



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:49 PM UTC

PDB ID : 8CGS / pdb_00008cgs
Title : Crystal structure of arsenite oxidase from *Alcaligenes faecalis* (Af Aio) bound to antimony oxyanion
Authors : Engrola, F.; Correia, M.A.S.; Romao, M.J.; Santos-Silva, T.
Deposited on : 2023-02-06
Resolution : 1.84 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

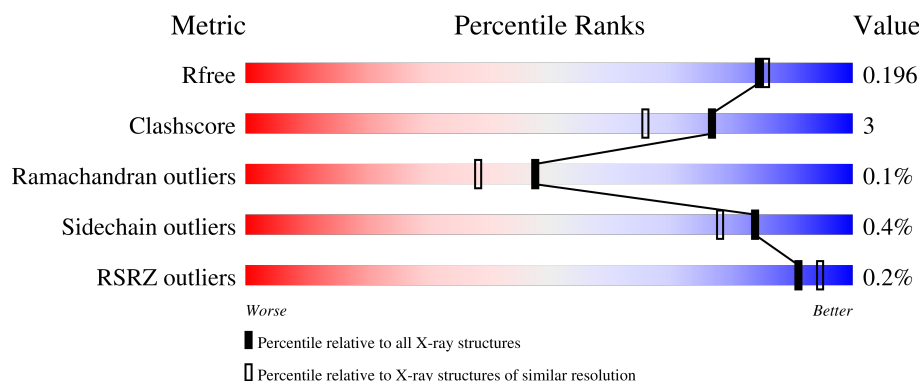
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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.



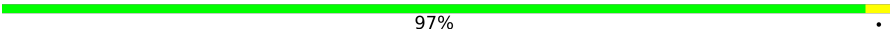
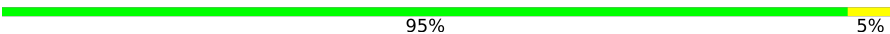
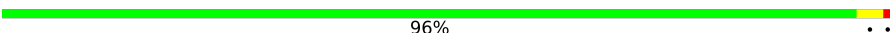
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	822	93% 7%
1	C	822	94% 6%
1	E	822	95% 5%
1	G	822	94% 6%
2	B	133	96% .

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Mol	Chain	Length	Quality of chain
2	D	133	 97% .
2	F	133	 95% 5%
2	H	133	 96% . .

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
13	TRS	A	5017	-	X	X	-
13	TRS	C	5112	-	X	X	-
13	TRS	G	5006	-	X	X	-
15	EDO	E	5010	-	-	X	-
15	EDO	E	5012	-	-	X	-
8	ACT	A	5009	-	-	X	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 33900 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.

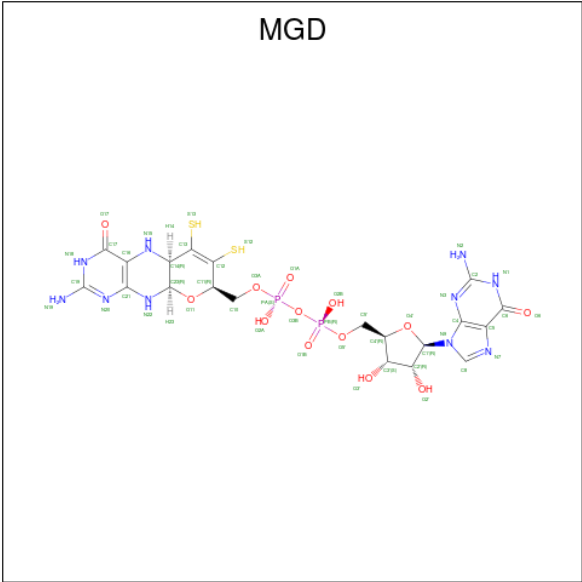
- Molecule 1 is a protein called Arsenite oxidase subunit AioA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	0	7	0
			6509	4096	1153	1219	41			
1	C	822	Total	C	N	O	S	0	4	0
			6491	4084	1152	1215	40			
1	E	822	Total	C	N	O	S	0	6	0
			6502	4093	1152	1215	42			
1	G	822	Total	C	N	O	S	0	3	0
			6484	4080	1147	1217	40			

- Molecule 2 is a protein called AioB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	2	0
			998	625	167	197	9			
2	D	133	Total	C	N	O	S	0	2	0
			1001	627	167	198	9			
2	F	133	Total	C	N	O	S	0	1	0
			995	623	167	196	9			
2	H	133	Total	C	N	O	S	0	1	0
			995	623	167	196	9			

- Molecule 3 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) (labeled as "Ligand of Interest" by depositor).



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

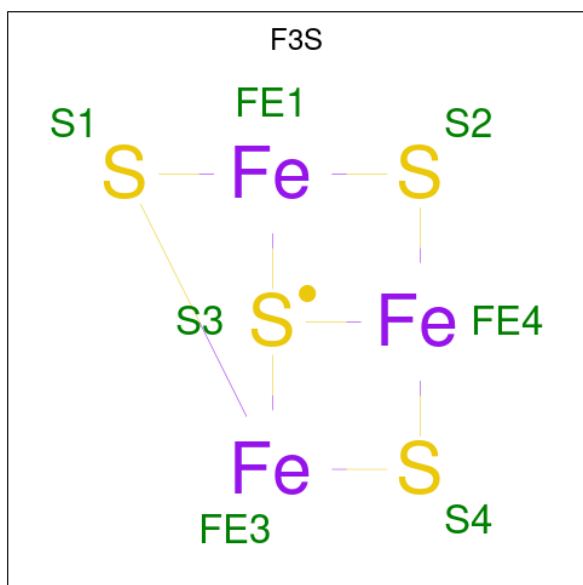
- Molecule 4 is OXYGEN ATOM (CCD ID: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		
4	G	1	Total	O	0	0
			1	1		

- Molecule 5 is MOLYBDENUM(IV) ION (CCD ID: 4MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

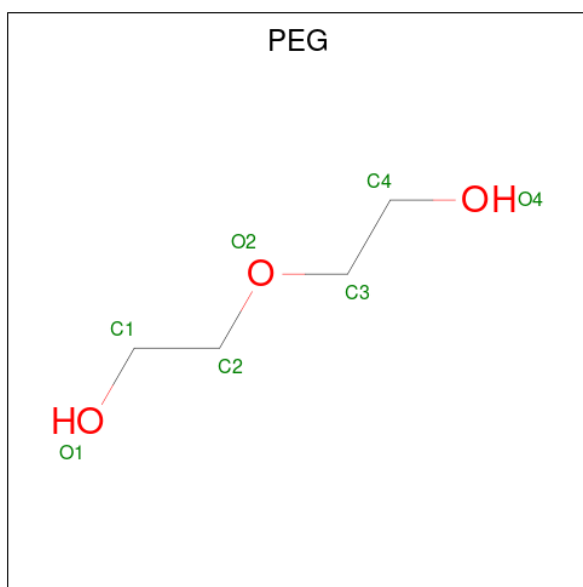
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mo	0	0
			1	1		
5	C	1	Total	Mo	0	0
			1	1		
5	E	1	Total	Mo	0	0
			1	1		
5	G	1	Total	Mo	0	0
			1	1		

- Molecule 6 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄) (labeled as "Ligand of Interest" by depositor).



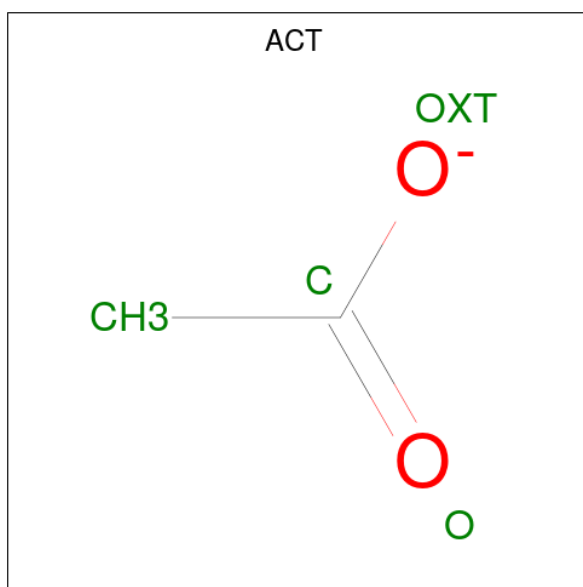
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			7	3	4		
6	C	1	Total	Fe	S	0	0
			7	3	4		
6	E	1	Total	Fe	S	0	0
			7	3	4		
6	G	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



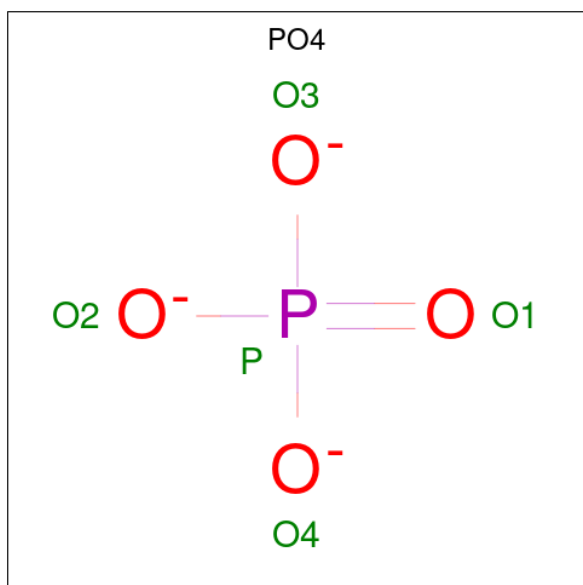
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	C	1	Total	C	O	0	0
			7	4	3		
7	E	1	Total	C	O	0	0
			7	4	3		
7	G	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



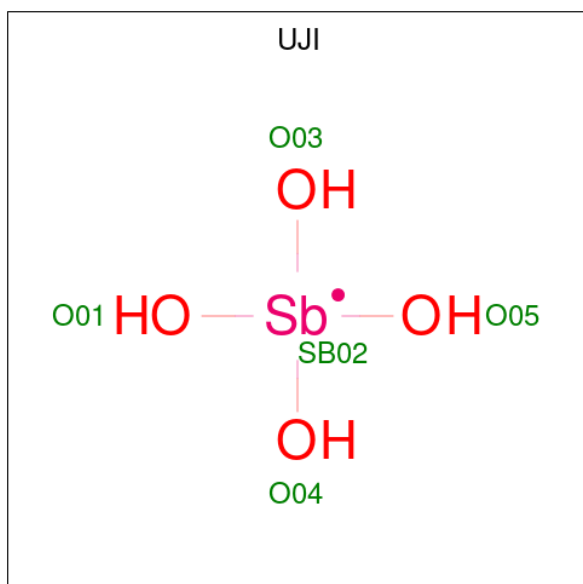
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	G	1	Total	C	O	0	0
			4	2	2		
8	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	P	0	0
			5	4	1		
9	C	1	Total	O	P	0	0
			5	4	1		
9	C	1	Total	O	P	0	0
			5	4	1		
9	E	1	Total	O	P	0	0
			5	4	1		
9	E	1	Total	O	P	0	0
			5	4	1		
9	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 10 is tetrakis(oxidanyl)antimony (CCD ID: UJI) (formula: $\text{H}_4\text{O}_4\text{Sb}$) (labeled as "Ligand of Interest" by depositor).

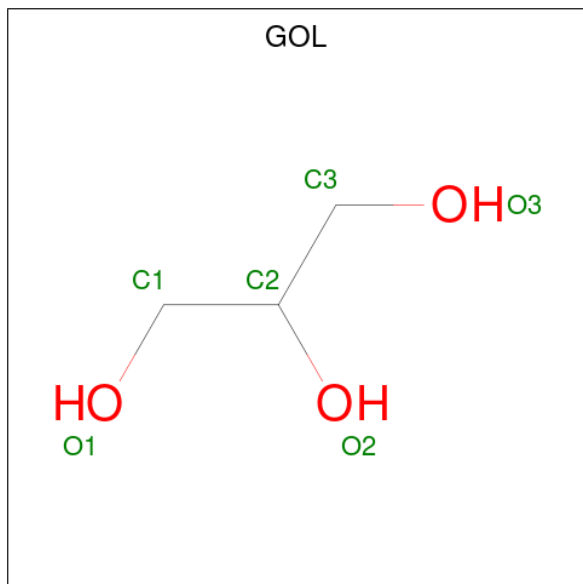


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	Sb	0	0
			5	4	1		
10	C	1	Total	O	Sb	0	0
			5	4	1		
10	E	1	Total	O	Sb	0	0
			5	4	1		
10	G	1	Total	O	Sb	0	0
			5	4	1		

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

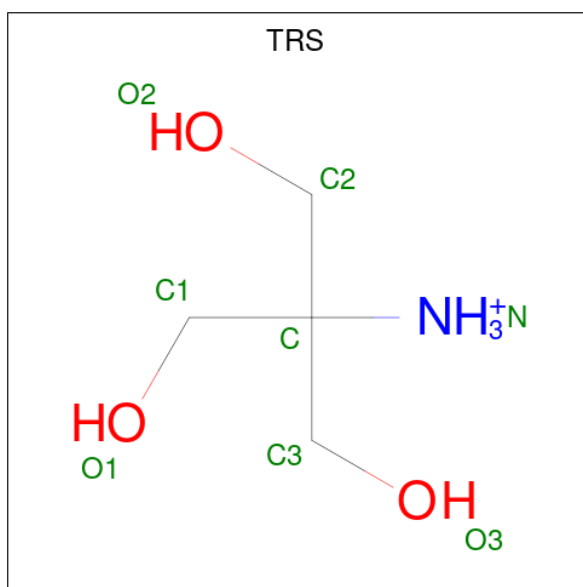
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total	Cl	0	0
			2	2		
11	C	1	Total	Cl	0	0
			1	1		
11	E	2	Total	Cl	0	0
			2	2		

- Molecule 12 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



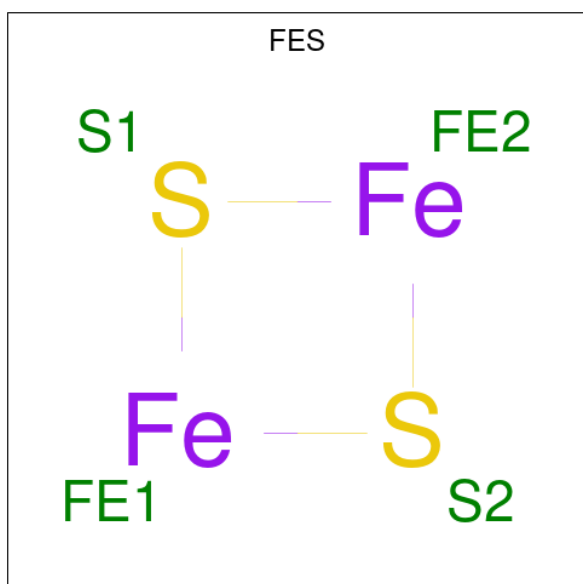
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			6	3	3		
12	A	1	Total	C	O	0	0
			6	3	3		
12	C	1	Total	C	O	0	0
			6	3	3		
12	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 13 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



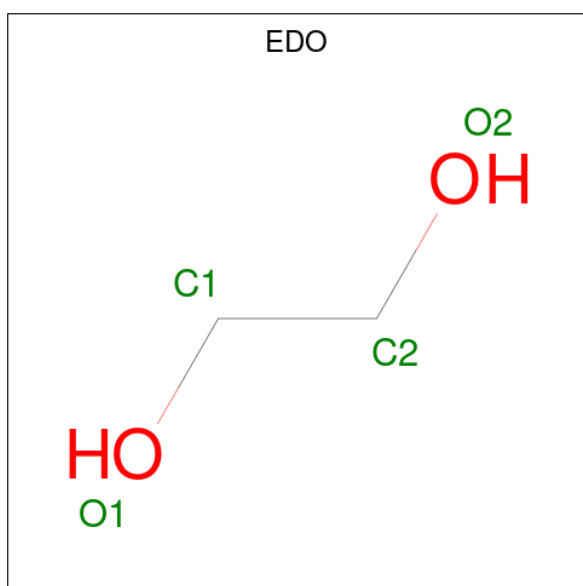
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	N	O	0	0
			8	4	1	3		
13	C	1	Total	C	N	O	0	0
			8	4	1	3		
13	G	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



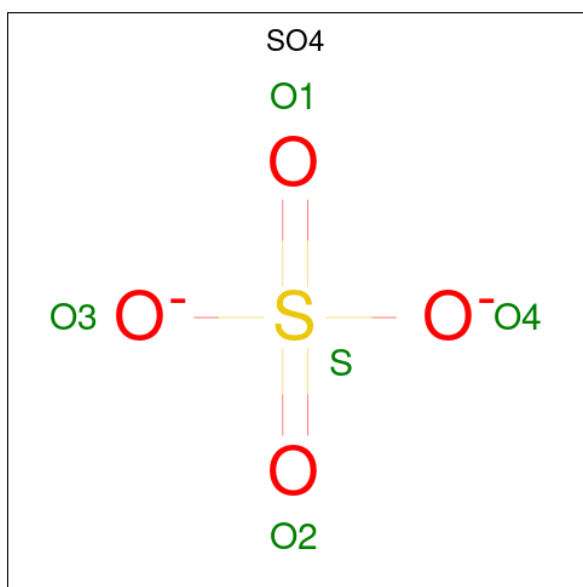
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	B	1	Total	Fe	S	0	0
			4	2	2		
14	D	1	Total	Fe	S	0	0
			4	2	2		
14	F	1	Total	Fe	S	0	0
			4	2	2		
14	H	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 15 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	E	1	Total	C	O	0	0
			4	2	2		
15	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 16 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 17 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	1	Total	Na	0	0
			1	1		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	738	Total	O	0	0
			738	738		
18	B	116	Total	O	0	0
			116	116		
18	C	726	Total	O	0	0
			726	726		
18	D	121	Total	O	0	0
			121	121		
18	E	692	Total	O	0	0
			692	692		
18	F	115	Total	O	0	0
			115	115		
18	G	687	Total	O	0	0
			687	687		

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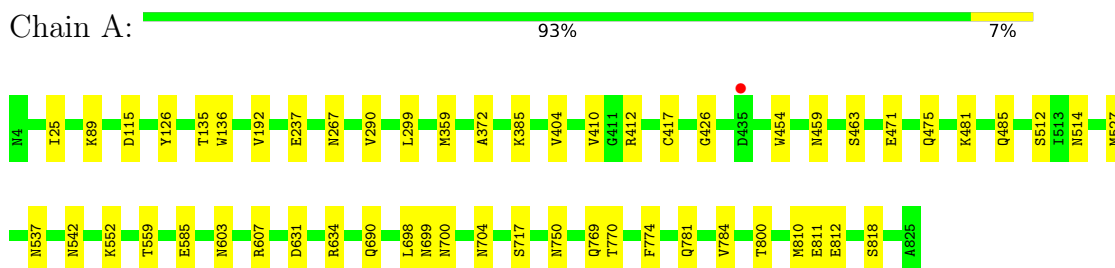
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	H	127	Total 127	O 127	0	0

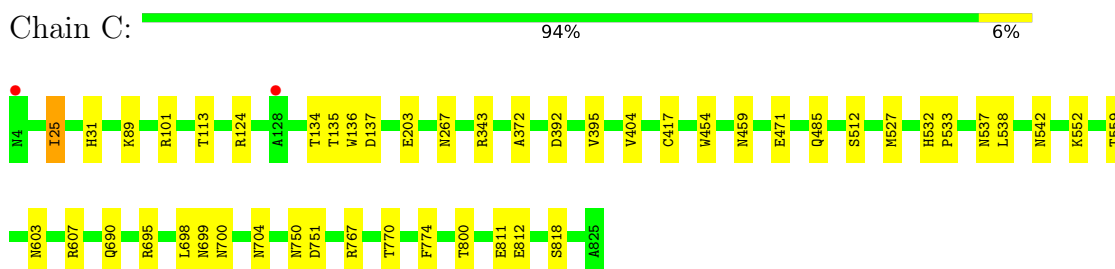
3 Residue-property plots

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.

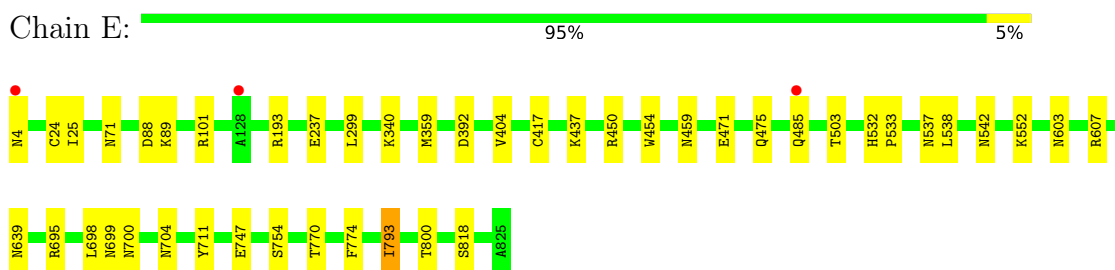
- Molecule 1: Arsenite oxidase subunit AioA



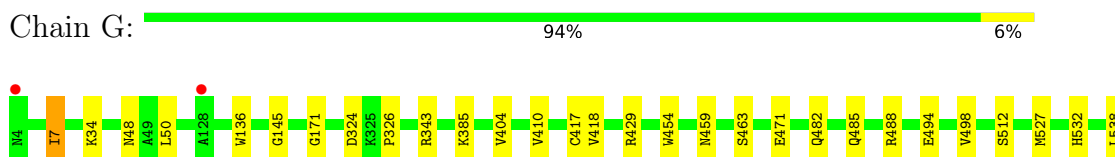
- Molecule 1: Arsenite oxidase subunit AioA



- Molecule 1: Arsenite oxidase subunit AioA



- Molecule 1: Arsenite oxidase subunit AioA

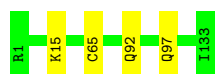




● Molecule 2: AioB



● Molecule 2: AioB



● Molecule 2: AioB



● Molecule 2: AioB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.38Å 109.21Å 117.34Å 97.71° 90.06° 96.28°	Depositor
Resolution (Å)	116.27 – 1.84 116.27 – 1.84	Depositor EDS
% Data completeness (in resolution range)	95.3 (116.27-1.84) 95.3 (116.27-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.154 , 0.189 0.165 , 0.196	Depositor DCC
R_{free} test set	18174 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33900	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, 4MO, PO4, NA, EDO, TRS, F3S, ACT, CL, MGD, UJI, O, SO4, GOL, FES

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	1.10	3/6688 (0.0%)	0.97	1/9063 (0.0%)
1	C	1.12	2/6664 (0.0%)	0.99	0/9032
1	E	1.09	2/6681 (0.0%)	0.98	2/9053 (0.0%)
1	G	1.11	2/6654 (0.0%)	0.98	1/9020 (0.0%)
2	B	1.10	0/1025	1.02	1/1396 (0.1%)
2	D	1.11	0/1028	1.02	0/1400
2	F	1.10	0/1019	1.04	2/1388 (0.1%)
2	H	1.11	0/1019	1.06	1/1388 (0.1%)
All	All	1.11	9/30778 (0.0%)	0.99	8/41740 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	488	ARG	CA-C	-7.00	1.44	1.52
1	A	514	ASN	C-O	6.77	1.31	1.23
1	E	193	ARG	C-O	6.17	1.32	1.23
1	A	192	VAL	C-O	5.81	1.30	1.24
1	A	290	VAL	C-O	-5.46	1.18	1.24
1	C	395	VAL	C-O	5.46	1.30	1.24
1	G	418	VAL	C-O	5.39	1.29	1.24
1	E	71	ASN	C-O	5.09	1.29	1.23
1	C	767	ARG	C-O	-5.00	1.17	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	71	LYS	N-CA-C	5.60	118.11	111.33
1	E	340	LYS	N-CA-C	5.47	117.05	111.14
2	H	104	ARG	N-CA-CB	5.34	118.89	110.23
2	F	78	CYS	CA-C-N	-5.31	114.84	121.00
2	F	78	CYS	C-N-CA	-5.31	114.84	121.00
1	A	585	GLU	N-CA-C	-5.31	105.40	111.14
1	E	24	CYS	N-CA-C	5.03	116.60	110.41
1	G	429	ARG	N-CA-C	5.01	114.06	108.25

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	4	ASN	Peptide

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	6509	0	6308	46	0
1	C	6491	0	6287	42	0
1	E	6502	0	6307	28	2
1	G	6484	0	6270	32	2
2	B	998	0	984	6	0
2	D	1001	0	985	5	0
2	F	995	0	979	7	0
2	H	995	0	979	7	0
3	A	94	0	44	2	0
3	C	94	0	44	2	0
3	E	94	0	44	3	0
3	G	94	0	44	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
6	A	7	0	0	0	0
6	C	7	0	0	0	0
6	E	7	0	0	0	0
6	G	7	0	0	0	0
7	A	21	0	30	5	0
7	C	7	0	10	1	0
7	E	7	0	10	2	0
7	G	7	0	10	0	0
8	A	8	0	6	3	0
8	G	8	0	6	0	0
9	A	5	0	0	0	0
9	C	10	0	0	0	0
9	E	10	0	0	1	0
9	G	5	0	0	0	0
10	A	5	0	0	0	0
10	C	5	0	0	1	0
10	E	5	0	0	0	0
10	G	5	0	0	0	0
11	A	2	0	0	1	0
11	C	1	0	0	0	0
11	E	2	0	0	1	0
12	A	12	0	16	0	0
12	C	6	0	8	0	0
12	E	6	0	8	2	0
13	A	8	0	11	14	0
13	C	8	0	12	7	0
13	G	8	0	12	7	0
14	B	4	0	0	0	0
14	D	4	0	0	0	0
14	F	4	0	0	0	0
14	H	4	0	0	0	0
15	E	8	0	8	9	0
16	E	5	0	0	0	0
17	G	1	0	0	0	0
18	A	738	0	0	5	0
18	B	116	0	0	2	0
18	C	726	0	0	4	0
18	D	121	0	0	2	0
18	E	692	0	0	5	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	F	115	0	0	3	0
18	G	687	0	0	5	0
18	H	127	0	0	2	1
All	All	33900	0	29422	171	3

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 3.

All (171) 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)
15:E:5010:EDO:C1	15:E:5012:EDO:O1	1.67	1.41
15:E:5010:EDO:C1	15:E:5012:EDO:C1	2.14	1.26
15:E:5010:EDO:C1	15:E:5012:EDO:C2	2.14	1.24
15:E:5010:EDO:C1	15:E:5012:EDO:H22	1.58	1.21
15:E:5010:EDO:C2	15:E:5012:EDO:C1	2.35	1.04
2:H:65:CYS:SG	18:H:414:HOH:O	2.16	1.02
15:E:5010:EDO:H12	15:E:5012:EDO:H22	1.44	1.00
13:A:5017:TRS:H31	18:A:5516:HOH:O	1.65	0.97
15:E:5010:EDO:O1	15:E:5012:EDO:O1	1.82	0.95
2:D:65:CYS:SG	18:D:410:HOH:O	2.26	0.92
2:B:65:CYS:SG	18:B:406:HOH:O	2.27	0.91
1:A:471[A]:GLU:OE2	1:C:485:GLN:HB2	1.72	0.90
2:F:65:CYS:SG	18:F:409:HOH:O	2.29	0.89
18:A:5583:HOH:O	13:C:5112:TRS:H11	1.73	0.88
1:C:124:ARG:HE	7:C:5106:PEG:H22	1.38	0.87
1:A:717:SER:H	8:A:5009:ACT:H2	1.44	0.81
1:A:115:ASP:OD1	8:A:5009:ACT:H1	1.83	0.79
1:G:745:ILE:HD11	1:G:810:MET:HE2	1.66	0.76
1:E:89:LYS:HE2	18:E:5483:HOH:O	1.86	0.75
1:E:704:ASN:HD21	2:F:97:GLN:HE22	1.37	0.73
1:G:695:ARG:NH2	18:G:5101:HOH:O	2.20	0.72
1:A:818:SER:H	2:B:92:GLN:HE22	1.39	0.70
13:G:5006:TRS:HO2	13:G:5006:TRS:HO1	1.42	0.68
1:C:704:ASN:HD21	2:D:97:GLN:HE22	1.41	0.68
1:G:136:TRP:H	13:G:5006:TRS:C3	2.08	0.66
1:E:818:SER:H	2:F:92:GLN:HE22	1.45	0.65
7:A:5012:PEG:H32	1:C:137:ASP:HB2	1.77	0.64
1:A:485:GLN:HB2	1:C:471:GLU:OE2	1.97	0.64
15:E:5010:EDO:C2	15:E:5012:EDO:O1	2.44	0.64
1:E:698:LEU:HB2	1:E:800:THR:HG23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:GLN:HE21	7:A:5011:PEG:H12	1.63	0.63
1:A:811[A]:GLU:HG2	13:A:5017:TRS:O3	2.00	0.62
1:E:695:ARG:NH2	18:E:5105:HOH:O	2.32	0.62
1:A:769:GLN:HE21	7:A:5011:PEG:C1	2.13	0.61
1:E:700:ASN:ND2	3:E:5001:MGD:H18	2.00	0.60
1:C:818:SER:H	2:D:92:GLN:HE22	1.50	0.60
7:E:5006:PEG:O4	18:E:5101:HOH:O	2.16	0.60
1:A:136:TRP:HB2	13:C:5112:TRS:H31	1.83	0.59
1:A:700:ASN:ND2	3:A:5001:MGD:H18	2.00	0.59
1:A:559:THR:HG21	13:C:5112:TRS:H21	1.86	0.58
1:G:649:ASP:OD2	1:G:652:LYS:NZ	2.36	0.58
1:G:704:ASN:HD21	2:H:97:GLN:HE22	1.51	0.58
1:C:700:ASN:ND2	3:C:5101:MGD:H18	2.02	0.58
1:E:704:ASN:ND2	2:F:97:GLN:HE22	2.01	0.57
13:A:5017:TRS:O2	1:C:135:THR:HA	2.05	0.57
1:A:812:GLU:HB2	13:A:5017:TRS:O1	2.05	0.56
1:E:699:ASN:HB3	1:E:770:THR:O	2.05	0.56
1:G:698:LEU:HB2	1:G:800:THR:HG23	1.88	0.55
13:G:5006:TRS:H12	18:G:5283:HOH:O	2.04	0.55
13:A:5017:TRS:O1	1:C:559:THR:HG21	2.07	0.55
1:C:31:HIS:HD2	18:C:5781:HOH:O	1.91	0.54
1:E:639:ASN:ND2	12:E:5008:GOL:H12	2.23	0.54
1:G:343:ARG:NH2	18:G:5106:HOH:O	2.39	0.54
13:G:5006:TRS:O2	13:G:5006:TRS:O1	2.25	0.54
1:A:698:LEU:HB2	1:A:800:THR:HG23	1.90	0.54
13:G:5006:TRS:H22	18:G:5634:HOH:O	2.07	0.54
1:A:704:ASN:HD21	2:B:97:GLN:HE22	1.57	0.53
7:A:5012:PEG:H41	18:A:5542:HOH:O	2.09	0.53
1:C:704:ASN:ND2	2:D:97:GLN:HE22	2.06	0.52
1:A:818:SER:H	2:B:92:GLN:NE2	2.05	0.52
1:E:818:SER:H	2:F:92:GLN:NE2	2.07	0.52
1:G:818:SER:H	2:H:92:GLN:HE22	1.57	0.52
1:C:454:TRP:HE1	1:C:459:ASN:HD22	1.57	0.51
1:A:471[B]:GLU:OE2	1:A:475:GLN:NE2	2.44	0.51
1:G:745:ILE:CD1	1:G:810:MET:HE2	2.37	0.51
1:A:471[B]:GLU:OE1	1:C:485:GLN:OE1	2.29	0.50
1:A:811[A]:GLU:H	13:A:5017:TRS:H11	1.74	0.50
1:C:533:PRO:HG3	1:C:538:LEU:HD13	1.93	0.50
1:G:136:TRP:HB2	13:G:5006:TRS:H32	1.93	0.50
1:A:25:ILE:O	1:A:542:ASN:HB2	2.11	0.50
1:E:101:ARG:HD3	3:E:5002:MGD:N19	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:10:GLN:NE2	18:F:301:HOH:O	2.29	0.50
11:A:5014:CL:CL	18:A:5396:HOH:O	2.57	0.50
1:G:454:TRP:HE1	1:G:459:ASN:HD22	1.58	0.50
1:C:698:LEU:HB2	1:C:800:THR:HG23	1.94	0.49
1:C:811:GLU:HB2	13:C:5112:TRS:H22	1.93	0.49
8:A:5009:ACT:H3	1:C:113:THR:HG22	1.94	0.49
1:A:812:GLU:H	13:A:5017:TRS:H11	1.78	0.48
1:E:454:TRP:HE1	1:E:459:ASN:HD22	1.61	0.48
1:A:267:ASN:ND2	1:A:372:ALA:HB3	2.28	0.48
1:C:267:ASN:ND2	1:C:372:ALA:HB3	2.28	0.48
15:E:5010:EDO:C2	15:E:5012:EDO:H11	2.36	0.48
2:H:104:ARG:HB3	18:H:362:HOH:O	2.12	0.48
1:A:454:TRP:HE1	1:A:459:ASN:HD22	1.61	0.48
1:A:812:GLU:H	13:A:5017:TRS:C1	2.27	0.48
1:E:25:ILE:O	1:E:542:ASN:HB2	2.14	0.48
13:A:5017:TRS:HO2	1:C:135:THR:HA	1.79	0.48
1:C:31:HIS:HE1	18:C:5736:HOH:O	1.97	0.48
1:A:471[B]:GLU:CD	1:C:485:GLN:OE1	2.57	0.47
1:G:699:ASN:HB3	1:G:770:THR:O	2.14	0.47
1:A:699:ASN:HB3	1:A:770:THR:O	2.13	0.47
1:C:699:ASN:HB3	1:C:770:THR:O	2.13	0.47
1:G:704:ASN:ND2	2:H:97:GLN:HE22	2.12	0.47
13:A:5017:TRS:H21	1:C:136:TRP:HB2	1.96	0.47
1:G:136:TRP:H	13:G:5006:TRS:H32	1.80	0.47
1:A:237:GLU:HA	1:A:704:ASN:HD22	1.79	0.47
1:E:437:LYS:HB3	1:E:793:ILE:HD12	1.97	0.46
1:C:25:ILE:O	1:C:542:ASN:HB2	2.15	0.46
1:A:299:LEU:HD23	1:A:359[B]:MET:SD	2.55	0.46
1:G:145:GLY:HA2	1:G:577:MET:HE1	1.96	0.46
1:E:404:VAL:HG11	1:E:417:CYS:HB2	1.98	0.46
1:A:704:ASN:ND2	2:B:97:GLN:HE22	2.14	0.46
1:C:404:VAL:HG11	1:C:417:CYS:HB2	1.98	0.46
1:C:537:ASN:ND2	1:C:552:LYS:H	2.13	0.45
1:A:810:MET:HE1	1:C:134:THR:O	2.17	0.45
1:E:747:GLU:OE2	1:E:754:SER:OG	2.33	0.45
1:G:690:GLN:HE21	1:G:750:ASN:HB2	1.82	0.45
1:A:810:MET:SD	13:A:5017:TRS:H12	2.57	0.45
1:E:533:PRO:HG3	1:E:538:LEU:HD13	1.98	0.45
1:G:690:GLN:HE22	1:G:751:ASP:H	1.64	0.45
1:A:404:VAL:HG11	1:A:417:CYS:HB2	1.98	0.44
1:E:711:TYR:CE1	3:E:5001:MGD:H8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:THR:HA	13:C:5112:TRS:O3	2.17	0.44
1:C:811:GLU:HG2	13:C:5112:TRS:O1	2.17	0.44
1:G:34:LYS:NZ	18:G:5124:HOH:O	2.50	0.44
1:G:818:SER:H	2:H:92:GLN:NE2	2.15	0.44
1:A:471[A]:GLU:OE2	1:C:485:GLN:CB	2.55	0.44
1:G:7:ILE:HG12	2:H:124:LEU:CD2	2.47	0.44
1:C:690:GLN:HE21	1:C:750:ASN:HB2	1.83	0.44
1:C:818:SER:H	2:D:92:GLN:NE2	2.15	0.44
1:G:171:GLY:O	1:G:538:LEU:HD11	2.18	0.44
1:A:631:ASP:OD1	1:A:634:ARG:NH1	2.51	0.43
1:C:690:GLN:HE22	1:C:751:ASP:H	1.66	0.43
1:G:459:ASN:HB3	1:G:463:SER:OG	2.17	0.43
1:C:603:ASN:OD1	1:C:607:ARG:HD3	2.18	0.43
1:A:385:LYS:HE2	3:A:5001:MGD:S13	2.58	0.43
1:G:494:GLU:O	1:G:498:VAL:HG23	2.18	0.43
1:G:48:ASN:HD22	1:G:50:LEU:H	1.66	0.43
1:E:475:GLN:NE2	18:E:5108:HOH:O	2.50	0.43
1:E:88:ASP:OD2	12:E:5008:GOL:H31	2.19	0.43
1:A:459:ASN:HB3	1:A:463:SER:OG	2.18	0.42
1:C:203:GLU:OE2	10:C:5109:UJI:O01	2.36	0.42
7:E:5006:PEG:H11	9:E:5011:PO4:O3	2.18	0.42
1:G:482:GLN:O	1:G:485[A]:GLN:HB3	2.18	0.42
1:C:343:ARG:NH1	18:C:5202:HOH:O	2.37	0.42
1:G:404:VAL:HG11	1:G:417:CYS:HB2	2.01	0.42
2:B:104:ARG:HG3	18:B:361:HOH:O	2.19	0.42
1:G:385:LYS:HE2	3:G:5001:MGD:S13	2.60	0.42
13:A:5017:TRS:O2	1:C:136:TRP:N	2.46	0.42
1:E:299:LEU:HD22	1:E:359[B]:MET:HG2	2.01	0.42
1:C:812:GLU:H	13:C:5112:TRS:C2	2.33	0.42
1:A:537:ASN:ND2	1:A:552:LYS:H	2.18	0.42
1:C:101:ARG:HD3	3:C:5102:MGD:N19	2.35	0.42
1:G:324:ASP:OD1	1:G:326:PRO:HD2	2.20	0.42
1:E:450:ARG:HD2	1:E:503:THR:OG1	2.20	0.41
1:A:126:TYR:CD2	1:A:481:LYS:HE2	2.55	0.41
1:A:412[A]:ARG:HH11	1:A:412[A]:ARG:HD3	1.68	0.41
1:E:537:ASN:ND2	1:E:552:LYS:H	2.17	0.41
1:A:603:ASN:OD1	1:A:607:ARG:HD3	2.20	0.41
1:G:698:LEU:HD13	1:G:784:VAL:HG21	2.02	0.41
18:D:334:HOH:O	1:G:652:LYS:HE3	2.21	0.41
1:E:237:GLU:HA	1:E:704:ASN:HD22	1.86	0.41
1:E:603:ASN:OD1	1:E:607:ARG:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:512:SER:O	1:C:527:MET:HA	2.21	0.41
1:E:299:LEU:CD2	1:E:359[B]:MET:HG2	2.51	0.41
7:A:5012:PEG:H42	1:C:135:THR:HG21	2.03	0.41
1:E:532:HIS:HB2	1:E:533:PRO:CD	2.51	0.41
1:A:690:GLN:HE21	1:A:750:ASN:HB2	1.86	0.41
13:A:5017:TRS:C2	1:C:136:TRP:H	2.34	0.41
1:C:89:LYS:HE3	18:C:5722:HOH:O	2.20	0.40
1:A:89:LYS:HE3	18:A:5556:HOH:O	2.21	0.40
1:A:299:LEU:CD2	1:A:359[B]:MET:HG2	2.51	0.40
1:A:299:LEU:CD2	1:A:359[B]:MET:SD	3.10	0.40
1:E:450:ARG:NH2	18:E:5122:HOH:O	2.50	0.40
2:F:104:ARG:HG3	18:F:383:HOH:O	2.20	0.40
1:A:512:SER:O	1:A:527:MET:HA	2.21	0.40
1:A:781:GLN:O	1:A:784:VAL:HG22	2.22	0.40
1:G:680:TRP:CZ2	1:G:682:GLY:HA2	2.56	0.40
1:G:512:SER:O	1:G:527:MET:HA	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:471:GLU:OE1	1:G:485[B]:GLN:OE1[1_654]	2.09	0.11
1:E:485:GLN:OE1	1:G:471:GLU:OE1[1_654]	2.13	0.07
18:E:5682:HOH:O	18:H:307:HOH:O[1_654]	2.14	0.06

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	827/822 (101%)	801 (97%)	25 (3%)	1 (0%)	48	38
1	C	824/822 (100%)	794 (96%)	28 (3%)	2 (0%)	43	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	826/822 (100%)	798 (97%)	26 (3%)	2 (0%)	43	34
1	G	823/822 (100%)	797 (97%)	26 (3%)	0	100	100
2	B	133/133 (100%)	128 (96%)	5 (4%)	0	100	100
2	D	133/133 (100%)	126 (95%)	7 (5%)	0	100	100
2	F	132/133 (99%)	128 (97%)	4 (3%)	0	100	100
2	H	132/133 (99%)	125 (95%)	7 (5%)	0	100	100
All	All	3830/3820 (100%)	3697 (96%)	128 (3%)	5 (0%)	48	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	392	ASP
1	E	392	ASP
1	C	25	ILE
1	E	793	ILE
1	A	426	GLY

5.3.2 Protein sidechains ⓘ

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	682/675 (101%)	680 (100%)	2 (0%)	86	81
1	C	679/675 (101%)	676 (100%)	3 (0%)	84	78
1	E	681/675 (101%)	680 (100%)	1 (0%)	88	85
1	G	678/675 (100%)	674 (99%)	4 (1%)	78	72
2	B	113/111 (102%)	113 (100%)	0	100	100
2	D	113/111 (102%)	112 (99%)	1 (1%)	70	60
2	F	112/111 (101%)	111 (99%)	1 (1%)	70	60
2	H	112/111 (101%)	111 (99%)	1 (1%)	70	60
All	All	3170/3144 (101%)	3157 (100%)	13 (0%)	84	78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	410	VAL
1	A	774	PHE
1	C	532	HIS
1	C	695	ARG
1	C	774	PHE
2	D	15	LYS
1	E	774	PHE
2	F	41	SER
1	G	7	ILE
1	G	410	VAL
1	G	532	HIS
1	G	774	PHE
2	H	104	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	31	HIS
1	A	216	ASN
1	A	267	ASN
1	A	270	GLN
1	A	459	ASN
1	A	537	ASN
1	A	572	ASN
1	A	611	GLN
1	A	638	ASN
1	A	642	GLN
1	A	681	ASN
1	A	688	GLN
1	A	690	GLN
1	A	700	ASN
1	A	704	ASN
1	A	769	GLN
2	B	10	GLN
2	B	62	HIS
2	B	92	GLN
1	C	31	HIS
1	C	82	ASN
1	C	233	ASN
1	C	267	ASN

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Mol	Chain	Res	Type
1	C	270	GLN
1	C	289	HIS
1	C	293	ASN
1	C	320	GLN
1	C	459	ASN
1	C	532	HIS
1	C	537	ASN
1	C	572	ASN
1	C	638	ASN
1	C	642	GLN
1	C	681	ASN
1	C	688	GLN
1	C	690	GLN
1	C	700	ASN
1	C	704	ASN
1	C	720	GLN
2	D	10	GLN
2	D	62	HIS
2	D	92	GLN
1	E	13	ASN
1	E	130	GLN
1	E	216	ASN
1	E	233	ASN
1	E	267	ASN
1	E	289	HIS
1	E	409	ASN
1	E	459	ASN
1	E	482	GLN
1	E	537	ASN
1	E	572	ASN
1	E	611	GLN
1	E	638	ASN
1	E	681	ASN
1	E	688	GLN
1	E	700	ASN
1	E	704	ASN
1	E	792	ASN
2	F	62	HIS
2	F	92	GLN
1	G	13	ASN
1	G	48	ASN
1	G	82	ASN

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Mol	Chain	Res	Type
1	G	233	ASN
1	G	289	HIS
1	G	442	GLN
1	G	459	ASN
1	G	475	GLN
1	G	532	HIS
1	G	537	ASN
1	G	572	ASN
1	G	611	GLN
1	G	638	ASN
1	G	681	ASN
1	G	688	GLN
1	G	690	GLN
1	G	704	ASN
1	G	720	GLN
1	G	792	ASN
2	H	62	HIS
2	H	92	GLN
2	H	101	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 60 ligands modelled in this entry, 14 are monoatomic - leaving 46 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	$\# Z > 2$
6	F3S	G	5005	1	0,9,9	-	-	-		
6	F3S	E	5005	1	0,9,9	-	-	-		
13	TRS	A	5017	-	7,7,7	2.24	4 (57%)	9,9,9	1.71	2 (22%)
13	TRS	C	5112	-	7,7,7	1.79	2 (28%)	9,9,9	2.35	4 (44%)
9	PO4	G	5008	-	4,4,4	0.83	0	6,6,6	0.77	0
7	PEG	A	5006	-	6,6,6	0.85	0	5,5,5	0.91	0
3	MGD	A	5001	5	47,52,52	1.61	10 (21%)	58,81,81	1.76	13 (22%)
8	ACT	G	5011	-	3,3,3	1.01	0	3,3,3	1.32	0
14	FES	D	201	2	0,4,4	-	-	-		
15	EDO	E	5012	-	3,3,3	1.25	0	2,2,2	0.55	0
8	ACT	G	5009	-	3,3,3	0.73	0	3,3,3	1.48	1 (33%)
14	FES	F	201	2	0,4,4	-	-	-		
3	MGD	E	5002	5	47,52,52	1.56	7 (14%)	58,81,81	1.71	14 (24%)
7	PEG	G	5007	-	6,6,6	0.52	0	5,5,5	0.74	0
8	ACT	A	5009	-	3,3,3	1.01	0	3,3,3	0.95	0
10	UJI	A	5010	-	0,4,4	-	-	-		
7	PEG	C	5106	-	6,6,6	1.09	0	5,5,5	1.46	1 (20%)
10	UJI	C	5109	-	0,4,4	-	-	-		
12	GOL	A	5015	-	5,5,5	0.26	0	5,5,5	0.20	0
3	MGD	G	5002	5	47,52,52	1.92	10 (21%)	58,81,81	1.75	14 (24%)
9	PO4	C	5110	-	4,4,4	1.13	0	6,6,6	0.72	0
9	PO4	E	5007	-	4,4,4	0.87	0	6,6,6	0.69	0
9	PO4	A	5008	-	4,4,4	0.88	0	6,6,6	0.85	0
9	PO4	C	5107	-	4,4,4	0.79	0	6,6,6	0.68	0
6	F3S	A	5005	1	0,9,9	-	-	-		
14	FES	H	201	2	0,4,4	-	-	-		
16	SO4	E	5015	-	4,4,4	1.23	1 (25%)	6,6,6	0.53	0
12	GOL	C	5108	-	5,5,5	0.17	0	5,5,5	0.51	0
12	GOL	E	5008	-	5,5,5	0.28	0	5,5,5	1.21	1 (20%)
6	F3S	C	5105	1	0,9,9	-	-	-		
3	MGD	C	5102	5	47,52,52	1.74	8 (17%)	58,81,81	1.90	14 (24%)
9	PO4	E	5011	-	4,4,4	1.41	0	6,6,6	0.96	0
10	UJI	G	5010	-	0,4,4	-	-	-		
13	TRS	G	5006	-	7,7,7	1.63	1 (14%)	9,9,9	2.47	4 (44%)
15	EDO	E	5010	-	3,3,3	1.32	0	2,2,2	1.48	1 (50%)
7	PEG	E	5006	-	6,6,6	0.29	0	5,5,5	0.78	0
7	PEG	A	5012	-	6,6,6	1.33	1 (16%)	5,5,5	1.90	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MGD	C	5101	5	47,52,52	1.74	11 (23%)	58,81,81	1.74	14 (24%)
3	MGD	E	5001	5	47,52,52	1.64	10 (21%)	58,81,81	2.12	17 (29%)
3	MGD	G	5001	5	47,52,52	1.34	5 (10%)	58,81,81	2.06	20 (34%)
8	ACT	A	5007	-	3,3,3	0.88	0	3,3,3	0.62	0
14	FES	B	201	2	0,4,4	-	-	-	-	-
7	PEG	A	5011	-	6,6,6	0.53	0	5,5,5	0.83	0
3	MGD	A	5002	5	47,52,52	1.77	10 (21%)	58,81,81	1.92	16 (27%)
10	UJI	E	5009	-	0,4,4	-	-	-	-	-
12	GOL	A	5016	-	5,5,5	0.85	0	5,5,5	1.59	1 (20%)

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
6	F3S	G	5005	1	-	-	0/3/3/3
13	TRS	A	5017	-	-	4/9/9/9	-
6	F3S	E	5005	1	-	-	0/3/3/3
13	TRS	C	5112	-	-	7/9/9/9	-
7	PEG	A	5006	-	-	2/4/4/4	-
3	MGD	A	5001	5	-	2/22/66/66	0/6/6/6
14	FES	D	201	2	-	-	0/1/1/1
15	EDO	E	5012	-	-	1/1/1/1	-
14	FES	F	201	2	-	-	0/1/1/1
3	MGD	E	5002	5	-	4/22/66/66	0/6/6/6
7	PEG	G	5007	-	-	4/4/4/4	-
7	PEG	C	5106	-	-	1/4/4/4	-
12	GOL	A	5015	-	-	2/4/4/4	-
3	MGD	G	5002	5	-	4/22/66/66	0/6/6/6
6	F3S	A	5005	1	-	-	0/3/3/3
14	FES	H	201	2	-	-	0/1/1/1
12	GOL	E	5008	-	-	4/4/4/4	-
12	GOL	C	5108	-	-	0/4/4/4	-
6	F3S	C	5105	1	-	-	0/3/3/3
3	MGD	C	5102	5	-	5/22/66/66	0/6/6/6
15	EDO	E	5010	-	-	1/1/1/1	-
13	TRS	G	5006	-	-	8/9/9/9	-
7	PEG	E	5006	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PEG	A	5012	-	-	1/4/4/4	-
3	MGD	C	5101	5	-	4/22/66/66	0/6/6/6
3	MGD	E	5001	5	-	4/22/66/66	0/6/6/6
3	MGD	G	5001	5	-	4/22/66/66	0/6/6/6
14	FES	B	201	2	-	-	0/1/1/1
7	PEG	A	5011	-	-	1/4/4/4	-
3	MGD	A	5002	5	-	4/22/66/66	0/6/6/6
12	GOL	A	5016	-	-	1/4/4/4	-

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5102	MGD	PA-O3B	7.62	1.67	1.59
3	G	5002	MGD	PA-O3B	6.33	1.66	1.59
3	G	5002	MGD	C16-C21	5.99	1.48	1.38
3	C	5101	MGD	PA-O3B	5.69	1.65	1.59
3	E	5002	MGD	C16-C21	5.32	1.47	1.38
3	A	5001	MGD	C16-C21	5.13	1.47	1.38
3	A	5002	MGD	PA-O3B	5.08	1.65	1.59
3	E	5001	MGD	PA-O3B	4.98	1.64	1.59
3	E	5001	MGD	C16-C21	4.95	1.47	1.38
3	G	5001	MGD	C16-C21	4.71	1.46	1.38
3	A	5002	MGD	C16-C21	4.50	1.46	1.38
13	A	5017	TRS	C2-C	-4.27	1.41	1.53
3	C	5101	MGD	C16-C21	4.26	1.45	1.38
3	E	5002	MGD	C6-N1	-4.03	1.31	1.38
3	A	5002	MGD	C6-N1	-3.82	1.31	1.38
3	A	5001	MGD	C6-N1	-3.80	1.31	1.38
13	C	5112	TRS	C3-C	-3.69	1.43	1.53
3	G	5002	MGD	C5-C4	3.48	1.48	1.38
3	G	5002	MGD	O6-C6	3.36	1.29	1.23
3	C	5102	MGD	O11-C23	-3.33	1.38	1.43
3	E	5001	MGD	C23-C14	3.22	1.56	1.53
3	A	5002	MGD	C5-N7	-3.17	1.32	1.39
3	G	5001	MGD	O11-C23	-3.13	1.39	1.43
3	A	5002	MGD	PB-O3B	3.09	1.62	1.59
3	C	5102	MGD	C16-C21	3.09	1.43	1.38
3	G	5002	MGD	C17-N18	-3.08	1.33	1.38
3	E	5002	MGD	O11-C23	-3.03	1.39	1.43
3	C	5101	MGD	C17-N18	-3.01	1.33	1.38
3	C	5102	MGD	C5-C4	3.00	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5001	MGD	C17-N18	-2.90	1.33	1.38
13	G	5006	TRS	C3-C	-2.86	1.45	1.53
3	C	5101	MGD	O17-C17	2.86	1.29	1.23
3	A	5002	MGD	C5-C4	2.81	1.46	1.38
3	G	5002	MGD	C6-N1	-2.81	1.33	1.38
3	G	5002	MGD	PB-O3B	2.74	1.62	1.59
3	A	5001	MGD	C23-C14	2.72	1.55	1.53
3	C	5101	MGD	C8-N9	-2.69	1.31	1.37
3	C	5101	MGD	C10-C11	-2.68	1.48	1.51
3	C	5101	MGD	C2-N3	2.67	1.39	1.33
3	A	5002	MGD	C14-N15	-2.64	1.43	1.46
3	E	5002	MGD	C5-N7	-2.64	1.33	1.39
3	C	5102	MGD	C6-N1	-2.61	1.34	1.38
3	E	5001	MGD	C2-N3	2.59	1.39	1.33
3	A	5001	MGD	PB-O3B	2.57	1.62	1.59
3	G	5001	MGD	C17-N18	-2.55	1.34	1.38
3	A	5001	MGD	C4-N9	-2.54	1.31	1.38
3	E	5001	MGD	C6-N1	-2.54	1.34	1.38
3	A	5001	MGD	C17-N18	-2.48	1.34	1.38
13	C	5112	TRS	C2-C	-2.47	1.46	1.53
13	A	5017	TRS	C1-C	-2.42	1.46	1.53
3	A	5002	MGD	C17-N18	-2.41	1.34	1.38
3	C	5101	MGD	C5-N7	-2.39	1.34	1.39
3	E	5002	MGD	C5-C4	2.38	1.45	1.38
3	G	5002	MGD	C23-C14	-2.37	1.51	1.53
3	G	5002	MGD	C16-C17	2.33	1.48	1.41
3	C	5102	MGD	C17-N18	-2.30	1.34	1.38
3	E	5002	MGD	PA-O3B	2.30	1.62	1.59
3	A	5002	MGD	C4-N9	-2.29	1.32	1.38
3	E	5001	MGD	O17-C17	2.29	1.27	1.23
3	G	5001	MGD	C16-N15	-2.27	1.32	1.37
3	G	5002	MGD	O11-C23	-2.26	1.40	1.43
16	E	5015	SO4	O1-S	2.23	1.58	1.44
3	A	5001	MGD	PA-O3B	2.19	1.61	1.59
3	C	5101	MGD	C21-N22	-2.17	1.33	1.35
3	E	5001	MGD	C16-N15	-2.15	1.32	1.37
13	A	5017	TRS	C3-C	-2.13	1.47	1.53
13	A	5017	TRS	O1-C1	-2.13	1.35	1.42
3	C	5102	MGD	C19-N18	-2.12	1.32	1.37
3	E	5002	MGD	C16-C17	2.11	1.48	1.41
3	C	5101	MGD	O3'-C3'	2.11	1.48	1.43
3	E	5001	MGD	C5-C4	2.10	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5001	MGD	C5-C4	2.07	1.44	1.38
3	A	5001	MGD	C16-C17	2.06	1.48	1.41
3	G	5001	MGD	C4-N3	2.05	1.38	1.34
3	A	5001	MGD	PA-O2A	-2.03	1.45	1.55
3	C	5101	MGD	PA-O2A	-2.03	1.45	1.55
3	A	5002	MGD	C8-N9	-2.02	1.33	1.37
3	E	5001	MGD	PB-O3B	2.02	1.61	1.59
7	A	5012	PEG	O2-C3	2.02	1.50	1.42
3	C	5102	MGD	C4-N9	-2.02	1.32	1.38

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5001	MGD	C23-C14-N15	8.47	116.19	107.87
3	G	5001	MGD	C23-C14-N15	5.78	113.54	107.87
3	A	5001	MGD	C23-C14-N15	5.54	113.31	107.87
3	C	5101	MGD	C23-C14-N15	5.34	113.11	107.87
3	A	5002	MGD	C5-C4-N3	-5.06	120.34	128.39
3	C	5102	MGD	O11-C23-N22	-4.90	104.16	108.61
3	E	5002	MGD	C5-C4-N3	-4.66	120.97	128.39
13	G	5006	TRS	C3-C-N	-4.57	96.52	108.17
3	E	5002	MGD	C23-C14-N15	4.52	112.31	107.87
3	A	5002	MGD	C23-C14-N15	4.42	112.21	107.87
3	E	5001	MGD	O11-C23-C14	4.41	111.91	108.96
3	E	5001	MGD	C5-C4-N3	-4.29	121.56	128.39
3	G	5002	MGD	C5-C4-N3	-4.24	121.64	128.39
3	G	5001	MGD	C5-C4-N3	-4.21	121.69	128.39
3	G	5002	MGD	C23-C14-N15	4.21	112.00	107.87
3	G	5001	MGD	N9-C4-N3	4.17	134.29	125.95
3	C	5102	MGD	N9-C4-N3	4.15	134.25	125.95
3	C	5102	MGD	C5-C4-N3	-3.99	122.03	128.39
3	C	5102	MGD	C19-N20-C21	3.96	120.35	113.36
3	G	5001	MGD	C2-N3-C4	3.95	119.10	112.30
3	G	5002	MGD	C19-N20-C21	3.94	120.31	113.36
3	C	5101	MGD	C5-C4-N3	-3.92	122.14	128.39
3	A	5002	MGD	O11-C23-C14	3.92	111.58	108.96
3	A	5001	MGD	C19-N20-C21	3.92	120.28	113.36
3	E	5002	MGD	N9-C4-N3	3.91	133.78	125.95
3	C	5102	MGD	C4'-O4'-C1'	-3.89	100.87	109.47
3	A	5002	MGD	C4'-O4'-C1'	-3.89	100.87	109.47
3	A	5002	MGD	N9-C4-N3	3.80	133.56	125.95
3	A	5001	MGD	C5-C4-N3	-3.77	122.38	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5102	MGD	O17-C17-C16	-3.69	118.36	127.26
3	A	5002	MGD	O17-C17-C16	-3.67	118.41	127.26
7	A	5012	PEG	O4-C4-C3	3.65	133.30	111.82
13	C	5112	TRS	C1-C-N	3.65	117.47	108.17
3	A	5002	MGD	C19-N20-C21	3.64	119.79	113.36
3	G	5001	MGD	O2B-PB-O3B	3.63	117.10	107.27
13	G	5006	TRS	C1-C-N	3.62	117.40	108.17
3	E	5001	MGD	N9-C4-N3	3.56	133.07	125.95
3	A	5001	MGD	N9-C4-N3	3.55	133.05	125.95
3	E	5001	MGD	C6-C5-N7	3.52	136.69	130.29
3	C	5102	MGD	C23-C14-N15	3.51	111.32	107.87
3	C	5102	MGD	C2-N3-C4	3.50	118.32	112.30
13	A	5017	TRS	C3-C-C2	-3.48	101.38	110.66
3	G	5002	MGD	N9-C4-N3	3.46	132.88	125.95
3	E	5001	MGD	C2-N3-C4	3.43	118.20	112.30
3	G	5001	MGD	C6-C5-N7	3.42	136.51	130.29
3	G	5001	MGD	O11-C23-N22	-3.40	105.52	108.61
3	E	5001	MGD	O3B-PB-O1B	-3.40	100.49	110.70
3	E	5002	MGD	O17-C17-C16	-3.38	119.12	127.26
3	G	5001	MGD	C19-N20-C21	3.36	119.29	113.36
3	G	5002	MGD	O2B-PB-O3B	3.35	116.32	107.27
3	G	5002	MGD	C4'-O4'-C1'	-3.35	102.08	109.47
3	C	5101	MGD	N9-C4-N3	3.33	132.60	125.95
3	C	5101	MGD	C6-C5-N7	3.30	136.30	130.29
13	C	5112	TRS	C3-C-C1	-3.28	101.91	110.66
3	G	5001	MGD	O3B-PB-O1B	-3.26	100.89	110.70
13	C	5112	TRS	C2-C-C1	3.23	119.26	110.66
3	E	5001	MGD	C1'-N9-C4	-3.18	117.10	126.49
13	G	5006	TRS	O3-C3-C	2.95	119.10	110.88
3	C	5102	MGD	O2A-PA-O1A	2.94	126.12	112.44
3	A	5002	MGD	O2A-PA-O1A	2.93	126.07	112.44
3	G	5001	MGD	O17-C17-C16	-2.88	120.31	127.26
3	A	5002	MGD	C2-N3-C4	2.88	117.27	112.30
3	G	5002	MGD	O17-C17-C16	-2.86	120.37	127.26
3	E	5002	MGD	C4'-O4'-C1'	-2.86	103.15	109.47
3	C	5101	MGD	C2-N3-C4	2.85	117.21	112.30
3	G	5001	MGD	C1'-N9-C4	-2.84	118.09	126.49
3	G	5002	MGD	O11-C23-N22	-2.82	106.05	108.61
3	A	5002	MGD	O6-C6-C5	-2.79	119.17	126.53
3	G	5002	MGD	O3B-PB-O1B	-2.79	102.32	110.70
3	A	5001	MGD	O3B-PB-O1B	-2.76	102.41	110.70
3	G	5001	MGD	O6-C6-C5	-2.76	119.26	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5002	MGD	O6-C6-C5	-2.74	119.31	126.53
3	A	5001	MGD	O4'-C4'-C3'	2.70	110.51	105.15
3	E	5002	MGD	O11-C23-N22	-2.70	106.16	108.61
3	E	5002	MGD	C2-N3-C4	2.68	116.92	112.30
3	E	5002	MGD	C19-N20-C21	2.66	118.04	113.36
3	G	5001	MGD	O11-C23-C14	2.65	110.73	108.96
13	C	5112	TRS	C2-C-N	-2.64	101.44	108.17
12	A	5016	GOL	O3-C3-C2	-2.62	98.57	110.38
3	E	5001	MGD	O3A-C10-C11	-2.62	102.11	108.58
3	C	5101	MGD	C4-C5-N7	-2.61	106.53	110.67
3	E	5001	MGD	O2B-PB-O3B	2.59	114.28	107.27
3	C	5101	MGD	C1'-N9-C4	-2.57	118.90	126.49
13	G	5006	TRS	O2-C2-C	2.56	118.01	110.88
3	G	5002	MGD	C17-C16-N15	2.53	123.17	116.27
3	E	5001	MGD	C8-N7-C5	2.52	108.75	104.26
7	C	5106	PEG	O2-C2-C1	2.52	121.23	110.11
3	E	5002	MGD	O6-C6-N1	2.50	124.81	120.11
3	C	5101	MGD	C19-N20-C21	2.47	117.72	113.36
13	A	5017	TRS	C3-C-N	2.45	114.42	108.17
3	A	5001	MGD	C2-N3-C4	2.44	116.50	112.30
3	G	5002	MGD	C6-C5-N7	2.44	134.73	130.29
3	E	5001	MGD	C4-C5-N7	-2.43	106.82	110.67
3	A	5001	MGD	O11-C23-C14	2.43	110.58	108.96
3	A	5001	MGD	C1'-N9-C4	-2.43	119.32	126.49
3	C	5101	MGD	O2A-PA-O1A	2.42	123.71	112.44
3	A	5002	MGD	C16-C17-N18	2.41	118.75	112.13
3	E	5001	MGD	N9-C8-N7	-2.40	108.94	113.40
3	C	5101	MGD	C8-N7-C5	2.36	108.46	104.26
3	A	5001	MGD	O6-C6-C5	-2.35	120.34	126.53
3	A	5001	MGD	C8-N9-C4	2.32	110.37	106.03
3	G	5001	MGD	C17-C16-N15	2.32	122.58	116.27
3	A	5002	MGD	C17-C16-N15	2.32	122.58	116.27
3	E	5001	MGD	O6-C6-C5	-2.31	120.43	126.53
3	E	5002	MGD	O3B-PB-O1B	-2.30	103.78	110.70
3	C	5102	MGD	C16-C17-N18	2.30	118.45	112.13
3	A	5001	MGD	C6-C5-N7	2.30	134.47	130.29
3	G	5001	MGD	O4'-C4'-C3'	2.30	109.71	105.15
3	A	5002	MGD	N2-C2-N3	-2.28	115.22	119.67
3	C	5102	MGD	O3B-PB-O1B	-2.27	103.88	110.70
3	C	5102	MGD	C6-C5-N7	2.26	134.40	130.29
3	G	5001	MGD	C8-N9-C4	2.24	110.22	106.03
3	G	5001	MGD	C2'-C1'-N9	2.24	119.48	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5001	MGD	C2'-C3'-C4'	-2.18	98.39	102.61
3	G	5001	MGD	C4-C5-N7	-2.16	107.24	110.67
3	C	5101	MGD	O6-C6-C5	-2.16	120.84	126.53
3	C	5101	MGD	O2B-PB-O3B	2.15	113.09	107.27
3	G	5002	MGD	C16-C17-N18	2.15	118.04	112.13
3	E	5001	MGD	C19-N20-C21	2.14	117.14	113.36
3	E	5001	MGD	C8-N9-C4	2.14	110.04	106.03
3	G	5001	MGD	C8-N7-C5	2.12	108.04	104.26
3	E	5001	MGD	C1'-N9-C8	2.12	132.75	126.73
3	G	5002	MGD	O2A-PA-O1A	2.12	122.28	112.44
3	E	5002	MGD	O17-C17-N18	2.11	124.08	120.11
3	E	5002	MGD	O2A-PA-O1A	2.10	122.20	112.44
3	G	5002	MGD	C2-N3-C4	2.09	115.90	112.30
3	C	5102	MGD	C8-N9-C4	2.08	109.92	106.03
8	G	5009	ACT	OXT-C-CH3	2.07	123.75	115.05
3	A	5002	MGD	O3B-PB-O1B	-2.07	104.47	110.70
12	E	5008	GOL	O1-C1-C2	2.06	119.66	110.38
3	C	5101	MGD	O17-C17-C16	-2.06	122.30	127.26
15	E	5010	EDO	O2-C2-C1	2.05	128.01	112.39
3	C	5101	MGD	C2'-C1'-N9	2.04	118.94	113.25
3	A	5002	MGD	C19-N18-C17	-2.04	121.41	125.11
3	A	5002	MGD	C4-C5-N7	-2.04	107.44	110.67
3	C	5102	MGD	O6-C6-C5	-2.02	121.21	126.53
3	E	5002	MGD	O2B-PB-O3B	2.00	112.68	107.27
3	G	5001	MGD	C16-C17-N18	2.00	117.63	112.13

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5001	MGD	C5'-O5'-PB-O1B
3	A	5002	MGD	C5'-O5'-PB-O1B
3	A	5002	MGD	C5'-O5'-PB-O3B
3	C	5101	MGD	C5'-O5'-PB-O1B
3	C	5102	MGD	PA-O3B-PB-O5'
3	C	5102	MGD	C5'-O5'-PB-O1B
3	E	5001	MGD	C5'-O5'-PB-O1B
3	E	5002	MGD	C5'-O5'-PB-O1B
3	E	5002	MGD	C5'-O5'-PB-O3B
3	G	5001	MGD	C5'-O5'-PB-O1B
3	G	5002	MGD	PA-O3B-PB-O5'
3	G	5002	MGD	C5'-O5'-PB-O1B

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Mol	Chain	Res	Type	Atoms
13	G	5006	TRS	N-C-C1-O1
13	G	5006	TRS	N-C-C2-O2
7	G	5007	PEG	O1-C1-C2-O2
7	A	5006	PEG	O1-C1-C2-O2
7	E	5006	PEG	O1-C1-C2-O2
12	A	5015	GOL	C1-C2-C3-O3
12	A	5016	GOL	O1-C1-C2-C3
12	E	5008	GOL	O1-C1-C2-C3
12	E	5008	GOL	C1-C2-C3-O3
7	G	5007	PEG	C4-C3-O2-C2
13	A	5017	TRS	C3-C-C2-O2
13	C	5112	TRS	C1-C-C3-O3
13	G	5006	TRS	C2-C-C1-O1
13	G	5006	TRS	C1-C-C3-O3
7	E	5006	PEG	O2-C3-C4-O4
15	E	5012	EDO	O1-C1-C2-O2
7	A	5011	PEG	O1-C1-C2-O2
12	A	5015	GOL	O2-C2-C3-O3
7	G	5007	PEG	O2-C3-C4-O4
7	A	5012	PEG	O2-C3-C4-O4
3	A	5001	MGD	O4'-C4'-C5'-O5'
13	A	5017	TRS	N-C-C1-O1
13	A	5017	TRS	N-C-C2-O2
13	C	5112	TRS	N-C-C1-O1
13	C	5112	TRS	N-C-C2-O2
13	C	5112	TRS	N-C-C3-O3
13	G	5006	TRS	N-C-C3-O3
7	C	5106	PEG	O2-C3-C4-O4
3	A	5002	MGD	PA-O3B-PB-O5'
3	C	5101	MGD	PA-O3B-PB-O5'
3	E	5001	MGD	PA-O3B-PB-O5'
3	E	5002	MGD	PA-O3B-PB-O5'
15	E	5010	EDO	O1-C1-C2-O2
3	C	5101	MGD	O4'-C4'-C5'-O5'
3	G	5001	MGD	O4'-C4'-C5'-O5'
12	E	5008	GOL	O2-C2-C3-O3
13	A	5017	TRS	C2-C-C1-O1
13	C	5112	TRS	C2-C-C3-O3
13	G	5006	TRS	C2-C-C3-O3
7	A	5006	PEG	C4-C3-O2-C2
3	C	5102	MGD	C5'-O5'-PB-O2B
3	C	5102	MGD	C5'-O5'-PB-O3B

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Mol	Chain	Res	Type	Atoms
3	G	5002	MGD	C5'-O5'-PB-O3B
3	E	5001	MGD	O4'-C4'-C5'-O5'
3	G	5002	MGD	PB-O3B-PA-O1A
13	C	5112	TRS	C2-C-C1-O1
13	C	5112	TRS	C3-C-C2-O2
13	G	5006	TRS	C3-C-C1-O1
13	G	5006	TRS	C1-C-C2-O2
12	E	5008	GOL	O1-C1-C2-O2
7	G	5007	PEG	C1-C2-O2-C3
3	C	5101	MGD	C3'-C4'-C5'-O5'
3	A	5002	MGD	PB-O3B-PA-O2A
3	C	5102	MGD	PB-O3B-PA-O2A
3	E	5001	MGD	PB-O3B-PA-O2A
3	E	5002	MGD	PB-O3B-PA-O2A
3	G	5001	MGD	PB-O3B-PA-O2A
3	G	5001	MGD	C3'-C4'-C5'-O5'

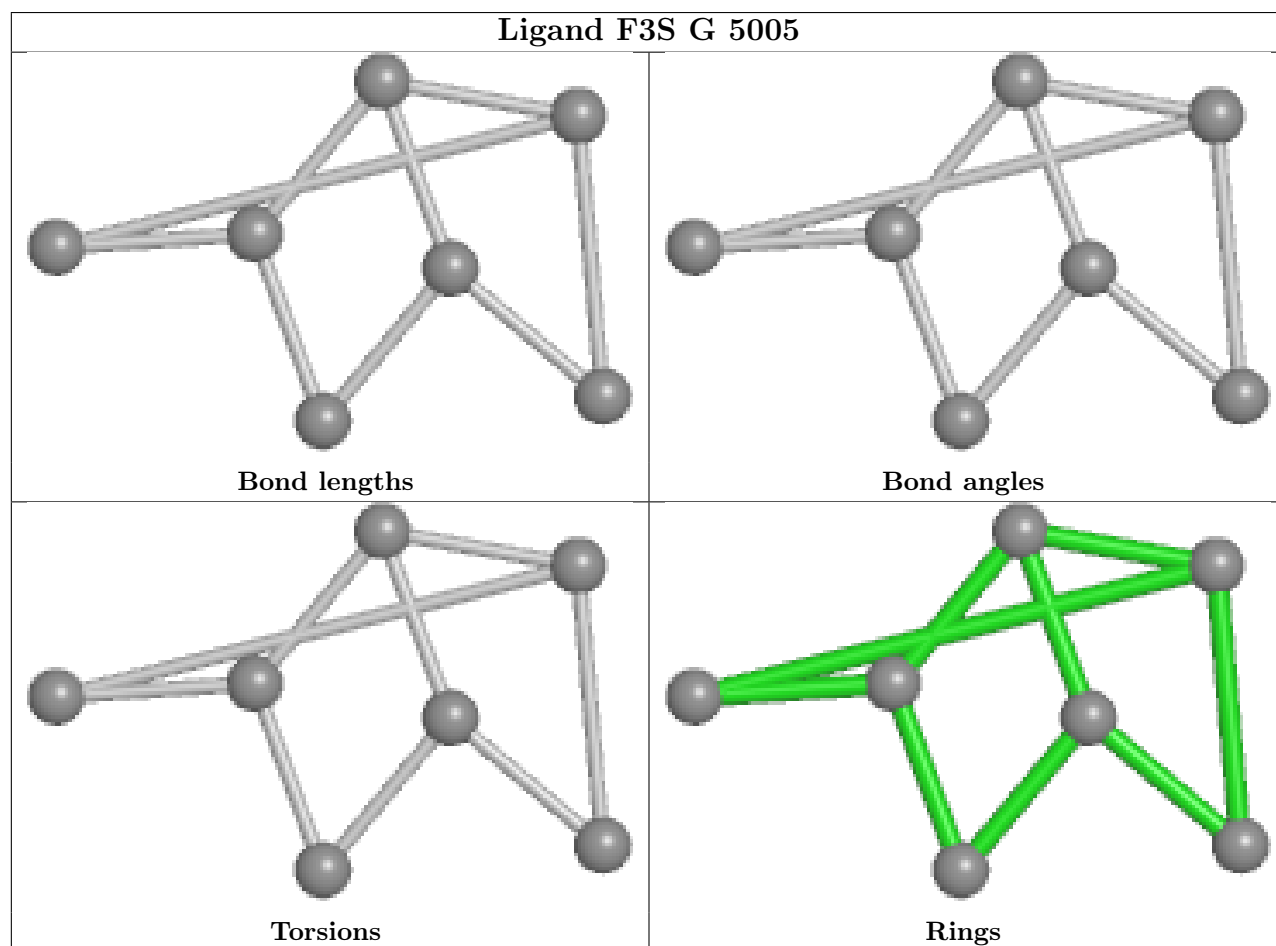
There are no ring outliers.

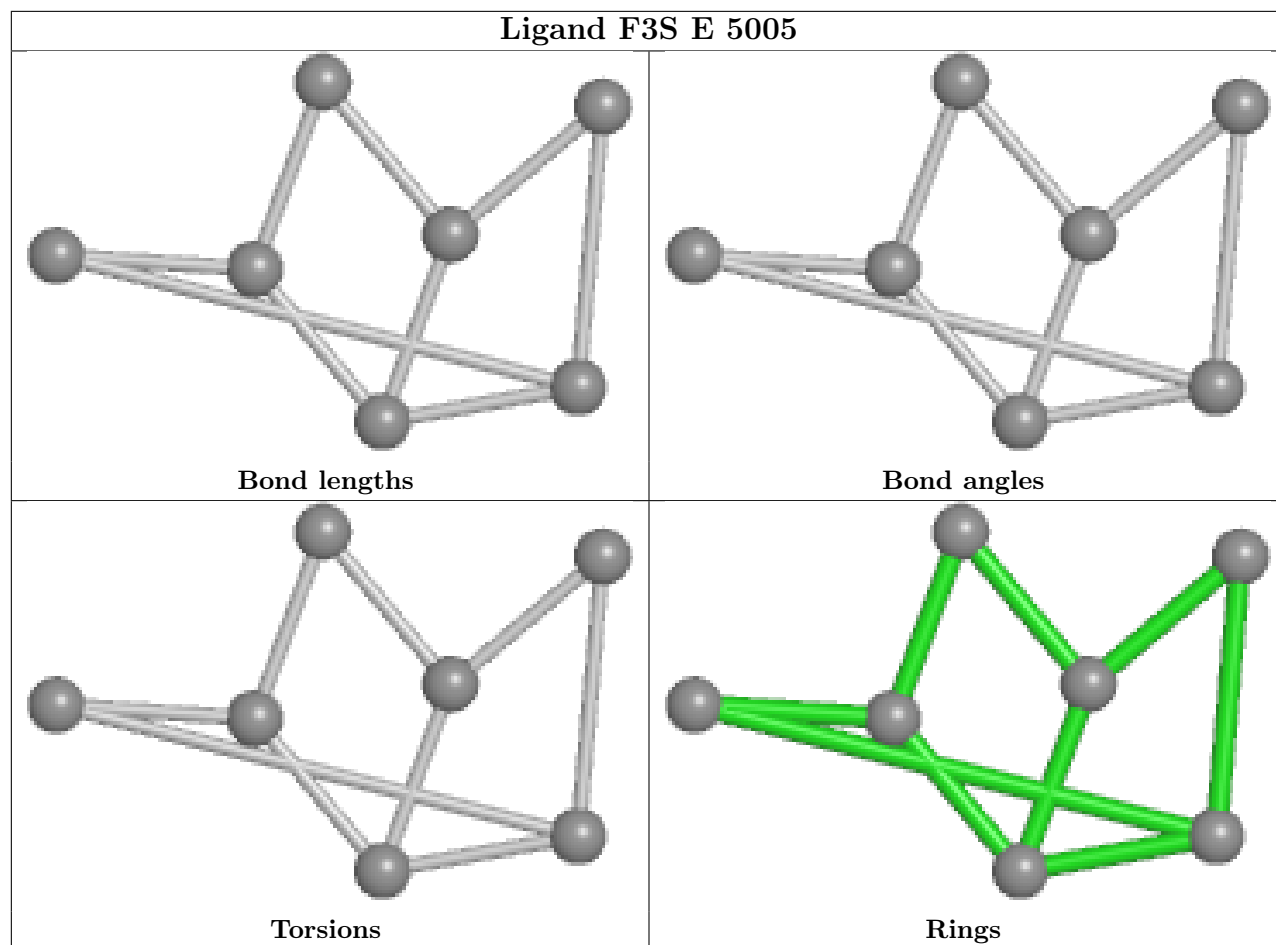
19 monomers are involved in 59 short contacts:

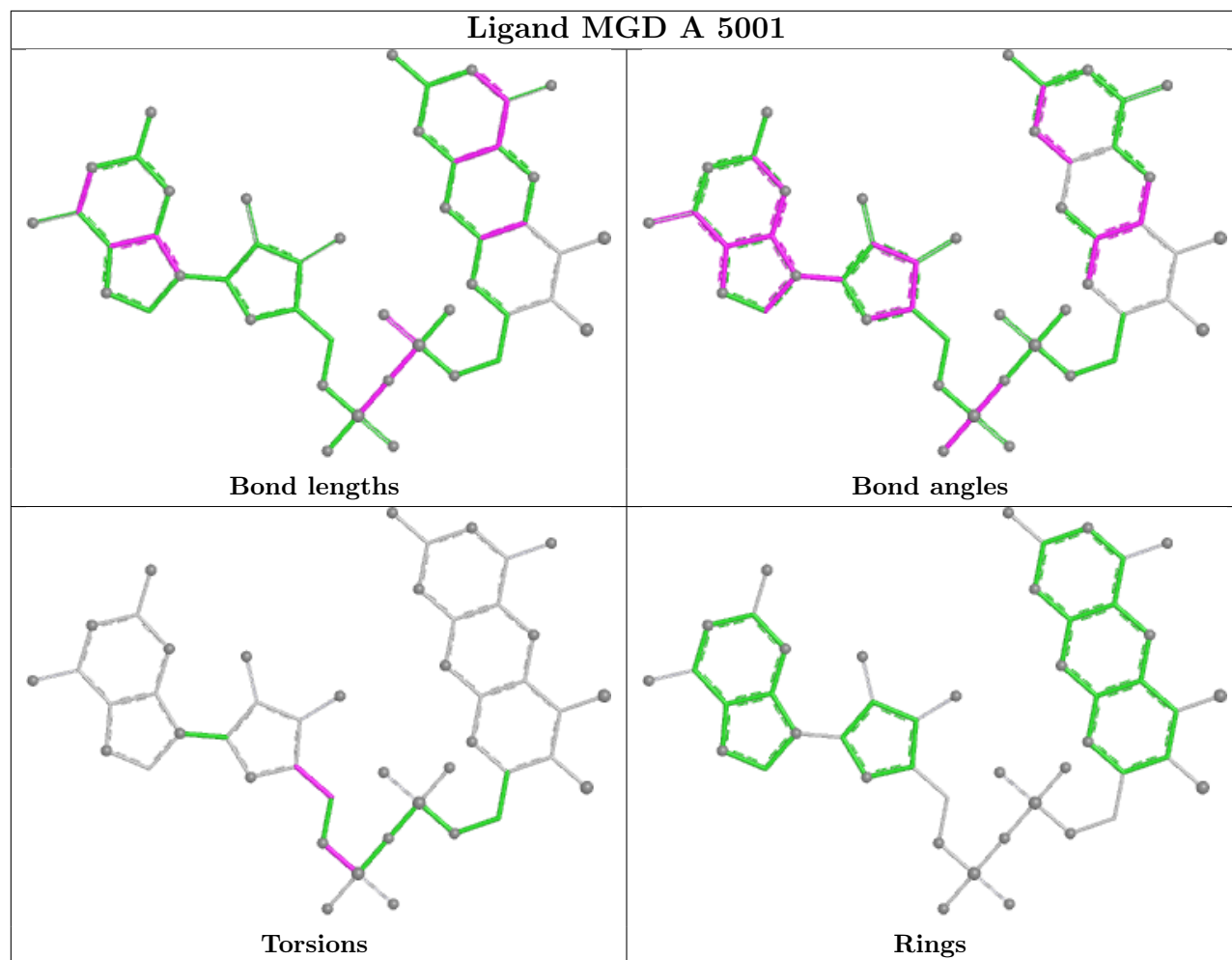
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	5017	TRS	14	0
13	C	5112	TRS	7	0
3	A	5001	MGD	2	0
15	E	5012	EDO	9	0
3	E	5002	MGD	1	0
8	A	5009	ACT	3	0
7	C	5106	PEG	1	0
10	C	5109	UJI	1	0
12	E	5008	GOL	2	0
3	C	5102	MGD	1	0
9	E	5011	PO4	1	0
13	G	5006	TRS	7	0
15	E	5010	EDO	9	0
7	E	5006	PEG	2	0
7	A	5012	PEG	3	0
3	C	5101	MGD	1	0
3	E	5001	MGD	2	0
3	G	5001	MGD	1	0
7	A	5011	PEG	2	0

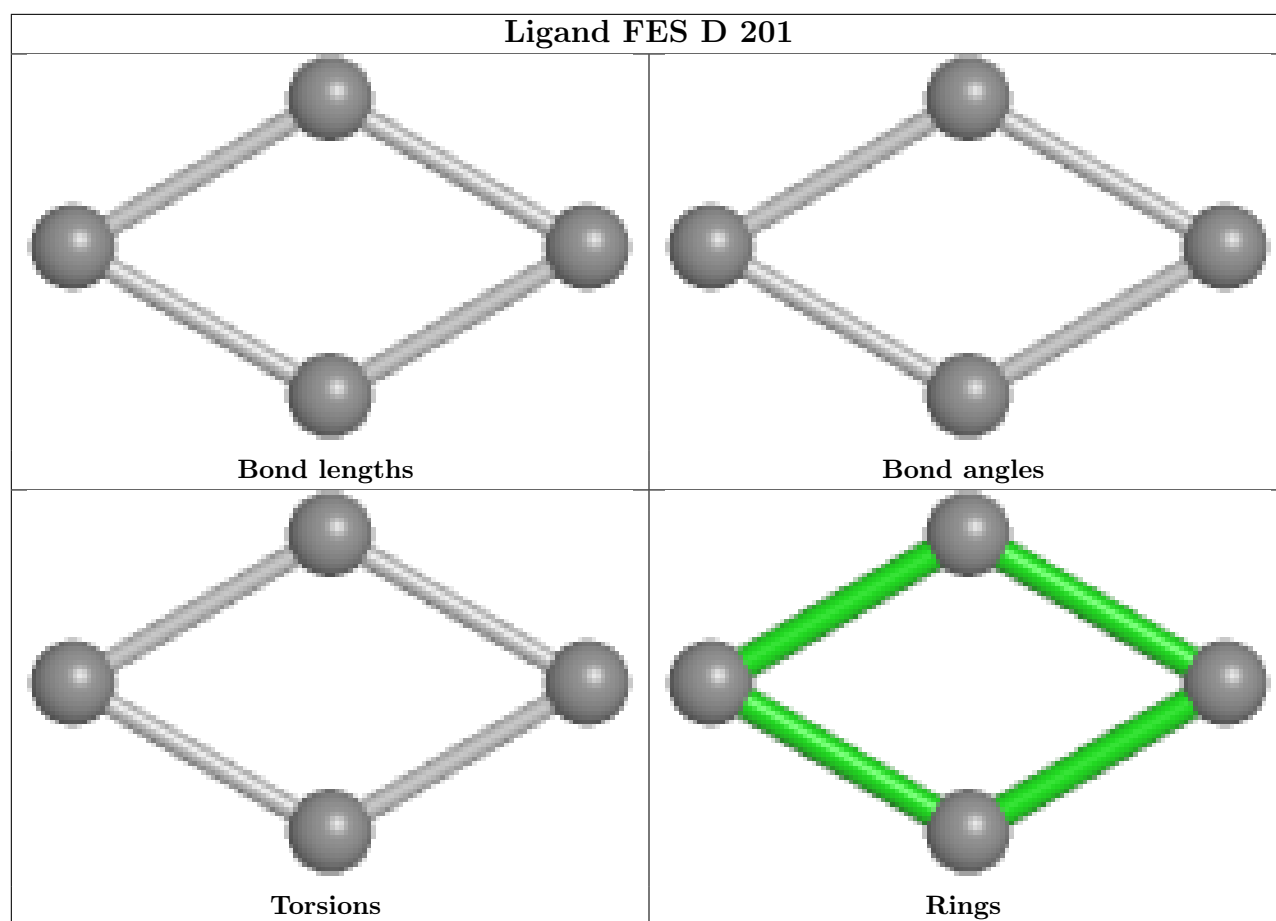
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

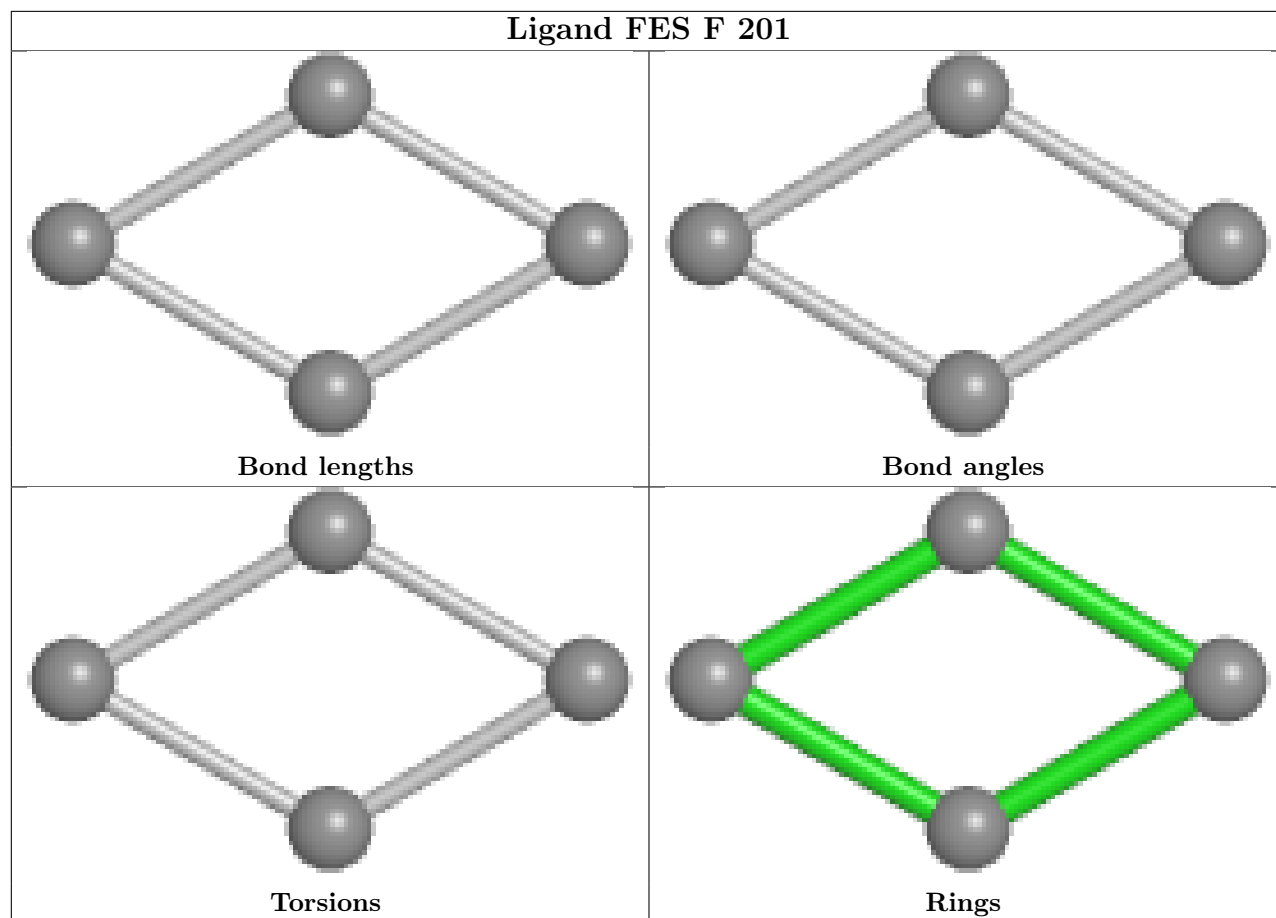
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

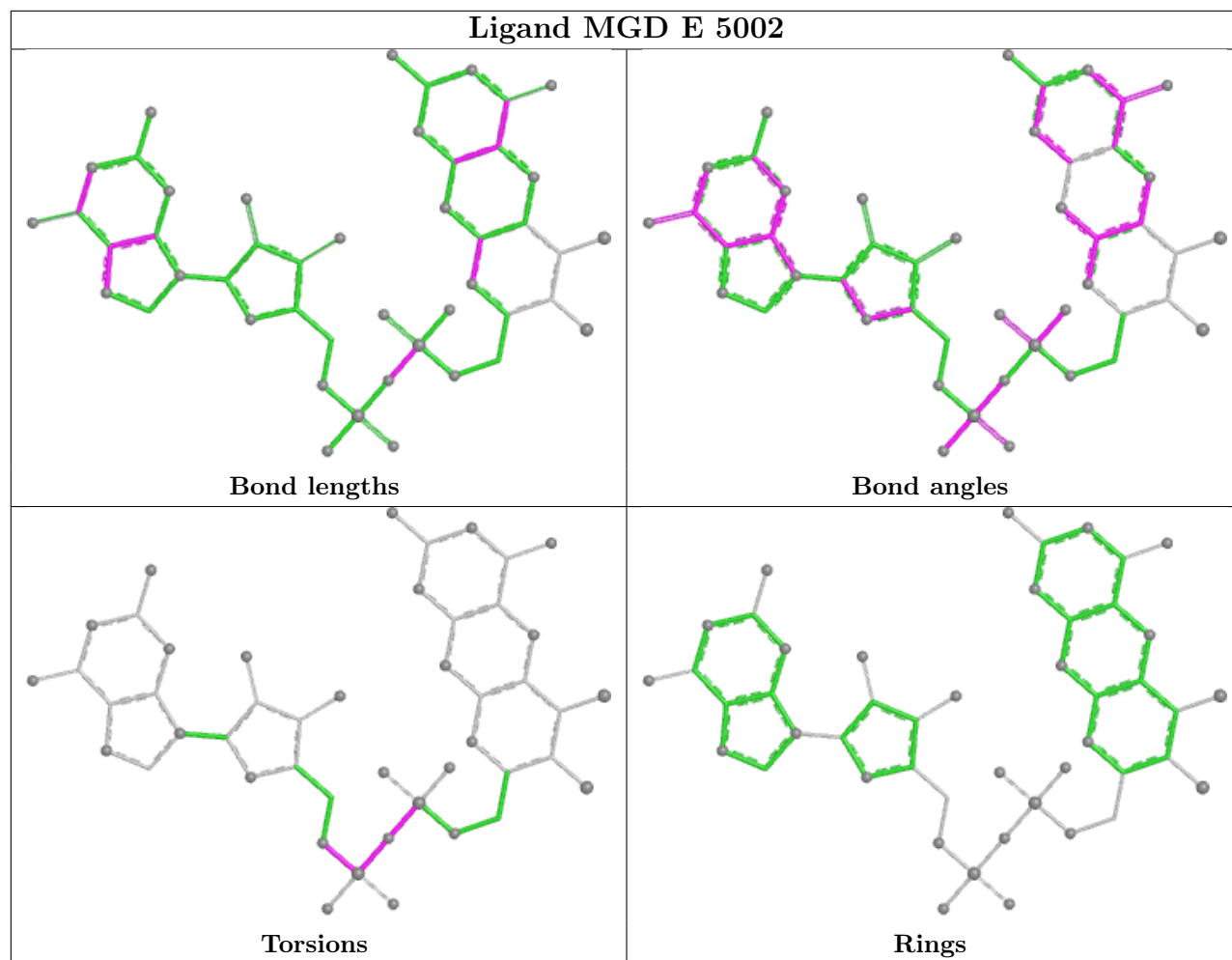


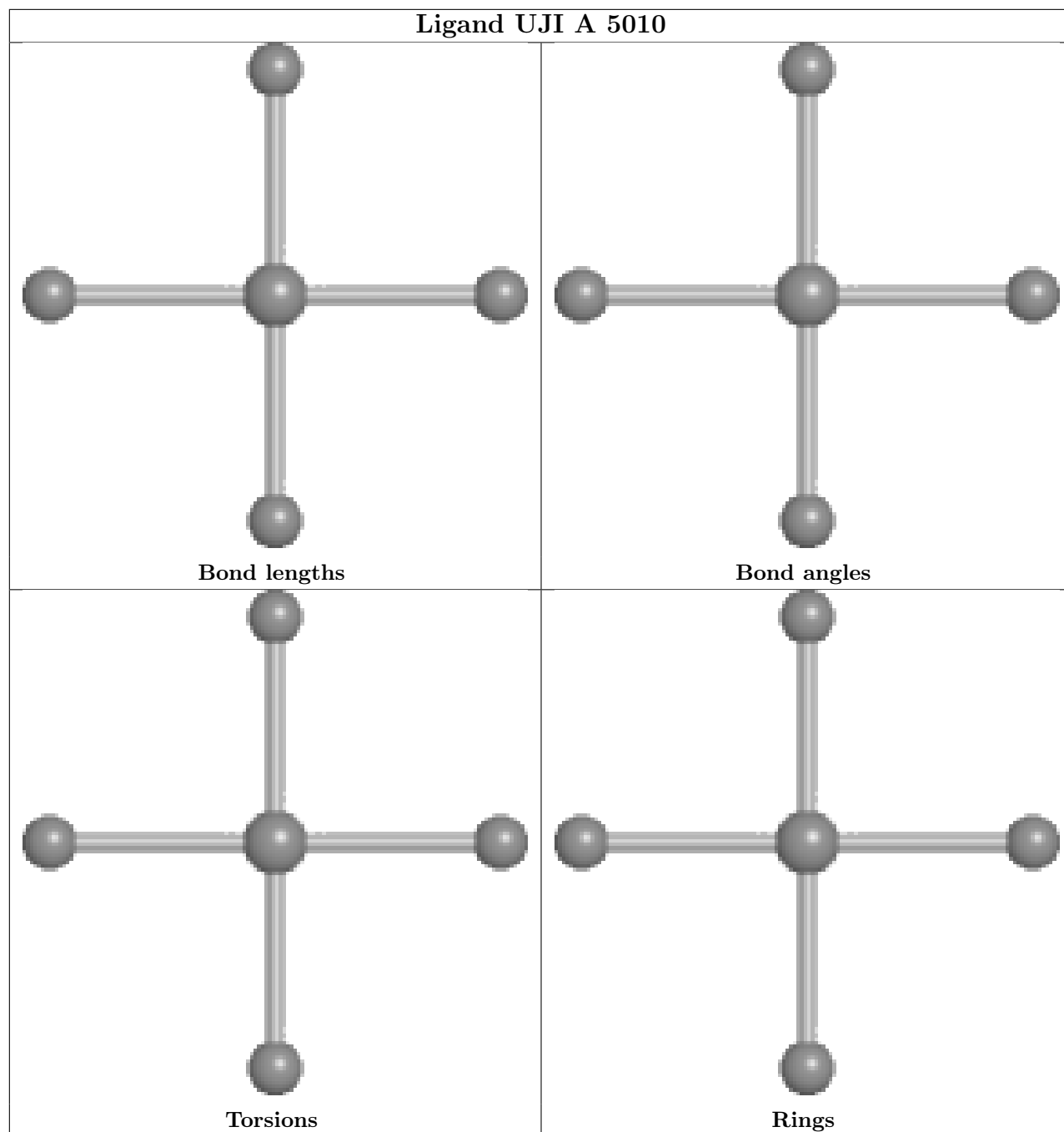


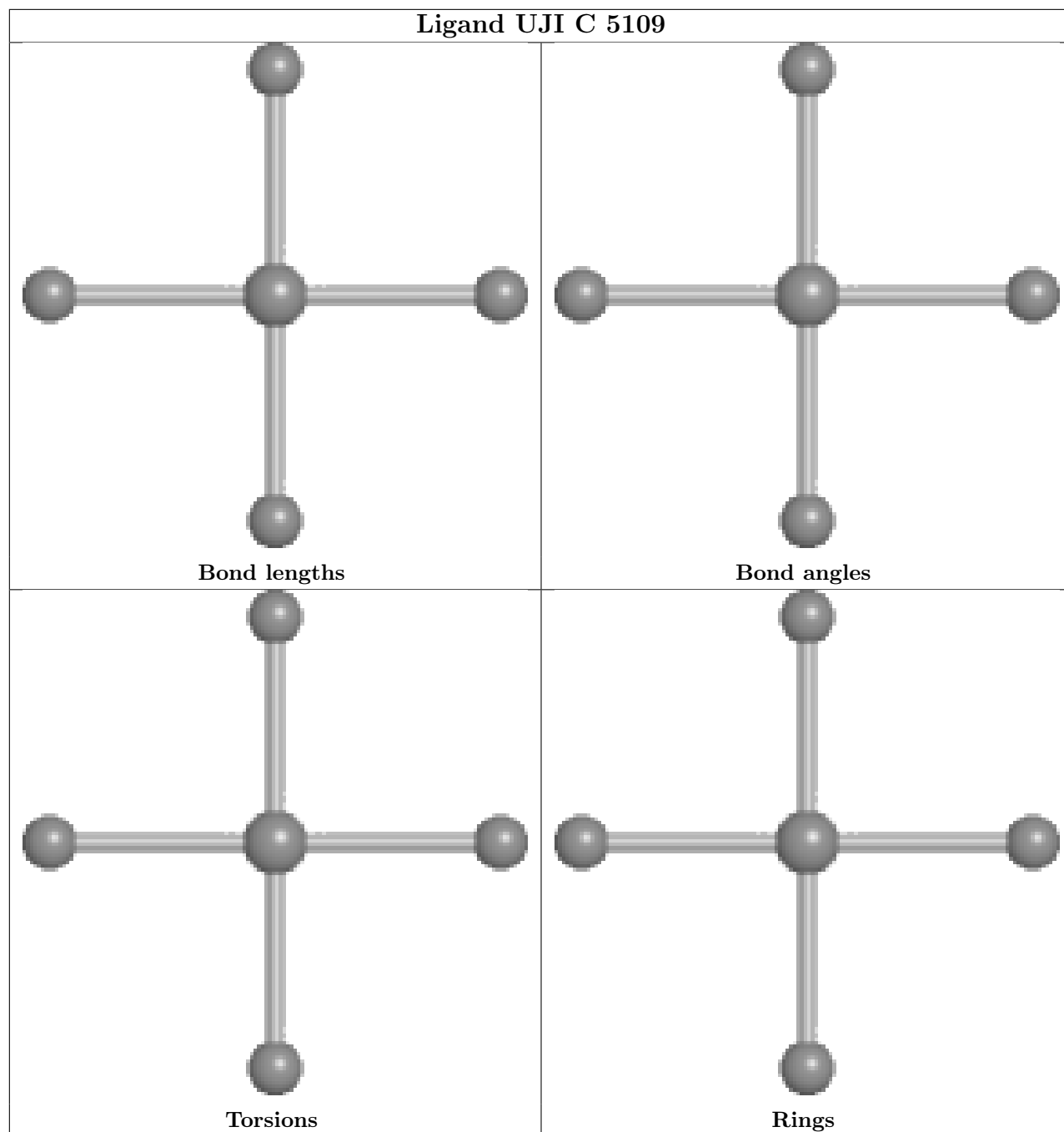


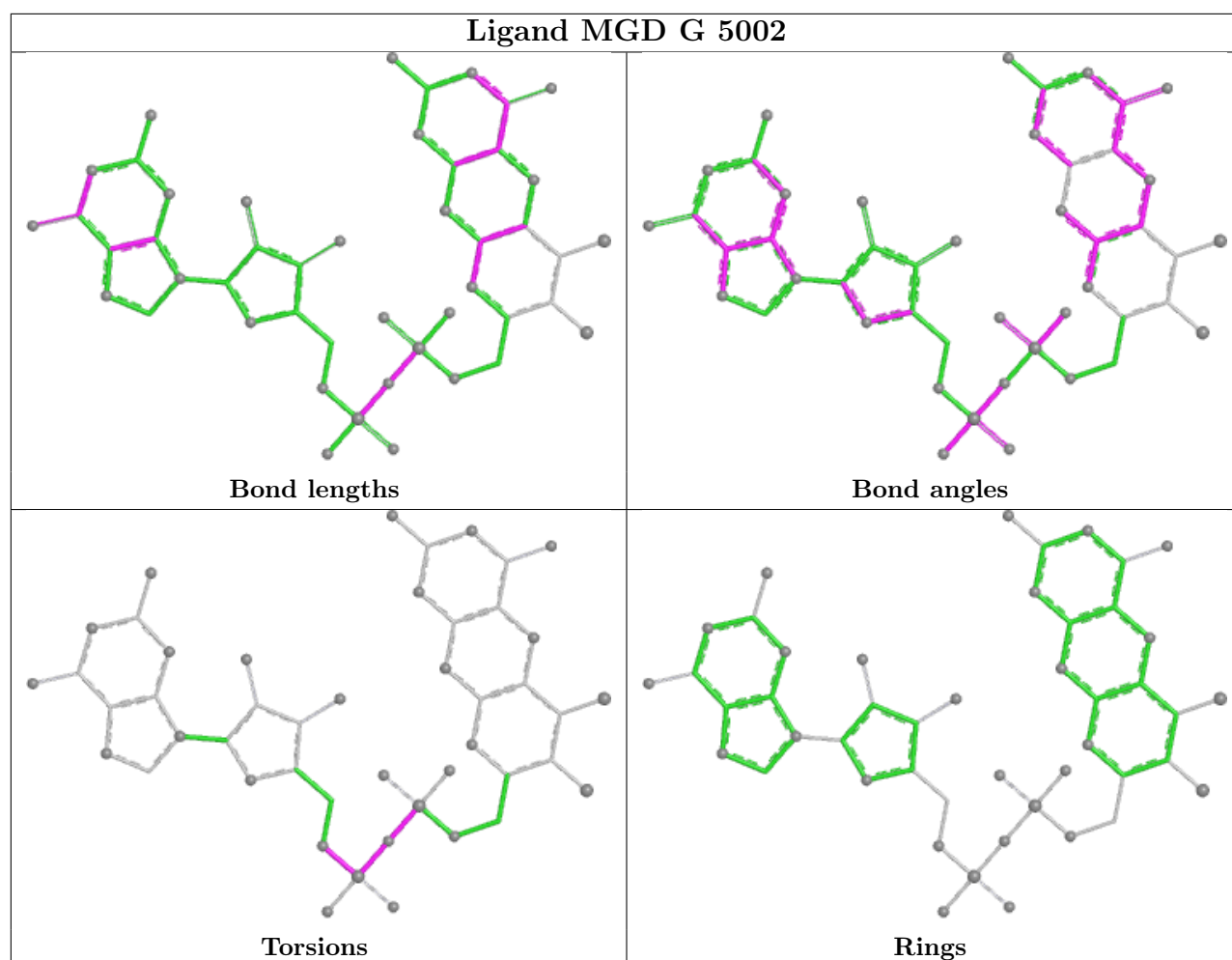


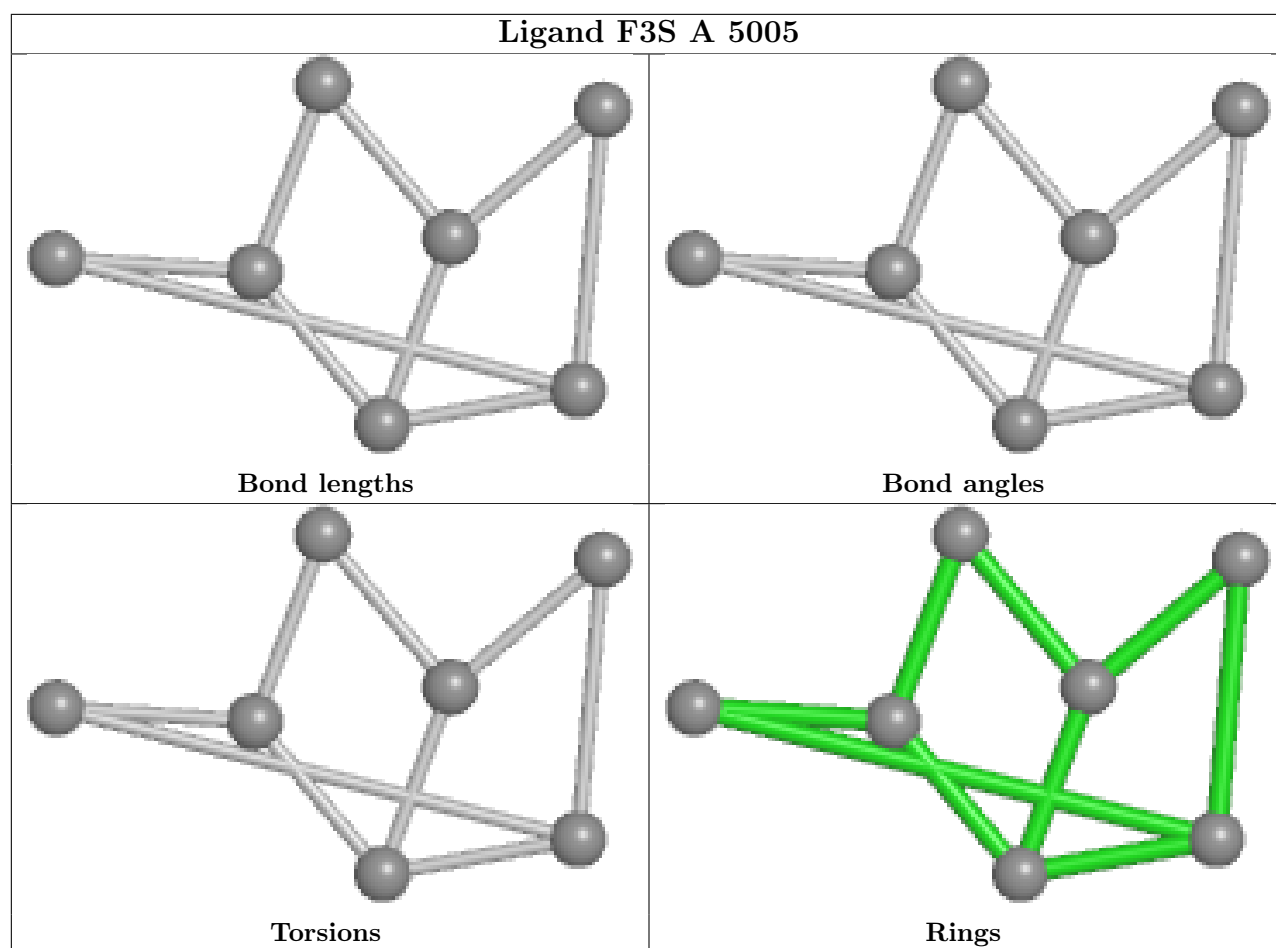


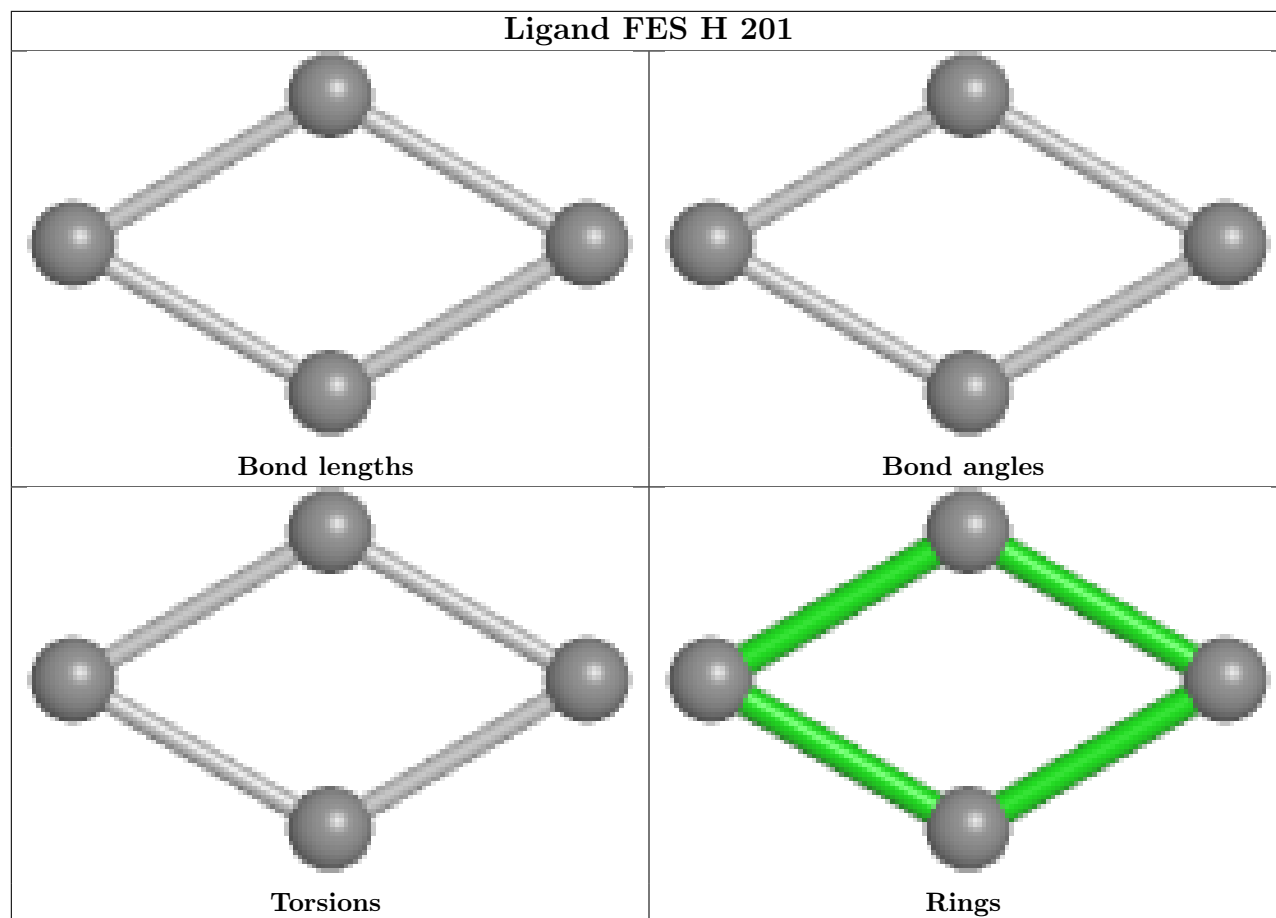


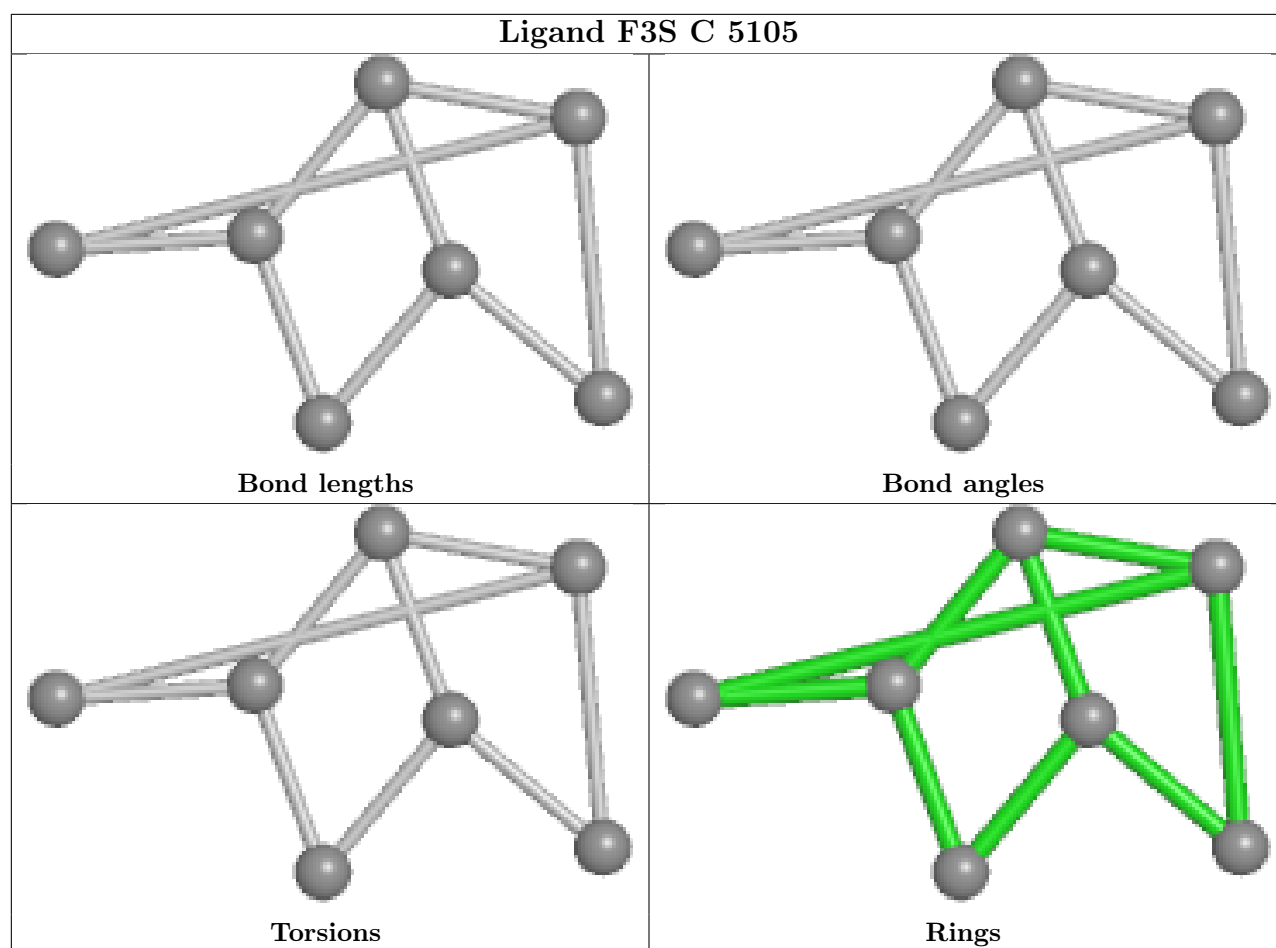




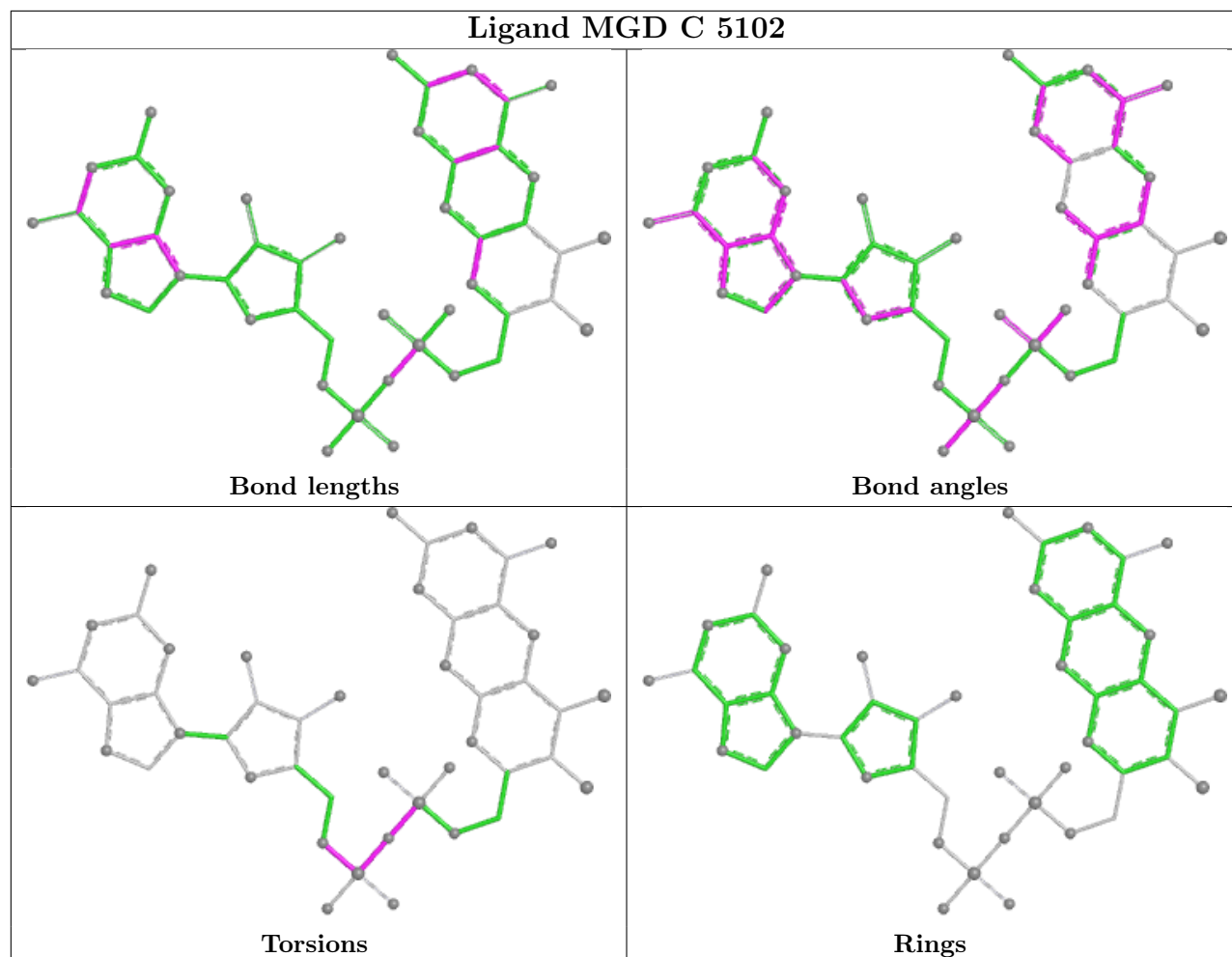


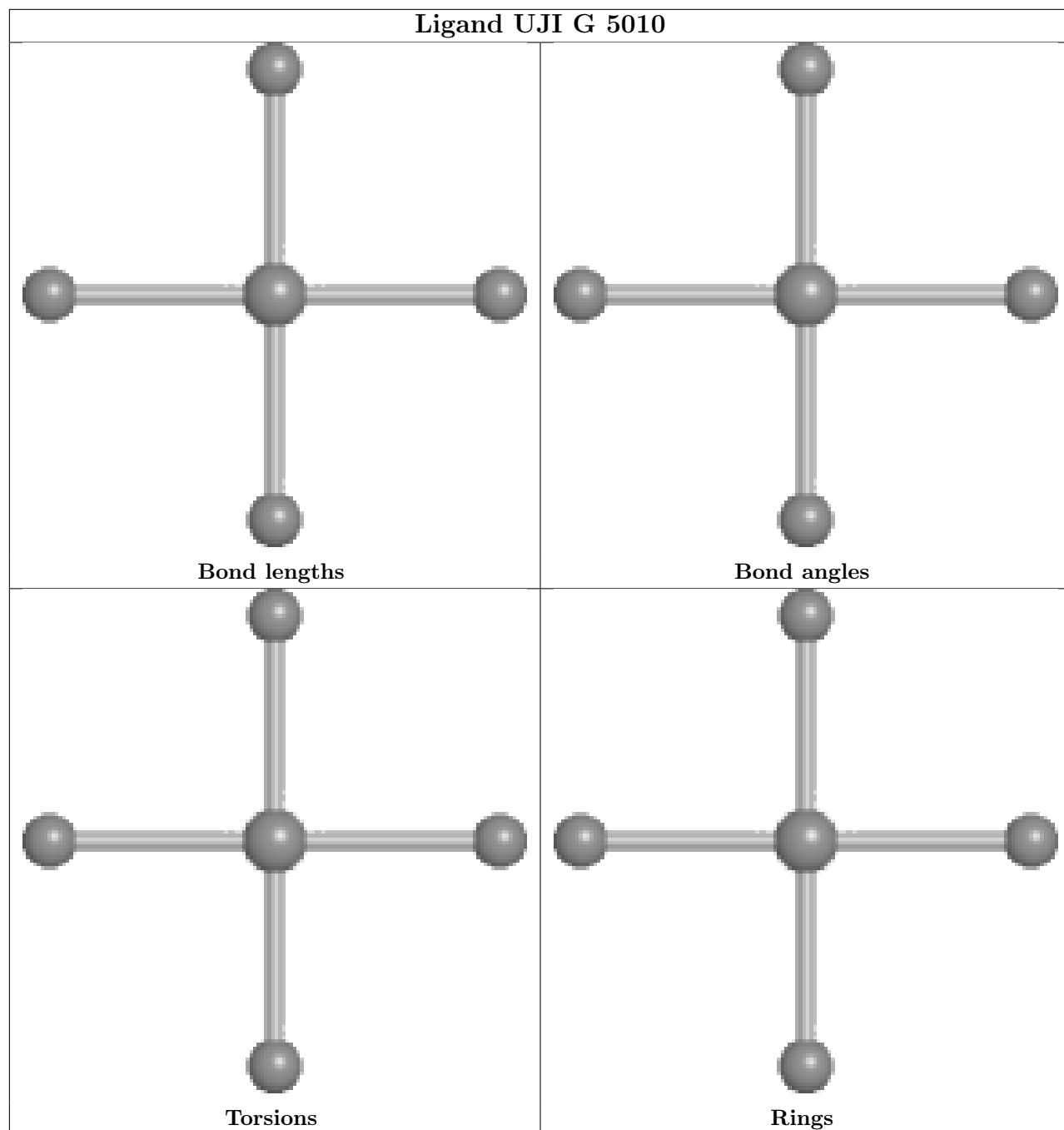


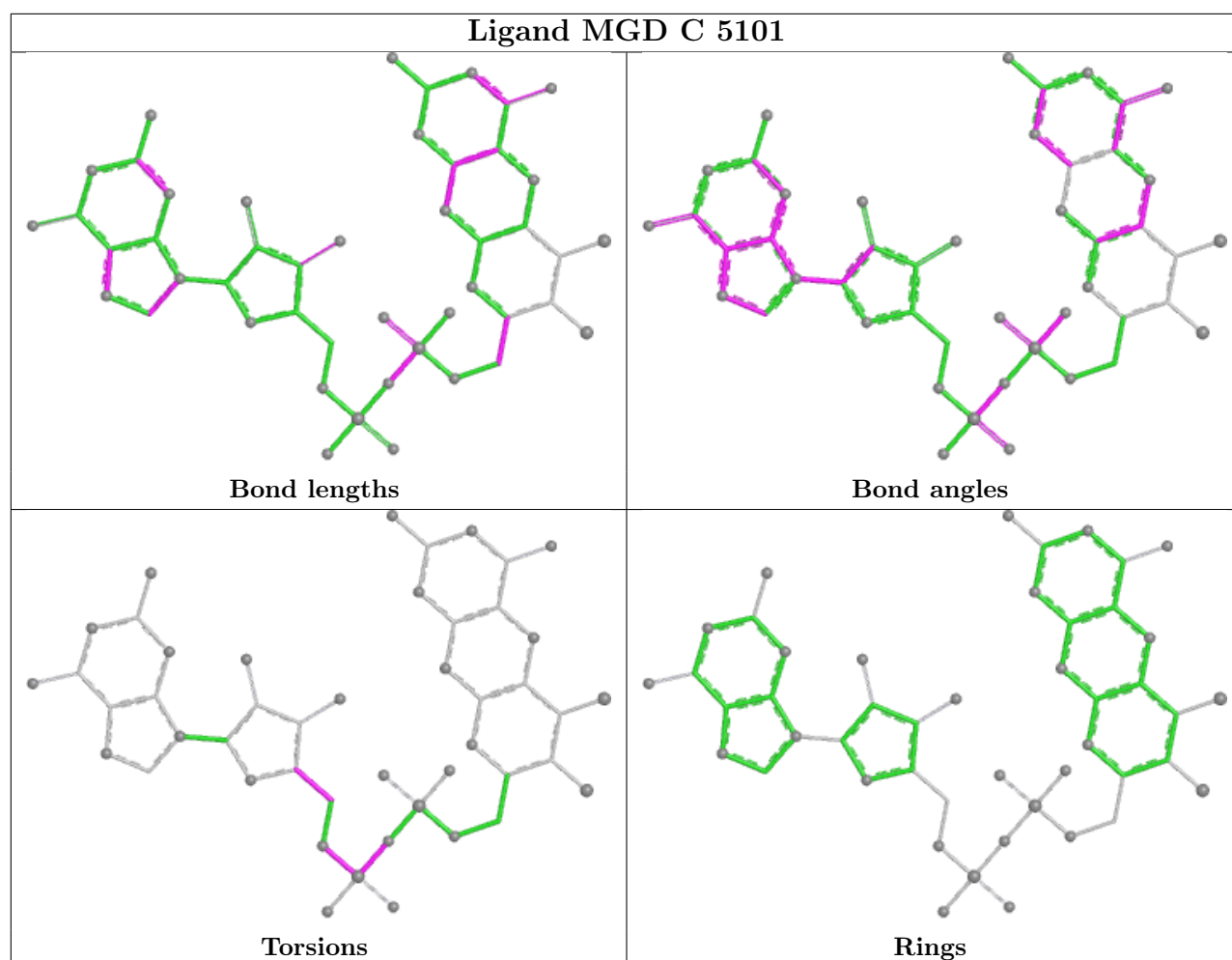


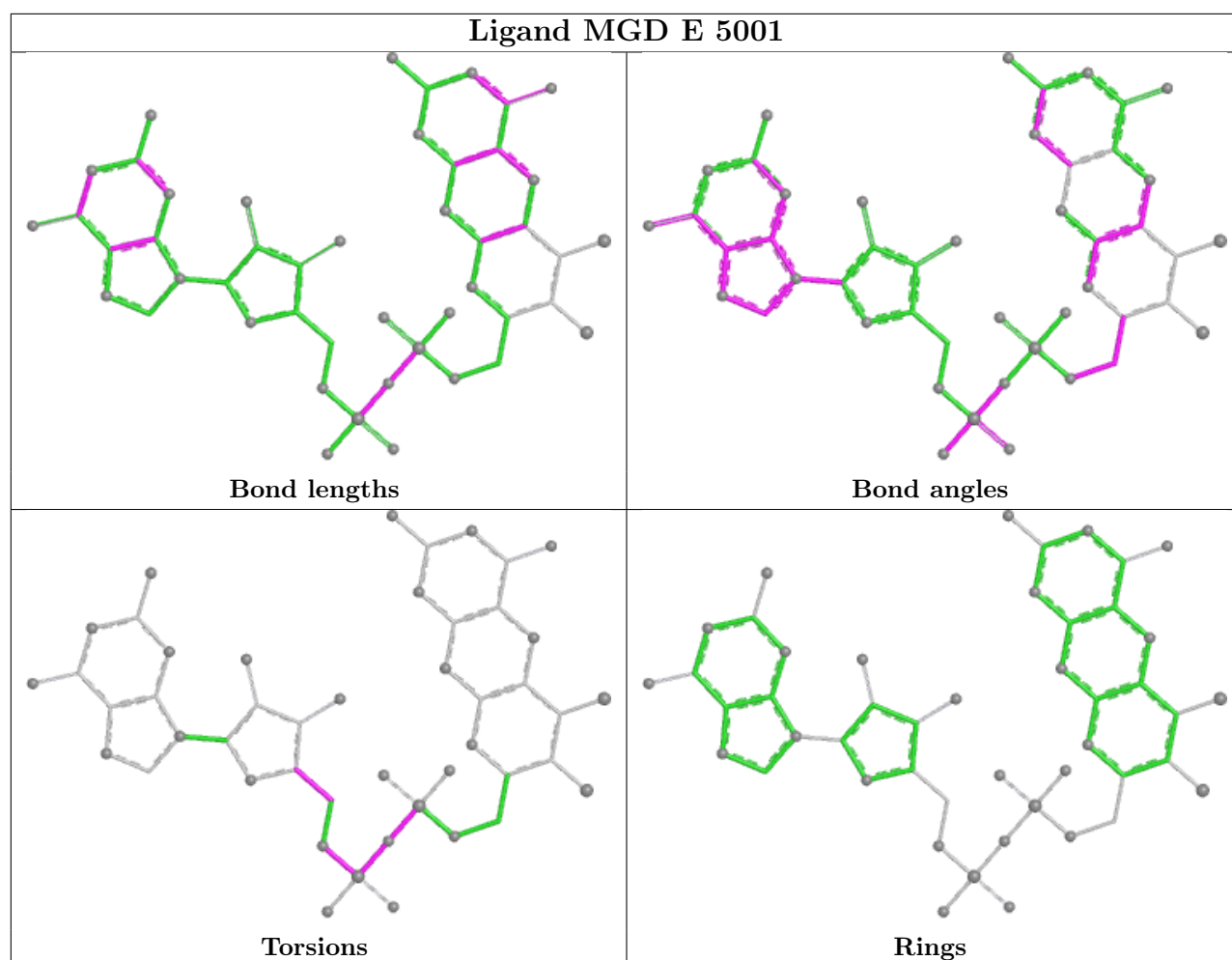


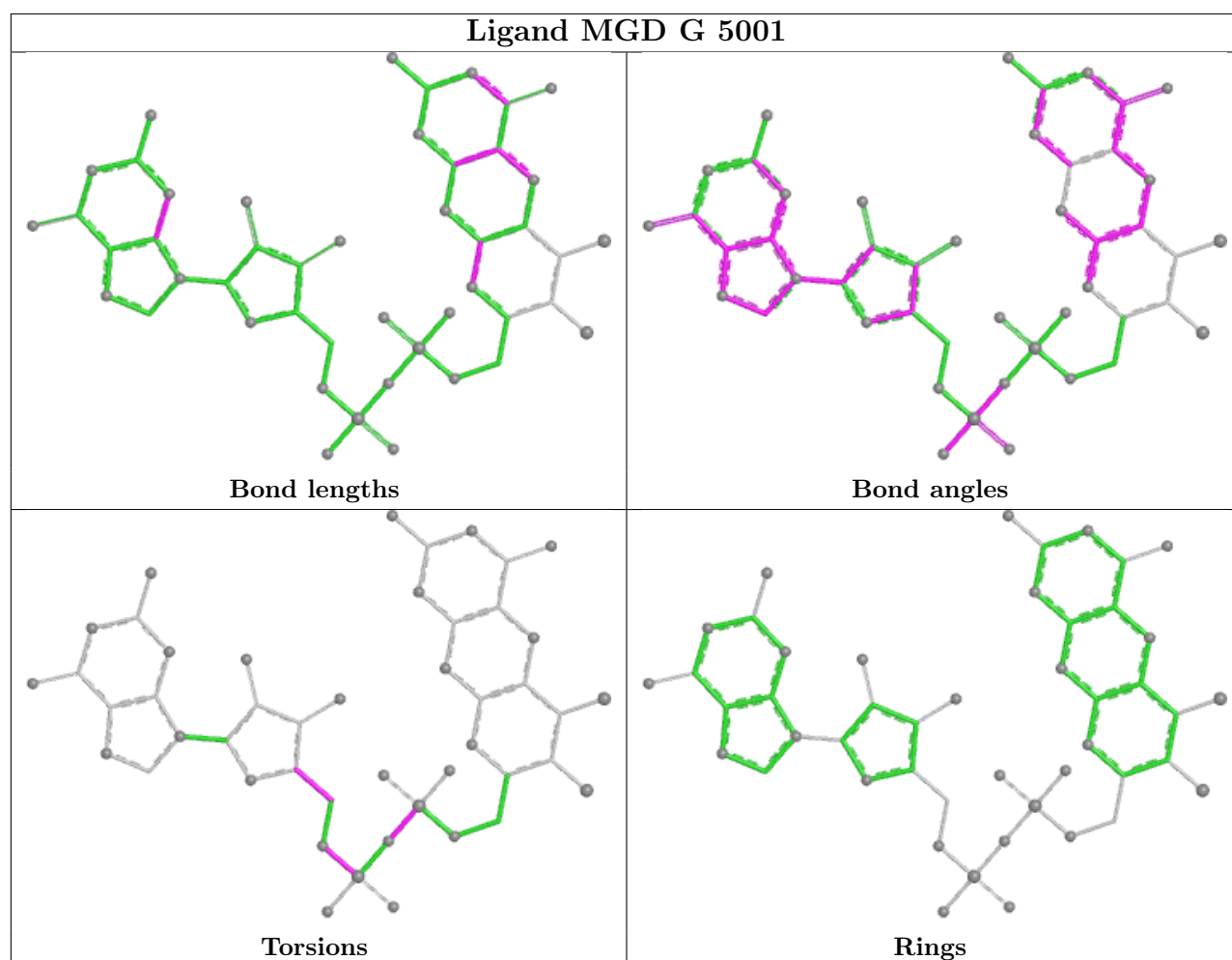
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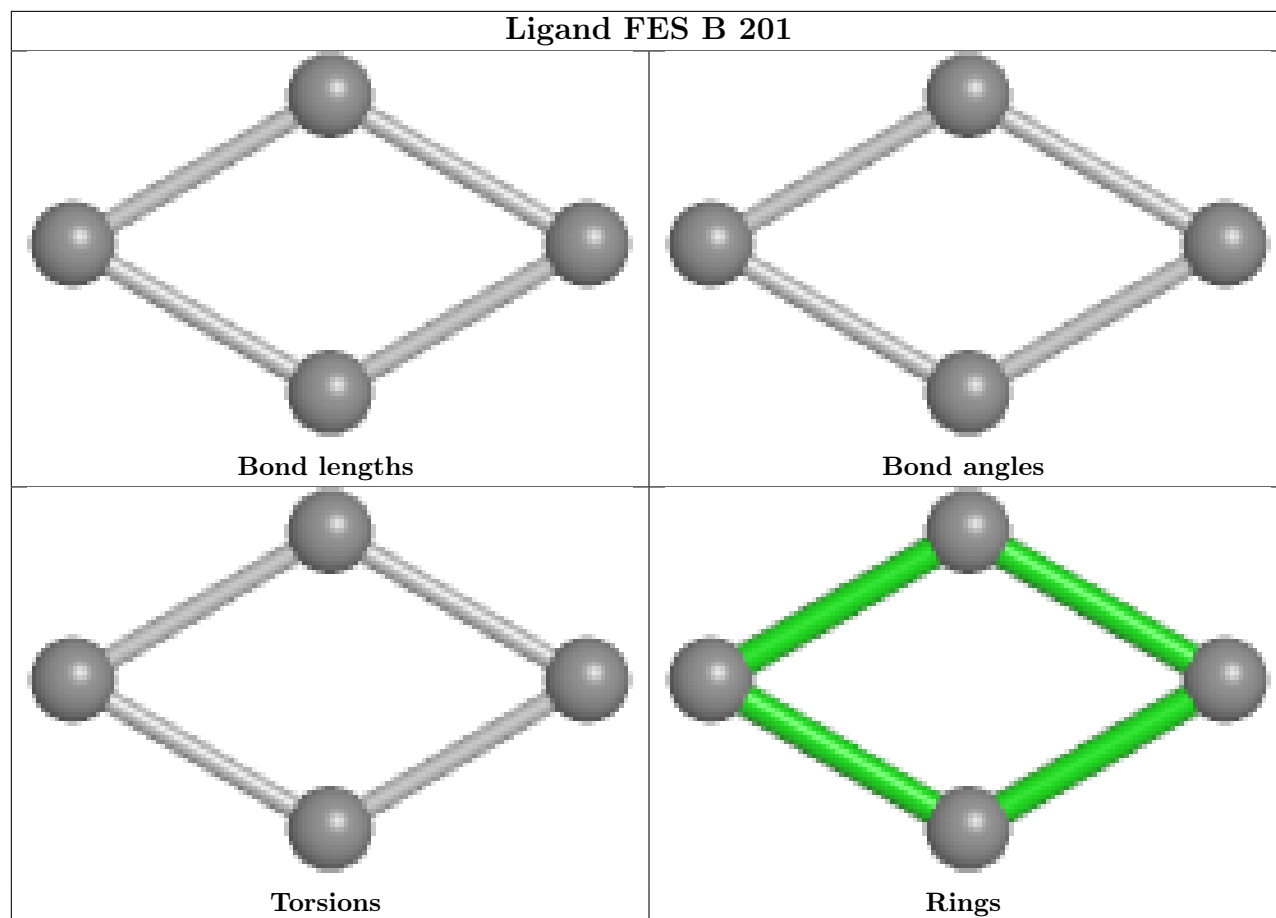


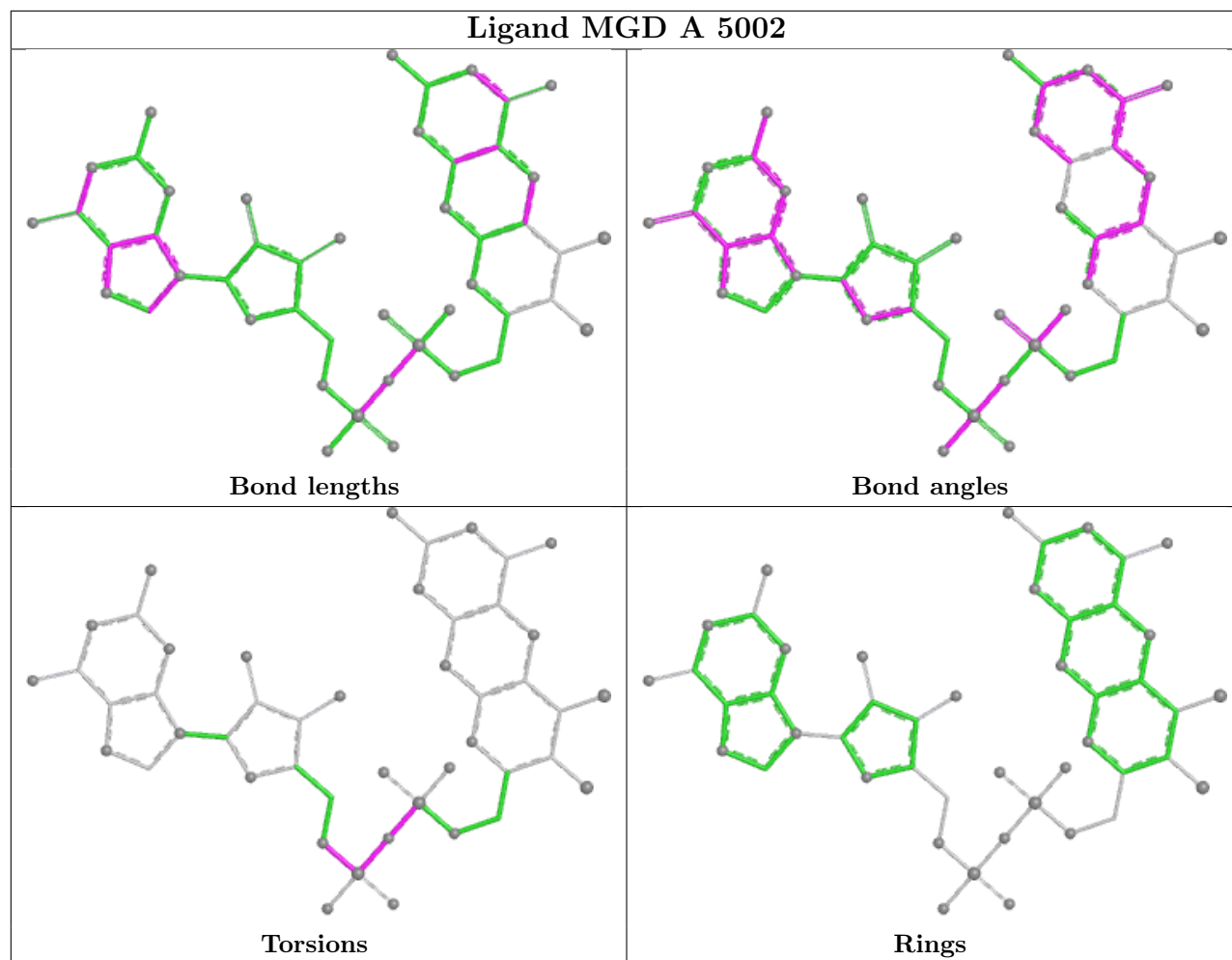


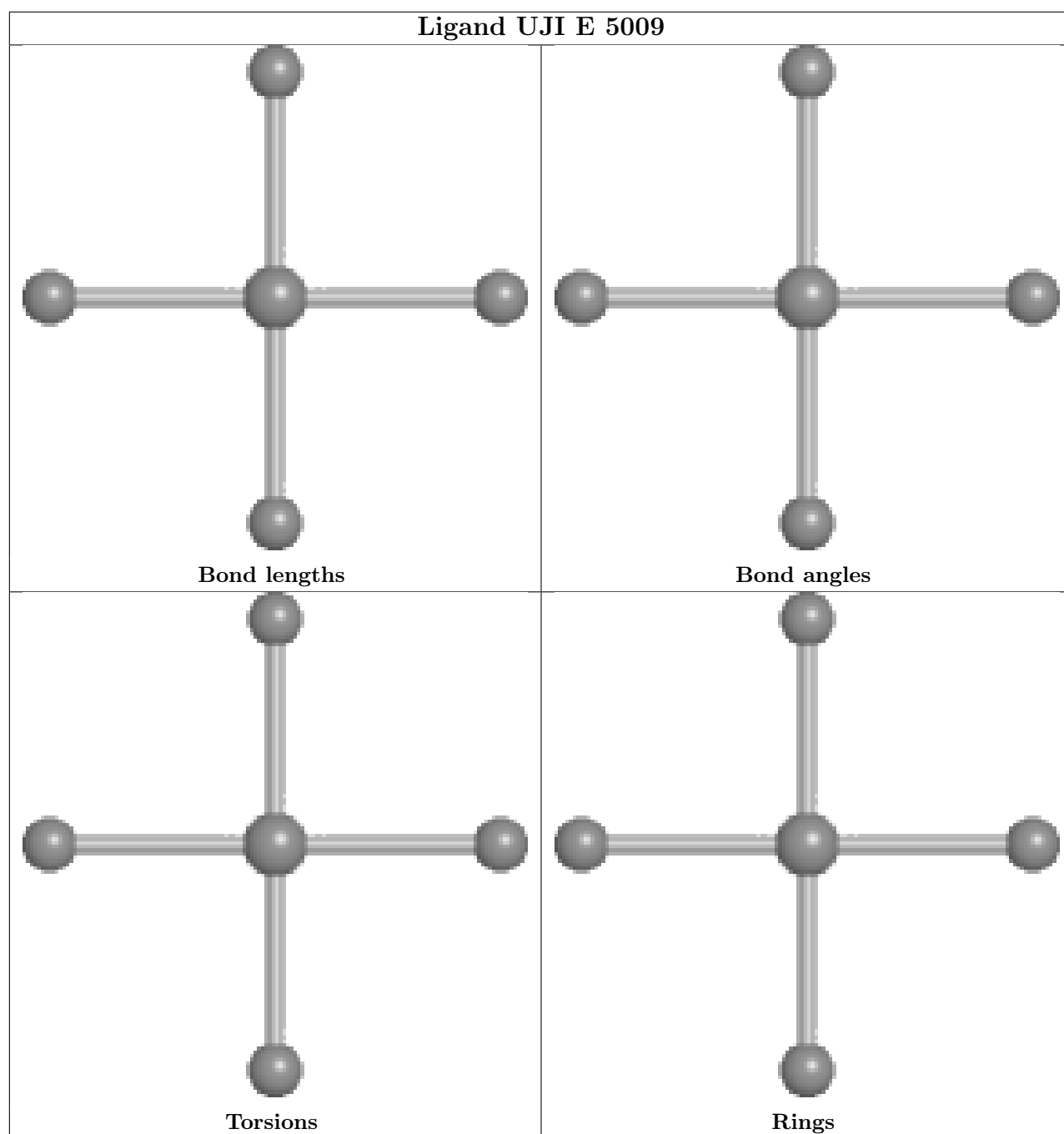












5.7 Other polymers [i](#)

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	822/822 (100%)	-0.45	1 (0%) 92 95	9, 18, 31, 53	8 (0%)
1	C	822/822 (100%)	-0.46	2 (0%) 91 94	11, 17, 29, 50	5 (0%)
1	E	822/822 (100%)	-0.39	3 (0%) 88 93	11, 18, 31, 54	7 (0%)
1	G	822/822 (100%)	-0.35	3 (0%) 88 93	12, 19, 32, 56	5 (0%)
2	B	133/133 (100%)	-0.34	0 100 100	13, 19, 30, 40	2 (1%)
2	D	133/133 (100%)	-0.34	0 100 100	13, 19, 32, 42	2 (1%)
2	F	133/133 (100%)	-0.32	0 100 100	12, 19, 31, 40	1 (0%)
2	H	133/133 (100%)	-0.29	0 100 100	14, 19, 30, 40	1 (0%)
All	All	3820/3820 (100%)	-0.40	9 (0%) 91 94	9, 18, 31, 56	31 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	128	ALA	3.5
1	G	4	ASN	3.1
1	E	128	ALA	2.6
1	C	4	ASN	2.5
1	A	435	ASP	2.5
1	G	128	ALA	2.4
1	E	4	ASN	2.1
1	E	485	GLN	2.0
1	G	582	GLY	2.0

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($\text{\AA}^2$)	Q<0.9
7	PEG	C	5106	7/7	0.75	0.20	35,37,41,46	0
8	ACT	G	5009	4/4	0.75	0.17	38,42,43,44	0
8	ACT	A	5009	4/4	0.77	0.20	28,39,40,46	0
7	PEG	A	5006	7/7	0.80	0.16	30,36,40,44	0
7	PEG	A	5011	7/7	0.81	0.18	46,48,51,53	0
7	PEG	G	5007	7/7	0.82	0.16	32,41,48,52	0
15	EDO	E	5012	4/4	0.83	0.19	40,43,46,51	0
13	TRS	G	5006	8/8	0.84	0.17	24,25,37,39	0
8	ACT	A	5007	4/4	0.86	0.16	51,56,57,58	0
7	PEG	A	5012	7/7	0.88	0.12	26,27,36,36	0
9	PO4	C	5107	5/5	0.89	0.10	53,54,57,61	0
9	PO4	G	5008	5/5	0.90	0.09	54,55,62,64	0
12	GOL	A	5016	6/6	0.90	0.14	27,31,34,40	0
7	PEG	E	5006	7/7	0.90	0.12	28,35,43,43	0
9	PO4	E	5007	5/5	0.90	0.10	56,59,68,69	0
13	TRS	C	5112	8/8	0.91	0.14	28,30,38,40	0
9	PO4	A	5008	5/5	0.91	0.10	55,58,61,62	0
13	TRS	A	5017	8/8	0.91	0.15	25,28,35,38	0
8	ACT	G	5011	4/4	0.92	0.17	37,37,40,44	0
12	GOL	C	5108	6/6	0.92	0.11	38,39,41,44	0
11	CL	E	5013	1/1	0.93	0.20	53,53,53,53	0
15	EDO	E	5010	4/4	0.93	0.11	31,33,33,35	0
12	GOL	E	5008	6/6	0.93	0.10	23,34,36,45	0
12	GOL	A	5015	6/6	0.94	0.09	38,41,42,46	0
16	SO4	E	5015	5/5	0.94	0.10	24,25,33,34	0
17	NA	G	5012	1/1	0.94	0.12	32,32,32,32	0
9	PO4	E	5011	5/5	0.95	0.08	44,44,46,48	0
11	CL	A	5013	1/1	0.95	0.13	42,42,42,42	0
11	CL	A	5014	1/1	0.95	0.12	61,61,61,61	0
10	UJI	C	5109	5/5	0.96	0.14	29,33,41,41	1
4	O	E	5003	1/1	0.97	0.08	26,26,26,26	0
11	CL	C	5111	1/1	0.97	0.14	42,42,42,42	0

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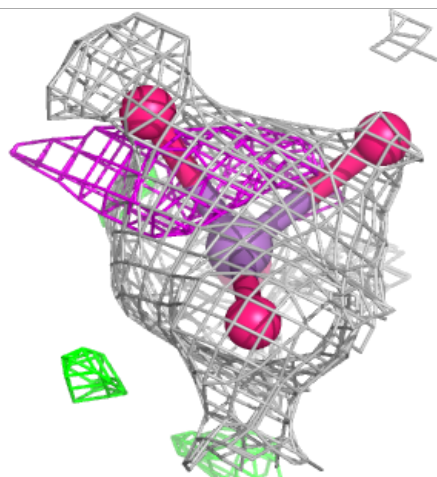
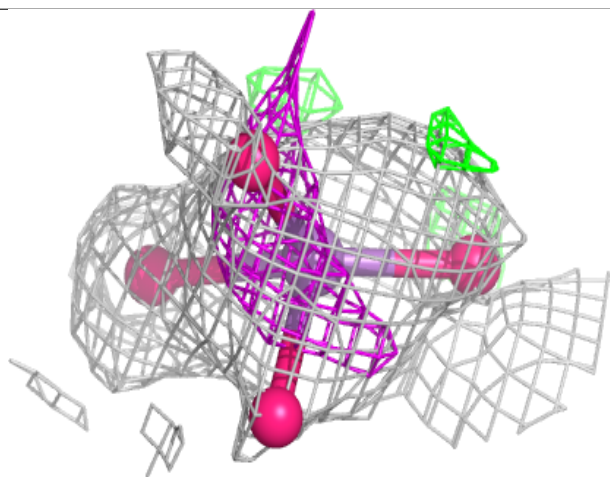
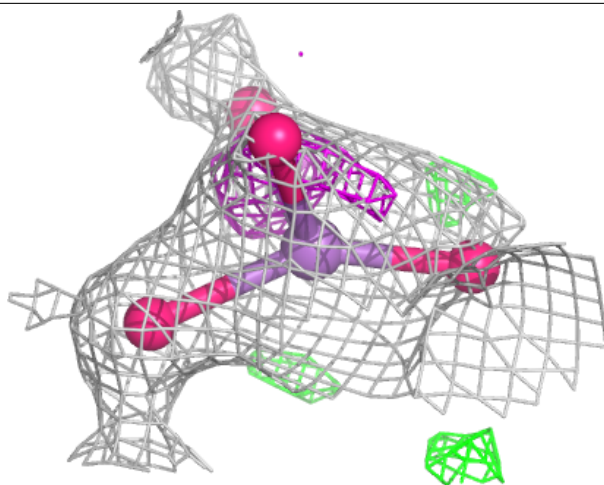
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	UJI	E	5009	5/5	0.97	0.11	25,28,33,37	1
11	CL	E	5014	1/1	0.97	0.18	40,40,40,40	0
10	UJI	A	5010	5/5	0.97	0.12	27,28,35,36	1
3	MGD	G	5002	47/47	0.98	0.04	13,15,16,17	0
4	O	A	5003	1/1	0.98	0.08	23,23,23,23	0
4	O	C	5103	1/1	0.98	0.08	28,28,28,28	0
3	MGD	A	5002	47/47	0.98	0.04	12,14,15,16	0
4	O	G	5003	1/1	0.98	0.06	25,25,25,25	0
10	UJI	G	5010	5/5	0.98	0.12	29,34,37,38	1
3	MGD	C	5101	47/47	0.98	0.05	11,14,16,17	0
3	MGD	E	5001	47/47	0.98	0.05	12,14,17,18	0
3	MGD	E	5002	47/47	0.98	0.04	12,14,16,18	0
9	PO4	C	5110	5/5	0.98	0.06	41,41,47,50	0
3	MGD	G	5001	47/47	0.98	0.04	13,15,18,19	0
6	F3S	A	5005	7/7	0.99	0.02	10,12,13,13	0
3	MGD	A	5001	47/47	0.99	0.04	12,14,16,17	0
3	MGD	C	5102	47/47	0.99	0.04	12,13,15,16	0
14	FES	D	201	4/4	0.99	0.03	17,17,18,18	0
5	4MO	G	5004	1/1	1.00	0.02	19,19,19,19	0
5	4MO	A	5004	1/1	1.00	0.02	19,19,19,19	0
14	FES	B	201	4/4	1.00	0.02	17,18,18,18	0
6	F3S	C	5105	7/7	1.00	0.02	12,13,14,15	0
14	FES	F	201	4/4	1.00	0.03	16,17,18,18	0
14	FES	H	201	4/4	1.00	0.03	18,18,19,19	0
6	F3S	E	5005	7/7	1.00	0.02	12,13,13,15	0
6	F3S	G	5005	7/7	1.00	0.02	13,14,15,17	0
5	4MO	C	5104	1/1	1.00	0.01	18,18,18,18	0
5	4MO	E	5004	1/1	1.00	0.01	19,19,19,19	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.

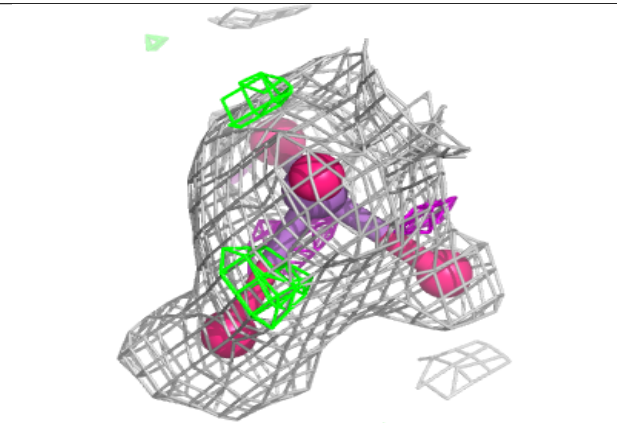
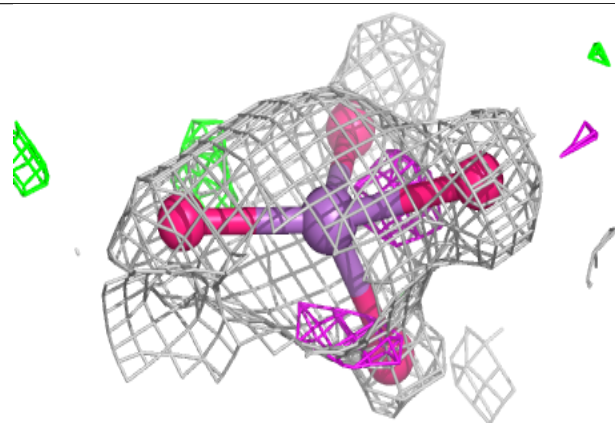
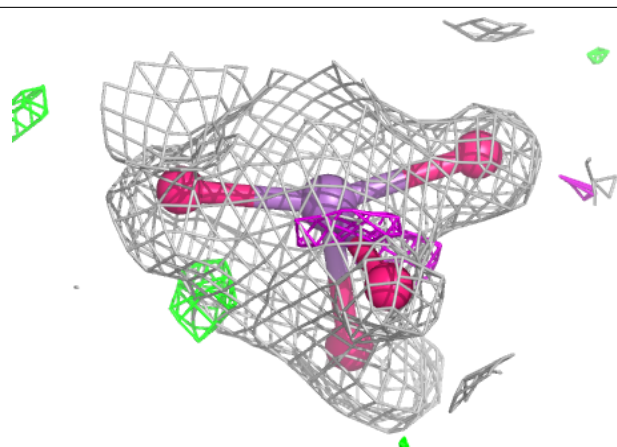
Electron density around UJI C 5109:

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



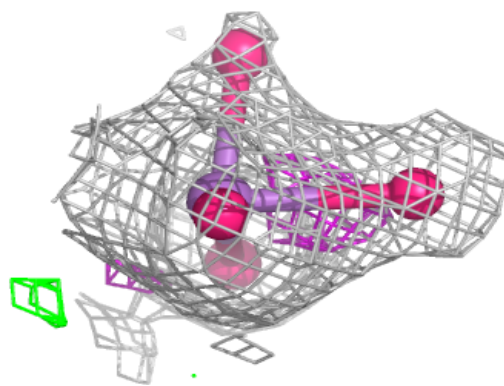
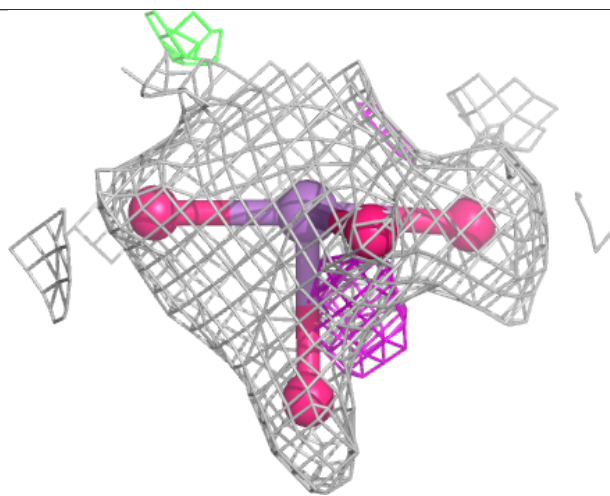
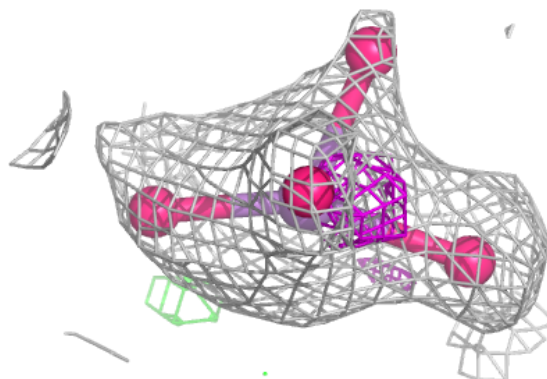
Electron density around UJI E 5009:

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



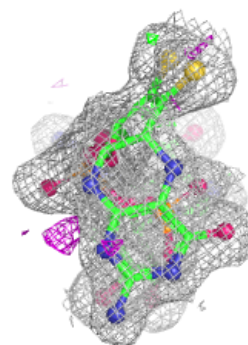
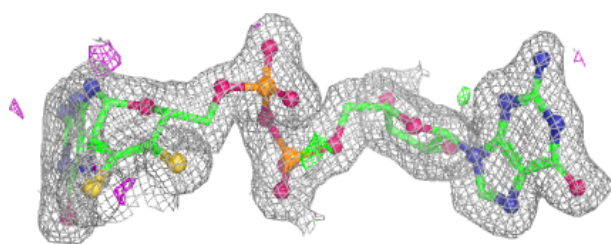
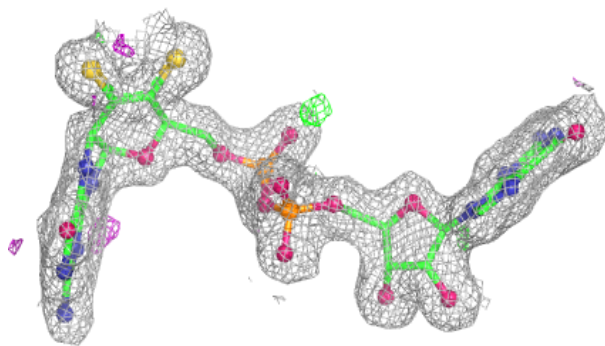
Electron density around UJI A 5010:

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

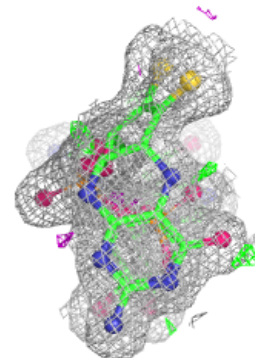
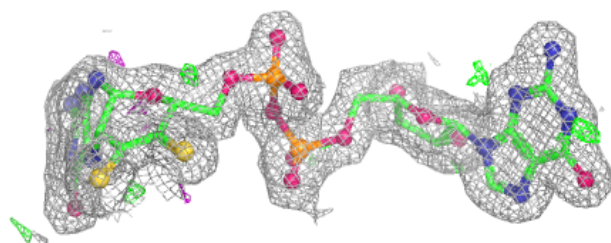
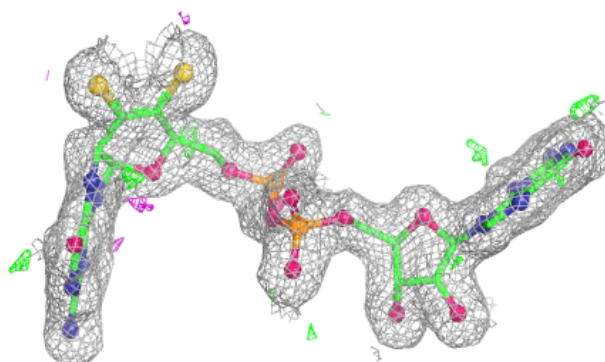


Electron density around MGD G 5002:

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

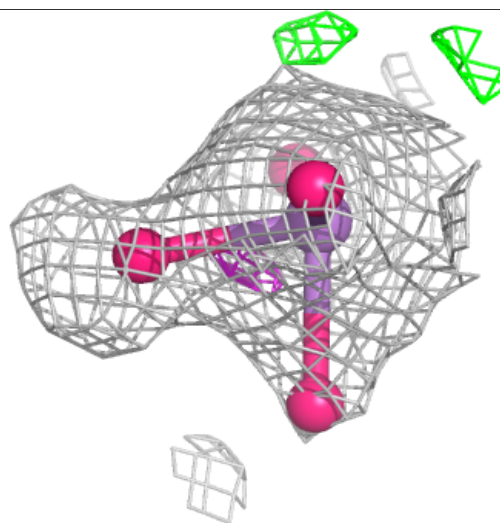
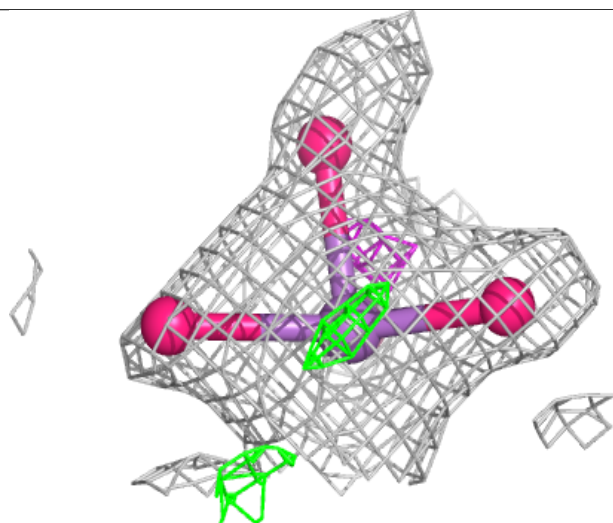
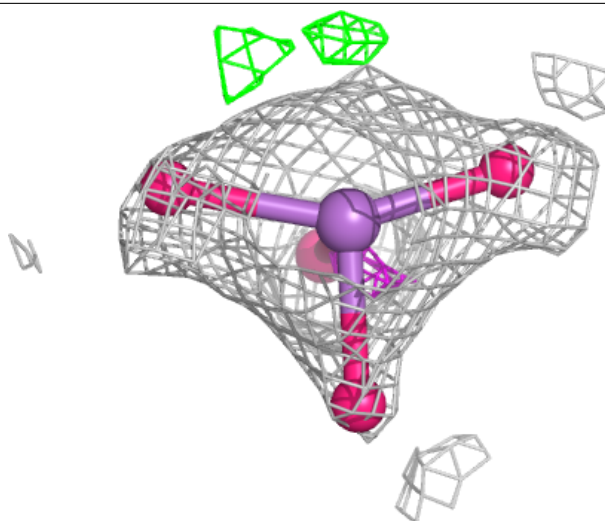
**Electron density around MGD A 5002:**

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



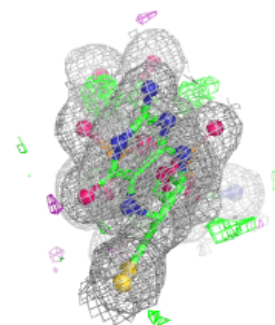
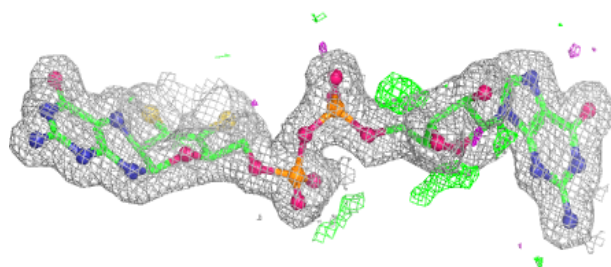
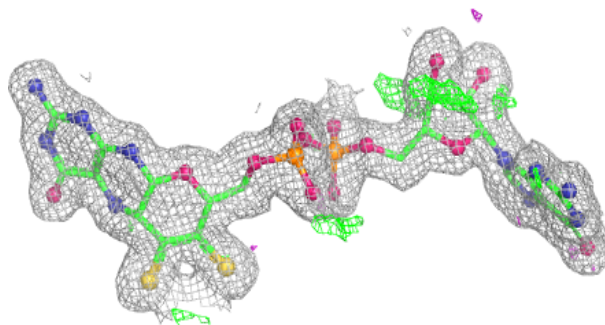
Electron density around UJI G 5010:

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

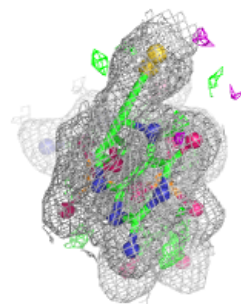
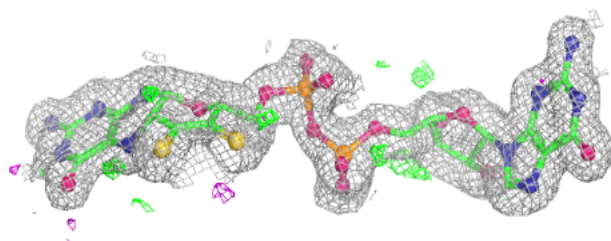
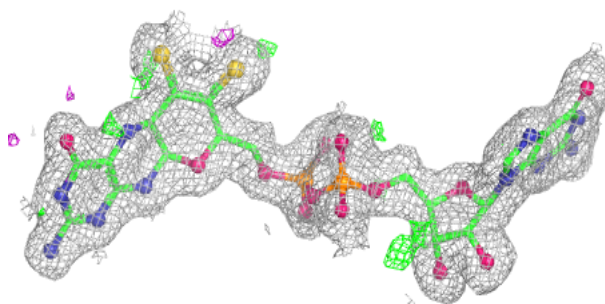


Electron density around MGD C 5101:

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

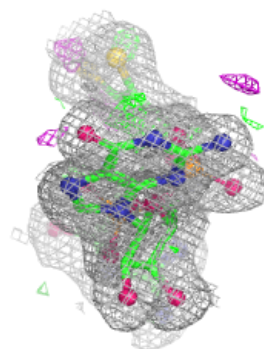
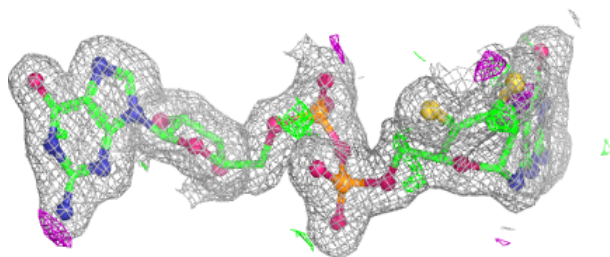
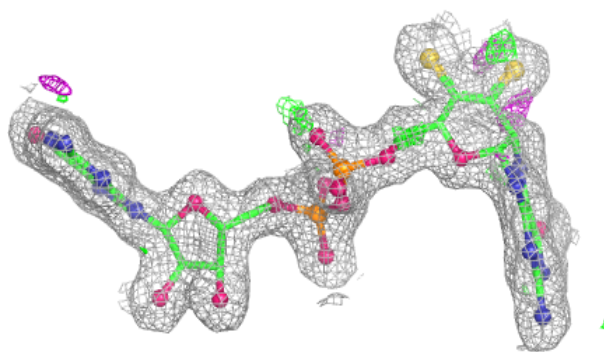
**Electron density around MGD E 5001:**

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

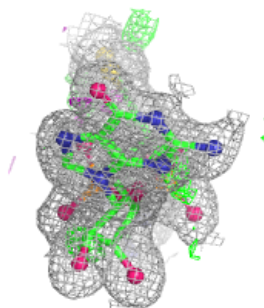
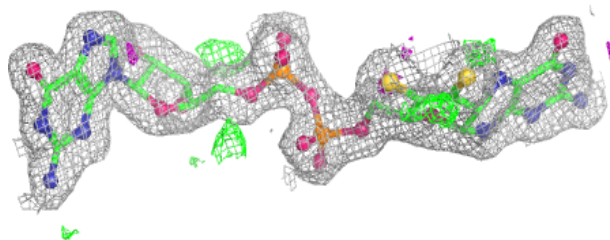
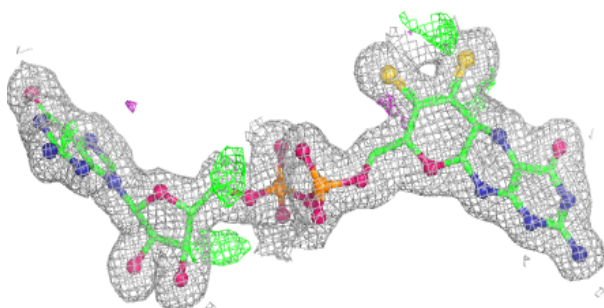


Electron density around MGD E 5002:

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

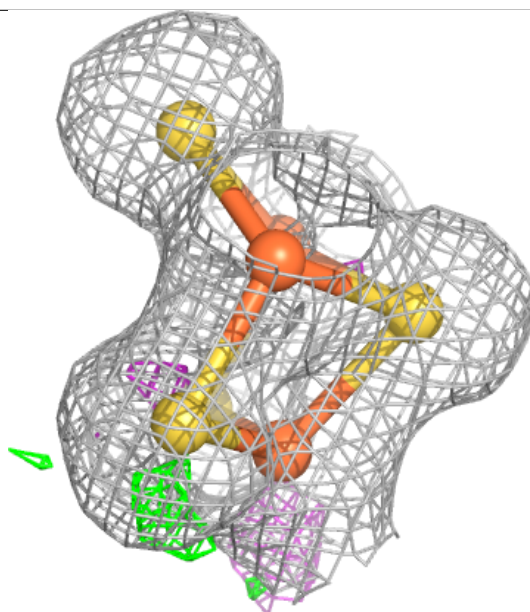
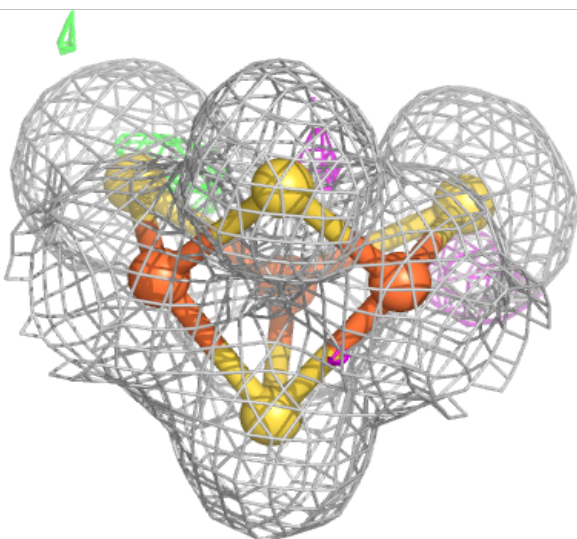
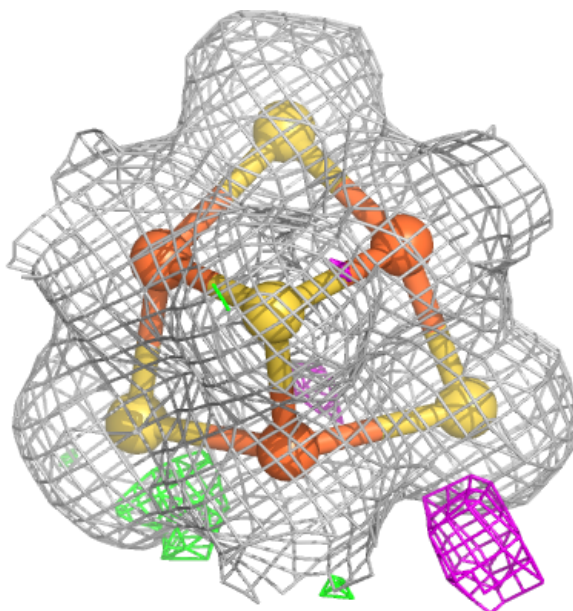
**Electron density around MGD G 5001:**

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



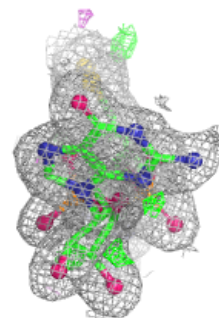
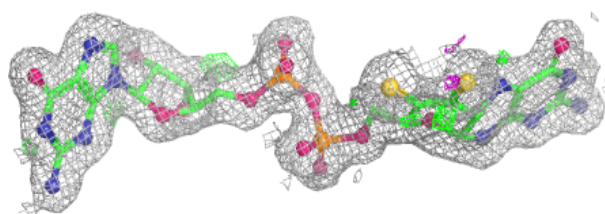
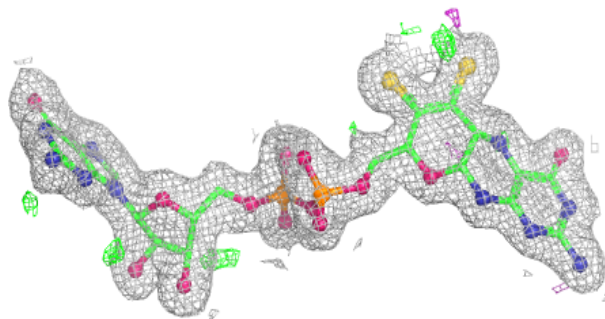
Electron density around F3S A 5005:

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

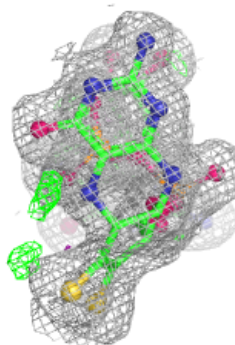
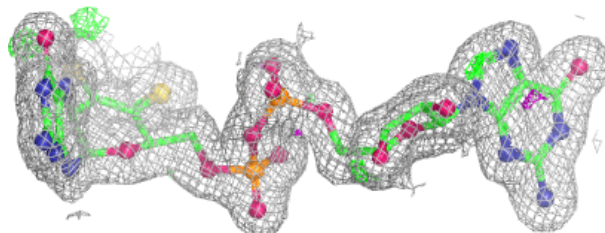
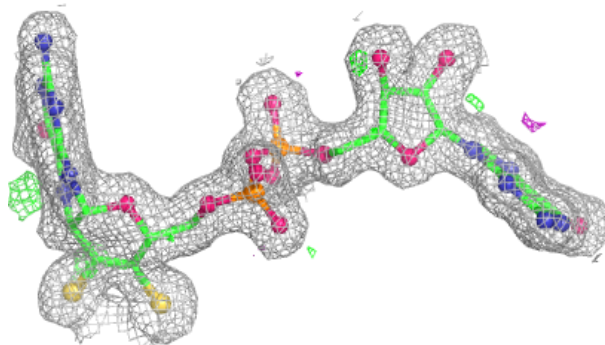


Electron density around MGD A 5001:

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

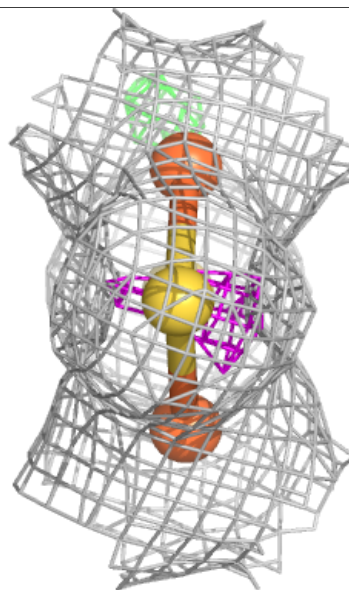
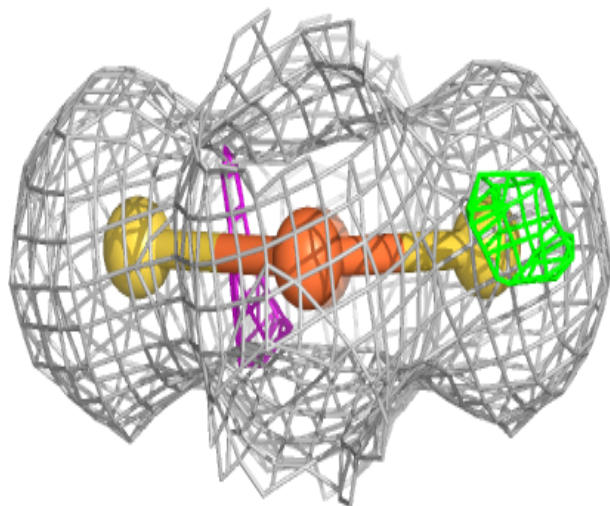
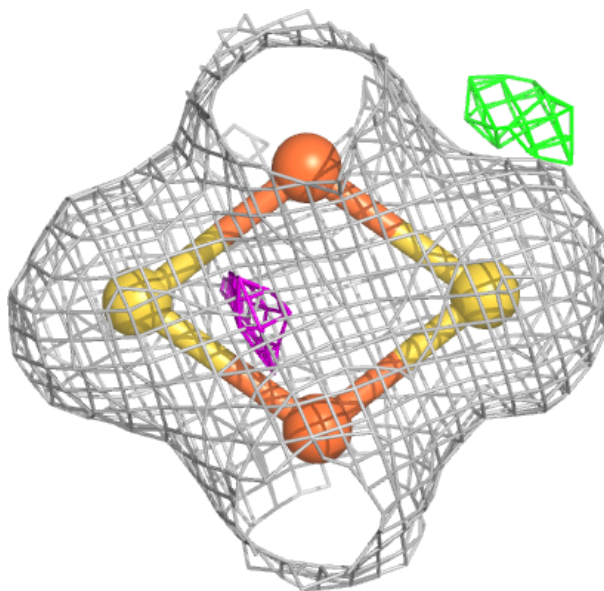
**Electron density around MGD C 5102:**

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



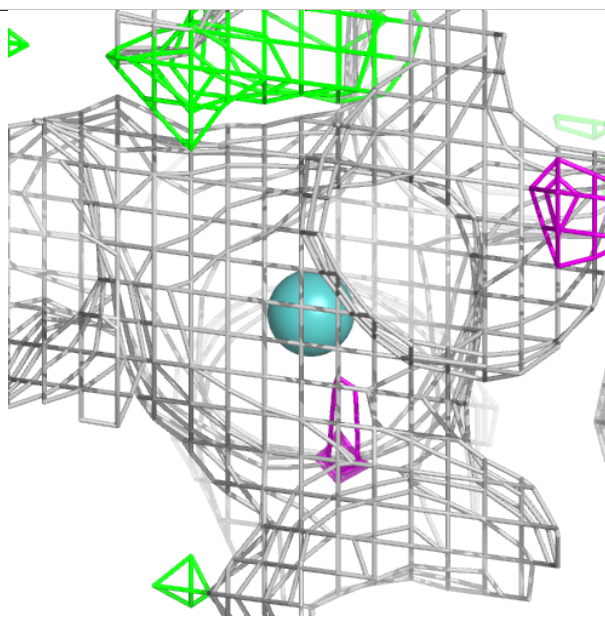
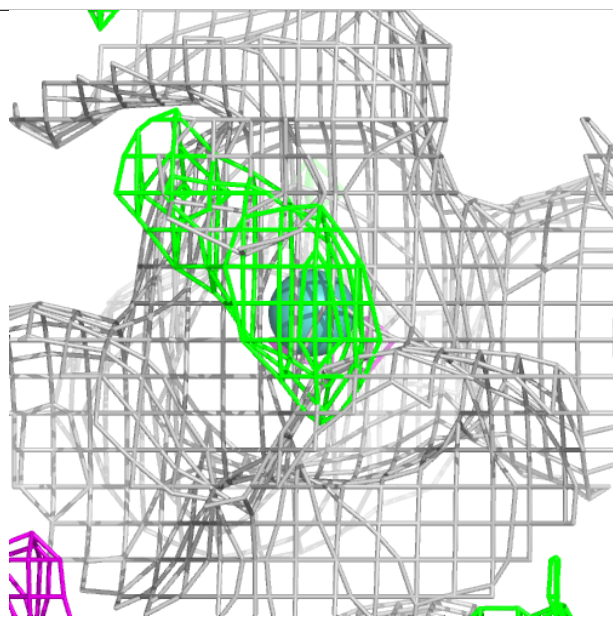
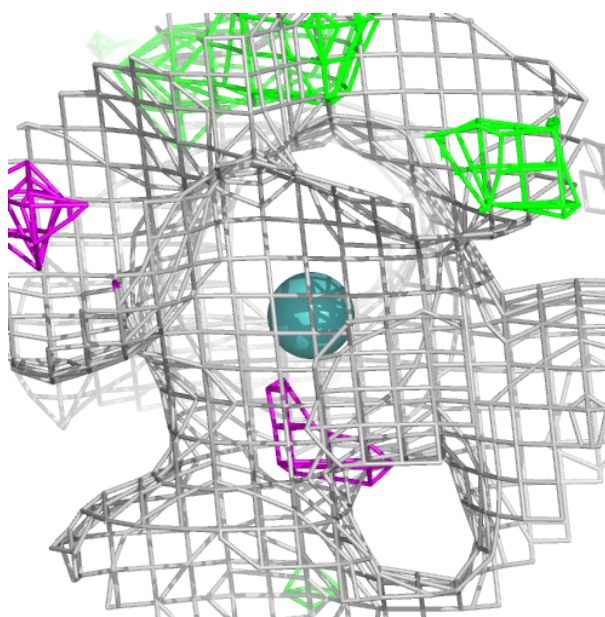
Electron density around FES D 201:

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



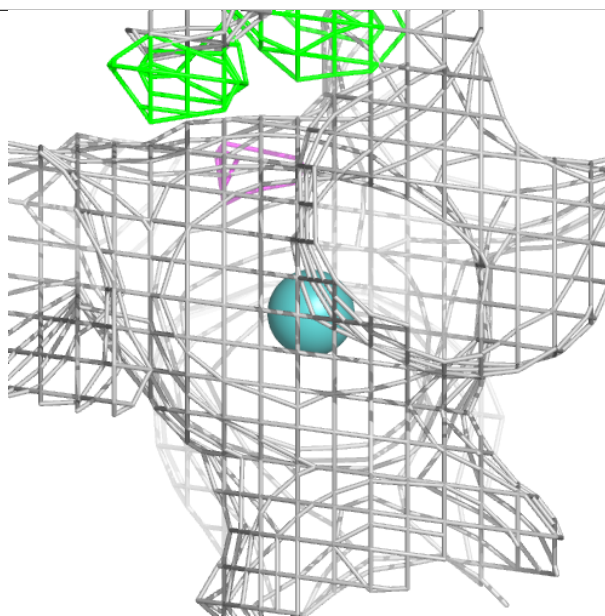
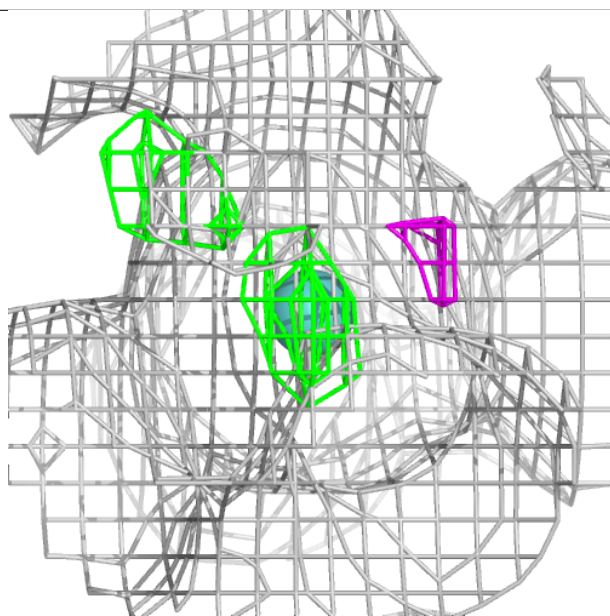
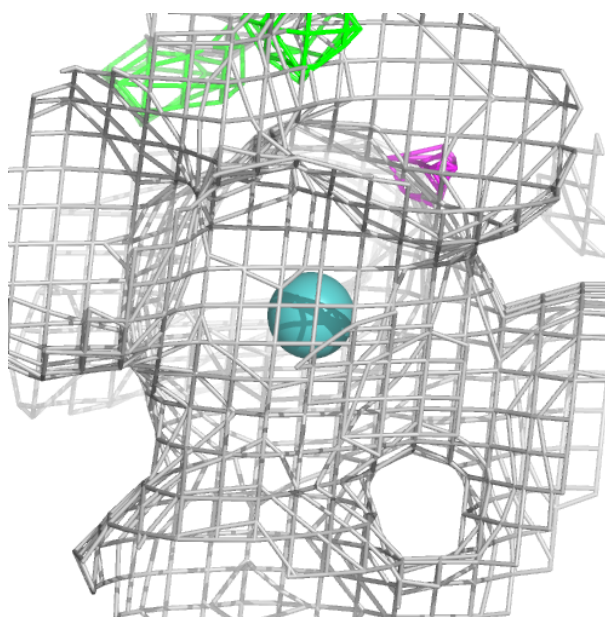
Electron density around 4MO G 5004:

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



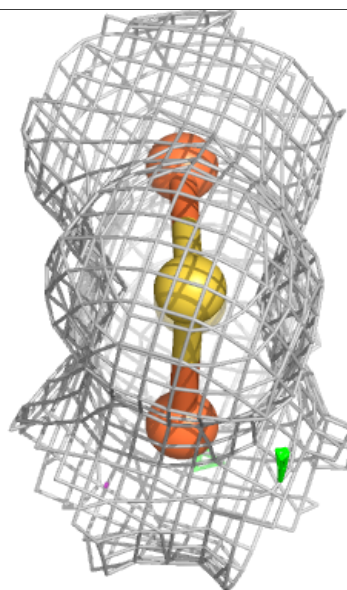
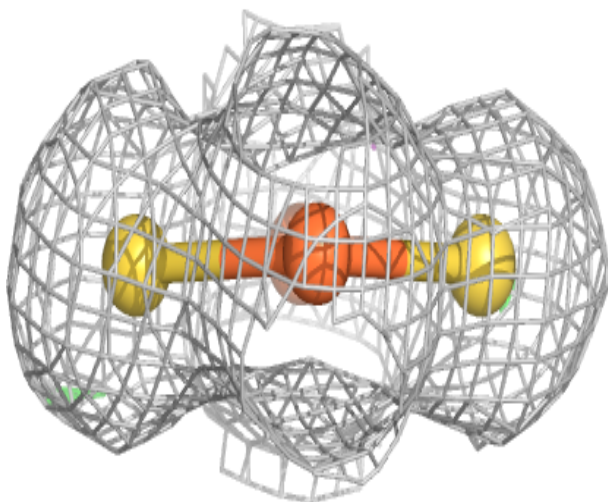
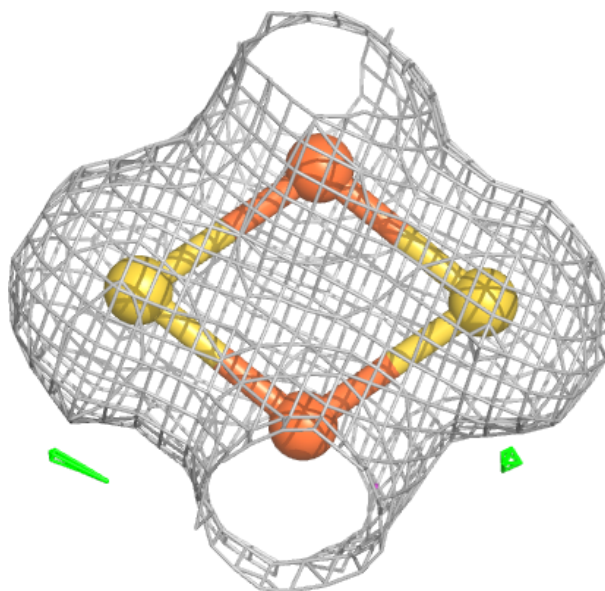
Electron density around 4MO A 5004:

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



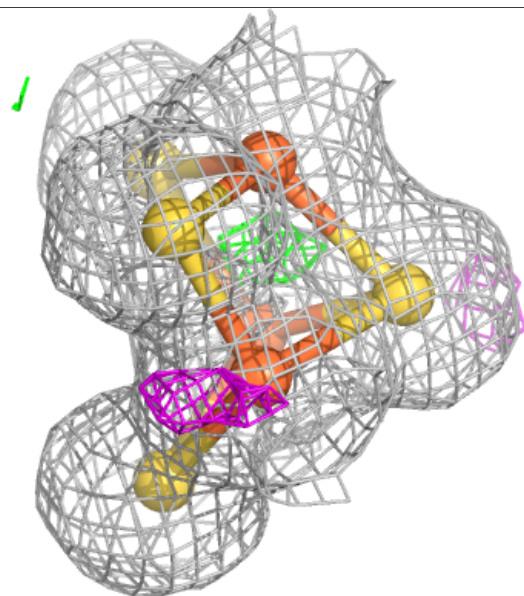
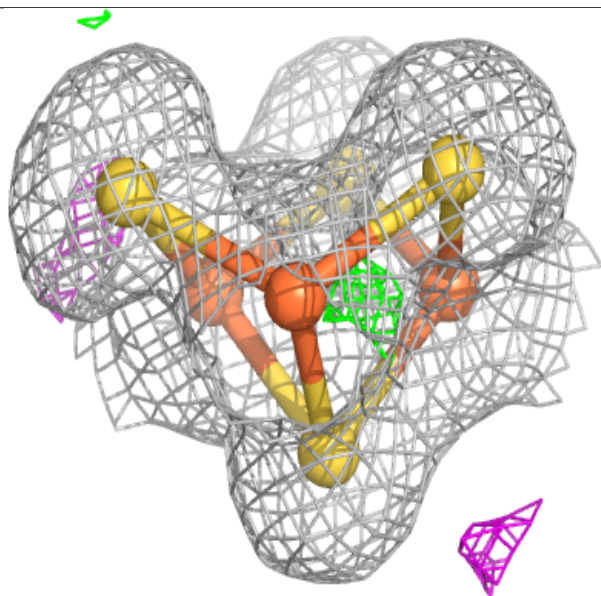
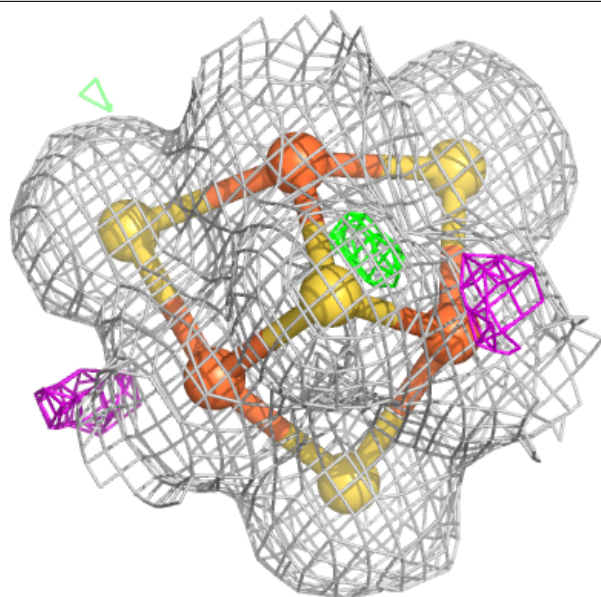
Electron density around FES B 201:

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



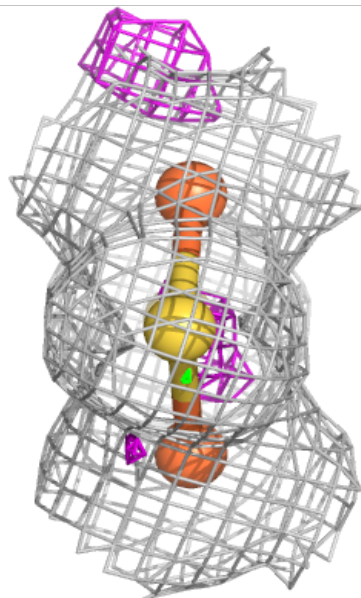
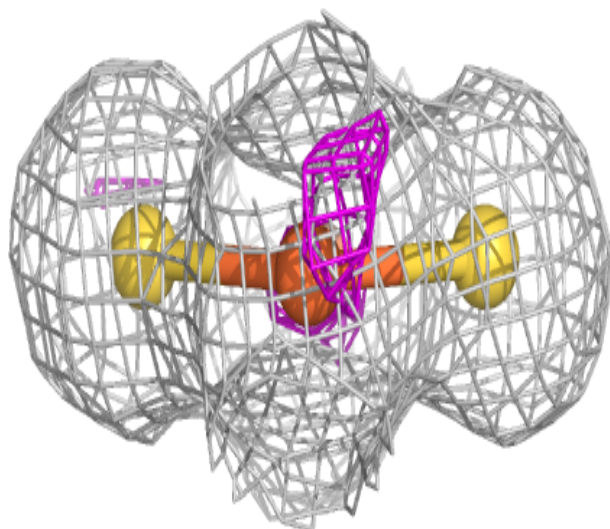
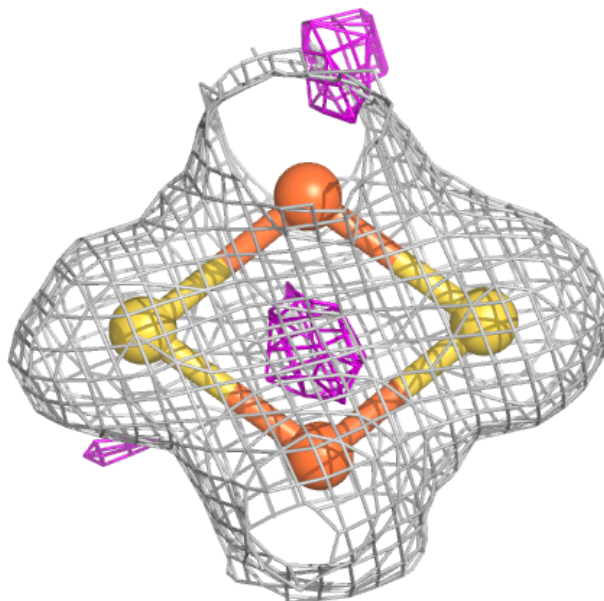
Electron density around F3S C 5105:

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



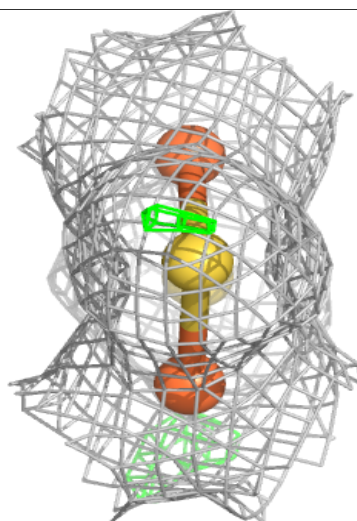
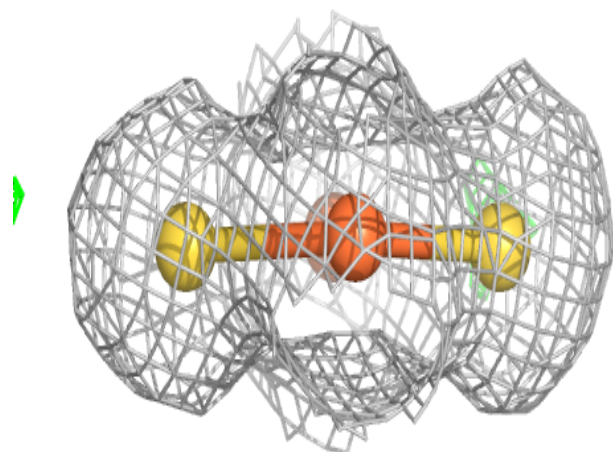
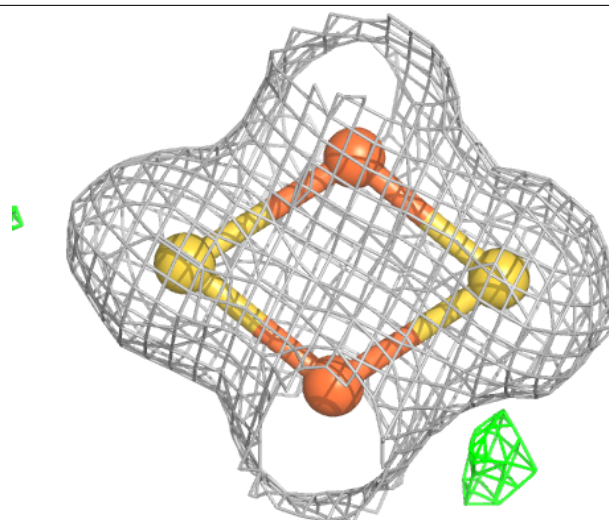
Electron density around FES F 201:

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



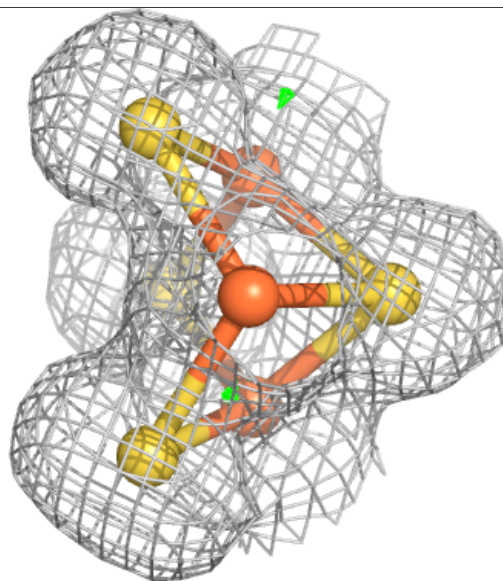
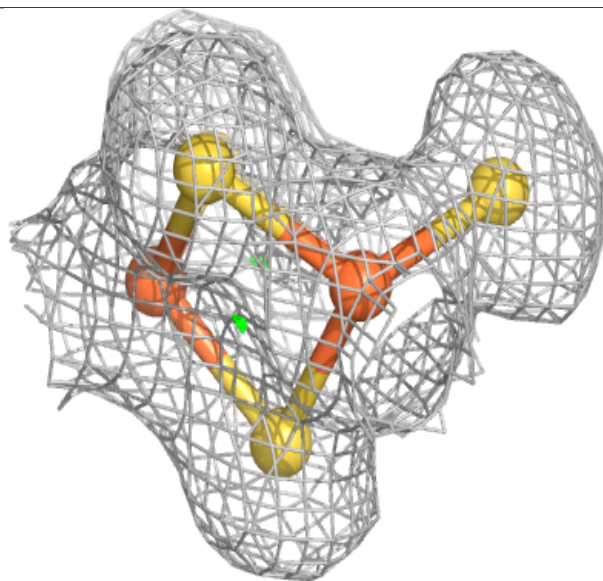
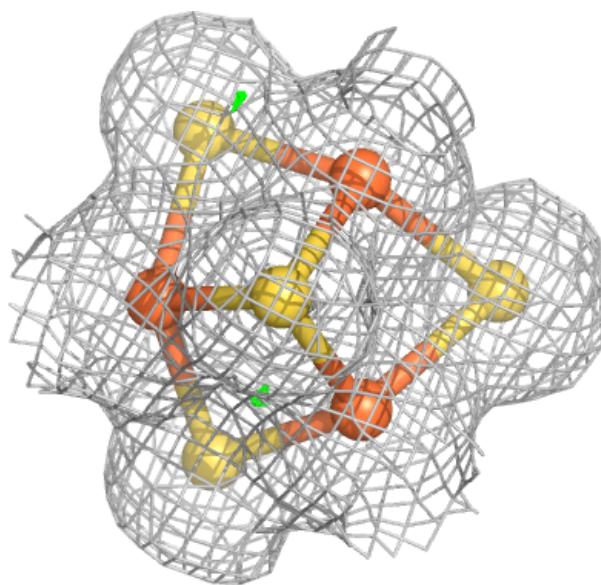
Electron density around FES H 201:

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



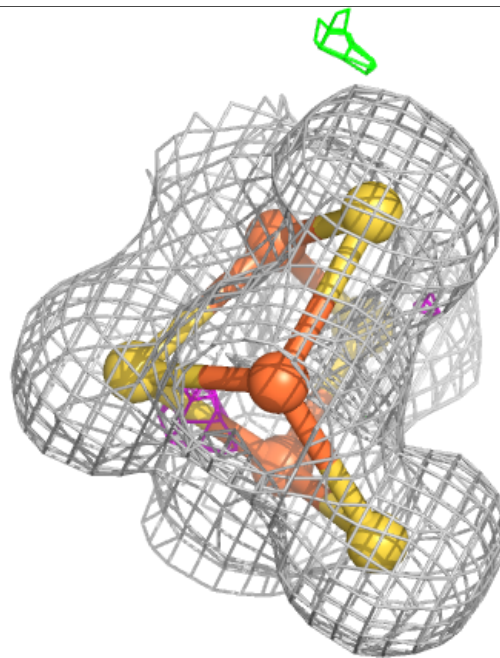
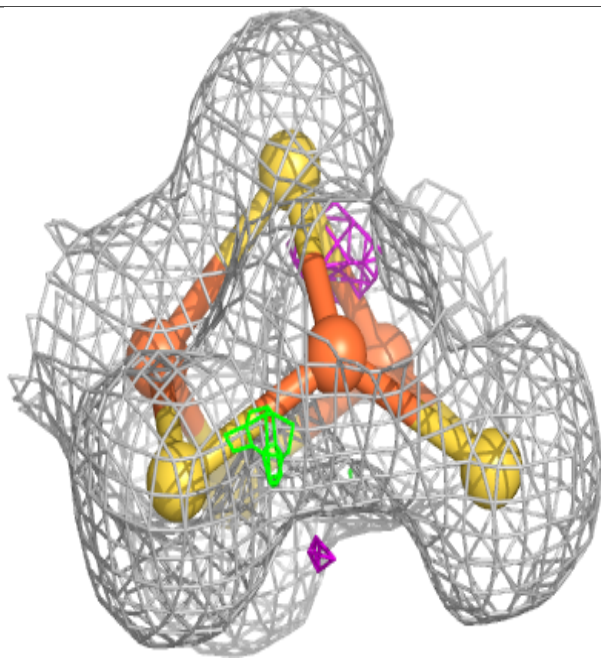
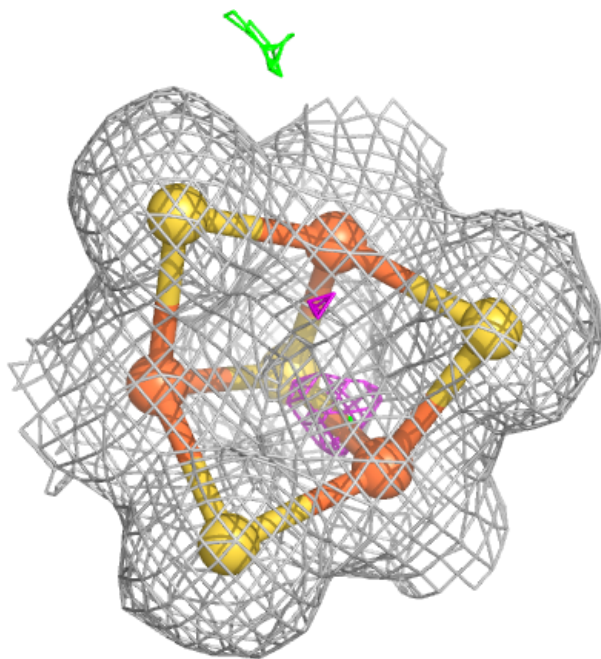
Electron density around F3S E 5005:

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



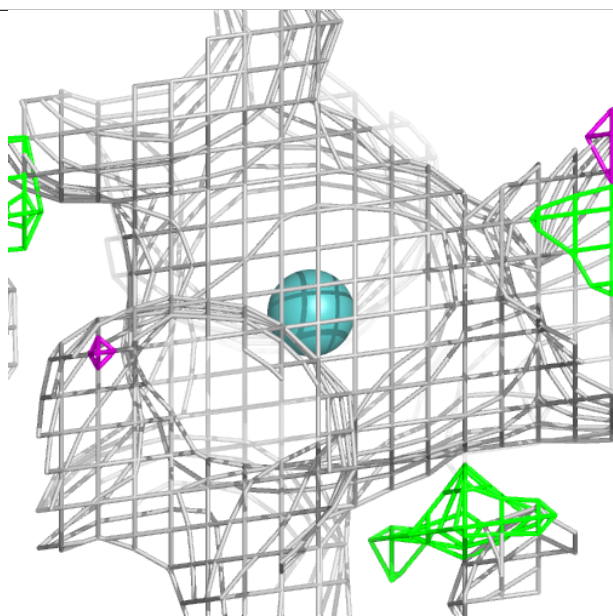
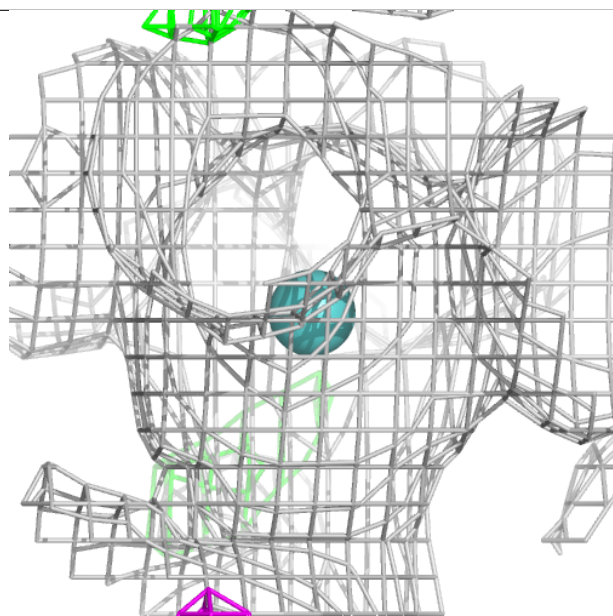
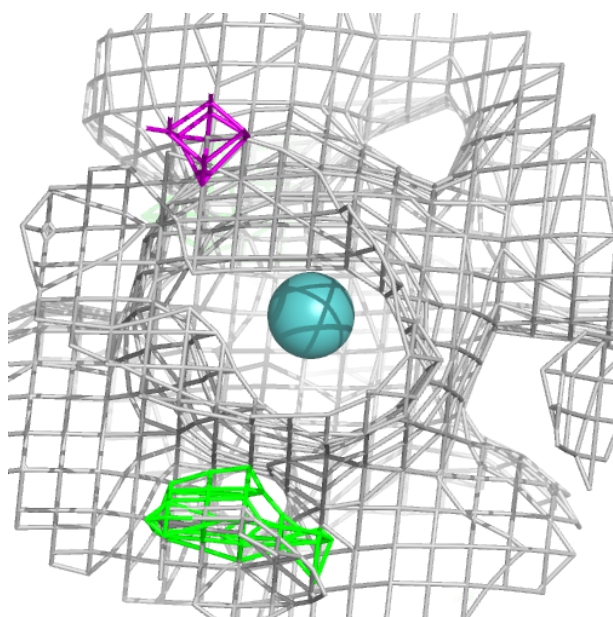
Electron density around F3S G 5005:

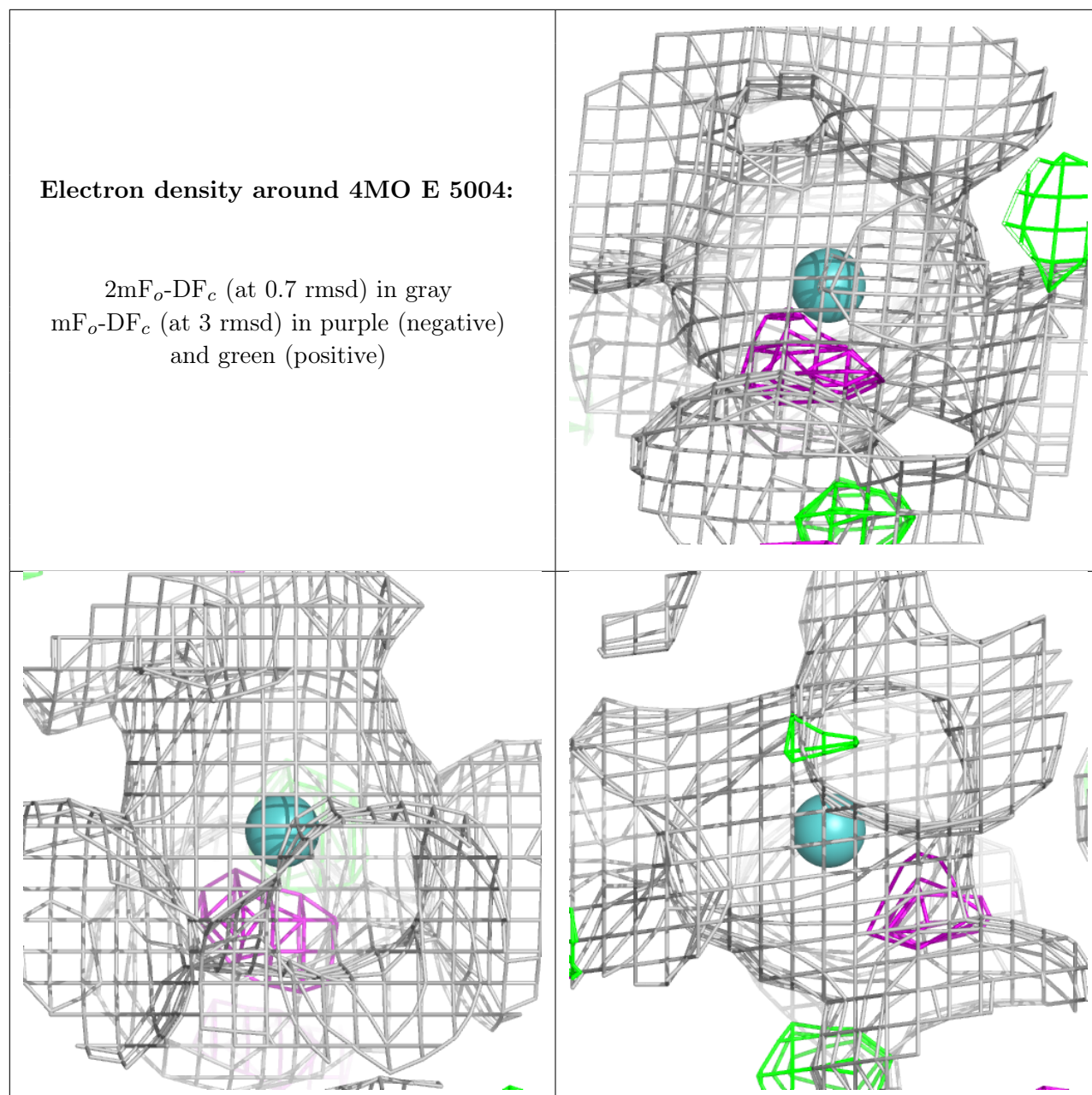
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 4MO C 5104:

$2mF_o-DF_c$ (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.