



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 28, 2025 – 01:45 pm BST

PDB ID : 8RQZ / pdb_00008rqz
Title : Crystal structure of Molybdenum bispyranopterin guanine dinucleotide formate dehydrogenases ForCE1 from Bacillus subtilis
Authors : Cherrier, M.V.; Arnoux, P.; Martin, L.; Nicolet, Y.; Schoehn, G.; Legrand, P.; Broc, M.; Seduk, F.; Brasseur, G.; Arias-Cartin, R.; Magalon, A.; Walburger, A.; Uzel, A.; Guigliarelli, B.; Grimaldi, S.; Pierrel, F.; Mate, M.
Deposited on : 2024-01-22
Resolution : 2.69 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

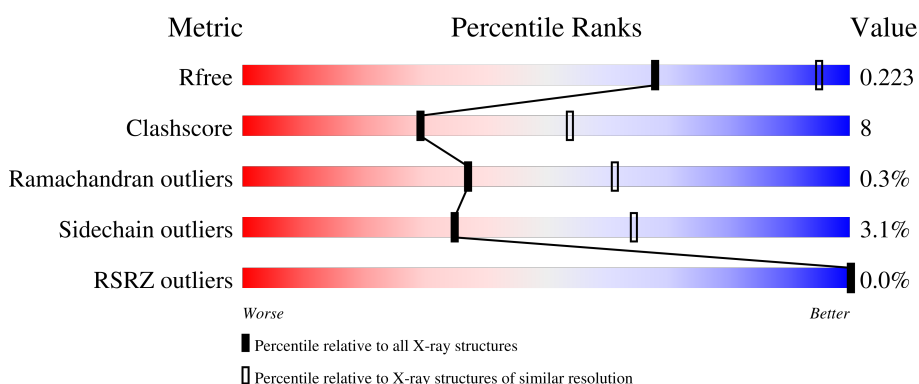
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.69 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	186	
1	B	186	
2	C	985	
2	D	985	

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	SF4	C	1004	-	-	X	-
7	SF4	D	1007	-	-	X	-
7	SF4	D	1008	-	-	X	-

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 18937 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

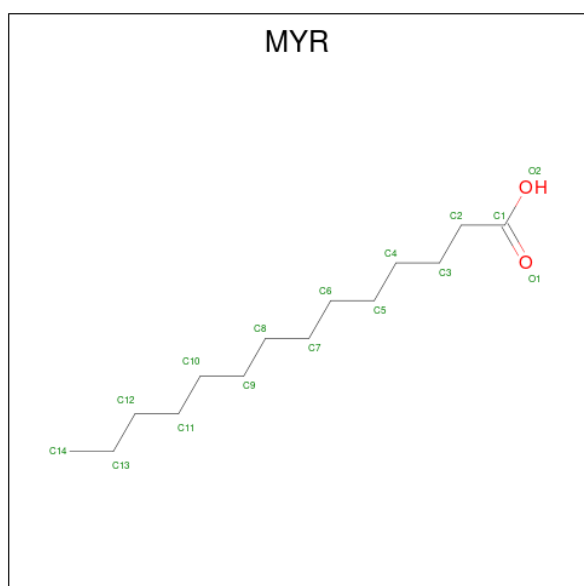
- Molecule 1 is a protein called Uncharacterized protein YjgD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1159	738	200	217	4			
1	B	147	Total	C	N	O	S	0	1	0
			1164	743	199	218	4			

- Molecule 2 is a protein called Probable oxidoreductase YjgC.

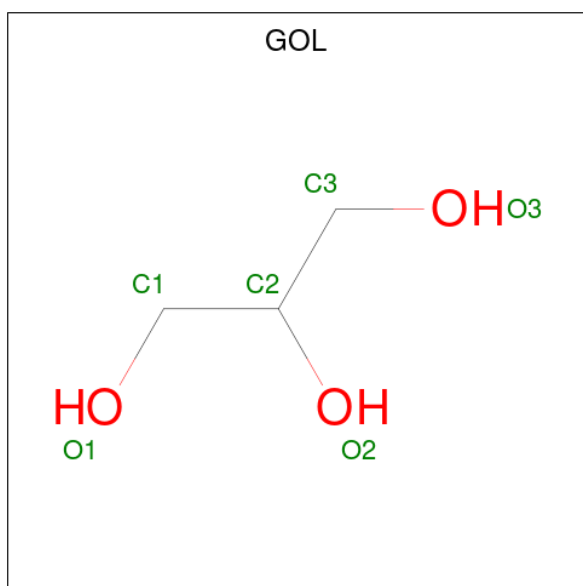
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	975	Total	C	N	O	S	0	4	0
			7664	4810	1314	1492	48			
2	D	975	Total	C	N	O	S	0	3	0
			7659	4808	1313	1490	48			

- Molecule 3 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	14	2		
3	A	1	Total	C	O	0	0
			14	12	2		
3	B	1	Total	C	O	0	0
			16	14	2		
3	B	1	Total	C	O	0	0
			14	12	2		
3	C	1	Total	C	O	0	0
			16	14	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



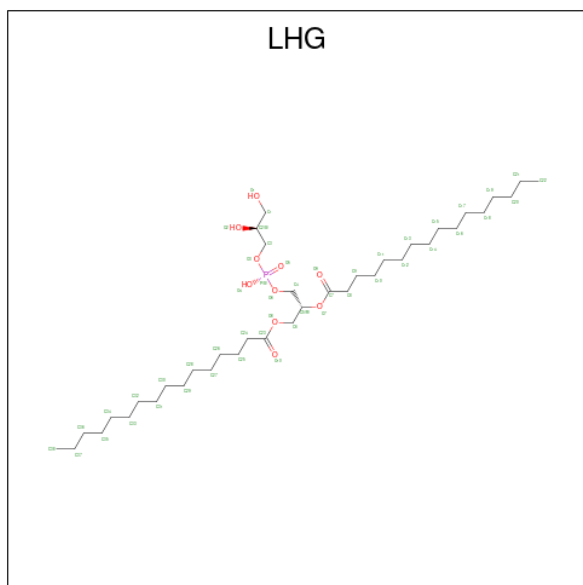
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



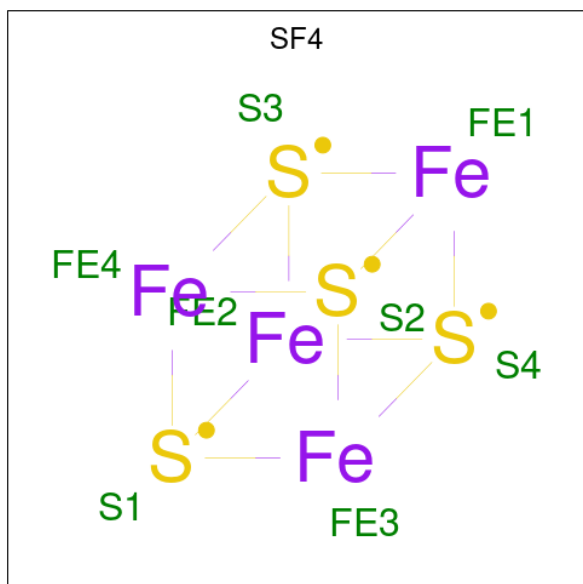
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	P	0	0
			45	34	10	1		
5	C	1	Total	C	O	P	0	0
			45	34	10	1		

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	Fe	S	0	0
			4	2	2		
6	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



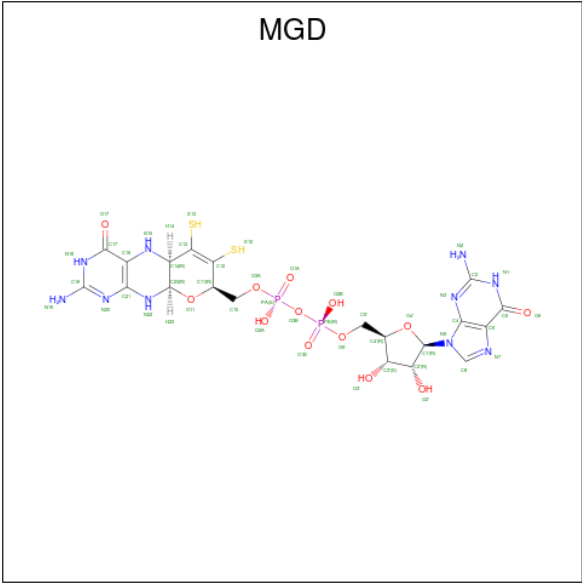
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	Fe	S	0	0
			8	4	4		
7	C	1	Total	Fe	S	0	0
			8	4	4		
7	C	1	Total	Fe	S	0	0
			8	4	4		
7	D	1	Total	Fe	S	0	0
			8	4	4		
7	D	1	Total	Fe	S	0	0
			8	4	4		
7	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 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 (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
8	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
8	D	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

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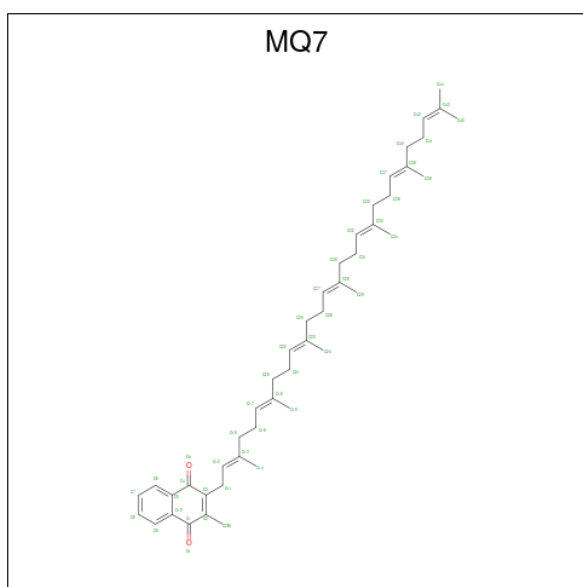
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	N	O	P	S	
			47	20	10	13	2	2	
								0	0

- Molecule 9 is MOLYBDENUM(IV) ION (CCD ID: 4MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

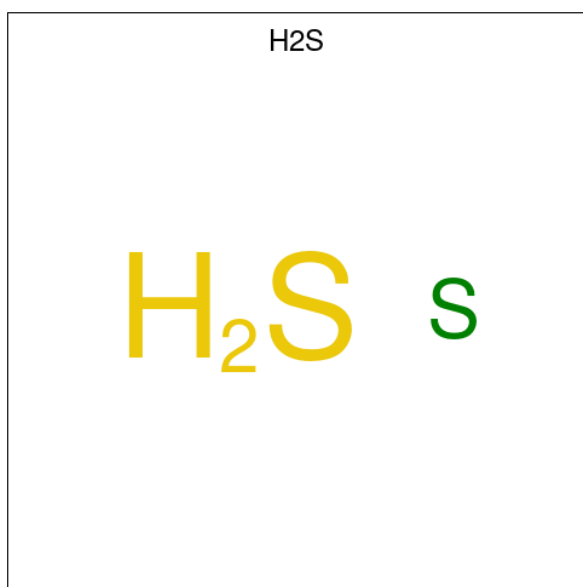
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Mo	0	0
			1	1		
9	D	1	Total	Mo	0	0
			1	1		

- Molecule 10 is MENAQUINONE-7 (CCD ID: MQ7) (formula: C₄₆H₆₄O₂) (labeled as "Ligand of Interest" by depositor).



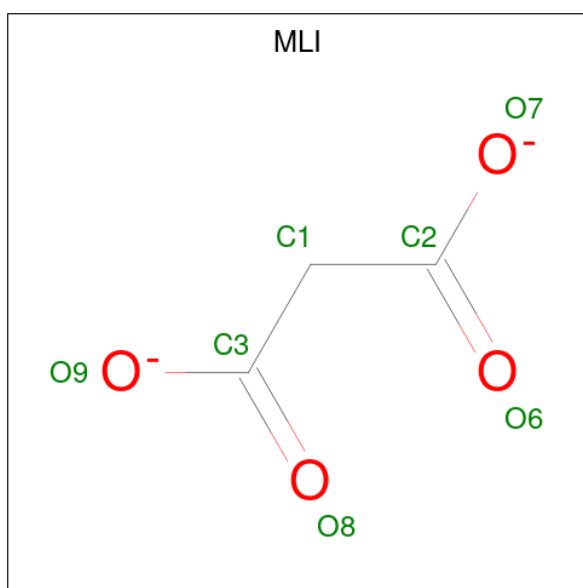
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			23	21	2		
10	D	1	Total	C	O	0	0
			23	21	2		

- Molecule 11 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total S 1 1	0	0
11	D	1	Total S 1 1	0	0

- Molecule 12 is MALONATE ION (CCD ID: MLI) (formula: C₃H₂O₄).



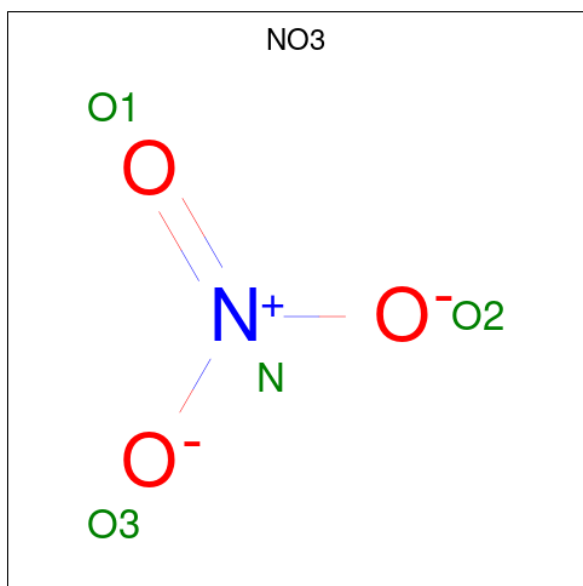
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C O 7 3 4	0	0
12	C	1	Total C O 7 3 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			7	3	4		
12	C	1	Total	C	O	0	0
			7	3	4		
12	C	1	Total	C	O	0	0
			7	3	4		
12	C	1	Total	C	O	0	0
			7	3	4		
12	D	1	Total	C	O	0	0
			7	3	4		
12	D	1	Total	C	O	0	0
			7	3	4		
12	D	1	Total	C	O	0	0
			7	3	4		

- Molecule 13 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	N	O	0	0
			4	1	3		
13	C	1	Total	N	O	0	0
			4	1	3		
13	D	1	Total	N	O	0	0
			4	1	3		
13	D	1	Total	N	O	0	0
			4	1	3		

- Molecule 14 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	D	1	Total	Na	0	0
			1	1		

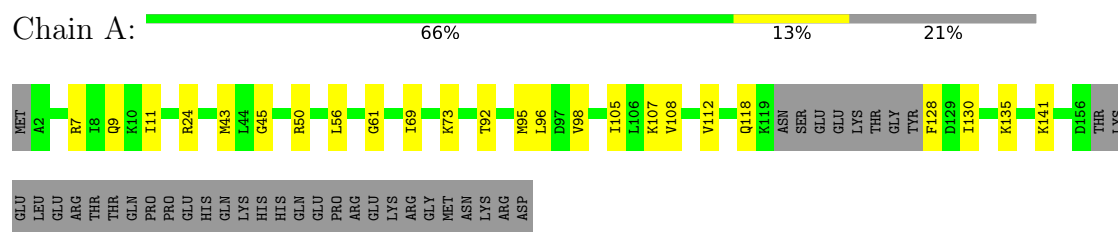
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	34	Total	O	0	0
			34	34		
15	B	24	Total	O	0	0
			24	24		
15	C	320	Total	O	0	0
			320	320		
15	D	309	Total	O	0	0
			309	309		

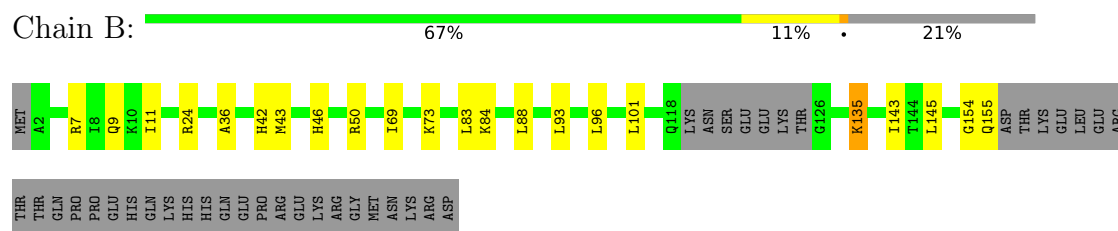
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

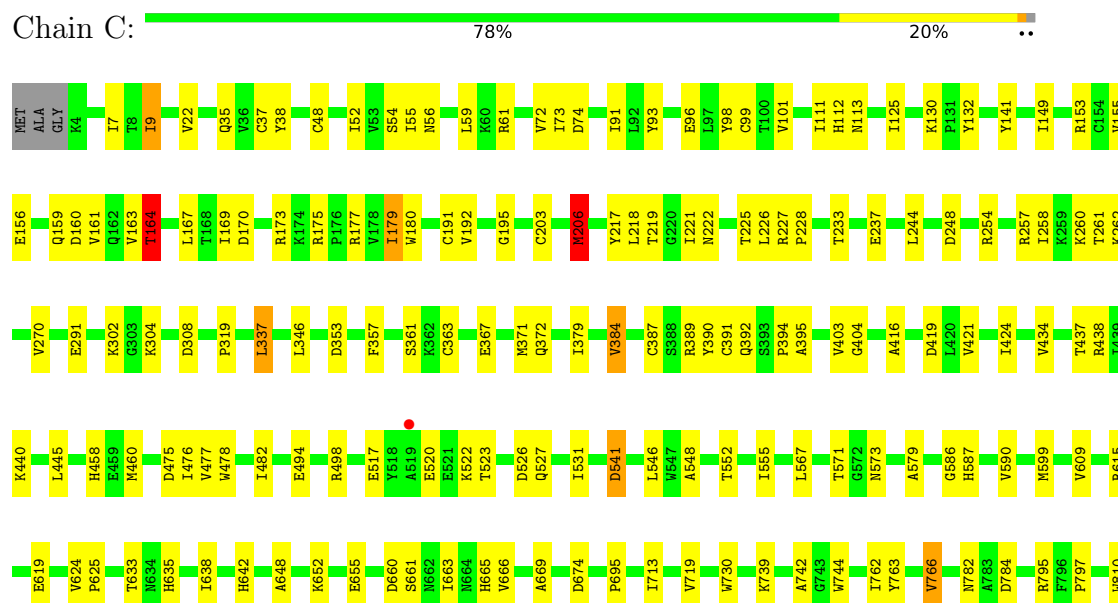
• Molecule 1: Uncharacterized protein YjgD

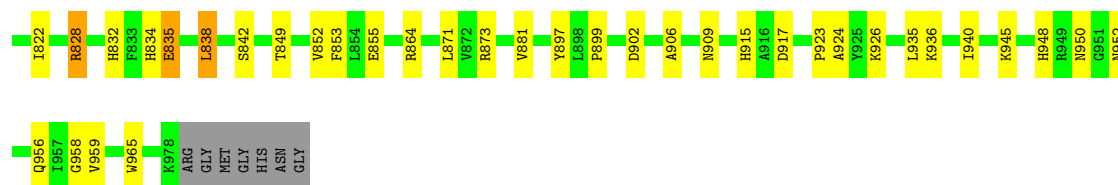


• Molecule 1: Uncharacterized protein YjgD

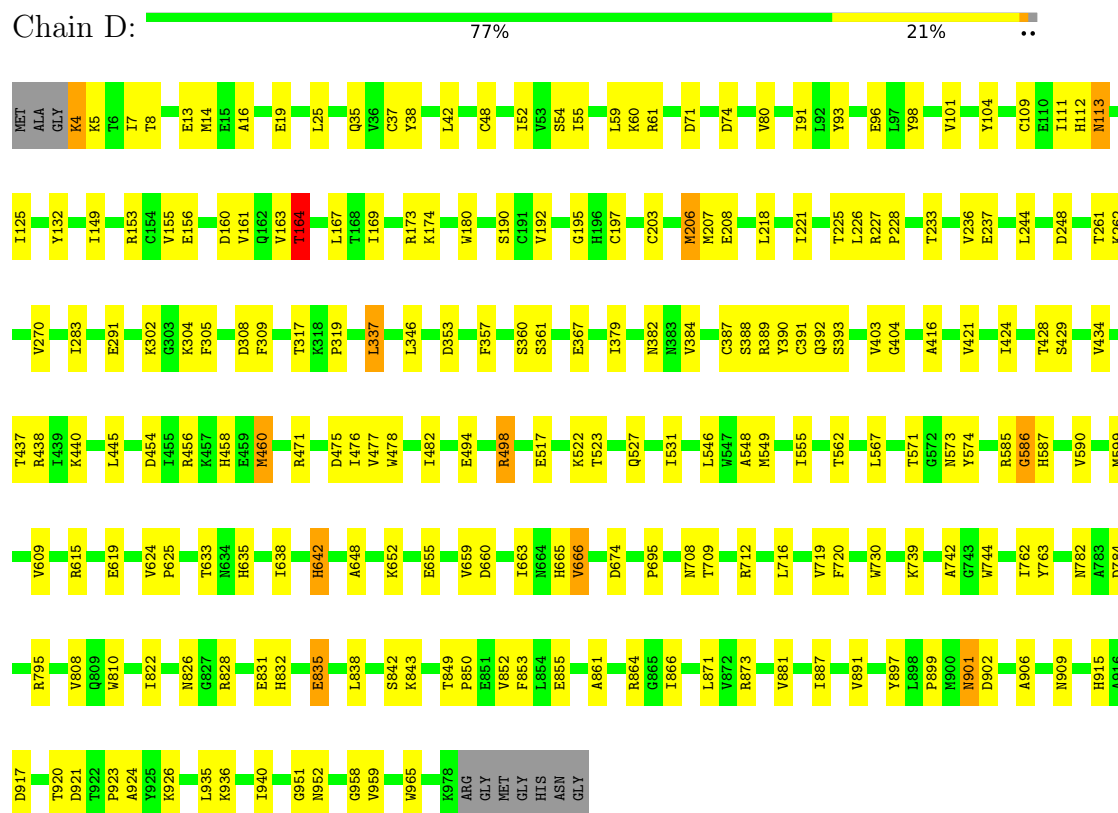


• Molecule 2: Probable oxidoreductase YjgC





• Molecule 2: Probable oxidoreductase YjgC



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	210.83Å 210.50Å 494.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.41 – 2.69 49.41 – 2.69	Depositor EDS
% Data completeness (in resolution range)	61.5 (49.41-2.69) 61.5 (49.41-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.4 (26-JUL-2023)	Depositor
R, R_{free}	0.196 , 0.231 0.191 , 0.223	Depositor DCC
R_{free} test set	4688 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.399 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18937	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: SF4, 4MO, H2S, FES, NA, MQ7, GOL, LHG, MYR, MLI, NO3, MGD

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	0.64	0/1168	1.10	0/1564
1	B	0.62	0/1177	1.08	0/1577
2	C	0.65	3/7832 (0.0%)	1.04	9/10606 (0.1%)
2	D	0.64	2/7828 (0.0%)	1.04	6/10599 (0.1%)
All	All	0.64	5/18005 (0.0%)	1.05	15/24346 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	460	MET	SD-CE	-7.52	1.60	1.79
2	C	391	CYS	N-CA	-6.12	1.42	1.46
2	D	548	ALA	CA-C	6.04	1.60	1.53
2	C	548	ALA	CA-C	5.93	1.60	1.52
2	C	206	MET	SD-CE	-5.36	1.66	1.79

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	541	ASP	CA-CB-CG	6.88	119.48	112.60
2	D	113	ASN	CA-CB-CG	6.16	118.76	112.60
2	D	98	TYR	CA-C-N	6.06	133.12	121.54
2	D	98	TYR	C-N-CA	6.06	133.12	121.54
2	C	113	ASN	CA-CB-CG	5.86	118.46	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1159	0	1230	18	0
1	B	1164	0	1231	23	0
2	C	7664	0	7487	130	0
2	D	7659	0	7488	149	0
3	A	30	0	47	3	0
3	B	30	0	47	4	0
3	C	16	0	27	3	0
4	A	6	0	8	0	0
4	B	6	0	8	1	0
4	C	12	0	16	0	0
4	D	24	0	32	5	0
5	B	45	0	60	1	0
5	C	45	0	60	1	0
6	C	4	0	0	0	0
6	D	4	0	0	0	0
7	C	32	0	0	3	0
7	D	32	0	0	4	0
8	C	94	0	44	8	0
8	D	94	0	44	14	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	C	23	0	21	1	0
10	D	23	0	21	1	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
12	C	42	0	12	1	0
12	D	21	0	6	0	0
13	C	8	0	0	0	0
13	D	8	0	0	0	0
14	D	1	0	0	0	0
15	A	34	0	0	0	0
15	B	24	0	0	0	0
15	C	320	0	0	3	0
15	D	309	0	0	3	0
All	All	18937	0	17889	307	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 8.

The worst 5 of 307 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:826:ASN:ND2	8:D:1010:MGD:H18	1.60	1.00
2:D:826:ASN:HD22	8:D:1010:MGD:H18	1.15	0.91
1:A:128:PHE:N	1:B:135:LYS:HZ2	1.70	0.88
1:B:42:HIS:NE2	4:B:201:GOL:H2	1.90	0.87
2:C:828:ARG:NH1	2:C:834:HIS:NE2	2.26	0.84

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 X-ray entries followed by that with respect to entries of similar resolution.

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	143/186 (77%)	139 (97%)	3 (2%)	1 (1%)	19	42
1	B	144/186 (77%)	142 (99%)	2 (1%)	0	100	100
2	C	977/985 (99%)	941 (96%)	34 (4%)	2 (0%)	44	68
2	D	976/985 (99%)	936 (96%)	37 (4%)	3 (0%)	37	61
All	All	2240/2342 (96%)	2158 (96%)	76 (3%)	6 (0%)	37	61

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	LYS
2	C	586	GLY
2	D	498	ARG
2	D	586	GLY
2	C	237	GLU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	128/165 (78%)	124 (97%)	4 (3%)	35	64
1	B	128/165 (78%)	122 (95%)	6 (5%)	22	49
2	C	843/845 (100%)	821 (97%)	22 (3%)	41	70
2	D	843/845 (100%)	816 (97%)	27 (3%)	34	63
All	All	1942/2020 (96%)	1883 (97%)	59 (3%)	35	65

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	828	ARG
2	D	891	VAL
2	D	164	THR
2	D	843	LYS
2	D	674	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	112	HIS
2	D	458	HIS
2	D	113	ASN
2	D	289	GLN
2	D	591	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 3 are monoatomic and 2 are modelled with single atom - leaving 44 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	$\# Z > 2$
5	LHG	B	204	-	44,44,48	0.38	0	47,50,54	0.39	0
3	MYR	A	202	-	13,13,15	0.67	0	13,13,15	1.09	0
12	MLI	C	1022	-	6,6,6	1.18	0	7,7,7	0.93	0
4	GOL	D	1016	-	5,5,5	0.07	0	5,5,5	0.22	0
12	MLI	D	1002	-	6,6,6	1.23	0	7,7,7	0.88	0
7	SF4	D	1009	2	0,12,12	-	-	-	-	-
12	MLI	C	1012	-	6,6,6	1.22	0	7,7,7	0.96	0
13	NO3	D	1004	-	1,3,3	0.01	0	0,3,3	-	-
7	SF4	D	1008	2	0,12,12	-	-	-	-	-
4	GOL	A	203	-	5,5,5	0.07	0	5,5,5	0.25	0
13	NO3	C	1014	-	1,3,3	0.11	0	0,3,3	-	-
13	NO3	C	1016	-	1,3,3	0.09	0	0,3,3	-	-
4	GOL	D	1018	-	5,5,5	0.04	0	5,5,5	0.27	0
3	MYR	C	1017	-	15,15,15	0.66	0	15,15,15	0.86	0
7	SF4	C	1005	2	0,12,12	-	-	-	-	-
12	MLI	C	1015	-	6,6,6	1.14	0	7,7,7	0.93	0
3	MYR	B	203	-	13,13,15	0.67	0	13,13,15	1.07	1 (7%)
8	MGD	D	1011	9	41,52,52	2.40	13 (31%)	40,81,81	1.76	9 (22%)
7	SF4	D	1007	2	0,12,12	-	-	-	-	-
10	MQ7	D	1013	-	24,24,49	0.39	0	30,33,63	0.58	1 (3%)
12	MLI	C	1020	-	6,6,6	1.18	0	7,7,7	0.86	0
4	GOL	C	1018	-	5,5,5	0.04	0	5,5,5	0.21	0
3	MYR	A	201	-	15,15,15	0.65	0	15,15,15	1.05	0
7	SF4	C	1004	2	0,12,12	-	-	-	-	-
4	GOL	C	1019	-	5,5,5	0.09	0	5,5,5	0.31	0
4	GOL	B	201	-	5,5,5	0.07	0	5,5,5	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FES	D	1005	2	0,4,4	-	-	-		
7	SF4	D	1006	2	0,12,12	-	-	-		
12	MLI	C	1021	-	6,6,6	1.22	0	7,7,7	0.96	0
7	SF4	C	1002	2	0,12,12	-	-	-		
12	MLI	D	1015	-	6,6,6	1.17	0	7,7,7	0.88	0
7	SF4	C	1003	2	0,12,12	-	-	-		
8	MGD	D	1010	9	41,52,52	2.37	13 (31%)	40,81,81	1.65	8 (20%)
8	MGD	C	1007	9	41,52,52	2.24	15 (36%)	40,81,81	1.99	10 (25%)
8	MGD	C	1006	9	41,52,52	2.29	13 (31%)	40,81,81	1.58	8 (20%)
5	LHG	C	1013	-	44,44,48	0.38	0	47,50,54	0.46	0
6	FES	C	1001	2	0,4,4	-	-	-		
3	MYR	B	202	-	15,15,15	0.66	0	15,15,15	1.01	0
4	GOL	D	1017	-	5,5,5	0.05	0	5,5,5	0.19	0
4	GOL	D	1003	-	5,5,5	0.16	0	5,5,5	0.41	0
10	MQ7	C	1009	-	24,24,49	0.39	0	30,33,63	0.51	1 (3%)
12	MLI	C	1011	-	6,6,6	1.16	0	7,7,7	0.88	0
12	MLI	D	1019	-	6,6,6	1.17	0	7,7,7	0.87	0
13	NO3	D	1001	-	1,3,3	0.14	0	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
5	LHG	B	204	-	-	19/49/49/53	-
3	MYR	A	202	-	-	4/11/11/13	-
12	MLI	C	1022	-	-	4/4/4/4	-
4	GOL	D	1016	-	-	0/4/4/4	-
12	MLI	D	1002	-	-	4/4/4/4	-
7	SF4	D	1009	2	-	-	0/6/5/5
12	MLI	C	1012	-	-	2/4/4/4	-
7	SF4	D	1008	2	-	-	0/6/5/5
4	GOL	A	203	-	-	0/4/4/4	-
4	GOL	D	1018	-	-	0/4/4/4	-
3	MYR	C	1017	-	-	7/13/13/13	-
7	SF4	C	1005	2	-	-	0/6/5/5
12	MLI	C	1015	-	-	2/4/4/4	-
3	MYR	B	203	-	-	5/11/11/13	-
8	MGD	D	1011	9	-	8/18/66/66	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	D	1007	2	-	-	0/6/5/5
10	MQ7	D	1013	-	-	1/11/31/61	0/2/2/2
12	MLI	C	1020	-	-	0/4/4/4	-
4	GOL	C	1018	-	-	0/4/4/4	-
3	MYR	A	201	-	-	1/13/13/13	-
7	SF4	C	1004	2	-	-	0/6/5/5
4	GOL	C	1019	-	-	0/4/4/4	-
4	GOL	B	201	-	-	0/4/4/4	-
12	MLI	C	1021	-	-	0/4/4/4	-
6	FES	D	1005	2	-	-	0/1/1/1
7	SF4	D	1006	2	-	-	0/6/5/5
12	MLI	D	1015	-	-	0/4/4/4	-
7	SF4	C	1002	2	-	-	0/6/5/5
7	SF4	C	1003	2	-	-	0/6/5/5
8	MGD	D	1010	9	-	7/18/66/66	0/6/6/6
8	MGD	C	1007	9	-	7/18/66/66	0/6/6/6
8	MGD	C	1006	9	-	6/18/66/66	0/6/6/6
5	LHG	C	1013	-	-	16/49/49/53	-
6	FES	C	1001	2	-	-	0/1/1/1
3	MYR	B	202	-	-	2/13/13/13	-
4	GOL	D	1017	-	-	1/4/4/4	-
4	GOL	D	1003	-	-	0/4/4/4	-
10	MQ7	C	1009	-	-	1/11/31/61	0/2/2/2
12	MLI	C	1011	-	-	0/4/4/4	-
12	MLI	D	1019	-	-	2/4/4/4	-

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	1011	MGD	C23-C14	8.72	1.60	1.53
8	D	1010	MGD	C23-C14	7.65	1.59	1.53
8	C	1007	MGD	C23-C14	7.32	1.59	1.53
8	C	1006	MGD	C23-C14	6.97	1.59	1.53
8	D	1011	MGD	C10-C11	5.87	1.59	1.52

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1007	MGD	O11-C23-N22	-6.63	101.75	108.57
8	C	1006	MGD	PA-O3B-PB	4.90	149.64	132.83
8	D	1010	MGD	PA-O3B-PB	4.87	149.55	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1007	MGD	PA-O3B-PB	4.64	148.75	132.83
8	C	1007	MGD	O6-C6-N1	-4.40	115.45	120.65

There are no chirality outliers.

5 of 99 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	204	LHG	C3-O3-P-O4
5	B	204	LHG	C3-O3-P-O5
5	B	204	LHG	C3-O3-P-O6
5	B	204	LHG	C4-O6-P-O5
5	B	204	LHG	O9-C7-O7-C5

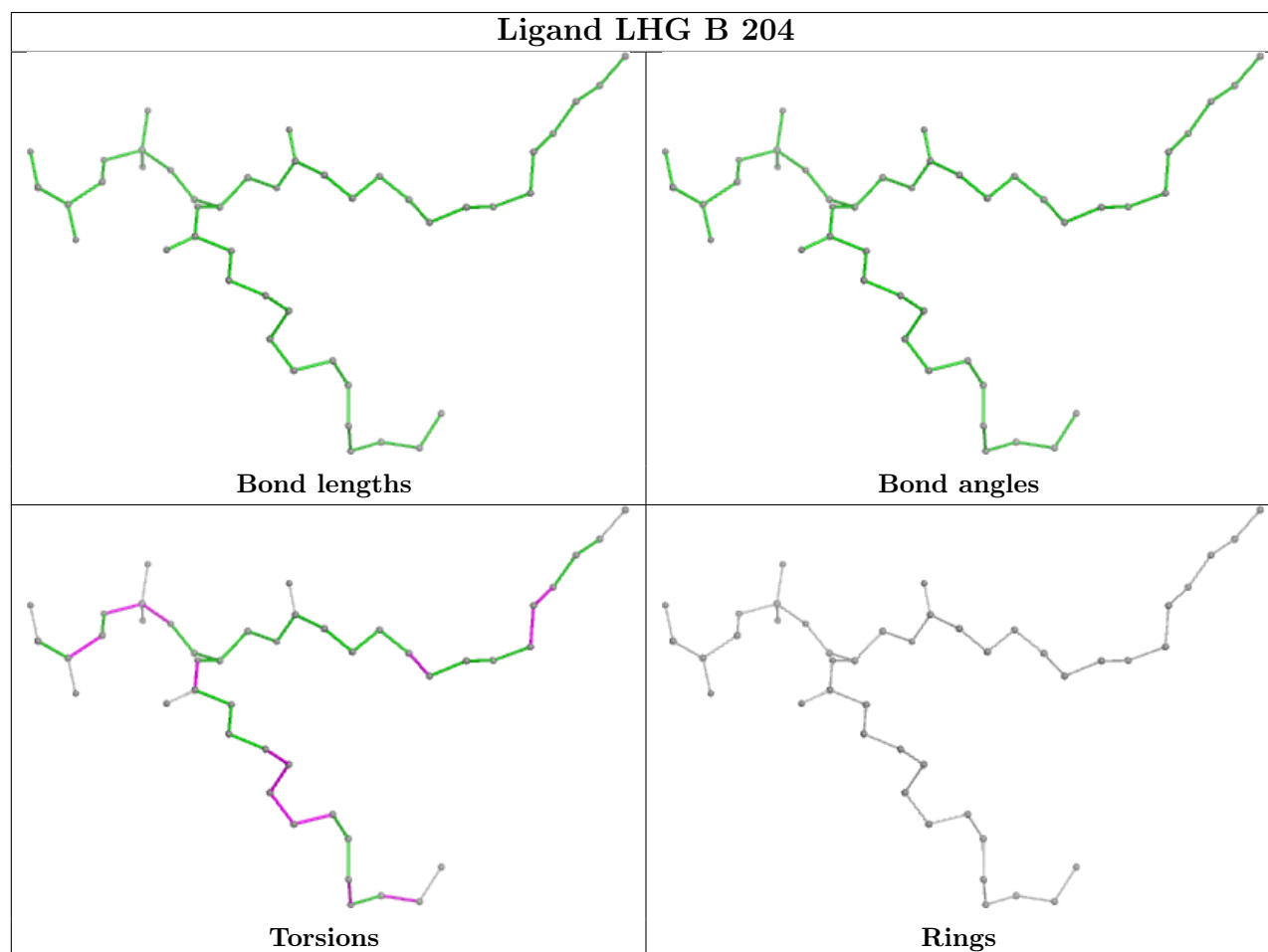
There are no ring outliers.

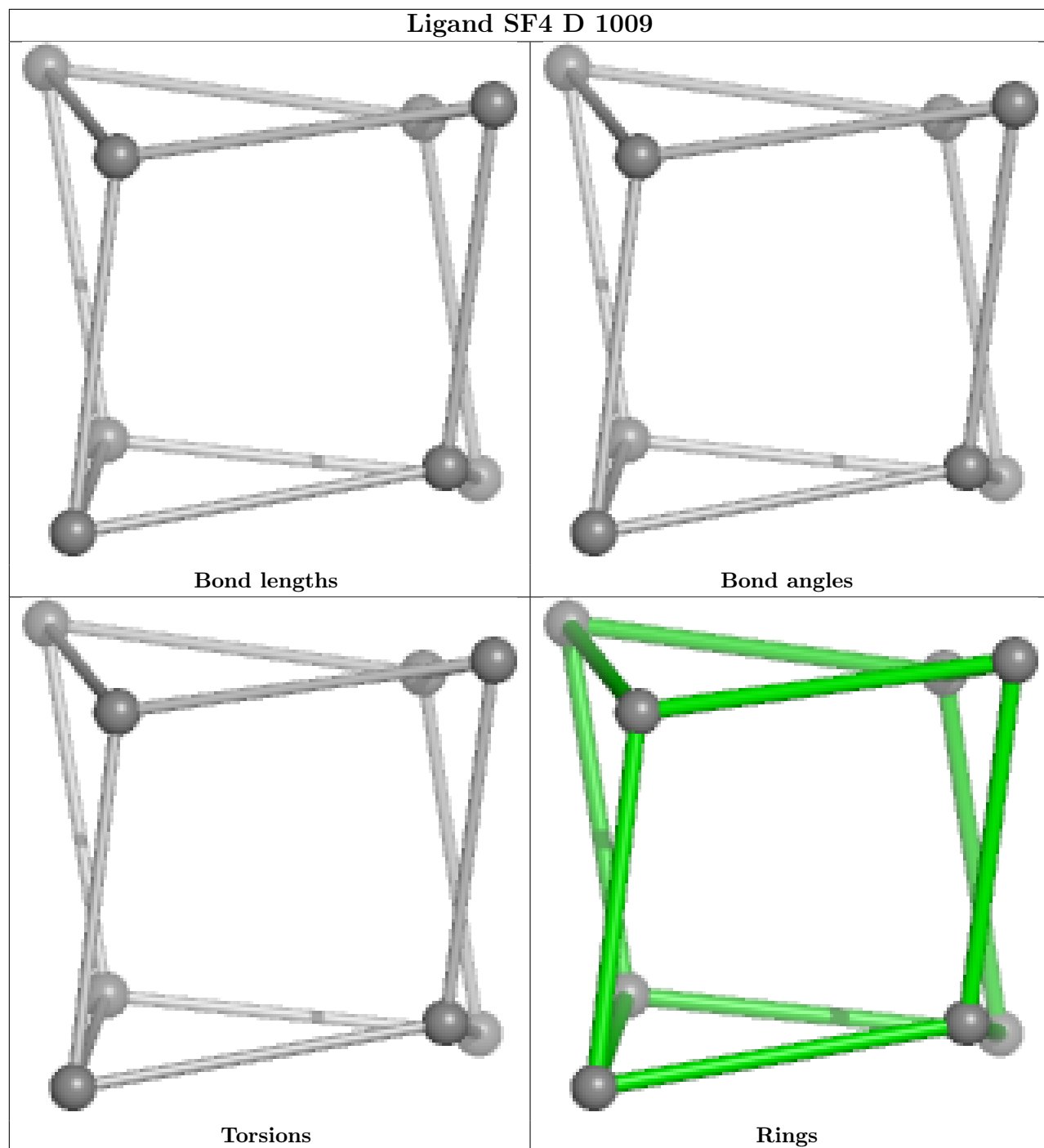
23 monomers are involved in 48 short contacts:

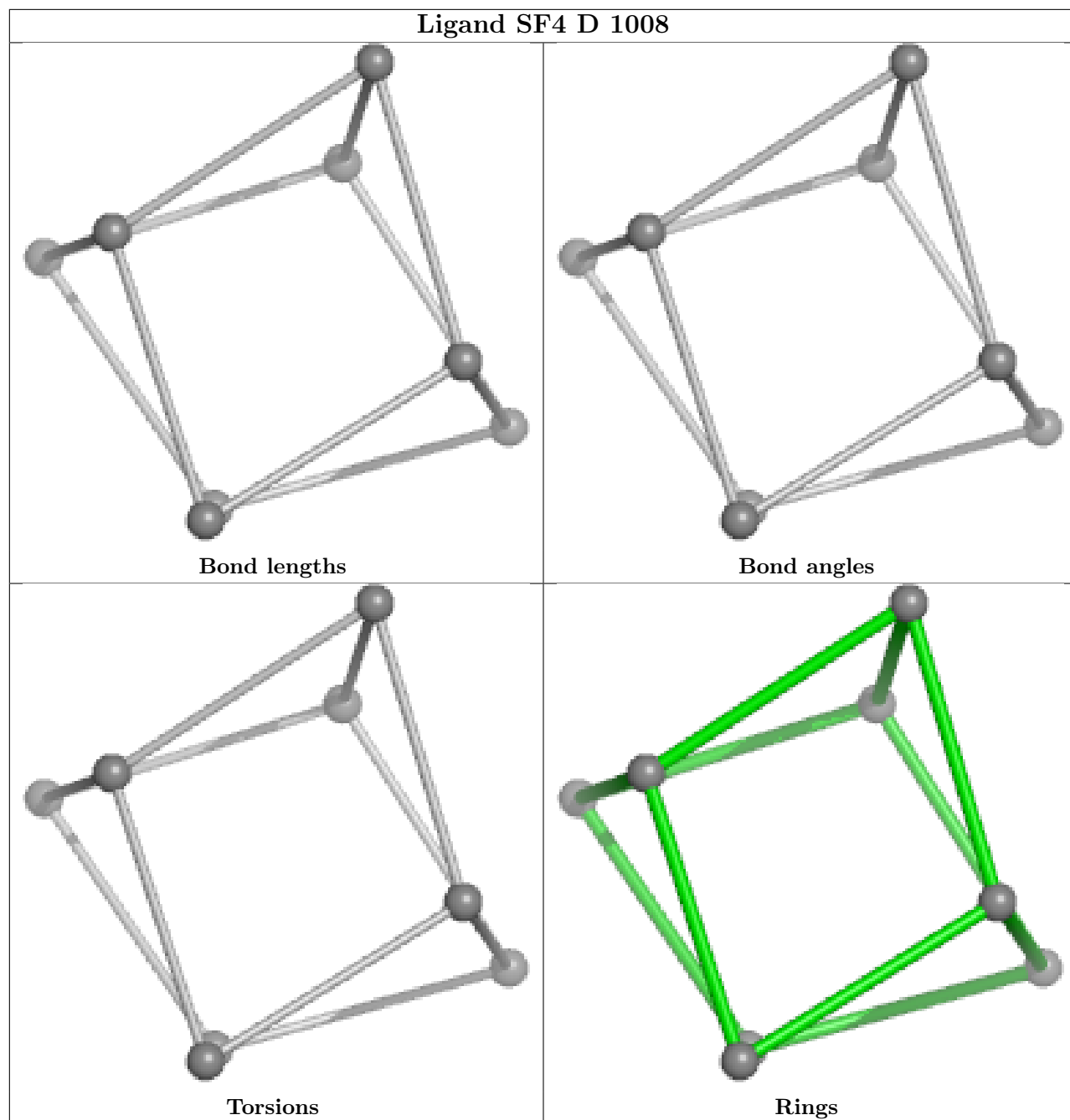
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	204	LHG	1	0
3	A	202	MYR	1	0
4	D	1016	GOL	1	0
12	C	1012	MLI	1	0
7	D	1008	SF4	2	0
4	D	1018	GOL	2	0
3	C	1017	MYR	3	0
3	B	203	MYR	2	0
8	D	1011	MGD	7	0
7	D	1007	SF4	2	0
10	D	1013	MQ7	1	0
3	A	201	MYR	2	0
7	C	1004	SF4	2	0
4	B	201	GOL	1	0
7	C	1003	SF4	1	0
8	D	1010	MGD	7	0
8	C	1007	MGD	3	0
8	C	1006	MGD	5	0
5	C	1013	LHG	1	0
3	B	202	MYR	2	0
4	D	1017	GOL	1	0
4	D	1003	GOL	1	0
10	C	1009	MQ7	1	0

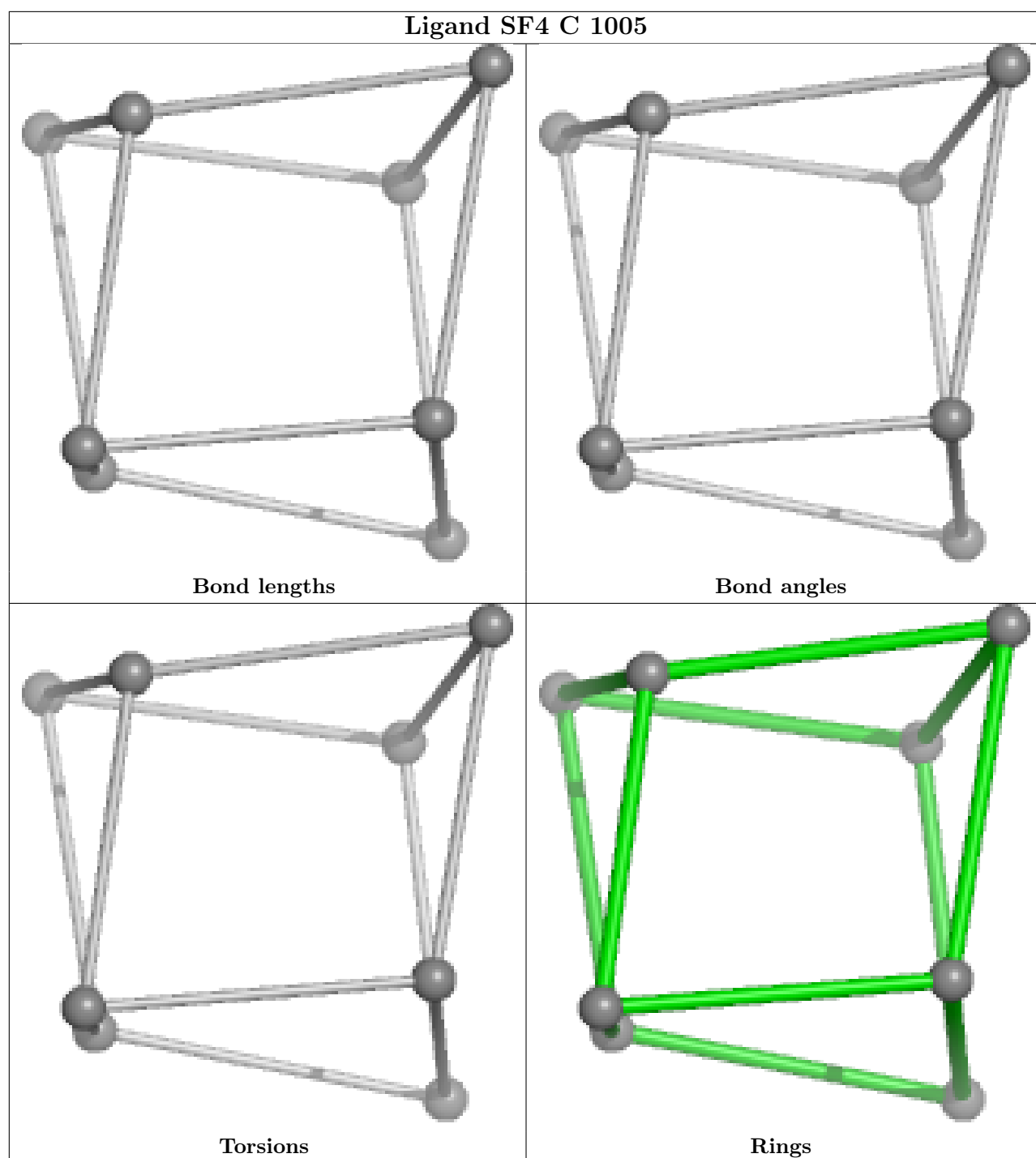
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

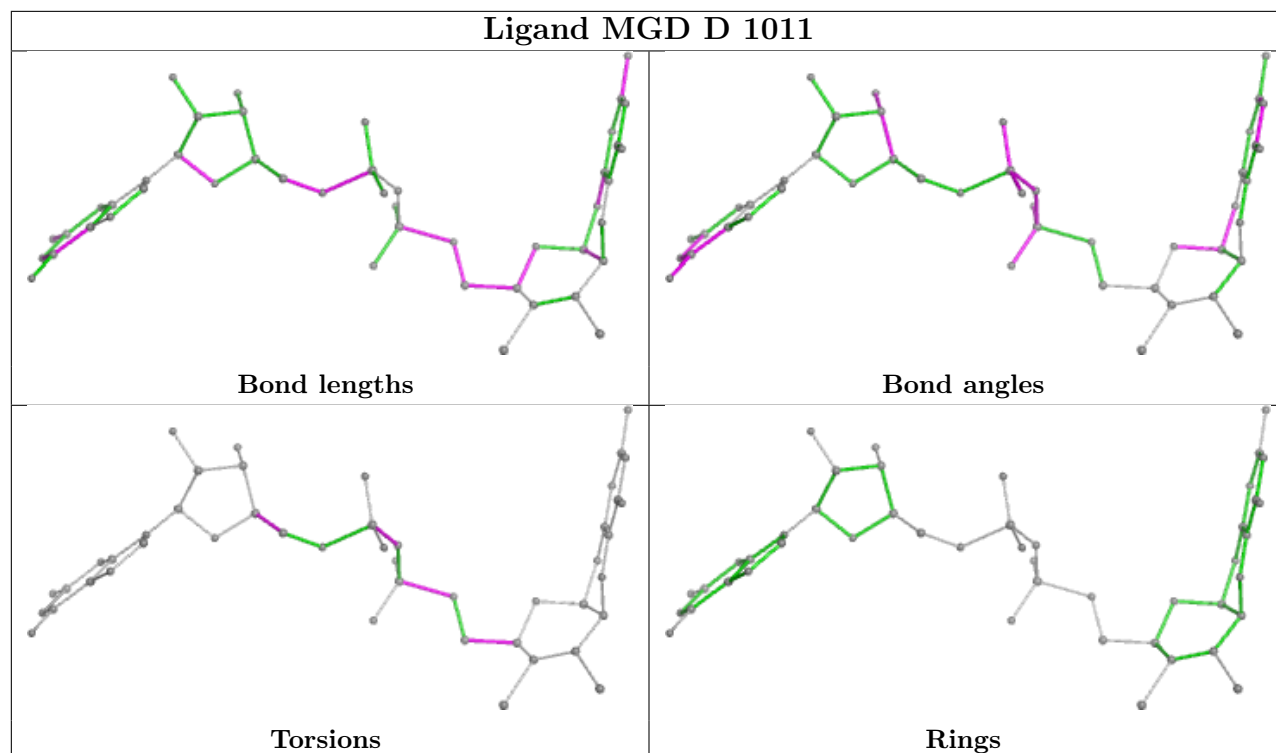


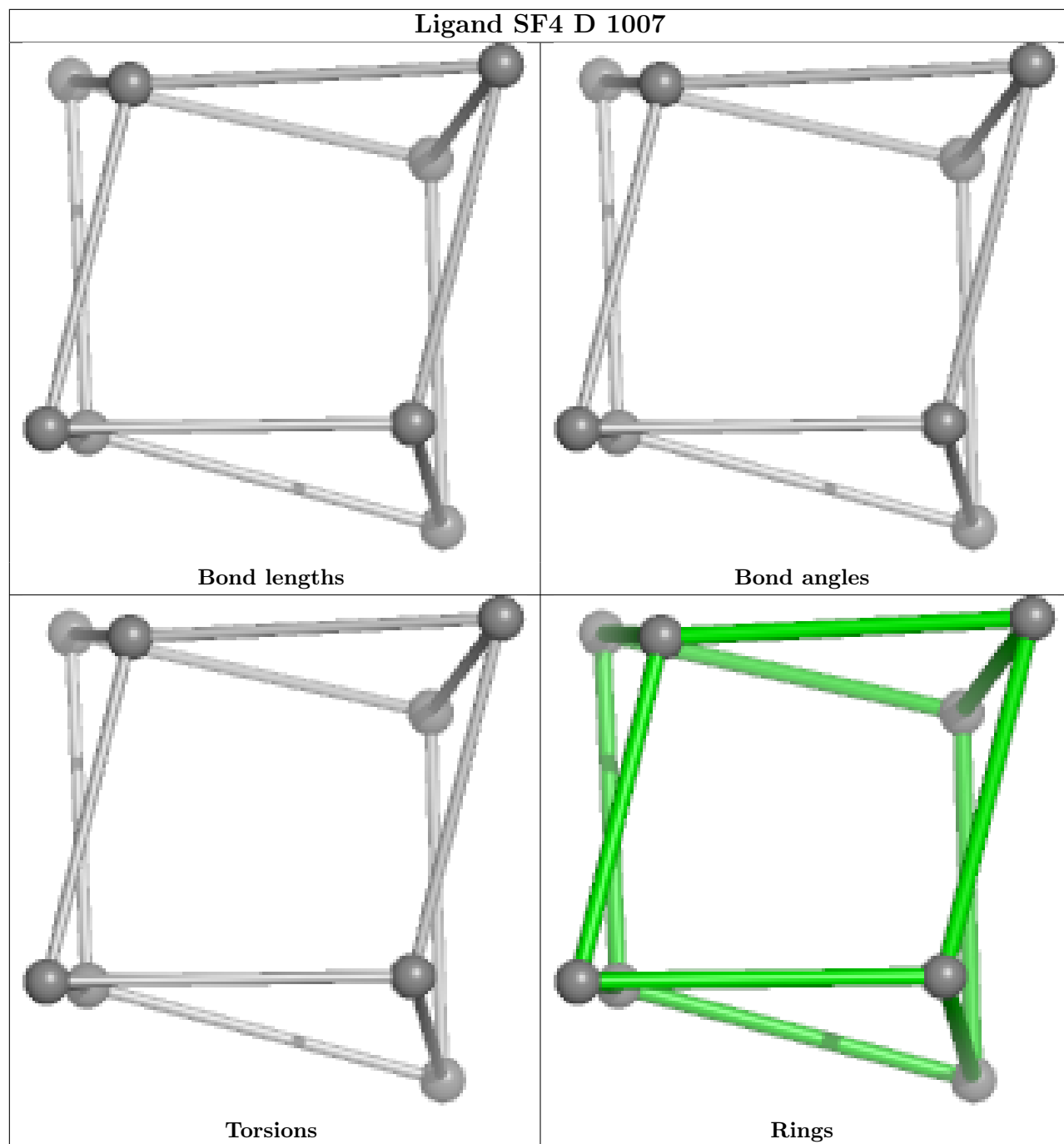


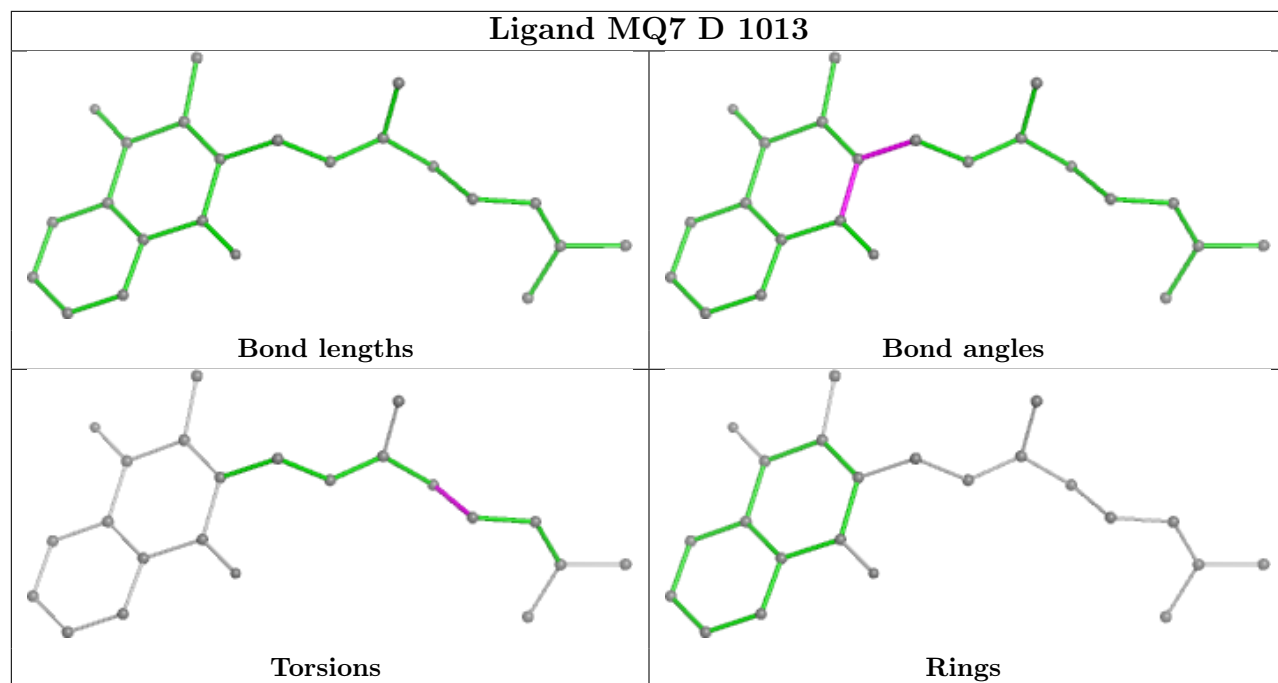


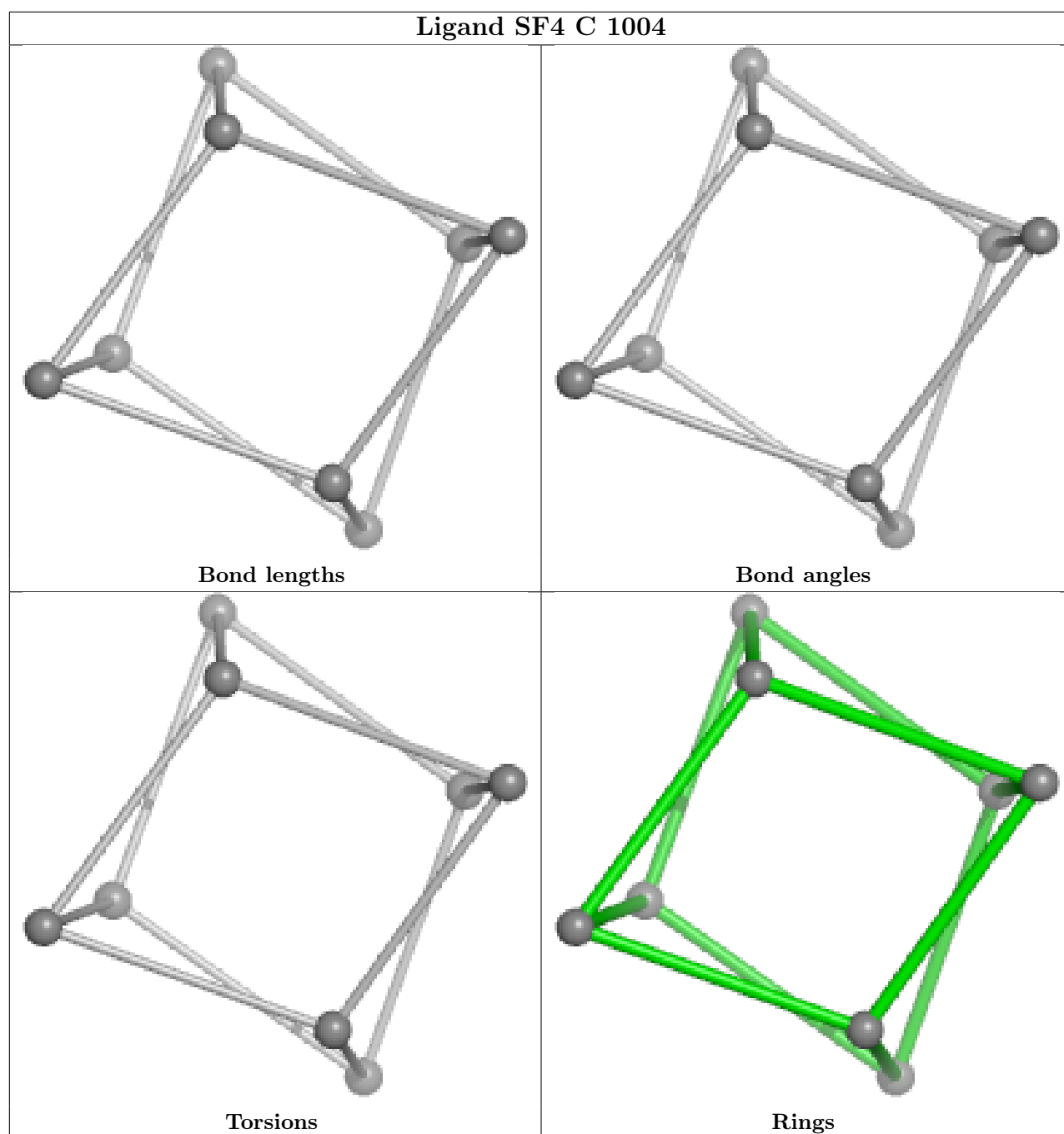


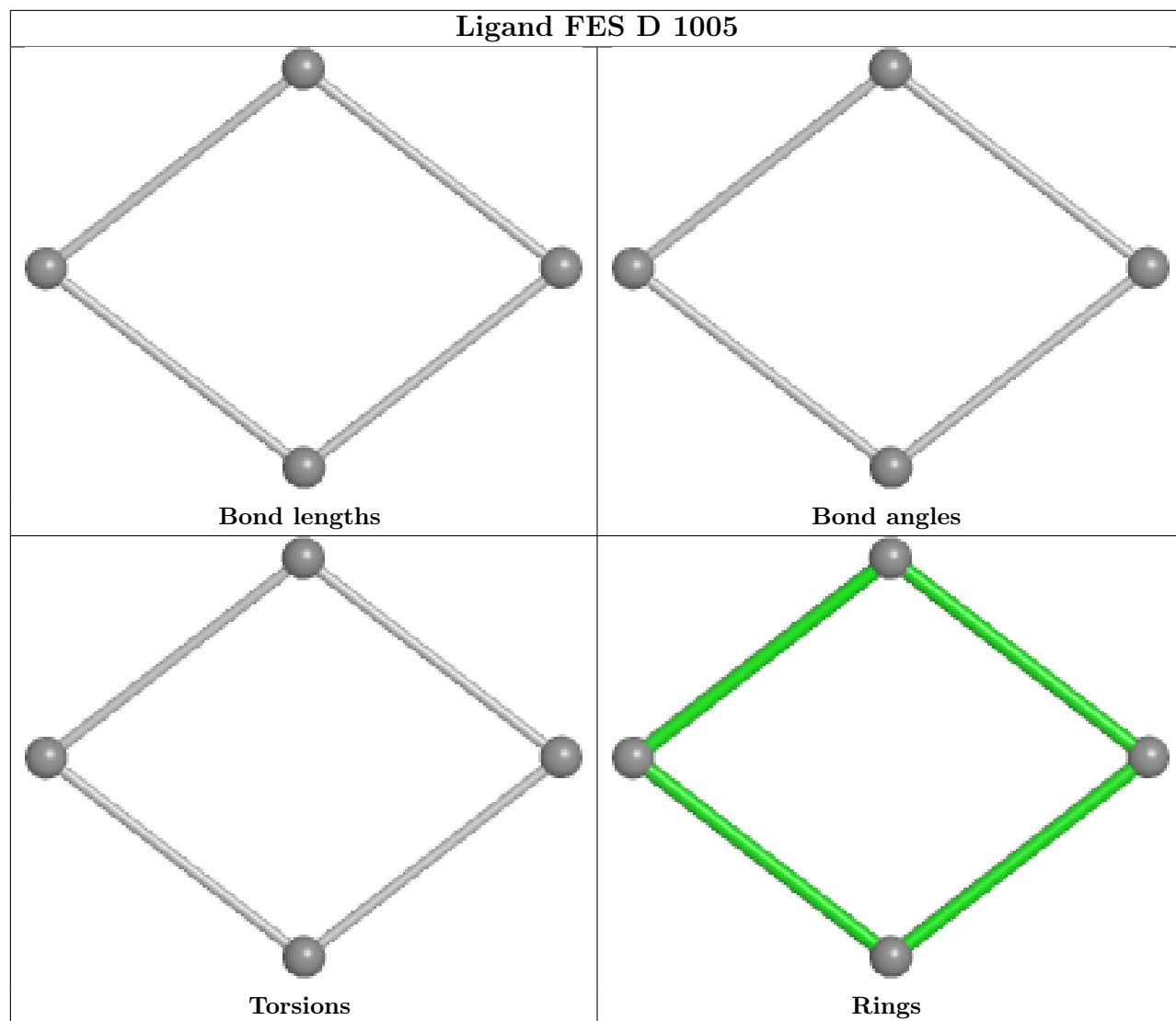
Ligand MGD D 1011

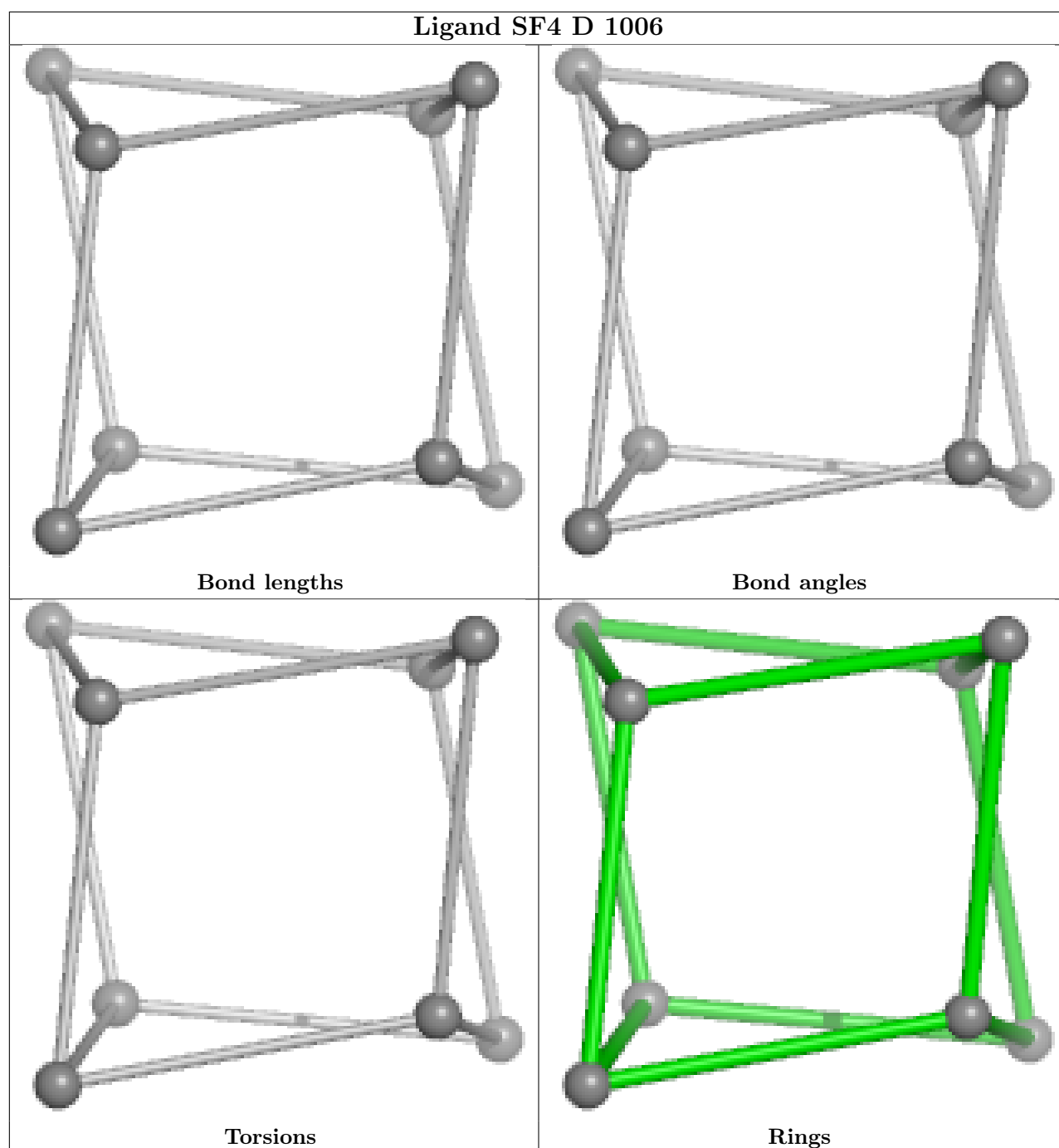


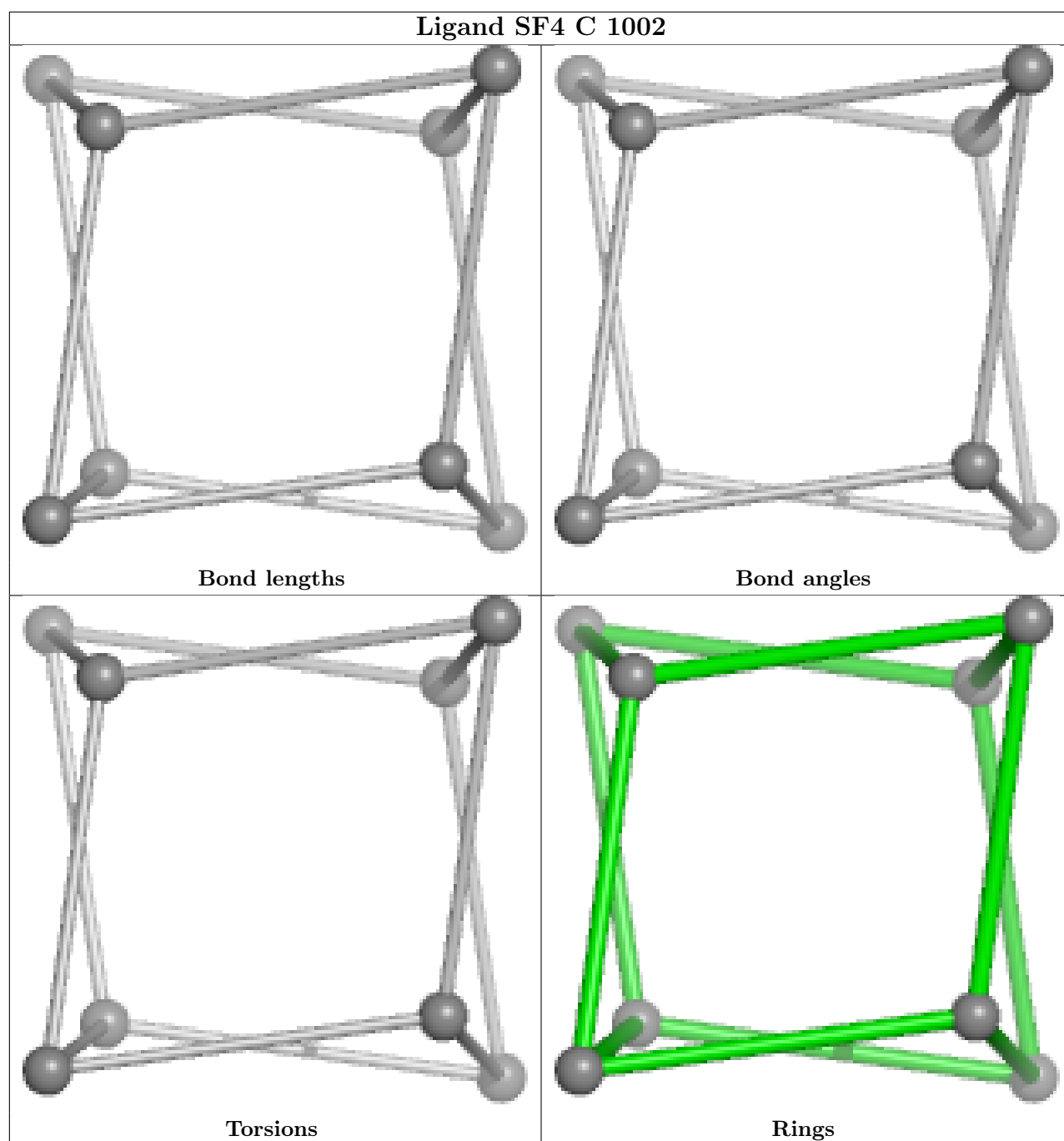


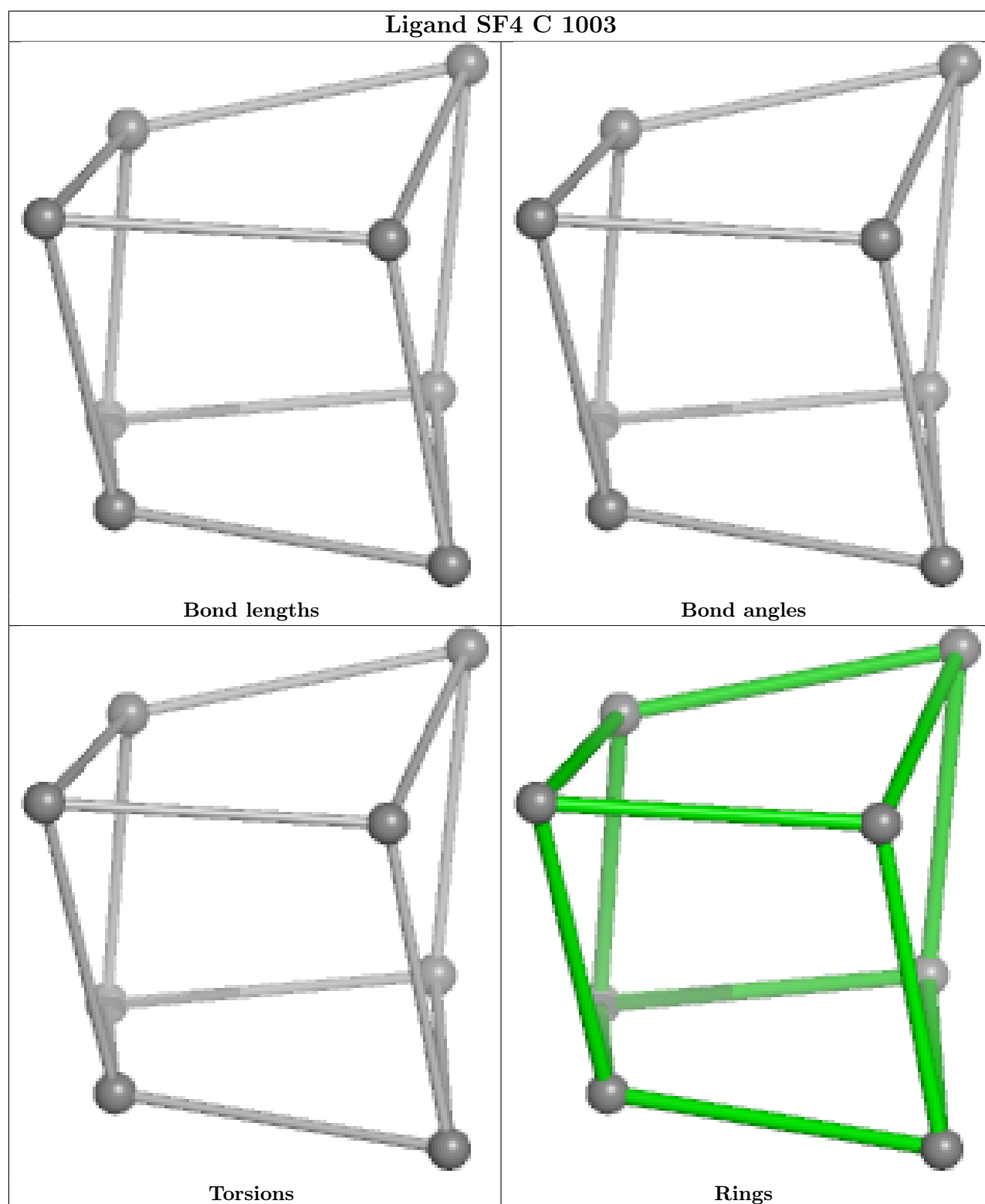




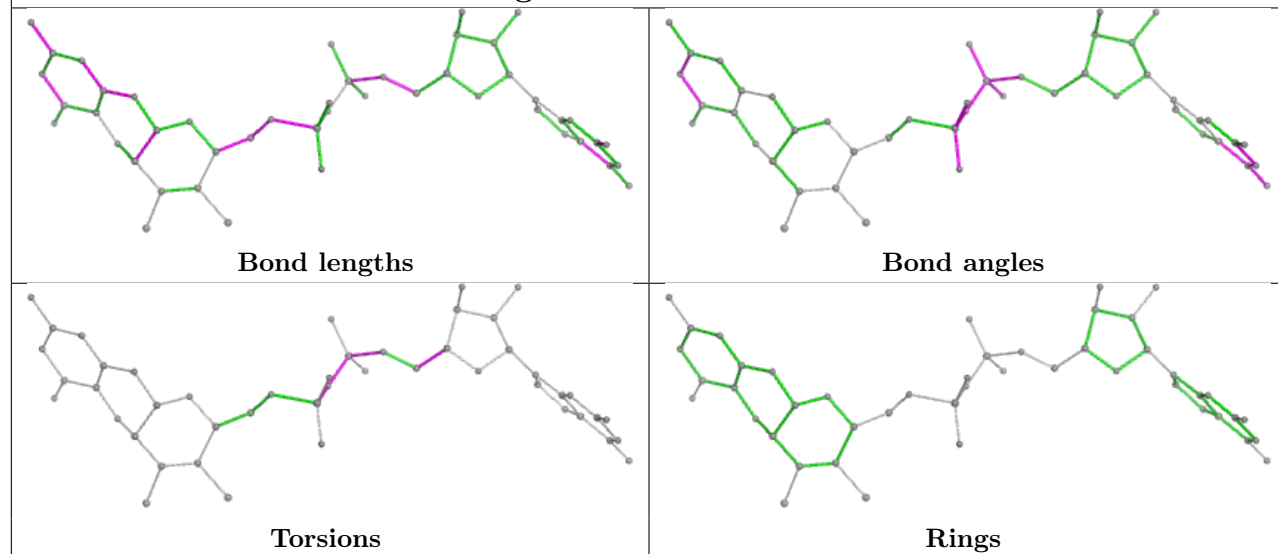




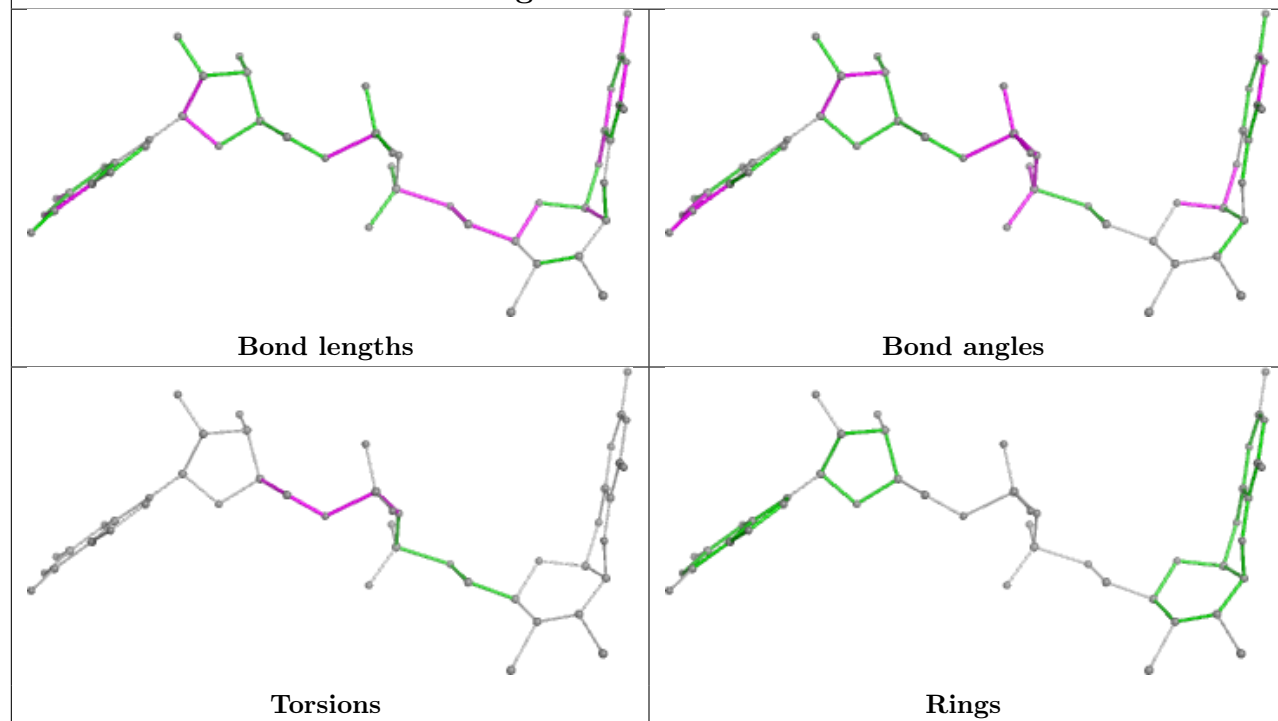




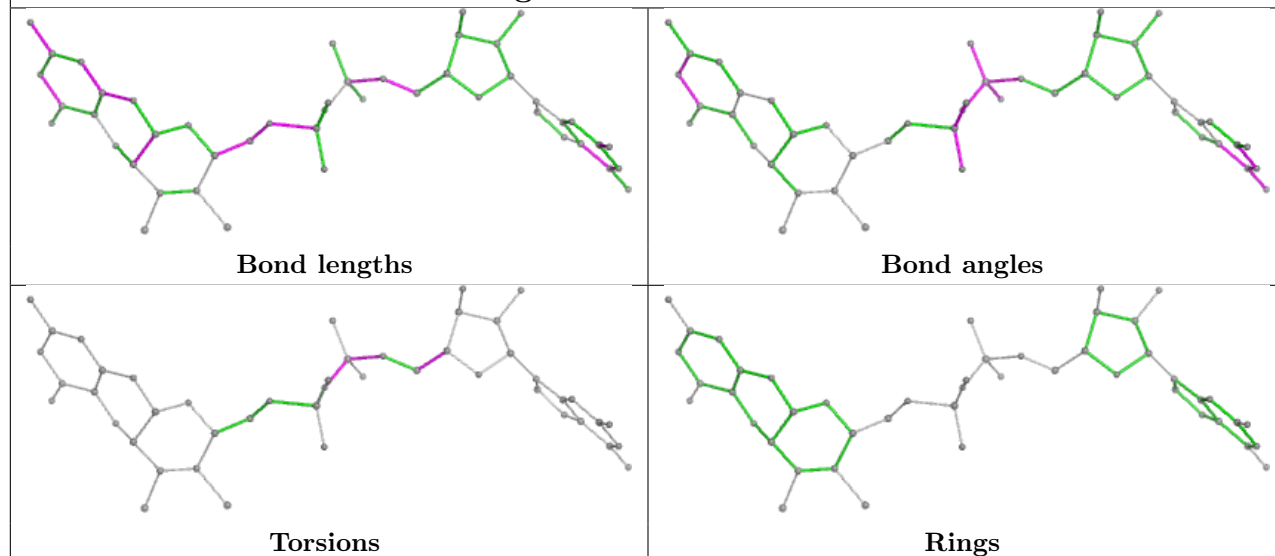
Ligand MGD D 1010



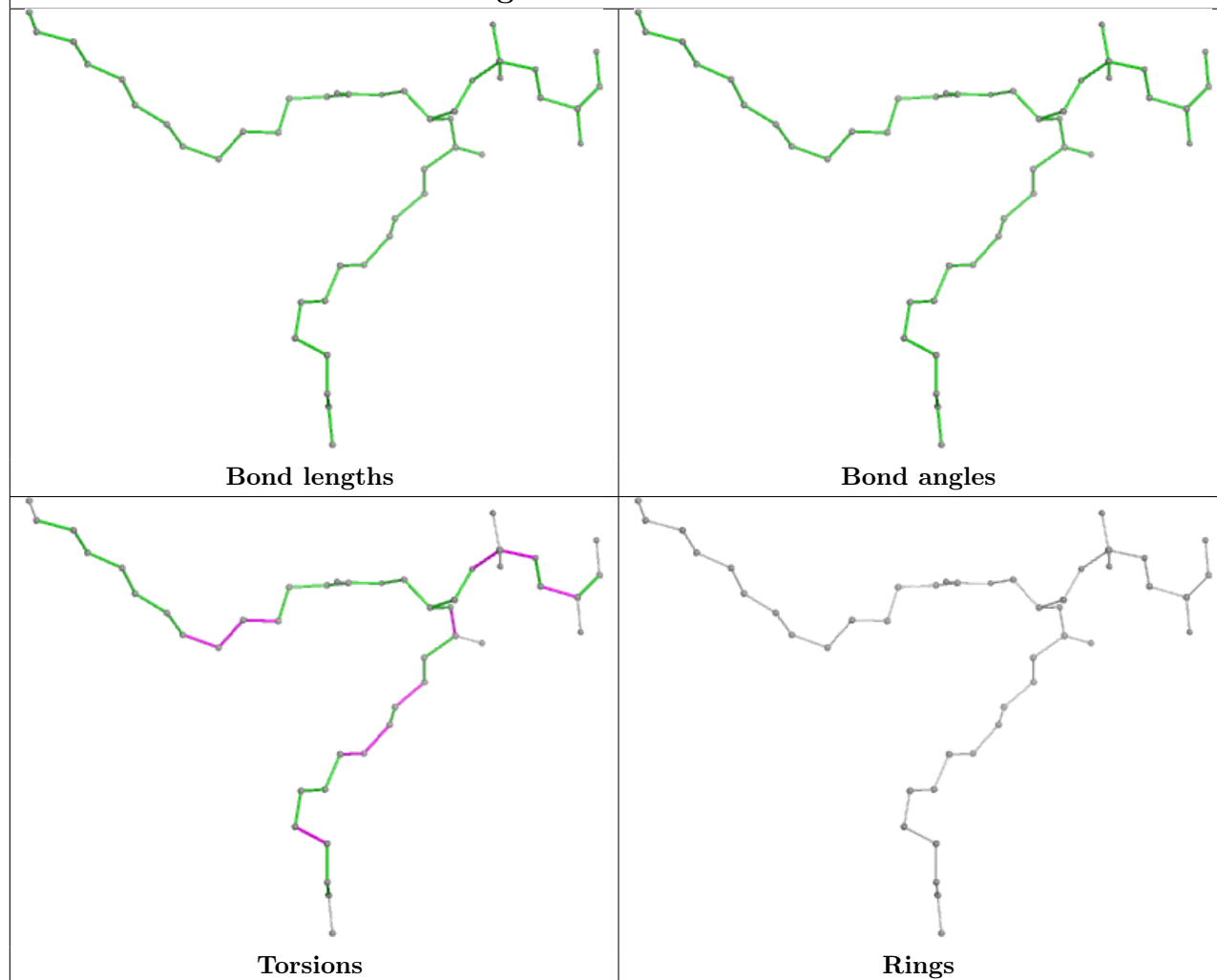
Ligand MGD C 1007

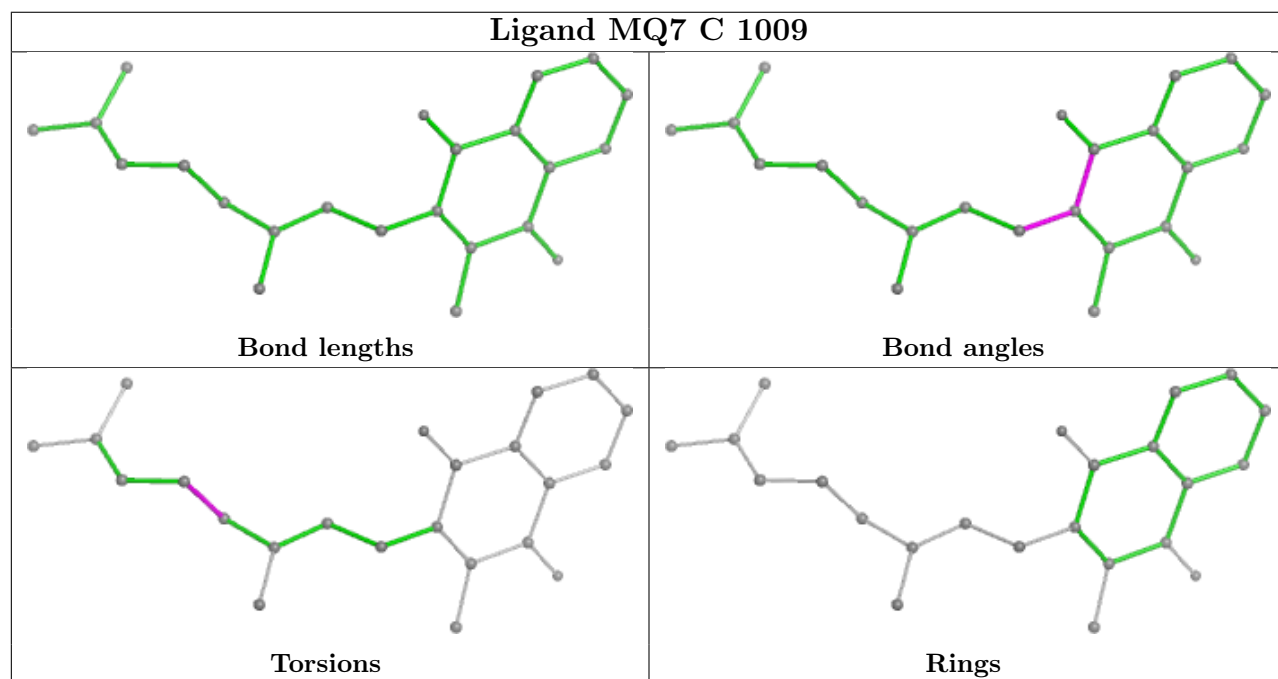
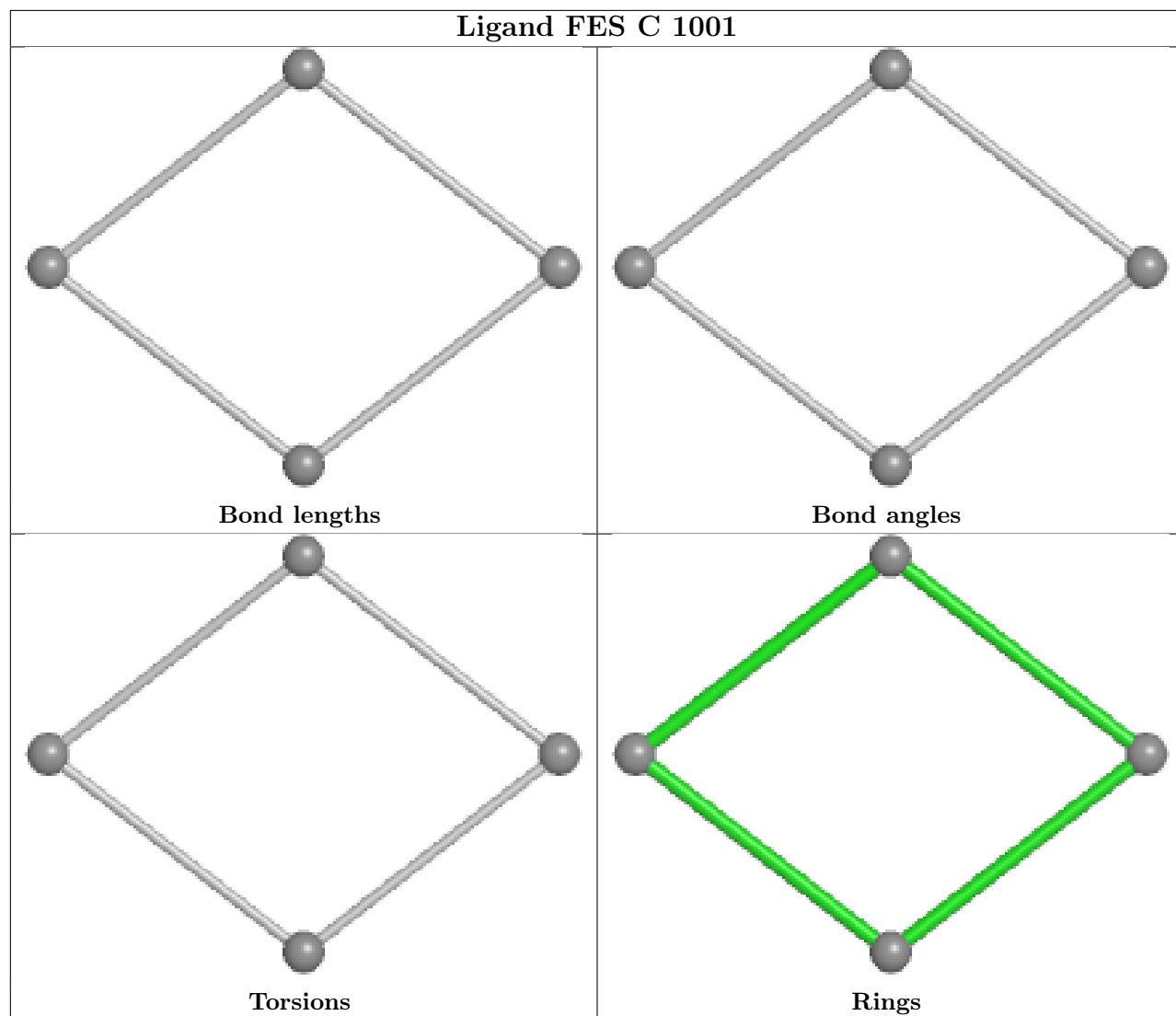


Ligand MGD C 1006



Ligand LHG C 1013





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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	147/186 (79%)	-1.53	0 100 100	13, 67, 149, 154	0
1	B	147/186 (79%)	-1.51	0 100 100	12, 68, 154, 160	1 (0%)
2	C	975/985 (98%)	-1.55	1 (0%) 92 92	16, 55, 91, 108	4 (0%)
2	D	975/985 (98%)	-1.55	0 100 100	20, 57, 97, 108	3 (0%)
All	All	2244/2342 (95%)	-1.54	1 (0%) 100 100	12, 57, 103, 160	8 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	519	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	203	6/6	0.98	0.06	57,58,58,58	0

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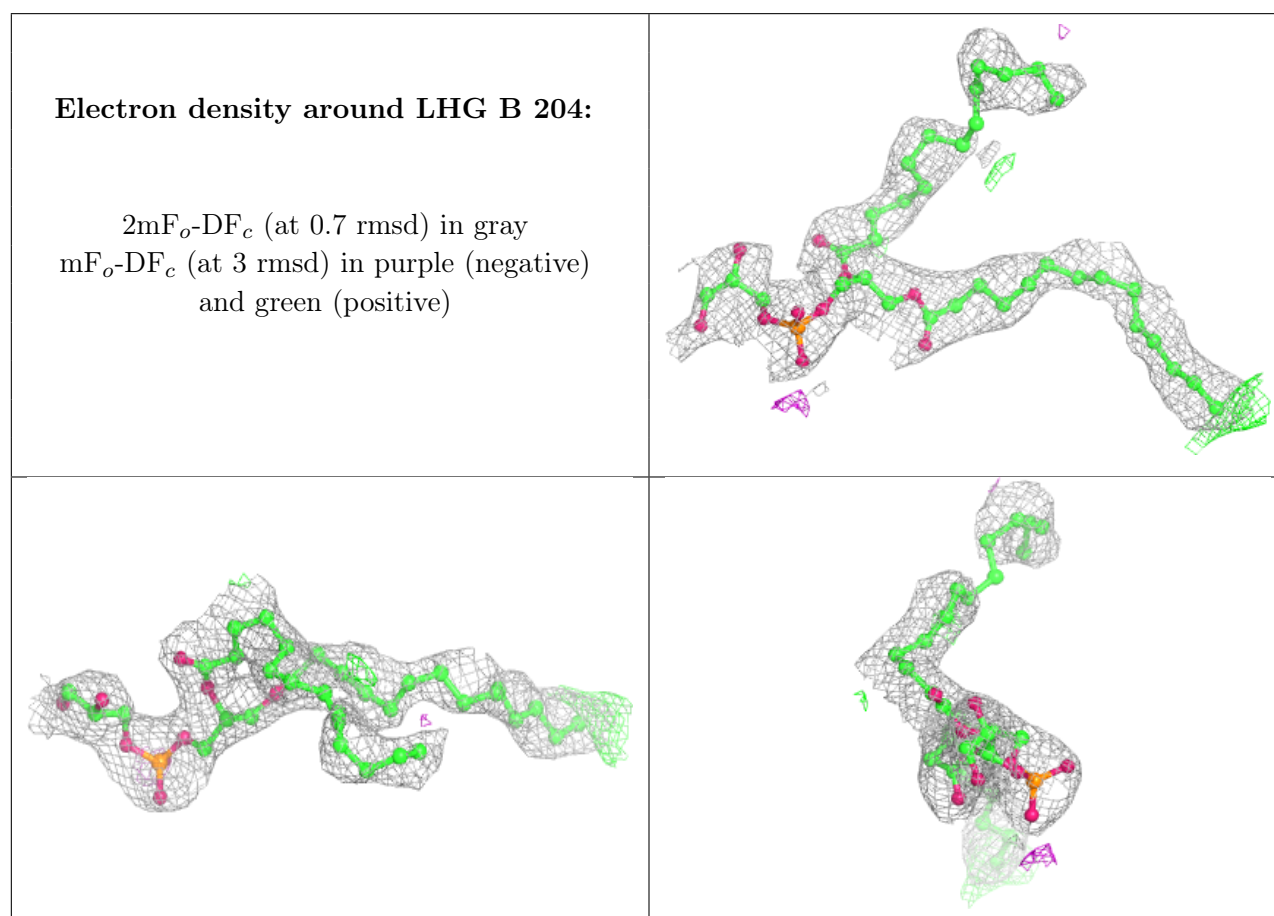
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	D	1016	6/6	0.98	0.11	120,120,120,121	0
12	MLI	C	1015	7/7	0.98	0.04	121,121,121,121	0
3	MYR	B	203	14/16	0.99	0.06	57,57,58,58	0
3	MYR	C	1017	16/16	0.99	0.07	75,76,77,77	0
3	MYR	A	201	16/16	0.99	0.05	53,54,55,55	0
4	GOL	B	201	6/6	0.99	0.04	52,52,52,52	0
4	GOL	D	1003	6/6	0.99	0.04	44,45,45,46	0
3	MYR	A	202	14/16	0.99	0.04	56,56,58,58	0
5	LHG	B	204	45/49	0.99	0.04	46,56,61,61	0
5	LHG	C	1013	45/49	0.99	0.04	46,57,59,59	0
10	MQ7	C	1009	23/48	0.99	0.05	64,66,67,67	0
10	MQ7	D	1013	23/48	0.99	0.04	65,65,65,65	0
12	MLI	C	1011	7/7	0.99	0.05	83,83,83,83	0
12	MLI	C	1012	7/7	0.99	0.05	97,97,97,97	0
3	MYR	B	202	16/16	0.99	0.05	55,55,58,58	0
12	MLI	C	1020	7/7	0.99	0.05	101,101,101,101	0
12	MLI	C	1022	7/7	0.99	0.06	74,74,75,75	0
12	MLI	D	1002	7/7	0.99	0.06	97,97,97,97	0
12	MLI	D	1015	7/7	0.99	0.06	99,99,99,99	0
12	MLI	D	1019	7/7	0.99	0.05	75,75,76,77	0
13	NO3	C	1014	4/4	0.99	0.05	67,67,67,67	0
13	NO3	C	1016	4/4	0.99	0.06	89,89,89,89	0
13	NO3	D	1001	4/4	0.99	0.08	79,79,79,79	0
13	NO3	D	1004	4/4	0.99	0.04	77,77,77,77	0
8	MGD	C	1006	47/47	1.00	0.03	34,43,49,49	0
8	MGD	C	1007	47/47	1.00	0.03	39,47,57,58	0
8	MGD	D	1010	47/47	1.00	0.03	33,43,51,51	0
8	MGD	D	1011	47/47	1.00	0.03	45,52,64,65	0
9	4MO	C	1008	1/1	1.00	0.00	49,49,49,49	0
9	4MO	D	1012	1/1	1.00	0.00	48,48,48,48	0
4	GOL	D	1017	6/6	1.00	0.04	82,83,83,83	0
4	GOL	D	1018	6/6	1.00	0.03	61,61,61,61	0
11	H2S	C	1010	1/1	1.00	0.08	41,41,41,41	1
11	H2S	D	1014	1/1	1.00	0.05	33,33,33,33	1
4	GOL	C	1018	6/6	1.00	0.05	74,74,74,75	0
4	GOL	C	1019	6/6	1.00	0.04	78,78,78,78	0
6	FES	C	1001	4/4	1.00	0.01	71,71,71,71	0
6	FES	D	1005	4/4	1.00	0.01	70,70,70,70	0
12	MLI	C	1021	7/7	1.00	0.04	86,86,87,87	0
7	SF4	C	1002	8/8	1.00	0.01	34,34,34,34	0
7	SF4	C	1003	8/8	1.00	0.01	45,45,45,46	0
7	SF4	C	1004	8/8	1.00	0.01	37,37,37,37	0

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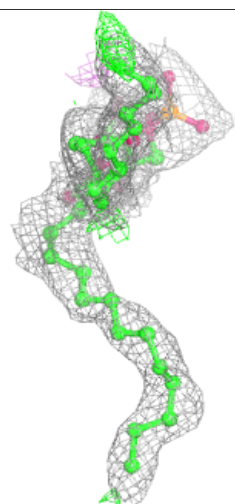
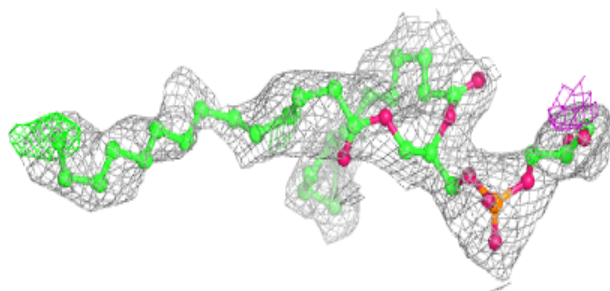
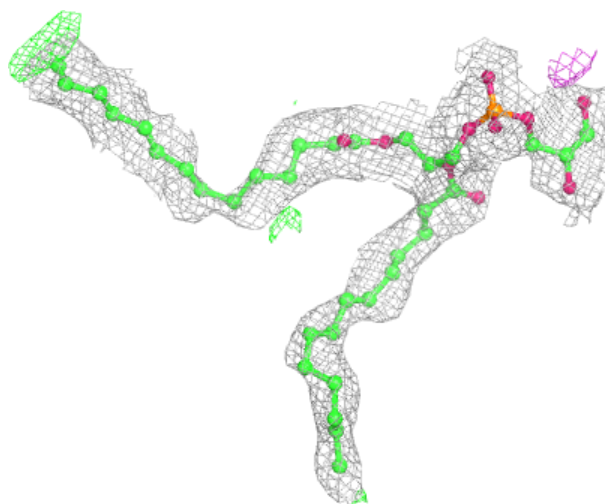
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	SF4	C	1005	8/8	1.00	0.01	33,33,33,33	0
7	SF4	D	1006	8/8	1.00	0.01	32,33,33,33	0
7	SF4	D	1007	8/8	1.00	0.01	45,45,46,46	0
7	SF4	D	1008	8/8	1.00	0.01	34,35,35,35	0
7	SF4	D	1009	8/8	1.00	0.01	33,34,34,34	0
14	NA	D	1020	1/1	1.00	0.03	28,28,28,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



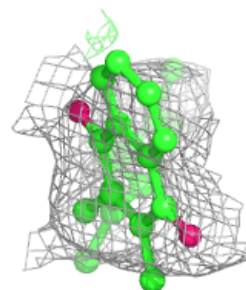
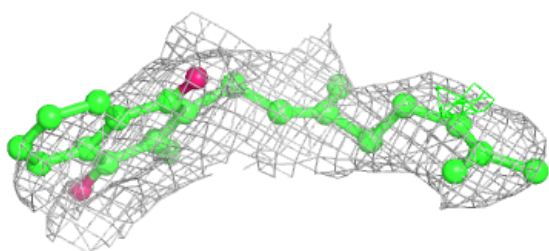
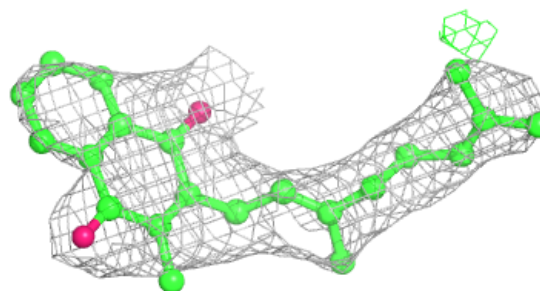
Electron density around LHG C 1013:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

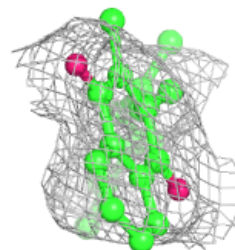
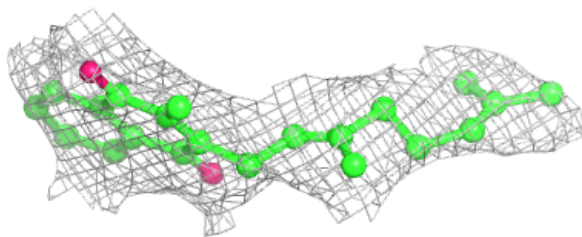
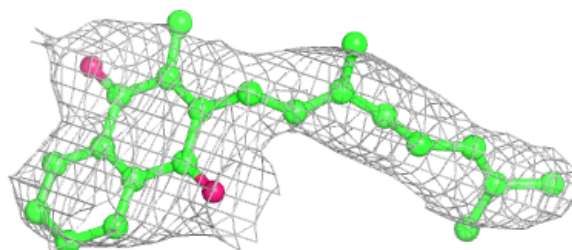


Electron density around MQ7 C 1009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

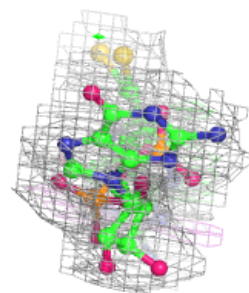
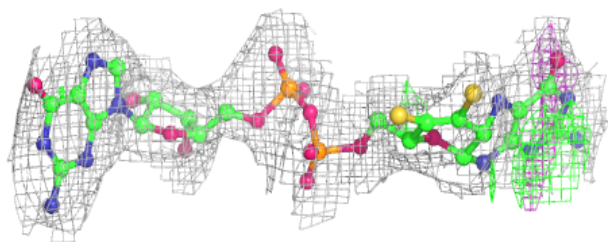
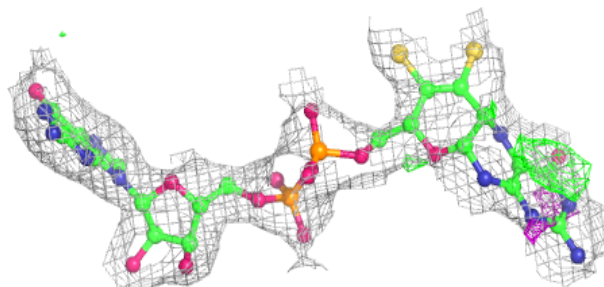
**Electron density around MQ7 D 1013:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

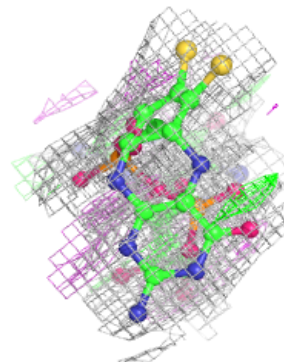
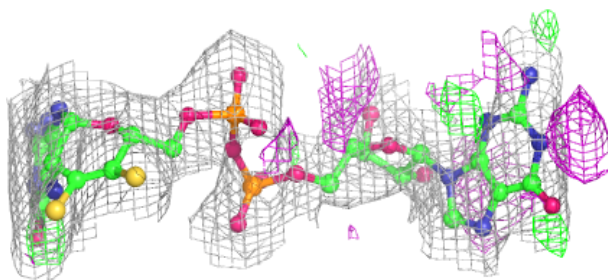
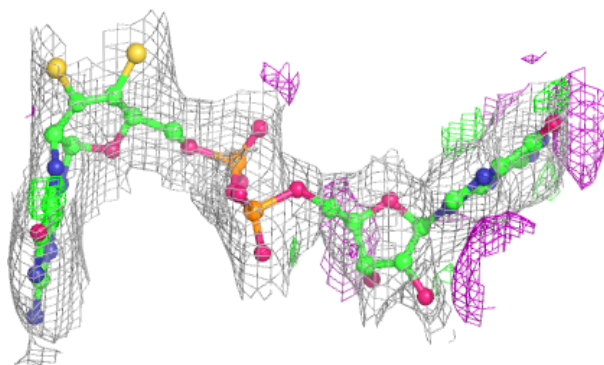


Electron density around MGD C 1006:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

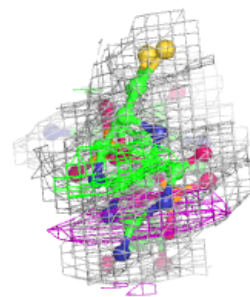
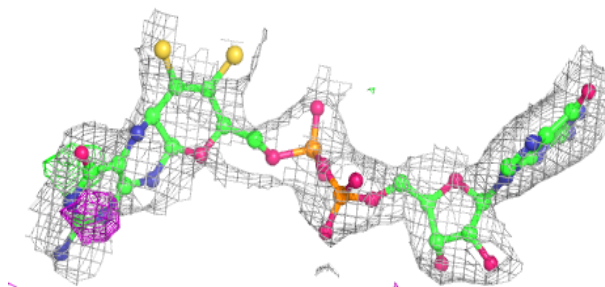
**Electron density around MGD C 1007:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

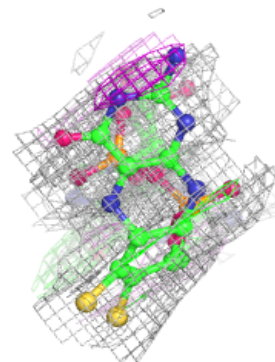
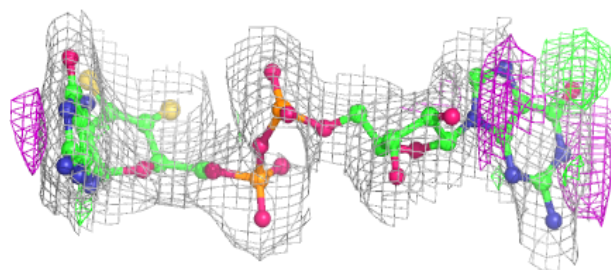
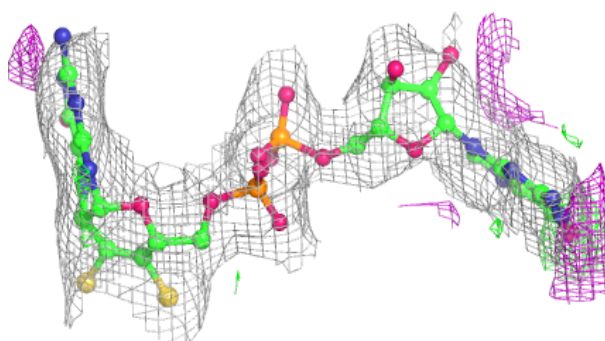


Electron density around MGD D 1010:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

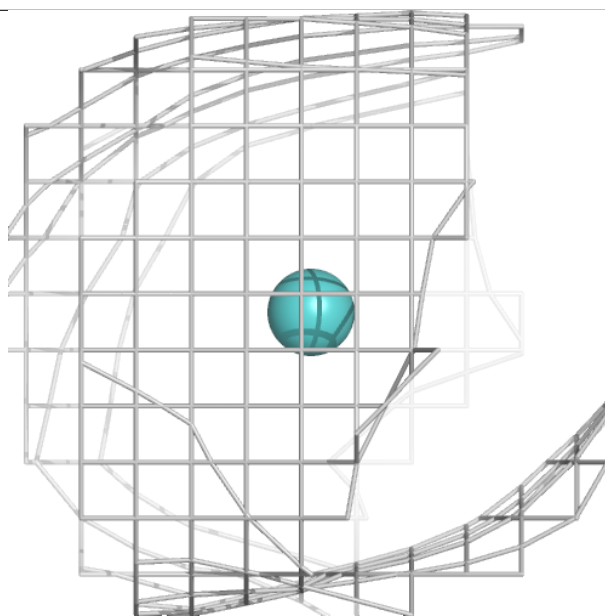
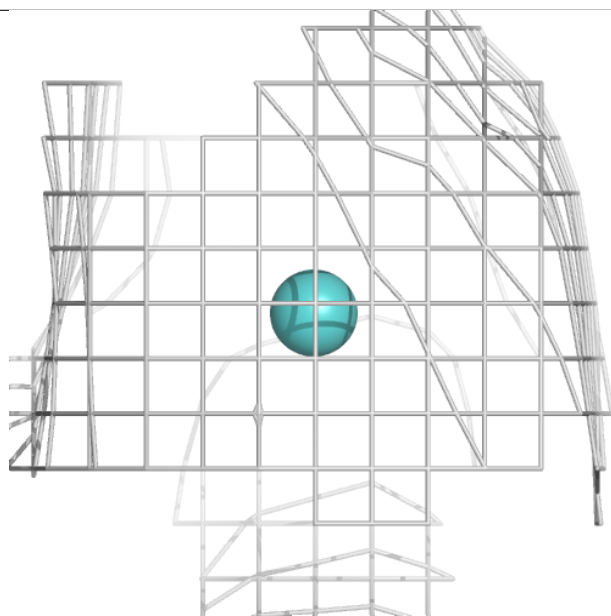
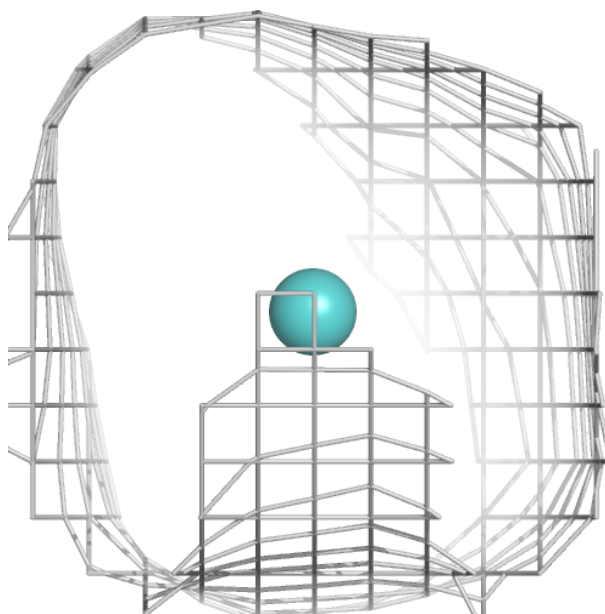
**Electron density around MGD D 1011:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



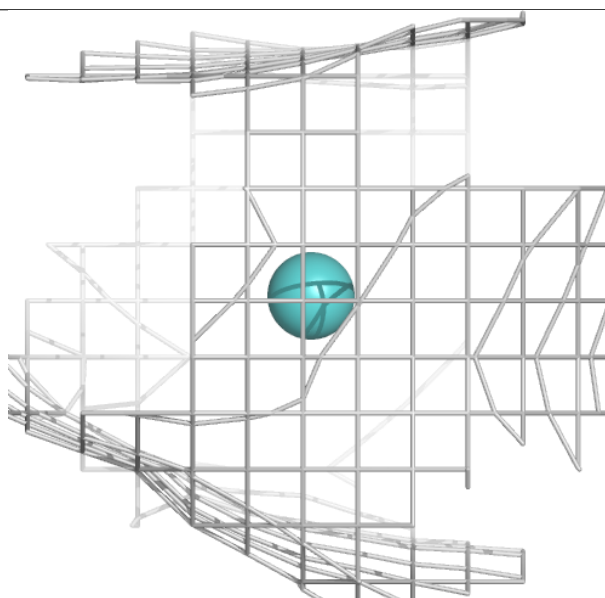
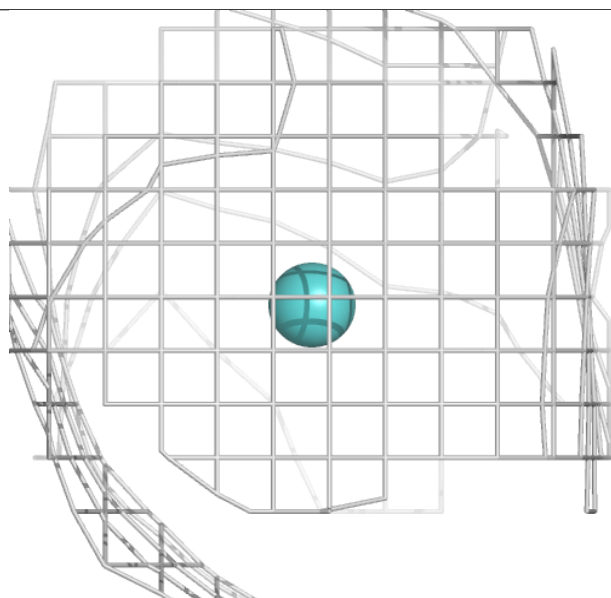
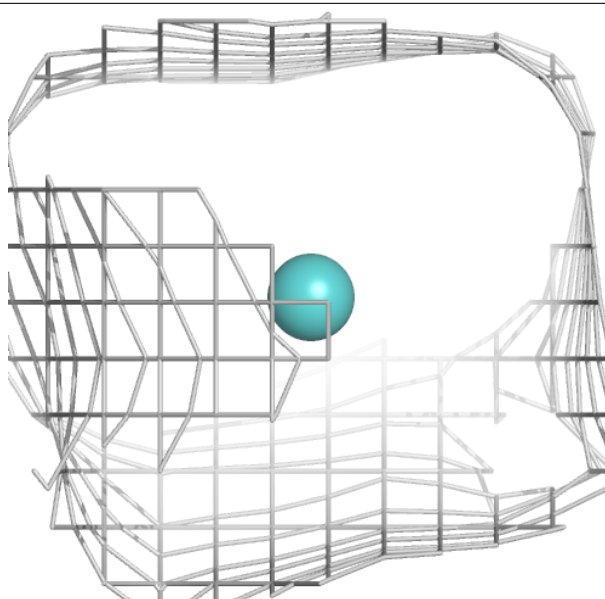
Electron density around 4MO C 1008:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



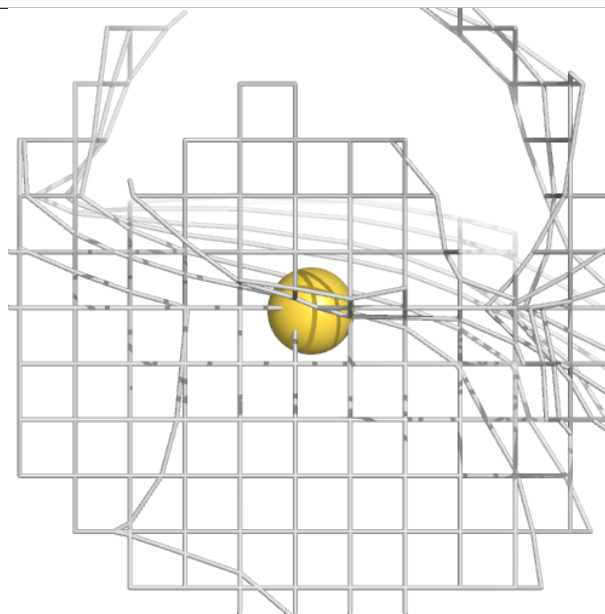
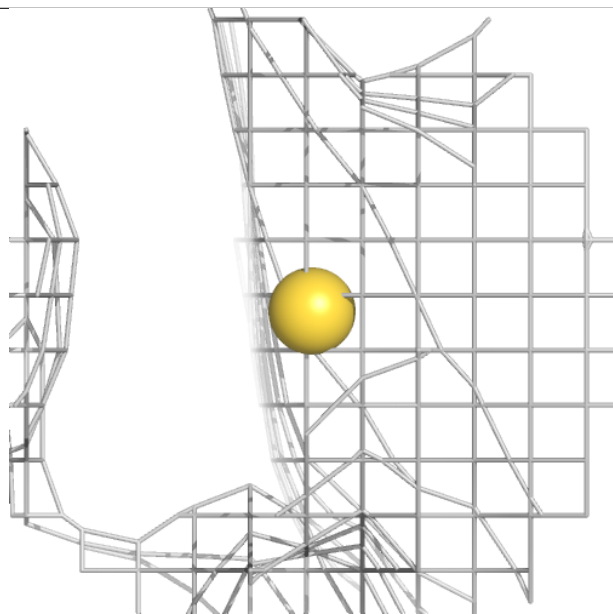
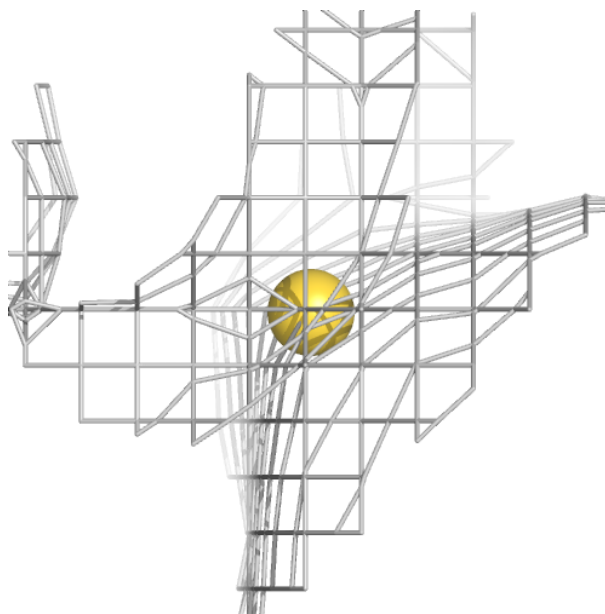
Electron density around 4MO D 1012:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



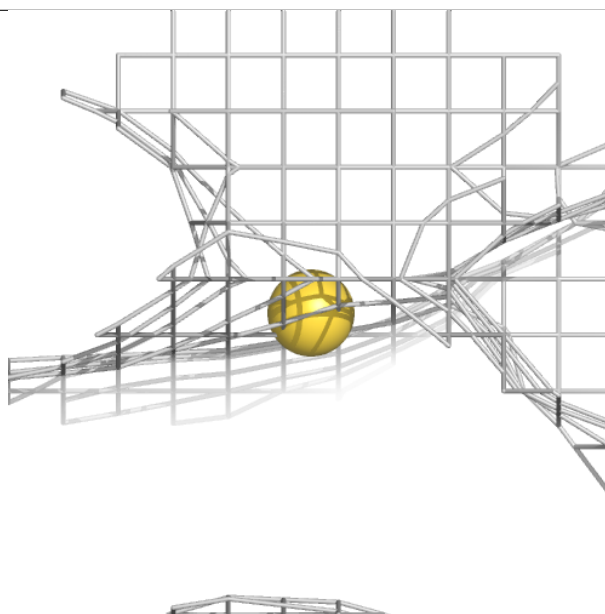
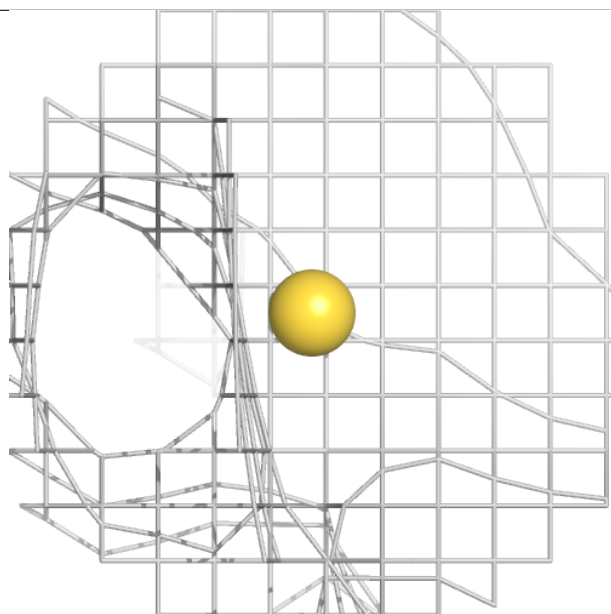
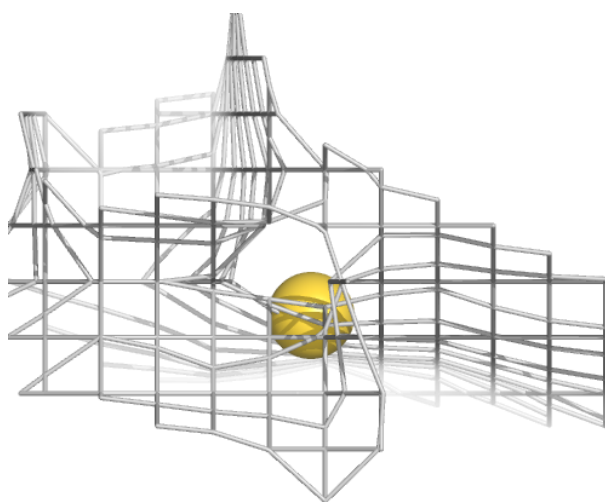
Electron density around H2S C 1010:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



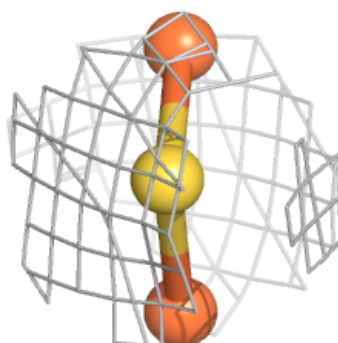
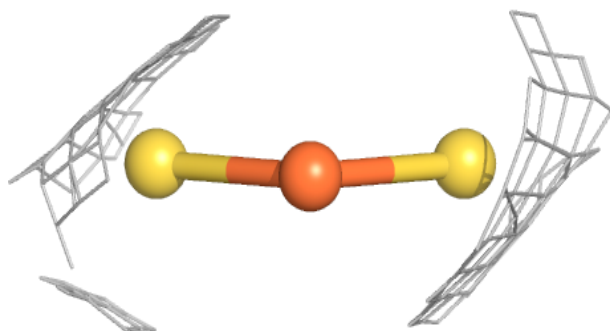
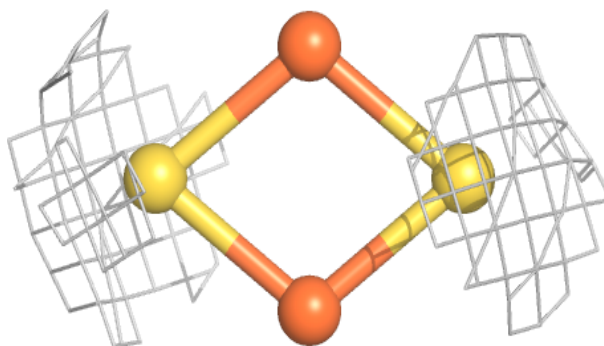
Electron density around H2S D 1014:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

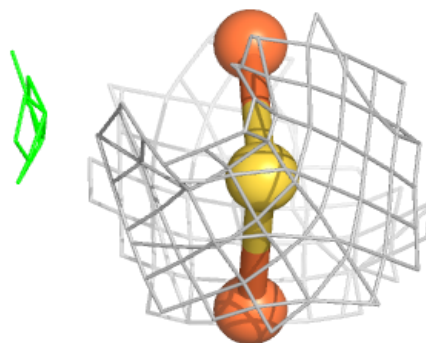
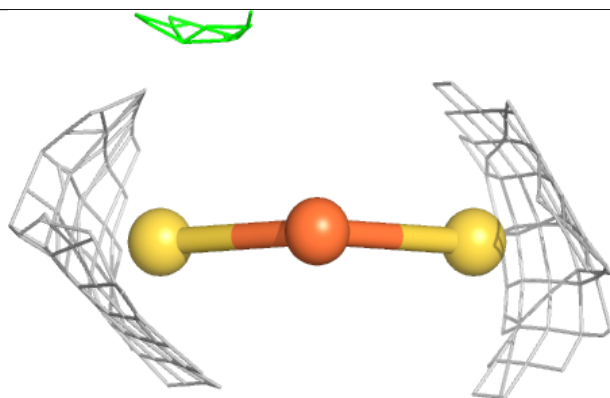
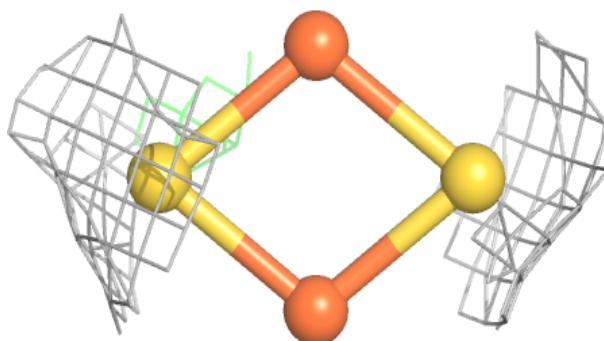


Electron density around FES C 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

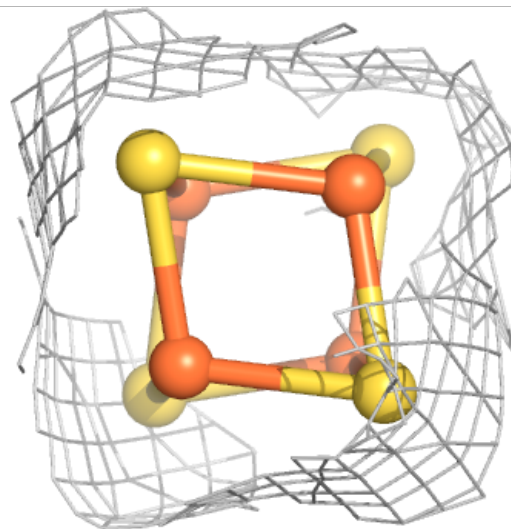
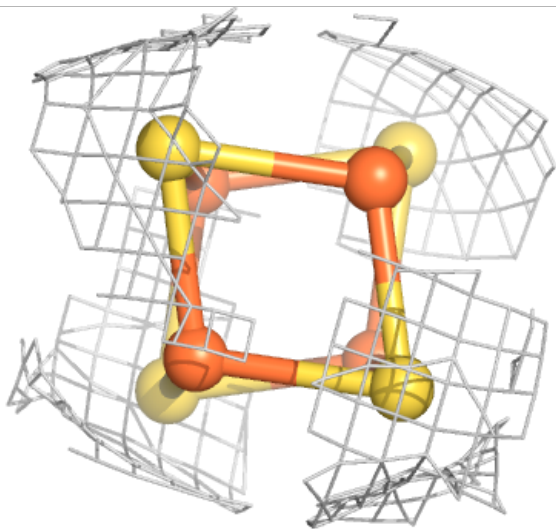
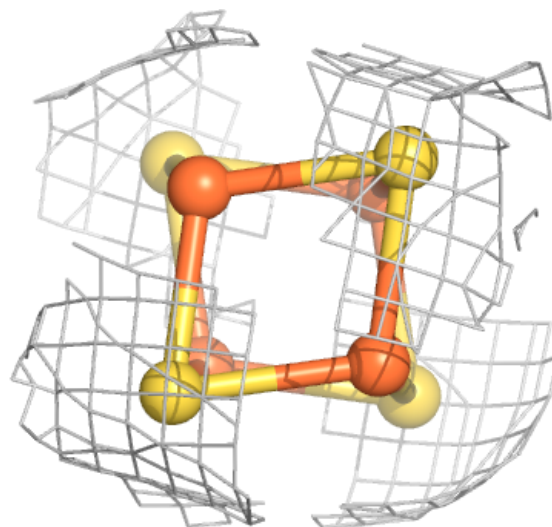
**Electron density around FES D 1005:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



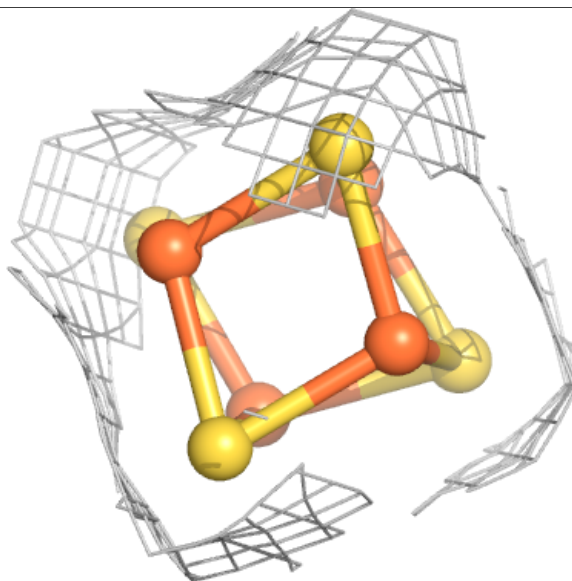
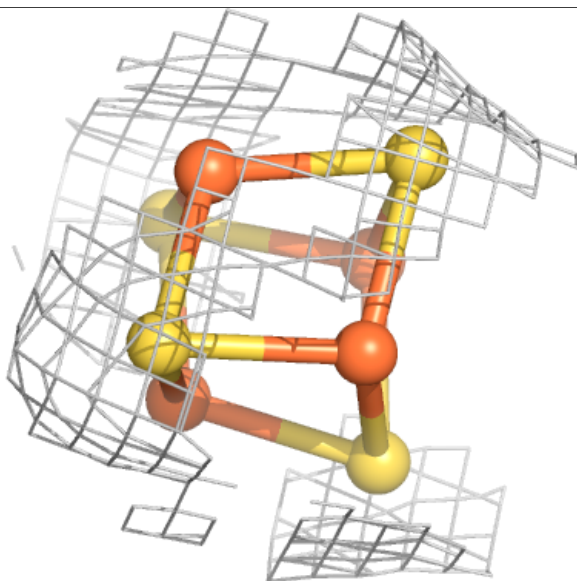
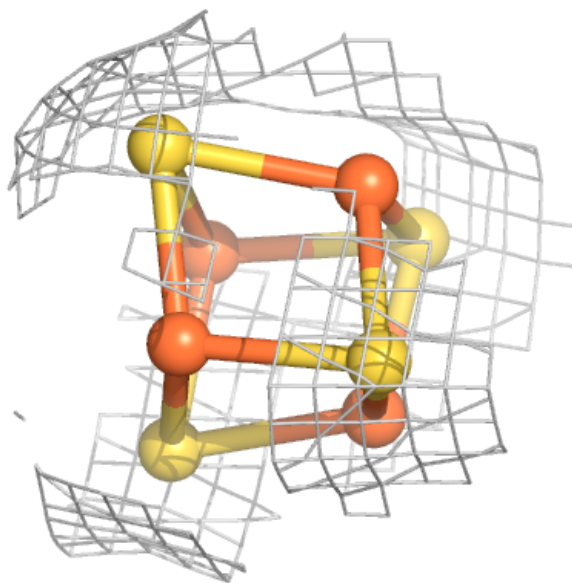
Electron density around SF4 C 1002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



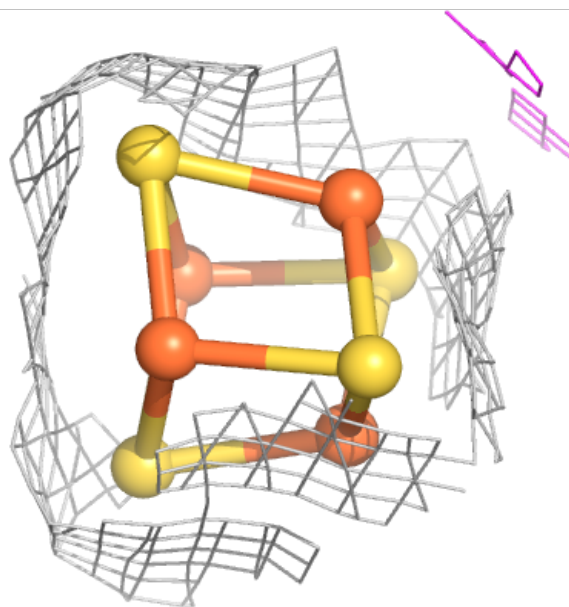
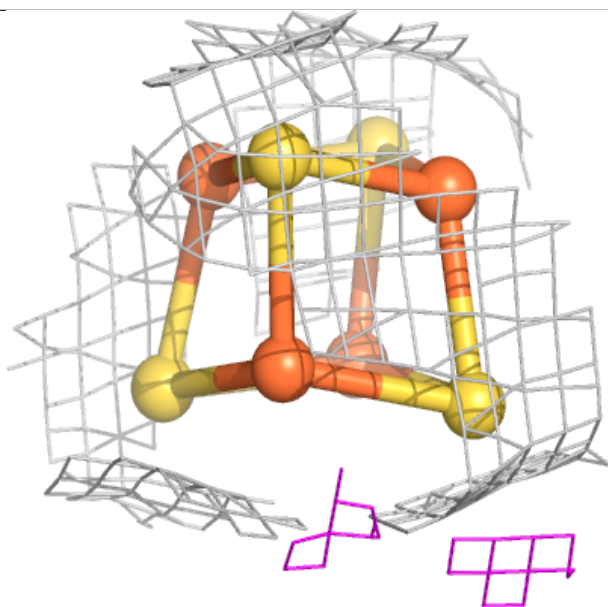
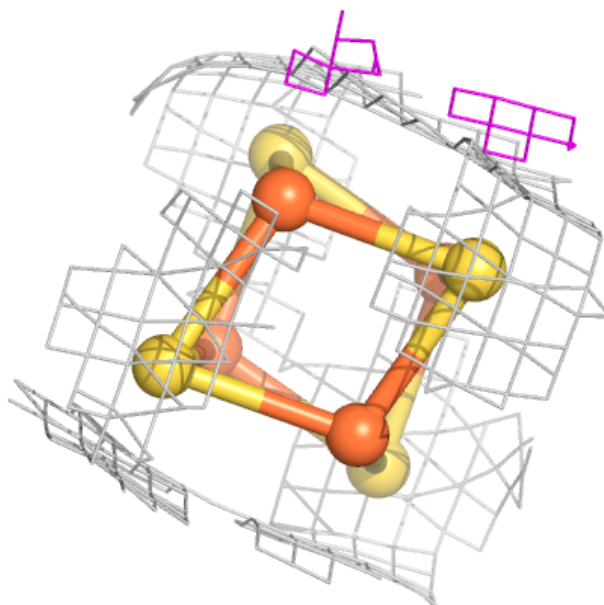
Electron density around SF4 C 1003:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



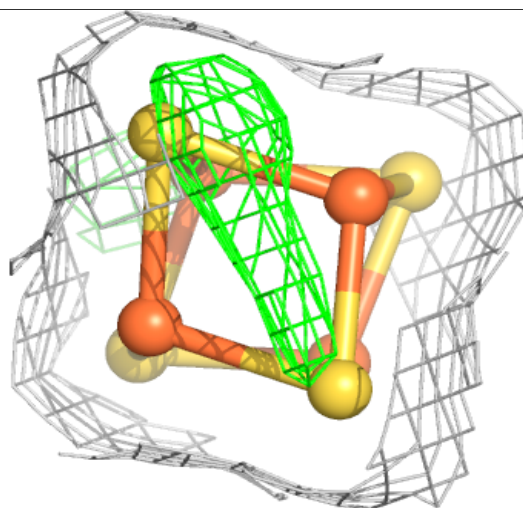
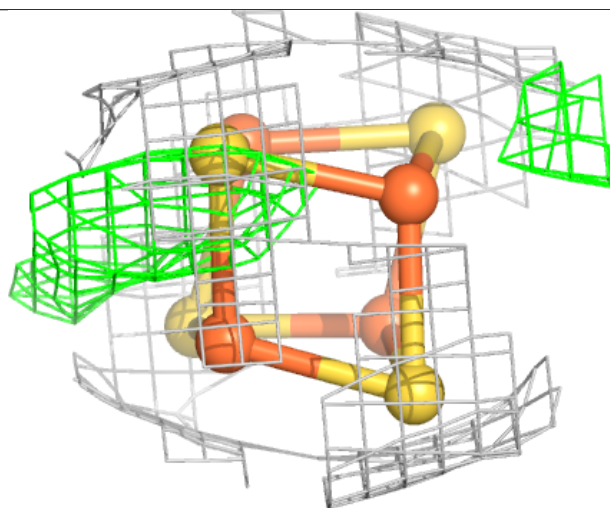
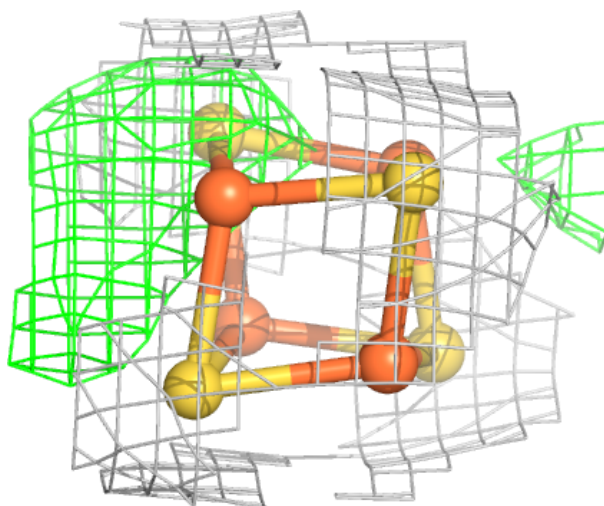
Electron density around SF4 C 1004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



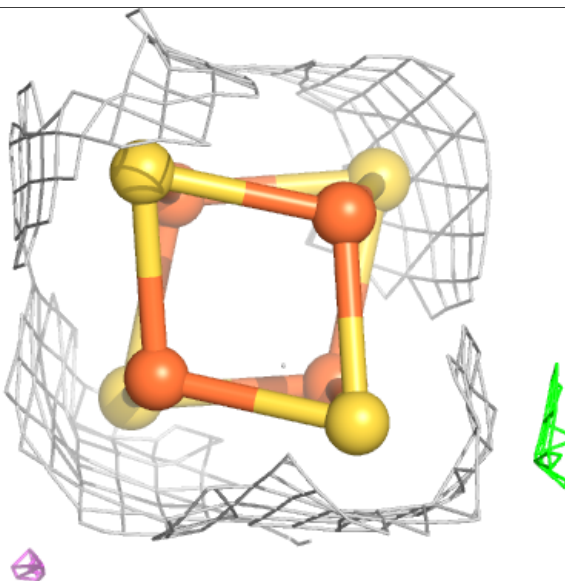
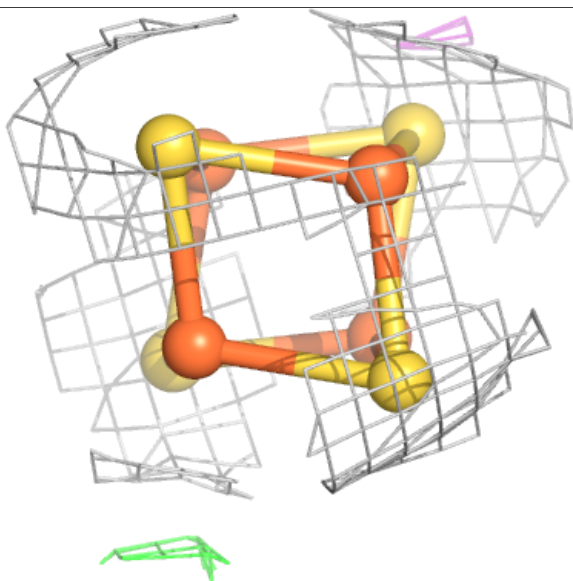
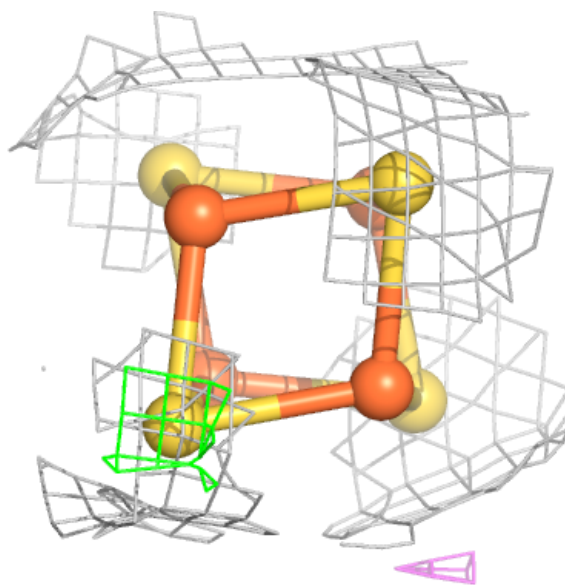
Electron density around SF4 C 1005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



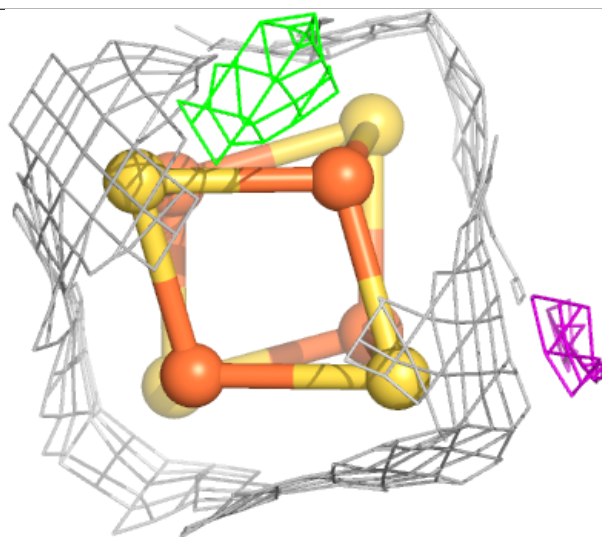
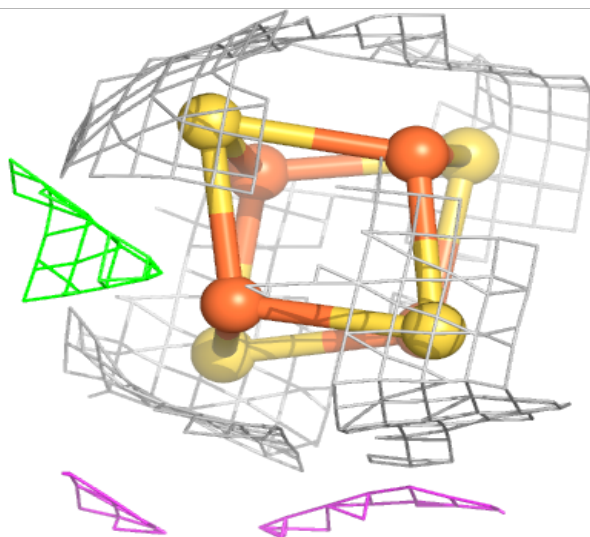
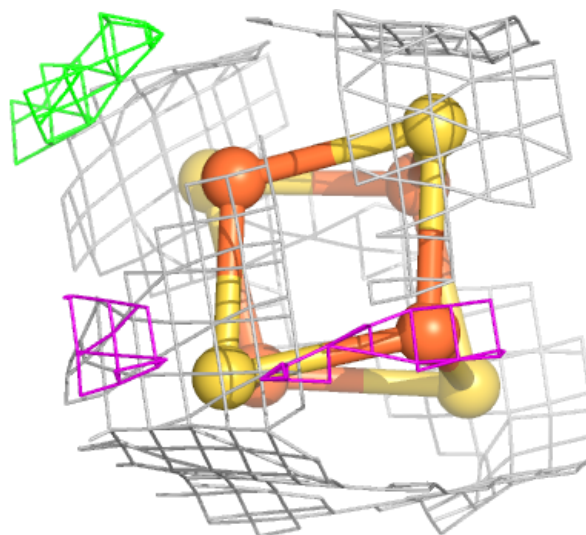
Electron density around SF4 D 1006:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



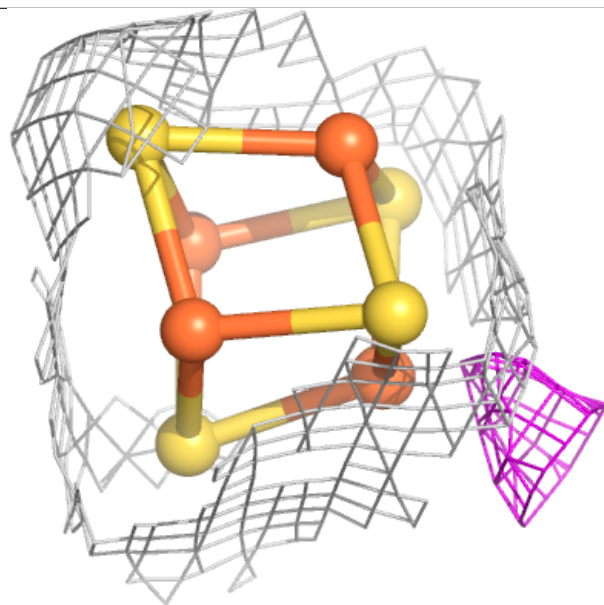
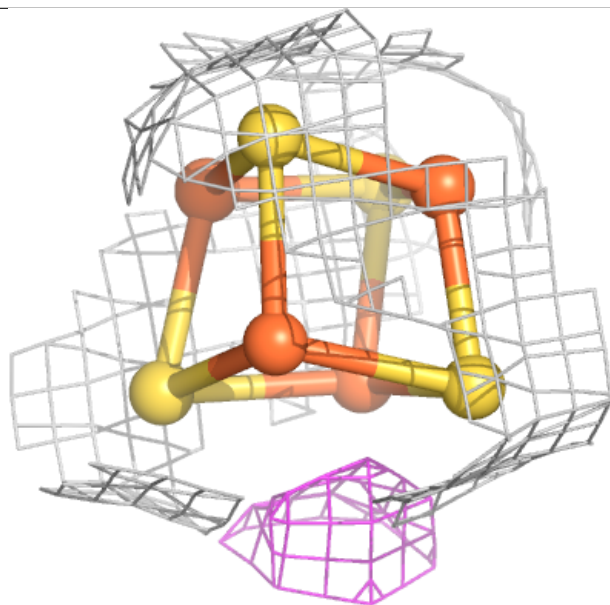
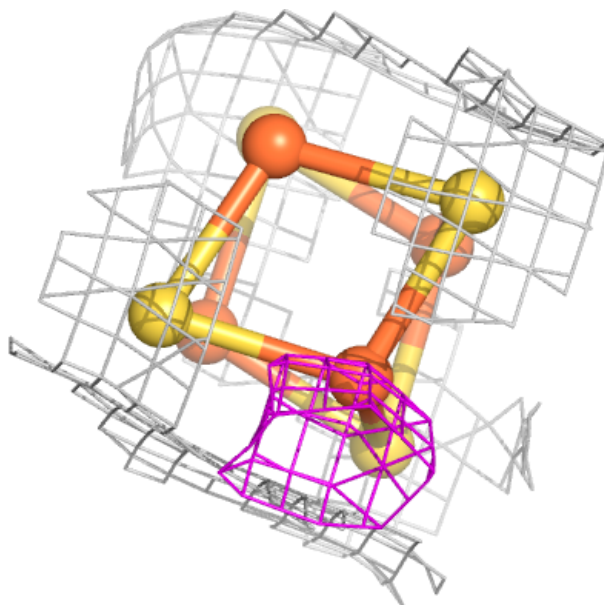
Electron density around SF4 D 1007:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



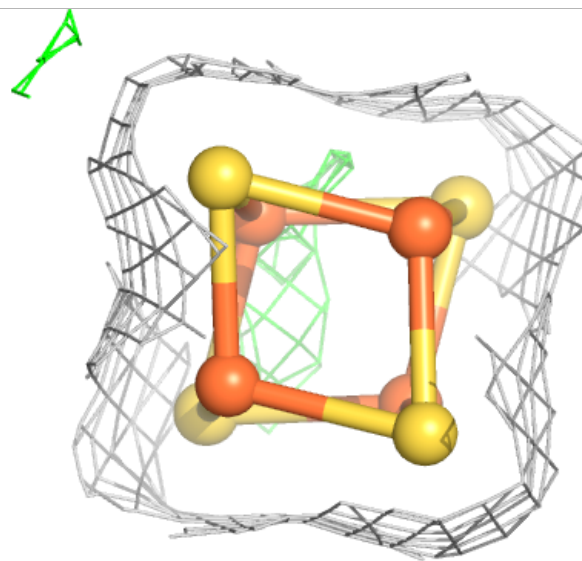
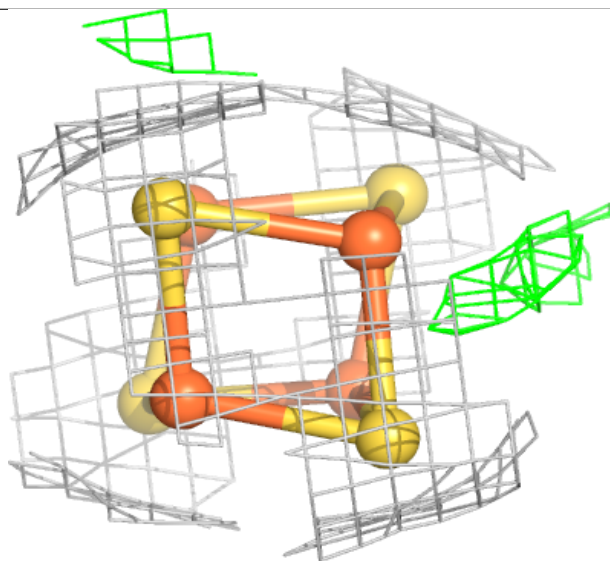
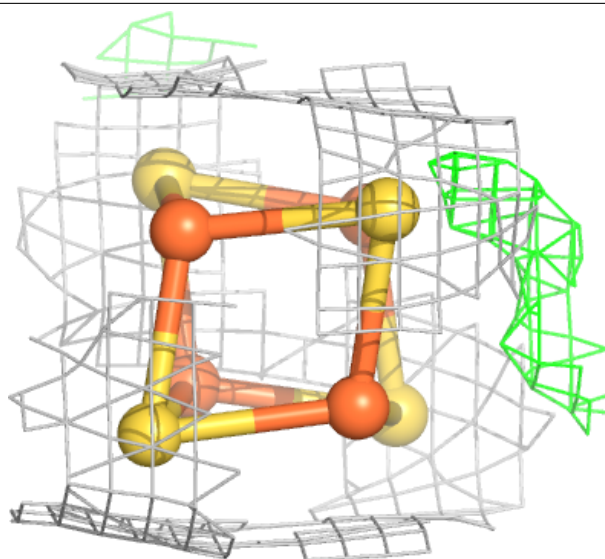
Electron density around SF4 D 1008:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SF4 D 1009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.