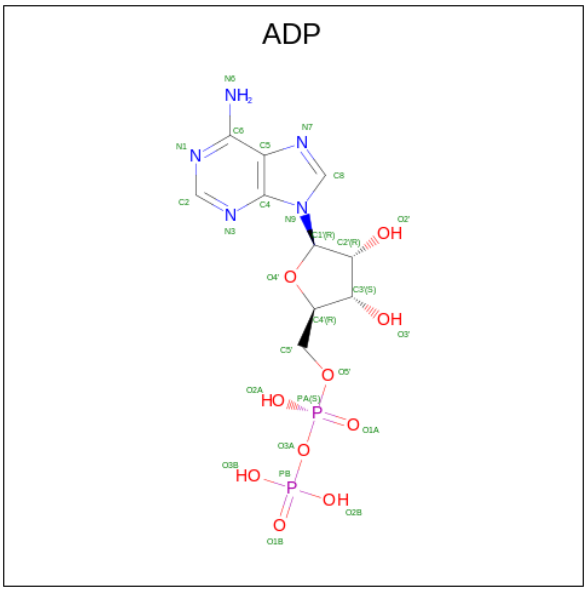
- Molecule 7 is a protein called T-complex protein 1 subunit theta.

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

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

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

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

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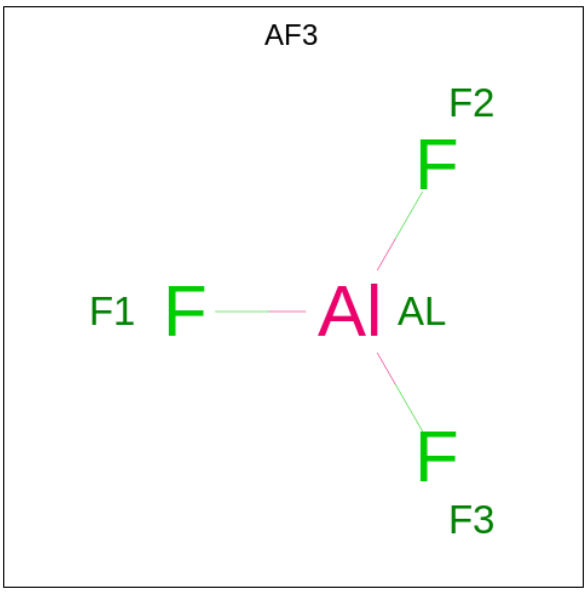
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	z	1	27	10	5	10	2	0
9	Z	1	27	10	5	10	2	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 11 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3) (labeled

as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
11	Z	1	4	1	3	0

- Molecule 12 is water.

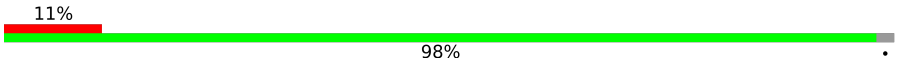
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
12	a	1	1	1	0
12	A	1	1	1	0
12	b	1	1	1	0
12	B	1	1	1	0
12	d	1	1	1	0
12	D	1	1	1	0
12	e	1	1	1	0
12	E	1	1	1	0
12	g	1	1	1	0
12	G	1	1	1	0
12	h	1	1	1	0
12	H	1	1	1	0
12	z	1	1	1	0
12	Z	1	1	1	0

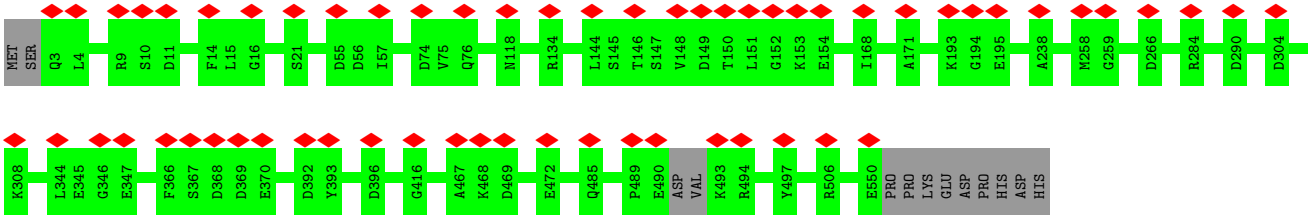
3 Residue-property plots (i)

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

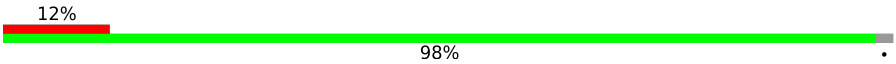
Chain a:

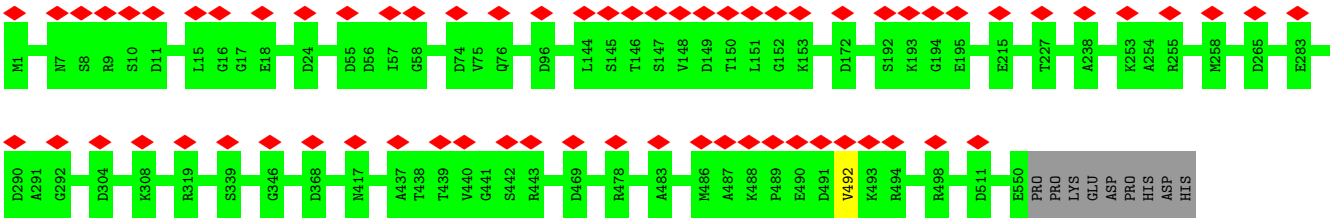




• Molecule 1: T-complex protein 1 subunit alpha

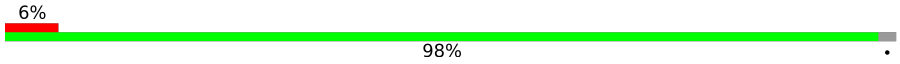
Chain A:

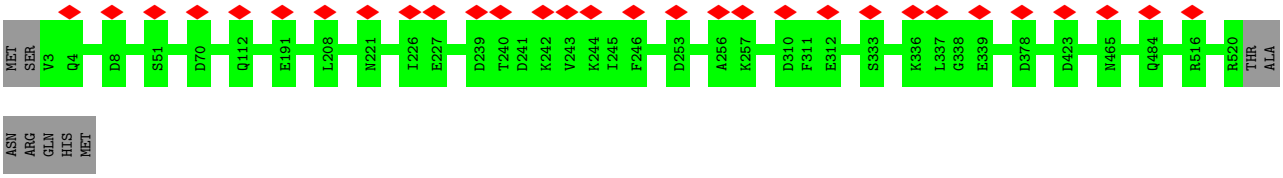




• Molecule 2: T-complex protein 1 subunit beta

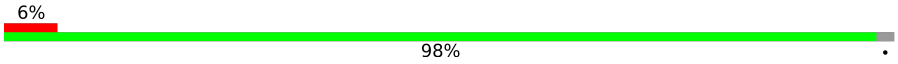
Chain b:

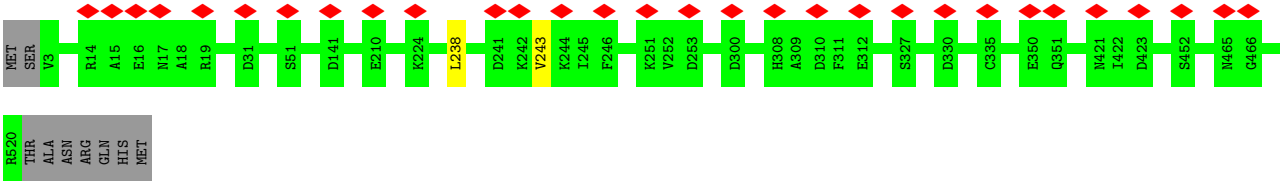




• Molecule 2: T-complex protein 1 subunit beta

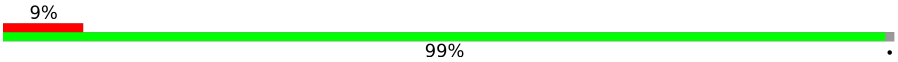
Chain B:

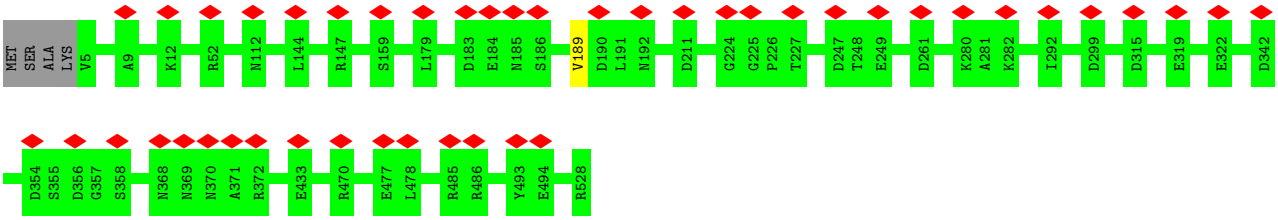




• Molecule 3: T-complex protein 1 subunit delta

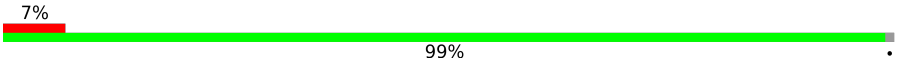
Chain d:

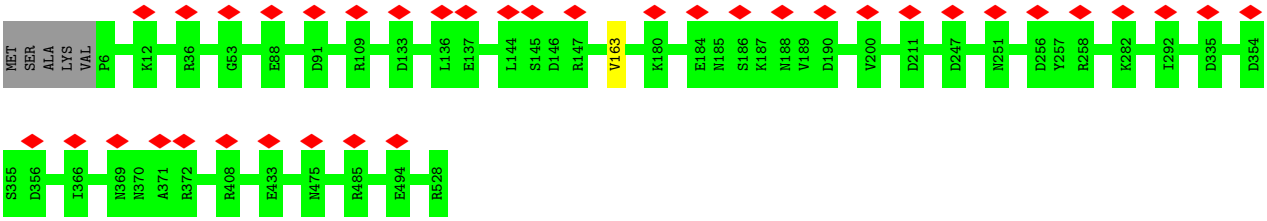




• Molecule 3: T-complex protein 1 subunit delta

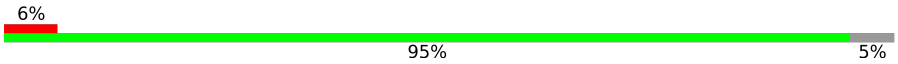
Chain D:

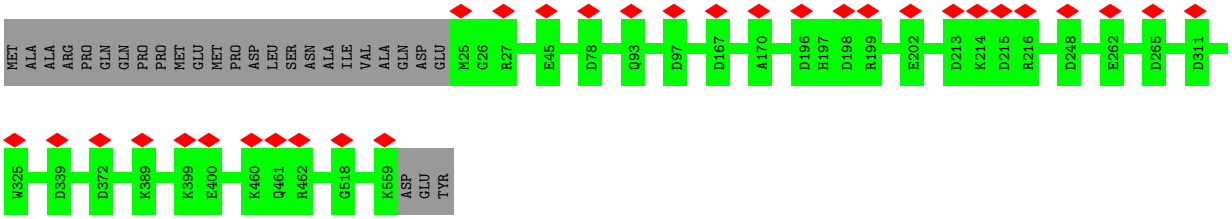




• Molecule 4: T-complex protein 1 subunit epsilon

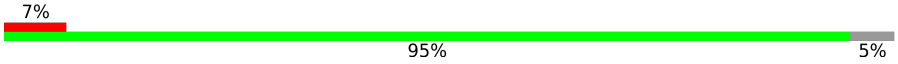
Chain e:

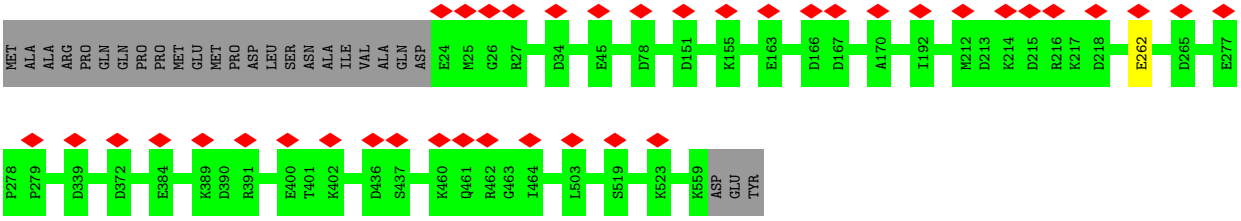




• Molecule 4: T-complex protein 1 subunit epsilon

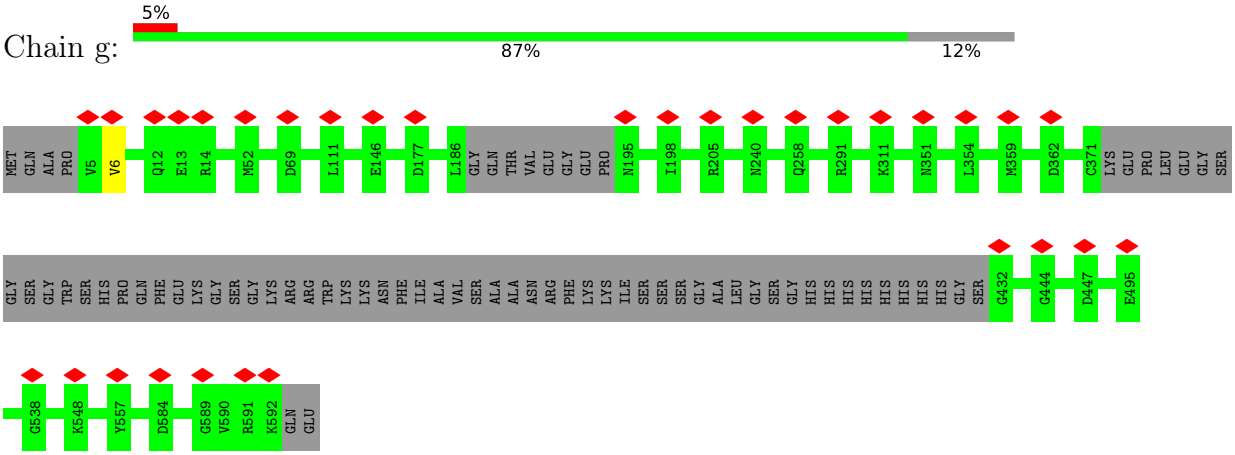
Chain E:





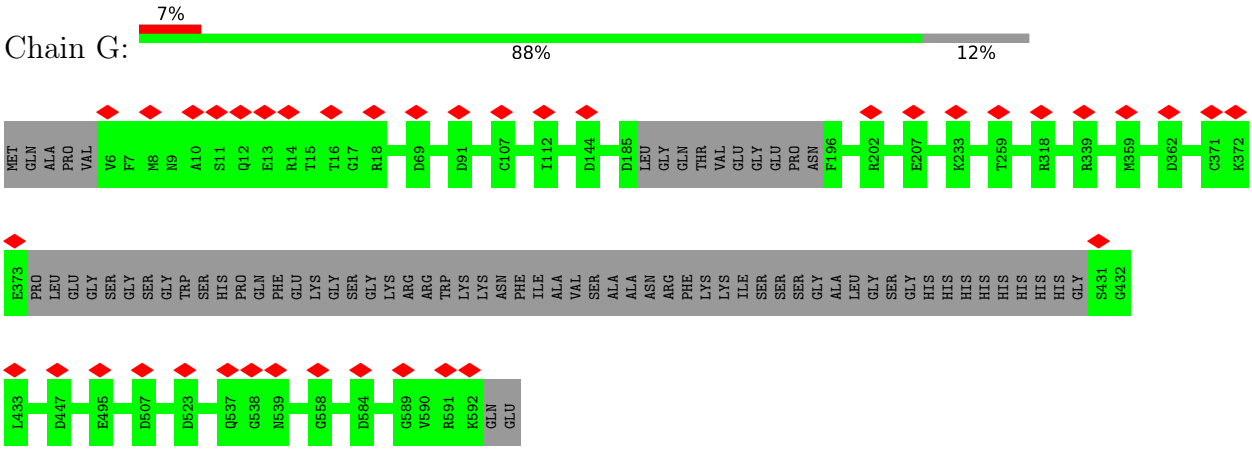
• Molecule 5: fusion protein of T-complex protein 1 subunit gamma,rep-His-CBP and T-complex protein 1 subunit gamma

Chain g:



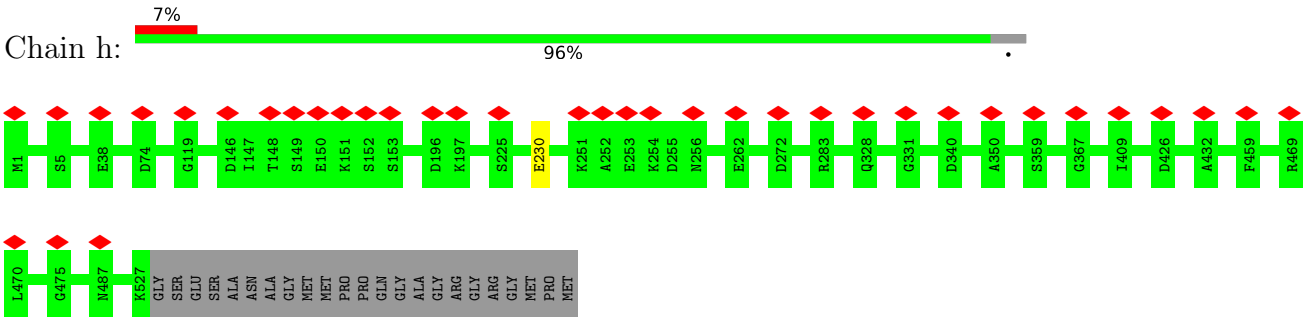
• Molecule 5: fusion protein of T-complex protein 1 subunit gamma,rep-His-CBP and T-complex protein 1 subunit gamma

Chain G:



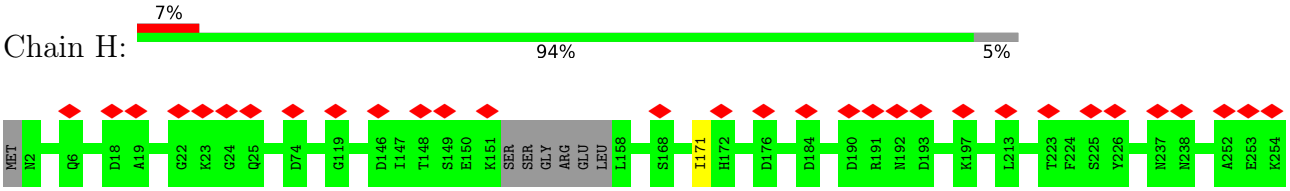
• Molecule 6: T-complex protein 1 subunit eta

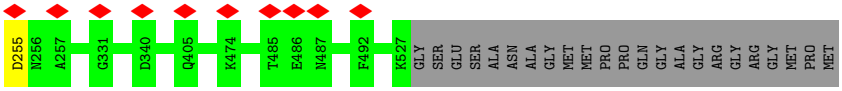
Chain h:



• Molecule 6: T-complex protein 1 subunit eta

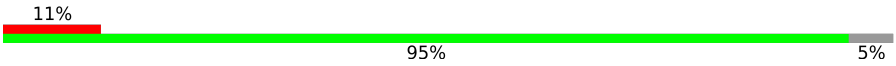
Chain H:

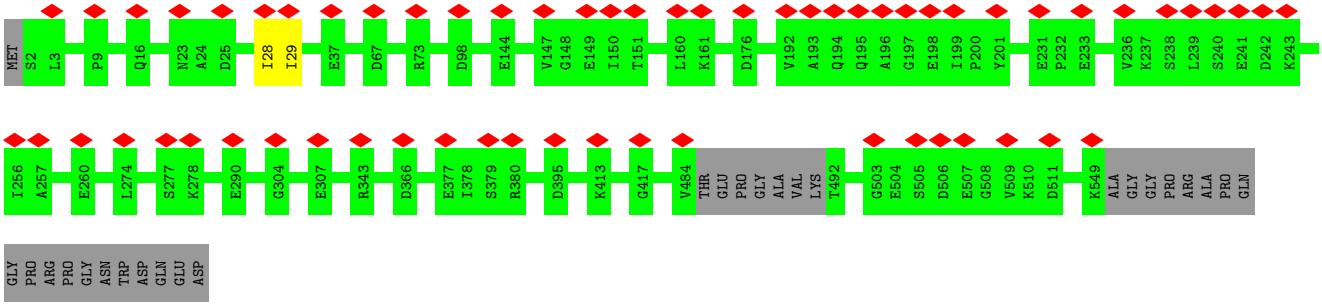




• Molecule 7: T-complex protein 1 subunit theta

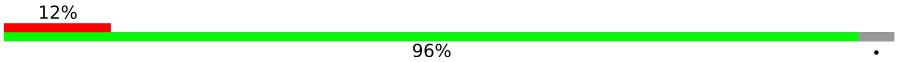
Chain q:

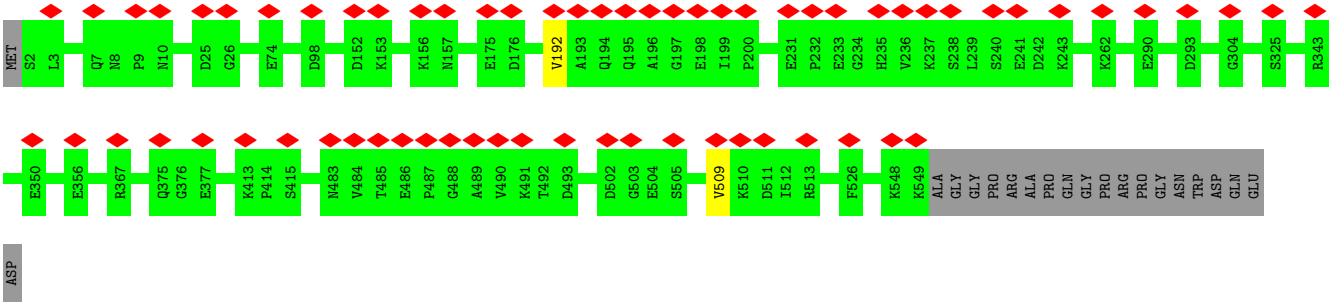




• Molecule 7: T-complex protein 1 subunit theta

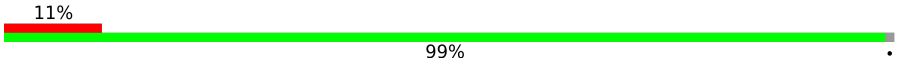
Chain Q:

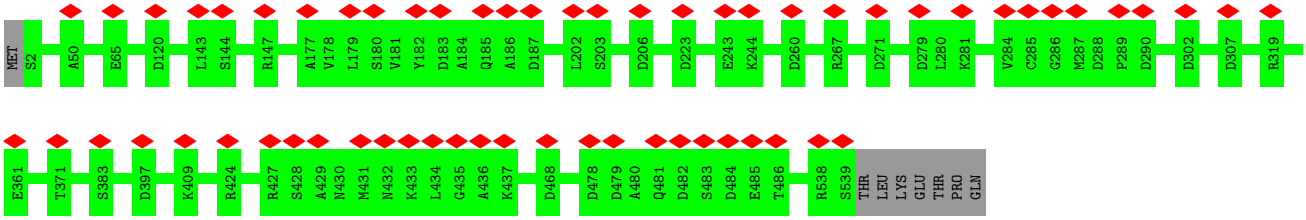




• Molecule 8: T-complex protein 1 subunit zeta

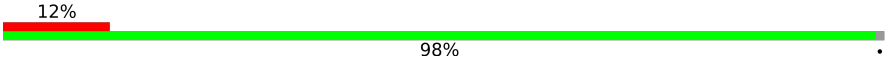
Chain z:

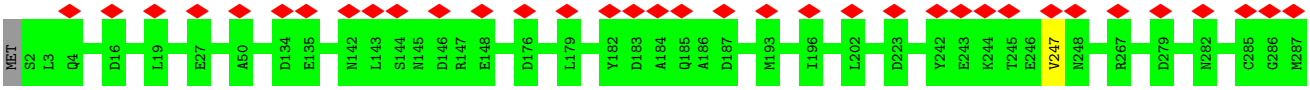


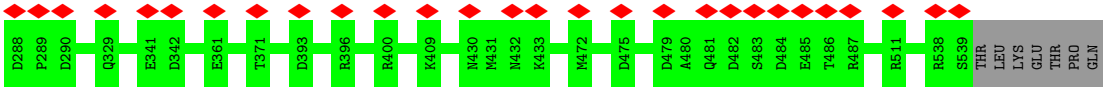


• Molecule 8: T-complex protein 1 subunit zeta

Chain Z:






D288
P289
D290
Q329
E341
D342
E361
T371
D393
R396
R400
K409
N430
M431
N432
K433
M472
D475
D479
A480
Q481
D482
S483
D484
E485
T486
R487
R511
R538
S539
THR
LEU
LYS
GLU
THR
PRO
GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	277360	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	337.408, 337.408, 337.408	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.659, 0.659, 0.659	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: AF3, MG, 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	0.23	0/4196	0.42	0/5661
1	a	0.23	0/4166	0.41	0/5619
2	B	0.23	0/3976	0.39	0/5358
2	b	0.23	0/3976	0.40	0/5358
3	D	0.23	0/4036	0.39	0/5440
3	d	0.23	0/4043	0.40	0/5451
4	E	0.23	0/4184	0.39	0/5629
4	e	0.23	0/4175	0.39	0/5617
5	G	0.23	0/4048	0.40	0/5459
5	g	0.23	0/4047	0.39	0/5460
6	H	0.24	0/4030	0.42	0/5440
6	h	0.23	0/4083	0.40	0/5511
7	Q	0.23	0/4214	0.42	0/5689
7	q	0.23	0/4164	0.41	0/5619
8	Z	0.23	0/4191	0.40	0/5663
8	z	0.23	0/4191	0.39	0/5663
All	All	0.23	0/65720	0.40	0/88637

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 (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	527 (96%)	20 (4%)	1 (0%)	47	82
1	a	542/559 (97%)	510 (94%)	32 (6%)	0	100	100
2	B	516/527 (98%)	501 (97%)	14 (3%)	1 (0%)	47	82
2	b	516/527 (98%)	503 (98%)	13 (2%)	0	100	100
3	D	521/528 (99%)	500 (96%)	20 (4%)	1 (0%)	47	82
3	d	522/528 (99%)	503 (96%)	18 (3%)	1 (0%)	47	82
4	E	534/562 (95%)	514 (96%)	19 (4%)	1 (0%)	47	82
4	e	533/562 (95%)	521 (98%)	12 (2%)	0	100	100
5	G	514/594 (86%)	501 (98%)	13 (2%)	0	100	100
5	g	514/594 (86%)	502 (98%)	11 (2%)	1 (0%)	47	82
6	H	516/550 (94%)	494 (96%)	20 (4%)	2 (0%)	34	72
6	h	525/550 (96%)	506 (96%)	18 (3%)	1 (0%)	47	82
7	Q	546/568 (96%)	516 (94%)	28 (5%)	2 (0%)	34	72
7	q	537/568 (94%)	512 (95%)	23 (4%)	2 (0%)	34	72
8	Z	536/546 (98%)	523 (98%)	12 (2%)	1 (0%)	47	82
8	z	536/546 (98%)	518 (97%)	18 (3%)	0	100	100
All	All	8456/8868 (95%)	8151 (96%)	291 (3%)	14 (0%)	50	82

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	163	VAL
5	g	6	VAL
7	q	29	ILE
6	H	171	ILE
8	Z	247	VAL
1	A	492	VAL

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Mol	Chain	Res	Type
2	B	243	VAL
7	Q	192	VAL
6	H	255	ASP
4	E	262	GLU
6	h	230	GLU
7	q	28	ILE
7	Q	509	VAL
3	d	189	VAL

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%)	462 (100%)	0	100	100
1	a	458/471 (97%)	458 (100%)	0	100	100
2	B	433/441 (98%)	432 (100%)	1 (0%)	93	98
2	b	433/441 (98%)	433 (100%)	0	100	100
3	D	449/453 (99%)	449 (100%)	0	100	100
3	d	450/453 (99%)	450 (100%)	0	100	100
4	E	461/483 (95%)	461 (100%)	0	100	100
4	e	460/483 (95%)	460 (100%)	0	100	100
5	G	443/501 (88%)	443 (100%)	0	100	100
5	g	443/501 (88%)	443 (100%)	0	100	100
6	H	434/454 (96%)	434 (100%)	0	100	100
6	h	440/454 (97%)	440 (100%)	0	100	100
7	Q	458/473 (97%)	458 (100%)	0	100	100
7	q	453/473 (96%)	453 (100%)	0	100	100
8	Z	455/463 (98%)	455 (100%)	0	100	100
8	z	455/463 (98%)	455 (100%)	0	100	100
All	All	7187/7478 (96%)	7186 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	238	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	7	ASN
1	a	64	ASN
1	a	89	GLN
1	a	90	GLN
1	a	430	ASN
1	A	64	ASN
1	A	90	GLN
1	A	261	GLN
1	A	363	GLN
2	b	4	GLN
2	b	144	HIS
2	b	221	ASN
2	b	351	GLN
2	B	118	GLN
2	B	286	ASN
2	B	288	GLN
2	B	351	GLN
3	d	8	ASN
3	d	188	ASN
3	d	303	HIS
3	d	499	GLN
3	D	125	GLN
3	D	240	GLN
3	D	303	HIS
3	D	395	HIS
4	e	41	GLN
4	e	299	GLN
4	e	303	GLN
4	e	353	HIS
4	e	397	GLN
4	E	35	GLN
4	E	42	HIS
4	E	253	GLN
4	E	299	GLN
4	E	353	HIS
4	E	397	GLN

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Mol	Chain	Res	Type
5	g	21	GLN
5	g	325	ASN
5	G	166	HIS
5	G	306	GLN
5	G	465	ASN
6	h	64	ASN
6	h	268	GLN
6	h	305	GLN
6	h	328	GLN
6	h	345	HIS
6	h	356	GLN
6	h	472	HIS
6	h	526	ASN
6	H	6	GLN
6	H	90	GLN
6	H	291	ASN
6	H	345	HIS
6	H	356	GLN
6	H	366	GLN
6	H	384	GLN
6	H	435	GLN
7	Q	154	ASN
7	Q	219	ASN
8	z	69	GLN
8	z	110	GLN
8	z	142	ASN
8	z	192	HIS
8	z	329	GLN
8	z	338	ASN
8	Z	7	ASN
8	Z	329	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	$\#\|Z\| > 2$
11	AF3	a	603	9	0,3,3	-	-	-		
11	AF3	Z	603	9	0,3,3	-	-	-		
9	ADP	A	601	11,10	24,29,29	0.95	1 (4%)	29,45,45	1.41	4 (13%)
11	AF3	G	603	5,9	0,3,3	-	-	-		
11	AF3	E	603	9	0,3,3	-	-	-		
9	ADP	Z	601	11,10	24,29,29	0.96	1 (4%)	29,45,45	1.41	4 (13%)
11	AF3	z	603	9	0,3,3	-	-	-		
9	ADP	G	601	11,10	24,29,29	0.95	1 (4%)	29,45,45	1.44	4 (13%)
11	AF3	e	603	9	0,3,3	-	-	-		
9	ADP	q	601	10	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
9	ADP	d	601	11,10	24,29,29	0.95	1 (4%)	29,45,45	1.41	4 (13%)
11	AF3	h	603	9	0,3,3	-	-	-		
9	ADP	z	601	11,10	24,29,29	0.96	1 (4%)	29,45,45	1.42	4 (13%)
9	ADP	H	601	11,10	24,29,29	0.96	1 (4%)	29,45,45	1.42	4 (13%)
9	ADP	B	601	10	24,29,29	0.95	1 (4%)	29,45,45	1.46	4 (13%)
11	AF3	b	603	9	0,3,3	-	-	-		
9	ADP	h	601	11,10	24,29,29	0.95	1 (4%)	29,45,45	1.38	4 (13%)
9	ADP	e	601	11,10	24,29,29	0.96	1 (4%)	29,45,45	1.37	4 (13%)
9	ADP	b	601	11,10	24,29,29	0.95	1 (4%)	29,45,45	1.40	4 (13%)
11	AF3	H	603	9	0,3,3	-	-	-		
11	AF3	D	603	3,9	0,3,3	-	-	-		
11	AF3	B	603	-	0,3,3	-	-	-		
9	ADP	a	601	11,10	24,29,29	0.95	1 (4%)	29,45,45	1.42	4 (13%)
11	AF3	d	603	9	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	AF3	g	603	-	0,3,3	-	-	-		
9	ADP	g	601	10	24,29,29	0.96	1 (4%)	29,45,45	1.41	4 (13%)
9	ADP	Q	602	10	24,29,29	0.96	1 (4%)	29,45,45	1.48	4 (13%)
9	ADP	D	601	11,10	24,29,29	0.95	1 (4%)	29,45,45	1.52	4 (13%)
9	ADP	E	601	11,10	24,29,29	0.95	1 (4%)	29,45,45	1.39	4 (13%)
11	AF3	A	603	9	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
9	ADP	A	601	11,10	-	2/12/32/32	0/3/3/3
9	ADP	q	601	10	-	2/12/32/32	0/3/3/3
9	ADP	b	601	11,10	-	3/12/32/32	0/3/3/3
9	ADP	d	601	11,10	-	0/12/32/32	0/3/3/3
9	ADP	g	601	10	-	6/12/32/32	0/3/3/3
9	ADP	Q	602	10	-	3/12/32/32	0/3/3/3
9	ADP	G	601	11,10	-	2/12/32/32	0/3/3/3
9	ADP	z	601	11,10	-	2/12/32/32	0/3/3/3
9	ADP	D	601	11,10	-	2/12/32/32	0/3/3/3
9	ADP	H	601	11,10	-	2/12/32/32	0/3/3/3
9	ADP	a	601	11,10	-	3/12/32/32	0/3/3/3
9	ADP	Z	601	11,10	-	2/12/32/32	0/3/3/3
9	ADP	E	601	11,10	-	2/12/32/32	0/3/3/3
9	ADP	B	601	10	-	3/12/32/32	0/3/3/3
9	ADP	h	601	11,10	-	2/12/32/32	0/3/3/3
9	ADP	e	601	11,10	-	1/12/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	601	ADP	C5-C4	2.54	1.47	1.40
9	Q	602	ADP	C5-C4	2.52	1.47	1.40
9	H	601	ADP	C5-C4	2.51	1.47	1.40
9	q	601	ADP	C5-C4	2.51	1.47	1.40
9	E	601	ADP	C5-C4	2.51	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	z	601	ADP	C5-C4	2.51	1.47	1.40
9	g	601	ADP	C5-C4	2.50	1.47	1.40
9	A	601	ADP	C5-C4	2.50	1.47	1.40
9	Z	601	ADP	C5-C4	2.49	1.47	1.40
9	G	601	ADP	C5-C4	2.49	1.47	1.40
9	b	601	ADP	C5-C4	2.49	1.47	1.40
9	d	601	ADP	C5-C4	2.49	1.47	1.40
9	e	601	ADP	C5-C4	2.49	1.47	1.40
9	B	601	ADP	C5-C4	2.48	1.47	1.40
9	h	601	ADP	C5-C4	2.48	1.47	1.40
9	a	601	ADP	C5-C4	2.48	1.47	1.40

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	601	ADP	PA-O3A-PB	-3.92	119.38	132.83
9	Q	602	ADP	PA-O3A-PB	-3.79	119.82	132.83
9	B	601	ADP	PA-O3A-PB	-3.58	120.54	132.83
9	q	601	ADP	PA-O3A-PB	-3.47	120.93	132.83
9	G	601	ADP	PA-O3A-PB	-3.42	121.10	132.83
9	D	601	ADP	C3'-C2'-C1'	3.35	106.03	100.98
9	z	601	ADP	PA-O3A-PB	-3.34	121.38	132.83
9	E	601	ADP	C3'-C2'-C1'	3.31	105.97	100.98
9	G	601	ADP	C3'-C2'-C1'	3.30	105.95	100.98
9	a	601	ADP	C3'-C2'-C1'	3.27	105.91	100.98
9	a	601	ADP	PA-O3A-PB	-3.25	121.67	132.83
9	e	601	ADP	C3'-C2'-C1'	3.25	105.87	100.98
9	Z	601	ADP	PA-O3A-PB	-3.25	121.69	132.83
9	h	601	ADP	C3'-C2'-C1'	3.24	105.86	100.98
9	H	601	ADP	PA-O3A-PB	-3.23	121.73	132.83
9	g	601	ADP	C3'-C2'-C1'	3.23	105.83	100.98
9	A	601	ADP	C3'-C2'-C1'	3.22	105.83	100.98
9	Q	602	ADP	C3'-C2'-C1'	3.22	105.83	100.98
9	B	601	ADP	C3'-C2'-C1'	3.22	105.83	100.98
9	Z	601	ADP	N3-C2-N1	-3.21	123.65	128.68
9	d	601	ADP	N3-C2-N1	-3.21	123.66	128.68
9	H	601	ADP	C3'-C2'-C1'	3.20	105.80	100.98
9	q	601	ADP	N3-C2-N1	-3.20	123.67	128.68
9	G	601	ADP	N3-C2-N1	-3.20	123.68	128.68
9	b	601	ADP	N3-C2-N1	-3.20	123.68	128.68
9	H	601	ADP	N3-C2-N1	-3.19	123.69	128.68
9	d	601	ADP	PA-O3A-PB	-3.19	121.88	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	z	601	ADP	C3'-C2'-C1'	3.19	105.78	100.98
9	e	601	ADP	N3-C2-N1	-3.19	123.69	128.68
9	h	601	ADP	N3-C2-N1	-3.19	123.70	128.68
9	z	601	ADP	N3-C2-N1	-3.19	123.70	128.68
9	b	601	ADP	C3'-C2'-C1'	3.18	105.76	100.98
9	A	601	ADP	N3-C2-N1	-3.18	123.71	128.68
9	a	601	ADP	N3-C2-N1	-3.18	123.72	128.68
9	E	601	ADP	N3-C2-N1	-3.18	123.72	128.68
9	Q	602	ADP	N3-C2-N1	-3.17	123.72	128.68
9	B	601	ADP	N3-C2-N1	-3.16	123.73	128.68
9	g	601	ADP	N3-C2-N1	-3.16	123.73	128.68
9	A	601	ADP	PA-O3A-PB	-3.16	121.98	132.83
9	g	601	ADP	PA-O3A-PB	-3.15	122.03	132.83
9	D	601	ADP	N3-C2-N1	-3.14	123.77	128.68
9	Z	601	ADP	C3'-C2'-C1'	3.13	105.69	100.98
9	b	601	ADP	PA-O3A-PB	-3.08	122.25	132.83
9	q	601	ADP	C3'-C2'-C1'	3.07	105.60	100.98
9	d	601	ADP	C3'-C2'-C1'	3.04	105.55	100.98
9	Q	602	ADP	C4-C5-N7	-2.74	106.54	109.40
9	E	601	ADP	PA-O3A-PB	-2.74	123.43	132.83
9	Z	601	ADP	C4-C5-N7	-2.73	106.55	109.40
9	z	601	ADP	C4-C5-N7	-2.73	106.56	109.40
9	b	601	ADP	C4-C5-N7	-2.72	106.56	109.40
9	A	601	ADP	C4-C5-N7	-2.71	106.58	109.40
9	h	601	ADP	C4-C5-N7	-2.70	106.58	109.40
9	E	601	ADP	C4-C5-N7	-2.70	106.59	109.40
9	q	601	ADP	C4-C5-N7	-2.70	106.59	109.40
9	H	601	ADP	C4-C5-N7	-2.70	106.59	109.40
9	B	601	ADP	C4-C5-N7	-2.68	106.61	109.40
9	h	601	ADP	PA-O3A-PB	-2.67	123.66	132.83
9	e	601	ADP	C4-C5-N7	-2.67	106.62	109.40
9	a	601	ADP	C4-C5-N7	-2.65	106.64	109.40
9	d	601	ADP	C4-C5-N7	-2.65	106.64	109.40
9	g	601	ADP	C4-C5-N7	-2.64	106.64	109.40
9	G	601	ADP	C4-C5-N7	-2.64	106.65	109.40
9	D	601	ADP	C4-C5-N7	-2.64	106.65	109.40
9	e	601	ADP	PA-O3A-PB	-2.60	123.89	132.83

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	b	601	ADP	C5'-O5'-PA-O1A
9	g	601	ADP	PB-O3A-PA-O5'
9	g	601	ADP	C5'-O5'-PA-O2A
9	h	601	ADP	C5'-O5'-PA-O1A
9	q	601	ADP	C5'-O5'-PA-O1A
9	Q	602	ADP	C5'-O5'-PA-O3A
9	g	601	ADP	O4'-C4'-C5'-O5'
9	g	601	ADP	C3'-C4'-C5'-O5'
9	e	601	ADP	PB-O3A-PA-O5'
9	E	601	ADP	PB-O3A-PA-O5'
9	B	601	ADP	O4'-C4'-C5'-O5'
9	b	601	ADP	C5'-O5'-PA-O3A
9	g	601	ADP	C5'-O5'-PA-O3A
9	h	601	ADP	C5'-O5'-PA-O3A
9	A	601	ADP	PB-O3A-PA-O1A
9	g	601	ADP	C5'-O5'-PA-O1A
9	Q	602	ADP	C5'-O5'-PA-O1A
9	A	601	ADP	PB-O3A-PA-O2A
9	G	601	ADP	PB-O3A-PA-O2A
9	H	601	ADP	PB-O3A-PA-O1A
9	H	601	ADP	PB-O3A-PA-O2A
9	z	601	ADP	PB-O3A-PA-O1A
9	z	601	ADP	PB-O3A-PA-O2A
9	Z	601	ADP	PB-O3A-PA-O1A
9	Z	601	ADP	PB-O3A-PA-O2A
9	Q	602	ADP	O4'-C4'-C5'-O5'
9	G	601	ADP	PB-O3A-PA-O1A
9	E	601	ADP	C5'-O5'-PA-O3A
9	B	601	ADP	C3'-C4'-C5'-O5'
9	D	601	ADP	O4'-C4'-C5'-O5'
9	q	601	ADP	O4'-C4'-C5'-O5'
9	a	601	ADP	PB-O3A-PA-O1A
9	a	601	ADP	PB-O3A-PA-O2A
9	b	601	ADP	PB-O3A-PA-O2A
9	a	601	ADP	C5'-O5'-PA-O1A
9	B	601	ADP	C5'-O5'-PA-O1A
9	D	601	ADP	C5'-O5'-PA-O1A

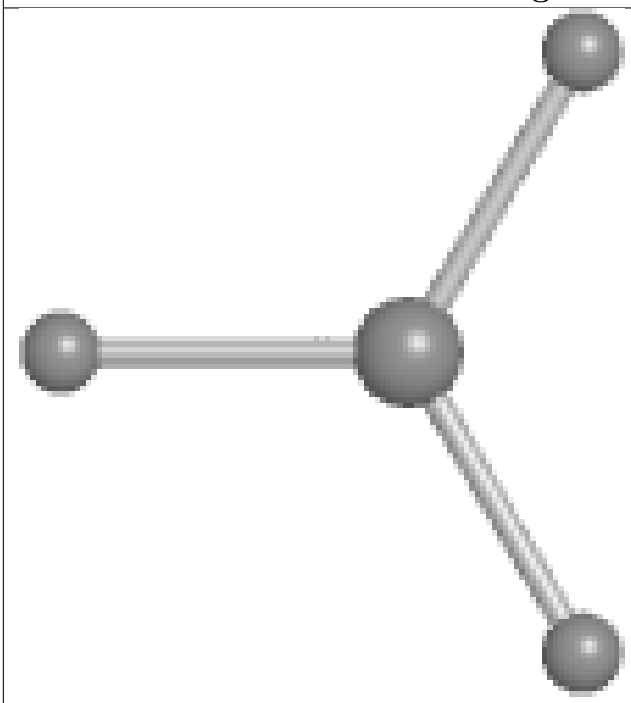
There are no ring outliers.

No monomer is involved in short contacts.

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 AF3 a 603



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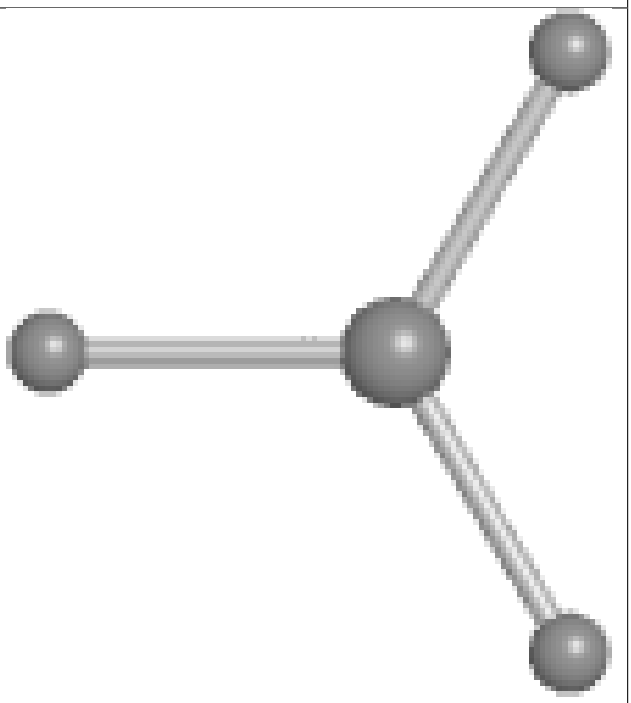

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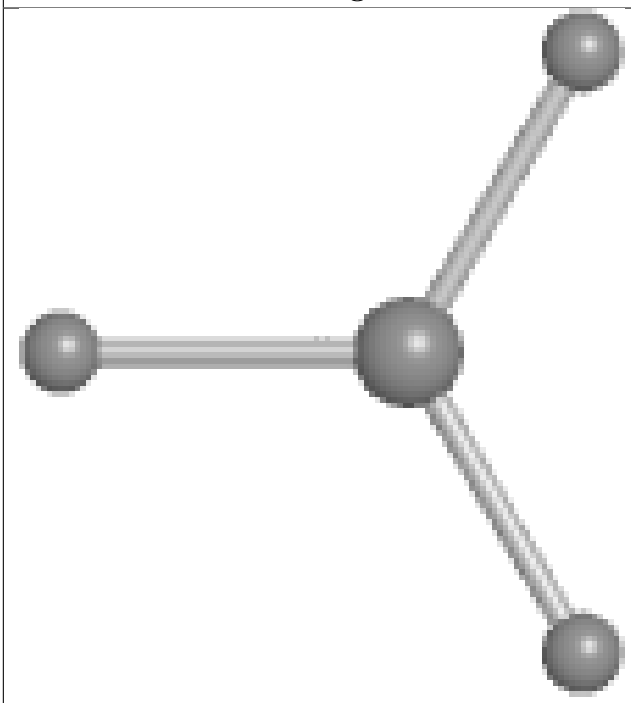

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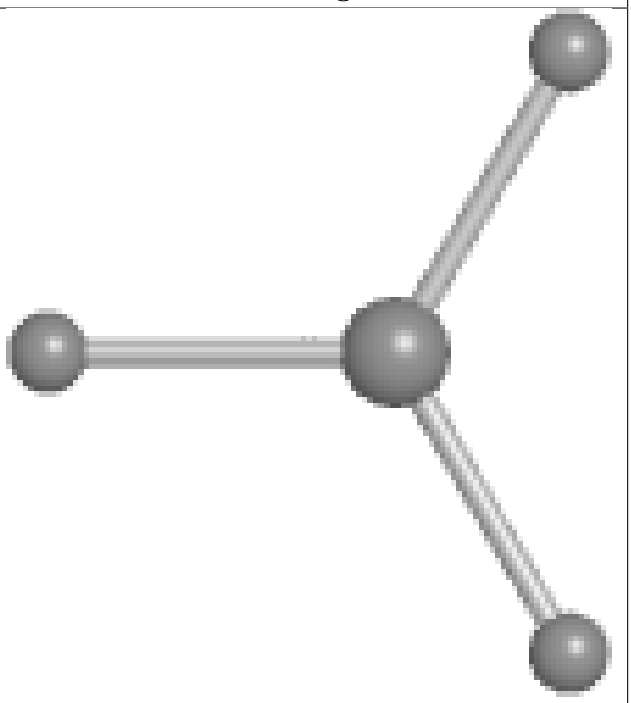
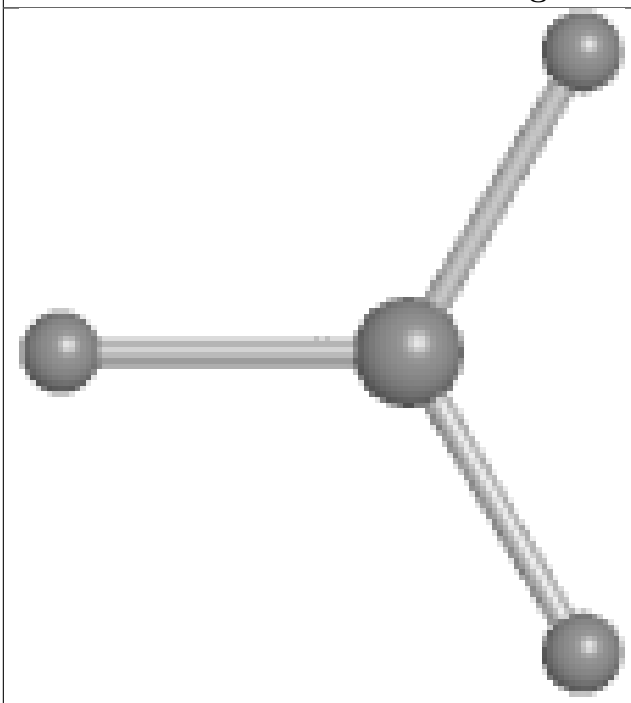


Rings

Ligand AF3 Z 603



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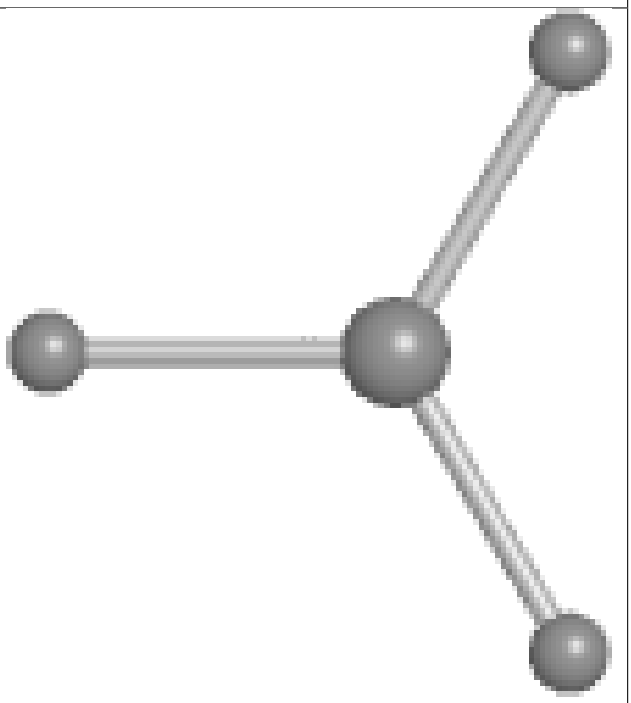

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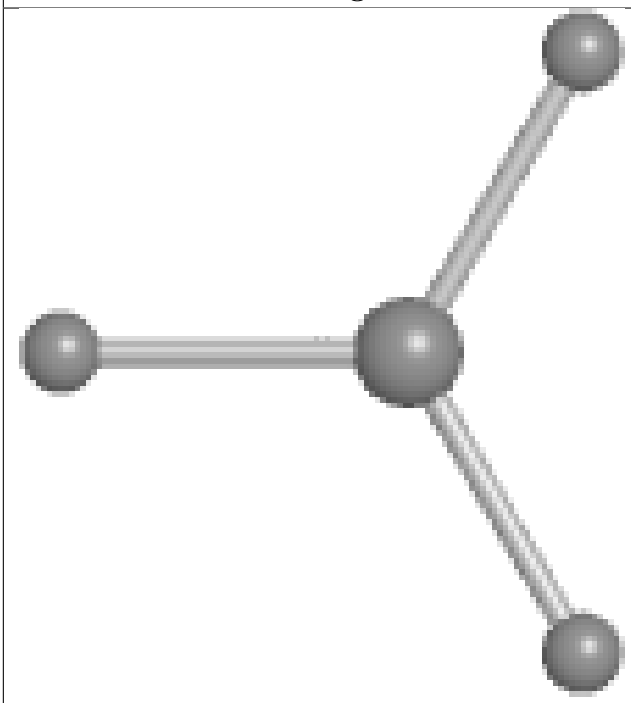

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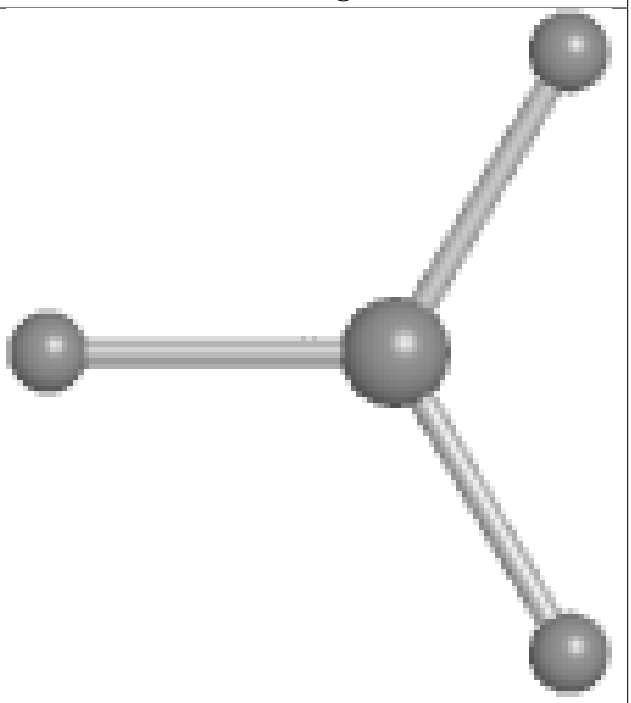

Rings

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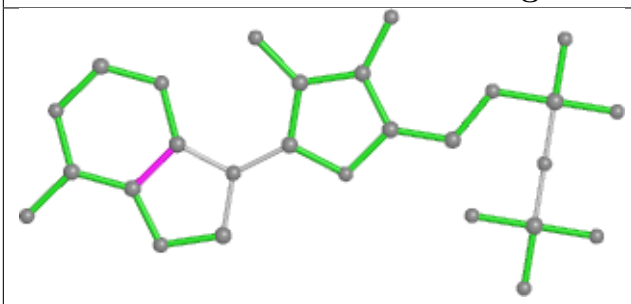
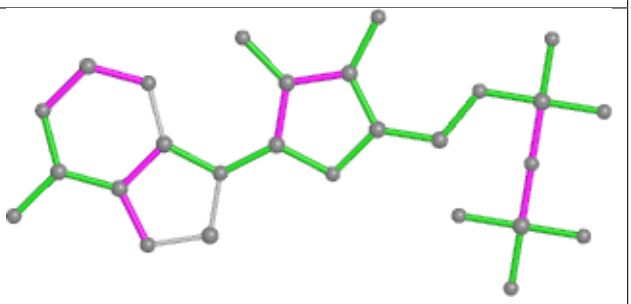
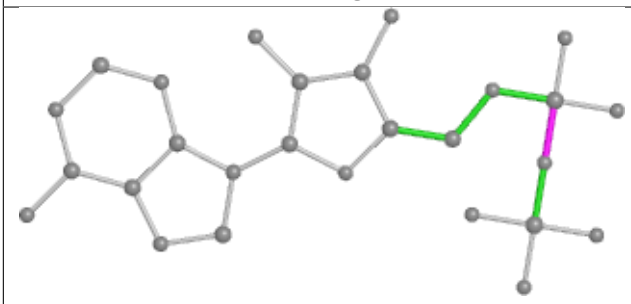
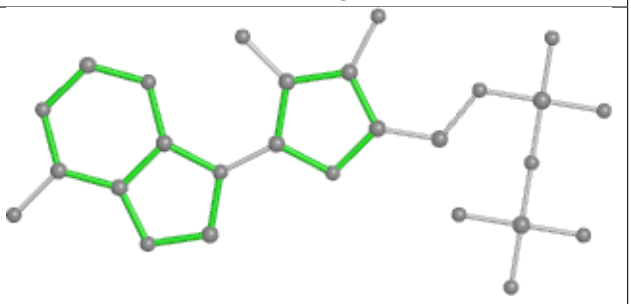
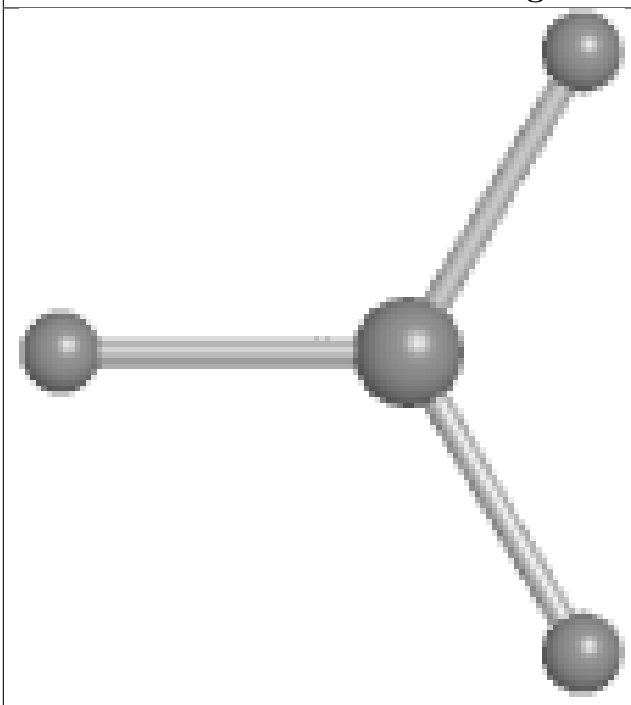
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AF3 G 603



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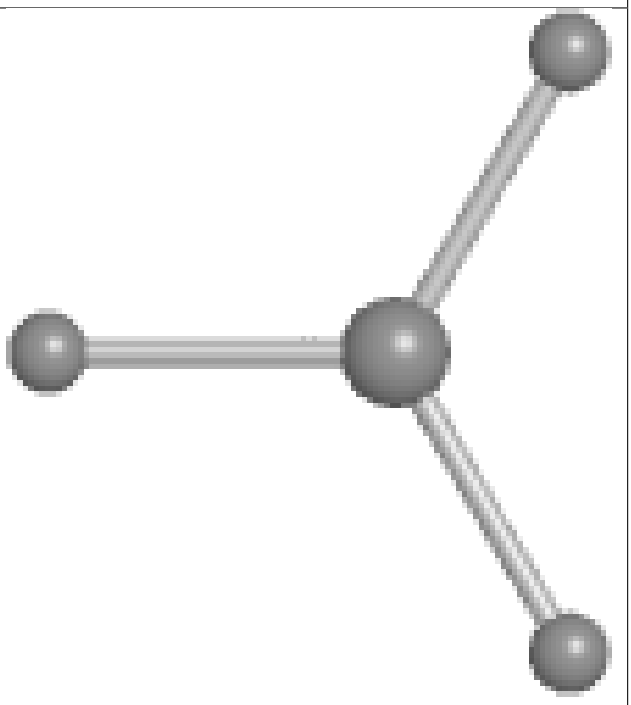

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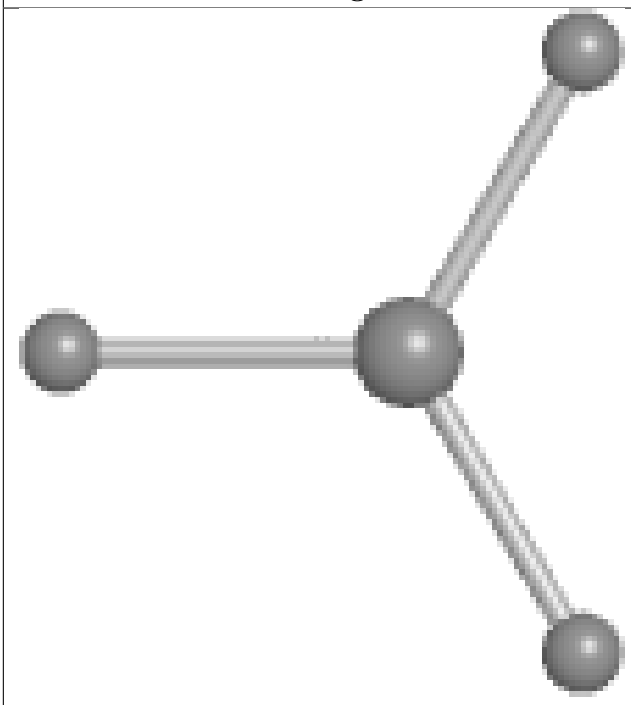

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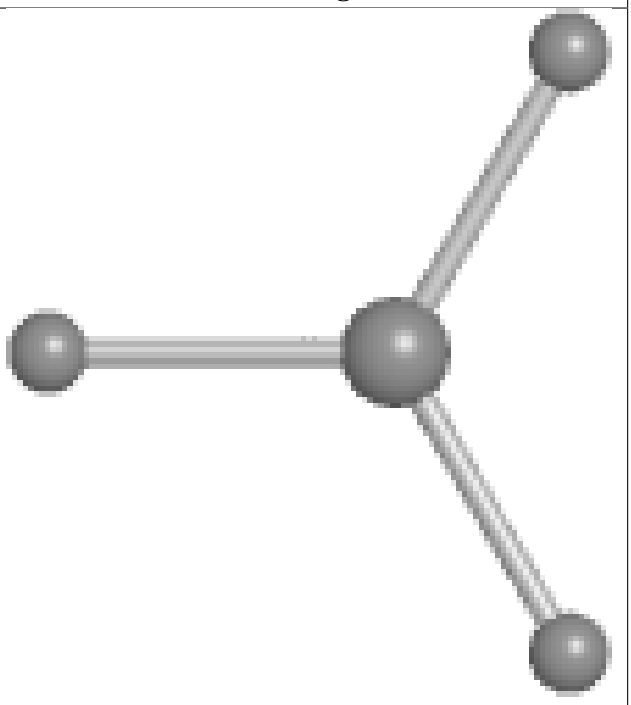
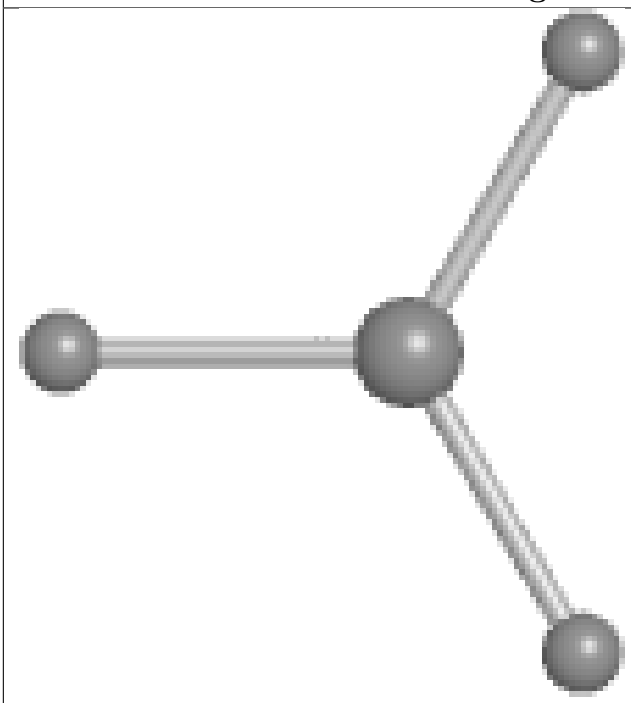


Rings

Ligand AF3 E 603



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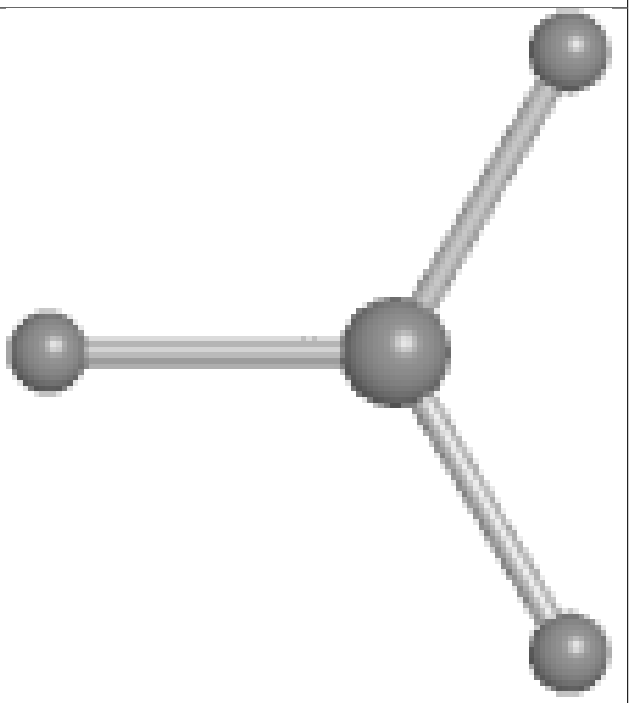

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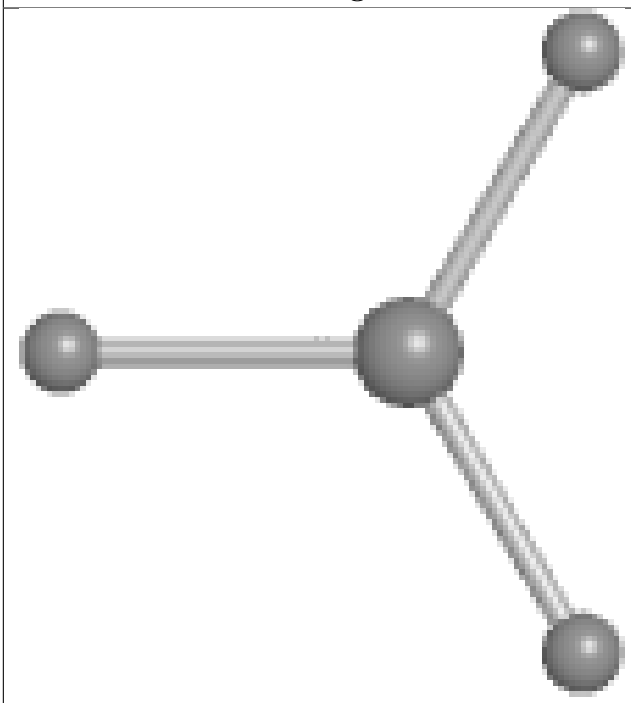

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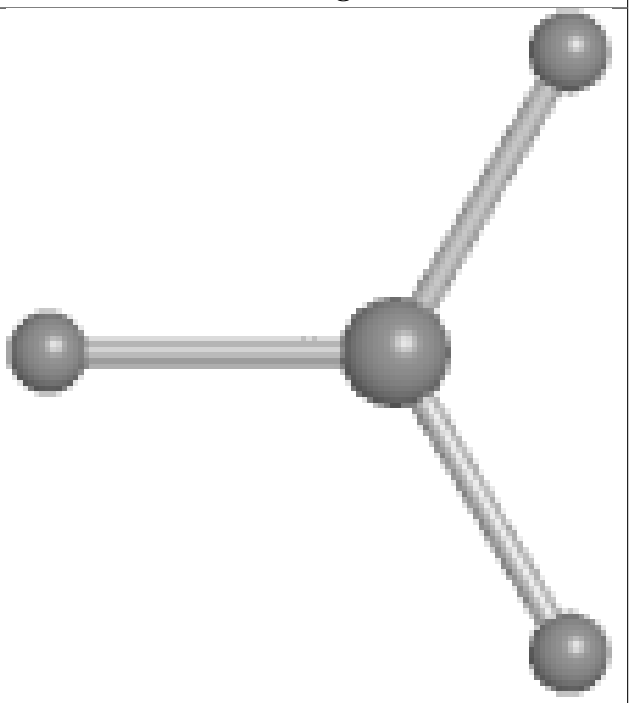
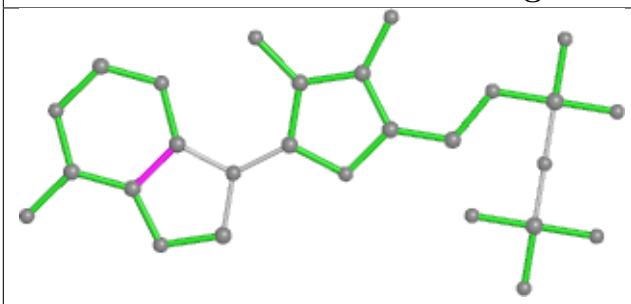
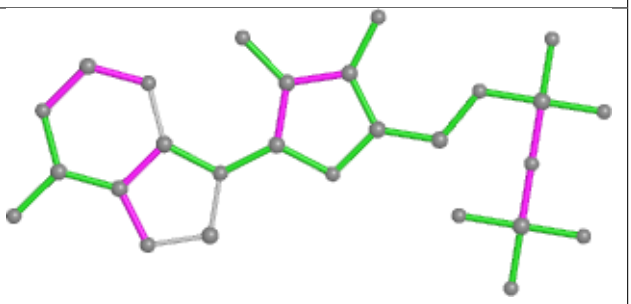
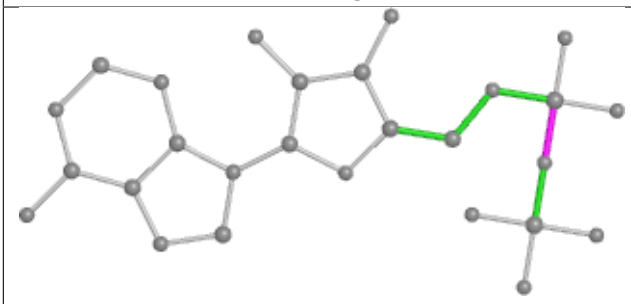
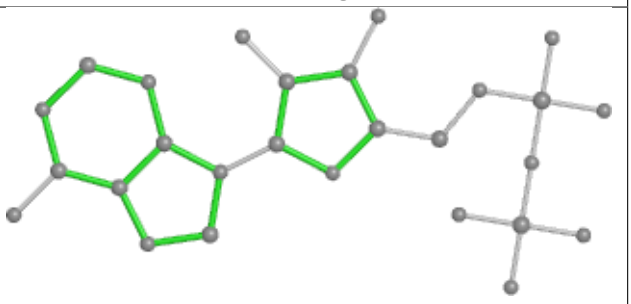
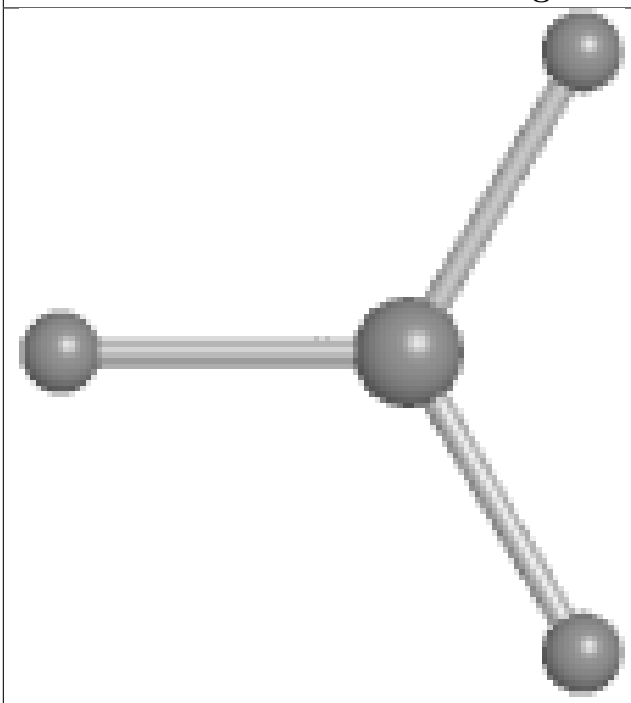


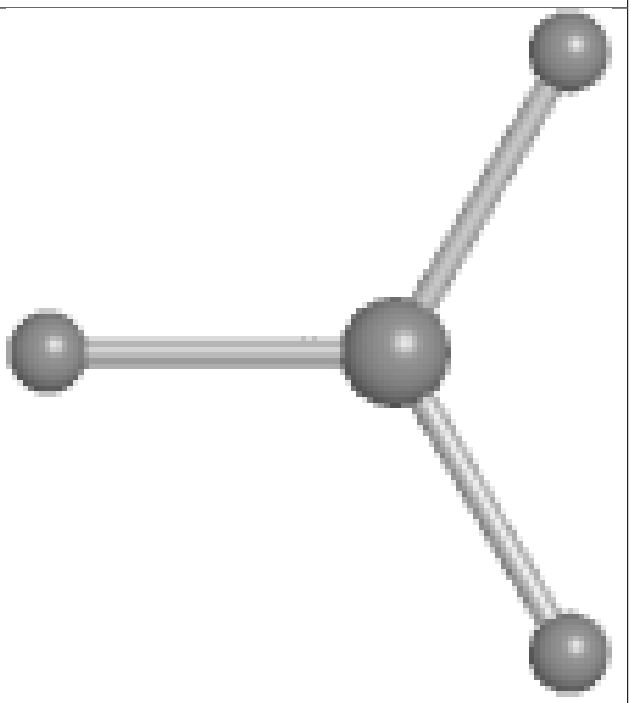
Rings

Ligand ADP Z 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

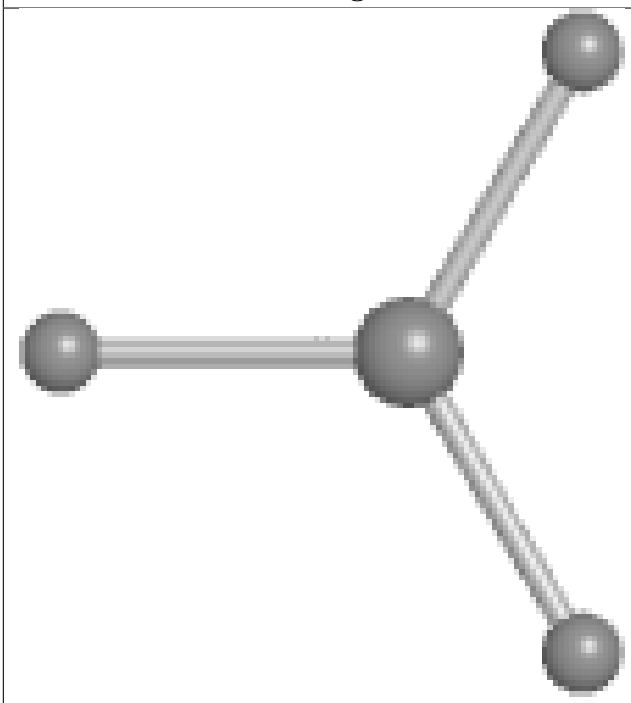
Ligand AF3 z 603



Bond lengths



Bond angles



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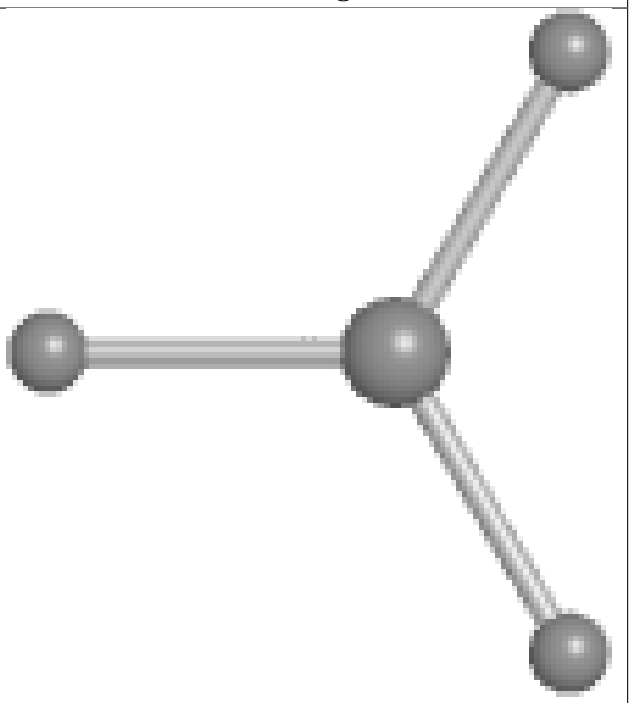
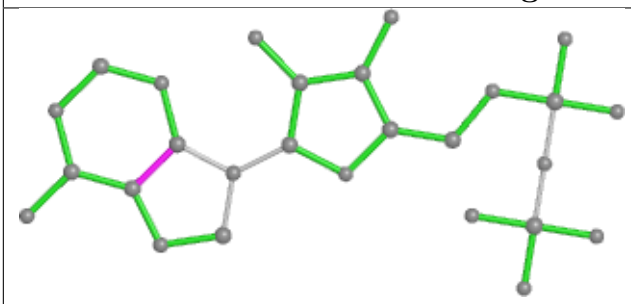
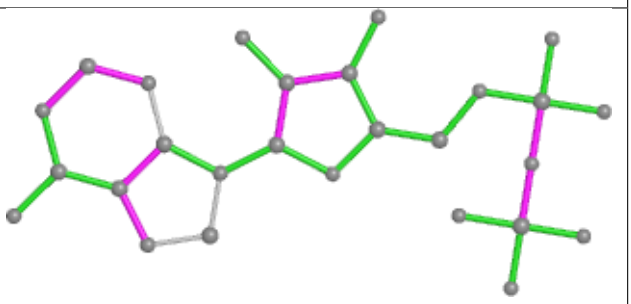
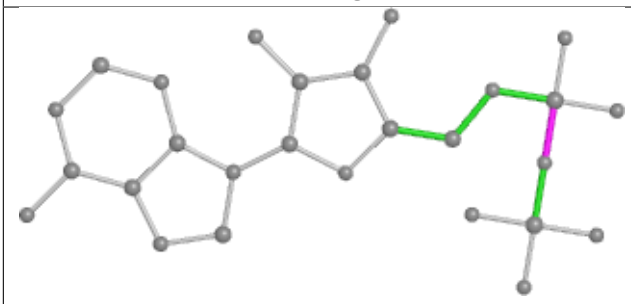
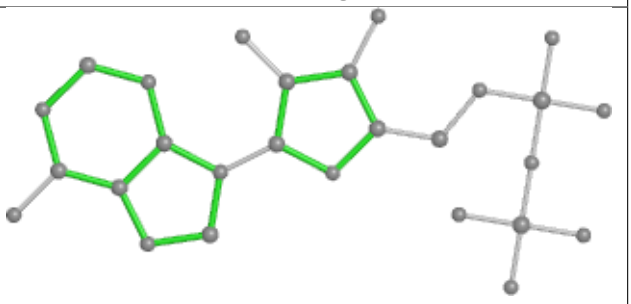
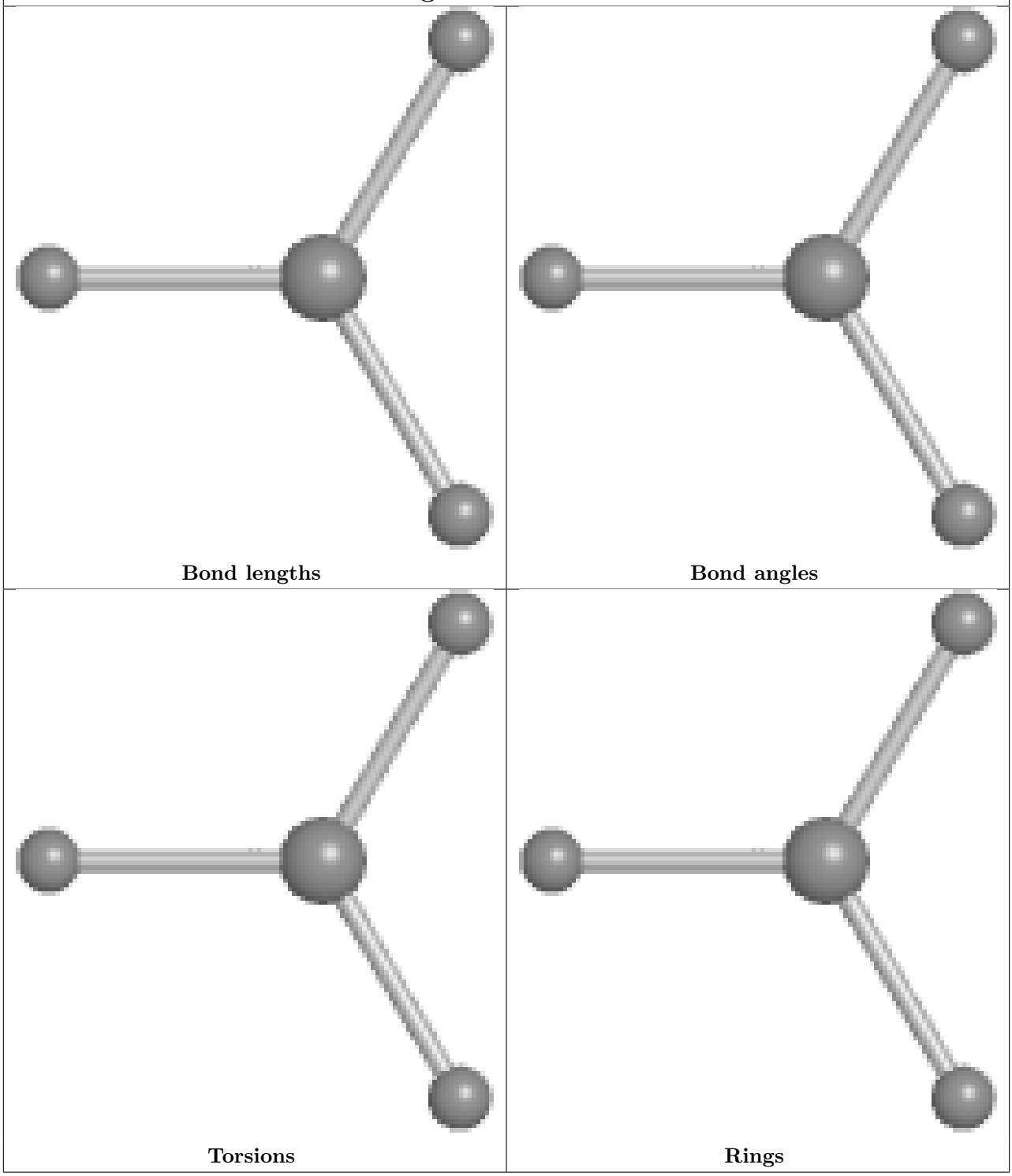


Rings

Ligand ADP G 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AF3 e 603



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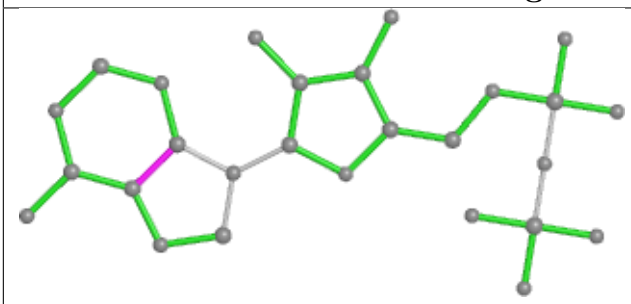
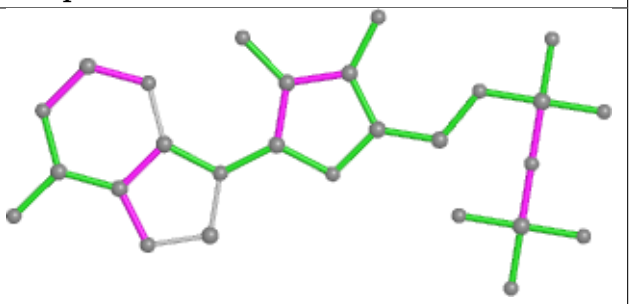
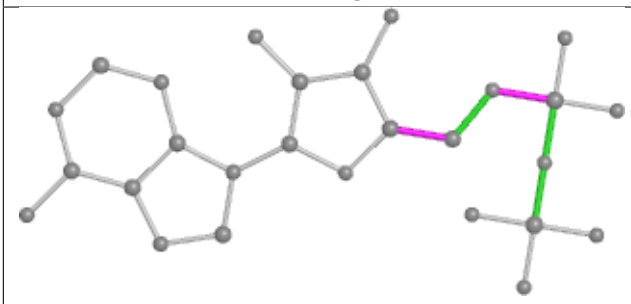
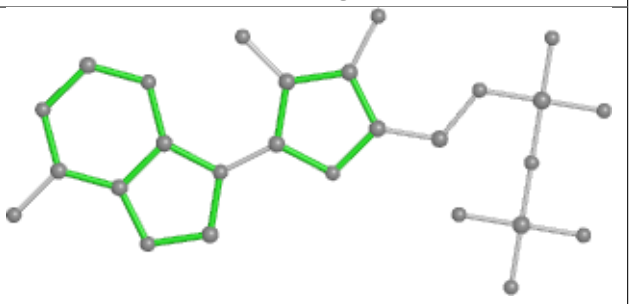
 Bond lengths	 Bond angles
 Torsions	 Rings

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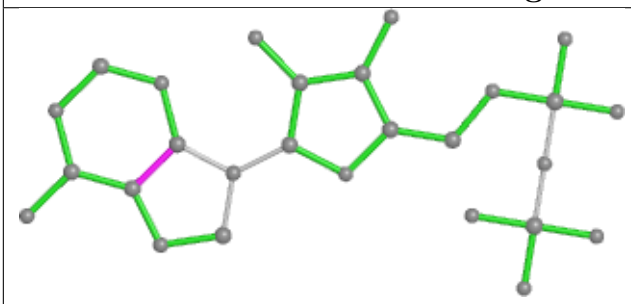
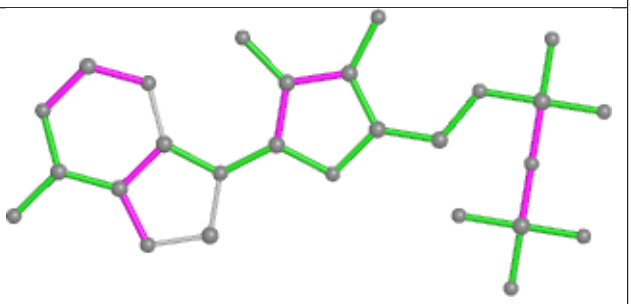
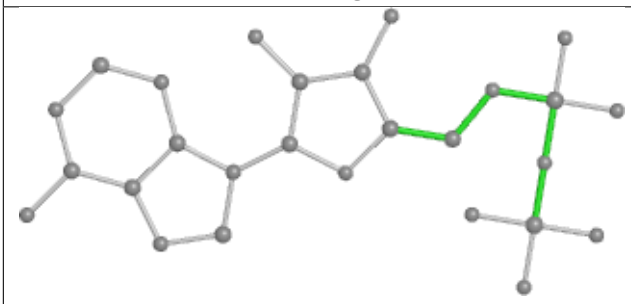
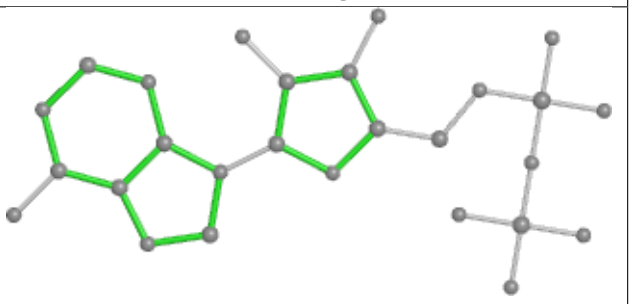
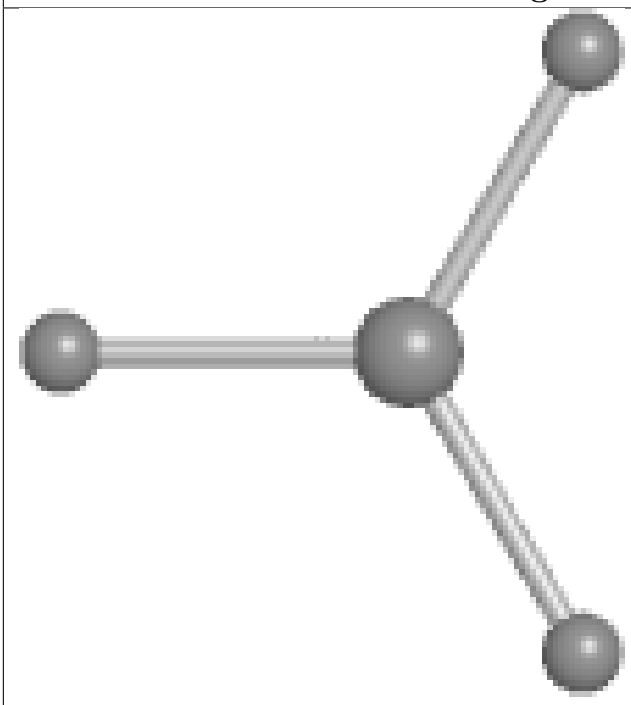
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AF3 h 603



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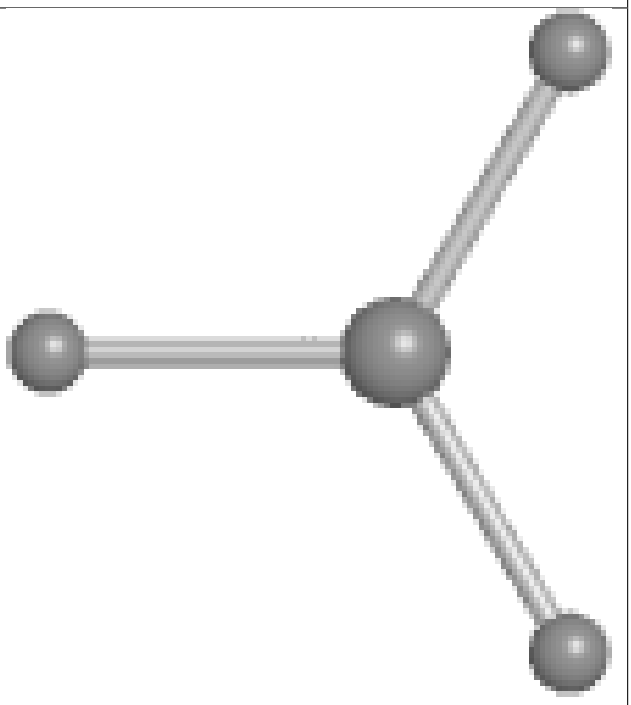

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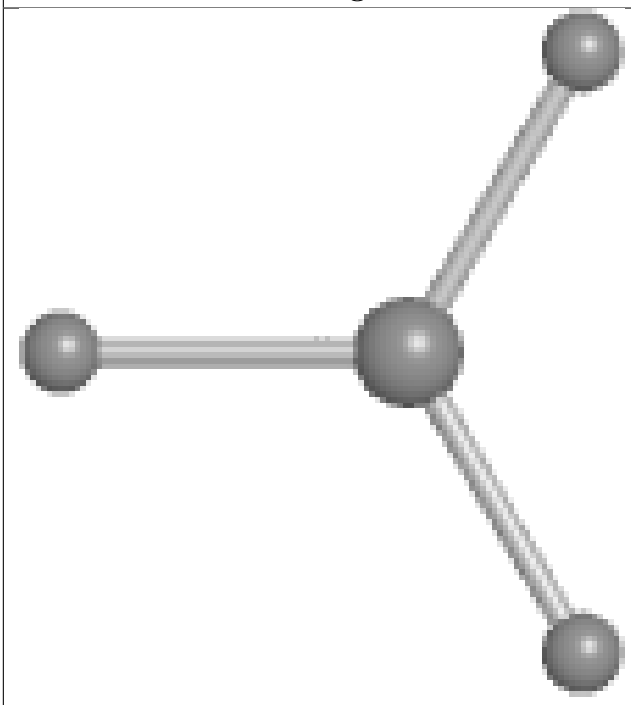

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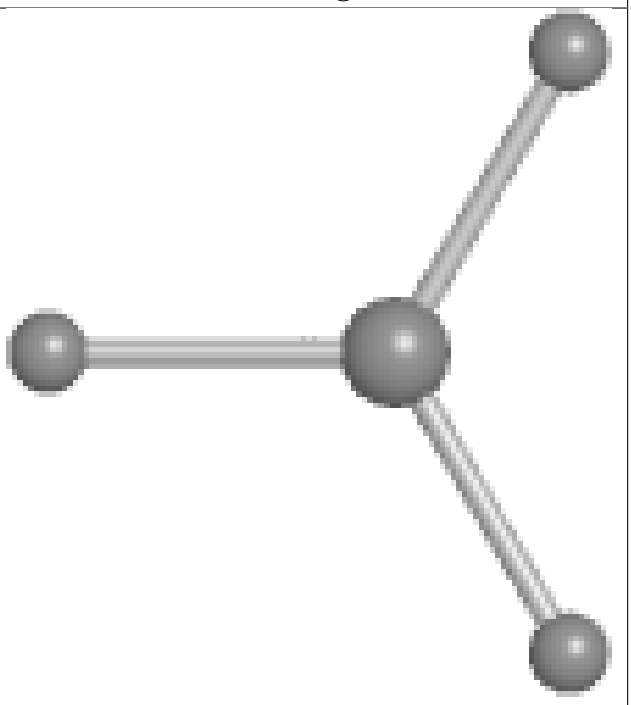
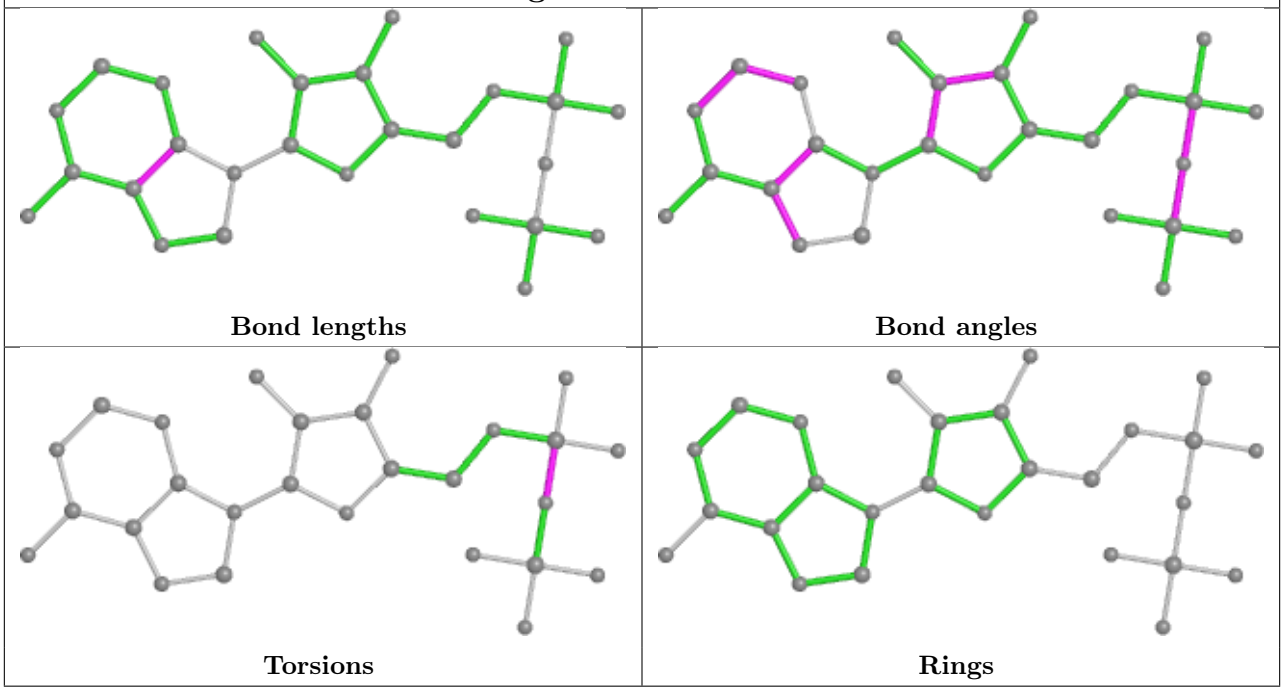


Rings

Ligand ADP z 601



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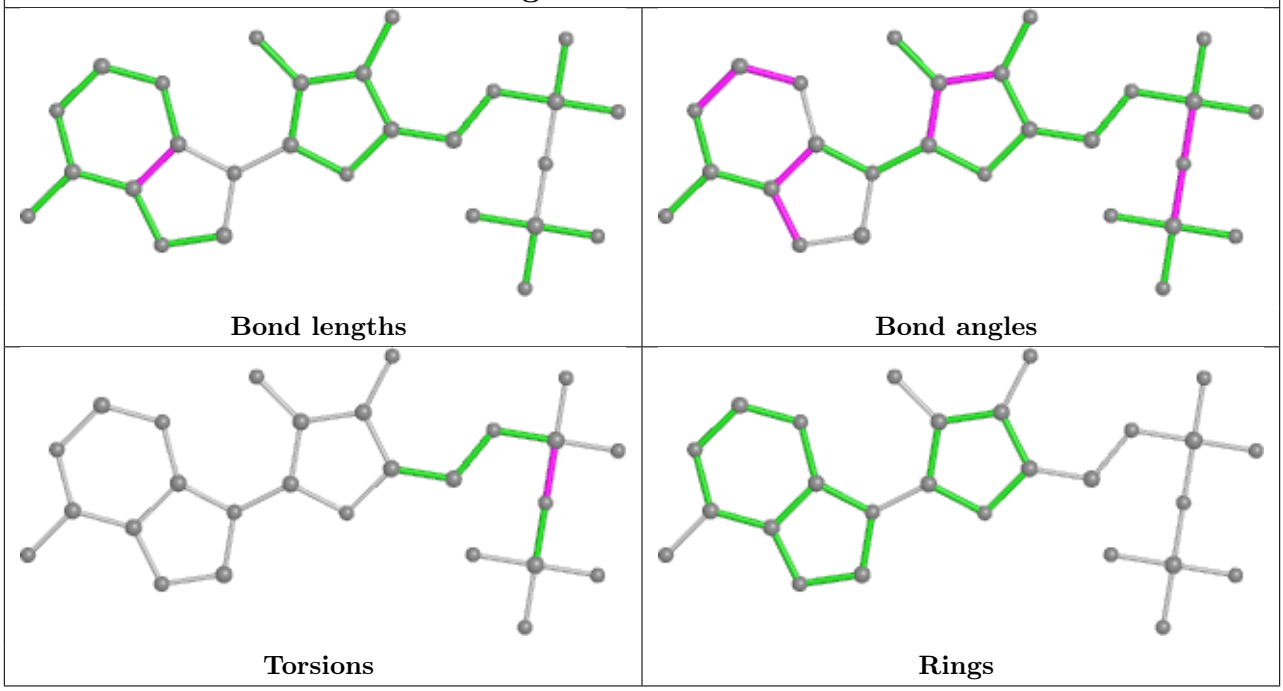

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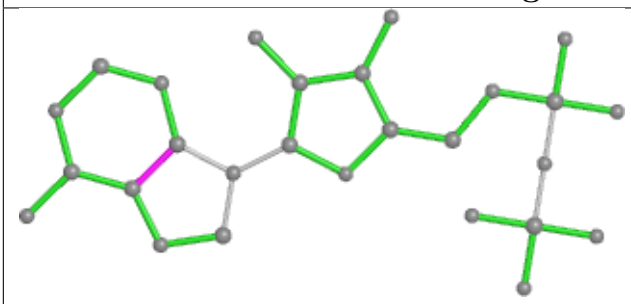
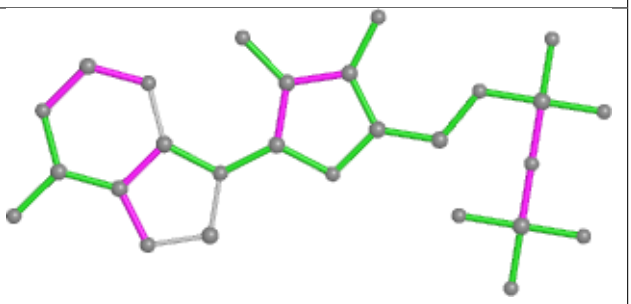
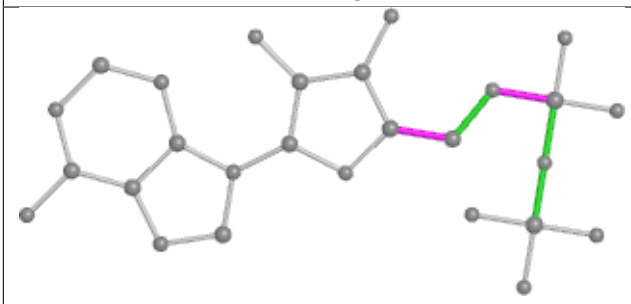
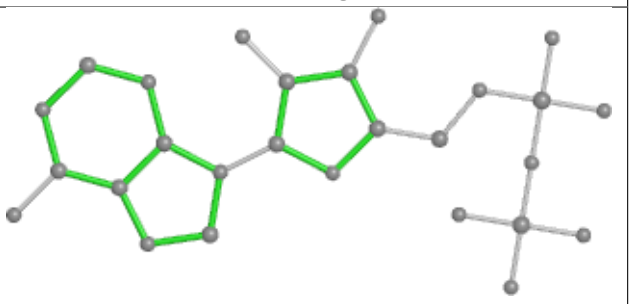
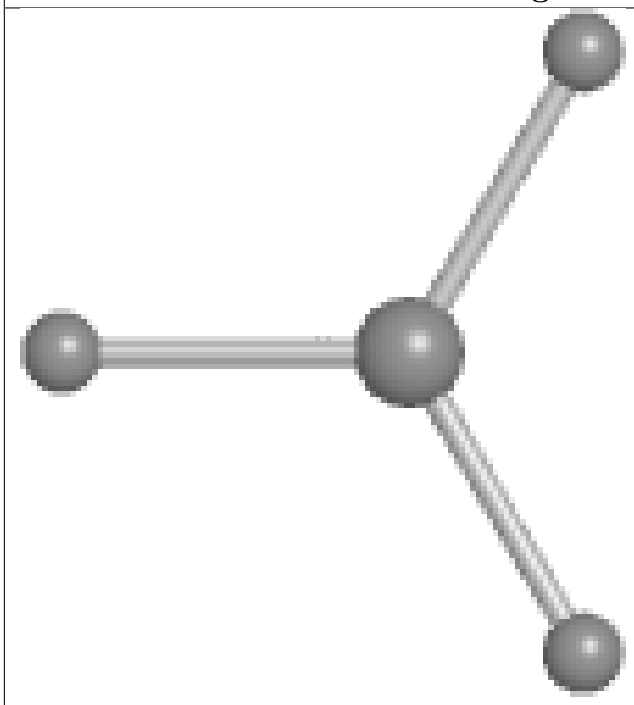
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AF3 b 603



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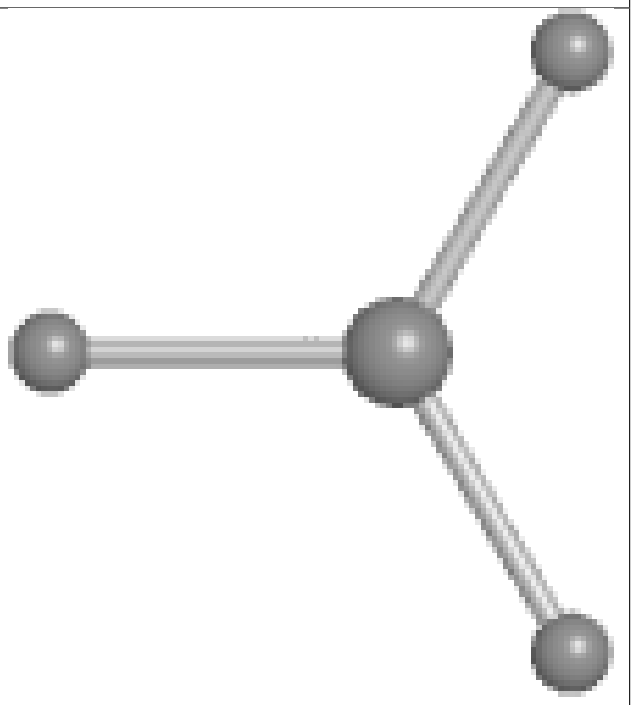
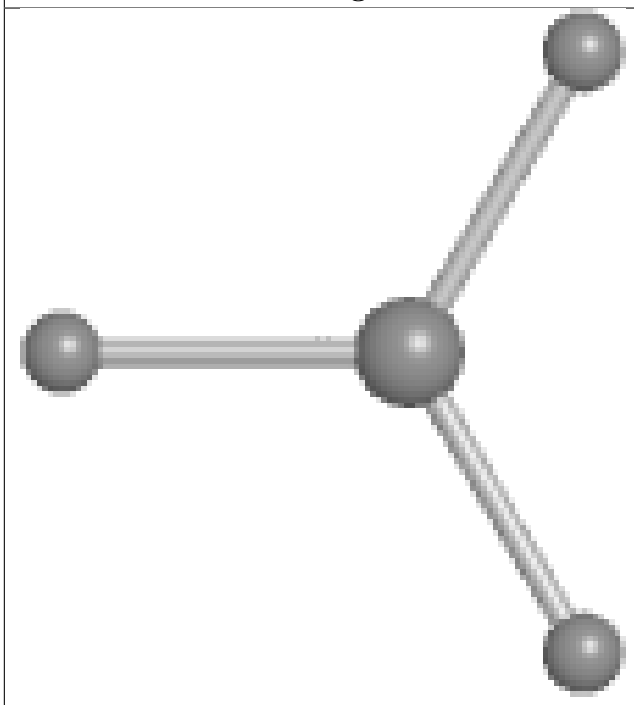


Bond angles



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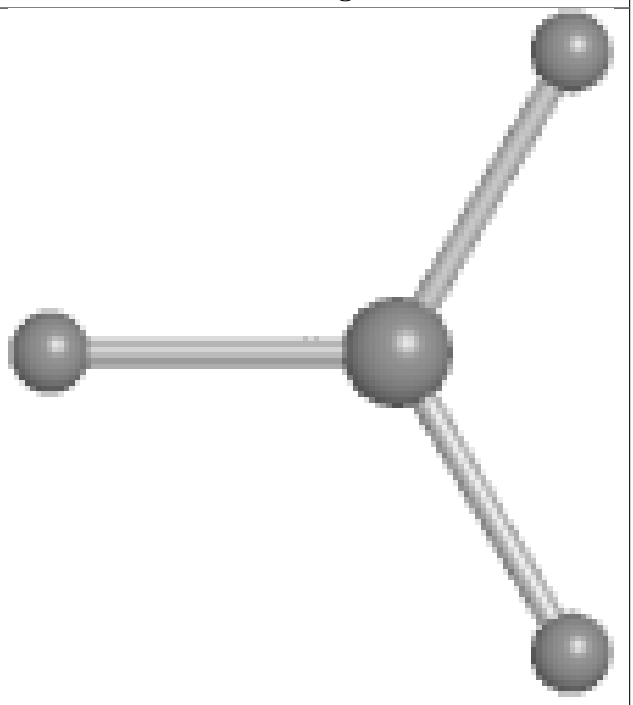
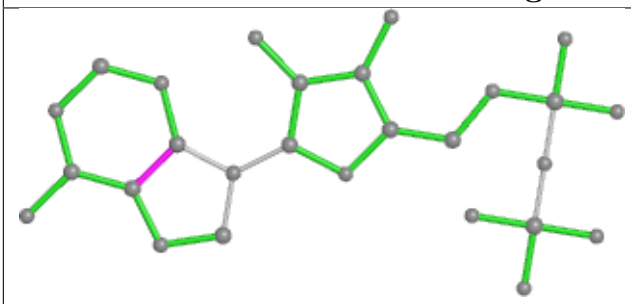


Rings

Ligand ADP h 601



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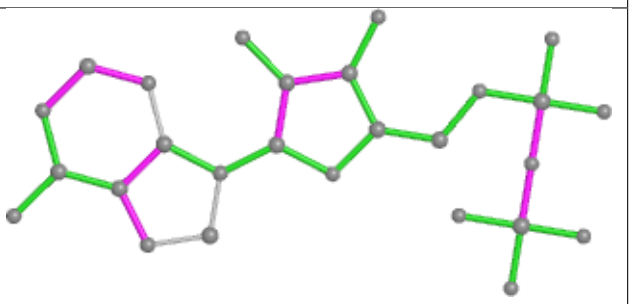

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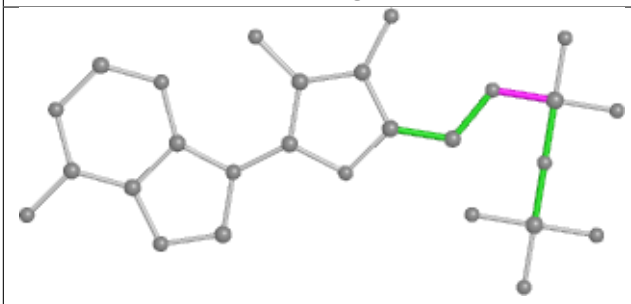

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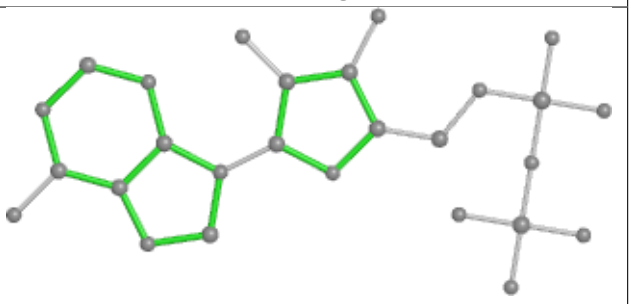
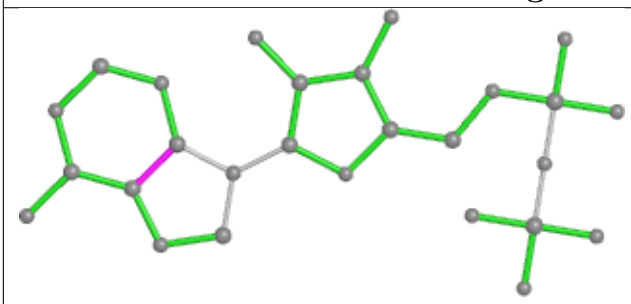


Rings

Ligand ADP e 601



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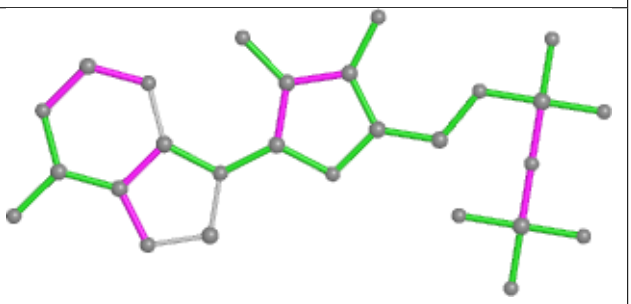

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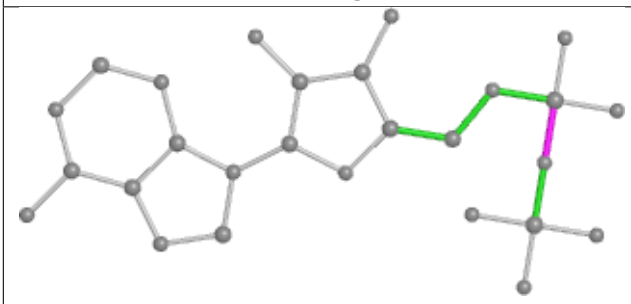

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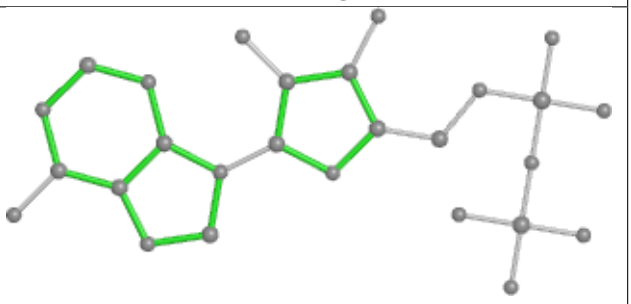

Rings

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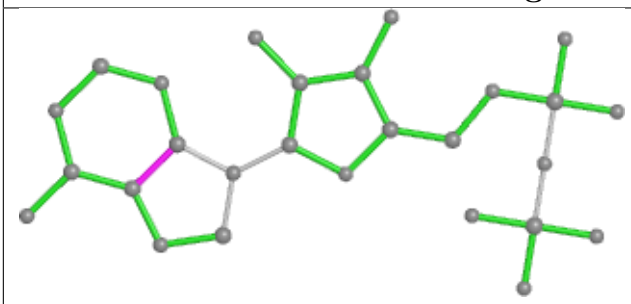
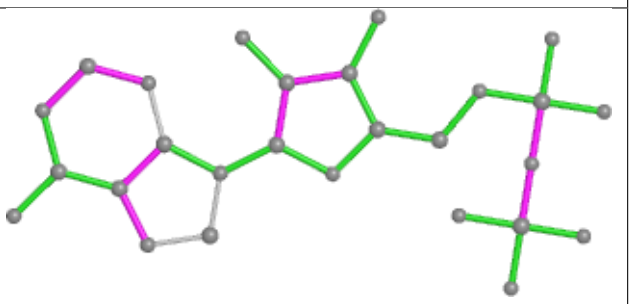
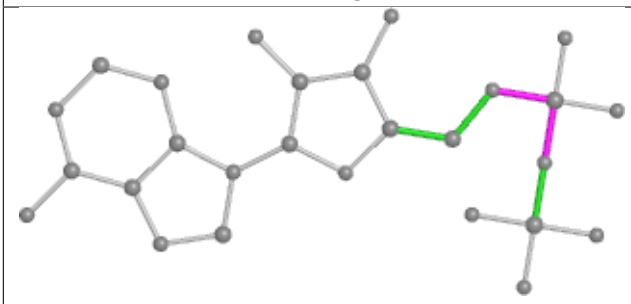
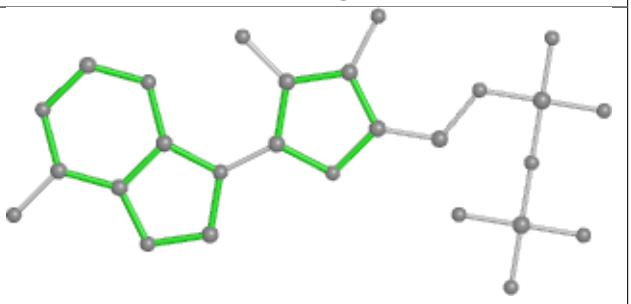
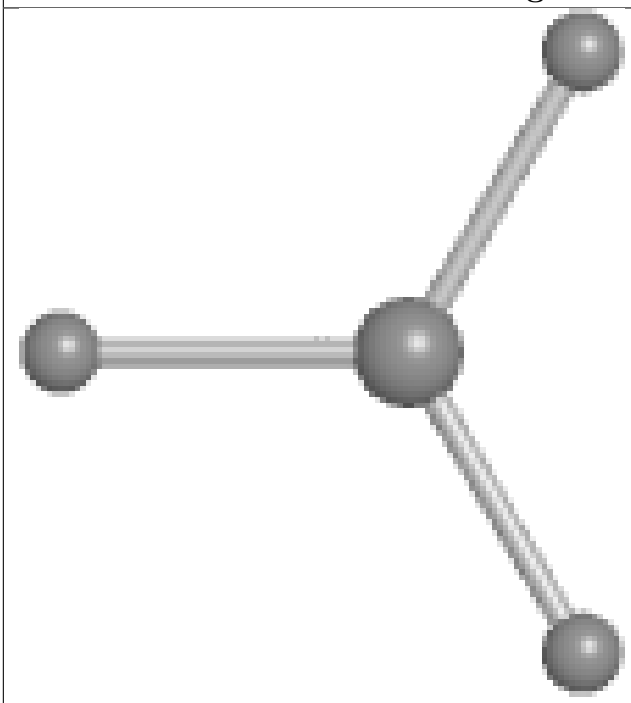
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AF3 H 603



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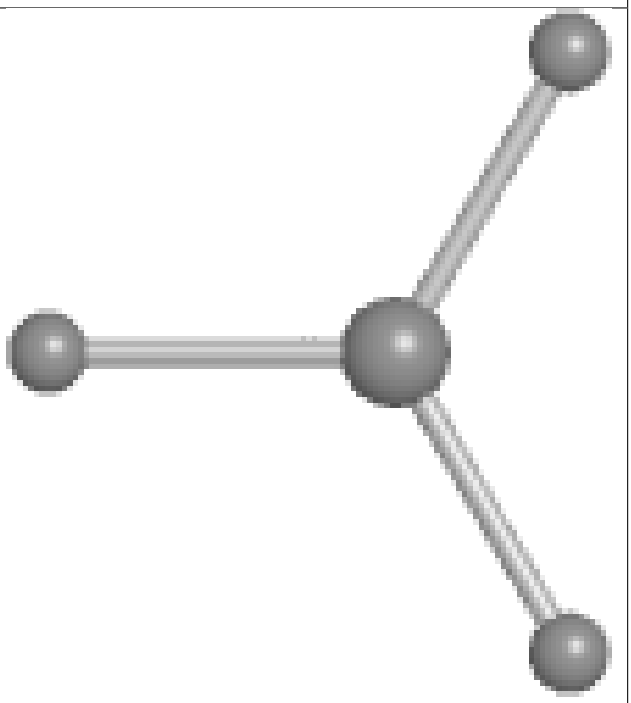

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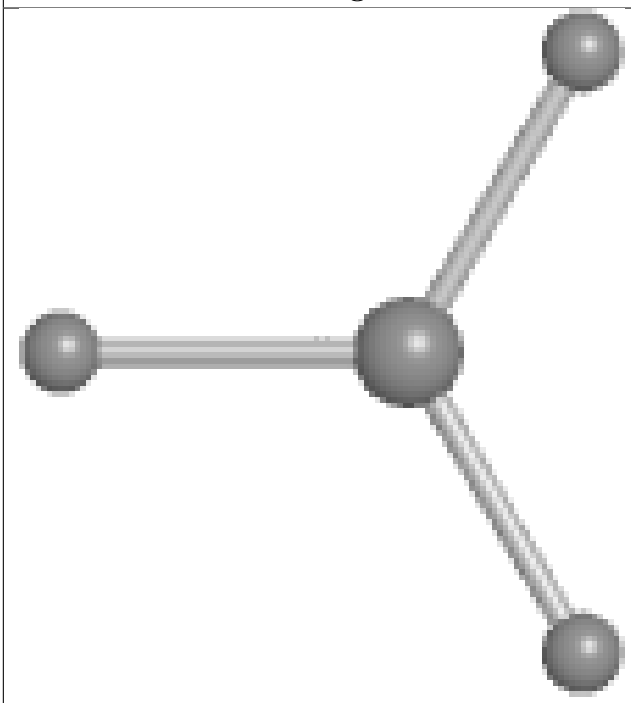

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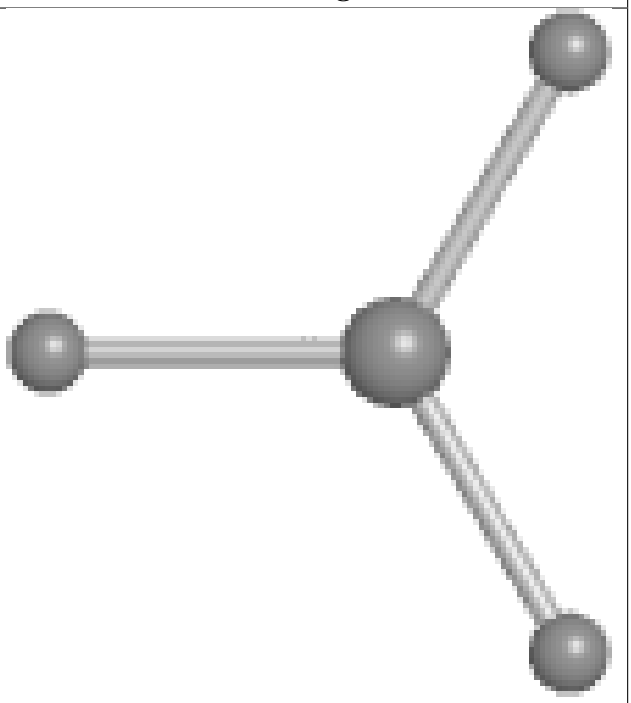
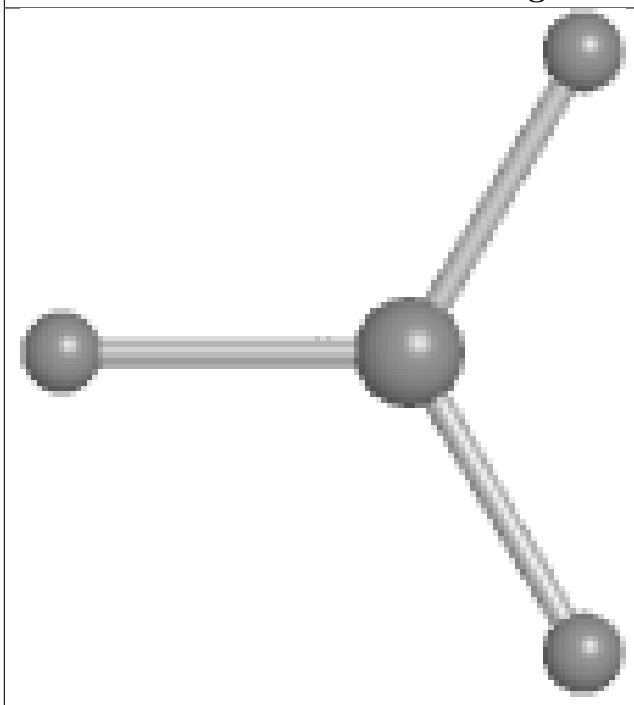


Rings

Ligand AF3 D 603



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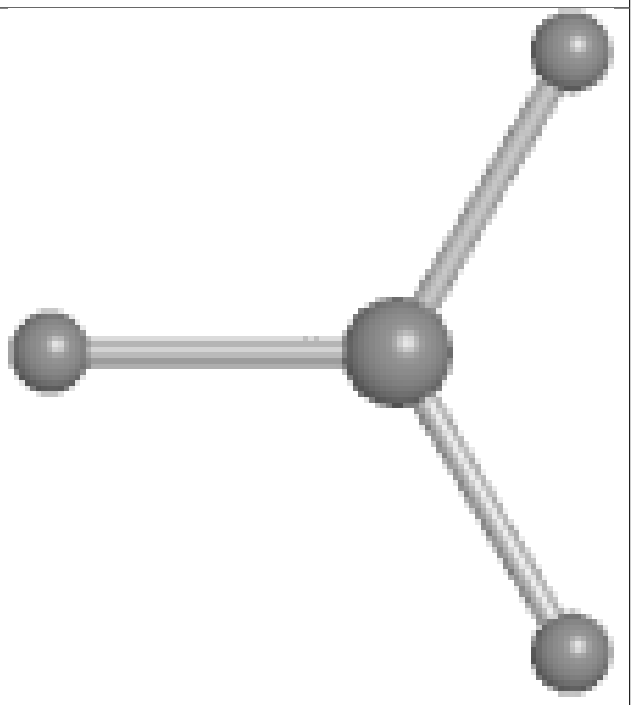

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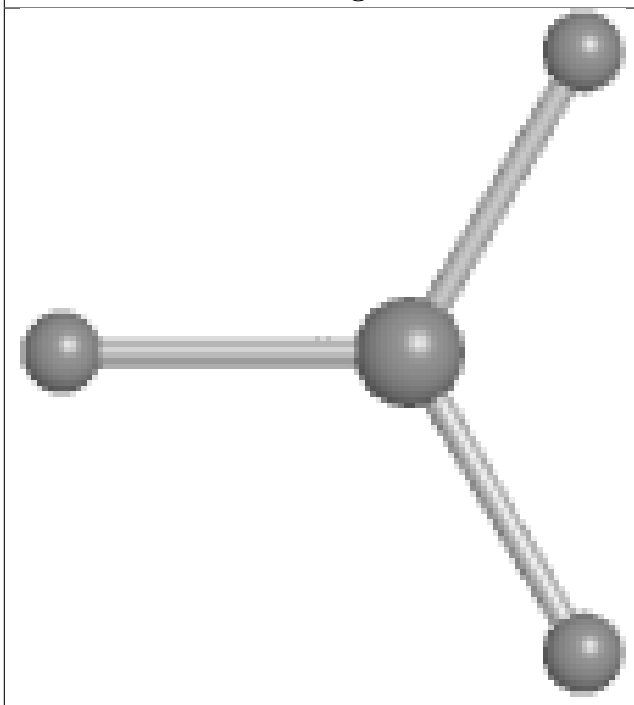

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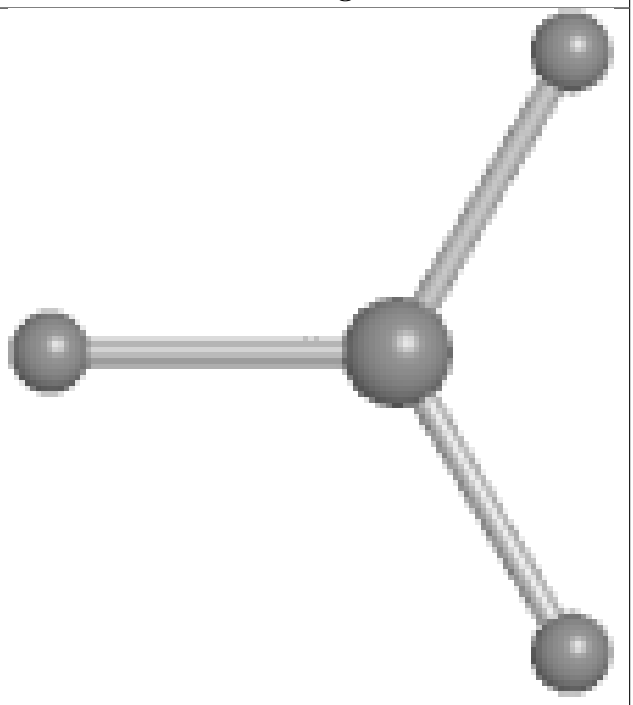
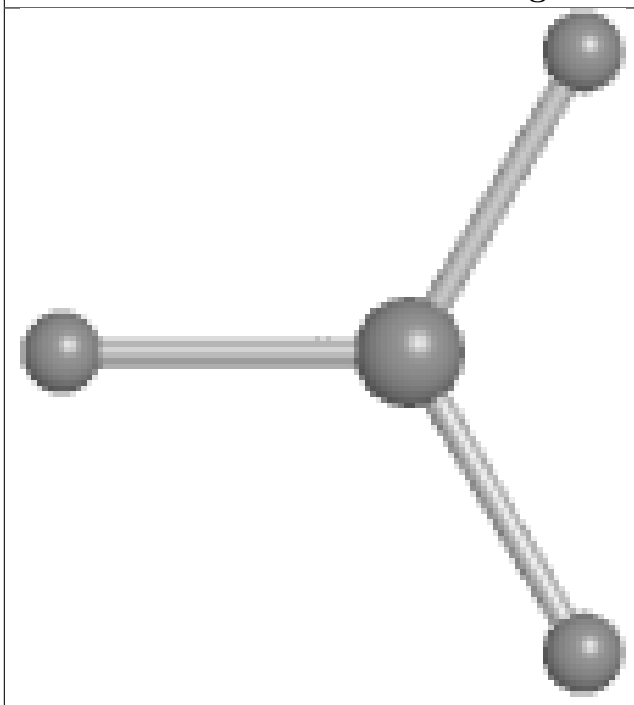


Rings

Ligand AF3 B 603



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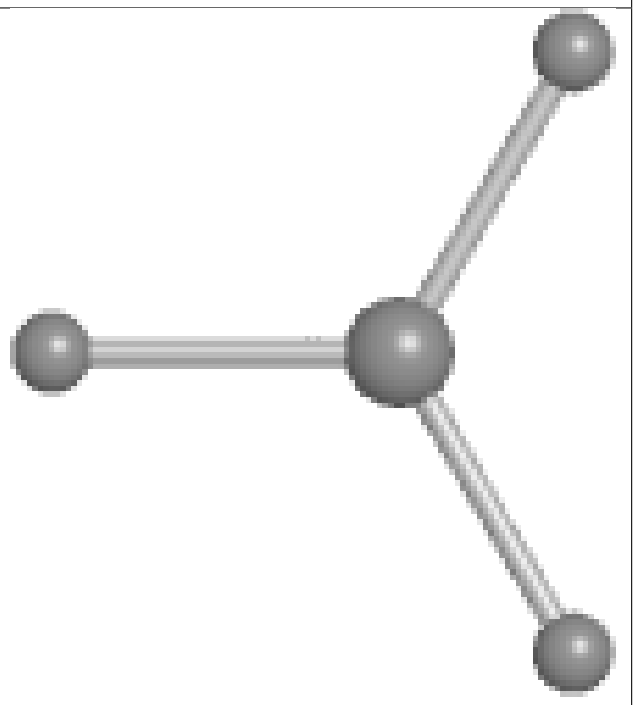

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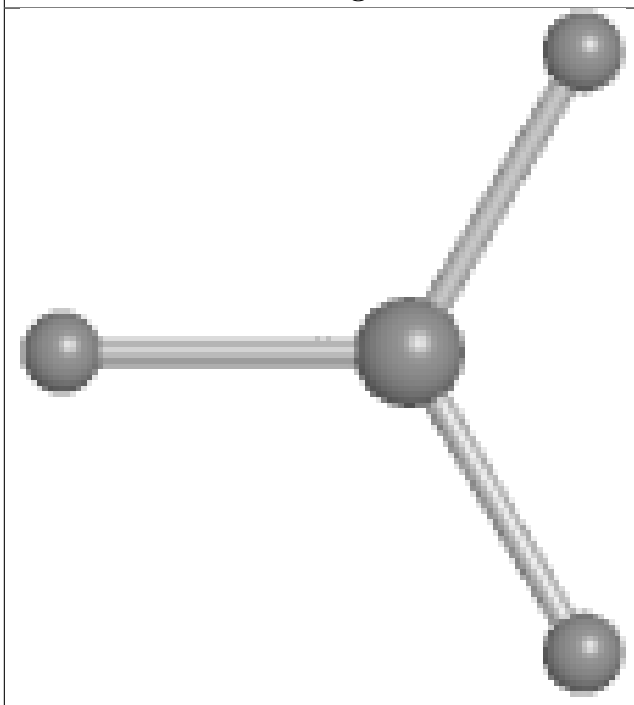

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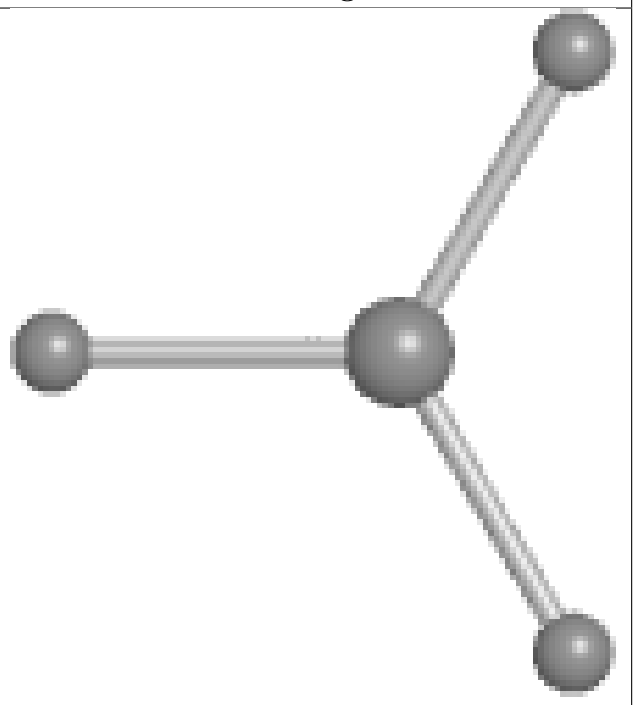
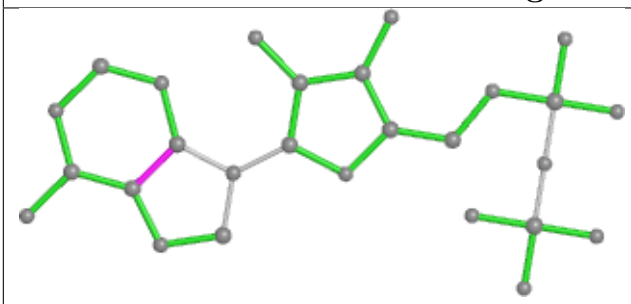
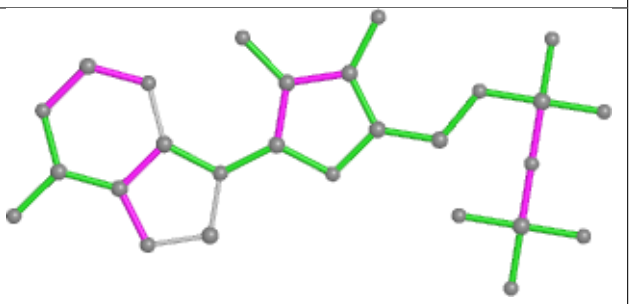
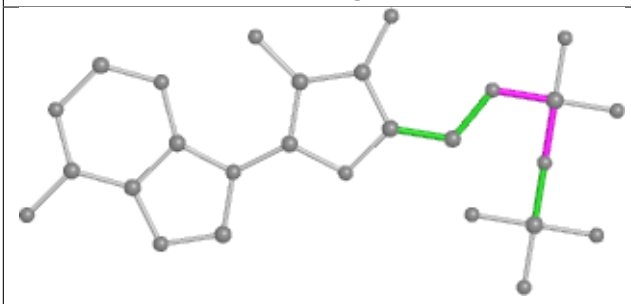
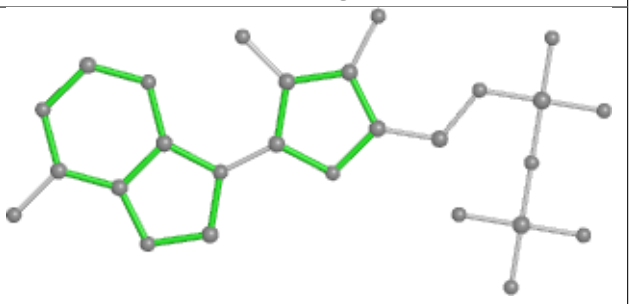
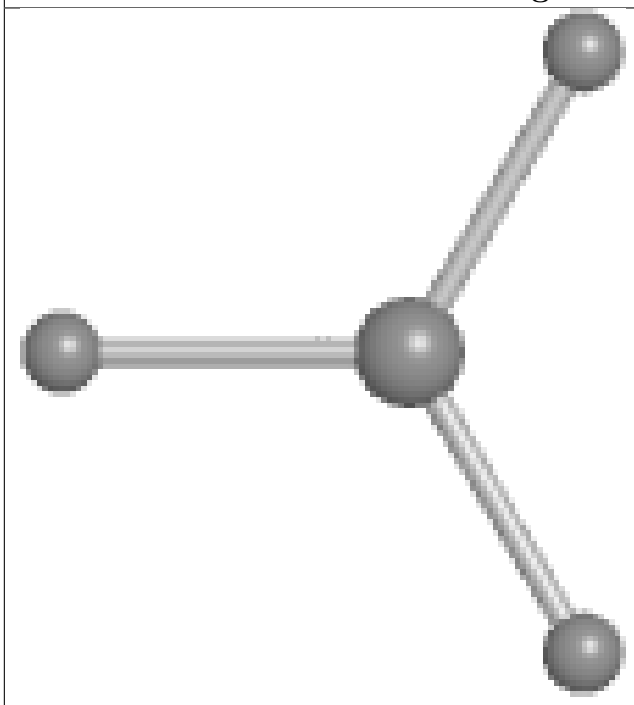


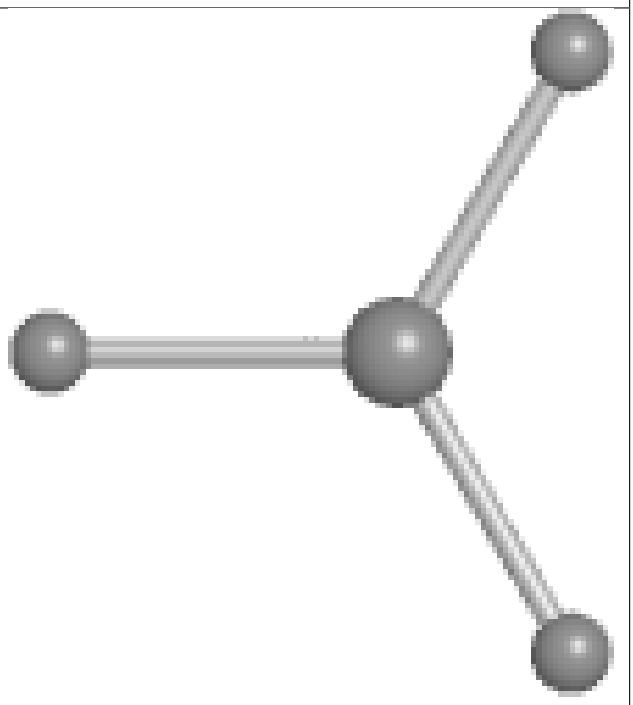
Rings

Ligand ADP a 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

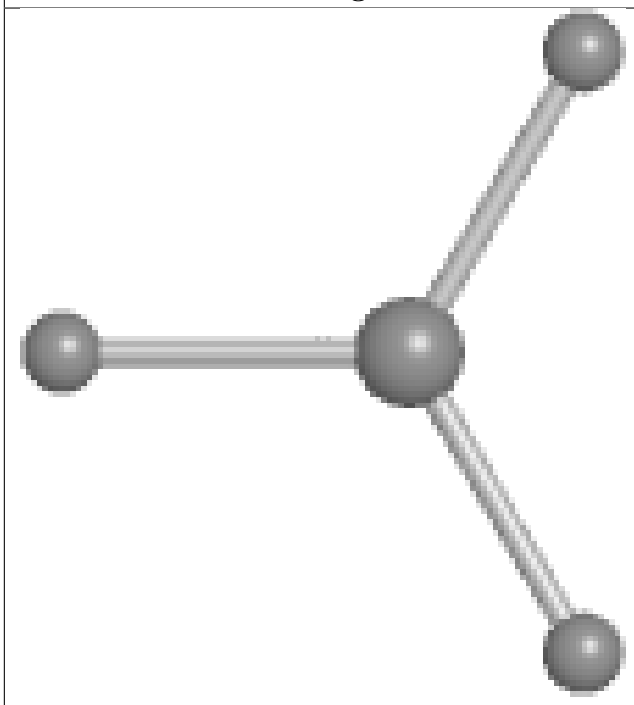
Ligand AF3 d 603



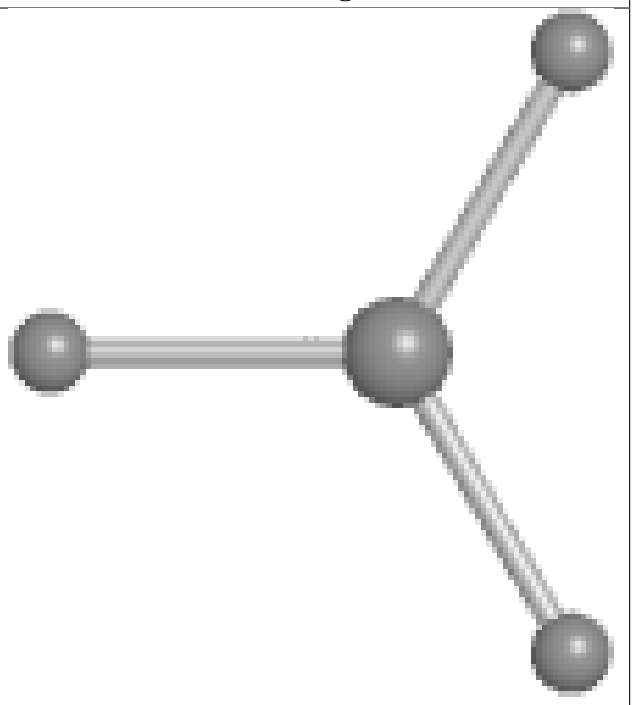
Bond lengths



Bond angles

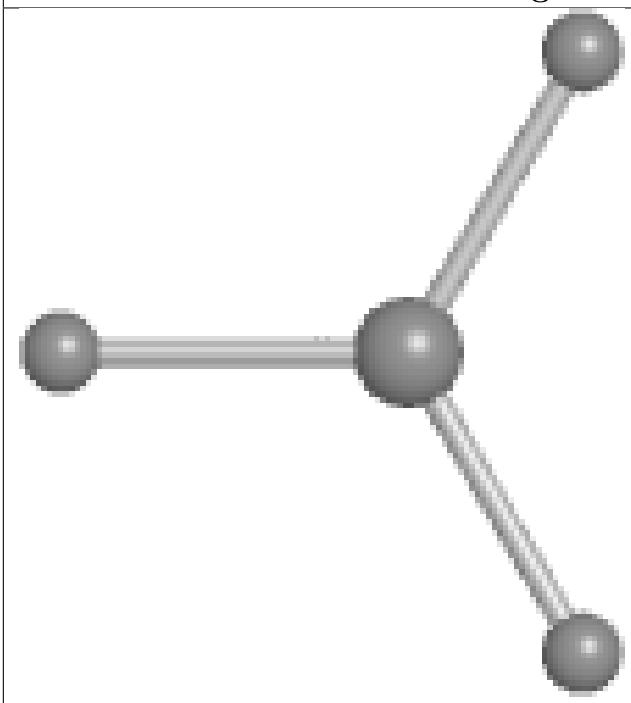


Torsions

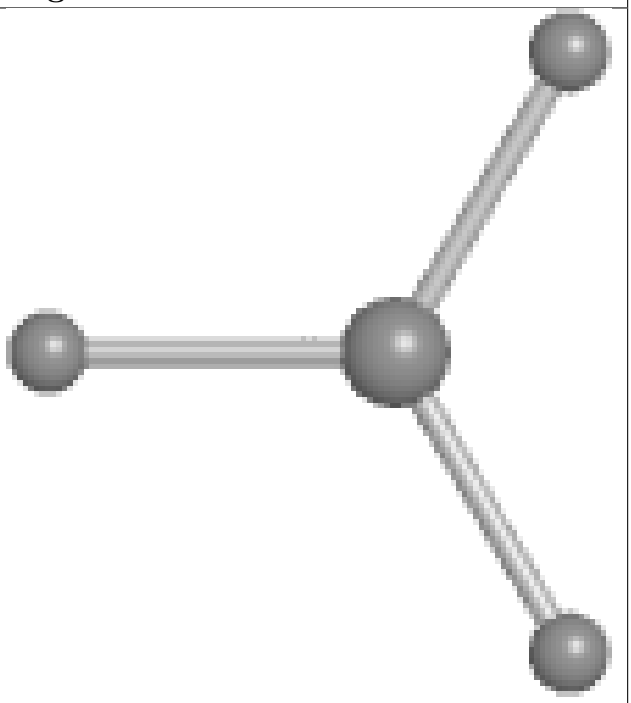


Rings

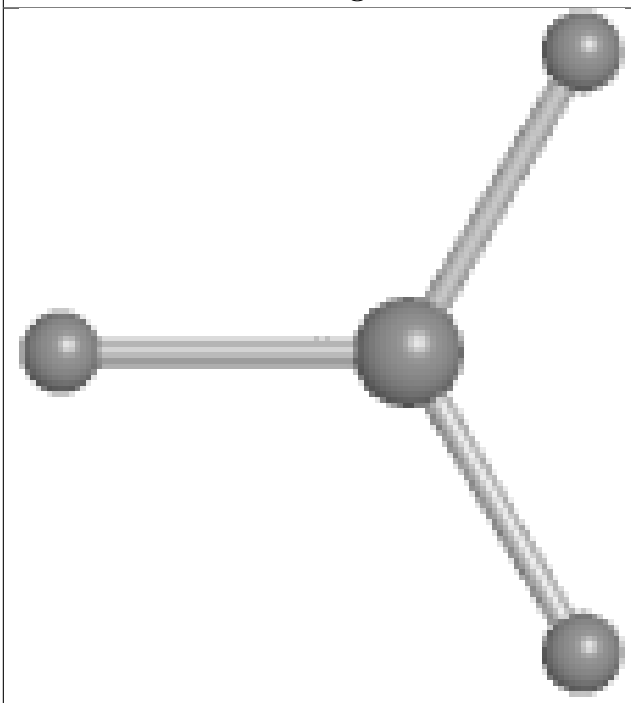
Ligand AF3 g 603



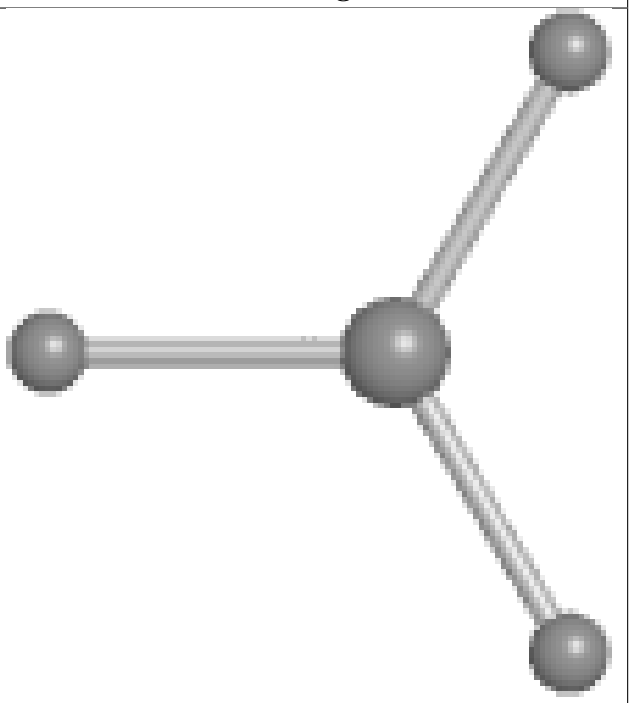
Bond lengths



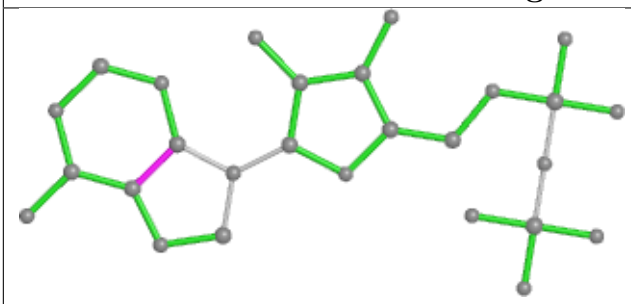
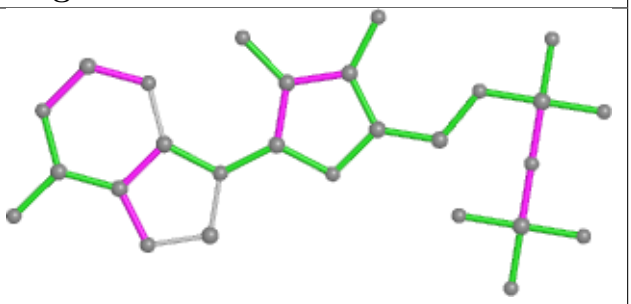
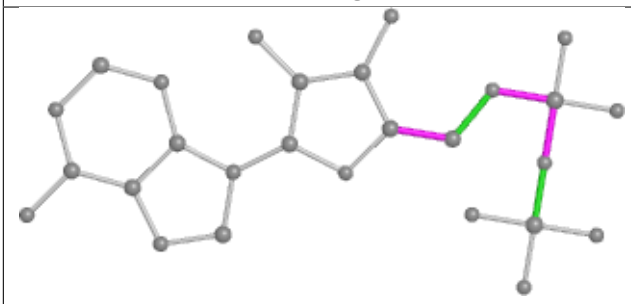
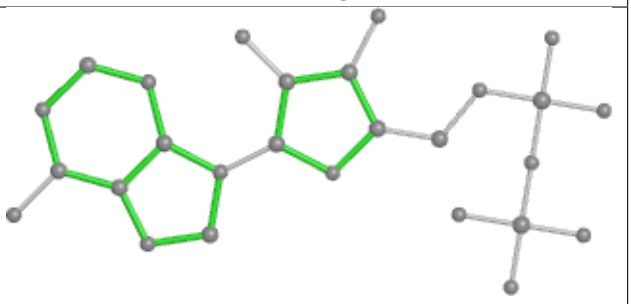
Bond angles

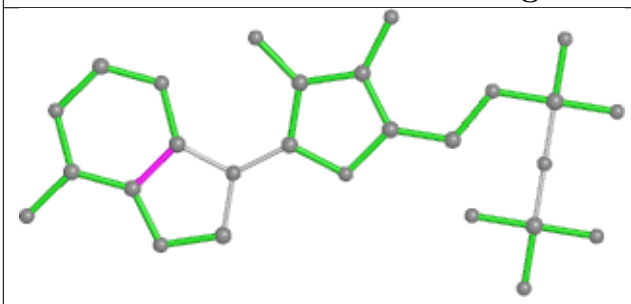
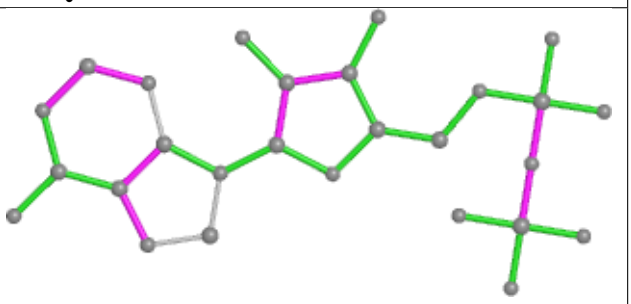
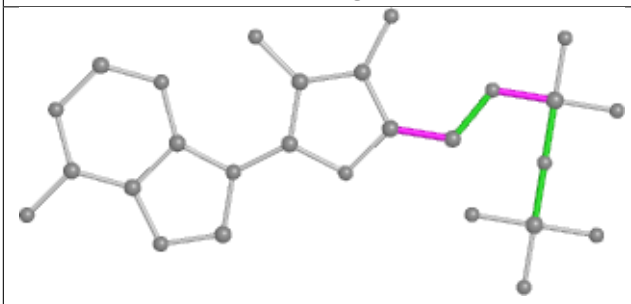
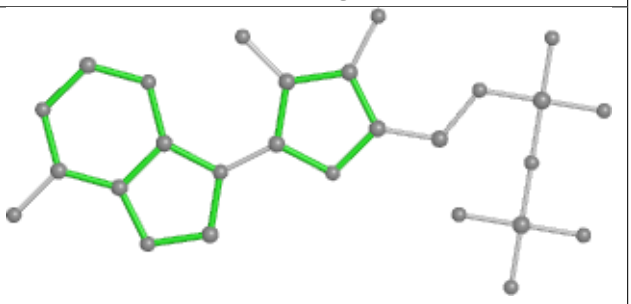


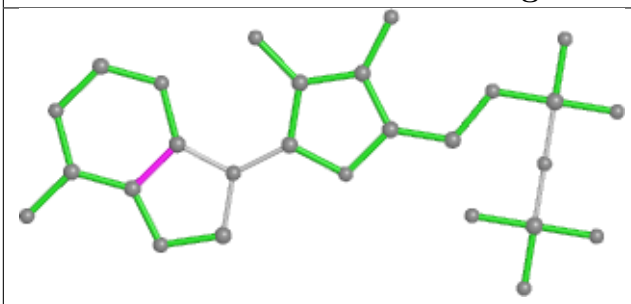
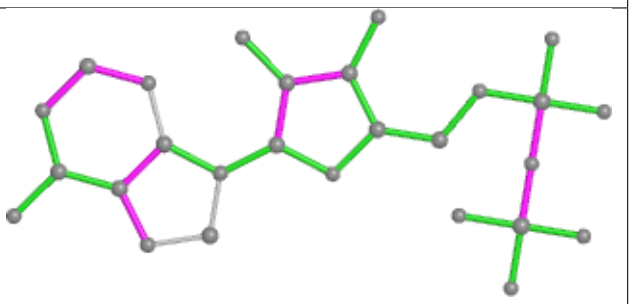
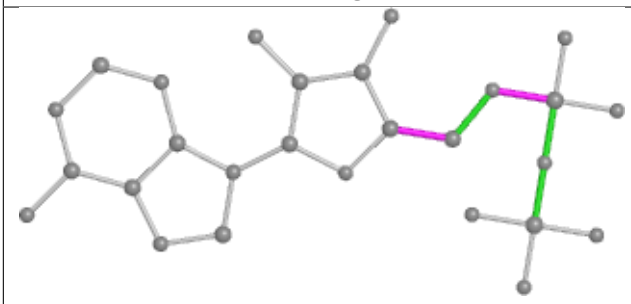
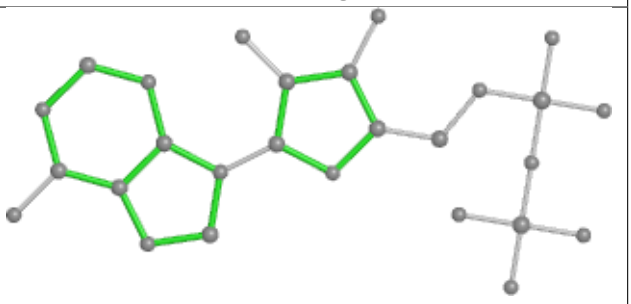
Torsions

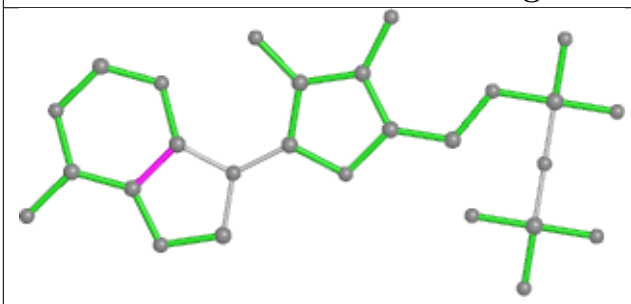
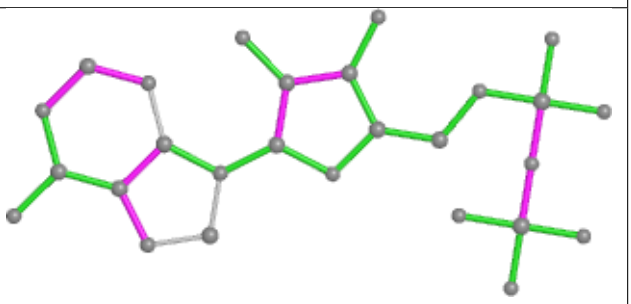
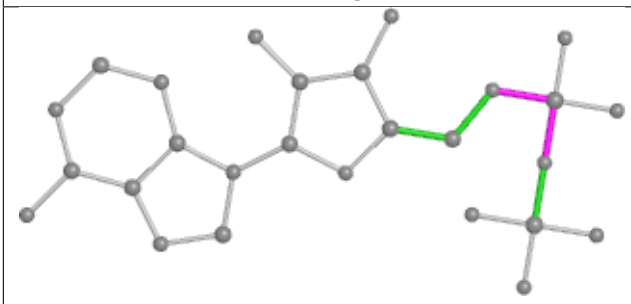
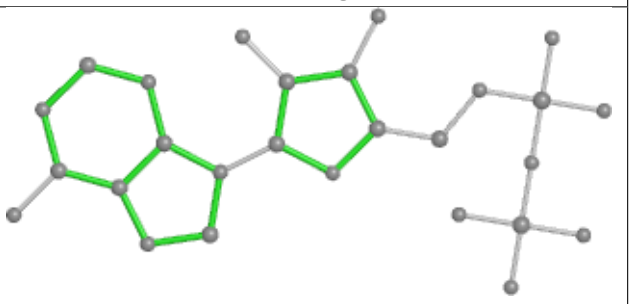


Rings

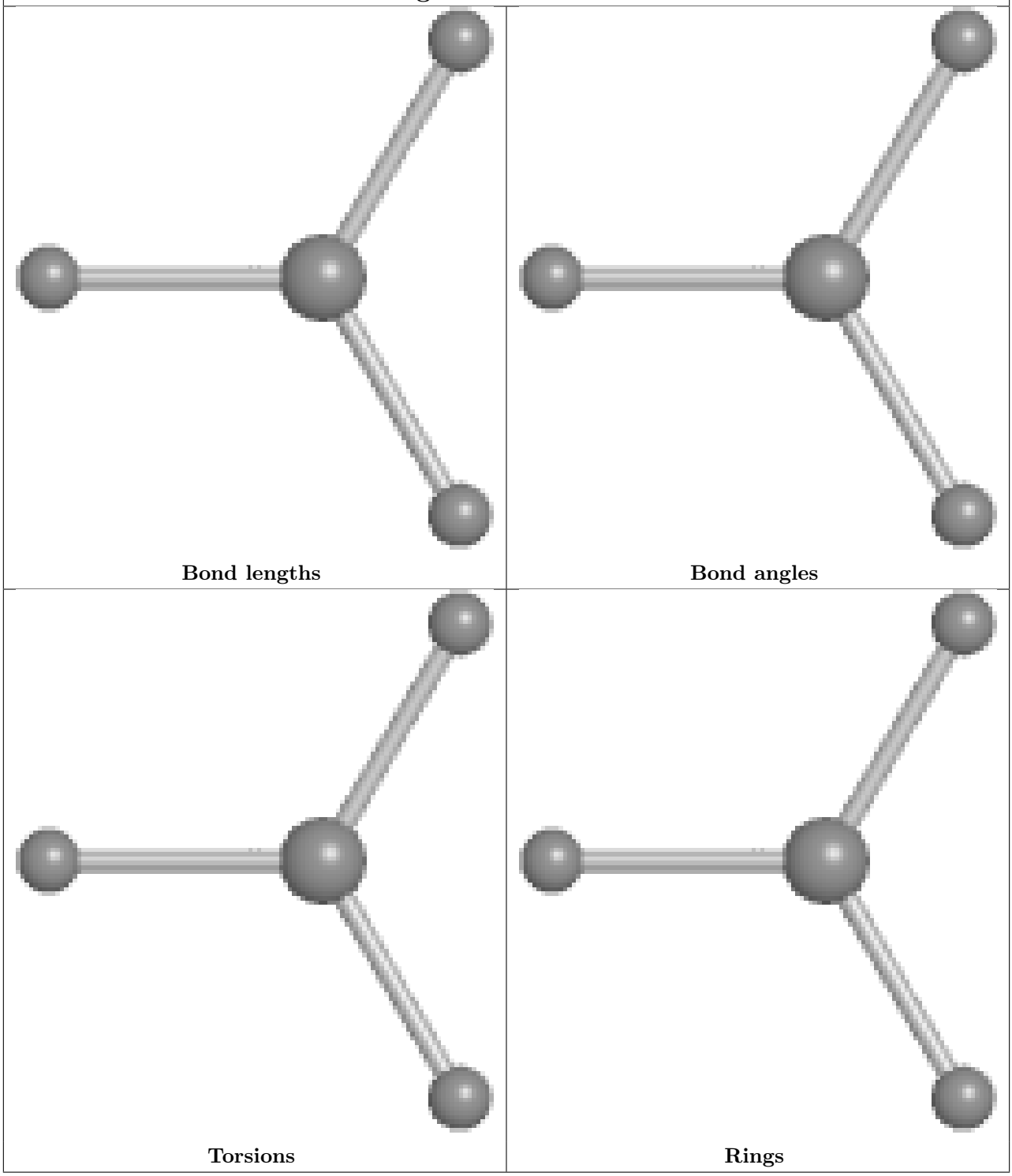
Ligand ADP g 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP Q 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP D 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP E 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AF3 A 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.

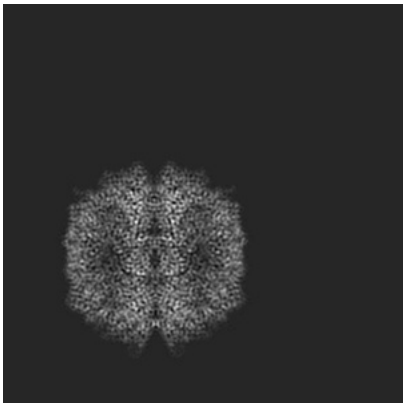
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0758. These allow visual inspection of the internal detail of the map and identification of artifacts.

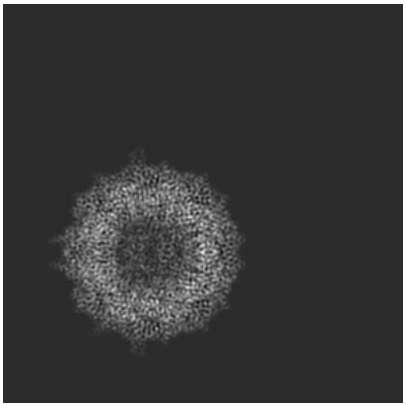
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

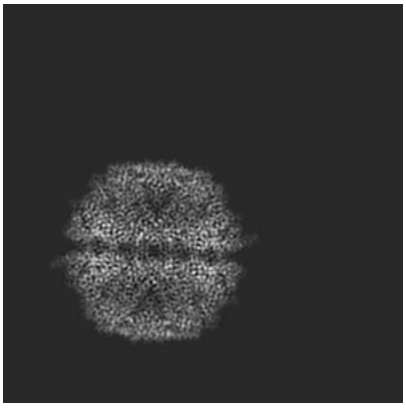
6.1.1 Primary map



X



Y

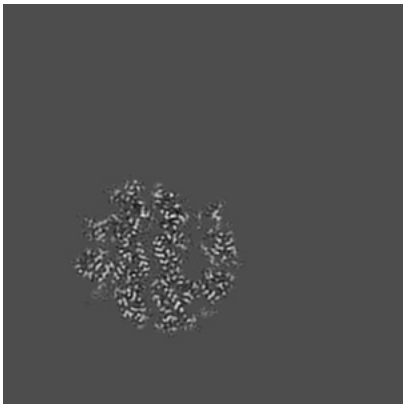


Z

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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 256

Y Index: 256

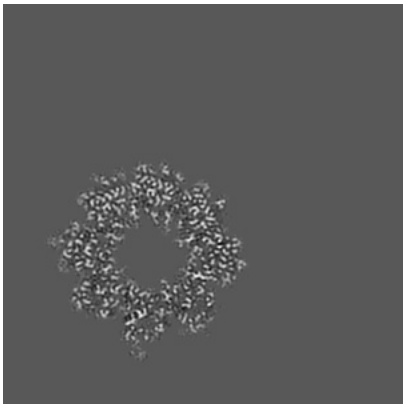
Z Index: 256

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

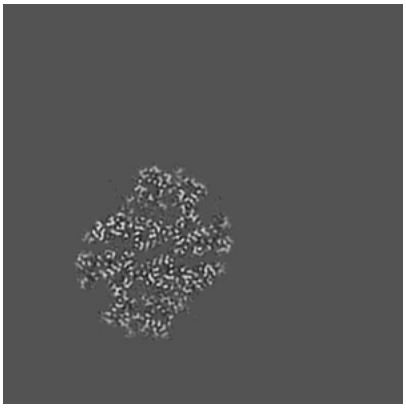
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 247



Y Index: 173

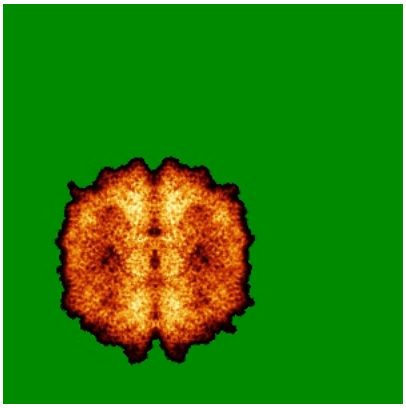


Z Index: 253

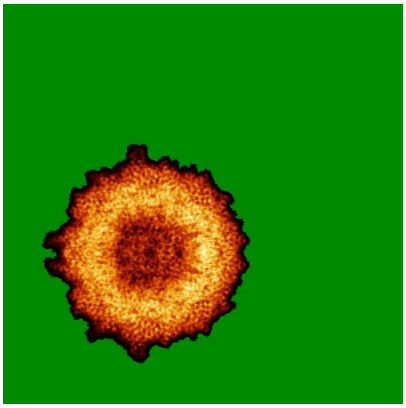
The images above show the largest variance slices of the map in three orthogonal directions.

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

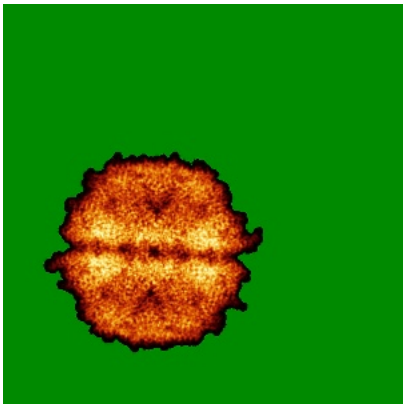
6.4.1 Primary map



X



Y

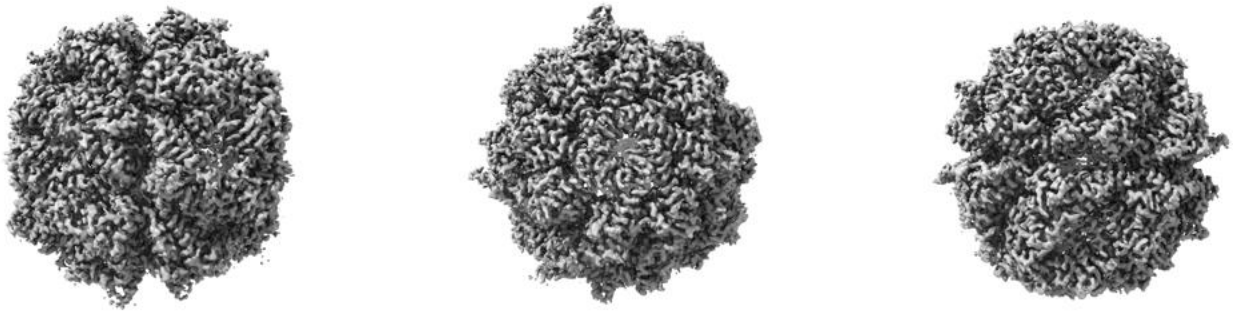


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

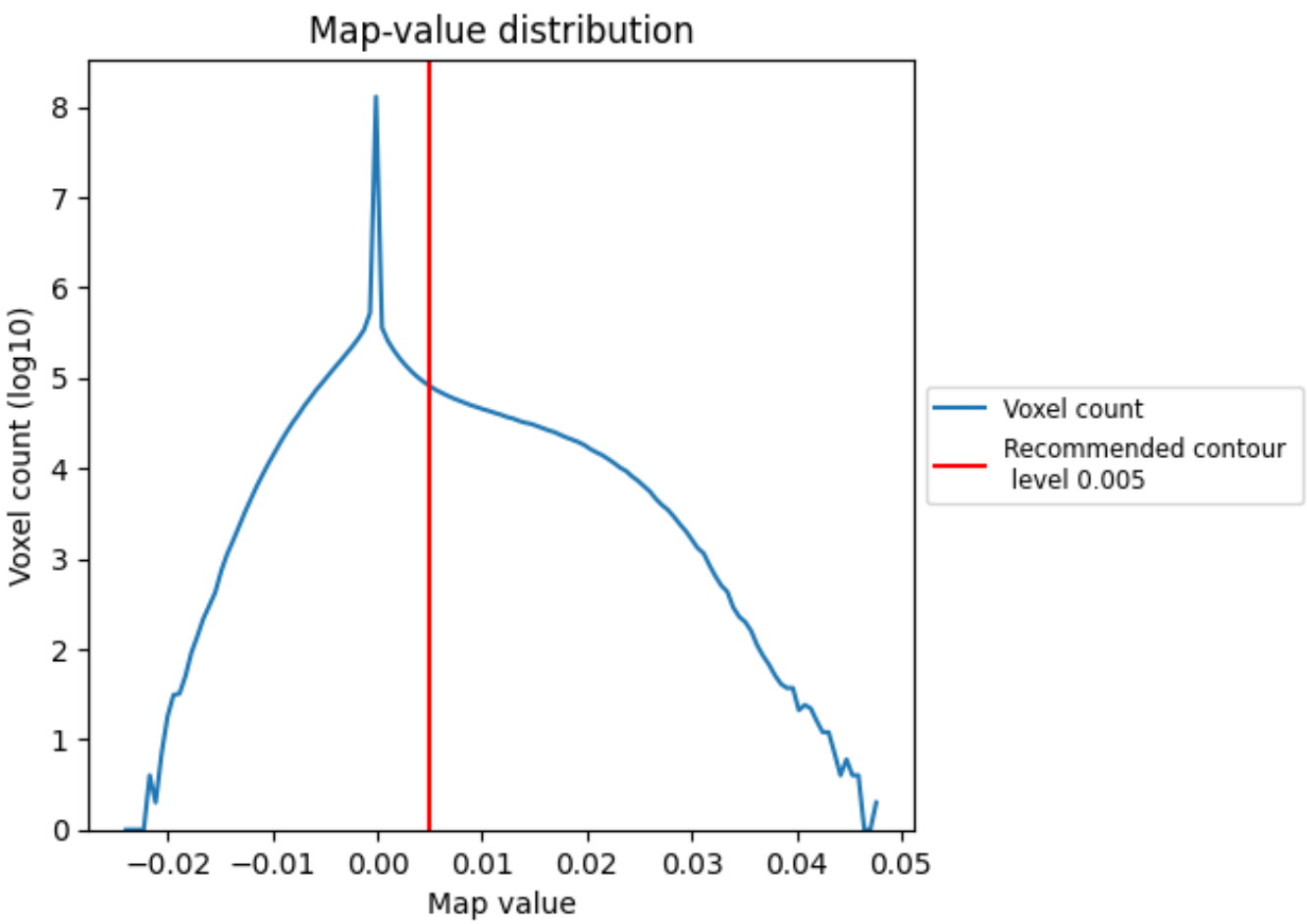
6.6 Mask visualisation (i)

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

7 Map analysis (i)

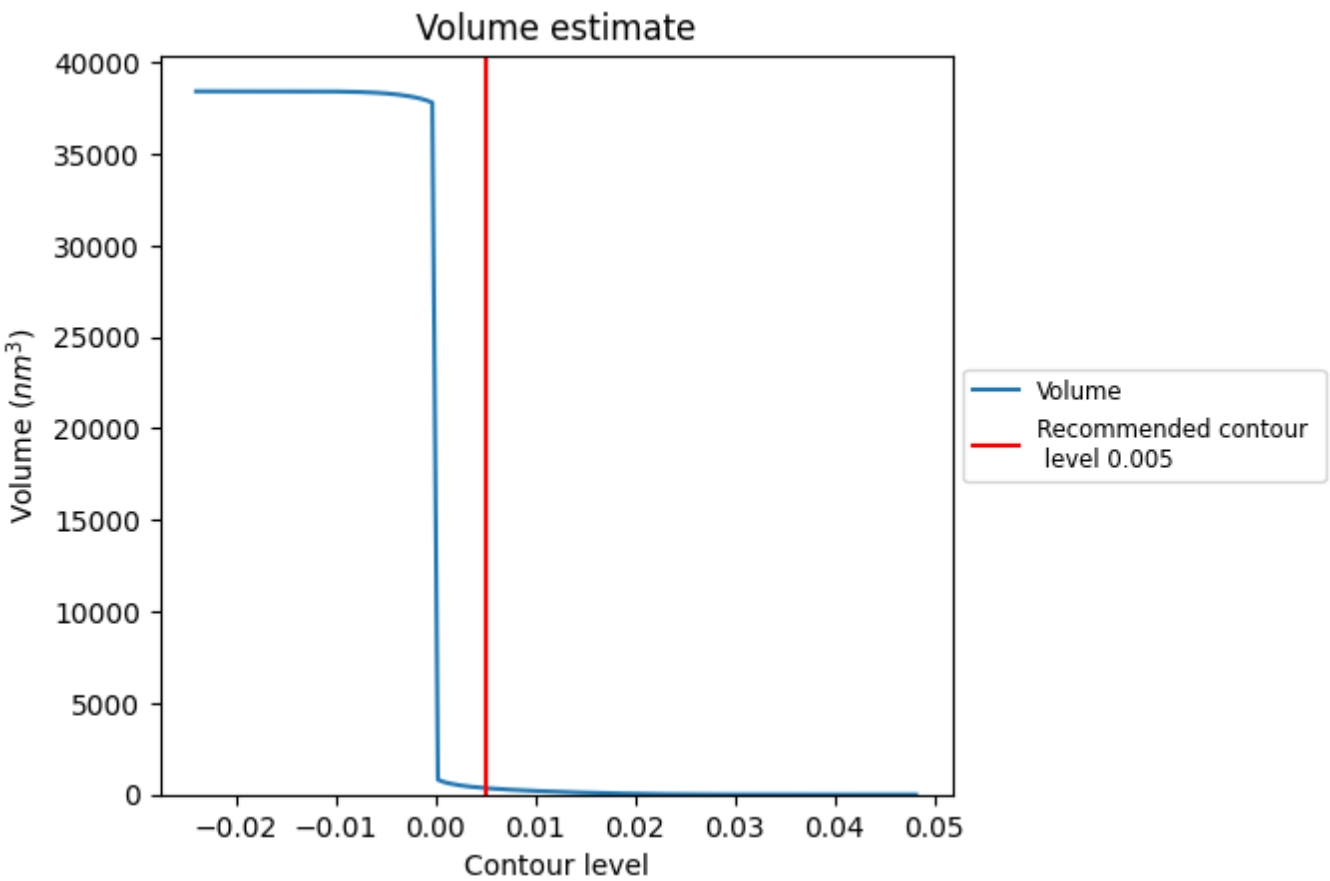
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

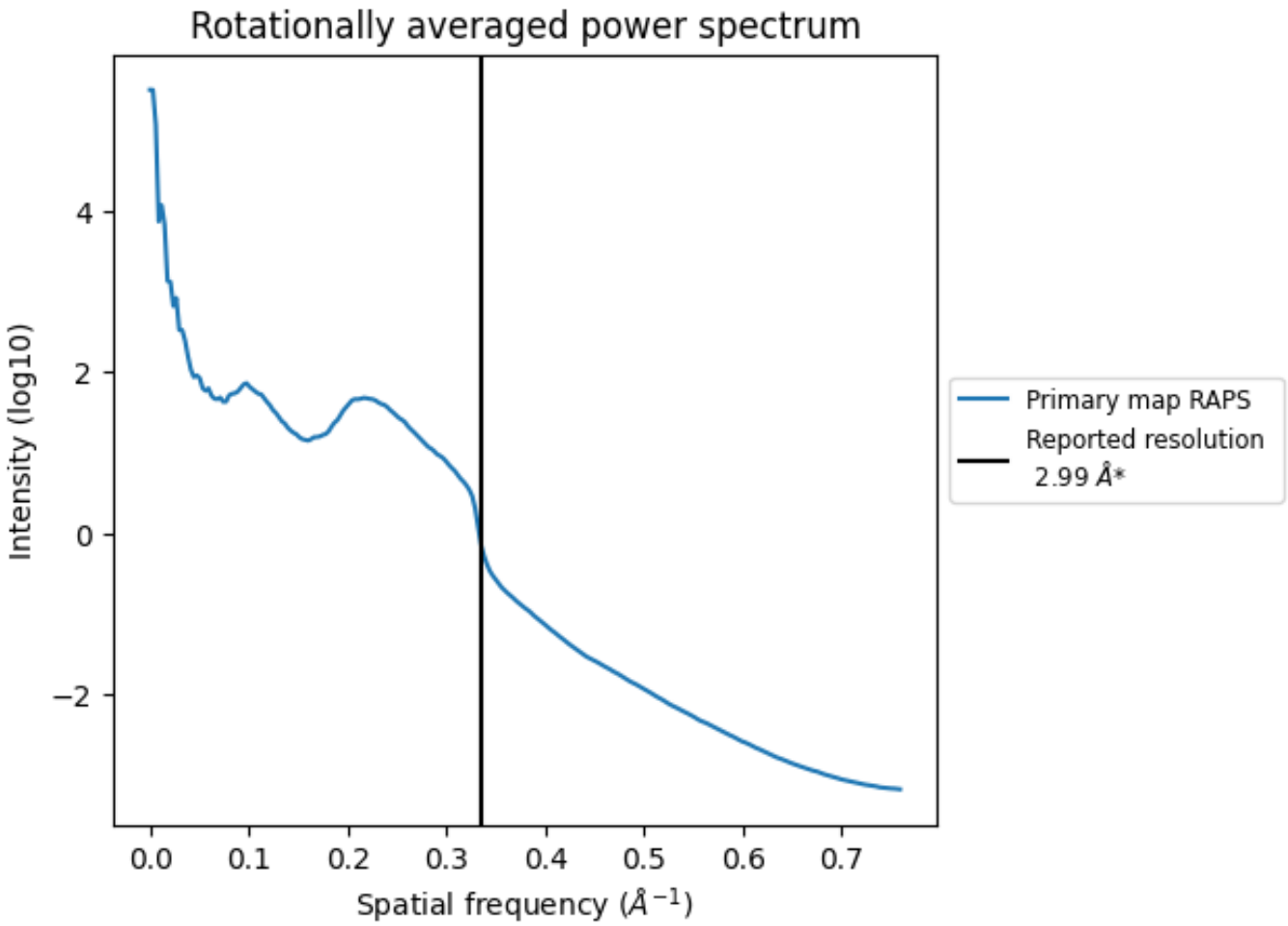
7.2 Volume estimate (i)



The volume at the recommended contour level is 355 nm^3; this corresponds to an approximate mass of 321 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 0.334 Å^{-1}

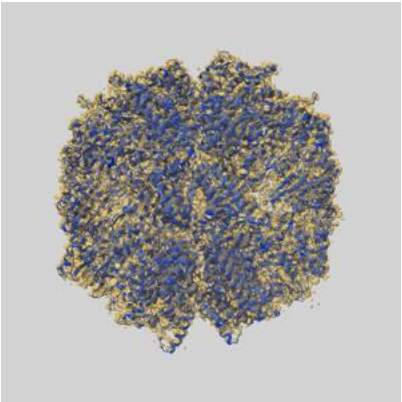
8 Fourier-Shell correlation (i)

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

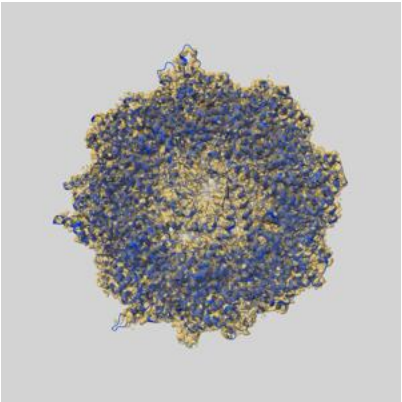
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0758 and PDB model 6KS6. Per-residue inclusion information can be found in section 3 on page 13.

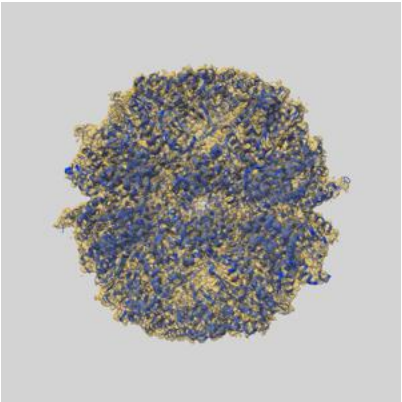
9.1 Map-model overlay (i)



X



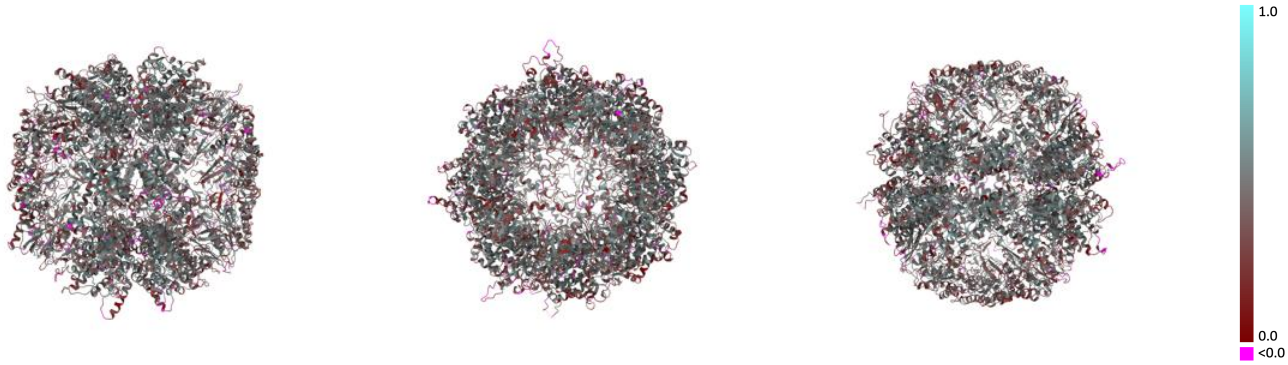
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 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.

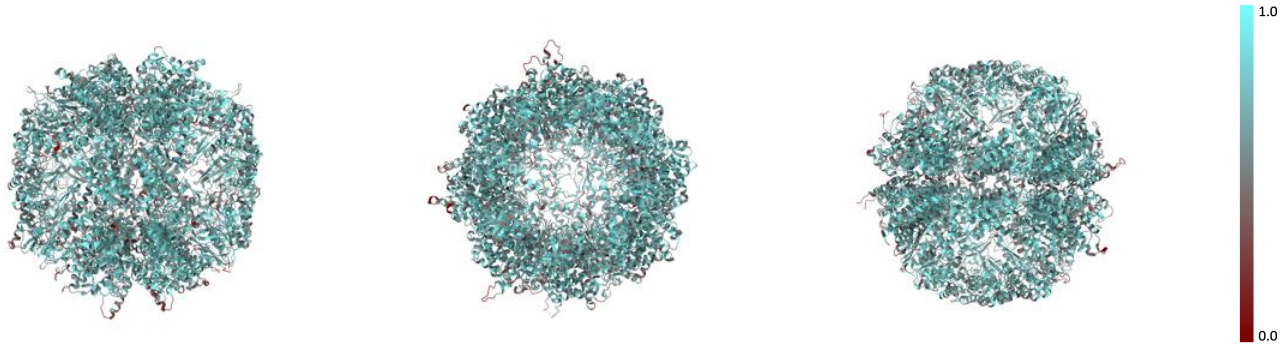
9.2 Q-score mapped to coordinate model (i)



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.

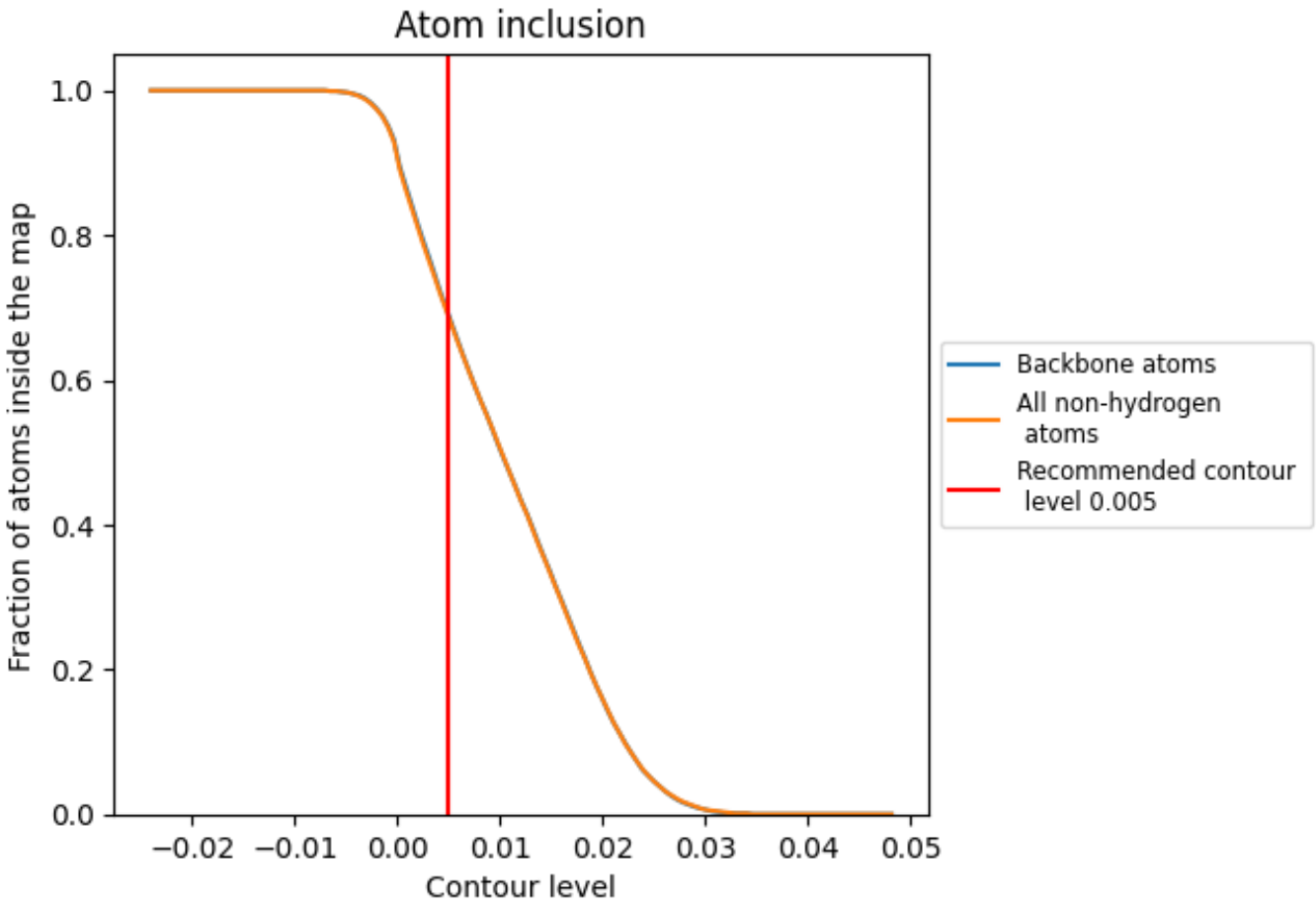
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6880	0.4000
A	0.6750	0.3790
B	0.7300	0.4290
D	0.7160	0.4160
E	0.7060	0.4090
G	0.7020	0.4020
H	0.6910	0.3870
Q	0.6580	0.3820
Z	0.6800	0.3870
a	0.6850	0.3930
b	0.7260	0.4210
d	0.6970	0.4040
e	0.6960	0.4090
g	0.7010	0.4120
h	0.7040	0.4000
q	0.6710	0.3850
z	0.6860	0.3980