wwPDB EM Validation Summary Report (i)

May 13, 2024 – 07:13 pm BST

PDB ID	:	6TG9
EMDB ID	:	EMD-10495
Title	:	Cryo-EM Structure of NADH reduced form of NAD+-dependent Formate Dehydrogenase from Rhodobacter capsulatus
Authors	:	Wendler, P.; Radon, C.; Mittelstaedt, G.
Deposited on	:	2019-11-15
Resolution	:	3.24 Å(reported)
Based on initial models	:	5XF9, 3IAM, 1FDO

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 (1)) were used in the production of this report:

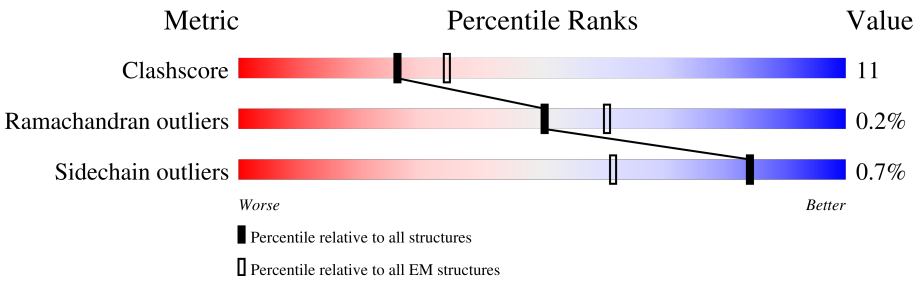
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.24 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	958	73% 25%
1	E	958	73% 26%
2	B	500	80% 19%
2	F	500	79% 19%
3	C	150	72% 25%
3	G	150	71% 26%
4	D	71	75% 23%
4	H	71	77% 20%

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
7	FES	A	1004	-	-	X	-
7	FES	C	201	-	-	X	-
7	FES	E	1004	-	-	X	-
7	FES	G	201	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 25412 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 Formate dehydrogenase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	949	7261	4518	1316	1378	49	0	0
1	E	949	7261	4518	1316	1378	49	0	0

- Molecule 2 is a protein called Formate dehydrogenase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	493	3645	2318	636	663	28	0	0
2	F	493	3645	2318	636	663	28	0	0

- Molecule 3 is a protein called Formate dehydrogenase subunit gamma.

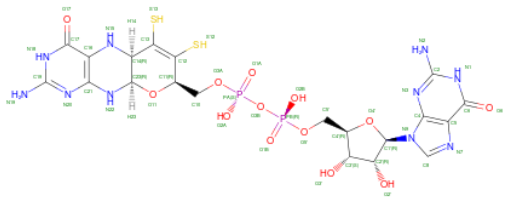
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	148	1076	674	197	197	8	0	0
3	C	148	1076	674	197	197	8	0	0

- Molecule 4 is a protein called NAD-dependent formate dehydrogenase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	69	505	321	93	89	2	0	0
4	H	69	505	321	93	89	2	0	0

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).

MGD

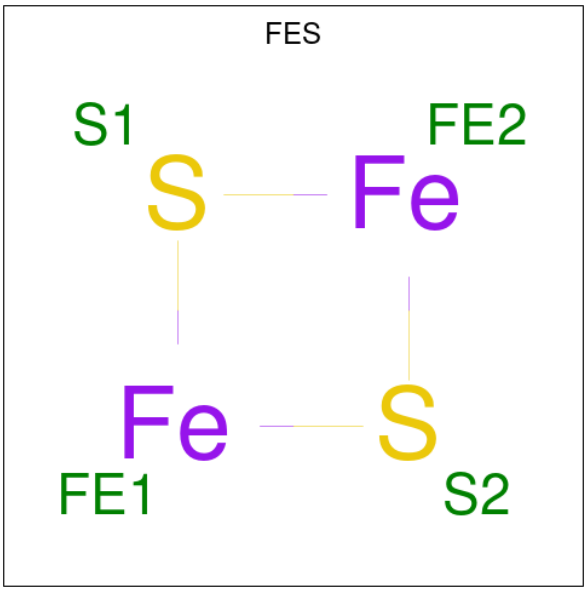


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
5	A	1	47	20	10	13	2	2	0
5	A	1	47	20	10	13	2	2	0
5	E	1	47	20	10	13	2	2	0
5	E	1	47	20	10	13	2	2	0

- Molecule 6 is MOLYBDENUM(VI) ION (three-letter code: 6MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

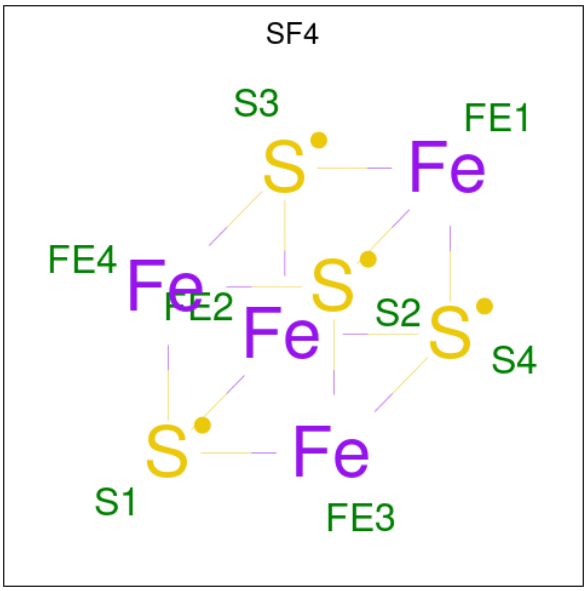
Mol	Chain	Residues	Atoms		AltConf
			Total	Mo	
6	A	1	1	1	0
6	E	1	1	1	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



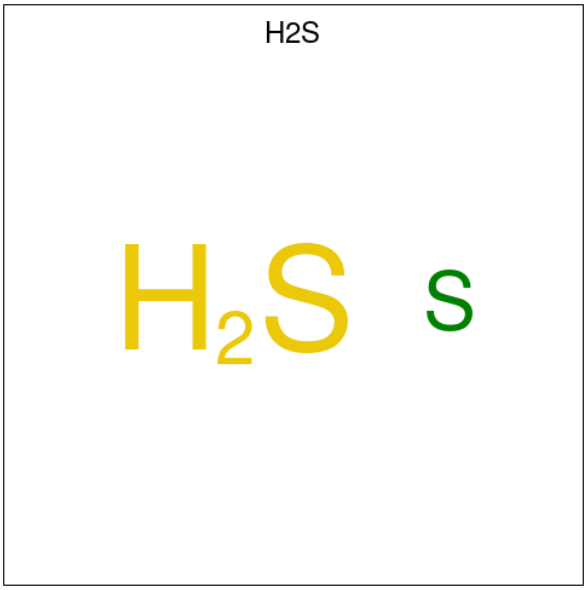
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
7	A	1	4	2	2	0
7	G	1	4	2	2	0
7	E	1	4	2	2	0
7	C	1	4	2	2	0

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
8	A	1	8	4	4	0
8	A	1	8	4	4	0
8	A	1	8	4	4	0
8	A	1	8	4	4	0
8	B	1	8	4	4	0
8	E	1	8	4	4	0
8	E	1	8	4	4	0
8	E	1	8	4	4	0
8	E	1	8	4	4	0
8	F	1	8	4	4	0

- Molecule 9 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H_2S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
			Total	S	
9	A	1	1	1	0

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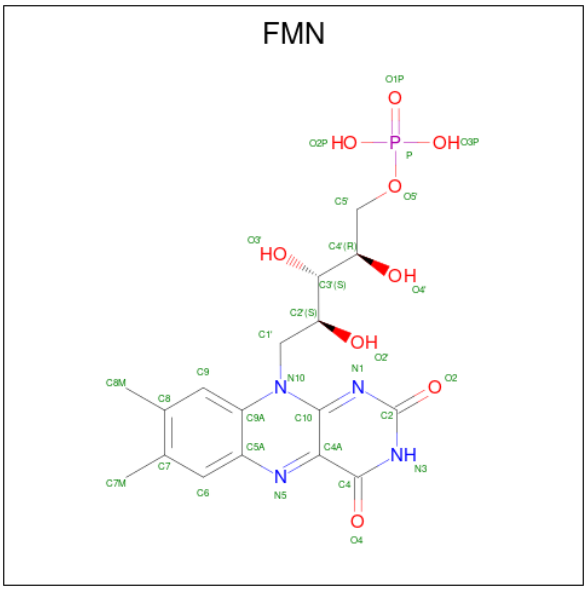
Mol	Chain	Residues	Atoms		AltConf
			Total	S	
9	E	1	1	1	0

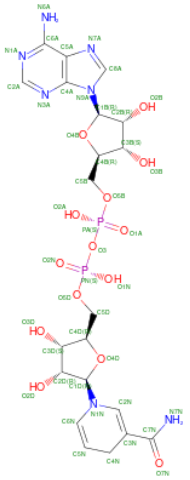
- Molecule 10 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	B	1	31	17	4	9	1	0
			Total	C	N	O	P	
10	F	1	31	17	4	9	1	0

- Molecule 11 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

NAI



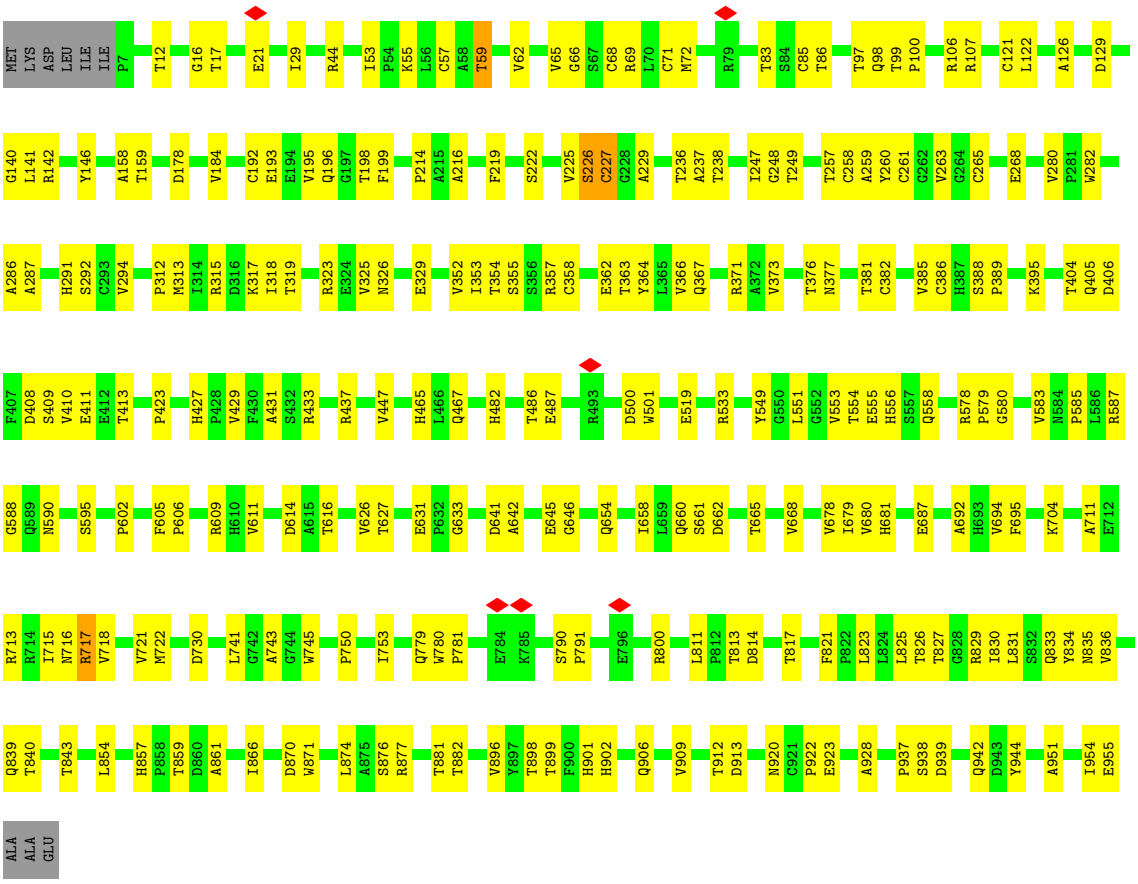
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	B	1	44	21	7	14	2	0
			Total	C	N	O	P	
11	F	1	44	21	7	14	2	0

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.

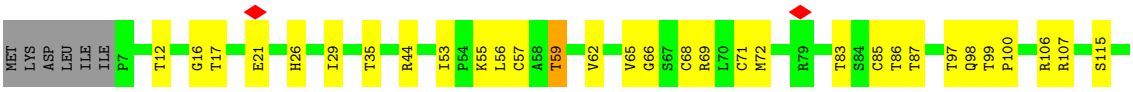
• Molecule 1: Formate dehydrogenase subunit alpha

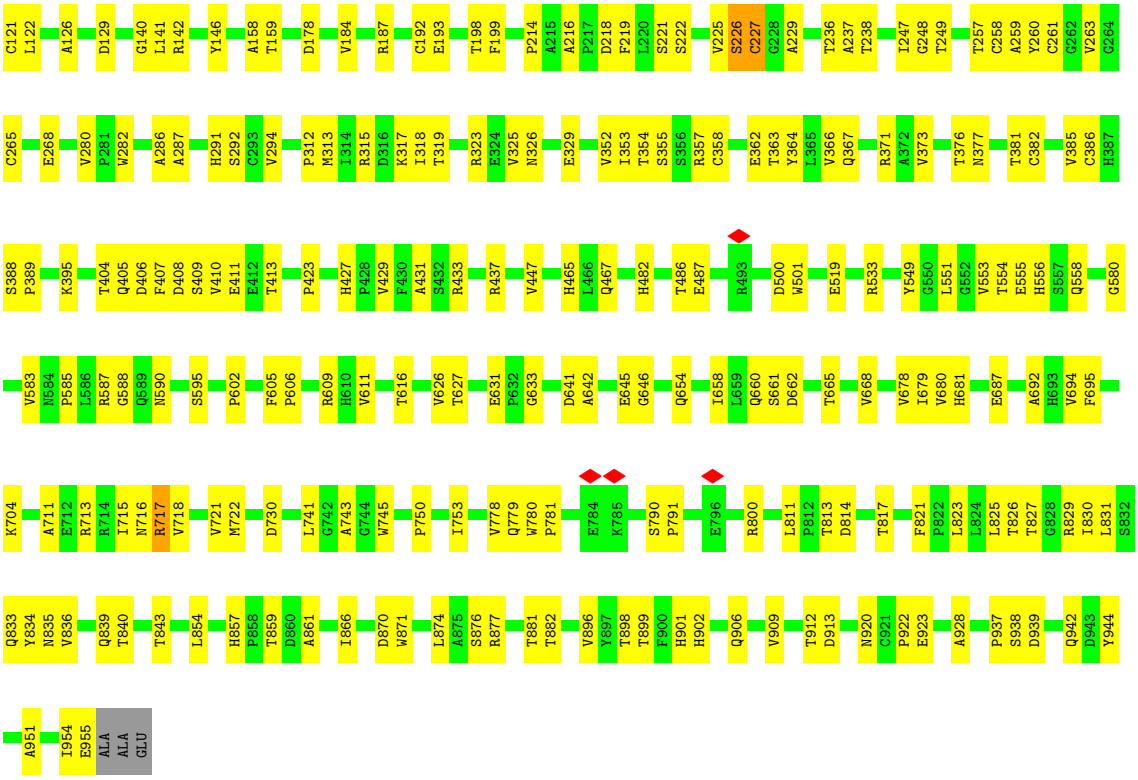
Chain A:



• Molecule 1: Formate dehydrogenase subunit alpha

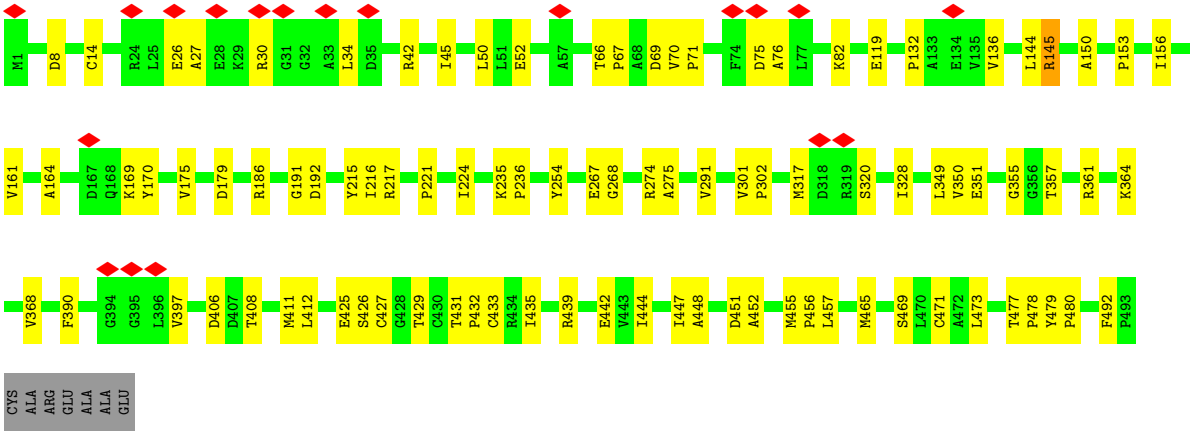
Chain E:





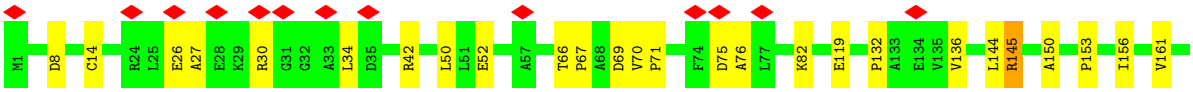
• Molecule 2: Formate dehydrogenase subunit beta

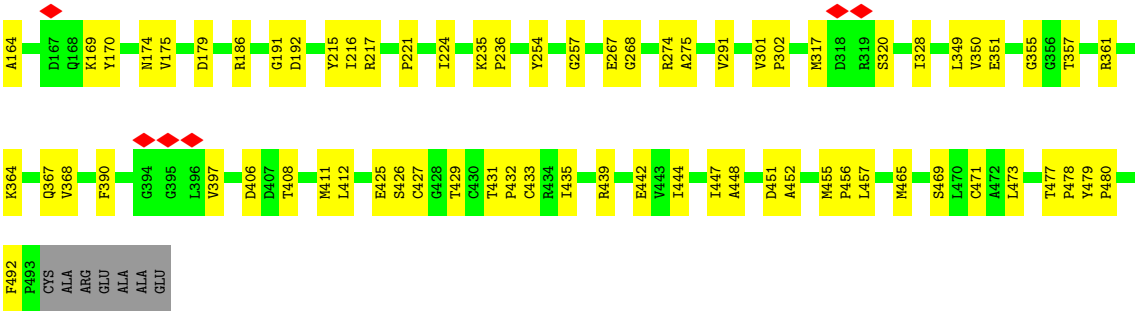
Chain B:



• Molecule 2: Formate dehydrogenase subunit beta

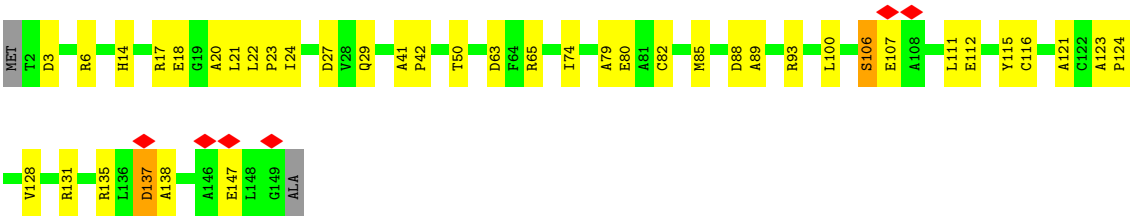
Chain F:





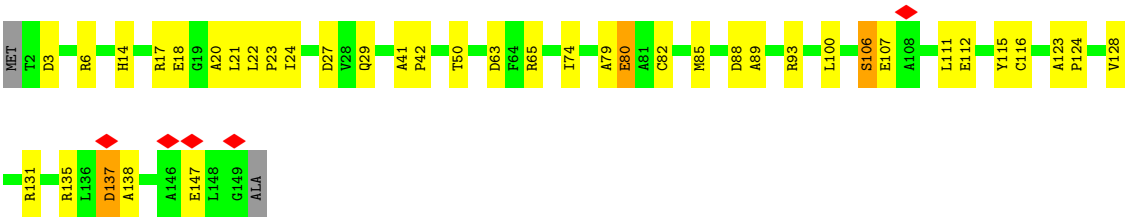
• Molecule 3: Formate dehydrogenase subunit gamma

Chain G:



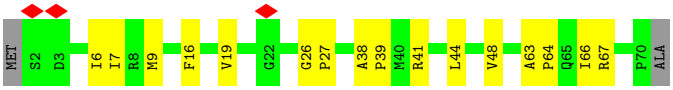
• Molecule 3: Formate dehydrogenase subunit gamma

Chain C:



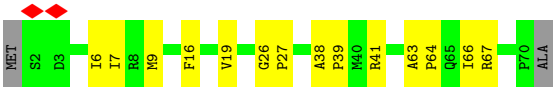
• Molecule 4: NAD-dependent formate dehydrogenase subunit delta

Chain D:



• Molecule 4: NAD-dependent formate dehydrogenase subunit delta

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	199229	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND4 was used to estimate contrast transfer function parameters. CTF correction was done in Relion 3.0.	Depositor
Microscope	FEI POLARA 300, FEI TITAN KRIOS	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ($e^-/Å^2$)	64, 40	Depositor
Minimum defocus (nm)	Not provided, Not provided	Depositor
Maximum defocus (nm)	Not provided, Not provided	Depositor
Magnification	Not provided, Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.348	Depositor
Minimum map value	-0.152	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0223	Depositor
Map size (Å)	239.68001, 239.68001, 239.68001	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: MGD, SF4, FMN, 6MO, FES, NAI, H2S

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	0.65	0/7426	0.52	0/10113
1	E	0.65	0/7426	0.52	0/10113
2	B	0.50	0/3724	0.47	0/5045
2	F	0.50	0/3724	0.47	0/5045
3	C	0.56	0/1091	0.49	0/1479
3	G	0.56	0/1091	0.49	0/1479
4	D	0.39	0/518	0.41	0/710
4	H	0.39	0/518	0.41	0/710
All	All	0.59	0/25518	0.50	0/34694

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)

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	7261	0	7057	184	0
1	E	7261	0	7057	188	0
2	B	3645	0	3659	62	0
2	F	3645	0	3659	66	0
3	C	1076	0	1085	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1076	0	1085	30	0
4	D	505	0	510	11	0
4	H	505	0	510	10	0
5	A	94	0	42	12	0
5	E	94	0	42	12	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	A	4	0	0	3	0
7	C	4	0	0	4	0
7	E	4	0	0	3	0
7	G	4	0	0	4	0
8	A	32	0	0	0	0
8	B	8	0	0	1	0
8	E	32	0	0	0	0
8	F	8	0	0	1	0
9	A	1	0	0	1	0
9	E	1	0	0	1	0
10	B	31	0	19	1	0
10	F	31	0	19	2	0
11	B	44	0	27	0	0
11	F	44	0	27	0	0
All	All	25412	0	24798	560	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 11.

The worst 5 of 560 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:CYS:HB3	9:A:1009:H2S:S	1.73	1.28
1:E:386:CYS:HB3	9:E:1009:H2S:S	1.73	1.27
1:E:882:THR:OG1	1:E:937:PRO:O	1.85	0.93
1:A:395:LYS:O	1:A:800:ARG:NH1	2.02	0.93
1:A:882:THR:OG1	1:A:937:PRO:O	1.85	0.92

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	947/958 (99%)	866 (91%)	79 (8%)	2 (0%)	47	78
1	E	947/958 (99%)	866 (91%)	79 (8%)	2 (0%)	47	78
2	B	491/500 (98%)	458 (93%)	31 (6%)	2 (0%)	34	68
2	F	491/500 (98%)	457 (93%)	32 (6%)	2 (0%)	34	68
3	C	146/150 (97%)	130 (89%)	16 (11%)	0	100	100
3	G	146/150 (97%)	130 (89%)	16 (11%)	0	100	100
4	D	67/71 (94%)	65 (97%)	2 (3%)	0	100	100
4	H	67/71 (94%)	65 (97%)	2 (3%)	0	100	100
All	All	3302/3358 (98%)	3037 (92%)	257 (8%)	8 (0%)	50	78

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	CYS
1	E	227	CYS
1	A	226	SER
2	B	144	LEU
2	B	145	ARG

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	765/772 (99%)	761 (100%)	4 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	765/772 (99%)	761 (100%)	4 (0%)	88	94
2	B	363/367 (99%)	361 (99%)	2 (1%)	86	93
2	F	363/367 (99%)	361 (99%)	2 (1%)	86	93
3	C	102/103 (99%)	99 (97%)	3 (3%)	42	71
3	G	102/103 (99%)	99 (97%)	3 (3%)	42	71
4	D	50/51 (98%)	50 (100%)	0	100	100
4	H	50/51 (98%)	50 (100%)	0	100	100
All	All	2560/2586 (99%)	2542 (99%)	18 (1%)	84	92

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	471	CYS
3	C	137	ASP
3	C	106	SER
3	G	137	ASP
2	F	119	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	686	ASN
2	F	168	GLN
2	F	382	HIS
2	B	168	GLN
2	B	382	HIS

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 26 ligands modelled in this entry, 2 are monoatomic and 2 are modelled with single atom - leaving 22 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	$\#\|Z\| > 2$
8	SF4	A	1006	1	0,12,12	-	-	-		
8	SF4	E	1006	1	0,12,12	-	-	-		
10	FMN	B	601	-	33,33,33	2.02	4 (12%)	48,50,50	1.24	7 (14%)
5	MGD	E	1001	6	41,52,52	4.28	22 (53%)	40,81,81	2.17	10 (25%)
11	NAI	B	603	-	42,48,48	1.84	10 (23%)	47,73,73	1.28	7 (14%)
8	SF4	F	602	2	0,12,12	-	-	-		
7	FES	C	201	3	0,4,4	-	-	-		
7	FES	G	201	3	0,4,4	-	-	-		
11	NAI	F	603	-	42,48,48	1.84	10 (23%)	47,73,73	1.29	7 (14%)
8	SF4	A	1005	1	0,12,12	-	-	-		
5	MGD	E	1002	6	41,52,52	4.20	21 (51%)	40,81,81	2.12	13 (32%)
8	SF4	E	1008	1	0,12,12	-	-	-		
8	SF4	A	1008	1	0,12,12	-	-	-		
5	MGD	A	1002	6	41,52,52	4.19	21 (51%)	40,81,81	2.12	13 (32%)
7	FES	A	1004	1	0,4,4	-	-	-		
8	SF4	B	602	2	0,12,12	-	-	-		
8	SF4	E	1005	1	0,12,12	-	-	-		
7	FES	E	1004	1	0,4,4	-	-	-		
5	MGD	A	1001	6	41,52,52	4.28	23 (56%)	40,81,81	2.17	10 (25%)
10	FMN	F	601	-	33,33,33	2.02	4 (12%)	48,50,50	1.24	7 (14%)
8	SF4	E	1007	1	0,12,12	-	-	-		
8	SF4	A	1007	1	0,12,12	-	-	-		

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
8	SF4	A	1006	1	-	-	0/6/5/5
8	SF4	E	1006	1	-	-	0/6/5/5
10	FMN	B	601	-	-	2/18/18/18	0/3/3/3
5	MGD	E	1001	6	-	5/18/66/66	0/6/6/6
11	NAI	B	603	-	-	9/25/72/72	0/5/5/5
8	SF4	F	602	2	-	-	0/6/5/5
7	FES	C	201	3	-	-	0/1/1/1
7	FES	G	201	3	-	-	0/1/1/1
11	NAI	F	603	-	-	9/25/72/72	0/5/5/5
8	SF4	A	1005	1	-	-	0/6/5/5
5	MGD	E	1002	6	-	10/18/66/66	0/6/6/6
8	SF4	E	1008	1	-	-	0/6/5/5
8	SF4	A	1008	1	-	-	0/6/5/5
5	MGD	A	1002	6	-	10/18/66/66	0/6/6/6
7	FES	A	1004	1	-	-	0/1/1/1
8	SF4	B	602	2	-	-	0/6/5/5
8	SF4	E	1005	1	-	-	0/6/5/5
7	FES	E	1004	1	-	-	0/1/1/1
5	MGD	A	1001	6	-	5/18/66/66	0/6/6/6
10	FMN	F	601	-	-	2/18/18/18	0/3/3/3
8	SF4	E	1007	1	-	-	0/6/5/5
8	SF4	A	1007	1	-	-	0/6/5/5

The worst 5 of 115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1002	MGD	C21-N20	10.24	1.51	1.36
5	A	1002	MGD	C21-N20	10.22	1.51	1.36
5	A	1001	MGD	C21-N20	9.98	1.50	1.36
5	E	1001	MGD	C21-N20	9.94	1.50	1.36
5	A	1002	MGD	C6-N1	9.16	1.51	1.37

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1001	MGD	O11-C23-N22	6.36	115.11	108.57
5	A	1001	MGD	O11-C23-N22	6.28	115.02	108.57
5	A	1001	MGD	C19-N20-C21	5.22	122.85	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1001	MGD	C19-N20-C21	5.22	122.85	113.43
5	A	1002	MGD	C19-N20-C21	4.92	122.32	113.43

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	MGD	C5'-O5'-PB-O3B
5	A	1002	MGD	C5'-O5'-PB-O1B
5	A	1002	MGD	C5'-O5'-PB-O3B
5	A	1002	MGD	C10-O3A-PA-O1A
5	A	1002	MGD	C10-O3A-PA-O2A

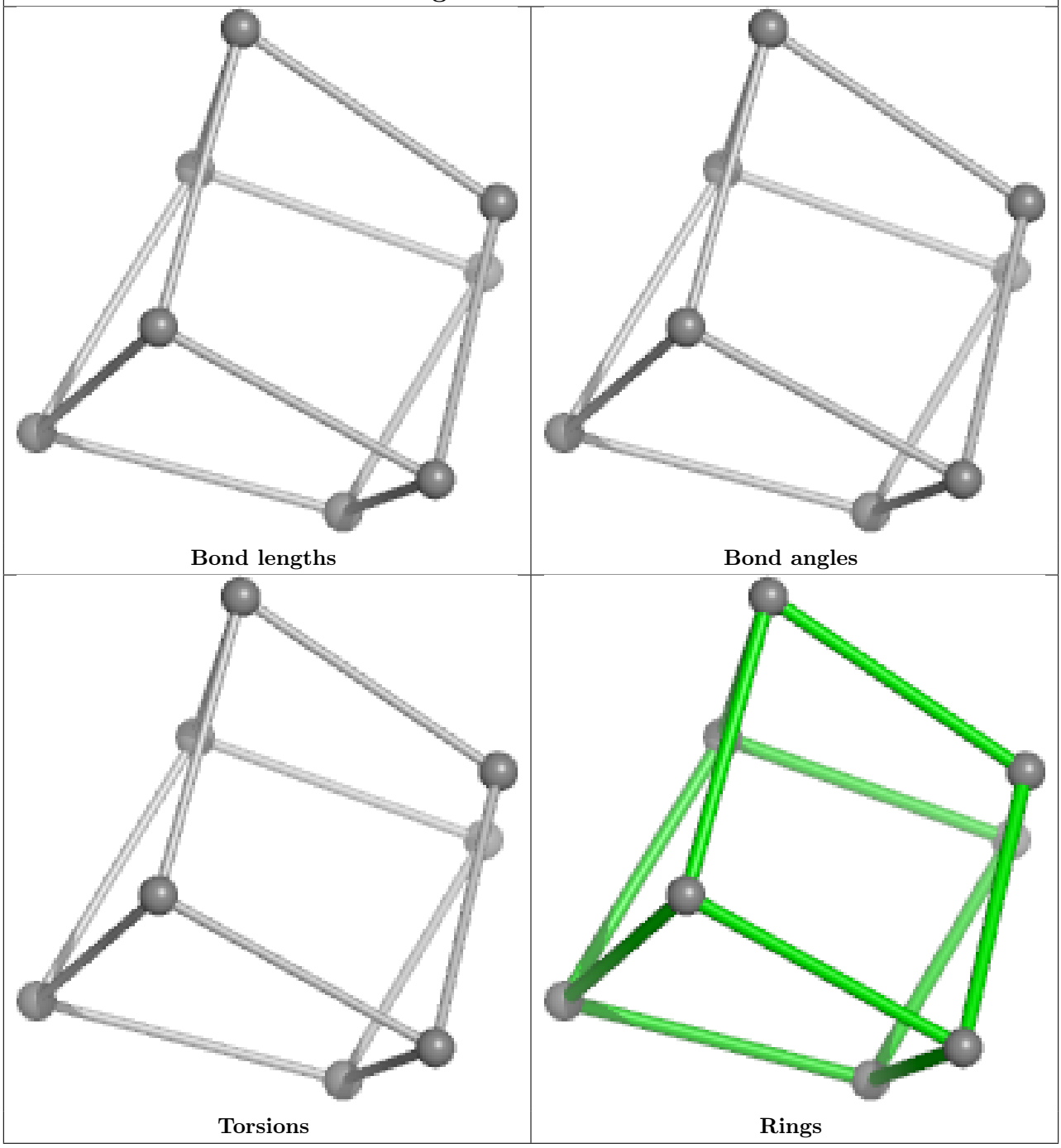
There are no ring outliers.

12 monomers are involved in 43 short contacts:

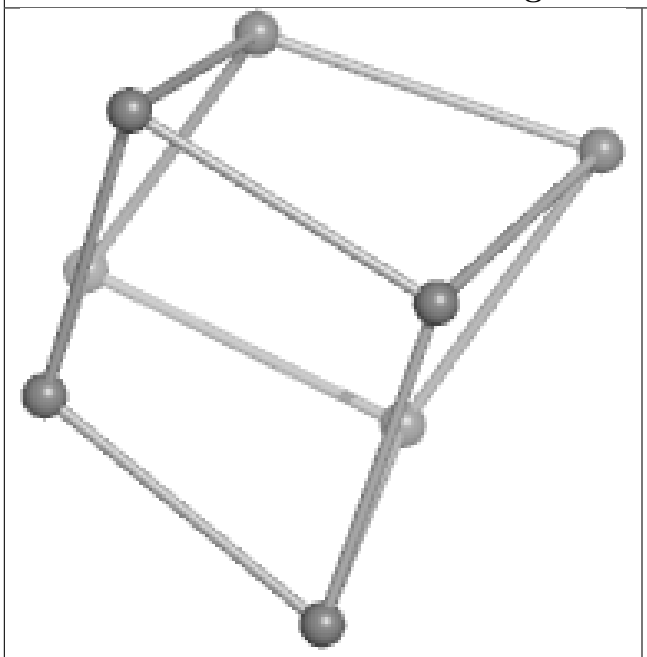
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	601	FMN	1	0
5	E	1001	MGD	5	0
8	F	602	SF4	1	0
7	C	201	FES	4	0
7	G	201	FES	4	0
5	E	1002	MGD	7	0
5	A	1002	MGD	7	0
7	A	1004	FES	3	0
8	B	602	SF4	1	0
7	E	1004	FES	3	0
5	A	1001	MGD	5	0
10	F	601	FMN	2	0

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 SF4 A 1006



Ligand SF4 E 1006



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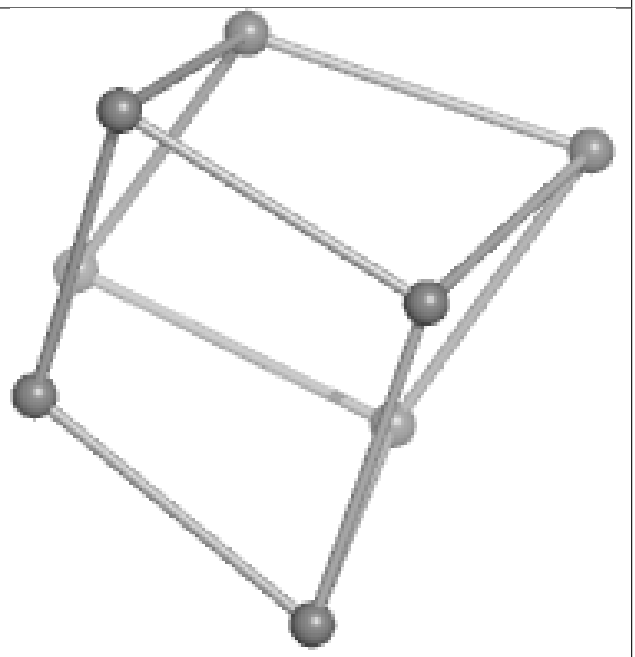
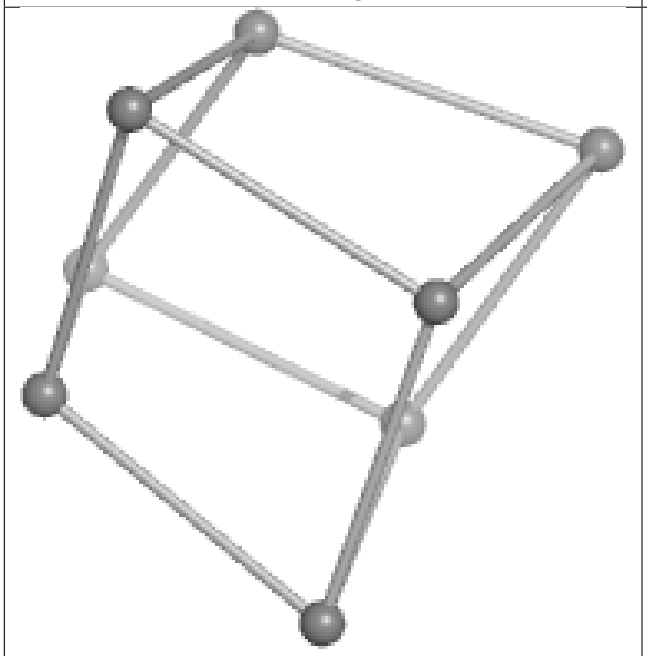
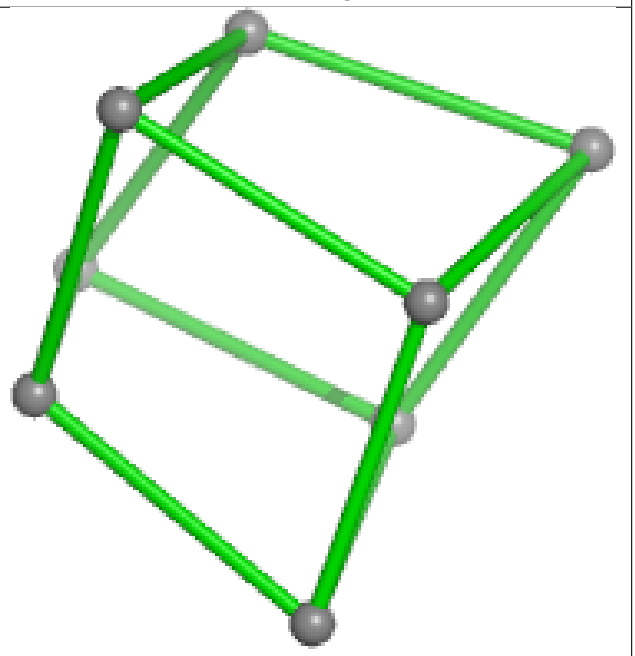


Bond angles

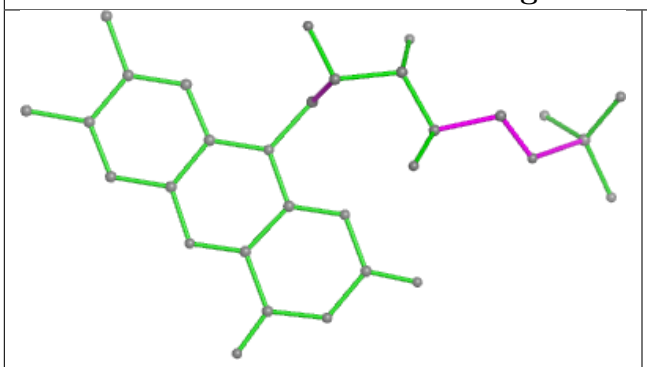


Torsions

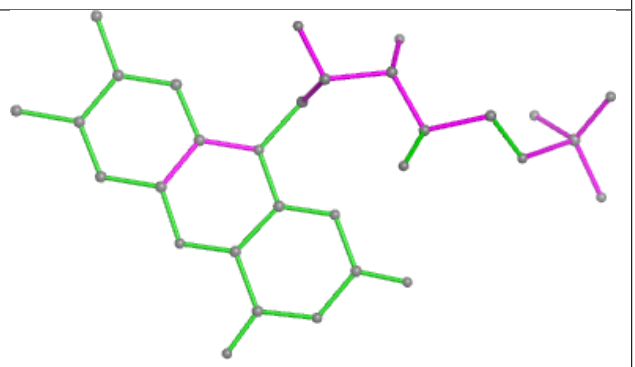


Rings

Ligand FMN B 601



Bond lengths



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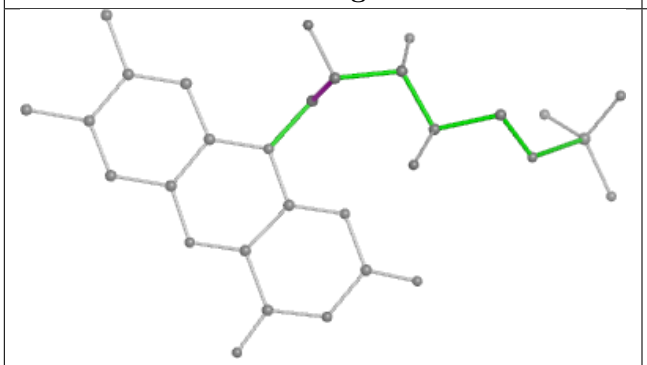
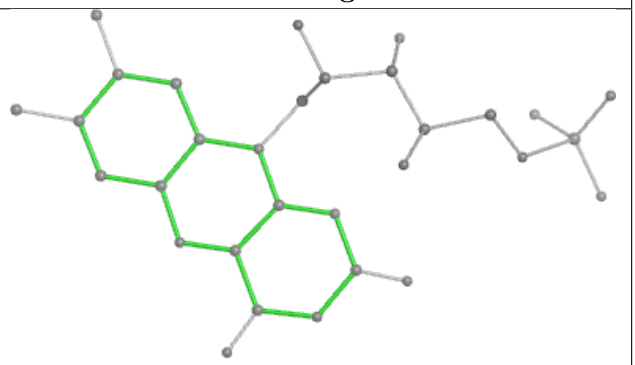
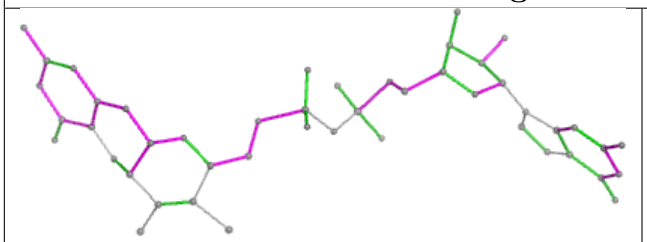


Torsions

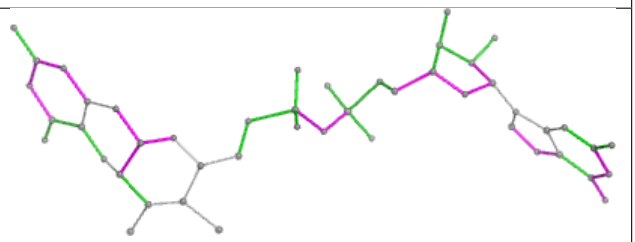


Rings

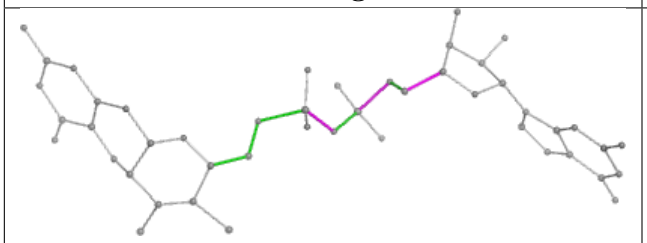
Ligand MGD E 1001



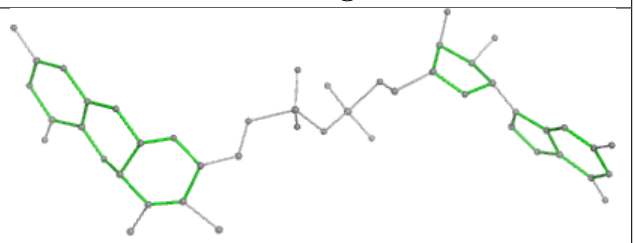
Bond lengths



Bond angles

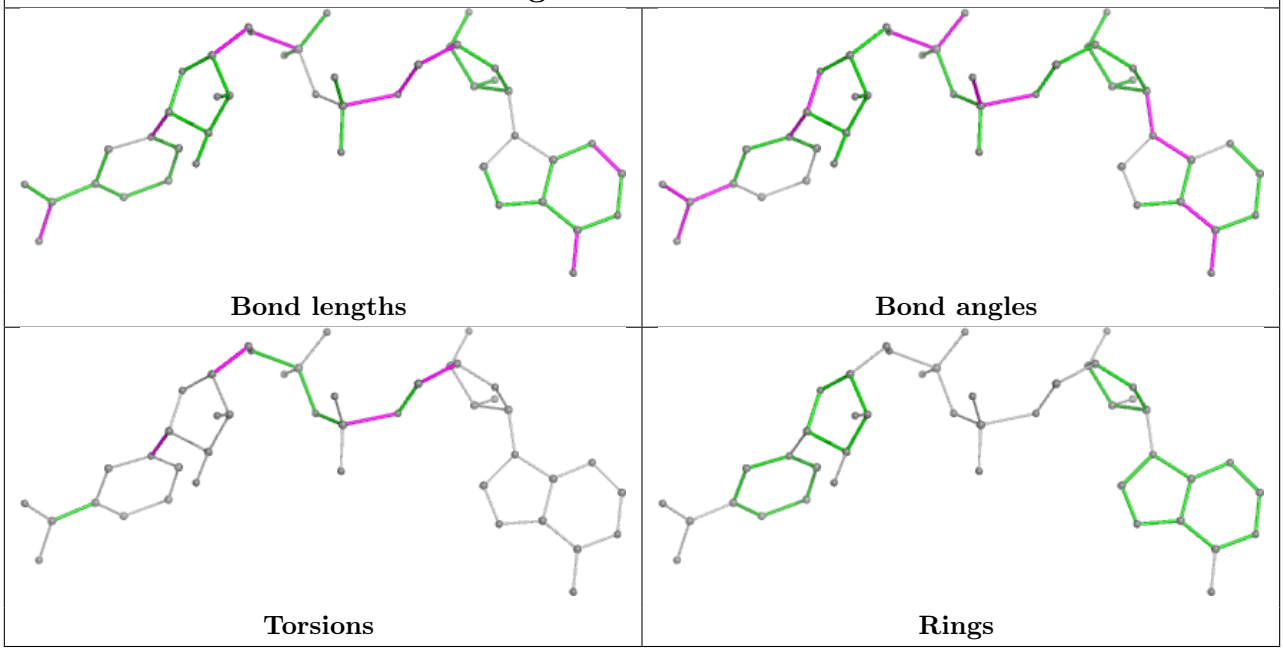


Torsions

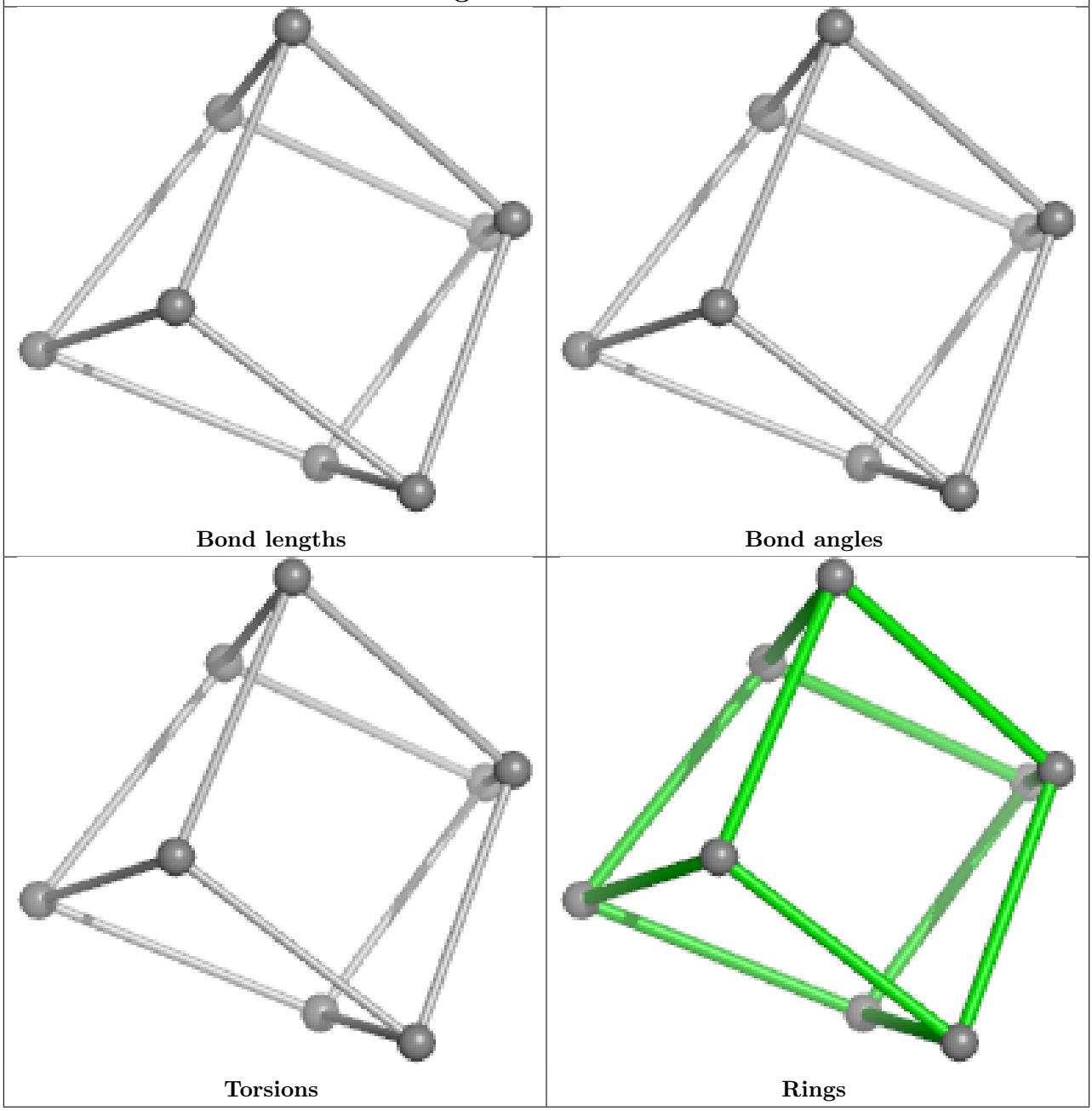


Rings

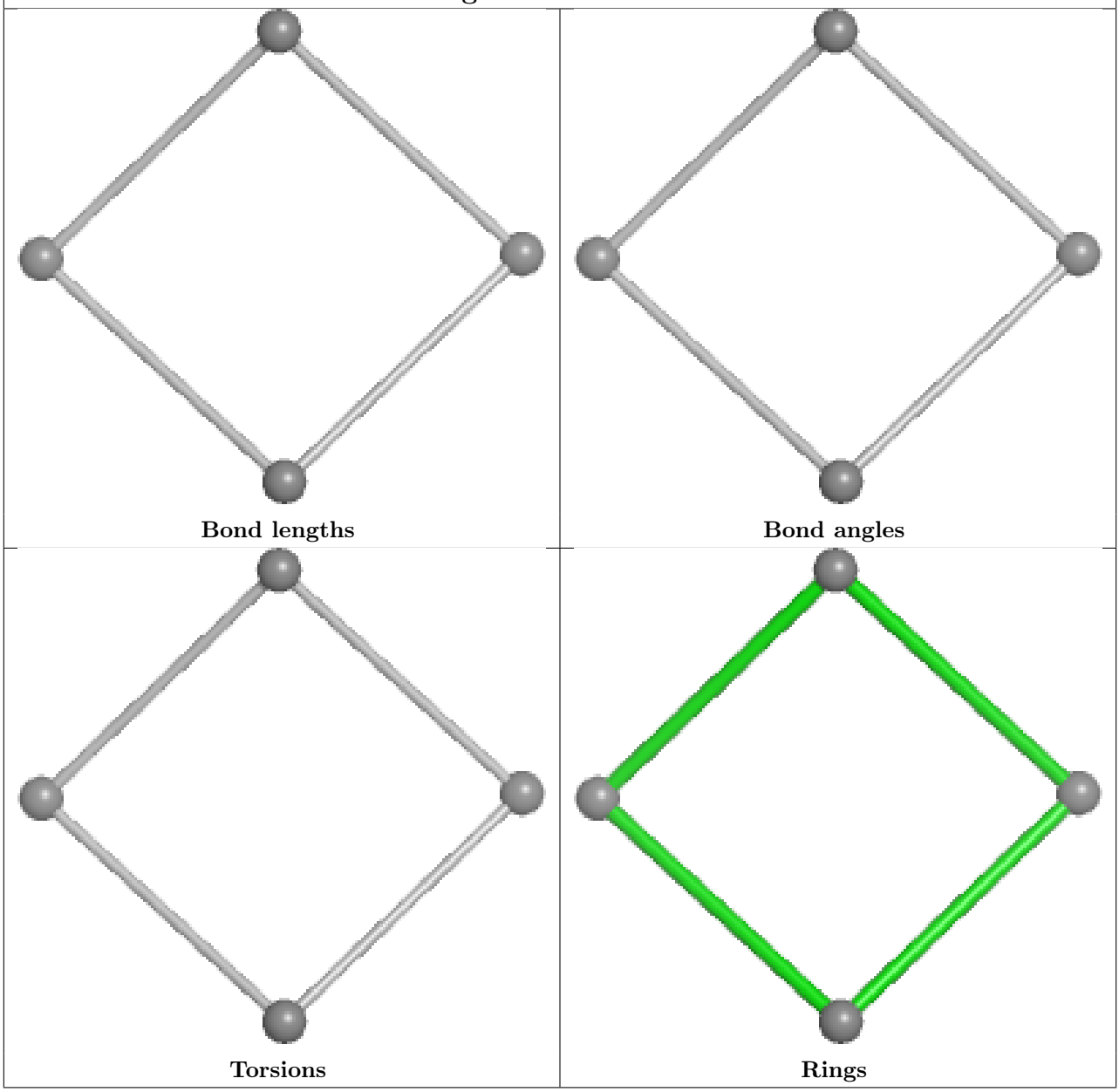
Ligand NAI B 603



Ligand SF4 F 602



Ligand FES C 201



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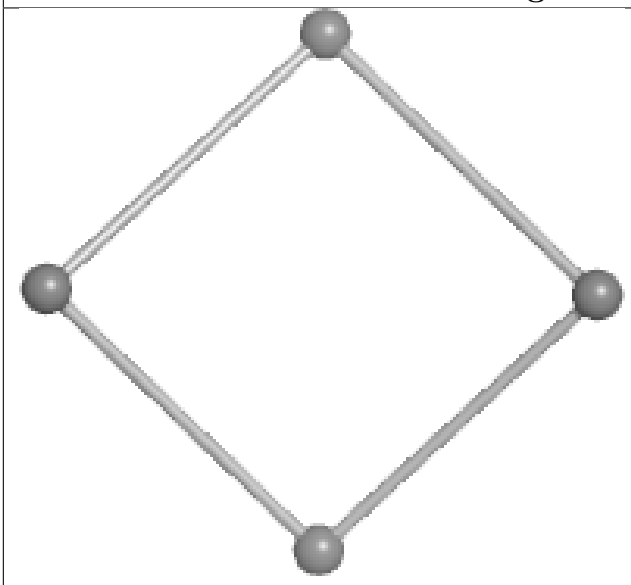
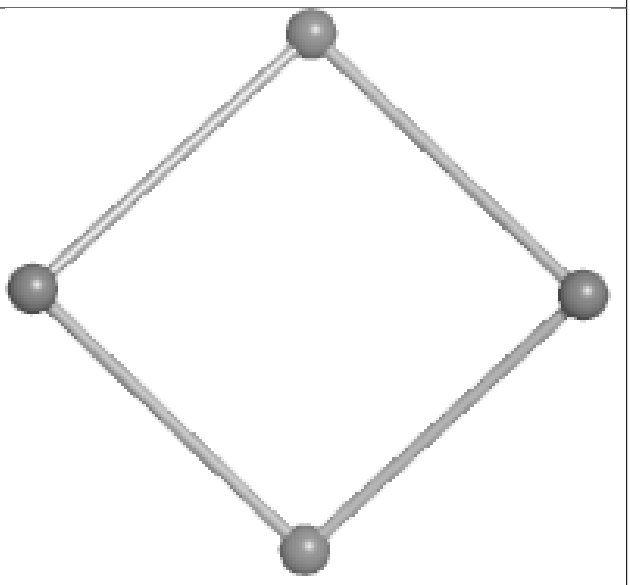
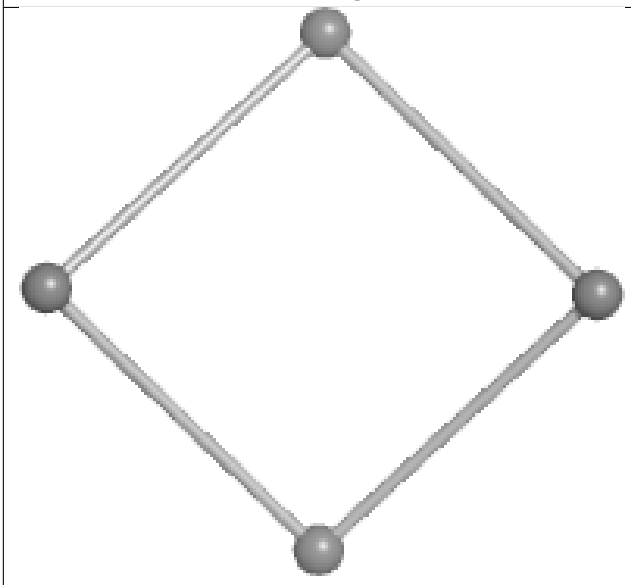


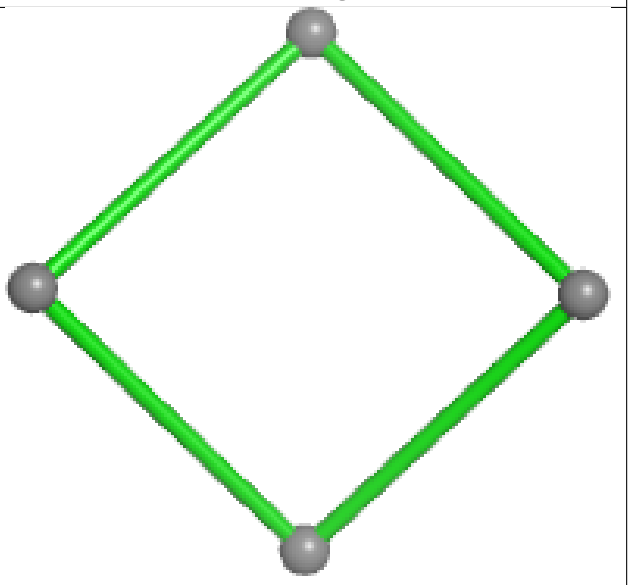
Bond lengths



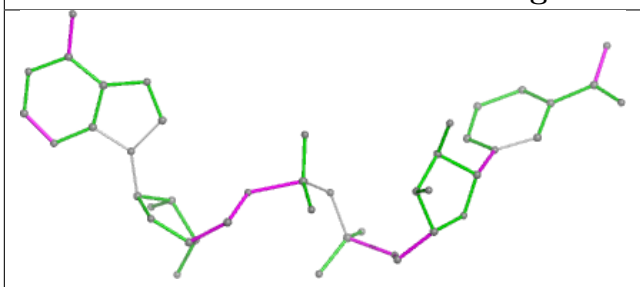
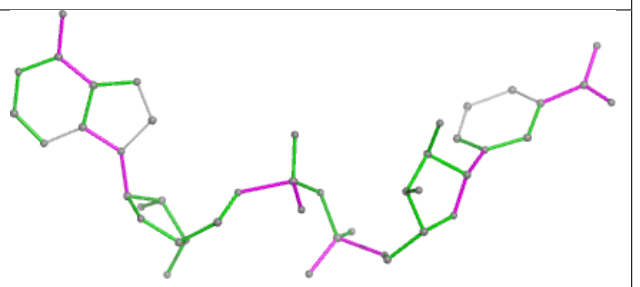
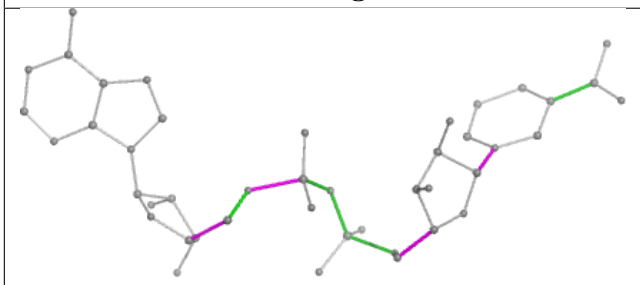
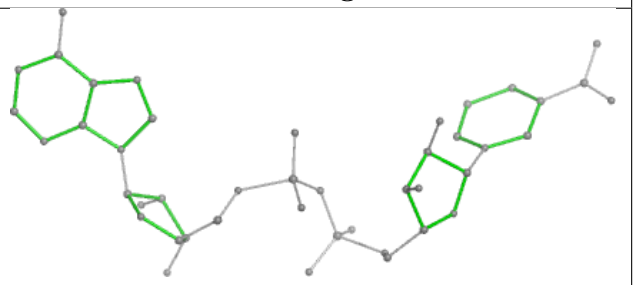
Bond angles



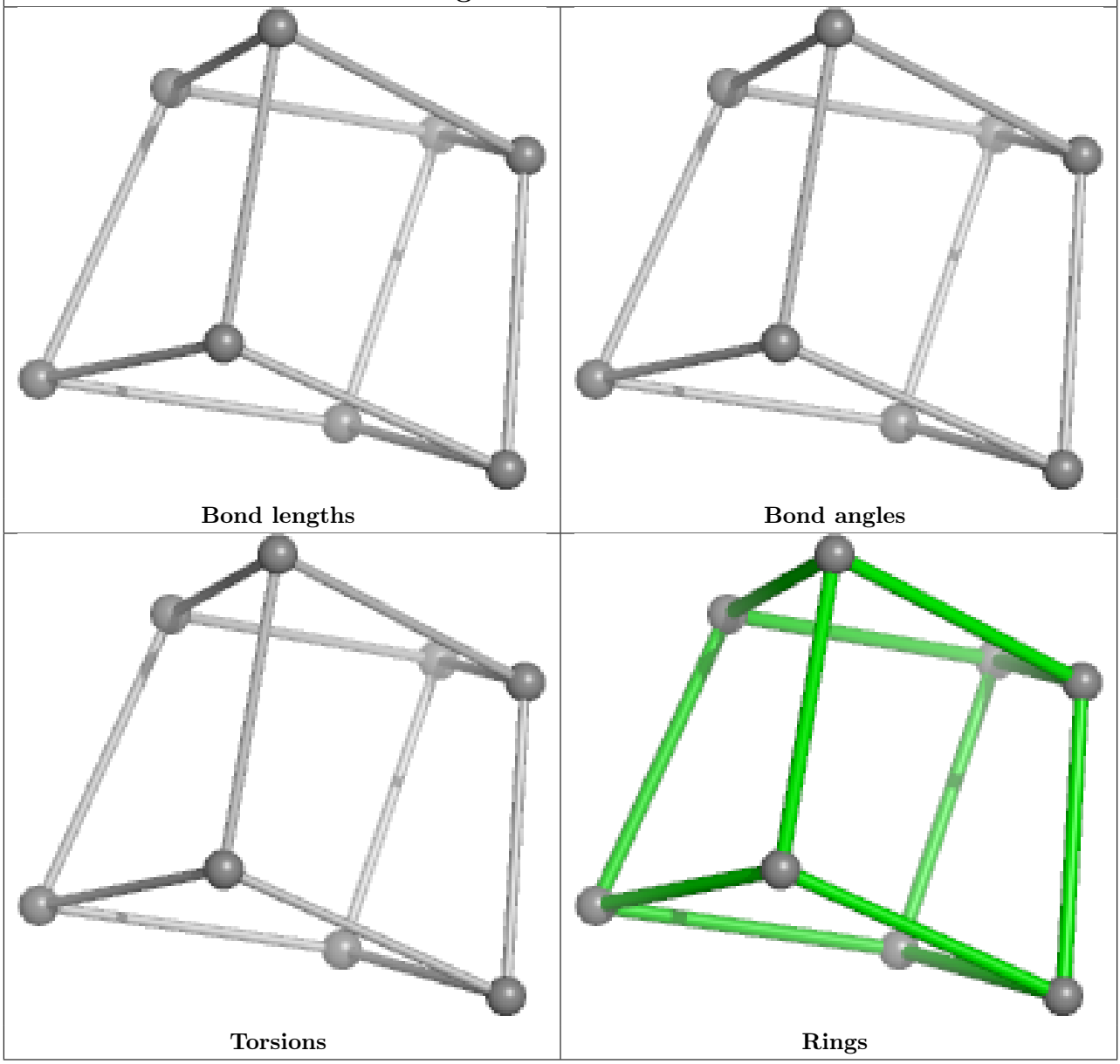
Torsions

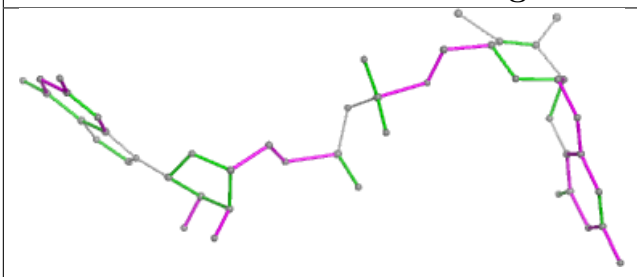
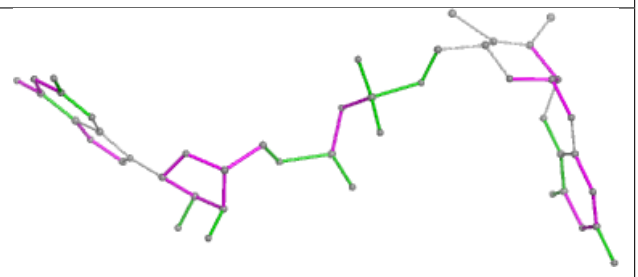
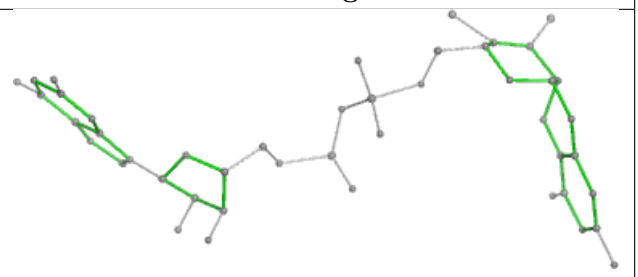


Rings

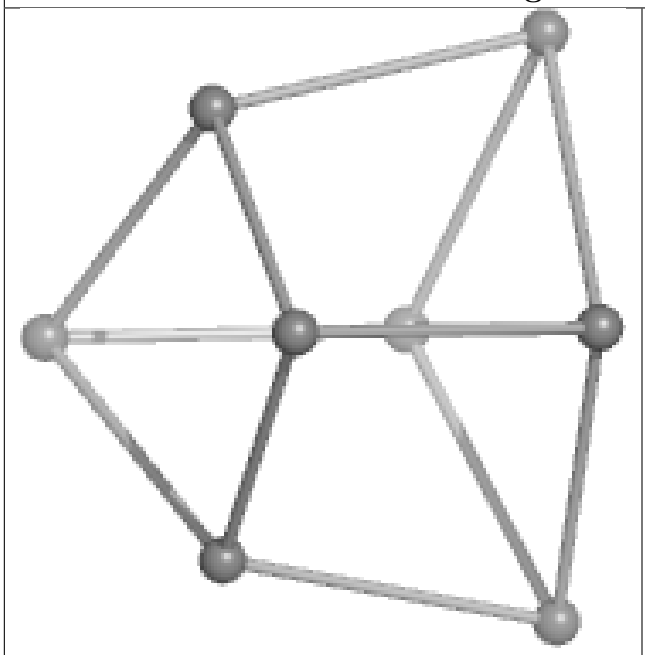
Ligand NAI F 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SF4 A 1005

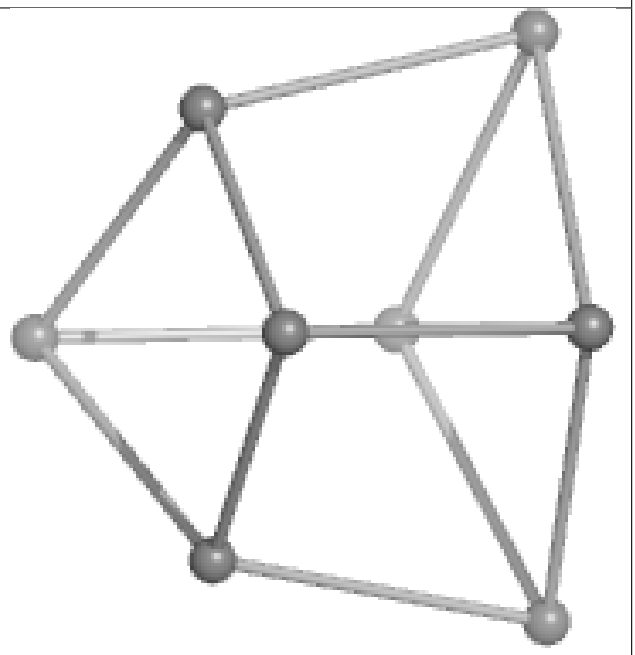


Ligand MGD E 1002	
 Bond lengths	 Bond angles
Torsions	 Rings

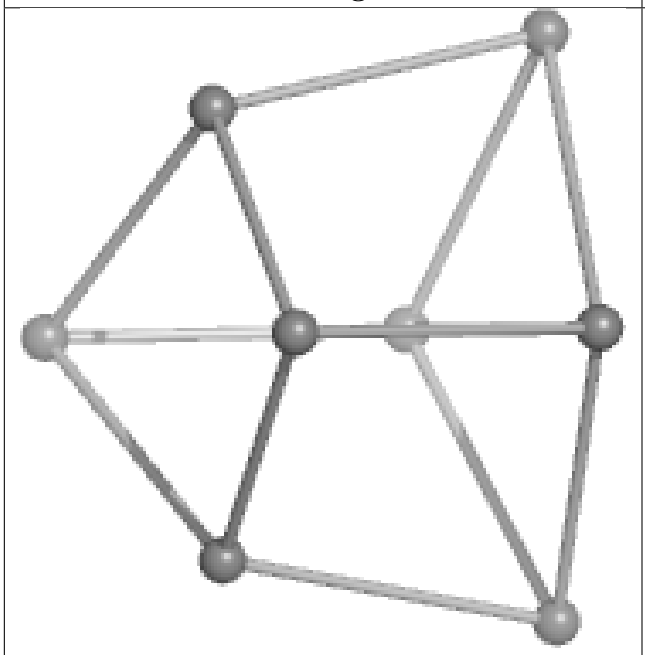
Ligand SF4 E 1008



Bond lengths



Bond angles



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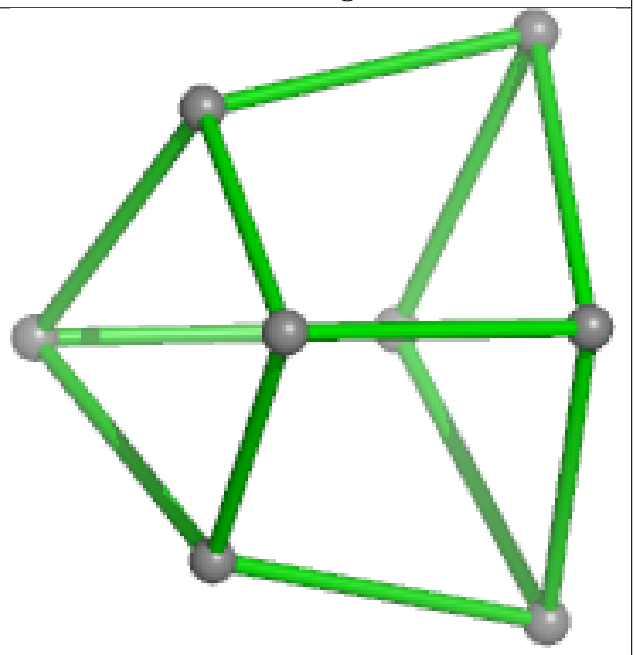
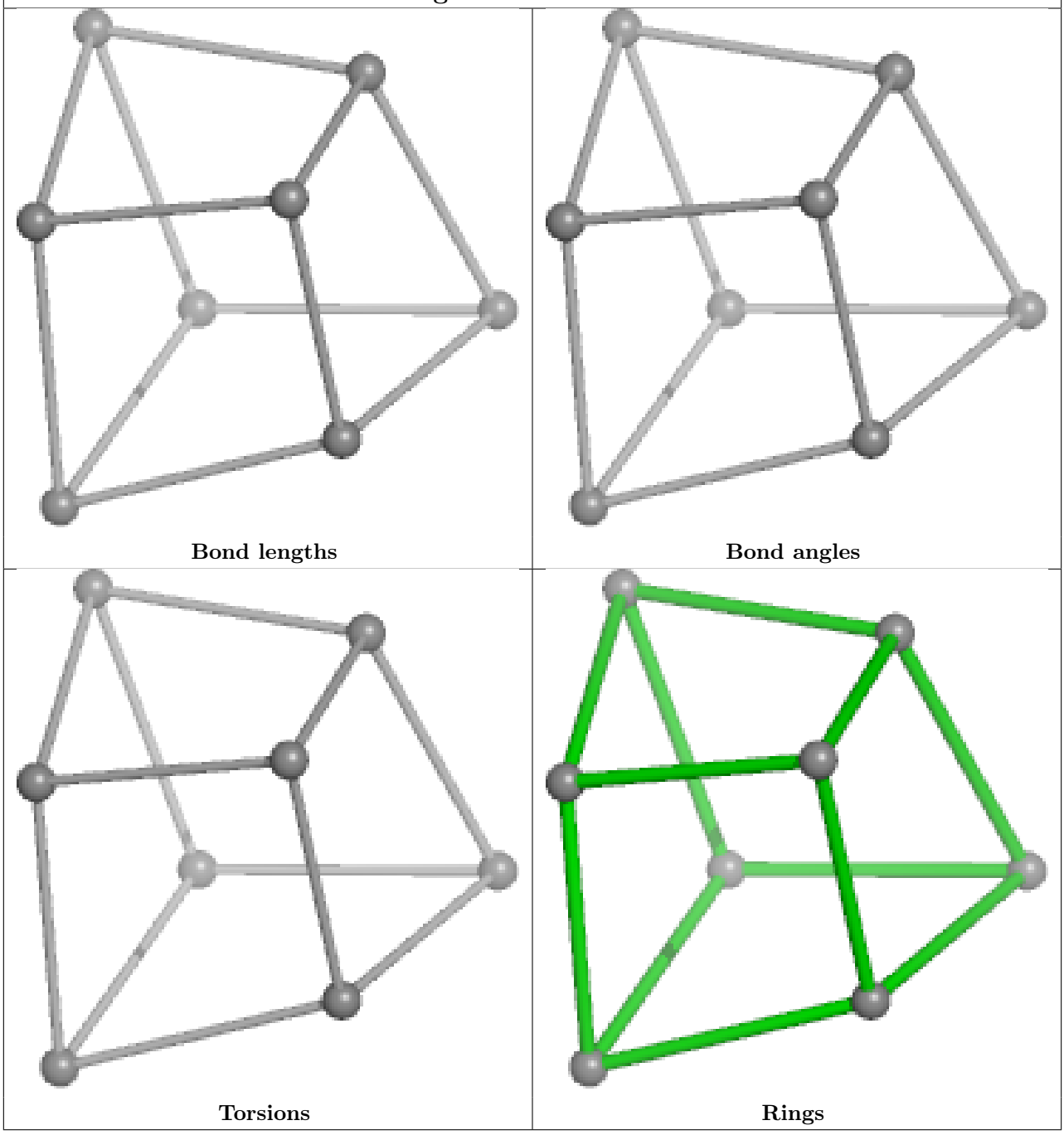
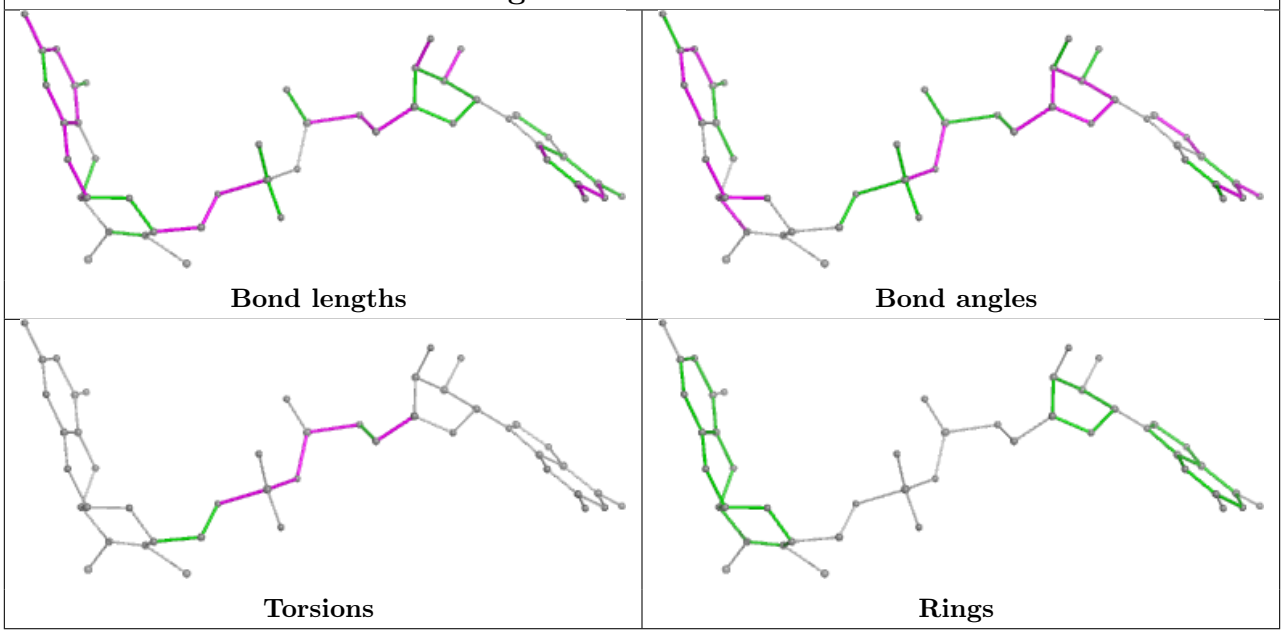


Rings

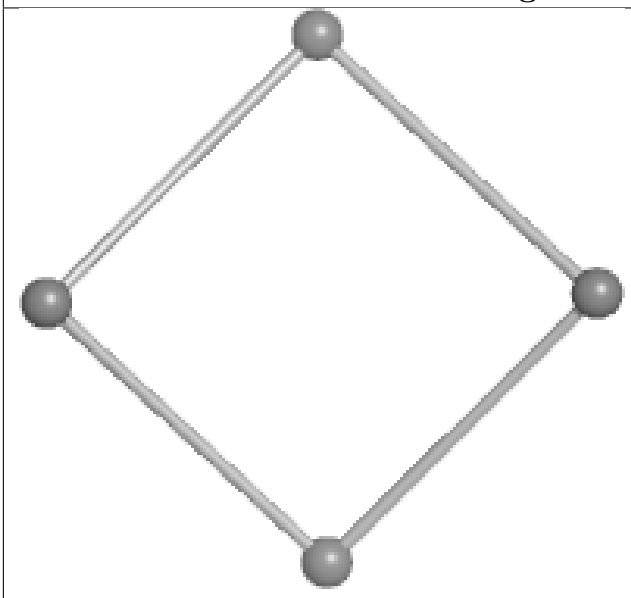
Ligand SF4 A 1008



Ligand MGD A 1002



Ligand FES A 1004



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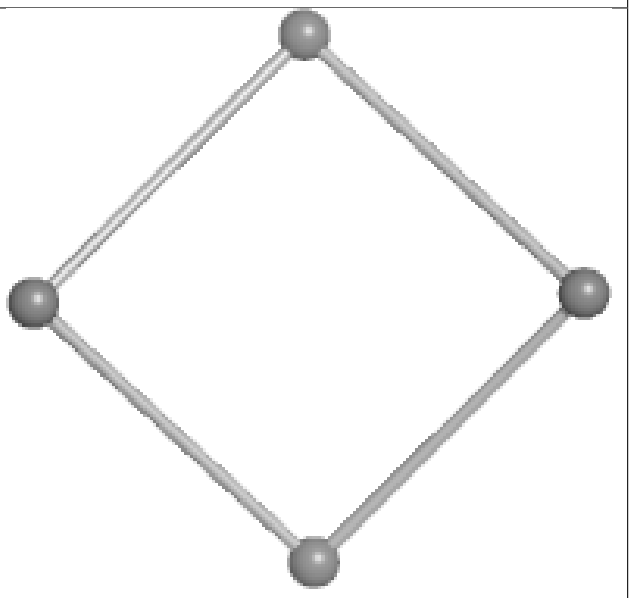
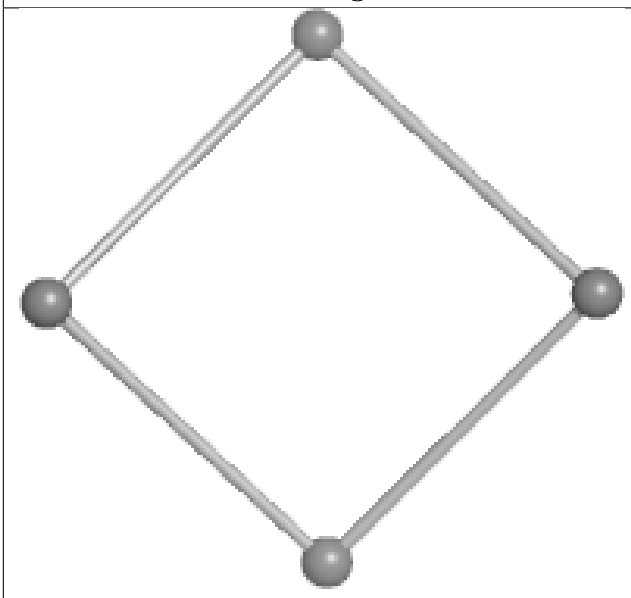
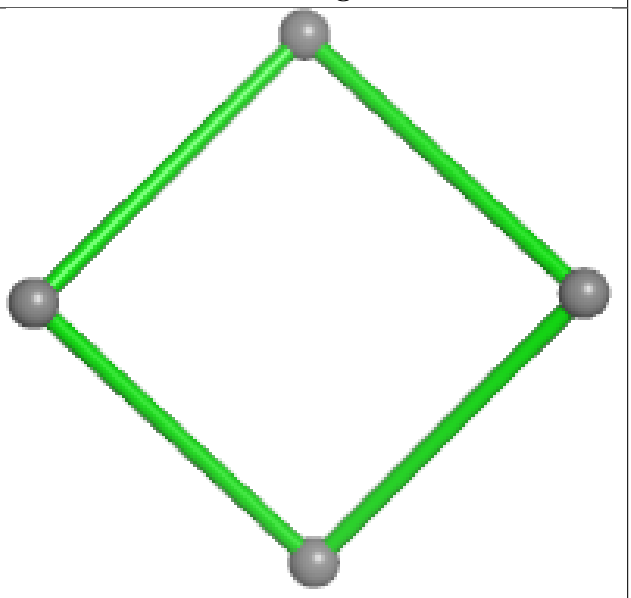


Bond angles

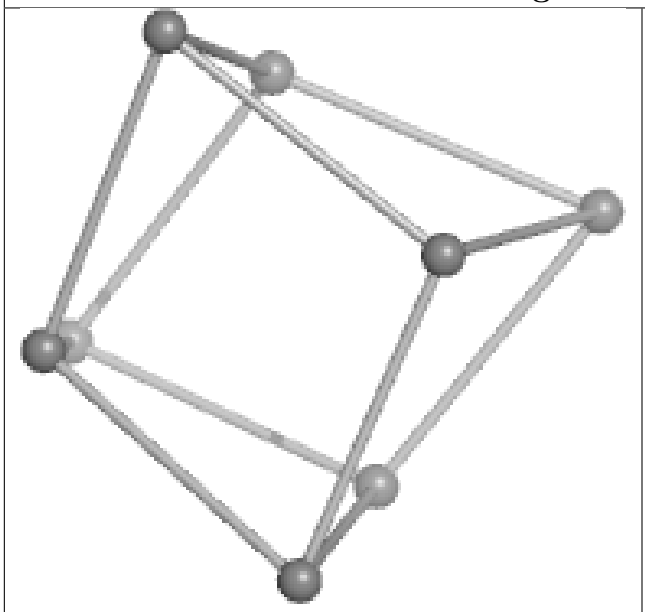


Torsions

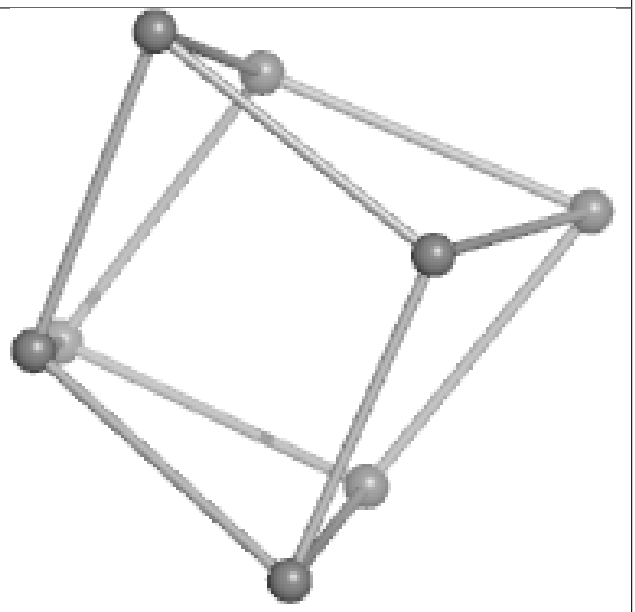


Rings

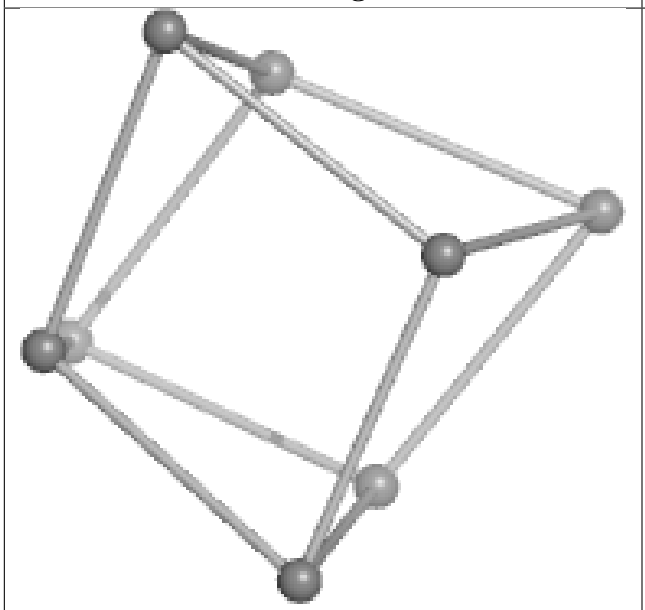
Ligand SF4 B 602



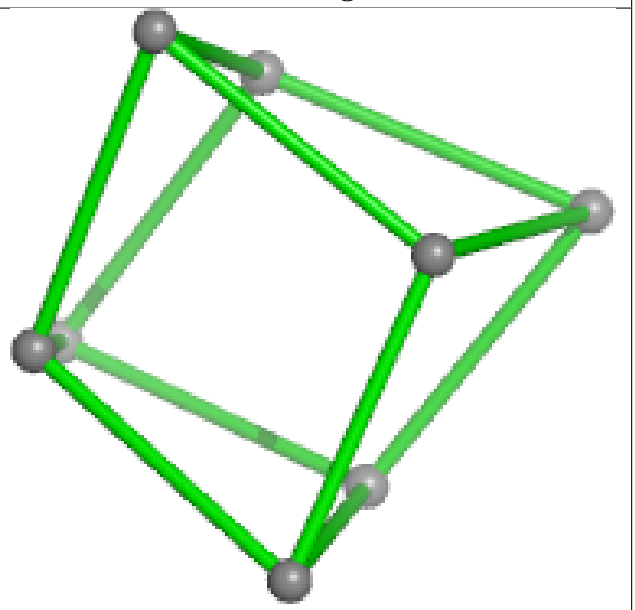
Bond lengths



Bond angles

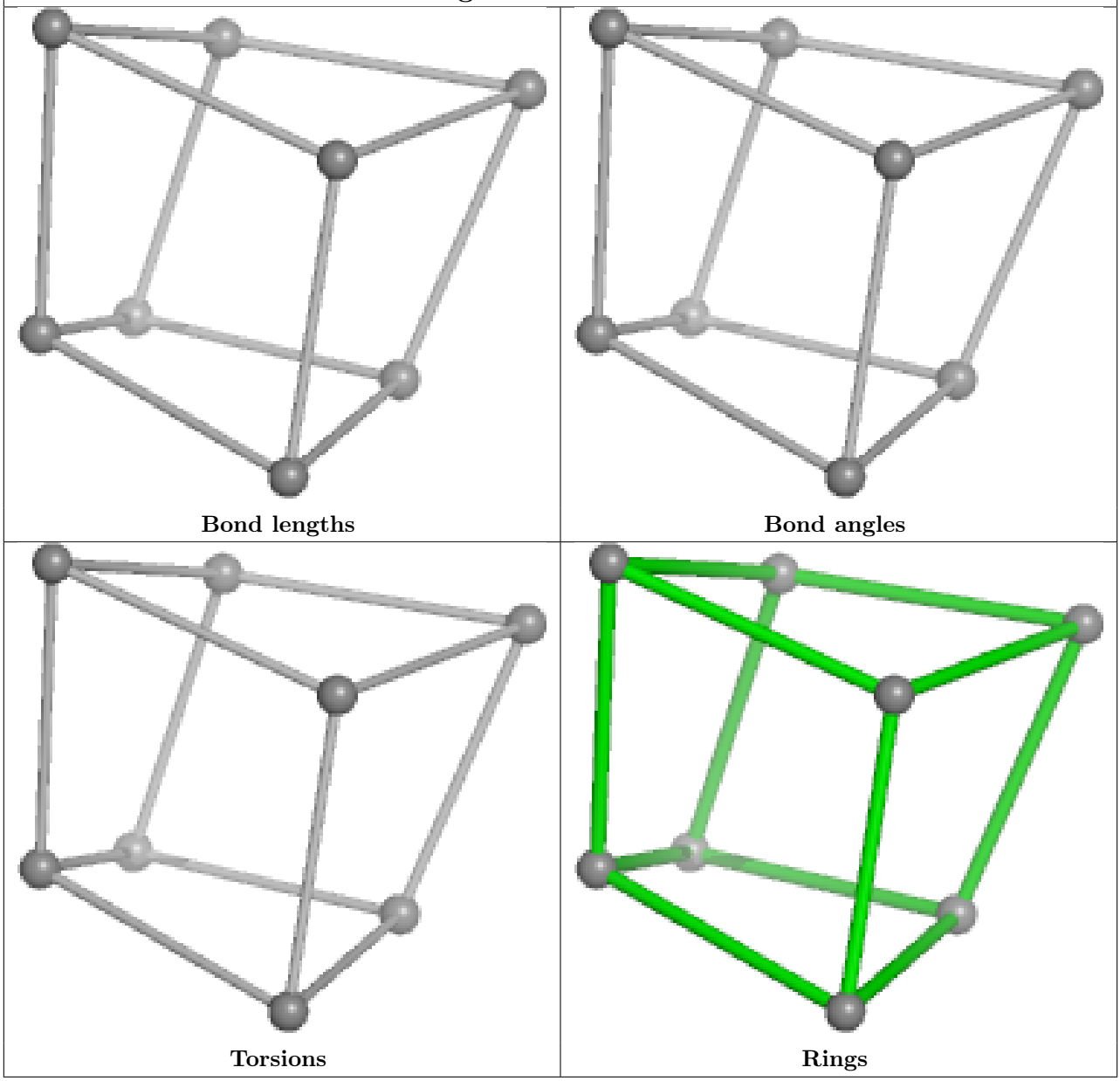


Torsions

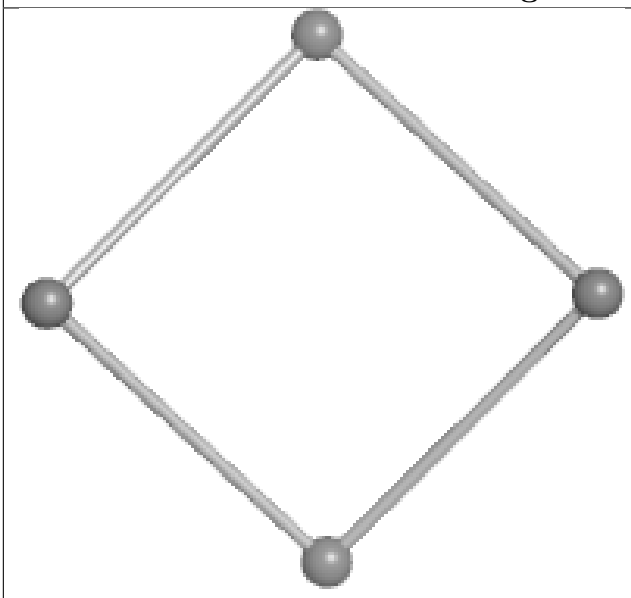


Rings

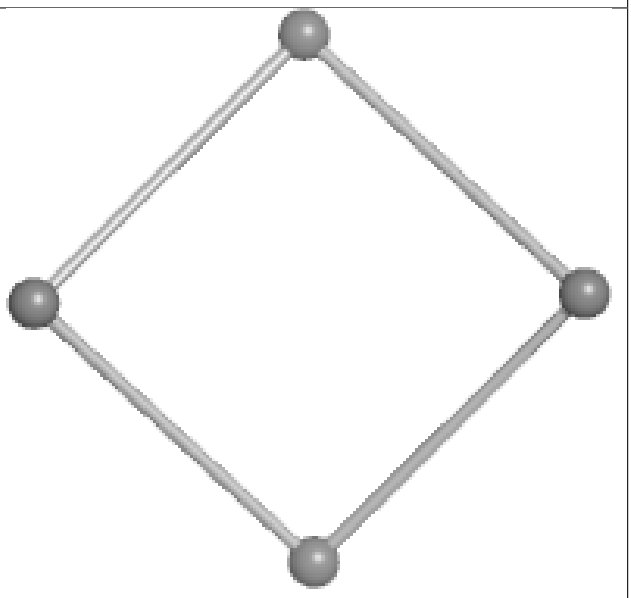
Ligand SF4 E 1005



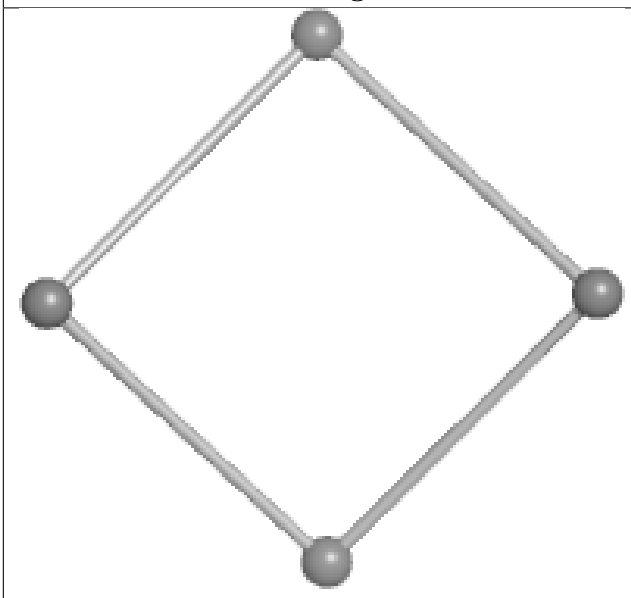
Ligand FES E 1004



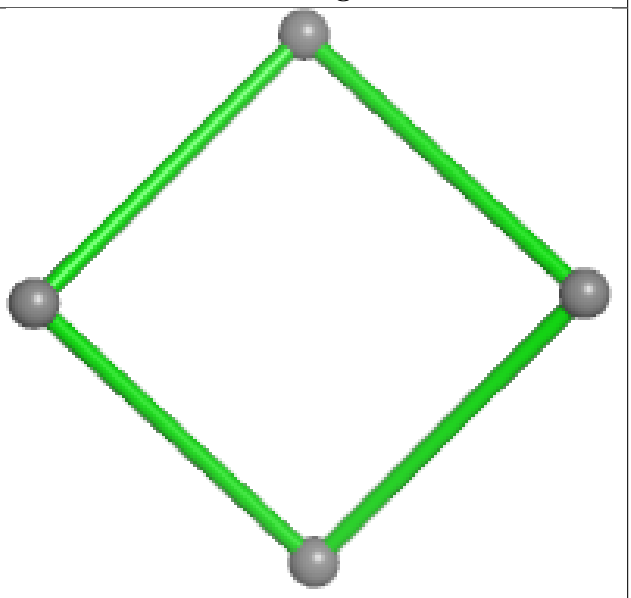
Bond lengths



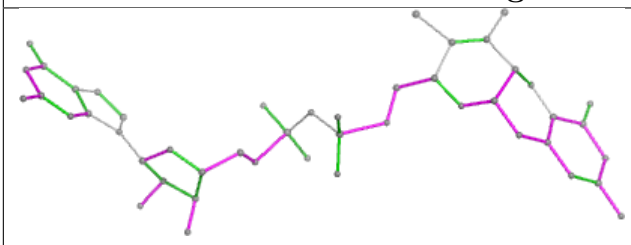
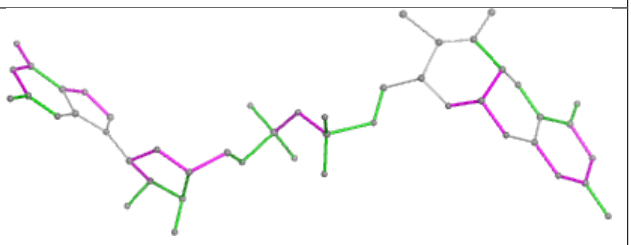
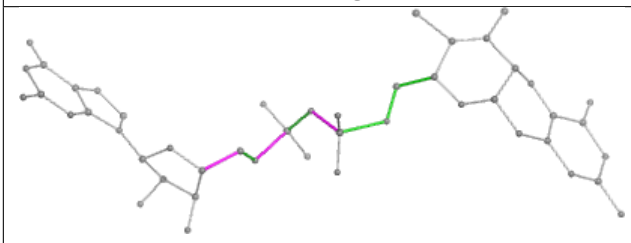
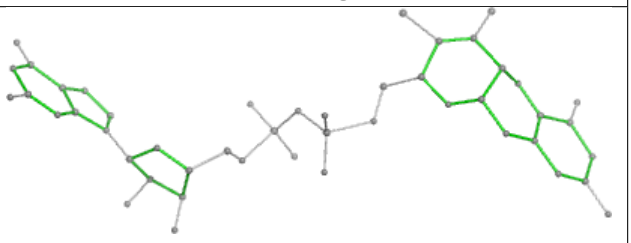
Bond angles

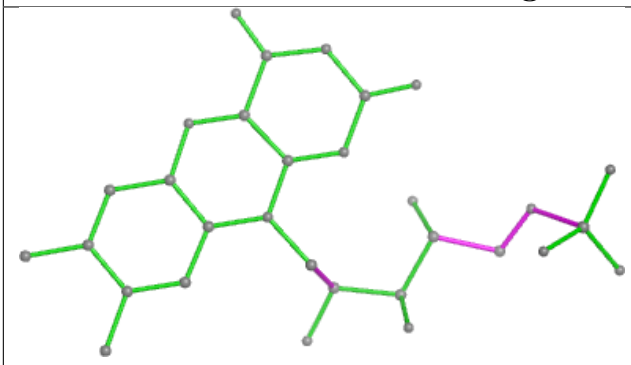
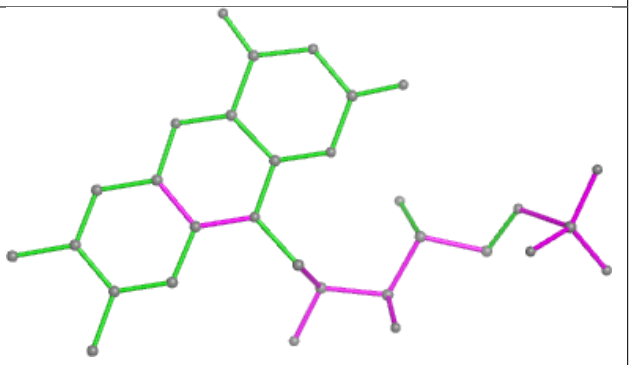
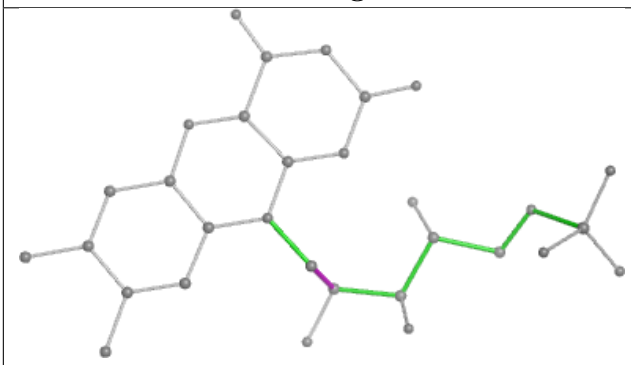
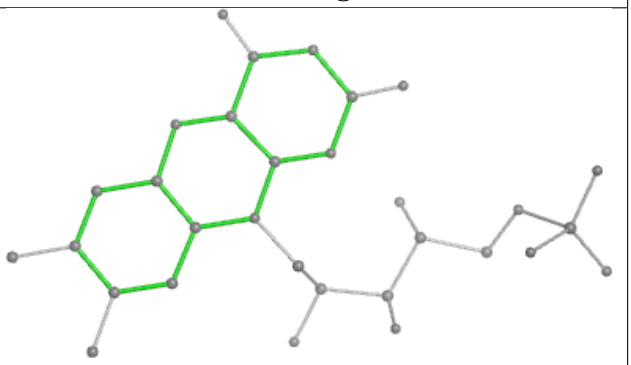


Torsions

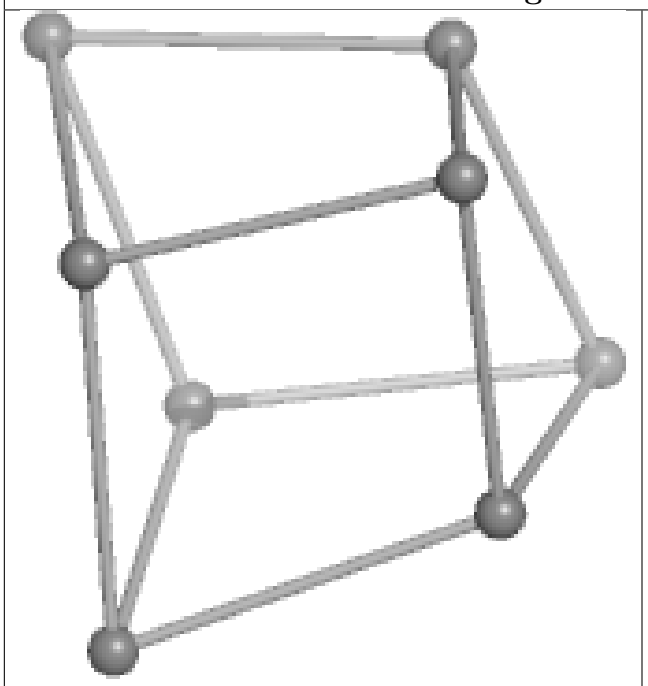


Rings

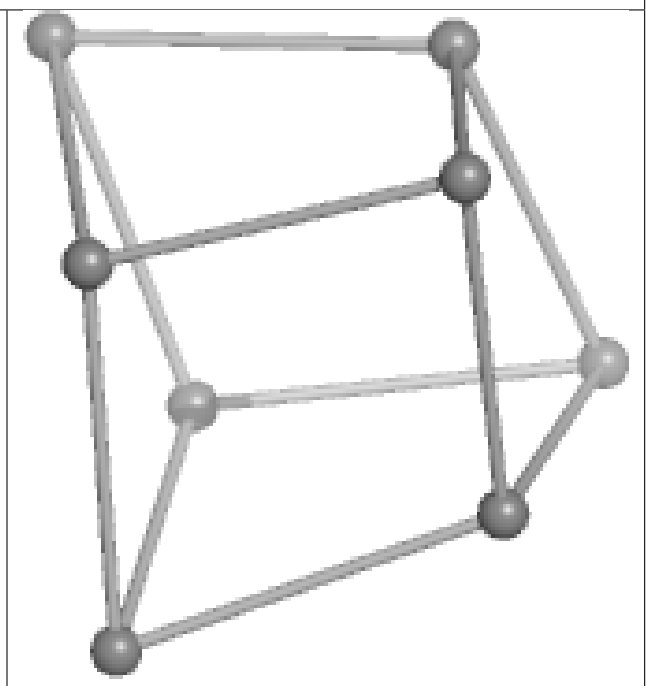
Ligand MGD A 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FMN F 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

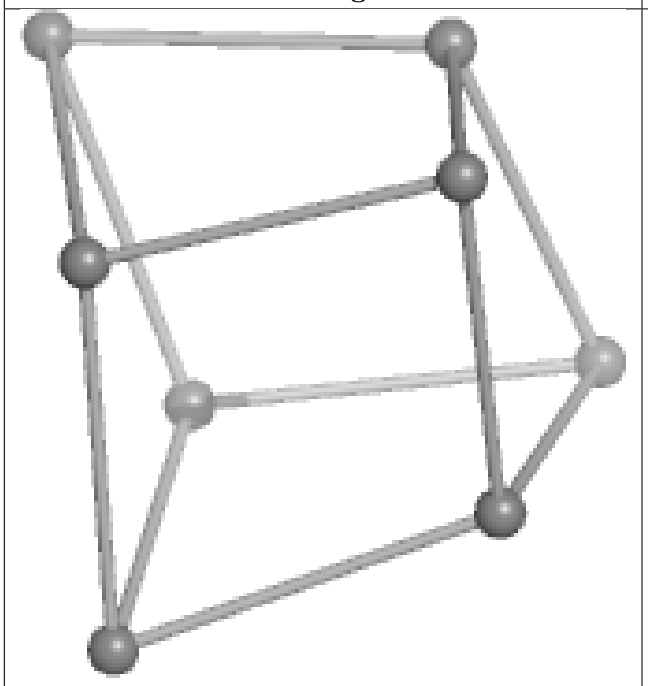
Ligand SF4 E 1007



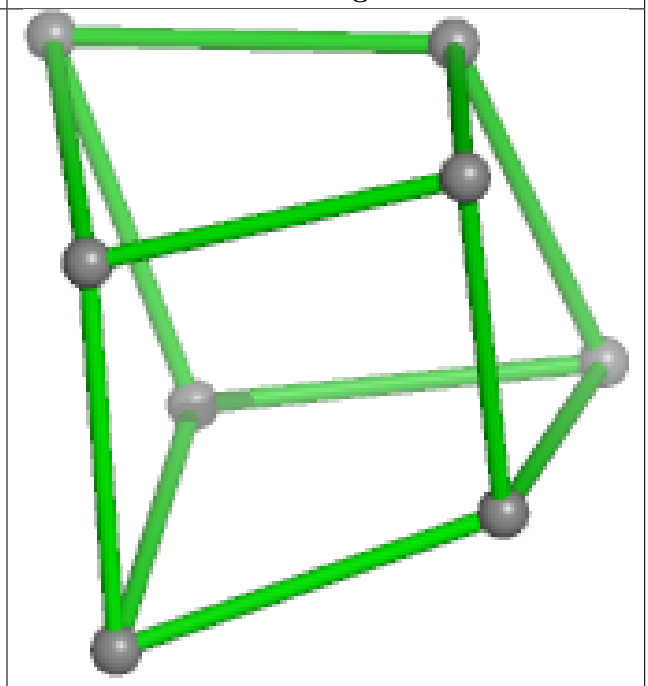
Bond lengths



Bond angles

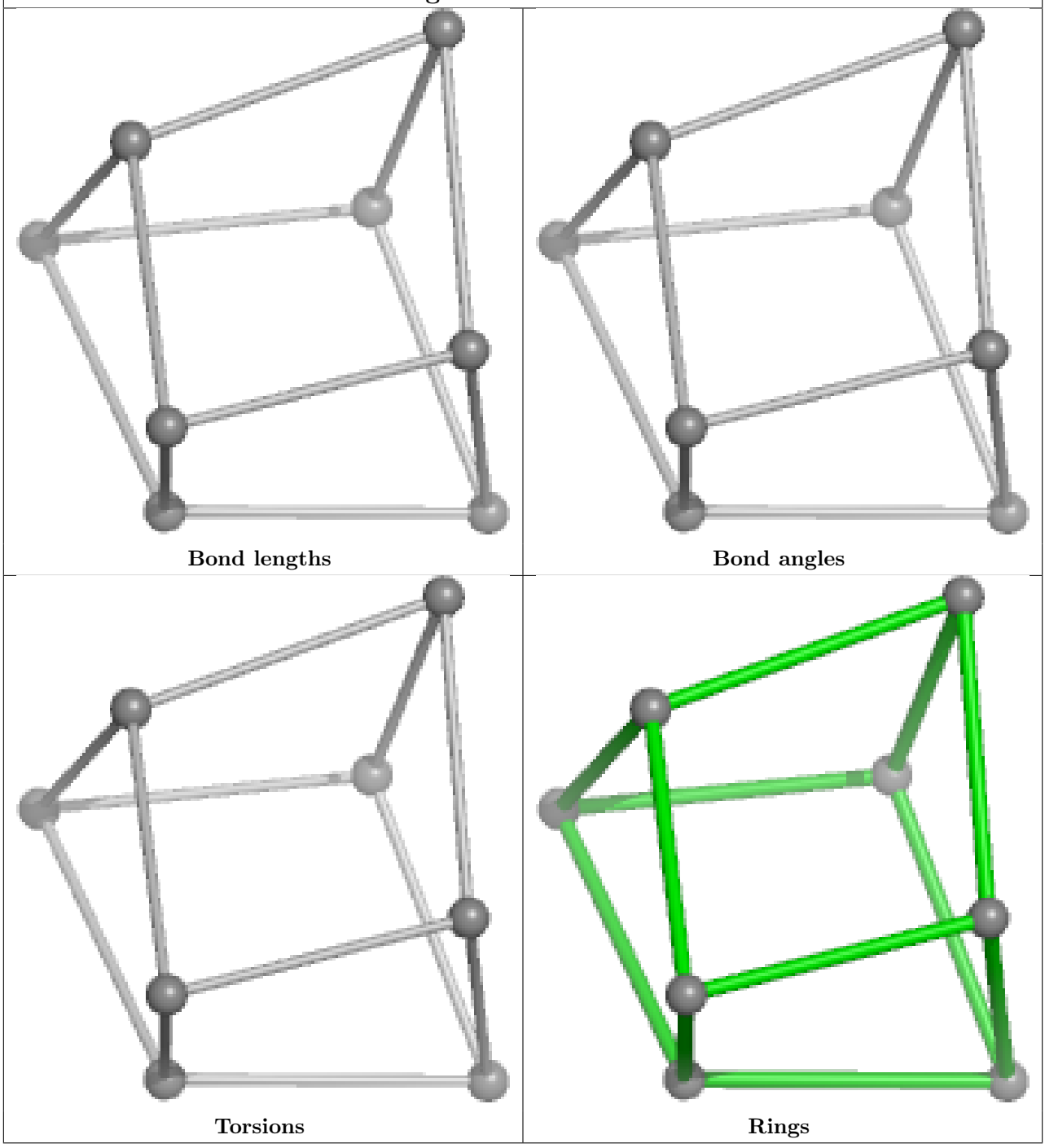


Torsions



Rings

Ligand SF4 A 1007



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.

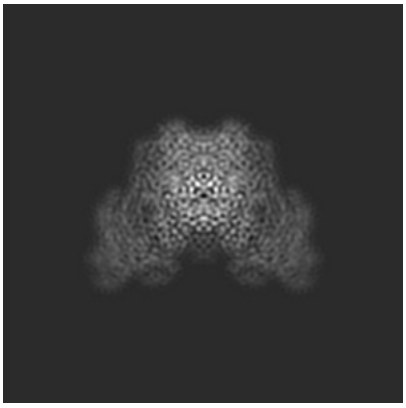
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10495. These allow visual inspection of the internal detail of the map and identification of artifacts.

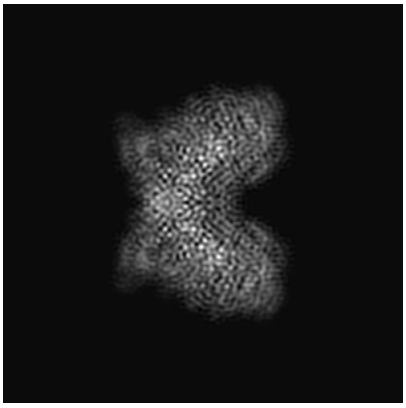
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

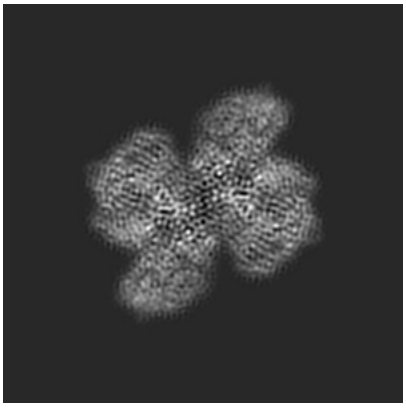
6.1.1 Primary map



X



Y



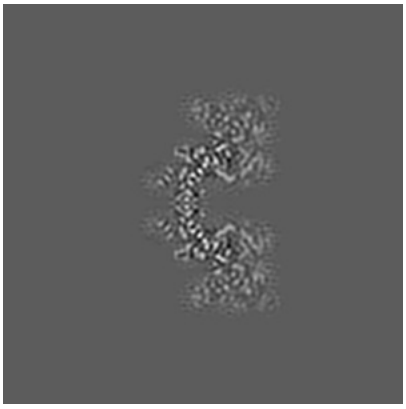
Z

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

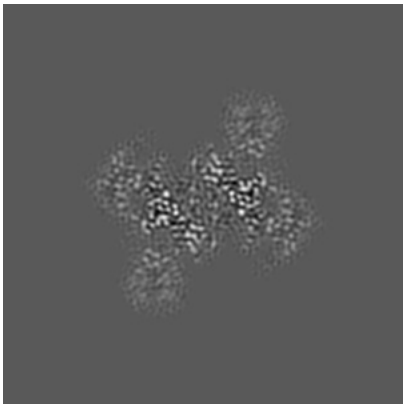
6.2 Central slices (i)

6.2.1 Primary map

X Index: 112



Y Index: 112



Z Index: 112

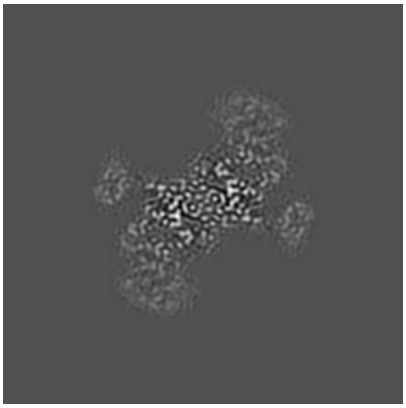
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 137

Y Index: 114

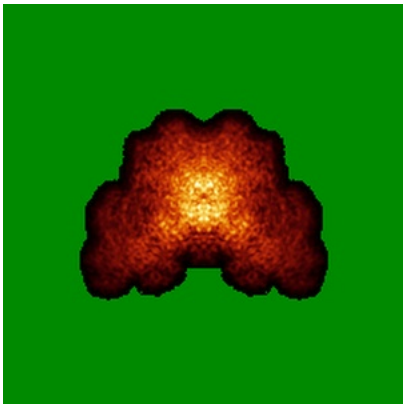


Z Index: 106

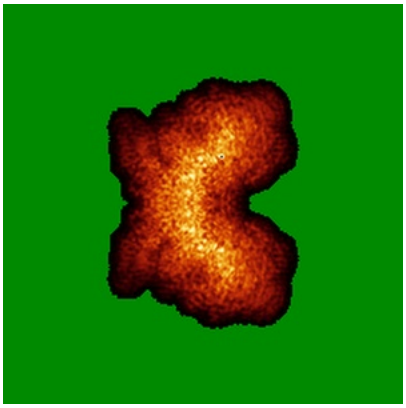
The images above show the largest variance slices of the map in three orthogonal directions.

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

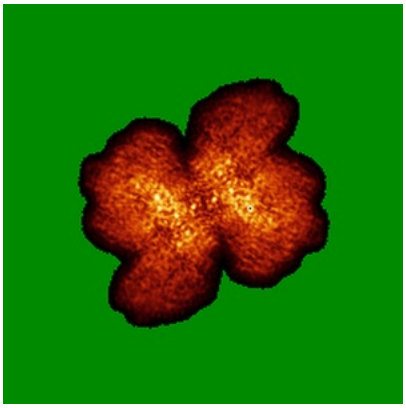
6.4.1 Primary map



X



Y

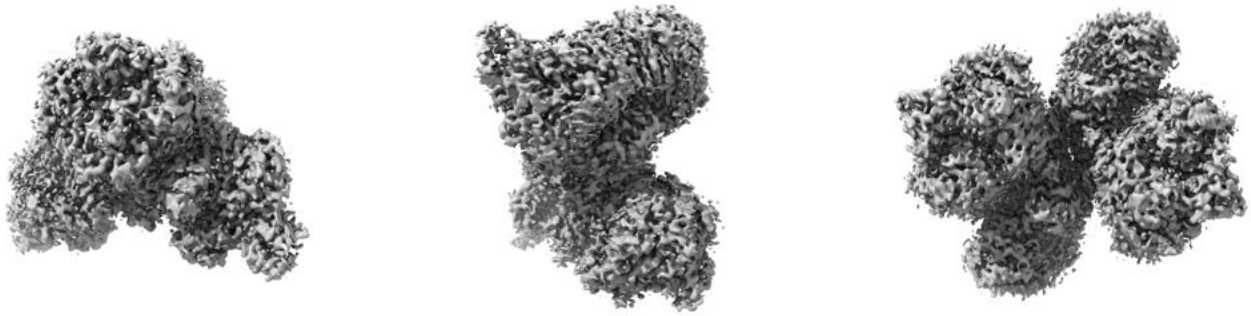


Z

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 0.0223. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

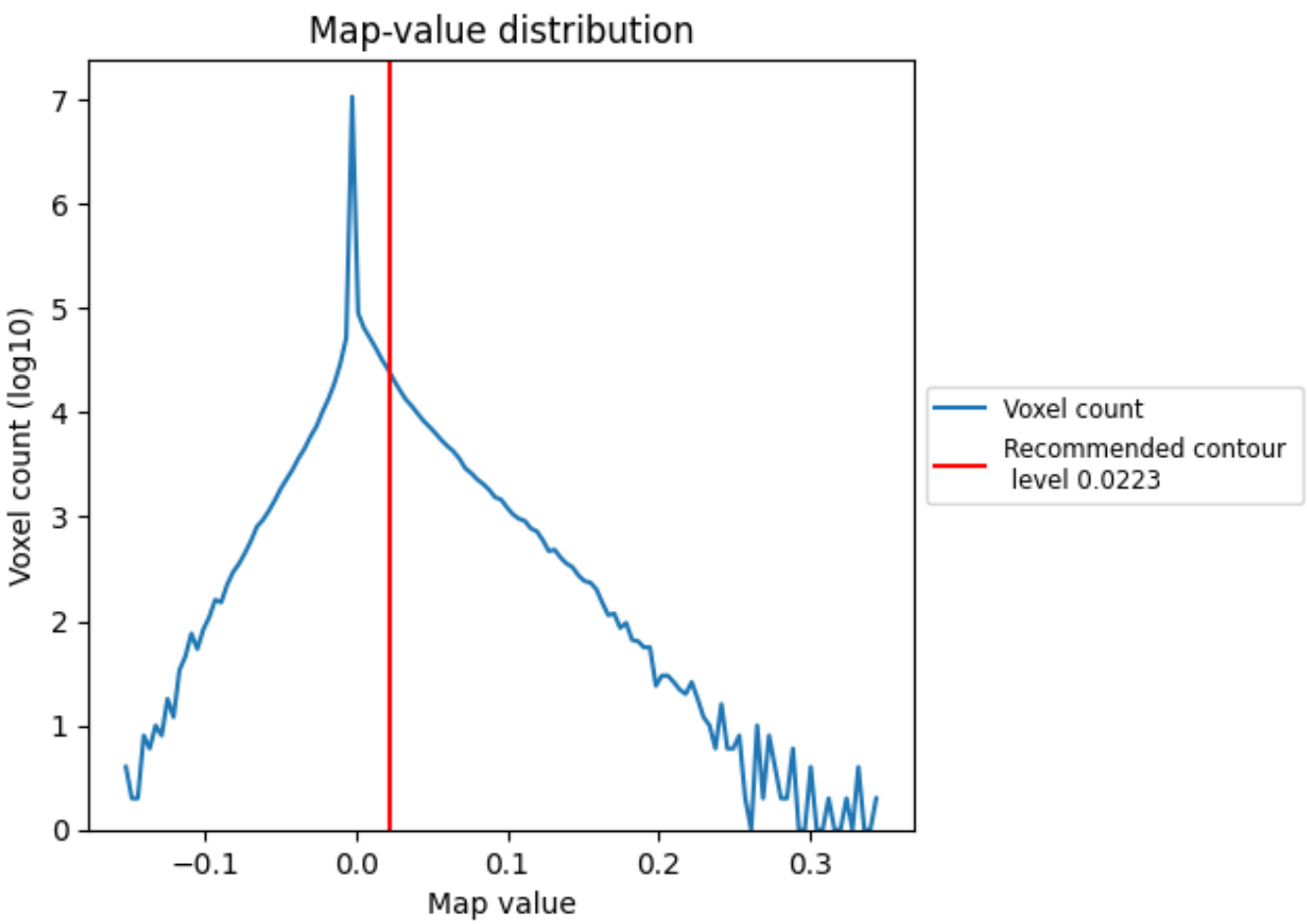
6.6 Mask visualisation (i)

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

7 Map analysis (i)

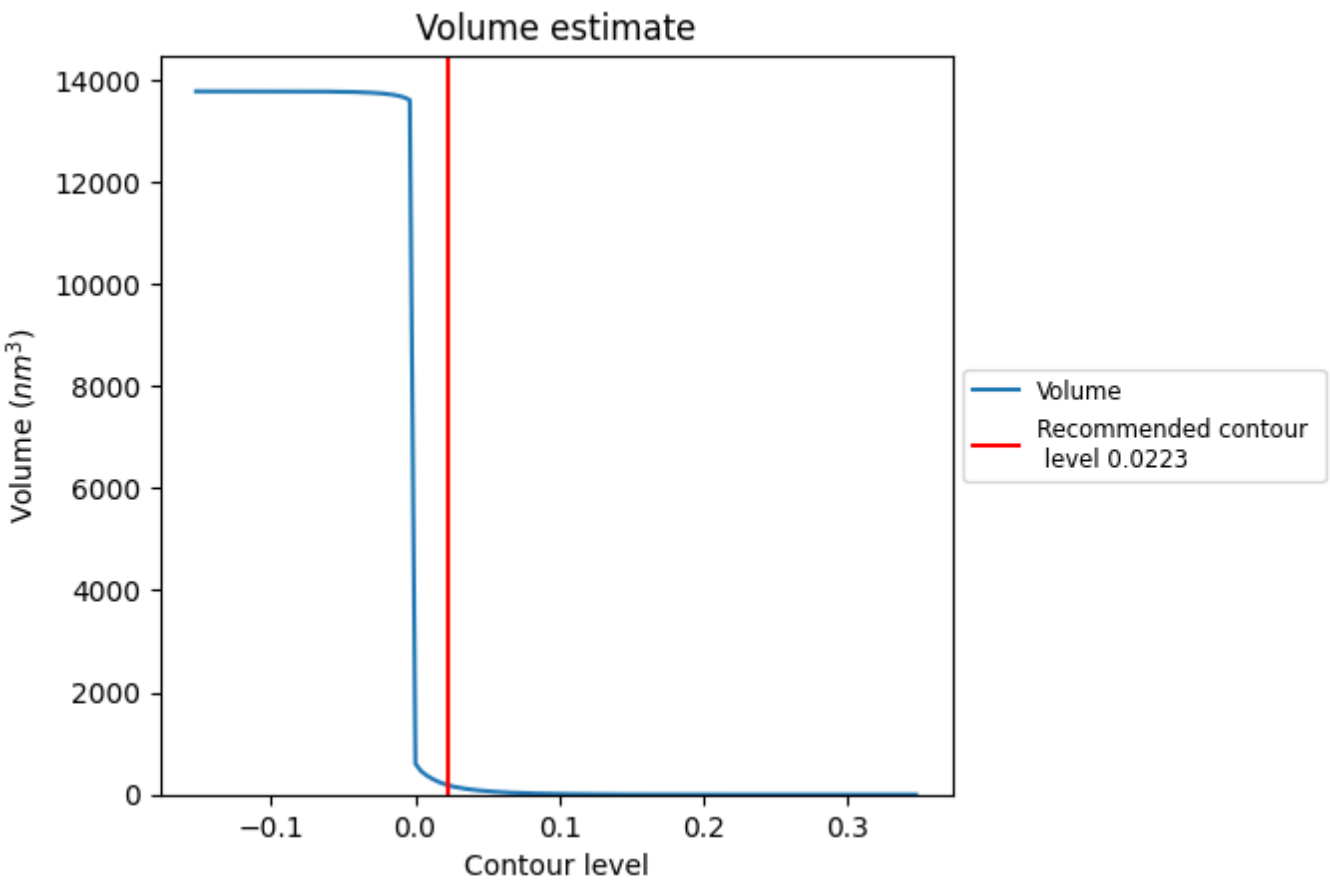
This section contains the results of statistical analysis of the map.

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.

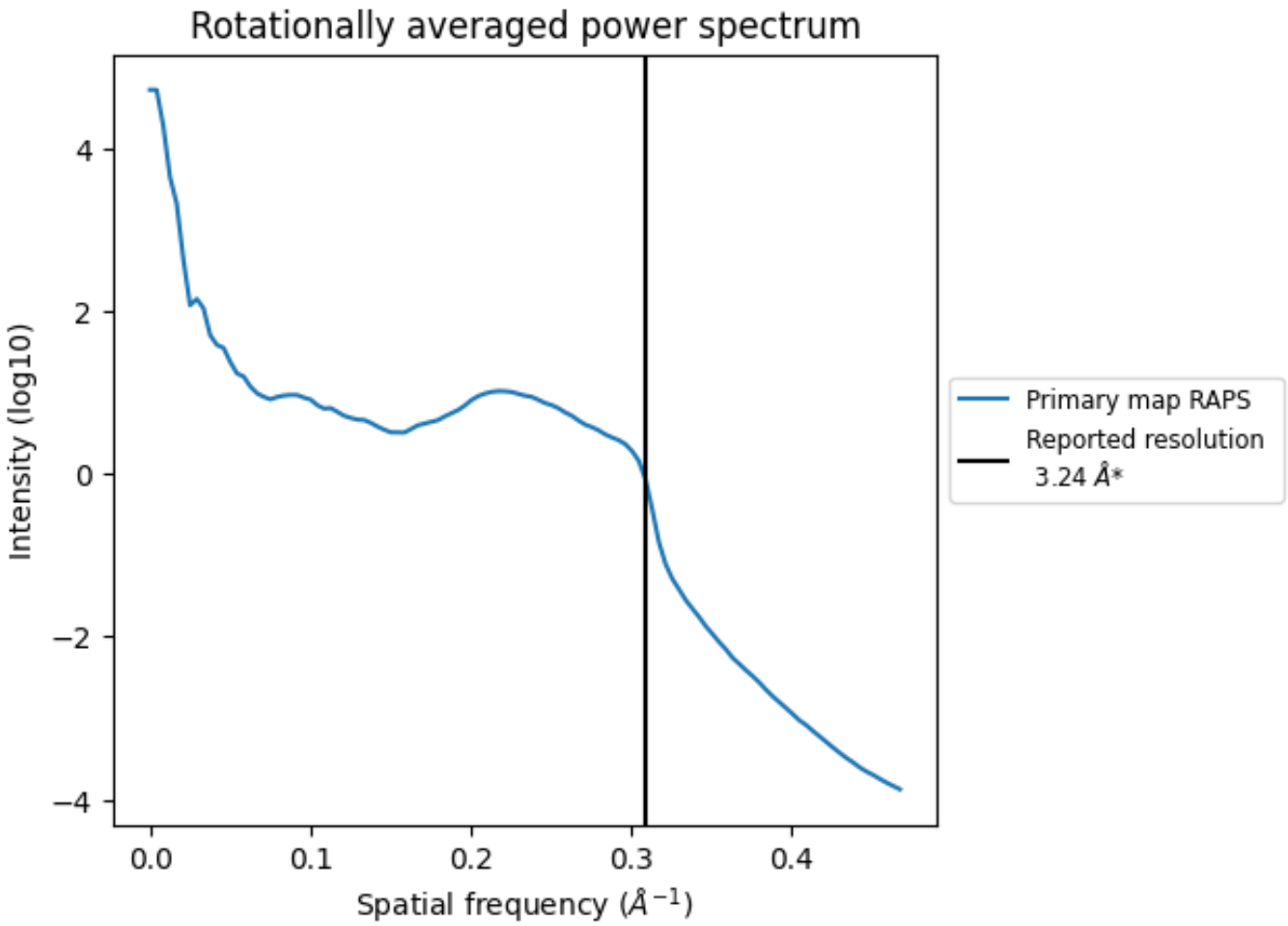
7.2 Volume estimate (i)



The volume at the recommended contour level is 189 nm^3; this corresponds to an approximate mass of 171 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)

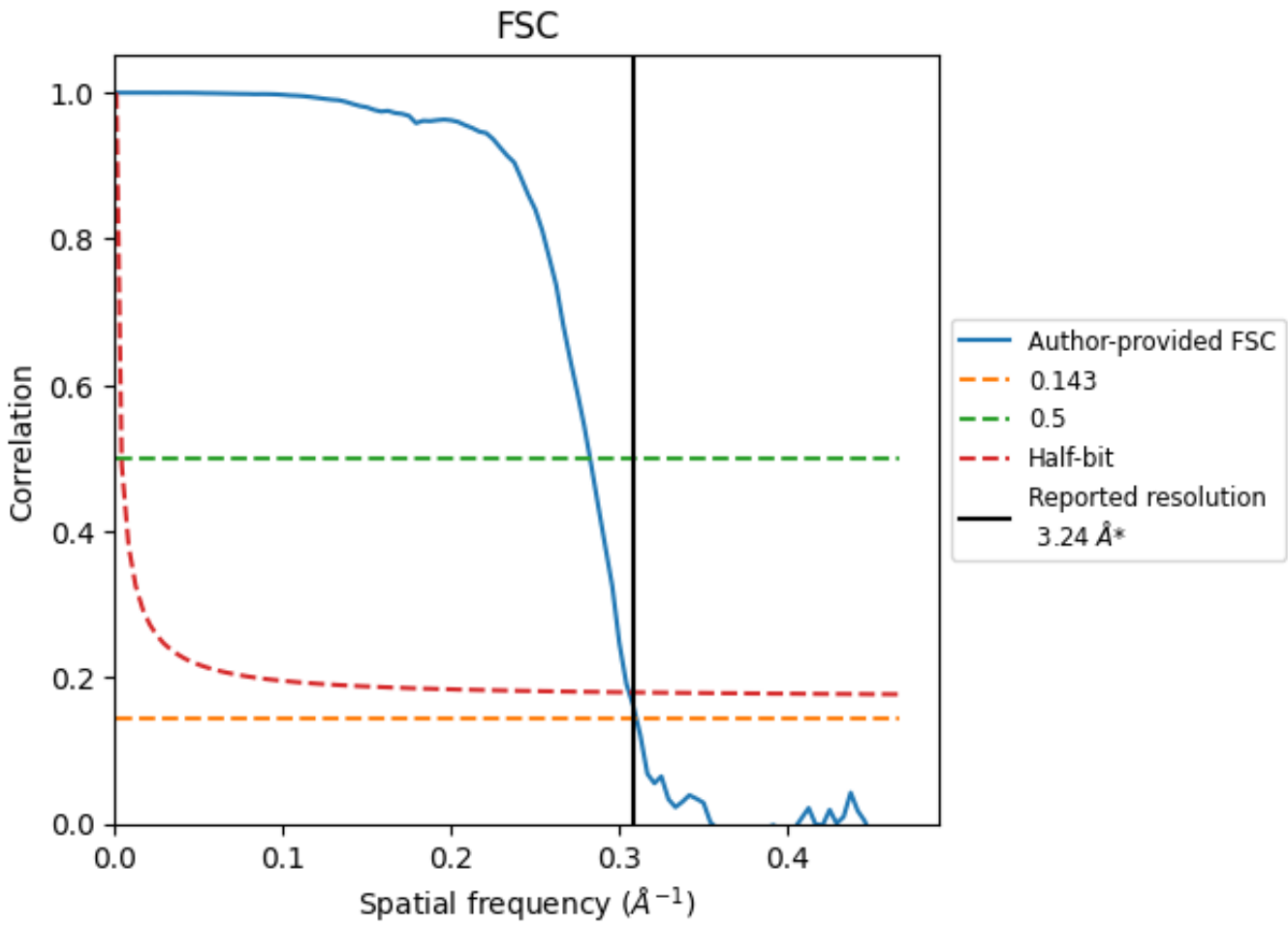


*Reported resolution corresponds to spatial frequency of 0.309 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.309 Å^{-1}

8.2 Resolution estimates (i)

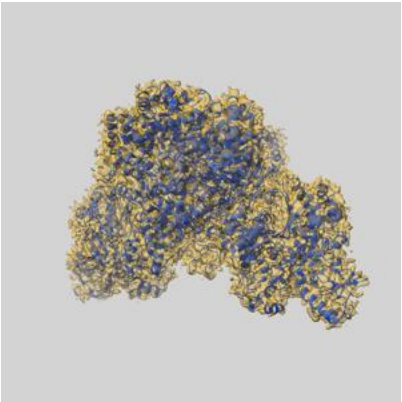
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	3.22	3.53	3.27
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

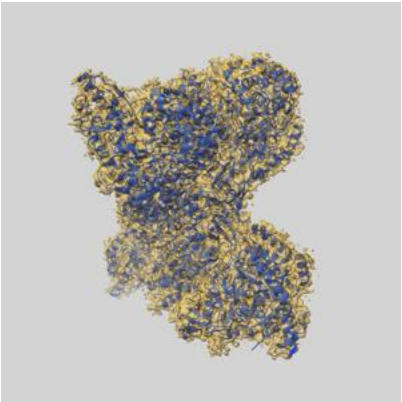
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10495 and PDB model 6TG9. Per-residue inclusion information can be found in section 3 on page 10.

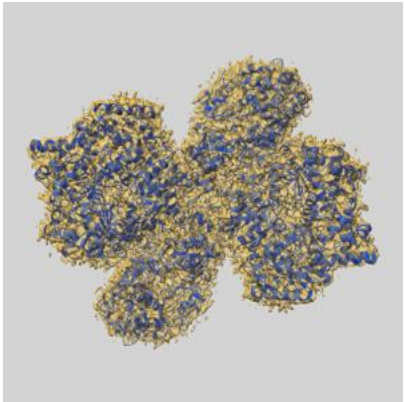
9.1 Map-model overlay (i)



X



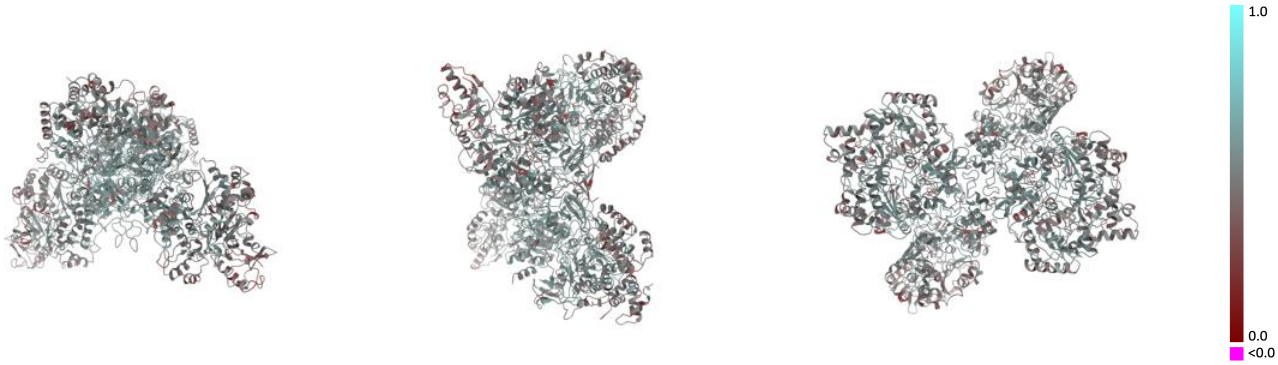
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0223 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.

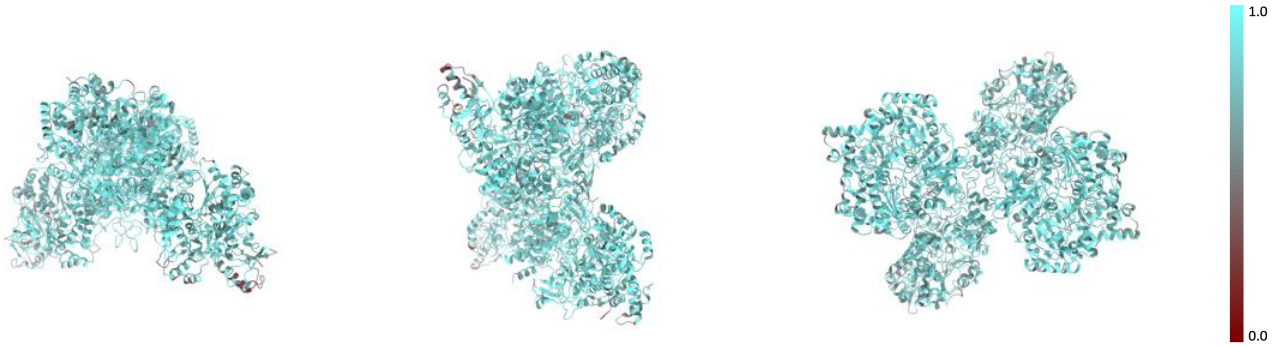
9.2 Q-score mapped to coordinate model (i)



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.

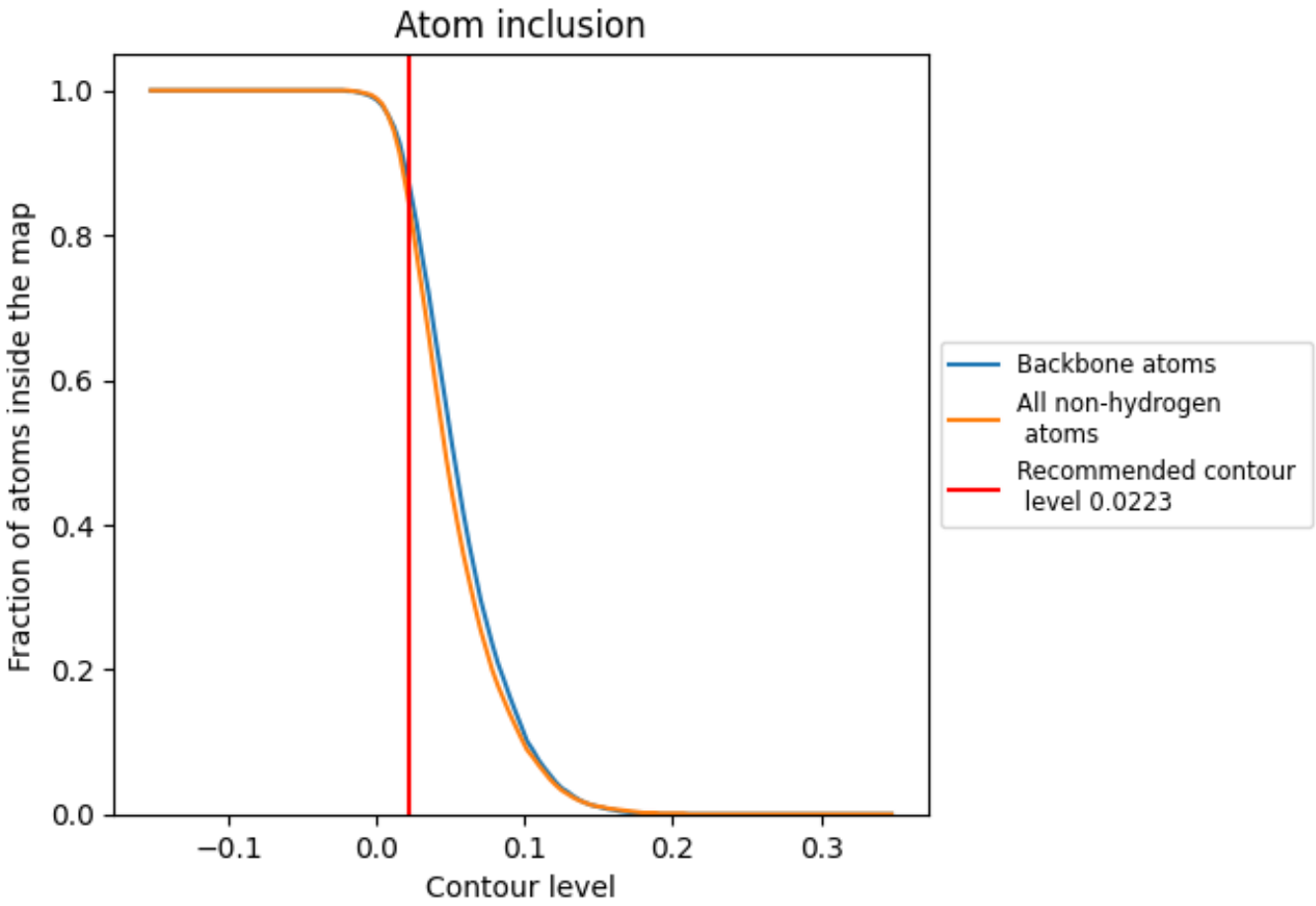
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0223).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 84% 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 (0.0223) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8410	0.4990
A	0.8690	0.5170
B	0.8040	0.4730
C	0.8290	0.4960
D	0.7440	0.4450
E	0.8690	0.5160
F	0.8040	0.4730
G	0.8200	0.4860
H	0.7560	0.4470