



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:31 AM UTC

PDB ID : 8CFF / pdb_00008cff
Title : Crystal structure of arsenite oxidase from *Alcaligenes faecalis* (Af Aio) bound to arsenite
Authors : Engrola, F.; Correia, M.A.S.; Romao, M.J.; Santos-Silva, T.
Deposited on : 2023-02-03
Resolution : 1.57 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

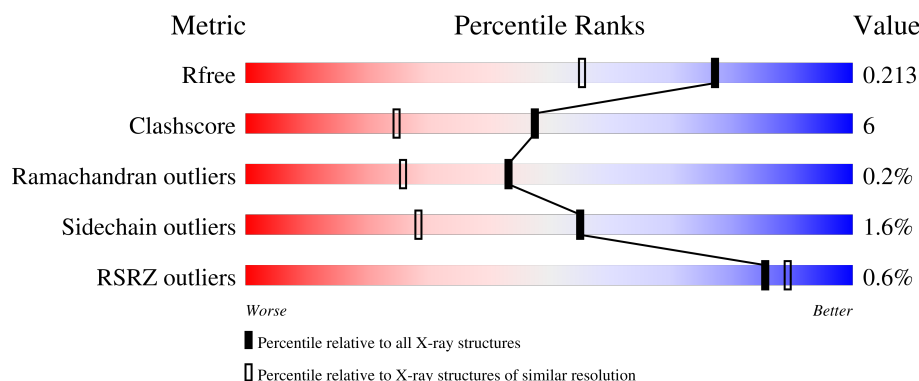
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.57 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.



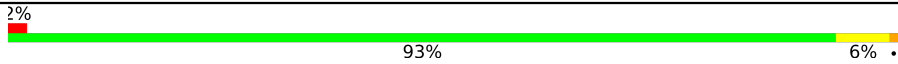
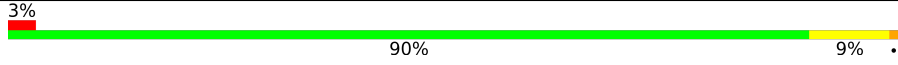
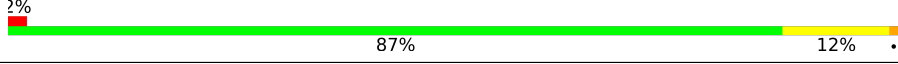
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	823	
1	C	823	
1	E	823	
1	G	823	
2	B	134	

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Mol	Chain	Length	Quality of chain
2	D	134	
2	F	134	
2	H	134	

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
10	PEG	B	2301	-	-	X	-
11	IPA	C	906	-	-	X	-
11	IPA	G	908	-	-	X	-
7	GOL	C	912	-	-	X	-
7	GOL	E	912	-	-	X	-
9	EDO	A	908[A]	-	-	X	-
9	EDO	A	908[B]	-	-	X	-
9	EDO	A	909	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 34530 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	823	Total	C	N	O	S	0	7	0
			6523	4106	1155	1220	42			
1	C	822	Total	C	N	O	S	5	10	0
			6555	4124	1161	1226	44			
1	E	822	Total	C	N	O	S	0	7	0
			6526	4108	1157	1218	43			
1	G	822	Total	C	N	O	S	1	8	0
			6517	4101	1153	1221	42			

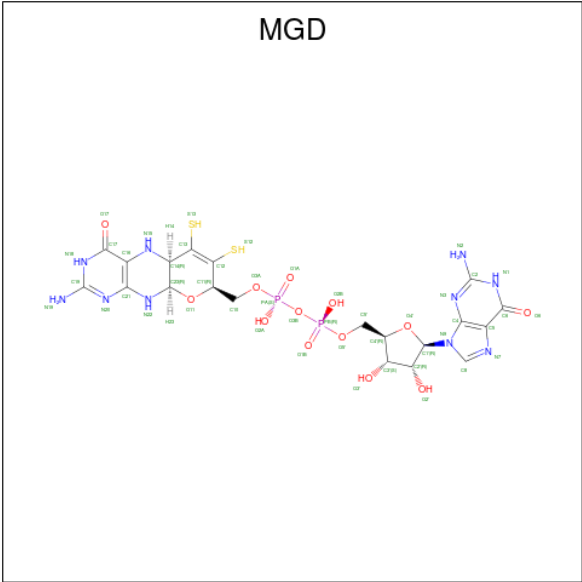
- Molecule 2 is a protein called Arsenite oxidase subunit AioB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	134	Total	C	N	O	S	0	3	0
			1018	637	170	202	9			
2	D	134	Total	C	N	O	S	2	2	0
			1015	635	170	201	9			
2	F	134	Total	C	N	O	S	1	2	0
			1009	632	169	199	9			
2	H	134	Total	C	N	O	S	2	3	0
			1018	637	170	202	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	LEU	-	expression tag	UNP Q7SIF3
D	0	LEU	-	expression tag	UNP Q7SIF3
F	0	LEU	-	expression tag	UNP Q7SIF3
H	0	LEU	-	expression tag	UNP Q7SIF3

- 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 MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

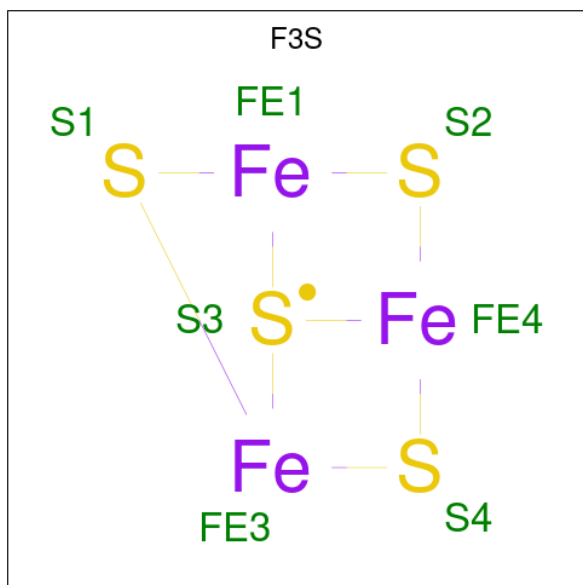
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mo	0	0
			1	1		
4	C	1	Total	Mo	0	0
			1	1		
4	E	1	Total	Mo	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mo	0	0
			1	1		

- Molecule 5 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4) (labeled as "Ligand of Interest" by depositor).



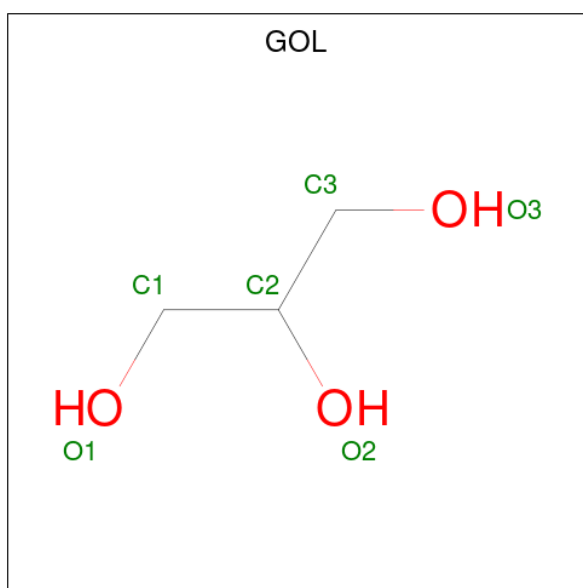
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			7	3	4		
5	C	1	Total	Fe	S	0	0
			7	3	4		
5	E	1	Total	Fe	S	0	0
			7	3	4		
5	G	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $\text{C}_6\text{H}_{14}\text{O}_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			20	12	8		
6	G	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



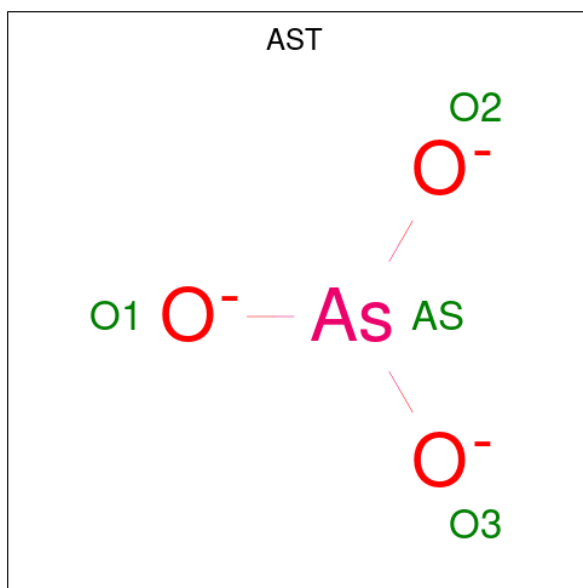
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		

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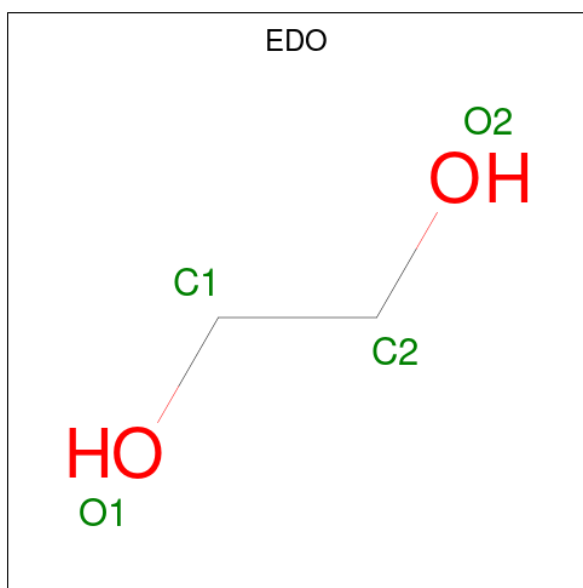
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is ARSENITE (CCD ID: AST) (formula: AsO₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



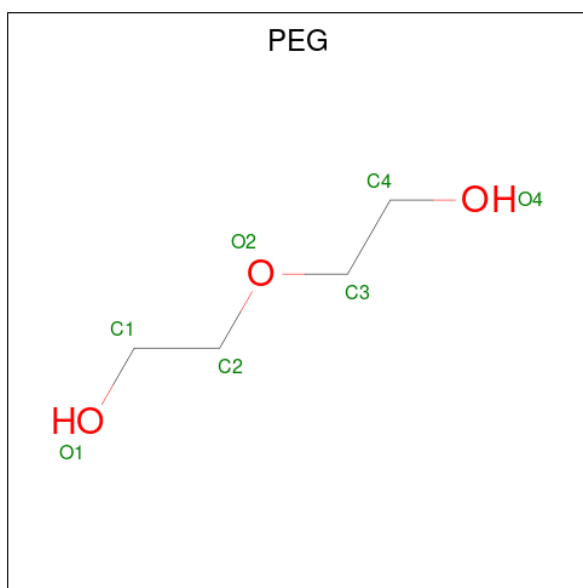
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	1
			8	4	4		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total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

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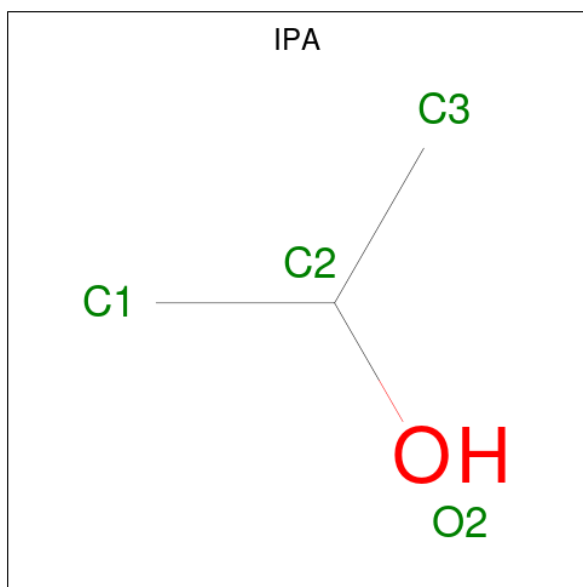
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			4	2	2		
9	E	1	Total	C	O	0	0
			4	2	2		
9	E	1	Total	C	O	0	0
			4	2	2		
9	E	1	Total	C	O	0	0
			4	2	2		
9	E	1	Total	C	O	0	0
			4	2	2		
9	E	1	Total	C	O	0	0
			4	2	2		
9	G	1	Total	C	O	0	1
			8	4	4		
9	G	1	Total	C	O	0	0
			4	2	2		
9	G	1	Total	C	O	0	0
			4	2	2		
9	G	1	Total	C	O	0	0
			4	2	2		
9	G	1	Total	C	O	0	0
			4	2	2		
9	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



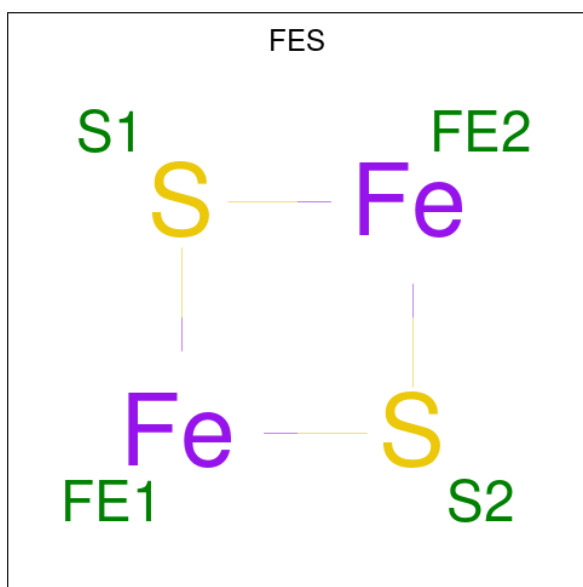
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		
10	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 11 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



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

- Molecule 12 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
12	B	1	Total	Fe	S	0	0
			4	2	2		
12	D	1	Total	Fe	S	0	0
			4	2	2		
12	F	1	Total	Fe	S	0	0
			4	2	2		
12	H	1	Total	Fe	S	0	0
			4	2	2		

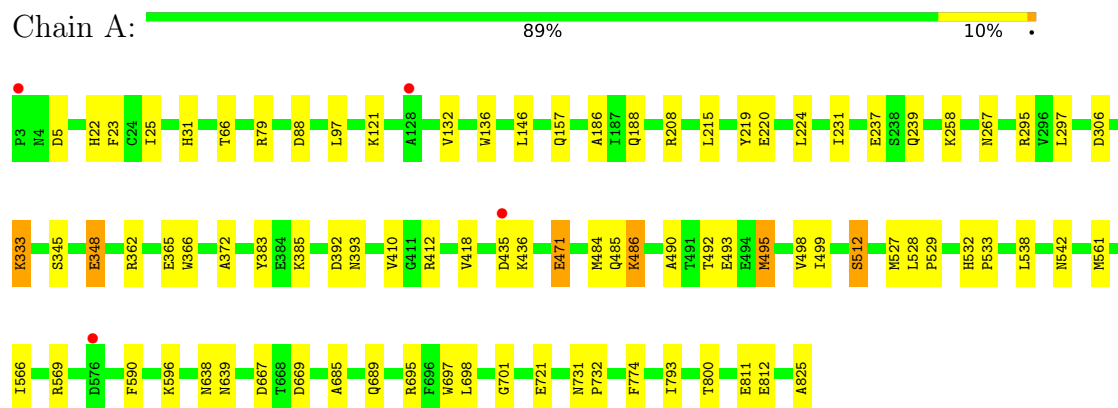
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	806	Total	O	0	0
			806	806		
13	B	137	Total	O	0	0
			137	137		
13	C	760	Total	O	0	0
			760	760		
13	D	148	Total	O	0	0
			148	148		
13	E	751	Total	O	0	0
			751	751		
13	F	129	Total	O	0	0
			129	129		
13	G	799	Total	O	0	0
			799	799		
13	H	153	Total	O	0	0
			153	153		

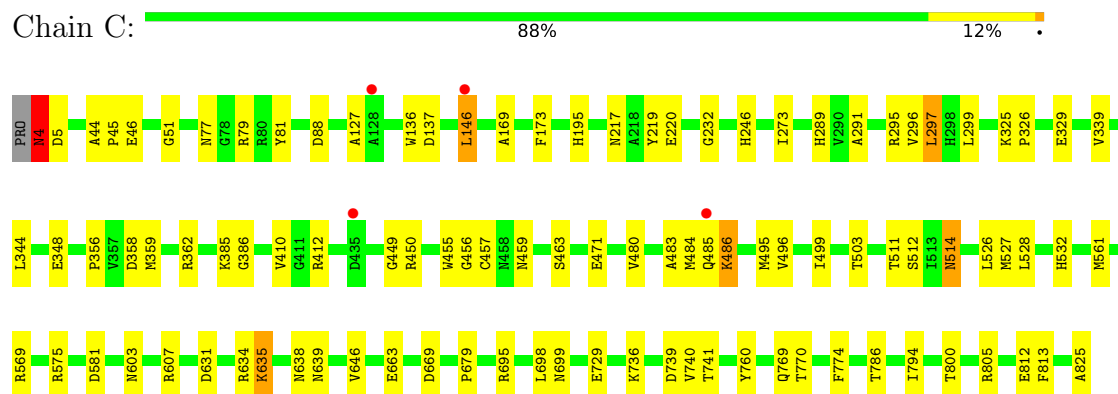
3 Residue-property plots

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.

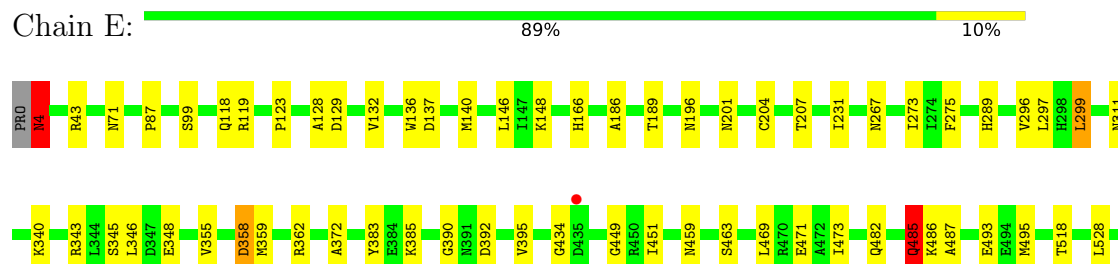
• Molecule 1: Arsenite oxidase subunit AioA

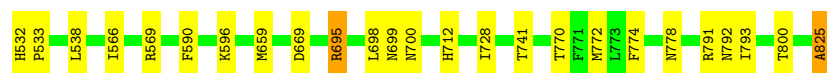


• Molecule 1: Arsenite oxidase subunit AioA



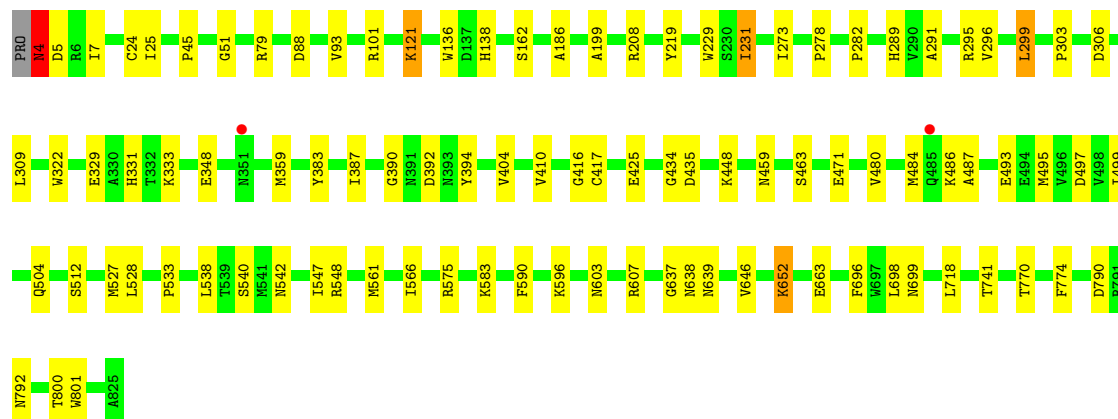
• Molecule 1: Arsenite oxidase subunit AioA





• Molecule 1: Arsenite oxidase subunit AioA

Chain G: 88% 11%



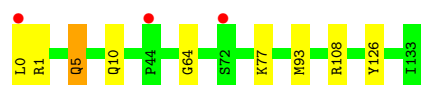
• Molecule 2: Arsenite oxidase subunit AioB

Chain B: 2% 90% 10%



• Molecule 2: Arsenite oxidase subunit AioB

Chain D: 2% 93% 6%



• Molecule 2: Arsenite oxidase subunit AioB

Chain F: 3% 90% 9%



• Molecule 2: Arsenite oxidase subunit AioB

Chain H: 2% 87% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.31Å 108.98Å 116.89Å 97.50° 90.21° 96.06°	Depositor
Resolution (Å)	65.62 – 1.57 65.62 – 1.57	Depositor EDS
% Data completeness (in resolution range)	73.2 (65.62-1.57) 73.7 (65.62-1.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.57Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.168 , 0.204 0.178 , 0.213	Depositor DCC
R_{free} test set	22459 reflections (3.63%)	wwPDB-VP
Wilson B-factor (Å ²)	12.4	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34530	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.54% 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: MGD, F3S, EDO, IPA, AST, GOL, MO, PEG, FES, PGE

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	1.19	10/6691 (0.1%)	1.30	12/9069 (0.1%)
1	C	1.17	14/6722 (0.2%)	1.32	12/9107 (0.1%)
1	E	1.19	16/6696 (0.2%)	1.31	13/9073 (0.1%)
1	G	1.21	15/6690 (0.2%)	1.31	9/9066 (0.1%)
2	B	1.17	2/1042 (0.2%)	1.26	0/1419
2	D	2.18	2/1036 (0.2%)	1.38	3/1412 (0.2%)
2	F	1.18	1/1033 (0.1%)	1.25	2/1407 (0.1%)
2	H	1.21	2/1042 (0.2%)	1.27	1/1419 (0.1%)
All	All	1.24	62/30952 (0.2%)	1.30	52/41972 (0.1%)

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	A	0	1

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5	GLN	CD-NE2	59.11	2.57	1.33
1	G	121	LYS	CE-NZ	-17.48	0.96	1.49
2	D	5	GLN	CD-OE1	-9.73	1.05	1.23
1	A	418	VAL	C-O	7.22	1.31	1.24
1	E	395	VAL	C-O	7.14	1.32	1.24
1	G	331	HIS	CE1-NE2	7.04	1.39	1.32
1	G	231	ILE	C-O	7.03	1.31	1.24
1	E	311	ASN	C-O	-6.91	1.15	1.24
2	H	54	VAL	C-O	6.67	1.30	1.23
1	E	123	PRO	C-O	6.63	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	712	HIS	CE1-NE2	6.55	1.39	1.32
1	E	778	ASN	C-O	6.51	1.31	1.23
1	C	455	TRP	C-O	6.47	1.31	1.24
1	G	416	GLY	C-O	-6.38	1.18	1.23
1	A	239	GLN	C-O	6.33	1.30	1.23
1	G	575	ARG	C-O	6.24	1.31	1.24
1	A	237	GLU	C-O	-6.19	1.16	1.24
1	G	93	VAL	C-O	6.18	1.31	1.24
1	A	512	SER	C-O	6.12	1.31	1.24
1	G	162	SER	CA-CB	-5.87	1.44	1.53
1	E	87	PRO	C-O	-5.86	1.17	1.23
1	G	199	ALA	C-O	5.85	1.30	1.23
2	F	127	GLY	C-O	5.84	1.32	1.24
1	E	289	HIS	CE1-NE2	5.81	1.38	1.32
1	G	448	LYS	C-O	5.75	1.31	1.23
1	C	195	HIS	CE1-NE2	5.74	1.38	1.32
1	C	740	VAL	C-O	5.69	1.29	1.24
1	G	322	TRP	C-O	5.66	1.31	1.24
1	A	23	PHE	CA-C	5.65	1.55	1.52
1	C	81	TYR	C-O	5.62	1.30	1.23
1	E	99	SER	C-O	5.57	1.31	1.23
1	C	514	ASN	C-O	5.49	1.30	1.23
1	G	278	PRO	C-O	-5.48	1.17	1.24
1	A	393	ASN	C-O	5.46	1.30	1.24
1	E	132	VAL	C-O	5.46	1.29	1.23
1	C	769	GLN	C-O	-5.45	1.16	1.23
1	G	229	TRP	C-O	-5.42	1.17	1.24
1	A	695	ARG	C-O	-5.41	1.17	1.24
1	G	289	HIS	CE1-NE2	5.38	1.38	1.32
1	C	813	PHE	C-O	5.36	1.30	1.24
1	C	289	HIS	CE1-NE2	5.32	1.37	1.32
1	E	128	ALA	C-O	5.30	1.30	1.24
1	A	697	TRP	C-O	5.28	1.30	1.24
1	C	786	THR	C-O	5.25	1.30	1.23
1	C	646	VAL	C-O	5.24	1.28	1.23
1	A	132	VAL	C-O	5.23	1.29	1.23
2	H	119	VAL	N-CA	5.22	1.50	1.46
1	C	169	ALA	C-O	5.19	1.30	1.23
1	E	71	ASN	C-O	5.16	1.29	1.23
1	G	663	GLU	CD-OE2	5.14	1.35	1.25
2	B	71	LYS	C-O	-5.11	1.18	1.24
2	B	117	THR	C-O	5.10	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	118	GLN	C-O	-5.10	1.17	1.24
1	E	728	ILE	C-O	5.10	1.29	1.24
1	A	721	GLU	CD-OE1	5.08	1.35	1.25
1	C	679	PRO	C-O	5.07	1.29	1.23
1	E	659	MET	C-O	-5.05	1.18	1.23
1	C	741	THR	C-O	5.03	1.29	1.23
1	E	148	LYS	C-O	5.03	1.29	1.24
1	C	794	ILE	N-CA	5.02	1.50	1.46
1	G	390	GLY	C-O	5.02	1.28	1.23
1	E	390	GLY	C-O	5.00	1.28	1.23

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5	GLN	OE1-CD-NE2	15.05	137.65	122.60
1	G	121	LYS	CD-CE-NZ	13.48	155.03	111.90
2	D	5	GLN	CB-CG-CD	-12.10	92.03	112.60
1	C	4	ASN	CA-CB-CG	10.01	122.61	112.60
1	A	669	ASP	CA-CB-CG	8.23	120.83	112.60
1	A	695	ARG	CB-CG-CD	7.26	128.00	111.30
1	G	4	ASN	CA-CB-CG	6.98	119.58	112.60
1	A	5	ASP	CA-CB-CG	6.86	119.46	112.60
1	G	79	ARG	CG-CD-NE	-6.72	97.22	112.00
1	E	825	ALA	CA-C-O	-6.42	109.89	120.80
1	A	295	ARG	CD-NE-CZ	6.39	133.34	124.40
1	C	669	ASP	CA-CB-CG	6.35	118.95	112.60
1	E	669	ASP	CA-CB-CG	6.13	118.73	112.60
1	E	4	ASN	CB-CA-C	6.08	121.66	110.10
2	F	123	GLY	CA-C-O	-5.90	118.38	122.22
1	A	812	GLU	CB-CG-CD	5.88	122.59	112.60
1	A	295	ARG	NE-CZ-NH2	-5.87	113.92	119.20
1	E	532	HIS	CB-CA-C	5.84	118.01	109.48
1	C	329	GLU	CB-CG-CD	5.71	122.31	112.60
1	G	5	ASP	CA-CB-CG	5.69	118.29	112.60
1	C	5	ASP	CA-CB-CG	5.68	118.28	112.60
1	E	189	THR	CA-CB-OG1	-5.64	101.14	109.60
1	E	358	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	173	PHE	CA-C-O	-5.58	114.64	120.55
1	C	812	GLU	CB-CG-CD	5.56	122.06	112.60
1	E	741	THR	CA-CB-OG1	-5.54	101.28	109.60
1	C	127	ALA	CA-C-O	-5.52	115.51	122.63
2	H	101	ASN	CB-CA-C	5.50	121.04	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	741	THR	CA-CB-OG1	-5.48	101.38	109.60
2	F	25	PHE	CA-C-O	-5.47	115.59	121.38
1	C	358	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	306	ASP	CA-CB-CG	-5.46	107.14	112.60
1	A	295	ARG	NE-CZ-NH1	5.43	126.93	121.50
1	C	217	ASN	CA-CB-CG	5.39	117.99	112.60
1	G	306	ASP	CA-CB-CG	-5.37	107.23	112.60
1	C	532	HIS	CB-CA-C	5.36	117.31	109.48
1	G	790	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	493	GLU	CB-CG-CD	5.27	121.56	112.60
1	A	701	GLY	CA-C-O	-5.25	117.28	120.91
1	A	532	HIS	CB-CA-C	5.22	117.11	109.48
1	E	493	GLU	CB-CG-CD	5.21	121.46	112.60
1	C	581	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	339	VAL	CA-C-O	-5.16	115.58	120.95
1	G	387	ILE	N-CA-C	-5.15	107.81	112.96
1	E	449	GLY	CA-C-O	-5.14	117.77	122.24
1	E	137	ASP	N-CA-C	-5.11	105.79	111.36
2	D	5	GLN	CG-CD-NE2	-5.09	108.77	116.40
1	A	471	GLU	CB-CG-CD	5.08	121.24	112.60
1	G	646	VAL	N-CA-C	-5.08	107.44	111.81
1	E	166	HIS	CA-C-N	5.04	126.91	122.43
1	E	166	HIS	C-N-CA	5.04	126.91	122.43
1	E	485	GLN	CB-CA-C	-5.00	102.48	110.79

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	HIS	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	6523	0	6319	80	0
1	C	6555	0	6342	72	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	6526	0	6328	66	0
1	G	6517	0	6311	66	1
2	B	1018	0	999	14	0
2	D	1015	0	995	8	0
2	F	1009	0	994	7	0
2	H	1018	0	999	10	0
3	A	94	0	44	1	0
3	C	94	0	44	3	0
3	E	94	0	44	2	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	1	0
4	G	1	0	0	0	0
5	A	7	0	0	0	0
5	C	7	0	0	0	0
5	E	7	0	0	0	0
5	G	7	0	0	0	0
6	A	20	0	28	5	0
6	G	10	0	14	1	0
7	A	6	0	8	2	0
7	C	18	0	24	6	0
7	E	18	0	24	8	0
7	G	12	0	16	4	0
8	A	4	0	0	0	0
8	C	4	0	0	0	0
8	E	4	0	0	1	0
8	G	4	0	0	0	0
9	A	32	0	45	18	0
9	C	28	0	42	7	0
9	D	4	0	6	1	0
9	E	20	0	30	0	0
9	G	28	0	41	8	0
10	A	7	0	10	3	0
10	B	7	0	10	4	0
11	A	4	0	8	3	0
11	C	4	0	8	4	0
11	E	4	0	8	0	0
11	G	4	0	8	7	0
12	B	4	0	0	0	0
12	D	4	0	0	0	0
12	F	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	H	4	0	0	0	0
13	A	806	0	0	19	3
13	B	137	0	0	4	0
13	C	760	0	0	28	11
13	D	148	0	0	2	1
13	E	751	0	0	14	4
13	F	129	0	0	3	0
13	G	799	0	0	30	7
13	H	153	0	0	4	4
All	All	34530	0	29793	337	16

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 6.

All (337) 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)
9:A:908[A]:EDO:O1	9:A:909:EDO:C1	1.91	1.19
9:A:908[A]:EDO:O1	9:A:909:EDO:H11	1.40	1.17
9:C:910:EDO:H21	13:C:1110:HOH:O	1.44	1.12
11:A:913:IPA:H33	13:A:1527:HOH:O	1.52	1.10
1:A:136:TRP:CH2	1:A:528[B]:LEU:HD21	1.88	1.09
1:A:136:TRP:HH2	1:A:528[B]:LEU:HD21	0.98	1.07
1:G:295:ARG:HB3	13:G:1009:HOH:O	1.50	1.07
1:A:495[A]:MET:HE2	1:A:495[A]:MET:HA	1.14	1.06
1:A:208:ARG:HH12	6:A:905[A]:PGE:H42	1.07	1.06
1:G:484[A]:MET:CE	13:G:1007:HOH:O	2.00	1.06
1:A:208:ARG:HH12	6:A:905[A]:PGE:C4	1.69	1.05
1:C:484[B]:MET:SD	13:C:1078:HOH:O	2.13	1.05
1:A:495[A]:MET:HA	1:A:495[A]:MET:CE	1.89	1.02
1:A:528[B]:LEU:HD22	1:A:566:ILE:HD13	1.37	1.02
1:A:495[A]:MET:HE2	1:A:495[A]:MET:CA	1.93	0.99
1:E:359[B]:MET:SD	1:E:362:ARG:NH1	2.36	0.98
1:A:471:GLU:HG3	1:E:485:GLN:CD	1.88	0.98
1:C:4:ASN:HA	13:C:1012:HOH:O	1.65	0.95
2:D:0:LEU:O	13:D:301:HOH:O	1.85	0.94
1:G:484[A]:MET:HE3	13:G:1007:HOH:O	1.63	0.94
1:E:273:ILE:HG22	13:E:1387:HOH:O	1.69	0.92
1:C:46[B]:GLU:OE2	13:C:1001:HOH:O	1.87	0.92
1:E:119:ARG:N	13:E:1001:HOH:O	1.87	0.92
1:C:136:TRP:HH2	13:C:1455:HOH:O	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:TRP:HH2	1:A:528[B]:LEU:CD2	1.83	0.90
1:E:296:VAL:HG22	13:E:1387:HOH:O	1.70	0.90
9:C:907:EDO:H11	13:C:1391:HOH:O	1.71	0.90
1:C:805:ARG:HD3	13:C:1157:HOH:O	1.72	0.88
1:A:208:ARG:NH1	6:A:905[A]:PGE:H42	1.88	0.88
1:A:492:THR:OG1	10:A:910:PEG:H32	1.73	0.87
1:E:359[B]:MET:HE1	1:E:362:ARG:HH12	1.40	0.86
1:G:484[A]:MET:HE1	13:G:1007:HOH:O	1.65	0.85
1:A:811:GLU:HG3	13:A:1533:HOH:O	1.77	0.85
1:A:436:LYS:HE3	13:A:1130:HOH:O	1.76	0.84
2:F:10:GLN:HG3	13:F:332:HOH:O	1.77	0.84
1:G:273:ILE:HG22	13:G:1243:HOH:O	1.77	0.83
1:C:79:ARG:NH1	13:C:1003:HOH:O	2.12	0.83
1:E:359[B]:MET:CE	1:E:362:ARG:HH12	1.90	0.83
1:G:136:TRP:HH2	13:G:1519:HOH:O	1.61	0.82
1:C:296:VAL:HG22	13:C:1559:HOH:O	1.79	0.81
13:A:1468:HOH:O	2:F:0:LEU:HD21	1.79	0.81
1:A:345:SER:OG	1:A:348:GLU:HG3	1.80	0.81
1:C:4:ASN:CA	13:C:1012:HOH:O	2.27	0.80
11:A:913:IPA:H12	13:A:1341:HOH:O	1.79	0.80
1:C:639:ASN:H	11:C:906:IPA:H32	1.47	0.80
1:C:638:ASN:H	11:C:906:IPA:H13	1.45	0.79
1:C:695:ARG:NH2	13:C:1004:HOH:O	2.14	0.79
1:E:136:TRP:HH2	13:E:1413:HOH:O	1.64	0.79
1:G:296:VAL:HG22	13:G:1243:HOH:O	1.84	0.78
1:E:4:ASN:OD1	13:E:1002:HOH:O	2.02	0.78
1:A:484:MET:HE3	1:A:499:ILE:HG12	1.65	0.77
1:G:652:LYS:HE3	13:G:1128:HOH:O	1.83	0.77
1:C:219:TYR:HB2	7:C:912:GOL:H11	1.66	0.76
1:C:136:TRP:CH2	13:C:1455:HOH:O	2.33	0.76
1:C:805:ARG:CD	13:C:1157:HOH:O	2.30	0.76
9:A:914:EDO:H21	13:A:1351:HOH:O	1.86	0.76
1:A:136:TRP:CH2	1:A:528[B]:LEU:CD2	2.63	0.75
1:A:528[B]:LEU:CD2	1:A:566:ILE:HD13	2.17	0.75
1:G:295:ARG:CB	13:G:1009:HOH:O	2.16	0.74
1:C:344:LEU:HD11	1:C:348:GLU:HG2	1.69	0.74
1:A:528[B]:LEU:HD22	1:A:566:ILE:CD1	2.16	0.73
1:C:471[A]:GLU:OE1	13:C:1002:HOH:O	2.05	0.73
1:E:792:ASN:ND2	7:E:912:GOL:O3	2.20	0.72
1:C:137:ASP:OD1	1:C:569[B]:ARG:NH1	2.22	0.72
1:C:273:ILE:HG22	13:C:1559:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138:HIS:ND1	6:G:907:PGE:H52	2.04	0.71
1:G:4:ASN:N	1:G:4:ASN:HD22	1.88	0.71
13:A:1483:HOH:O	10:B:2301:PEG:H22	1.91	0.71
1:E:792:ASN:HD21	7:E:912:GOL:C3	2.04	0.70
1:A:88:ASP:OD2	9:A:908[B]:EDO:C2	2.39	0.69
1:A:219:TYR:HB2	7:A:906:GOL:H2	1.73	0.69
1:G:638:ASN:HB2	11:G:908:IPA:H33	1.74	0.69
1:C:356:PRO:HG2	1:C:359[A]:MET:HE3	1.75	0.68
2:D:5:GLN:HB3	2:D:5:GLN:NE2	2.09	0.68
4:E:902:MO:MO	8:E:906:AST:O3	1.65	0.67
1:A:484:MET:HE2	1:A:499:ILE:HD11	1.76	0.66
1:G:495:MET:HE2	1:G:495:MET:HA	1.77	0.66
9:A:908[A]:EDO:C1	9:A:909:EDO:H11	2.24	0.66
1:A:88:ASP:OD2	9:A:908[B]:EDO:O2	2.14	0.66
1:C:88:ASP:OD2	11:C:906:IPA:H11	1.96	0.66
1:A:208:ARG:NH1	6:A:905[A]:PGE:C4	2.52	0.65
2:F:0:LEU:O	13:F:301:HOH:O	2.13	0.65
1:C:495[A]:MET:HA	1:C:495[A]:MET:HE2	1.78	0.65
1:G:480:VAL:HG12	1:G:484[A]:MET:HE2	1.78	0.65
1:E:698:LEU:HB2	1:E:800:THR:HG23	1.79	0.65
2:H:5:GLN:HE21	2:H:5:GLN:HA	1.60	0.65
9:G:914:EDO:H11	13:G:1551:HOH:O	1.96	0.65
1:E:273:ILE:CG2	13:E:1387:HOH:O	2.36	0.64
1:G:348:GLU:OE2	13:G:1003:HOH:O	2.15	0.64
1:A:495[A]:MET:HE1	1:A:498:VAL:HG21	1.78	0.64
1:G:583:LYS:HE3	13:G:1647:HOH:O	1.95	0.64
9:G:915:EDO:H21	2:H:63:MET:HE1	1.78	0.64
1:A:485:GLN:HG2	1:E:471:GLU:OE2	1.98	0.64
9:A:908[A]:EDO:O1	9:A:909:EDO:O1	2.15	0.64
1:E:566:ILE:HD13	13:E:1413:HOH:O	1.98	0.63
1:C:575:ARG:HD3	13:C:1413:HOH:O	1.98	0.63
11:C:906:IPA:H33	13:C:1575:HOH:O	1.98	0.63
9:A:914:EDO:C2	13:A:1351:HOH:O	2.43	0.63
1:C:296:VAL:CG2	13:C:1559:HOH:O	2.40	0.63
1:E:129:ASP:OD2	1:E:485:GLN:NE2	2.32	0.63
1:G:639:ASN:H	11:G:908:IPA:H12	1.63	0.63
1:E:267:ASN:ND2	1:E:372:ALA:HB3	2.13	0.62
1:C:46[B]:GLU:CD	1:C:46[B]:GLU:H	2.07	0.62
1:E:136:TRP:CH2	13:E:1413:HOH:O	2.47	0.62
1:A:490:ALA:HB1	1:A:495[A]:MET:HE3	1.80	0.62
1:C:736:LYS:O	9:C:911[A]:EDO:C2	2.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:652:LYS:NZ	13:G:1001:HOH:O	2.03	0.62
2:B:63:MET:HE1	10:B:2301:PEG:H21	1.80	0.61
9:G:915:EDO:H22	13:G:1115:HOH:O	2.00	0.61
1:E:791:ARG:CD	7:E:912:GOL:H11	2.30	0.61
1:E:791:ARG:HD3	7:E:912:GOL:H11	1.83	0.61
1:G:219:TYR:HB2	7:G:905:GOL:H2	1.82	0.61
1:C:4:ASN:N	13:C:1012:HOH:O	2.33	0.60
1:C:146[A]:LEU:HD22	1:C:496:VAL:HG13	1.84	0.60
1:A:471:GLU:HG3	1:E:485:GLN:CG	2.30	0.60
1:C:698:LEU:HB2	1:C:800:THR:HG23	1.83	0.60
1:E:296:VAL:CG2	13:E:1387:HOH:O	2.38	0.60
1:E:825:ALA:O	2:F:77:LYS:NZ	2.25	0.60
1:G:136:TRP:CH2	13:G:1519:HOH:O	2.44	0.60
1:A:811:GLU:CG	13:A:1533:HOH:O	2.42	0.59
1:E:201:ASN:O	7:E:914:GOL:H2	2.01	0.59
1:E:566:ILE:CD1	13:E:1413:HOH:O	2.51	0.59
9:A:916:EDO:H22	2:B:93:MET:HB3	1.85	0.59
1:G:638:ASN:H	11:G:908:IPA:H32	1.67	0.59
2:D:93:MET:HB3	9:D:202:EDO:H22	1.84	0.59
9:G:914:EDO:C1	13:G:1551:HOH:O	2.51	0.59
1:A:436:LYS:CE	13:A:1130:HOH:O	2.41	0.59
9:A:908[A]:EDO:O1	9:A:909:EDO:C2	2.49	0.58
1:C:449:GLY:H	7:C:909:GOL:C1	2.16	0.58
1:C:805:ARG:NH1	13:C:1014:HOH:O	2.36	0.58
1:C:297[A]:LEU:HD12	1:C:299:LEU:CD2	2.33	0.58
1:C:449:GLY:H	7:C:909:GOL:H12	1.69	0.57
1:G:299[A]:LEU:HD21	1:G:309:LEU:HD11	1.85	0.57
1:E:345:SER:OG	1:E:348:GLU:HG3	2.04	0.57
1:A:208:ARG:HH12	6:A:905[A]:PGE:H4	1.66	0.57
1:A:495[A]:MET:CE	1:A:495[A]:MET:CA	2.67	0.57
1:E:791:ARG:HD2	7:E:912:GOL:C1	2.35	0.57
1:G:528:LEU:HB3	13:G:1519:HOH:O	2.04	0.57
1:C:412[A]:ARG:NH2	13:C:1009:HOH:O	2.32	0.56
1:C:736:LYS:O	9:C:911[A]:EDO:H22	2.05	0.56
1:A:267:ASN:OD1	1:A:372:ALA:HB3	2.05	0.56
2:B:0:LEU:HD13	1:E:43:ARG:HD2	1.87	0.56
1:C:273:ILE:CG2	13:C:1559:HOH:O	2.48	0.56
1:C:825:ALA:C	2:D:77:LYS:HZ3	2.13	0.56
1:G:637:GLY:HA3	11:G:908:IPA:H13	1.87	0.56
1:C:297[A]:LEU:HD12	1:C:299:LEU:HD23	1.87	0.56
1:E:359[B]:MET:CE	1:E:362:ARG:NH1	2.63	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:333:LYS:HE3	13:G:1121:HOH:O	2.05	0.55
1:E:359[B]:MET:HE1	1:E:362:ARG:NH1	2.15	0.55
1:A:471:GLU:HG3	1:E:485:GLN:NE2	2.20	0.55
1:C:495[A]:MET:HE2	1:C:495[A]:MET:CA	2.34	0.55
1:G:291:ALA:HB1	13:G:1009:HOH:O	2.06	0.55
1:G:638:ASN:H	11:G:908:IPA:C3	2.19	0.54
1:A:490:ALA:CB	1:A:495[A]:MET:HE3	2.37	0.54
1:A:639:ASN:CG	9:A:909:EDO:H22	2.33	0.54
1:C:291:ALA:O	1:C:295:ARG:HD3	2.08	0.54
1:A:528[B]:LEU:HD23	1:A:529:PRO:N	2.23	0.54
1:C:514:ASN:ND2	13:C:1006:HOH:O	2.40	0.54
1:G:299[B]:LEU:HD22	1:G:359[B]:MET:HG2	1.89	0.54
1:C:825:ALA:C	2:D:77:LYS:NZ	2.66	0.54
1:E:299[B]:LEU:HD13	1:E:355:VAL:HG21	1.90	0.54
1:G:7:ILE:HG22	13:G:1482:HOH:O	2.07	0.54
1:A:667:ASP:OD2	9:A:912:EDO:H21	2.08	0.53
1:G:504:GLN:NE2	13:G:1013:HOH:O	2.41	0.53
1:G:698:LEU:HB2	1:G:800:THR:HG23	1.89	0.53
1:E:146:LEU:HD23	1:E:451:ILE:HD12	1.92	0.52
1:A:685:ALA:O	1:A:689:GLN:HG3	2.09	0.52
1:A:297[A]:LEU:HG	1:A:366:TRP:CH2	2.45	0.52
1:C:739:ASP:OD1	9:C:911[B]:EDO:H21	2.09	0.52
1:A:31:HIS:HD2	13:A:1600:HOH:O	1.91	0.52
1:E:495[A]:MET:HE2	1:E:495[A]:MET:HA	1.92	0.52
1:E:791:ARG:HD2	7:E:912:GOL:H12	1.92	0.52
2:D:1:ARG:CZ	2:D:5:GLN:HG2	2.39	0.52
9:G:915:EDO:C2	13:G:1115:HOH:O	2.56	0.52
2:F:104:ARG:HG3	13:F:376:HOH:O	2.09	0.52
1:A:484:MET:CE	1:A:499:ILE:HD11	2.41	0.51
1:G:208:ARG:HH22	9:G:909[B]:EDO:H12	1.75	0.51
1:E:297:LEU:HD21	1:E:362:ARG:HD2	1.91	0.51
1:C:220:GLU:N	7:C:912:GOL:H12	2.26	0.51
1:A:345:SER:OG	1:A:348:GLU:CG	2.56	0.51
1:G:299[A]:LEU:HD21	1:G:309:LEU:CD1	2.41	0.51
1:C:359[B]:MET:HE1	1:C:362:ARG:HH12	1.75	0.51
1:A:528[B]:LEU:CD2	1:A:566:ILE:CD1	2.84	0.50
2:H:122:ASP:OD2	13:H:301:HOH:O	2.19	0.50
1:A:385:LYS:HE2	3:A:901:MGD:S13	2.52	0.50
1:A:698:LEU:HB2	1:A:800:THR:HG23	1.94	0.50
1:A:333:LYS:HE2	13:A:1138:HOH:O	2.10	0.49
1:E:695:ARG:NH1	13:E:1018:HOH:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LEU:HD21	10:B:2301:PEG:H41	1.93	0.49
1:C:44:ALA:HB1	1:C:46[B]:GLU:OE1	2.12	0.49
2:H:5:GLN:HA	2:H:5:GLN:NE2	2.28	0.49
1:A:136:TRP:CH2	1:A:528[B]:LEU:CG	2.95	0.49
9:A:908[A]:EDO:C2	9:A:909:EDO:H21	2.43	0.49
1:E:482:GLN:O	1:E:485:GLN:HB2	2.13	0.49
1:G:186:ALA:HB1	1:G:590:PHE:CD1	2.48	0.48
1:C:561:MET:HE2	13:C:1024:HOH:O	2.13	0.48
9:C:907:EDO:C1	13:C:1391:HOH:O	2.45	0.48
1:G:639:ASN:N	11:G:908:IPA:H12	2.26	0.48
1:E:267:ASN:HD21	1:E:372:ALA:HB3	1.77	0.48
1:E:533:PRO:HG3	1:E:538:LEU:HD13	1.94	0.48
1:C:729:GLU:HA	1:C:760:TYR:O	2.13	0.48
1:E:487:ALA:CB	1:E:495[A]:MET:HE1	2.43	0.48
1:G:296:VAL:CG2	13:G:1243:HOH:O	2.54	0.48
1:E:358:ASP:CG	1:E:359[B]:MET:HE2	2.39	0.47
1:A:25:ILE:O	1:A:542:ASN:HB2	2.14	0.47
1:A:825:ALA:C	2:B:77:LYS:NZ	2.72	0.47
1:A:484:MET:HE3	1:A:499:ILE:CG1	2.39	0.47
1:C:495[A]:MET:HA	1:C:495[A]:MET:CE	2.45	0.47
1:E:231:ILE:O	1:E:383:TYR:HA	2.13	0.47
1:G:273:ILE:CG2	13:G:1243:HOH:O	2.49	0.47
1:C:483:ALA:O	1:C:486:LYS:HE2	2.15	0.47
1:E:528:LEU:HB3	13:E:1413:HOH:O	2.14	0.47
1:G:231:ILE:O	1:G:383:TYR:HA	2.15	0.47
9:G:912:EDO:H11	13:G:1673:HOH:O	2.13	0.47
1:C:457:CYS:C	13:C:1006:HOH:O	2.58	0.47
1:E:140:MET:SD	1:E:569[A]:ARG:HG2	2.55	0.47
1:C:561:MET:HE1	1:C:569[A]:ARG:HH11	1.79	0.47
1:G:566:ILE:HD13	13:G:1519:HOH:O	2.15	0.46
1:C:232:GLY:CA	1:C:386:GLY:HA3	2.46	0.46
2:D:108:ARG:HD3	13:D:307:HOH:O	2.14	0.46
1:G:25:ILE:O	1:G:542:ASN:HB2	2.16	0.46
1:A:157:GLN:HG2	13:A:1076:HOH:O	2.15	0.46
1:A:220:GLU:HB2	7:A:906:GOL:H32	1.98	0.46
1:C:499:ILE:O	1:C:503:THR:HG23	2.16	0.46
1:G:459:ASN:HB3	1:G:463:SER:OG	2.16	0.46
1:A:224:LEU:HD21	1:A:258:LYS:HD3	1.97	0.46
3:C:903:MGD:O3'	13:C:1006:HOH:O	2.21	0.46
1:A:31:HIS:CE1	9:A:908[B]:EDO:H21	2.50	0.46
1:A:533:PRO:HG3	1:A:538:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:ASN:HB3	1:C:463:SER:OG	2.15	0.46
1:A:495[A]:MET:HE2	1:A:495[A]:MET:N	2.30	0.45
1:E:791:ARG:CD	7:E:912:GOL:C1	2.92	0.45
1:G:696:PHE:O	1:G:801:TRP:HA	2.16	0.45
1:A:561:MET:HE1	1:A:569:ARG:HH11	1.81	0.45
1:C:480:VAL:O	1:C:484[A]:MET:HG3	2.17	0.45
1:A:79:ARG:HH11	1:A:79:ARG:HG2	1.80	0.45
1:A:471:GLU:OE2	1:E:485:GLN:HG3	2.16	0.45
1:C:246:HIS:CE1	7:C:912:GOL:H31	2.51	0.45
1:C:631:ASP:OD1	1:C:634:ARG:NH1	2.49	0.45
2:B:64:GLY:HA3	2:B:126:TYR:CD2	2.52	0.45
1:E:275:PHE:O	1:E:299[A]:LEU:HB2	2.17	0.45
1:E:434:GLY:HA3	13:E:1393:HOH:O	2.16	0.45
2:H:44:PRO:HG3	13:H:425:HOH:O	2.16	0.45
1:A:486:LYS:H	1:A:486:LYS:HD3	1.80	0.45
1:G:404:VAL:HG11	1:G:417:CYS:HB2	1.99	0.45
1:G:566:ILE:CD1	13:G:1519:HOH:O	2.64	0.45
9:A:912:EDO:H12	13:A:1541:HOH:O	2.16	0.45
1:E:186:ALA:HB1	1:E:590:PHE:CD1	2.51	0.45
1:C:385:LYS:HE2	3:C:903:MGD:S13	2.56	0.45
1:E:385:LYS:HE2	3:E:901:MGD:S13	2.56	0.45
2:H:51:ASN:ND2	13:H:303:HOH:O	2.50	0.45
1:C:528:LEU:HB3	13:C:1455:HOH:O	2.16	0.45
1:A:484:MET:CE	1:A:499:ILE:CD1	2.96	0.44
1:E:459:ASN:HB3	1:E:463:SER:OG	2.16	0.44
1:A:297[A]:LEU:HD21	1:A:362:ARG:HD2	1.98	0.44
1:A:486:LYS:N	1:A:486:LYS:CD	2.81	0.44
1:G:495:MET:HE2	1:G:495:MET:CA	2.43	0.44
1:A:825:ALA:C	2:B:77:LYS:HZ1	2.24	0.44
1:G:435:ASP:OD1	1:G:435:ASP:N	2.49	0.44
1:G:497:ASP:OD2	13:G:1004:HOH:O	2.21	0.44
1:A:512:SER:O	1:A:527:MET:HA	2.18	0.44
2:B:108:ARG:HD3	13:B:2414:HOH:O	2.17	0.44
1:E:495[A]:MET:HE2	1:E:495[A]:MET:CA	2.47	0.44
1:A:31:HIS:HE1	9:A:908[B]:EDO:O1	2.00	0.44
1:A:188:GLN:OE1	13:A:1003:HOH:O	2.21	0.44
1:C:635:LYS:HD2	1:C:635:LYS:N	2.32	0.44
2:F:64:GLY:HA3	2:F:126:TYR:CD2	2.53	0.44
1:G:45:PRO:O	1:G:51:GLY:HA2	2.18	0.44
1:G:394:TYR:CE1	7:G:913:GOL:H32	2.53	0.44
1:A:215:LEU:HB2	11:A:913:IPA:H32	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ASP:OD1	1:A:435:ASP:N	2.50	0.43
1:E:700:ASN:HA	1:E:772:MET:O	2.17	0.43
1:G:484[B]:MET:HE3	1:G:499:ILE:HD11	1.99	0.43
2:B:84:GLU:OE2	13:B:2401:HOH:O	2.21	0.43
2:H:64:GLY:HA3	2:H:126:TYR:CD2	2.54	0.43
2:B:61:THR:CG2	2:B:103:PRO:HD3	2.49	0.43
1:E:136:TRP:HB3	1:E:569[A]:ARG:CZ	2.48	0.43
2:H:104:ARG:HG3	13:H:379:HOH:O	2.18	0.43
1:G:561:MET:HE2	1:G:561:MET:HB3	1.80	0.43
10:A:910:PEG:C1	13:A:1012:HOH:O	2.67	0.43
1:C:511:THR:HA	1:C:526:LEU:O	2.18	0.43
1:E:204:CYS:HB3	1:E:207:THR:HG22	2.01	0.43
1:G:434:GLY:HA3	13:G:1458:HOH:O	2.16	0.43
1:G:792:ASN:OD1	7:G:913:GOL:H31	2.18	0.43
1:A:638:ASN:ND2	9:A:908[B]:EDO:H21	2.33	0.43
1:C:699:ASN:HB3	1:C:770:THR:O	2.18	0.43
1:G:4:ASN:CG	13:G:1061:HOH:O	2.61	0.43
1:C:45:PRO:O	1:C:51:GLY:HA2	2.19	0.43
1:C:603:ASN:OD1	1:C:607:ARG:HD3	2.19	0.43
1:E:196:ASN:HB2	3:E:901:MGD:C12	2.49	0.43
1:G:699:ASN:HB3	1:G:770:THR:O	2.18	0.43
1:A:79:ARG:HG2	13:A:1448:HOH:O	2.19	0.42
1:A:121:LYS:NZ	13:A:1034:HOH:O	2.52	0.42
1:C:512:SER:O	1:C:527:MET:HA	2.19	0.42
1:G:88:ASP:OD2	11:G:908:IPA:C3	2.67	0.42
1:G:512:SER:O	1:G:527:MET:HA	2.19	0.42
1:G:394:TYR:CE1	7:G:913:GOL:C3	3.02	0.42
1:E:358:ASP:OD1	1:E:359[B]:MET:HE2	2.19	0.42
1:G:101:ARG:HD3	3:G:903:MGD:N19	2.34	0.42
2:H:12[B]:SER:OG	2:H:13:VAL:N	2.53	0.42
1:A:66:THR:HB	2:B:100[B]:GLU:HG2	2.00	0.42
1:A:186:ALA:HB1	1:A:590:PHE:CD1	2.55	0.42
2:B:0:LEU:HD11	13:E:1430:HOH:O	2.19	0.42
1:C:297[A]:LEU:HD12	1:C:299:LEU:HD21	2.02	0.42
1:C:736:LYS:O	9:C:911[A]:EDO:H21	2.20	0.42
1:E:136:TRP:CE3	1:E:569[A]:ARG:HD3	2.55	0.42
1:E:469:LEU:O	1:E:473:ILE:HG12	2.19	0.42
1:G:603:ASN:OD1	1:G:607:ARG:HD3	2.20	0.42
1:A:731:ASN:HA	1:A:732:PRO:HD3	1.94	0.41
1:C:359[B]:MET:HE1	1:C:362:ARG:NH1	2.34	0.41
1:A:231:ILE:O	1:A:383:TYR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:64:GLY:HA3	2:D:126:TYR:CD2	2.54	0.41
2:F:81:HIS:C	2:F:82:PHE:CD2	2.98	0.41
1:E:204:CYS:HB3	1:E:207:THR:CG2	2.50	0.41
10:A:910:PEG:C4	10:A:910:PEG:H12	2.50	0.41
1:C:450:ARG:HD2	1:C:503:THR:OG1	2.21	0.41
1:G:533:PRO:HG3	1:G:538:LEU:HD13	2.02	0.41
1:A:412[A]:ARG:HH11	1:A:412[A]:ARG:HD3	1.76	0.41
2:B:0:LEU:HB2	13:B:2402:HOH:O	2.21	0.41
1:G:425:GLU:O	1:G:540[B]:SER:HB2	2.20	0.41
2:B:0:LEU:HD13	1:E:43:ARG:CD	2.49	0.41
1:G:291:ALA:O	1:G:295:ARG:HD3	2.21	0.41
9:A:908[A]:EDO:O2	9:A:909:EDO:C2	2.69	0.41
1:E:346:LEU:HD23	1:E:346:LEU:HA	1.89	0.41
1:E:699:ASN:HB3	1:E:770:THR:O	2.20	0.41
2:B:66:PRO:HD2	13:B:2422:HOH:O	2.21	0.41
1:C:456:GLY:HA2	3:C:903:MGD:N3	2.36	0.41
1:G:208:ARG:HH22	9:G:909[B]:EDO:C1	2.33	0.41
1:G:487:ALA:CB	1:G:495:MET:HE1	2.51	0.41
1:A:136:TRP:CH2	1:A:528[B]:LEU:HG	2.56	0.40
1:C:246:HIS:HE1	7:C:912:GOL:H31	1.86	0.40
13:A:1483:HOH:O	10:B:2301:PEG:H31	2.21	0.40
1:G:547:ILE:C	1:G:548:ARG:HD3	2.46	0.40
1:C:325:LYS:N	1:C:326:PRO:CD	2.85	0.40
1:E:275:PHE:O	1:E:299[B]:LEU:HB2	2.22	0.40
1:E:362:ARG:HD2	1:E:362:ARG:HH11	1.68	0.40
2:H:61:THR:CG2	2:H:103:PRO:HD3	2.52	0.40

All (16) 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:C:485:GLN:NE2	1:G:471[A]:GLU:OE2[1_455]	1.51	0.69
13:C:1758:HOH:O	13:G:1797:HOH:O[1_455]	1.64	0.56
13:C:1642:HOH:O	13:G:1732:HOH:O[1_455]	1.68	0.52
13:A:1806:HOH:O	13:G:1799:HOH:O[1_465]	1.69	0.51
13:A:1788:HOH:O	13:E:1744:HOH:O[1_455]	1.70	0.50
13:C:1760:HOH:O	13:H:447:HOH:O[1_455]	1.81	0.39
13:C:1363:HOH:O	13:H:301:HOH:O[1_455]	1.83	0.37
13:C:1709:HOH:O	13:G:1657:HOH:O[1_455]	1.94	0.26
13:E:1067:HOH:O	13:H:409:HOH:O[1_566]	2.04	0.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:C:1456:HOH:O	13:G:1625:HOH:O[1_455]	2.05	0.15
13:C:1125:HOH:O	13:G:1633:HOH:O[1_455]	2.10	0.10
13:C:1554:HOH:O	13:E:1522:HOH:O[1_544]	2.13	0.07
13:A:1239:HOH:O	13:D:400:HOH:O[1_565]	2.15	0.05
13:C:1473:HOH:O	13:G:1485:HOH:O[1_455]	2.15	0.05
13:C:1554:HOH:O	13:E:1601:HOH:O[1_544]	2.15	0.05
13:C:1363:HOH:O	13:H:424:HOH:O[1_455]	2.17	0.03

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	828/823 (101%)	796 (96%)	30 (4%)	2 (0%)	43	26
1	C	831/823 (101%)	802 (96%)	29 (4%)	0	100	100
1	E	828/823 (101%)	797 (96%)	28 (3%)	3 (0%)	30	12
1	G	828/823 (101%)	801 (97%)	26 (3%)	1 (0%)	48	28
2	B	135/134 (101%)	130 (96%)	5 (4%)	0	100	100
2	D	134/134 (100%)	128 (96%)	6 (4%)	0	100	100
2	F	134/134 (100%)	128 (96%)	6 (4%)	0	100	100
2	H	135/134 (101%)	126 (93%)	9 (7%)	0	100	100
All	All	3853/3828 (101%)	3708 (96%)	139 (4%)	6 (0%)	43	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	392	ASP
1	A	392	ASP
1	G	392	ASP
1	E	518	THR
1	A	793	ILE

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Mol	Chain	Res	Type
1	E	793	ILE

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	683/676 (101%)	673 (98%)	10 (2%)	57	31
1	C	686/676 (102%)	675 (98%)	11 (2%)	55	28
1	E	683/676 (101%)	672 (98%)	11 (2%)	55	28
1	G	683/676 (101%)	668 (98%)	15 (2%)	45	15
2	B	115/112 (103%)	114 (99%)	1 (1%)	70	52
2	D	114/112 (102%)	113 (99%)	1 (1%)	70	52
2	F	114/112 (102%)	111 (97%)	3 (3%)	40	11
2	H	115/112 (103%)	112 (97%)	3 (3%)	40	11
All	All	3193/3152 (101%)	3138 (98%)	55 (2%)	55	25

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	LEU
1	A	333	LYS
1	A	348	GLU
1	A	365	GLU
1	A	410	VAL
1	A	486	LYS
1	A	495[A]	MET
1	A	495[B]	MET
1	A	596	LYS
1	A	774	PHE
2	B	0	LEU
1	C	4	ASN
1	C	77	ASN
1	C	146[A]	LEU

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Mol	Chain	Res	Type
1	C	146[B]	LEU
1	C	297[A]	LEU
1	C	297[B]	LEU
1	C	410	VAL
1	C	486	LYS
1	C	635	LYS
1	C	663	GLU
1	C	774	PHE
2	D	10	GLN
1	E	4	ASN
1	E	299[A]	LEU
1	E	299[B]	LEU
1	E	299[C]	LEU
1	E	340	LYS
1	E	343	ARG
1	E	485	GLN
1	E	486	LYS
1	E	596	LYS
1	E	695	ARG
1	E	774	PHE
2	F	0	LEU
2	F	35	VAL
2	F	128	ARG
1	G	4	ASN
1	G	24	CYS
1	G	121	LYS
1	G	282	PRO
1	G	299[A]	LEU
1	G	299[B]	LEU
1	G	303	PRO
1	G	329	GLU
1	G	410	VAL
1	G	486	LYS
1	G	493	GLU
1	G	596	LYS
1	G	652	LYS
1	G	718	LEU
1	G	774	PHE
2	H	5	GLN
2	H	10	GLN
2	H	128	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	216	ASN
1	A	233	ASN
1	A	252	GLN
1	A	270	GLN
1	A	461	GLN
1	A	611	GLN
1	A	792	ASN
2	B	51	ASN
1	C	4	ASN
1	C	77	ASN
1	C	138	HIS
1	C	442	GLN
1	C	688	GLN
1	C	792	ASN
1	E	4	ASN
1	E	216	ASN
1	E	267	ASN
1	E	485	GLN
1	E	505	ASN
1	E	611	GLN
1	E	681	ASN
1	E	688	GLN
1	E	792	ASN
2	F	51	ASN
1	G	216	ASN
1	G	293	ASN
1	G	311	ASN
1	G	504	GLN
2	H	5	GLN
2	H	51	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 70 ligands modelled in this entry, 4 are monoatomic - leaving 66 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	$\# Z > 2$
12	FES	B	2302	2	0,4,4	-	-	-		
9	EDO	E	907	-	3,3,3	0.93	0	2,2,2	0.48	0
3	MGD	E	903	4	47,52,52	0.91	3 (6%)	58,81,81	1.20	5 (8%)
9	EDO	A	914	-	3,3,3	0.58	0	2,2,2	0.60	0
9	EDO	A	912	-	3,3,3	0.42	0	2,2,2	0.23	0
3	MGD	A	902	4	47,52,52	0.92	1 (2%)	58,81,81	1.30	5 (8%)
7	GOL	G	913	-	5,5,5	0.28	0	5,5,5	1.13	0
6	PGE	G	907	-	9,9,9	0.84	0	8,8,8	0.33	0
9	EDO	C	915	-	3,3,3	0.16	0	2,2,2	0.45	0
9	EDO	A	916	-	3,3,3	1.04	0	2,2,2	0.78	0
3	MGD	G	902	4	47,52,52	0.91	1 (2%)	58,81,81	1.22	7 (12%)
9	EDO	C	911[A]	-	3,3,3	0.34	0	2,2,2	0.71	0
7	GOL	E	914	-	5,5,5	0.22	0	5,5,5	0.24	0
9	EDO	D	202	-	3,3,3	0.73	0	2,2,2	0.44	0
9	EDO	G	912	-	3,3,3	0.76	0	2,2,2	0.36	0
8	AST	G	906	-	0,3,3	-	-	0,3,3	-	-
9	EDO	C	913	-	3,3,3	0.28	0	2,2,2	0.33	0
7	GOL	C	912	-	5,5,5	0.41	0	5,5,5	1.03	0
7	GOL	E	913	-	5,5,5	0.21	0	5,5,5	0.64	0
3	MGD	C	902	4	47,52,52	0.95	3 (6%)	58,81,81	1.15	5 (8%)
9	EDO	A	908[A]	-	3,3,3	0.26	0	2,2,2	0.41	0
9	EDO	E	909	-	3,3,3	0.79	0	2,2,2	0.44	0
11	IPA	A	913	-	3,3,3	0.42	0	3,3,3	0.41	0
7	GOL	C	908	-	5,5,5	0.20	0	5,5,5	0.30	0
9	EDO	E	910	-	3,3,3	0.92	0	2,2,2	0.72	0
9	EDO	E	911	-	3,3,3	0.52	0	2,2,2	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	IPA	C	906	-	3,3,3	0.98	0	3,3,3	0.66	0
5	F3S	G	904	1	0,9,9	-	-	-		
9	EDO	A	915	-	3,3,3	0.69	0	2,2,2	0.54	0
12	FES	D	201	2	0,4,4	-	-	-		
11	IPA	G	908	-	3,3,3	0.88	0	3,3,3	1.22	0
7	GOL	G	905	-	5,5,5	0.52	0	5,5,5	0.92	0
3	MGD	G	903	4	47,52,52	0.90	3 (6%)	58,81,81	1.01	4 (6%)
5	F3S	E	904	1	0,9,9	-	-	-		
9	EDO	A	909	-	3,3,3	0.70	0	2,2,2	0.84	0
9	EDO	C	911[B]	-	3,3,3	0.28	0	2,2,2	0.30	0
12	FES	H	201	2	0,4,4	-	-	-		
9	EDO	G	911	-	3,3,3	0.17	0	2,2,2	0.54	0
8	AST	A	907	-	0,3,3	-	-	0,3,3	-	-
7	GOL	E	912	-	5,5,5	0.14	0	5,5,5	0.57	0
9	EDO	G	915	-	3,3,3	0.28	0	2,2,2	0.26	0
5	F3S	C	904	1	0,9,9	-	-	-		
10	PEG	A	910	-	6,6,6	0.32	0	5,5,5	0.24	0
7	GOL	C	909	-	5,5,5	0.25	0	5,5,5	0.88	0
9	EDO	G	914	-	3,3,3	0.71	0	2,2,2	0.41	0
8	AST	C	905	-	0,3,3	-	-	0,3,3	-	-
3	MGD	A	901	4	47,52,52	0.89	2 (4%)	58,81,81	1.45	5 (8%)
6	PGE	A	905[A]	-	9,9,9	0.61	0	8,8,8	0.58	0
9	EDO	G	909[A]	-	3,3,3	0.23	0	2,2,2	0.52	0
9	EDO	A	911	-	3,3,3	0.19	0	2,2,2	0.73	0
9	EDO	A	908[B]	-	3,3,3	1.05	0	2,2,2	0.83	0
9	EDO	E	908	-	3,3,3	0.73	0	2,2,2	1.01	0
11	IPA	E	905	-	3,3,3	0.45	0	3,3,3	0.60	0
5	F3S	A	904	1	0,9,9	-	-	-		
9	EDO	G	910	-	3,3,3	0.14	0	2,2,2	0.38	0
12	FES	F	201	2	0,4,4	-	-	-		
3	MGD	E	901	4	47,52,52	0.97	2 (4%)	58,81,81	1.15	5 (8%)
7	GOL	A	906	-	5,5,5	0.50	0	5,5,5	1.00	0
9	EDO	C	910	-	3,3,3	0.57	0	2,2,2	0.61	0
9	EDO	C	914	-	3,3,3	1.02	0	2,2,2	0.80	0
8	AST	E	906	-	0,3,3	-	-	0,3,3	-	-
9	EDO	C	907	-	3,3,3	0.70	0	2,2,2	1.06	0
10	PEG	B	2301	-	6,6,6	0.31	0	5,5,5	0.25	0
6	PGE	A	905[B]	-	9,9,9	0.18	0	8,8,8	0.25	0
9	EDO	G	909[B]	-	3,3,3	0.34	0	2,2,2	0.51	0
3	MGD	C	903	4	47,52,52	0.96	3 (6%)	58,81,81	1.24	5 (8%)

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
12	FES	B	2302	2	-	-	0/1/1/1
9	EDO	E	907	-	-	1/1/1/1	-
3	MGD	E	903	4	-	4/22/66/66	0/6/6/6
9	EDO	A	914	-	-	0/1/1/1	-
9	EDO	A	912	-	-	0/1/1/1	-
3	MGD	A	902	4	-	5/22/66/66	0/6/6/6
7	GOL	G	913	-	-	4/4/4/4	-
6	PGE	G	907	-	-	5/7/7/7	-
9	EDO	C	915	-	-	0/1/1/1	-
9	EDO	A	916	-	-	0/1/1/1	-
3	MGD	G	902	4	-	5/22/66/66	0/6/6/6
9	EDO	C	911[A]	-	-	0/1/1/1	-
7	GOL	E	914	-	-	0/4/4/4	-
9	EDO	D	202	-	-	0/1/1/1	-
9	EDO	G	912	-	-	1/1/1/1	-
9	EDO	C	913	-	-	1/1/1/1	-
7	GOL	C	912	-	-	4/4/4/4	-
7	GOL	E	913	-	-	0/4/4/4	-
3	MGD	C	902	4	-	5/22/66/66	0/6/6/6
9	EDO	A	908[A]	-	-	1/1/1/1	-
9	EDO	E	909	-	-	0/1/1/1	-
7	GOL	C	908	-	-	4/4/4/4	-
9	EDO	E	910	-	-	1/1/1/1	-
9	EDO	E	911	-	-	1/1/1/1	-
5	F3S	G	904	1	-	-	0/3/3/3
9	EDO	A	915	-	-	1/1/1/1	-
12	FES	D	201	2	-	-	0/1/1/1
3	MGD	G	903	4	-	5/22/66/66	0/6/6/6
9	EDO	A	909	-	-	1/1/1/1	-
9	EDO	C	911[B]	-	-	1/1/1/1	-
5	F3S	E	904	1	-	-	0/3/3/3
12	FES	H	201	2	-	-	0/1/1/1
3	MGD	C	903	4	-	5/22/66/66	0/6/6/6
9	EDO	G	911	-	-	0/1/1/1	-
7	GOL	E	912	-	-	4/4/4/4	-
9	EDO	G	915	-	-	1/1/1/1	-
10	PEG	A	910	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	F3S	C	904	1	-	-	0/3/3/3
7	GOL	C	909	-	-	4/4/4/4	-
9	EDO	G	914	-	-	0/1/1/1	-
3	MGD	A	901	4	-	5/22/66/66	0/6/6/6
6	PGE	A	905[A]	-	-	3/7/7/7	-
9	EDO	G	909[A]	-	-	1/1/1/1	-
9	EDO	A	911	-	-	0/1/1/1	-
9	EDO	A	908[B]	-	-	0/1/1/1	-
9	EDO	E	908	-	-	1/1/1/1	-
5	F3S	A	904	1	-	-	0/3/3/3
9	EDO	G	910	-	-	1/1/1/1	-
12	FES	F	201	2	-	-	0/1/1/1
3	MGD	E	901	4	-	5/22/66/66	0/6/6/6
7	GOL	A	906	-	-	2/4/4/4	-
9	EDO	C	910	-	-	1/1/1/1	-
9	EDO	C	914	-	-	1/1/1/1	-
9	EDO	C	907	-	-	0/1/1/1	-
10	PEG	B	2301	-	-	3/4/4/4	-
6	PGE	A	905[B]	-	-	5/7/7/7	-
9	EDO	G	909[B]	-	-	1/1/1/1	-
7	GOL	G	905	-	-	4/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	902	MGD	PA-O3B	4.14	1.64	1.59
3	E	901	MGD	C23-C14	4.02	1.56	1.53
3	A	902	MGD	PA-O3B	3.44	1.63	1.59
3	C	903	MGD	C23-C14	3.40	1.56	1.53
3	A	901	MGD	PA-O3B	3.20	1.62	1.59
3	C	902	MGD	PA-O3B	3.00	1.62	1.59
3	G	903	MGD	PA-O3B	2.83	1.62	1.59
3	C	902	MGD	C23-C14	-2.82	1.51	1.53
3	C	903	MGD	PA-O3B	2.55	1.62	1.59
3	C	902	MGD	PB-O3B	2.52	1.62	1.59
3	E	903	MGD	C10-C11	-2.45	1.48	1.51
3	E	903	MGD	PA-O3B	2.42	1.62	1.59
3	E	901	MGD	PA-O3B	2.42	1.62	1.59
3	A	901	MGD	C23-C14	2.40	1.55	1.53
3	G	903	MGD	C10-C11	-2.23	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	903	MGD	C21-N20	2.11	1.39	1.36
3	E	903	MGD	PB-O3B	2.08	1.61	1.59
3	C	903	MGD	PB-O3B	2.06	1.61	1.59

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	MGD	O11-C23-C14	6.18	113.08	108.96
3	C	903	MGD	O11-C23-C14	5.35	112.53	108.96
3	A	901	MGD	C23-C14-N15	5.17	112.94	107.87
3	A	902	MGD	O11-C23-C14	4.19	111.76	108.96
3	E	901	MGD	C19-N20-C21	3.78	120.04	113.36
3	G	902	MGD	C23-C14-N15	3.78	111.58	107.87
3	C	903	MGD	C23-C14-N15	3.51	111.32	107.87
3	G	903	MGD	C23-C14-N15	3.48	111.28	107.87
3	A	902	MGD	C19-N20-C21	3.46	119.47	113.36
3	C	902	MGD	C19-N20-C21	3.42	119.39	113.36
3	A	902	MGD	C23-C14-N15	3.36	111.17	107.87
3	E	903	MGD	C19-N20-C21	3.35	119.27	113.36
3	G	902	MGD	O11-C23-C14	3.22	111.11	108.96
3	C	902	MGD	C23-C14-N15	3.22	111.03	107.87
3	A	902	MGD	C4'-O4'-C1'	-3.04	102.76	109.47
3	G	902	MGD	C19-N20-C21	3.03	118.71	113.36
3	C	902	MGD	C4'-O4'-C1'	-2.90	103.07	109.47
3	E	903	MGD	O11-C23-C14	2.80	110.83	108.96
3	A	901	MGD	O2B-PB-O3B	2.80	114.84	107.27
3	G	902	MGD	O2B-PB-O3B	2.80	114.84	107.27
3	E	903	MGD	C4'-O4'-C1'	-2.76	103.37	109.47
3	G	902	MGD	C17-C16-N15	2.73	123.70	116.27
3	G	903	MGD	C4'-O4'-C1'	-2.70	103.52	109.47
3	C	903	MGD	O2B-PB-O3B	2.68	114.52	107.27
3	E	901	MGD	C23-C14-N15	2.66	110.48	107.87
3	E	901	MGD	O2B-PB-O3B	2.59	114.27	107.27
3	E	903	MGD	C23-C14-N15	2.54	110.36	107.87
3	A	901	MGD	O2A-PA-O1A	2.48	123.98	112.44
3	A	902	MGD	O11-C23-N22	-2.44	106.39	108.61
3	G	902	MGD	O2A-PA-O1A	2.39	123.57	112.44
3	E	901	MGD	O11-C23-N22	-2.39	106.44	108.61
3	G	903	MGD	O11-C23-N22	-2.35	106.47	108.61
3	C	902	MGD	O11-C23-C14	2.32	110.51	108.96
3	E	901	MGD	C17-C16-N15	2.27	122.47	116.27
3	G	903	MGD	C19-N20-C21	2.27	117.36	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	903	MGD	O11-C23-N22	-2.22	106.59	108.61
3	E	903	MGD	O2B-PB-O1B	2.20	122.69	112.44
3	C	903	MGD	C19-N20-C21	2.20	117.24	113.36
3	A	901	MGD	C17-C16-N15	2.09	121.95	116.27
3	C	902	MGD	C17-C16-N15	2.04	121.84	116.27
3	G	902	MGD	O4'-C1'-N9	-2.03	103.76	108.36

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	MGD	C5'-O5'-PB-O1B
3	A	902	MGD	C5'-O5'-PB-O1B
3	A	902	MGD	C5'-O5'-PB-O3B
3	C	902	MGD	C5'-O5'-PB-O1B
3	C	903	MGD	C5'-O5'-PB-O1B
3	E	901	MGD	C5'-O5'-PB-O1B
3	E	903	MGD	PA-O3B-PB-O5'
3	E	903	MGD	C5'-O5'-PB-O1B
3	E	903	MGD	C5'-O5'-PB-O3B
7	A	906	GOL	O1-C1-C2-C3
7	C	912	GOL	O1-C1-C2-C3
7	E	912	GOL	O1-C1-C2-C3
7	E	912	GOL	C1-C2-C3-O3
7	G	905	GOL	C1-C2-C3-O3
7	G	913	GOL	C1-C2-C3-O3
6	A	905[B]	PGE	O2-C3-C4-O3
7	C	909	GOL	O2-C2-C3-O3
7	C	912	GOL	O2-C2-C3-O3
7	E	912	GOL	O1-C1-C2-O2
7	G	905	GOL	O2-C2-C3-O3
6	A	905[A]	PGE	O2-C3-C4-O3
6	A	905[B]	PGE	O3-C5-C6-O4
7	C	908	GOL	O1-C1-C2-C3
7	C	909	GOL	O1-C1-C2-C3
7	C	909	GOL	C1-C2-C3-O3
7	C	912	GOL	C1-C2-C3-O3
7	G	905	GOL	O1-C1-C2-C3
7	G	913	GOL	O1-C1-C2-C3
7	A	906	GOL	O1-C1-C2-O2
7	C	908	GOL	O1-C1-C2-O2
7	C	912	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	G	913	GOL	O1-C1-C2-O2
9	C	911[B]	EDO	O1-C1-C2-O2
9	G	912	EDO	O1-C1-C2-O2
6	G	907	PGE	O3-C5-C6-O4
7	E	912	GOL	O2-C2-C3-O3
7	G	913	GOL	O2-C2-C3-O3
3	A	901	MGD	O4'-C4'-C5'-O5'
3	E	901	MGD	O4'-C4'-C5'-O5'
9	C	914	EDO	O1-C1-C2-O2
9	E	910	EDO	O1-C1-C2-O2
9	G	909[B]	EDO	O1-C1-C2-O2
3	G	902	MGD	O4'-C4'-C5'-O5'
7	C	909	GOL	O1-C1-C2-O2
3	A	901	MGD	C3'-C4'-C5'-O5'
3	G	902	MGD	C3'-C4'-C5'-O5'
3	A	901	MGD	PA-O3B-PB-O5'
3	A	902	MGD	PA-O3B-PB-O5'
3	C	902	MGD	PA-O3B-PB-O5'
3	C	903	MGD	PA-O3B-PB-O5'
3	E	901	MGD	PA-O3B-PB-O5'
3	G	902	MGD	PA-O3B-PB-O5'
3	G	903	MGD	PA-O3B-PB-O5'
7	G	905	GOL	O1-C1-C2-O2
6	A	905[A]	PGE	O1-C1-C2-O2
6	A	905[A]	PGE	C6-C5-O3-C4
6	A	905[B]	PGE	C6-C5-O3-C4
7	C	908	GOL	C1-C2-C3-O3
6	A	905[B]	PGE	C1-C2-O2-C3
6	G	907	PGE	C4-C3-O2-C2
6	G	907	PGE	C6-C5-O3-C4
6	A	905[B]	PGE	C4-C3-O2-C2
3	C	903	MGD	O4'-C4'-C5'-O5'
10	B	2301	PEG	C1-C2-O2-C3
3	A	902	MGD	C5'-O5'-PB-O2B
3	C	902	MGD	C5'-O5'-PB-O2B
3	C	902	MGD	C5'-O5'-PB-O3B
3	G	902	MGD	C5'-O5'-PB-O1B
3	G	903	MGD	C5'-O5'-PB-O1B
3	G	903	MGD	C5'-O5'-PB-O2B
3	G	903	MGD	C5'-O5'-PB-O3B
10	A	910	PEG	O2-C3-C4-O4
6	G	907	PGE	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
9	A	909	EDO	O1-C1-C2-O2
3	C	903	MGD	C3'-C4'-C5'-O5'
9	C	910	EDO	O1-C1-C2-O2
9	C	913	EDO	O1-C1-C2-O2
9	E	907	EDO	O1-C1-C2-O2
9	E	908	EDO	O1-C1-C2-O2
9	G	915	EDO	O1-C1-C2-O2
3	E	901	MGD	C3'-C4'-C5'-O5'
3	E	903	MGD	PB-O3B-PA-O1A
9	E	911	EDO	O1-C1-C2-O2
9	G	909[A]	EDO	O1-C1-C2-O2
6	G	907	PGE	C3-C4-O3-C5
10	B	2301	PEG	C4-C3-O2-C2
9	A	908[A]	EDO	O1-C1-C2-O2
9	G	910	EDO	O1-C1-C2-O2
3	C	903	MGD	PB-O3B-PA-O2A
3	G	903	MGD	PB-O3B-PA-O2A
10	A	910	PEG	C4-C3-O2-C2
10	B	2301	PEG	O1-C1-C2-O2
7	C	908	GOL	O2-C2-C3-O3
10	A	910	PEG	C1-C2-O2-C3
9	A	915	EDO	O1-C1-C2-O2
3	A	901	MGD	PB-O3B-PA-O2A
3	A	902	MGD	PB-O3B-PA-O2A
3	C	902	MGD	PB-O3B-PA-O2A
3	E	901	MGD	PB-O3B-PA-O2A
3	G	902	MGD	PB-O3B-PA-O2A

There are no ring outliers.

34 monomers are involved in 89 short contacts:

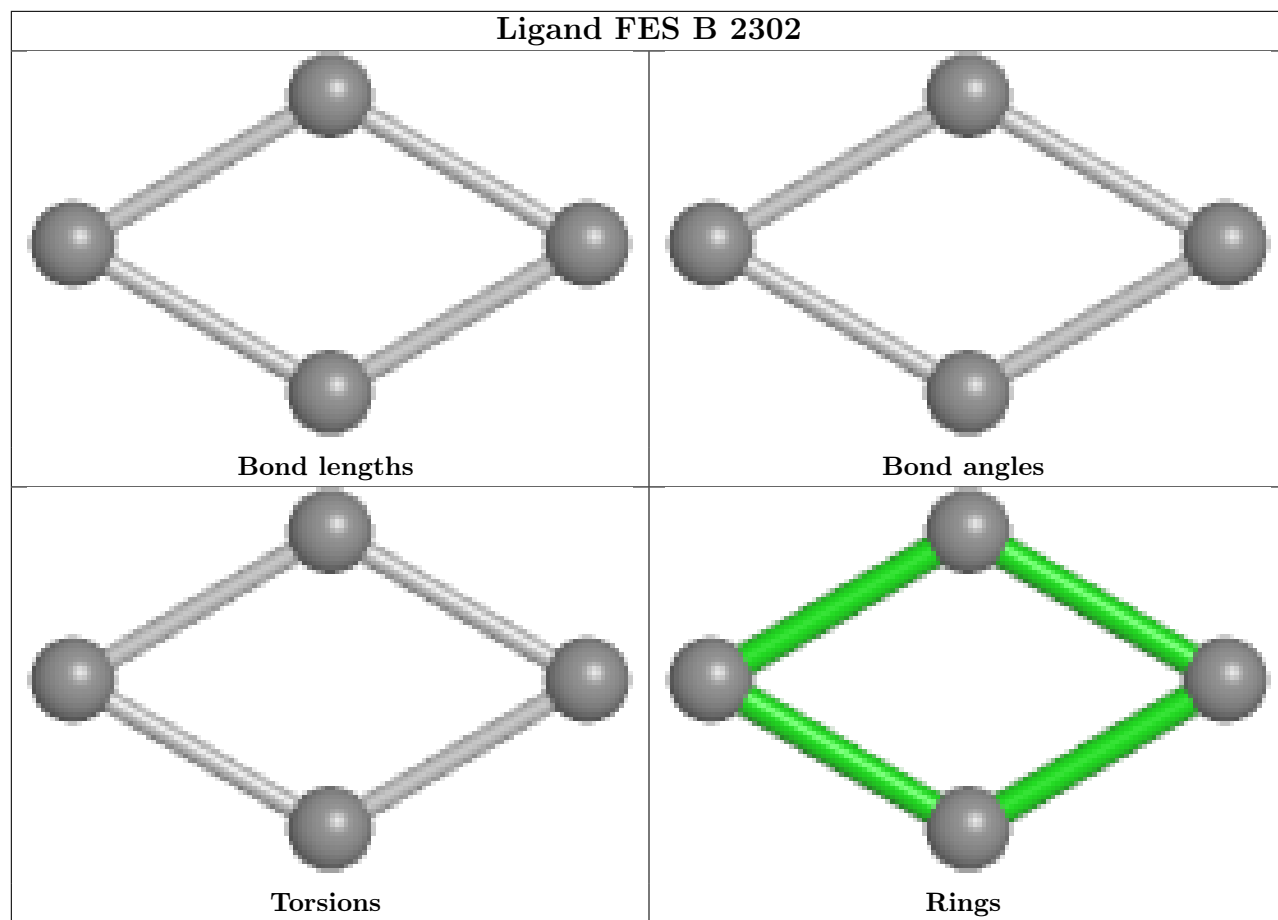
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	914	EDO	2	0
9	A	912	EDO	2	0
7	G	913	GOL	3	0
6	G	907	PGE	1	0
9	A	916	EDO	1	0
9	C	911[A]	EDO	3	0
7	E	914	GOL	1	0
9	D	202	EDO	1	0
9	G	912	EDO	1	0
7	C	912	GOL	4	0

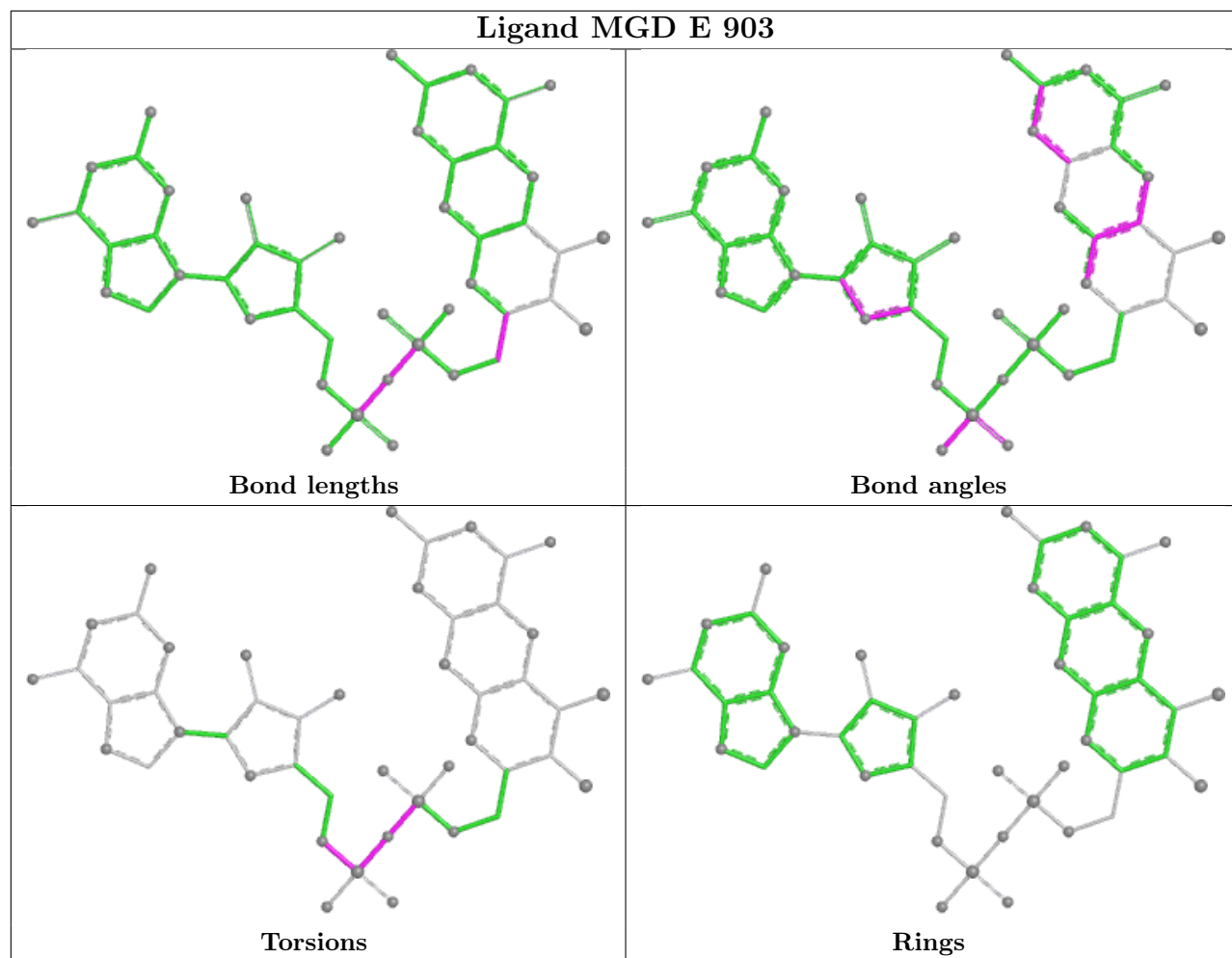
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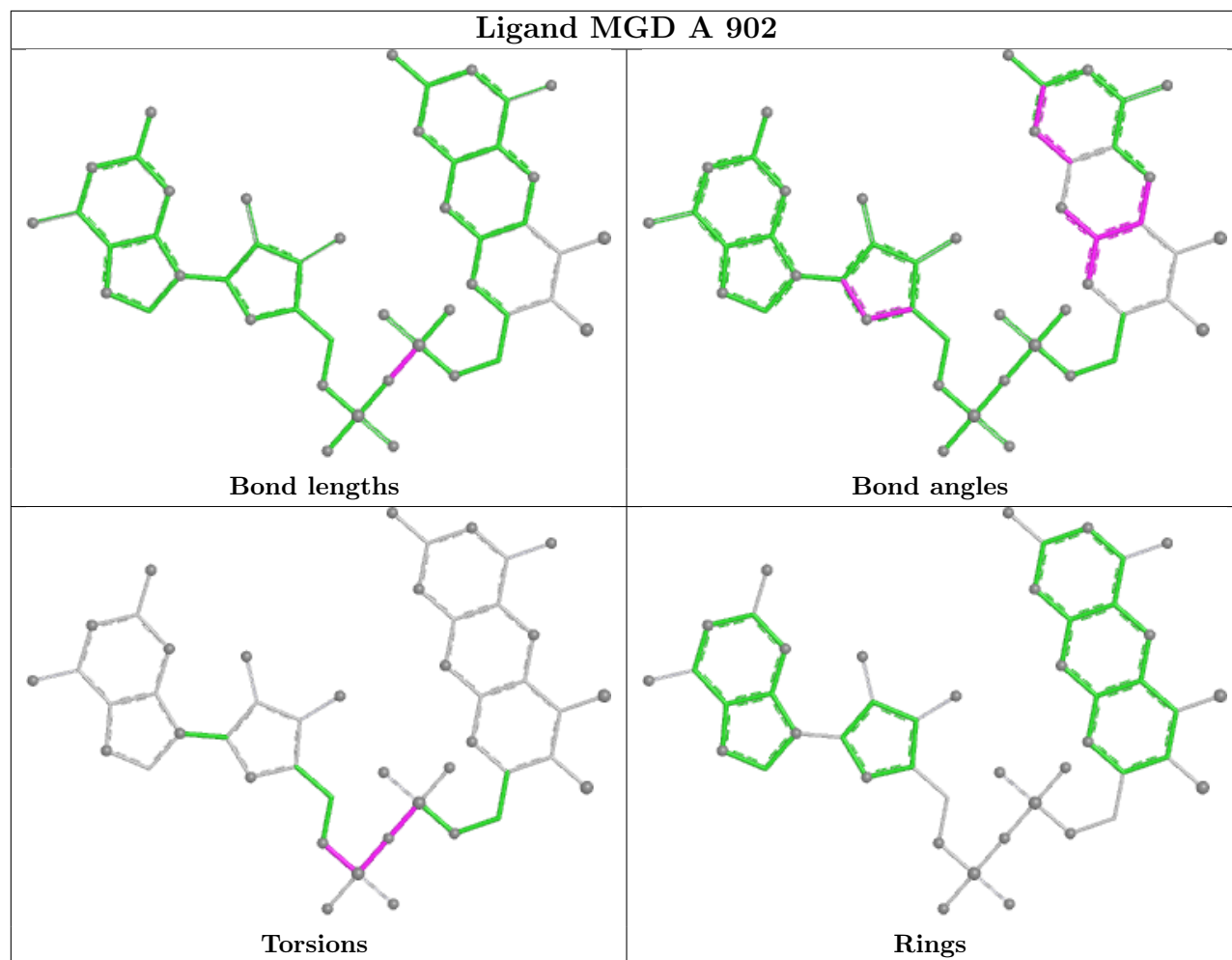
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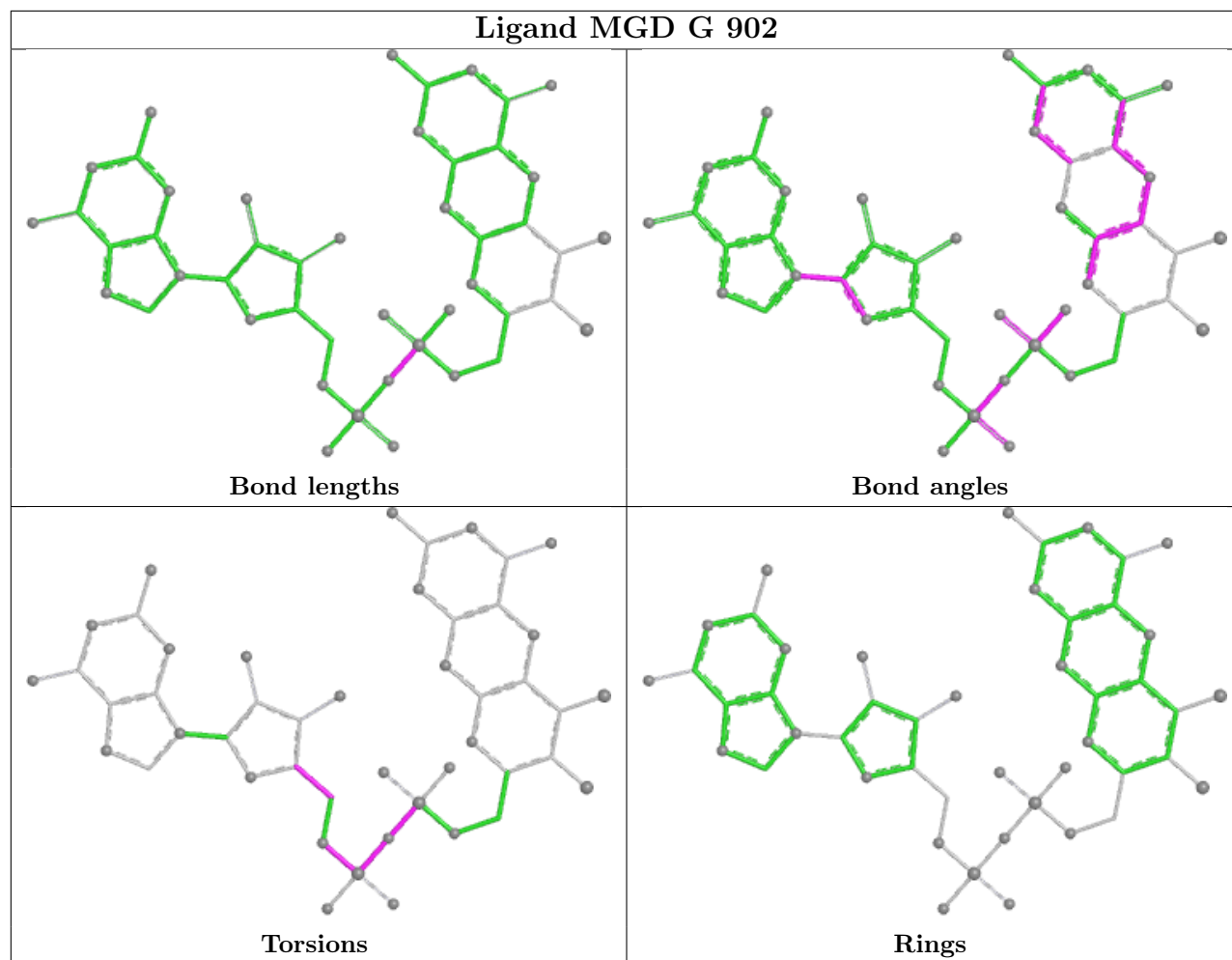
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	908[A]	EDO	7	0
11	A	913	IPA	3	0
11	C	906	IPA	4	0
11	G	908	IPA	7	0
7	G	905	GOL	1	0
3	G	903	MGD	1	0
9	A	909	EDO	8	0
9	C	911[B]	EDO	1	0
7	E	912	GOL	7	0
9	G	915	EDO	3	0
10	A	910	PEG	3	0
7	C	909	GOL	2	0
9	G	914	EDO	2	0
3	A	901	MGD	1	0
6	A	905[A]	PGE	5	0
9	A	908[B]	EDO	5	0
3	E	901	MGD	2	0
7	A	906	GOL	2	0
9	C	910	EDO	1	0
8	E	906	AST	1	0
9	C	907	EDO	2	0
10	B	2301	PEG	4	0
9	G	909[B]	EDO	2	0
3	C	903	MGD	3	0

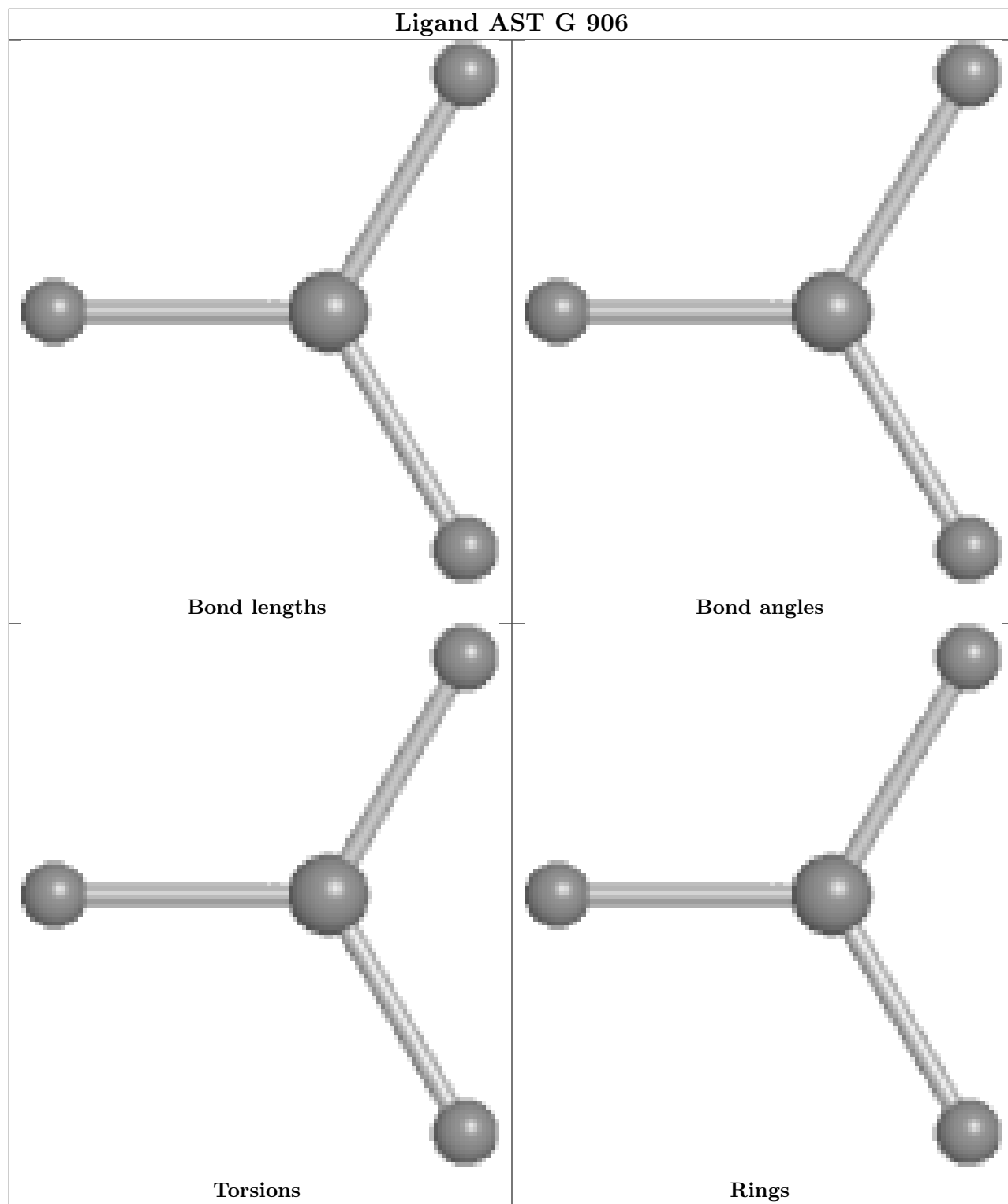
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

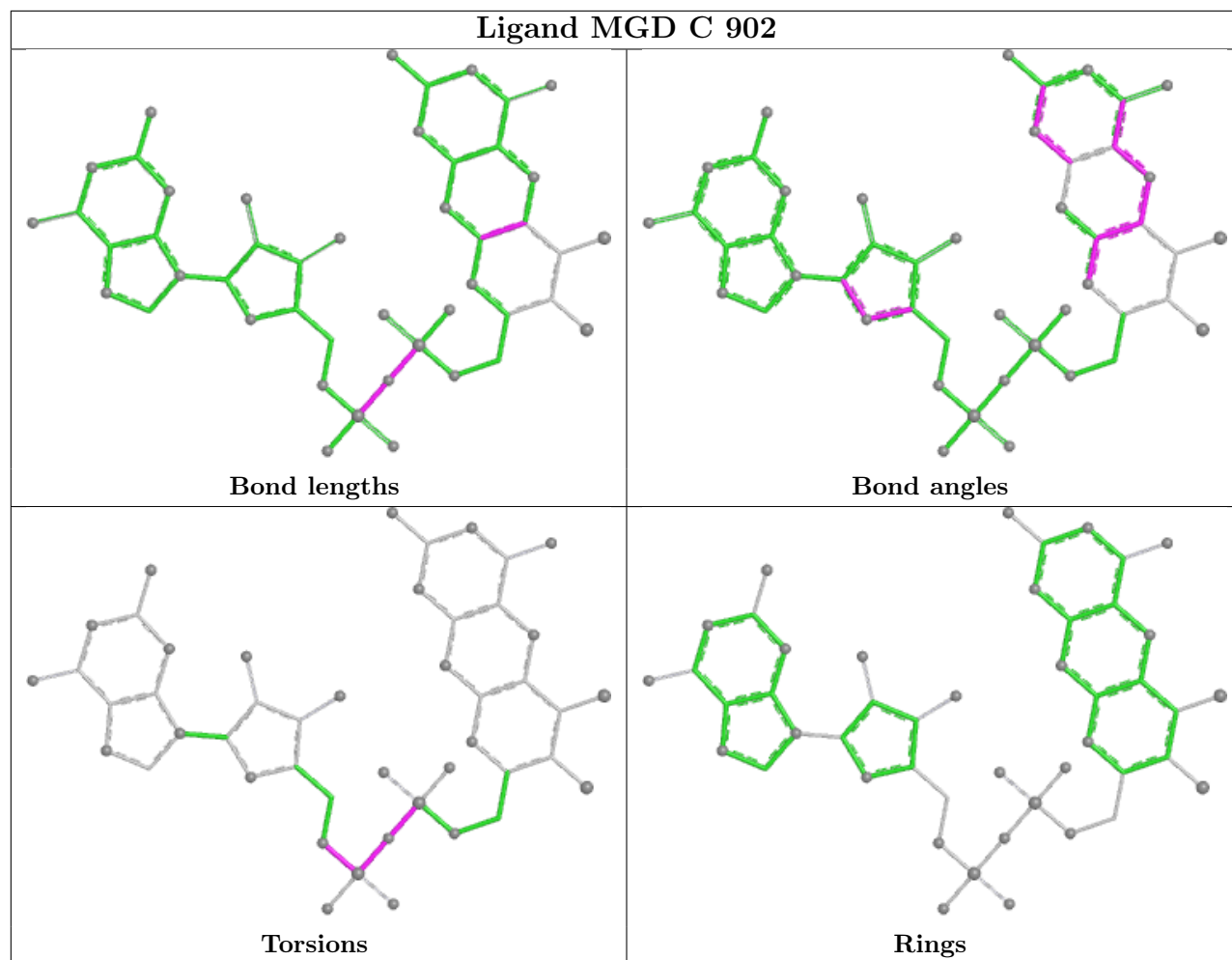


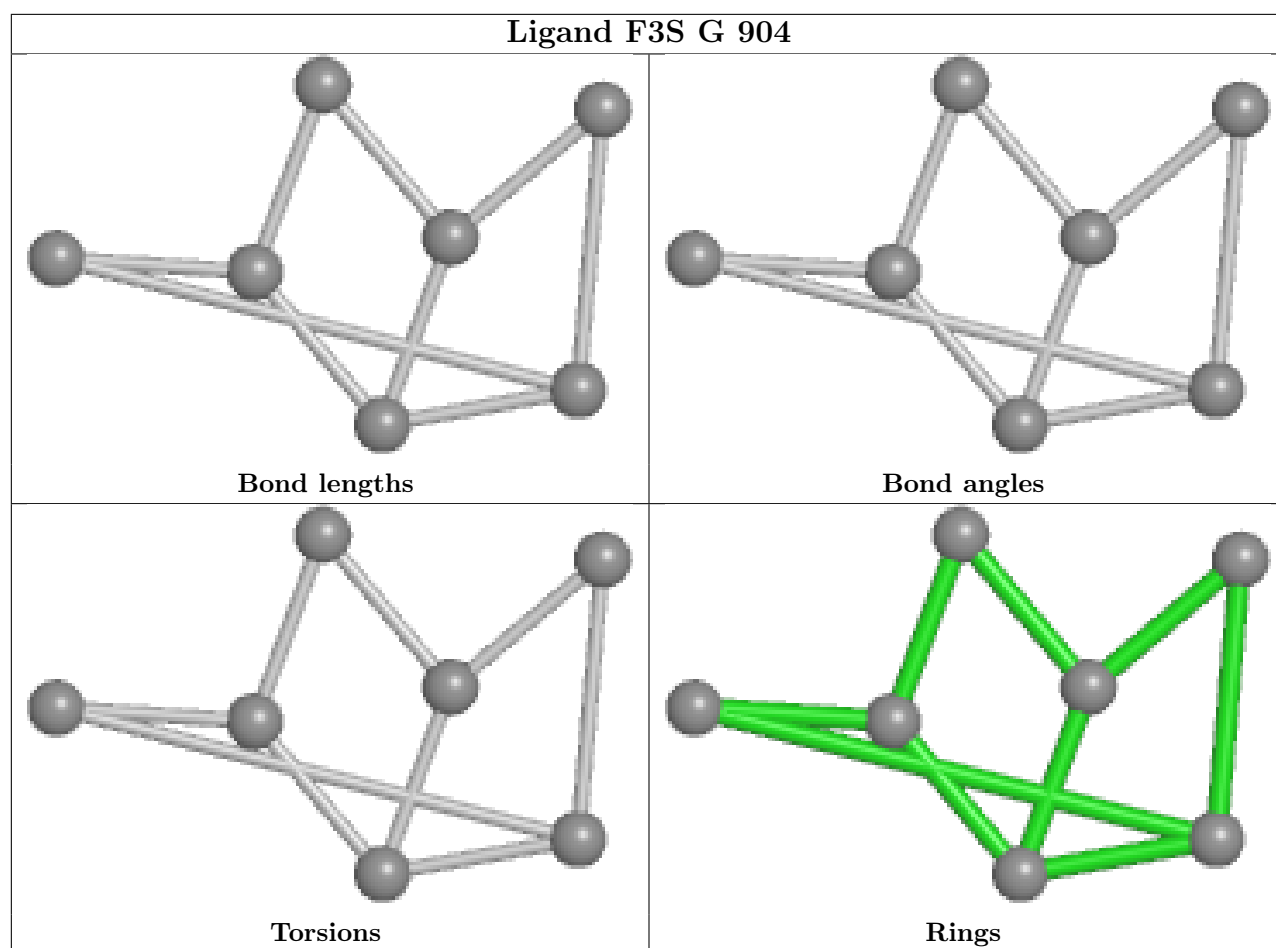


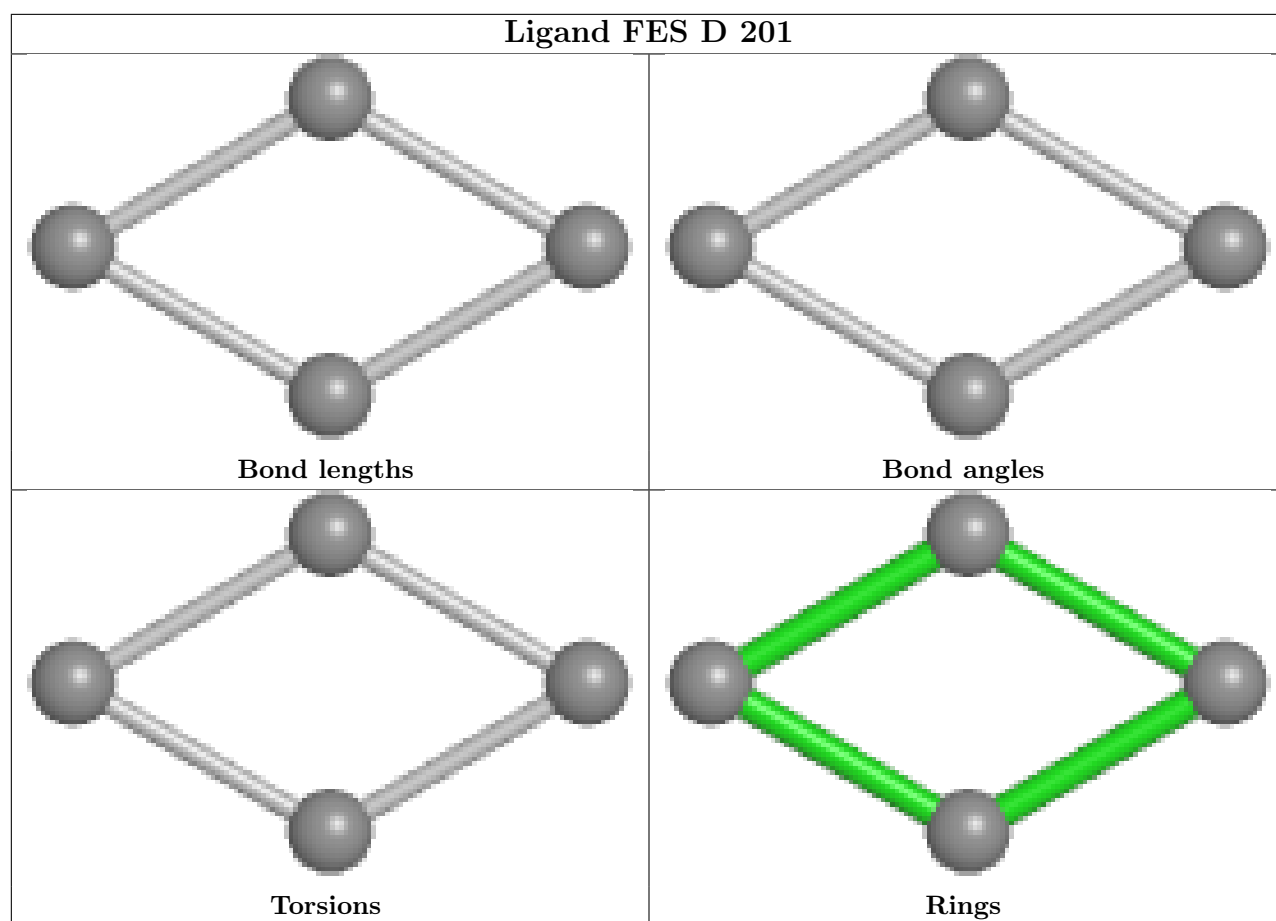


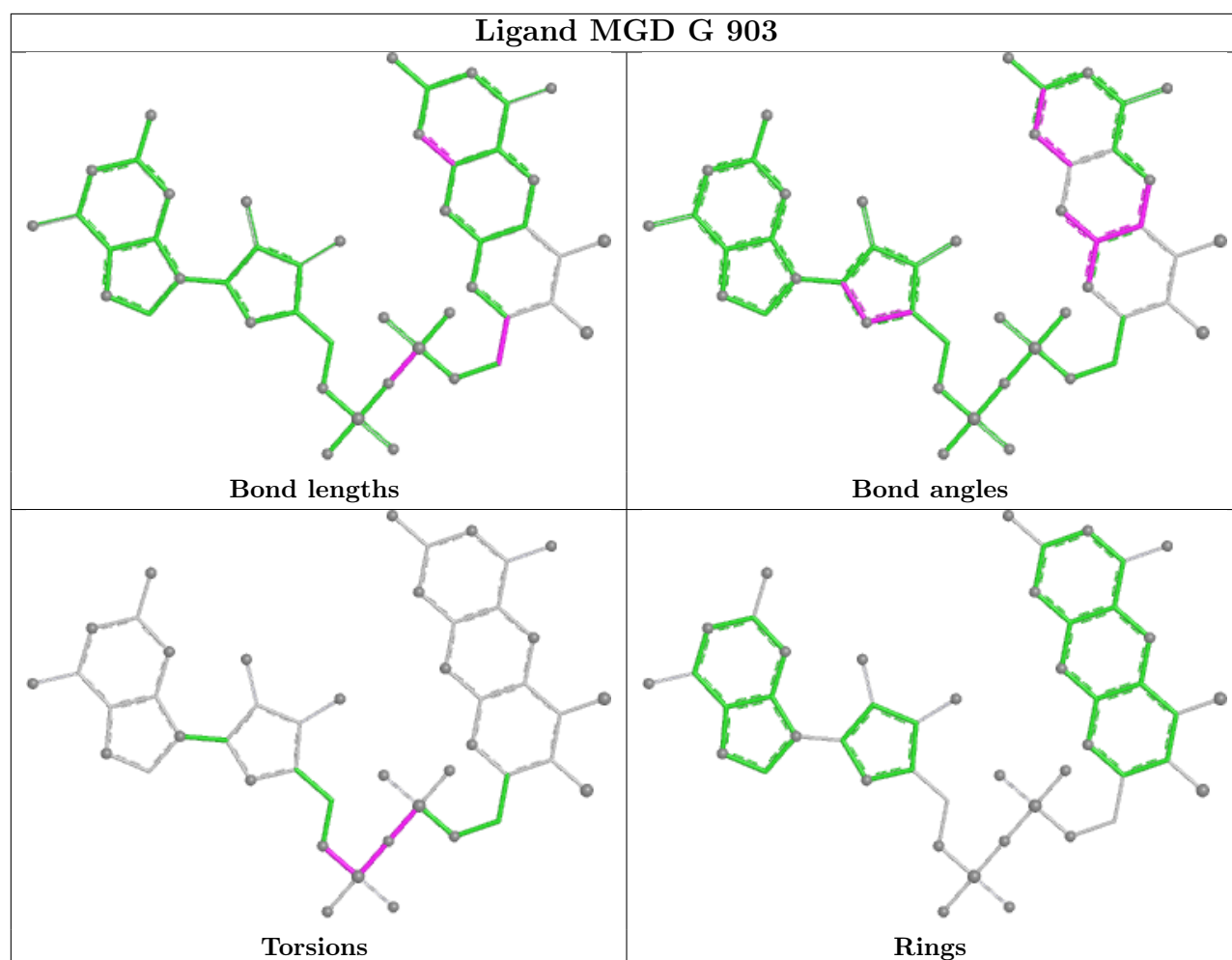


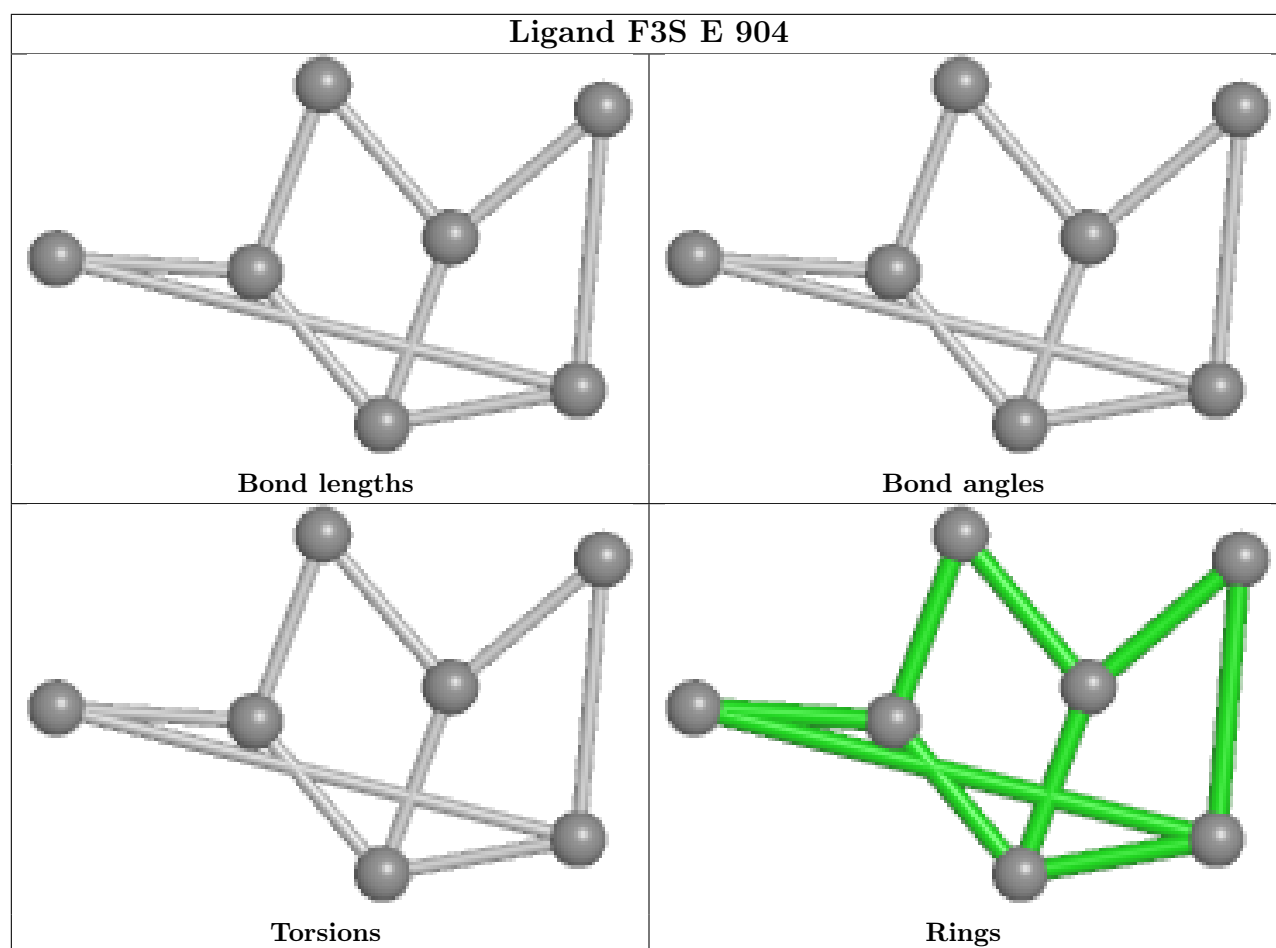


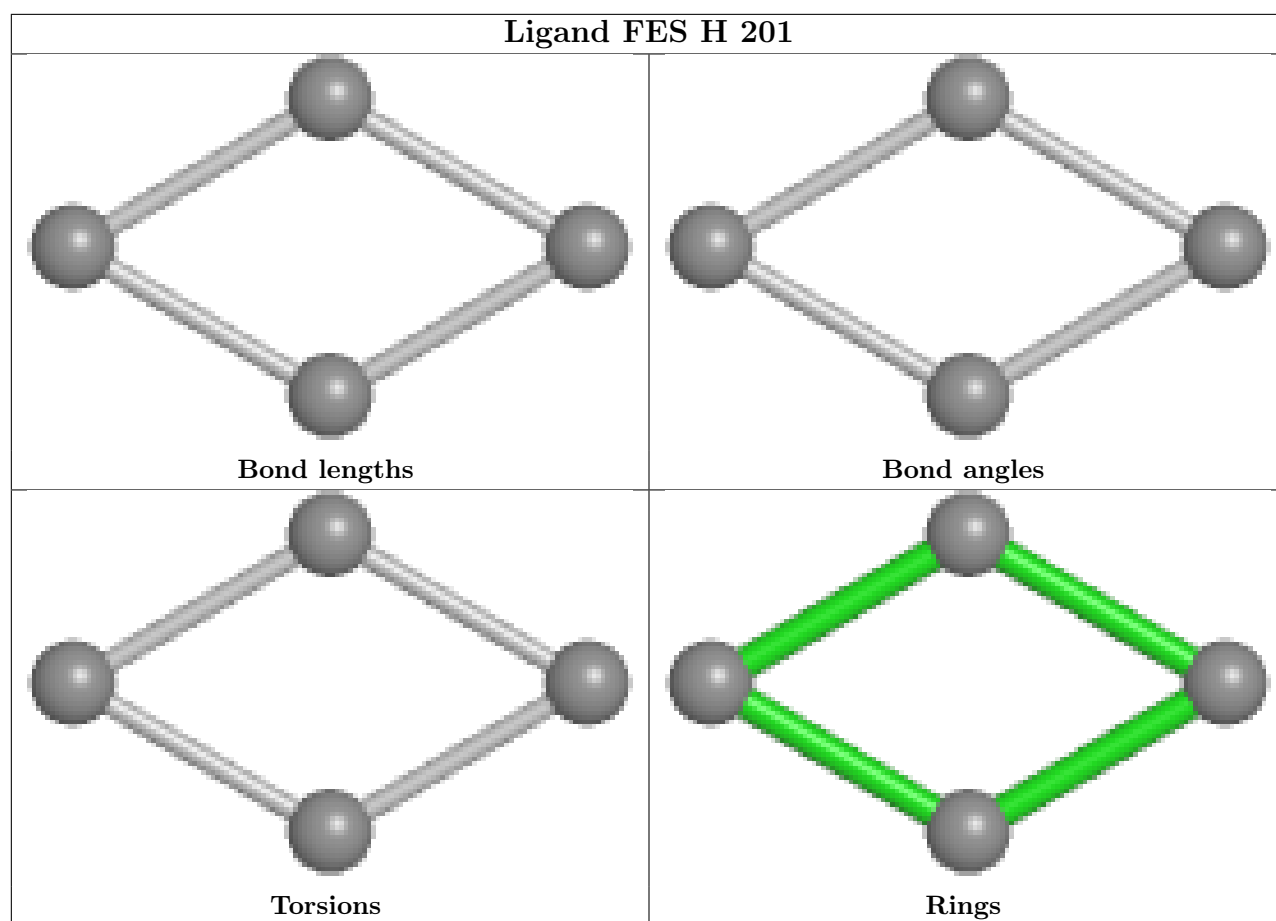


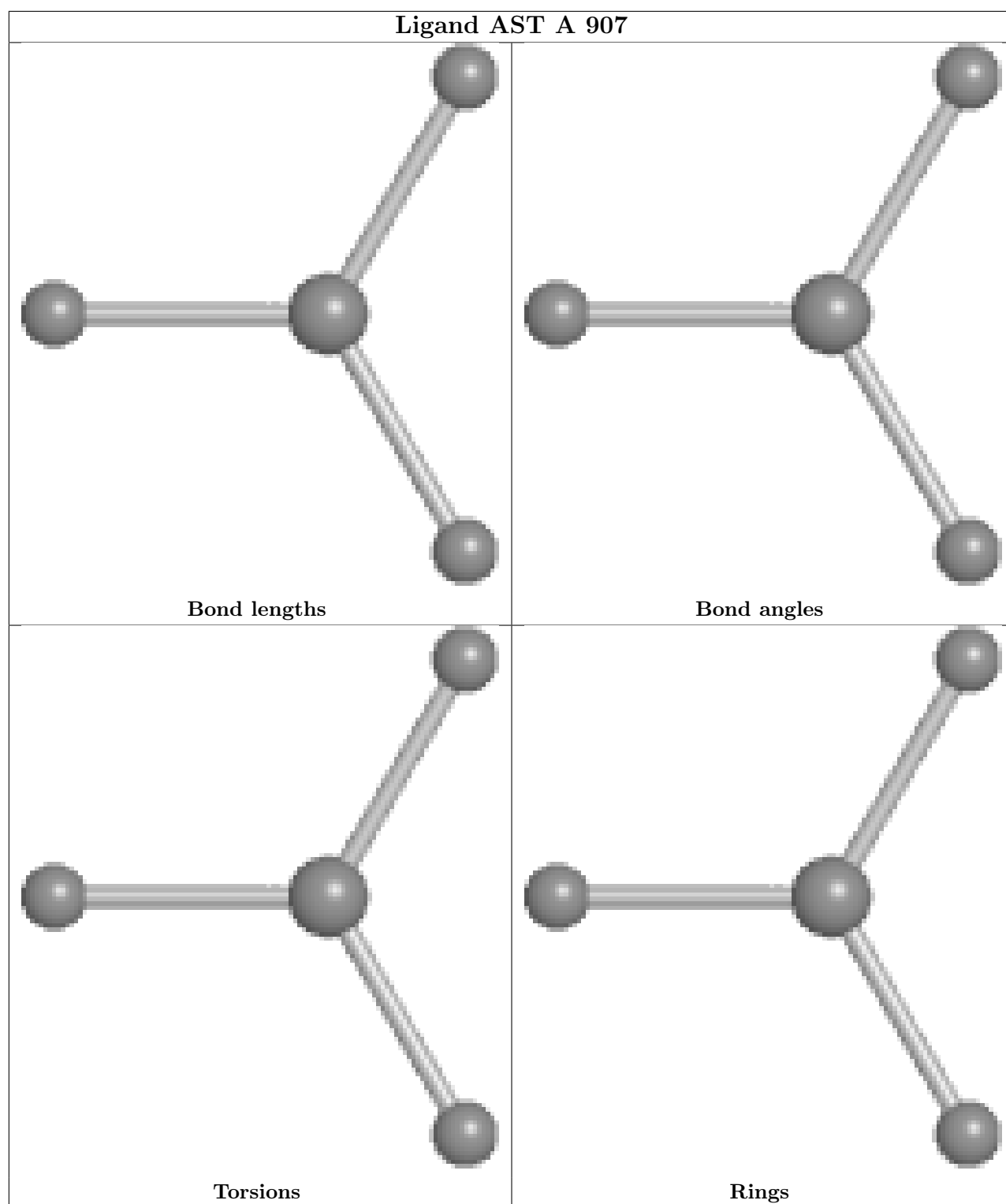


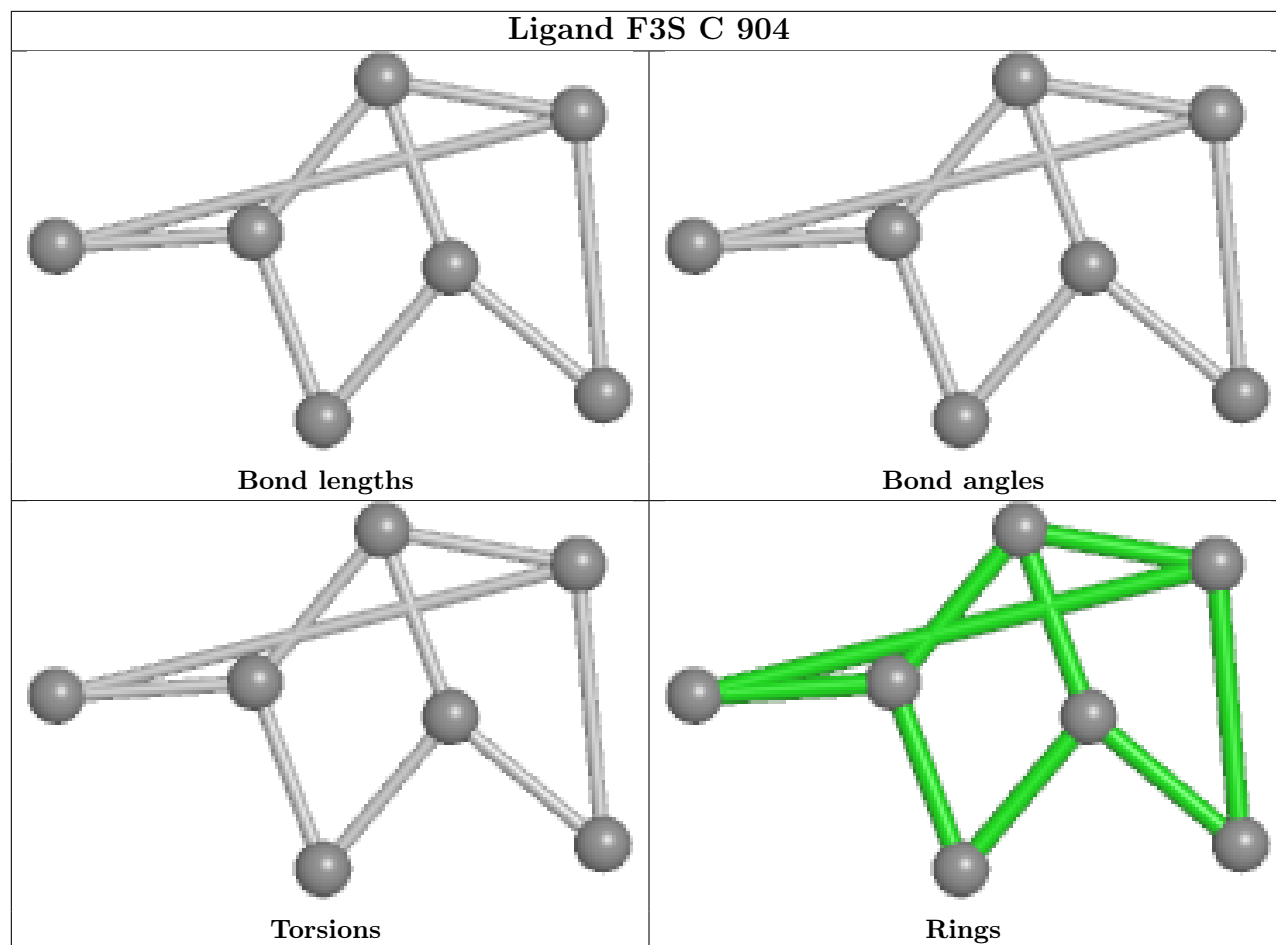


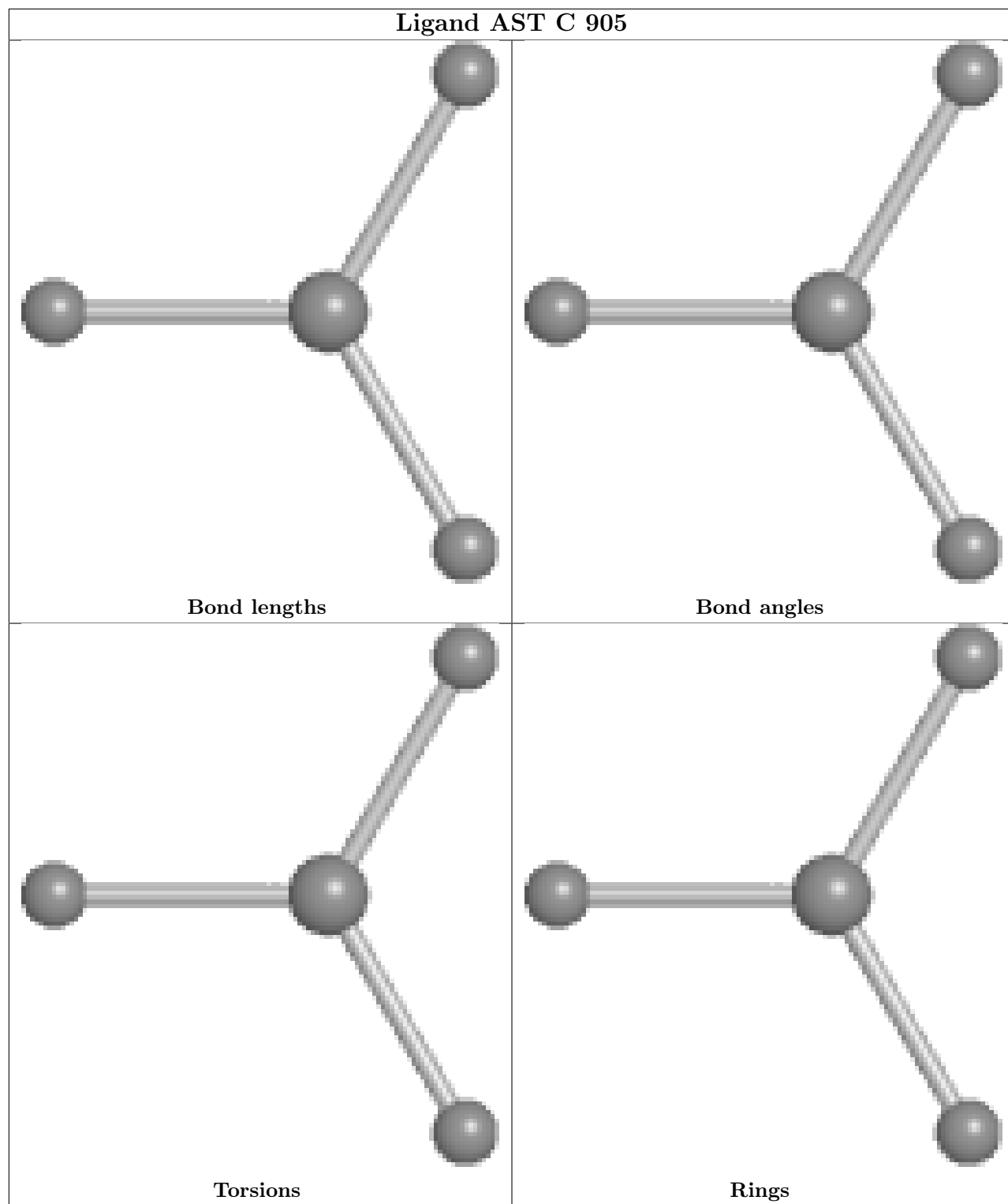


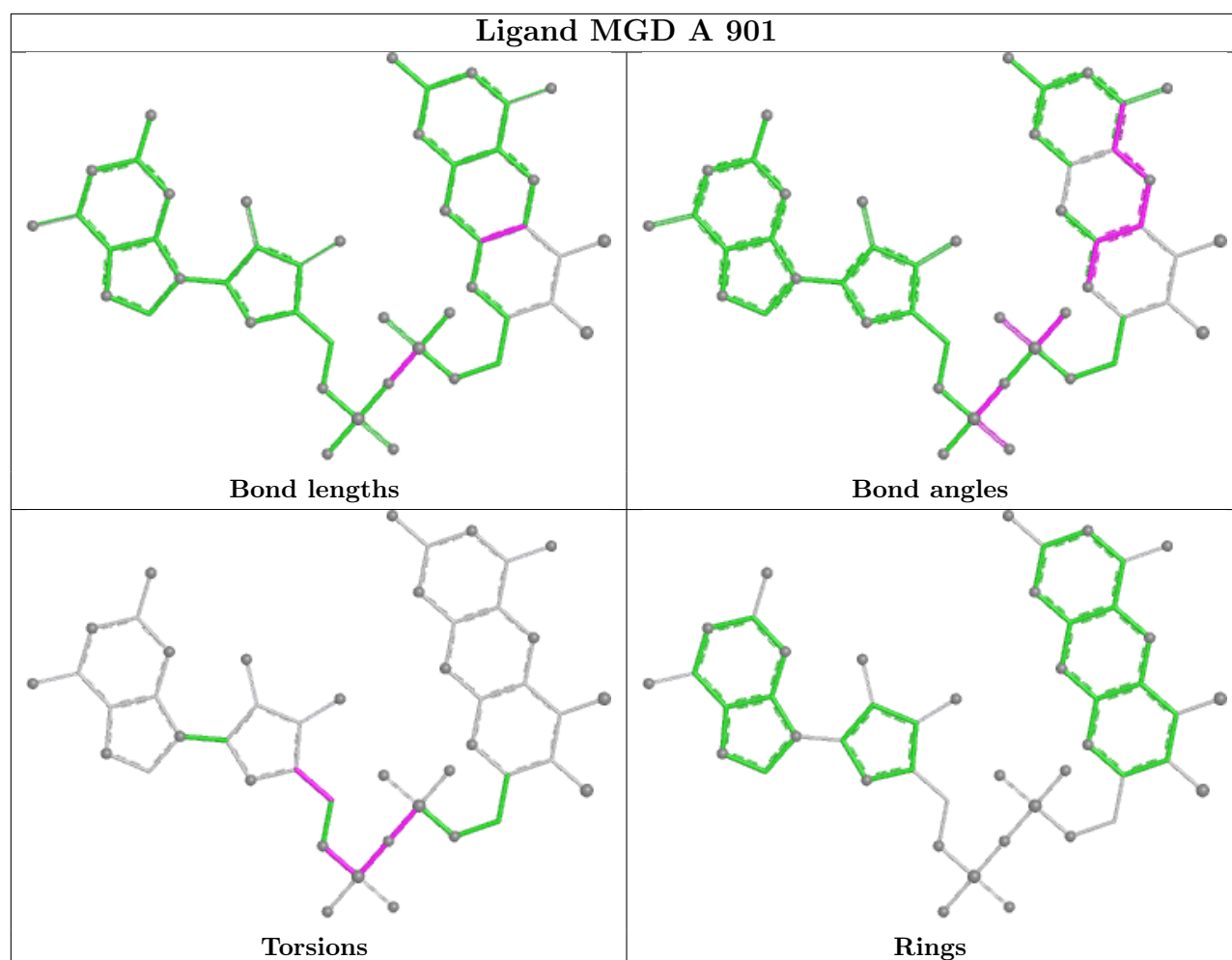




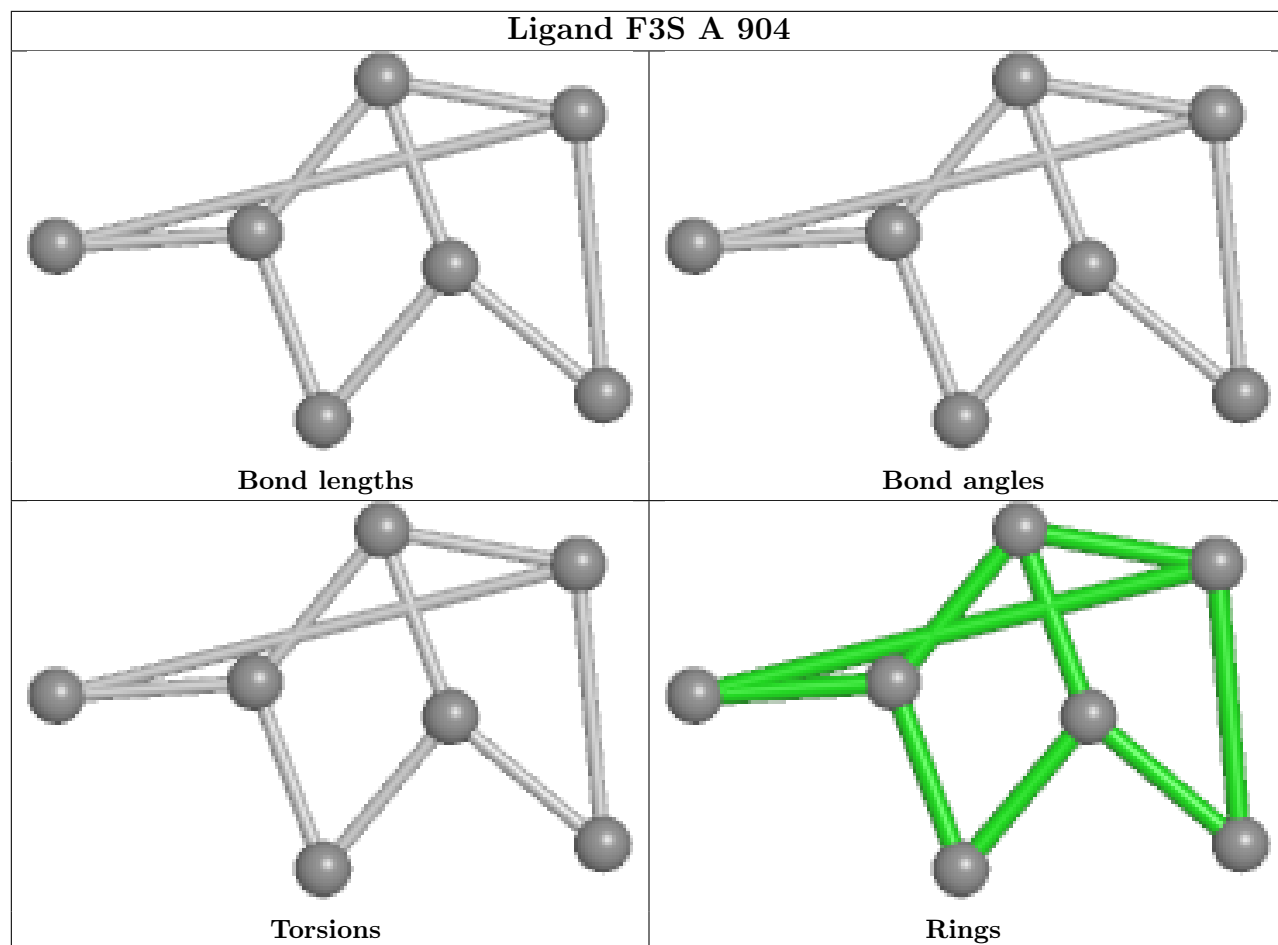


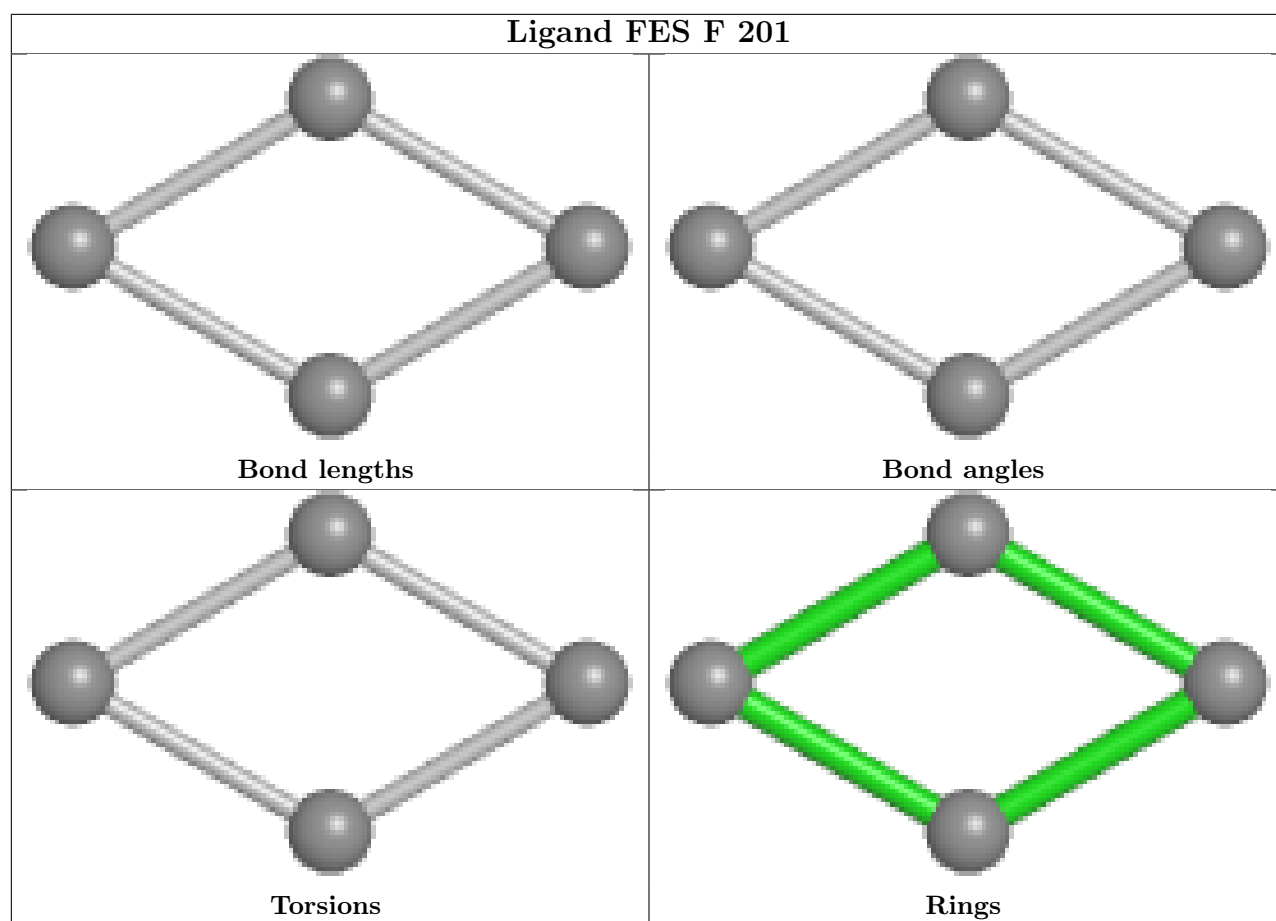


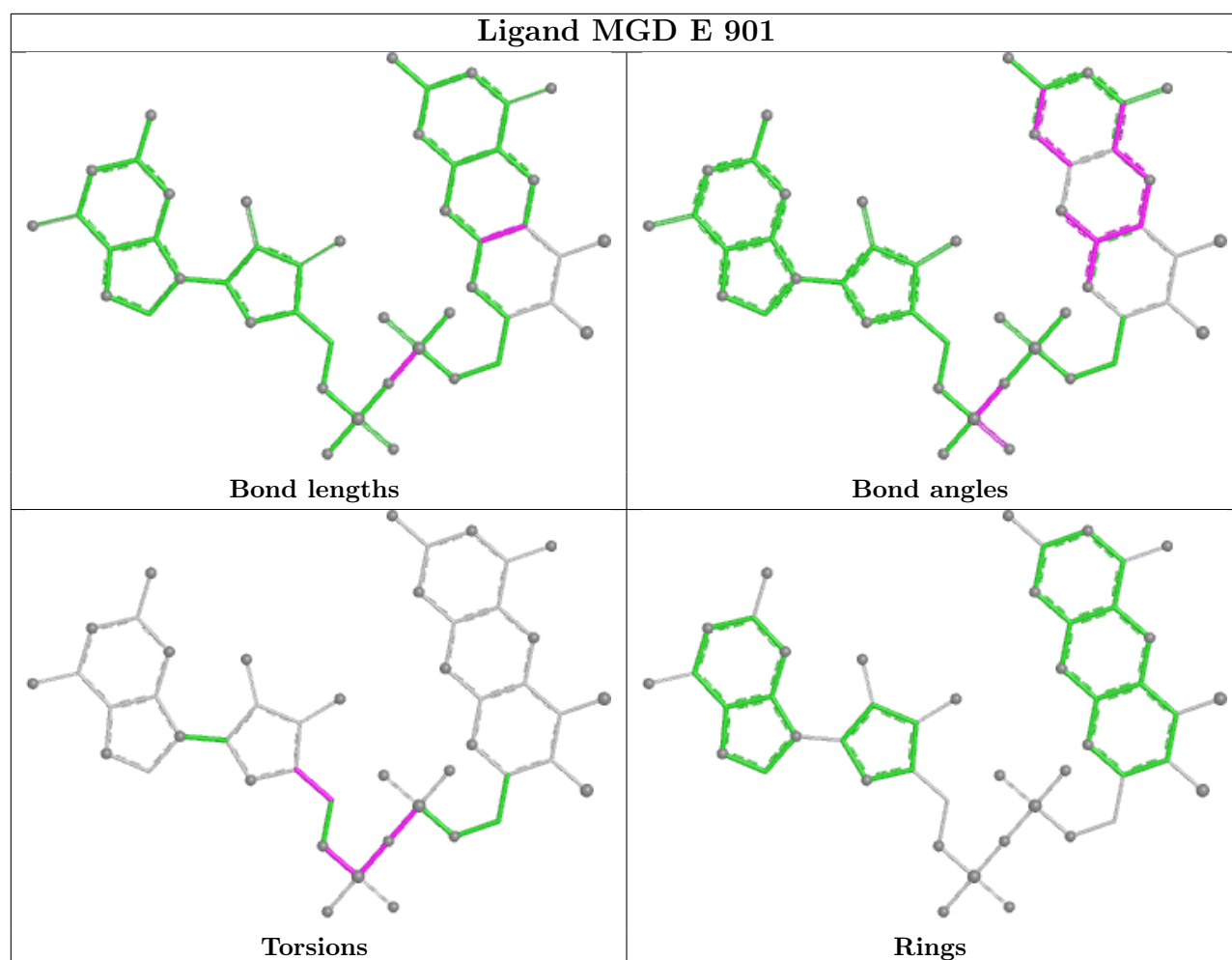


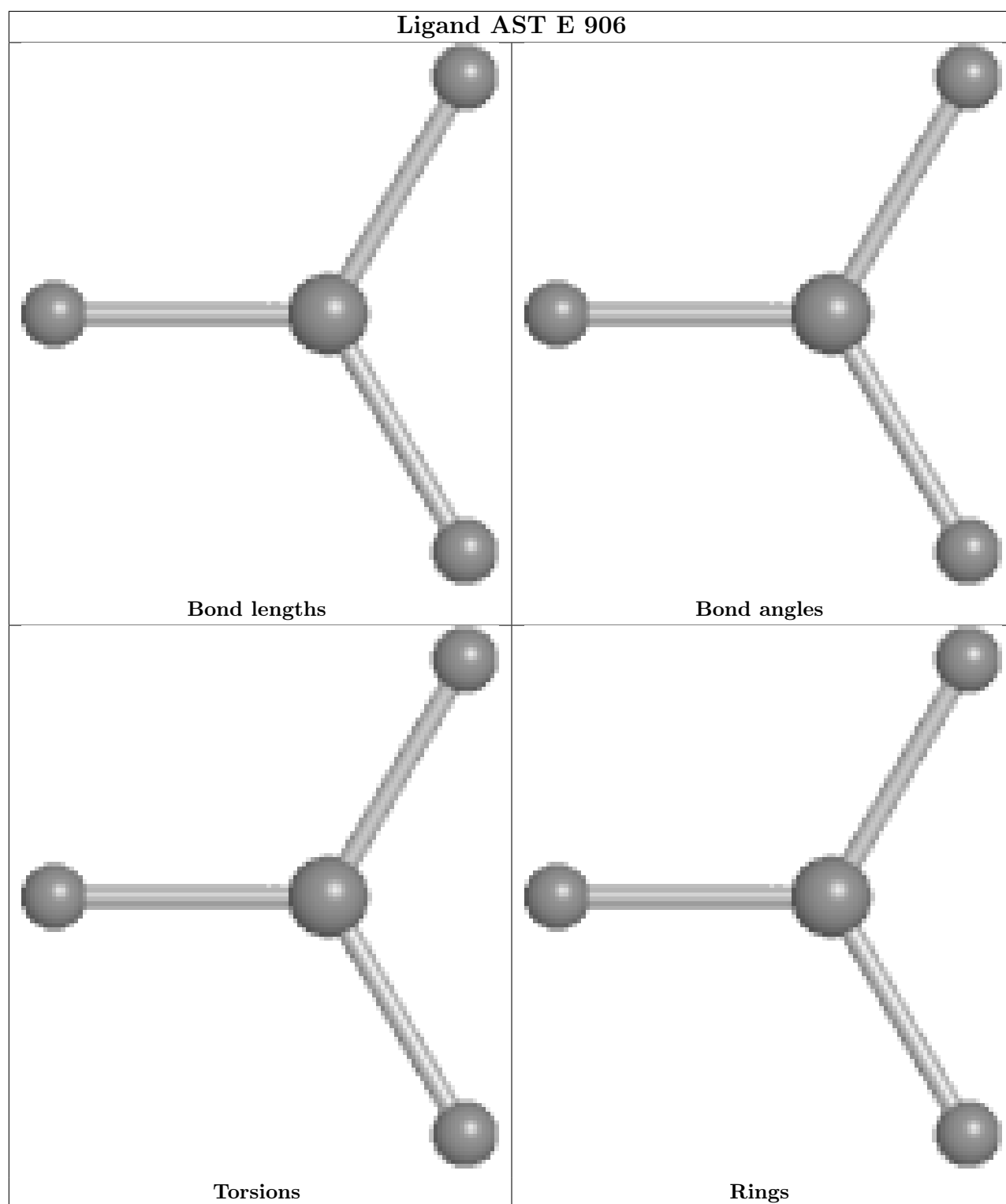


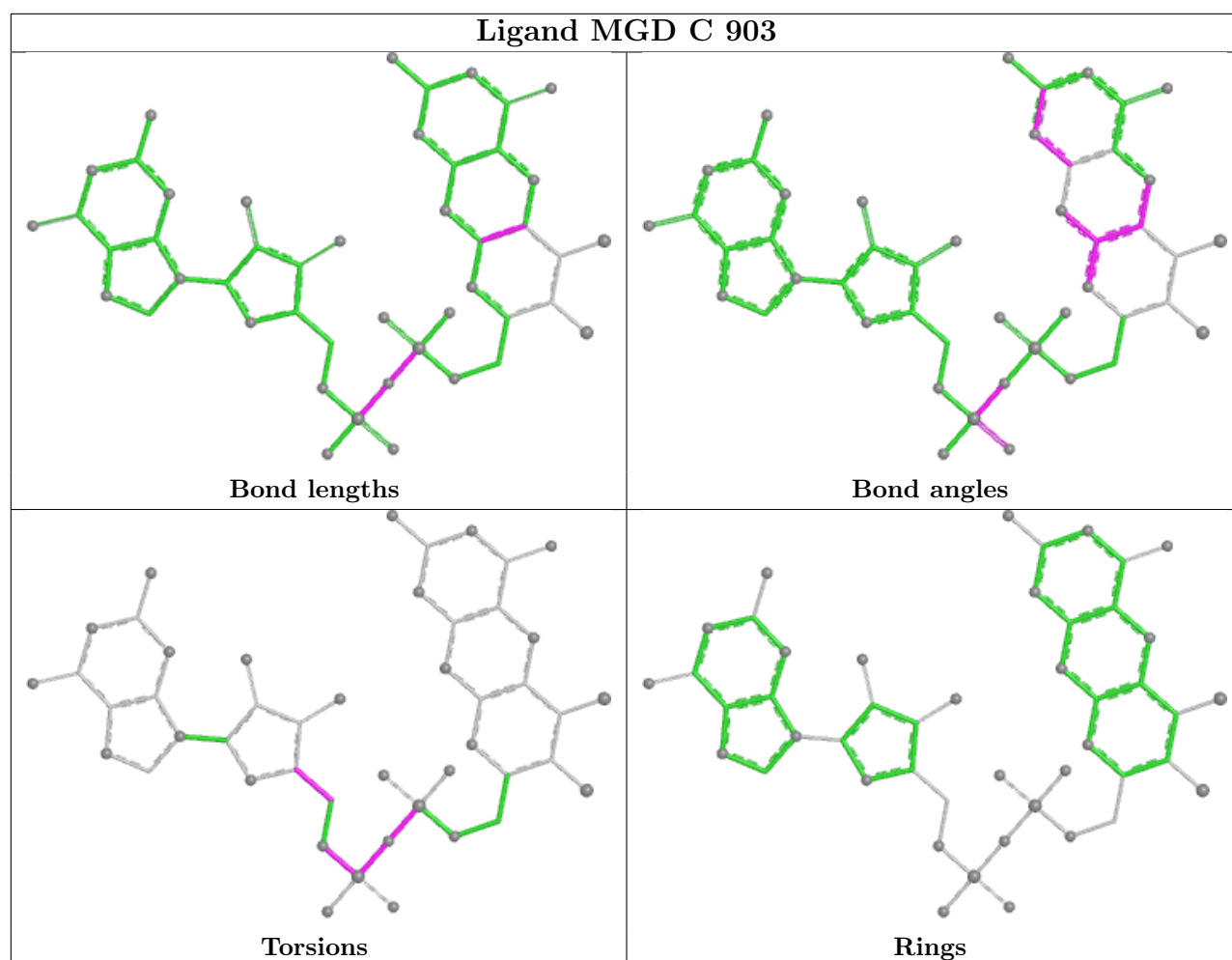
Ligand F3S A 904











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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9	
1	A	823/823 (100%)	-0.18	4 (0%)	87	90	5, 13, 22, 33	8 (0%)
1	C	822/823 (99%)	-0.15	4 (0%)	87	90	6, 13, 22, 36	13 (1%)
1	E	822/823 (99%)	-0.18	1 (0%)	92	92	4, 13, 22, 33	8 (0%)
1	G	822/823 (99%)	-0.16	2 (0%)	91	92	5, 13, 22, 34	10 (1%)
2	B	134/134 (100%)	-0.02	3 (2%)	62	73	5, 13, 22, 35	3 (2%)
2	D	134/134 (100%)	-0.04	3 (2%)	62	73	5, 14, 20, 34	4 (2%)
2	F	134/134 (100%)	0.01	4 (2%)	52	65	6, 14, 22, 32	3 (2%)
2	H	134/134 (100%)	0.01	3 (2%)	62	73	6, 13, 23, 39	5 (3%)
All	All	3825/3828 (99%)	-0.14	24 (0%)	85	89	4, 13, 22, 39	54 (1%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	0	LEU	6.1
1	A	3	PRO	4.4
2	B	0	LEU	4.2
2	D	0	LEU	3.9
2	F	0	LEU	3.4
1	C	485	GLN	3.2
2	F	44	PRO	3.0
2	B	45	GLY	3.0
1	C	435	ASP	2.9
1	A	128	ALA	2.8
2	H	44	PRO	2.8
1	G	485	GLN	2.6
1	C	146[A]	LEU	2.5
1	E	435	ASP	2.5
2	D	44	PRO	2.4
2	D	72	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	128	ALA	2.3
2	B	44	PRO	2.3
2	F	45	GLY	2.3
1	A	576	ASP	2.2
1	A	435	ASP	2.2
1	G	351	ASN	2.2
2	H	111	GLU	2.1
2	F	72	SER	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(Å ²)	Q<0.9
11	IPA	G	908	4/4	0.64	0.21	15,16,19,23	0
6	PGE	G	907	10/10	0.65	0.21	29,32,36,36	0
11	IPA	C	906	4/4	0.67	0.19	16,16,18,21	0
9	EDO	C	911[A]	4/4	0.72	0.20	28,28,28,29	4
9	EDO	C	911[B]	4/4	0.72	0.20	23,24,25,25	4
9	EDO	A	908[A]	4/4	0.73	0.29	24,25,26,26	4
9	EDO	A	908[B]	4/4	0.73	0.29	20,21,23,24	4
11	IPA	A	913	4/4	0.74	0.17	23,24,24,26	0
9	EDO	G	911	4/4	0.77	0.18	31,32,32,33	0
7	GOL	E	912	6/6	0.78	0.20	16,17,18,18	0
11	IPA	E	905	4/4	0.80	0.17	27,28,28,29	0
9	EDO	C	913	4/4	0.83	0.12	32,32,33,35	0
9	EDO	G	912	4/4	0.84	0.15	34,35,35,36	0
10	PEG	A	910	7/7	0.84	0.15	28,28,29,32	0
9	EDO	G	915	4/4	0.85	0.16	25,25,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	EDO	C	910	4/4	0.85	0.14	25,28,29,32	0
9	EDO	E	910	4/4	0.85	0.12	26,26,26,27	0
9	EDO	G	910	4/4	0.85	0.13	30,30,30,31	0
7	GOL	C	908	6/6	0.85	0.13	32,33,34,34	0
9	EDO	A	914	4/4	0.85	0.14	20,24,24,26	0
6	PGE	A	905[B]	10/10	0.86	0.13	14,14,15,15	10
6	PGE	A	905[A]	10/10	0.86	0.13	16,19,22,22	10
9	EDO	A	911	4/4	0.86	0.12	30,32,33,34	0
9	EDO	A	912	4/4	0.86	0.14	26,26,28,28	0
9	EDO	D	202	4/4	0.86	0.20	22,22,24,24	0
7	GOL	E	913	6/6	0.86	0.11	23,24,25,25	0
9	EDO	E	911	4/4	0.86	0.15	24,25,27,28	0
9	EDO	C	907	4/4	0.86	0.14	25,26,27,28	0
9	EDO	E	909	4/4	0.87	0.13	23,26,27,27	0
7	GOL	E	914	6/6	0.87	0.11	21,23,25,26	0
9	EDO	A	916	4/4	0.88	0.18	22,22,23,25	0
9	EDO	C	914	4/4	0.89	0.10	19,20,21,22	0
7	GOL	C	909	6/6	0.89	0.11	28,29,31,32	0
7	GOL	G	913	6/6	0.90	0.11	21,25,27,27	0
7	GOL	G	905	6/6	0.90	0.14	14,16,18,22	0
9	EDO	E	907	4/4	0.90	0.10	24,27,27,28	0
9	EDO	G	909[B]	4/4	0.91	0.09	15,15,15,16	4
10	PEG	B	2301	7/7	0.91	0.11	23,24,24,25	0
9	EDO	A	909	4/4	0.91	0.11	14,15,17,17	0
7	GOL	A	906	6/6	0.91	0.15	13,16,19,25	0
9	EDO	A	915	4/4	0.91	0.11	15,17,17,18	0
9	EDO	G	909[A]	4/4	0.91	0.09	15,16,16,17	4
9	EDO	G	914	4/4	0.92	0.09	21,22,22,24	0
7	GOL	C	912	6/6	0.93	0.14	15,18,19,23	0
9	EDO	C	915	4/4	0.93	0.10	20,20,21,21	0
9	EDO	E	908	4/4	0.95	0.07	14,15,16,16	0
8	AST	A	907	4/4	0.96	0.08	13,14,14,15	1
8	AST	G	906	4/4	0.96	0.07	12,12,12,13	1
8	AST	C	905	4/4	0.97	0.07	11,12,13,13	1
3	MGD	C	902	47/47	0.98	0.04	8,9,10,12	0
3	MGD	C	903	47/47	0.98	0.04	9,9,10,10	0
3	MGD	E	901	47/47	0.98	0.04	9,9,10,10	0
3	MGD	G	902	47/47	0.98	0.04	8,9,10,11	0
3	MGD	A	901	47/47	0.98	0.04	8,9,10,11	0
3	MGD	A	902	47/47	0.98	0.04	7,9,10,10	0
8	AST	E	906	4/4	0.98	0.07	12,13,14,14	1
3	MGD	E	903	47/47	0.99	0.04	8,9,10,10	0

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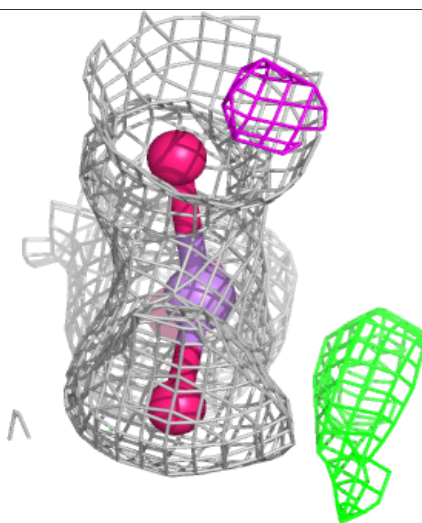
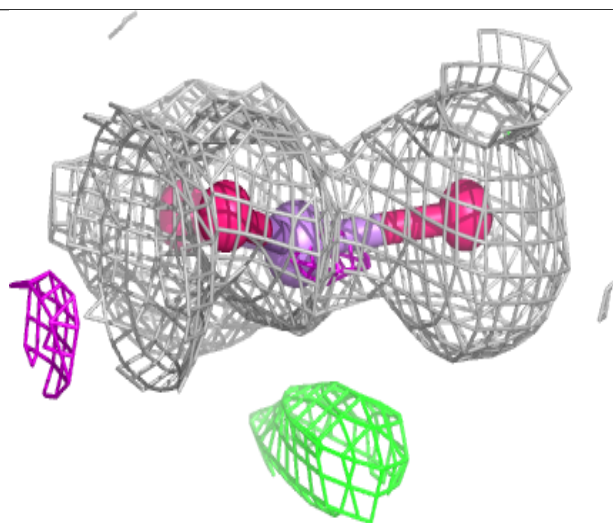
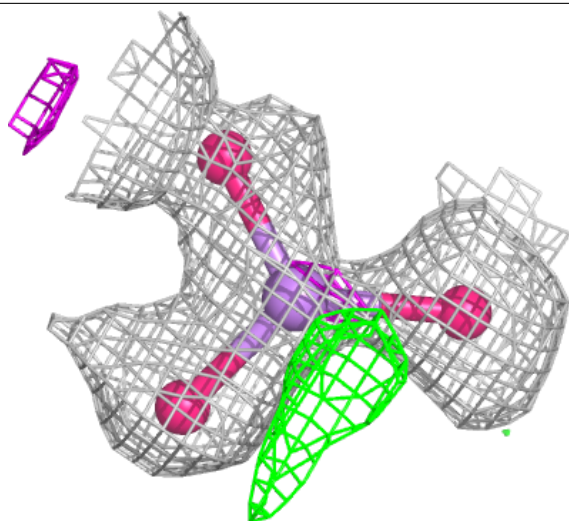
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MGD	G	903	47/47	0.99	0.04	7,9,10,10	0
12	FES	B	2302	4/4	0.99	0.03	10,11,11,12	0
12	FES	H	201	4/4	0.99	0.03	10,11,11,11	0
5	F3S	A	904	7/7	1.00	0.02	8,9,9,9	0
5	F3S	C	904	7/7	1.00	0.02	9,9,9,9	0
5	F3S	E	904	7/7	1.00	0.02	8,9,9,10	0
5	F3S	G	904	7/7	1.00	0.02	8,8,8,8	0
4	MO	A	903	1/1	1.00	0.02	9,9,9,9	0
4	MO	C	901	1/1	1.00	0.02	10,10,10,10	0
4	MO	E	902	1/1	1.00	0.02	10,10,10,10	0
12	FES	D	201	4/4	1.00	0.03	11,11,11,12	0
12	FES	F	201	4/4	1.00	0.03	11,12,12,12	0
4	MO	G	901	1/1	1.00	0.01	9,9,9,9	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.

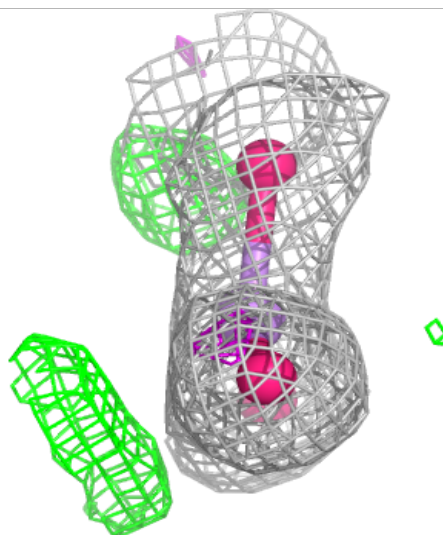
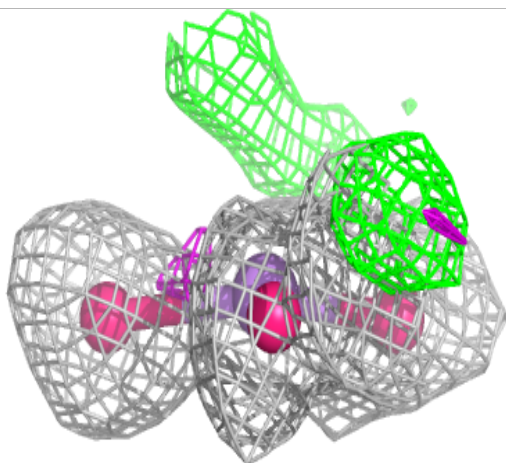
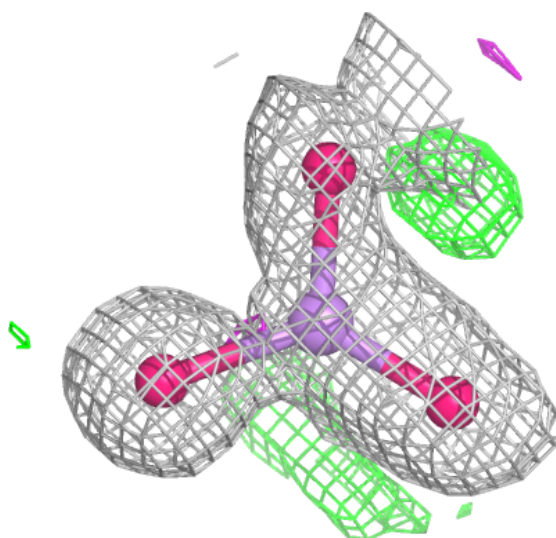
Electron density around AST A 907:

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



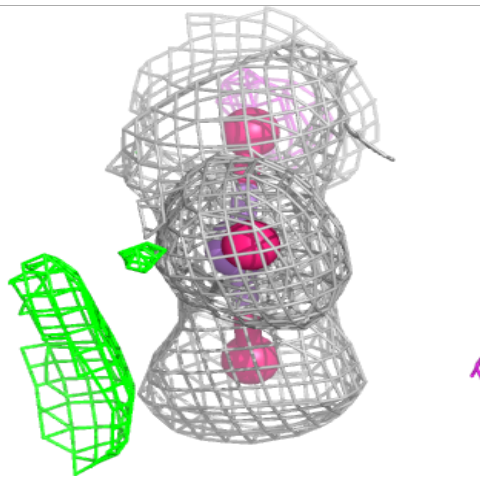
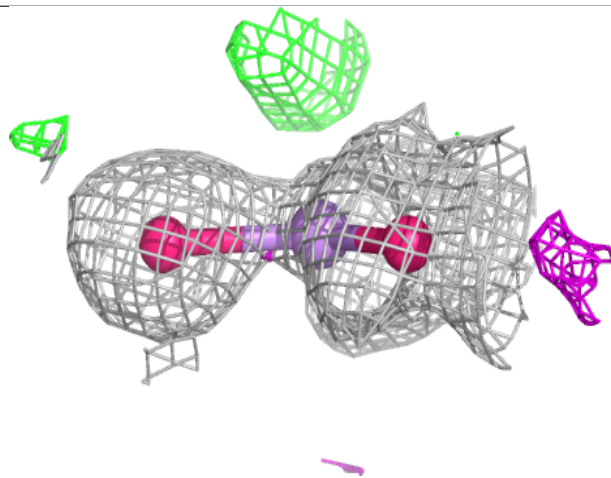
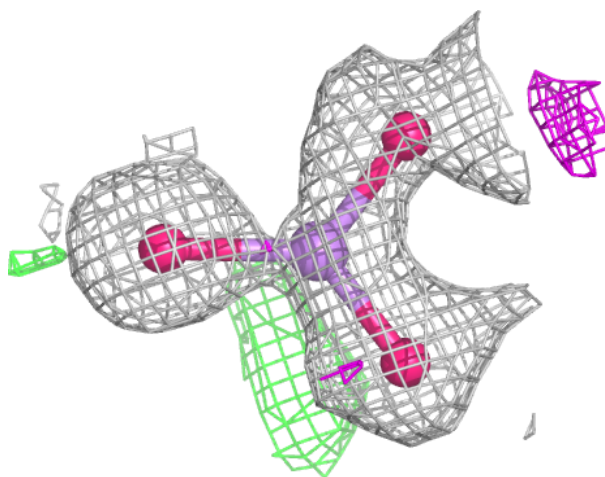
Electron density around AST G 906:

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



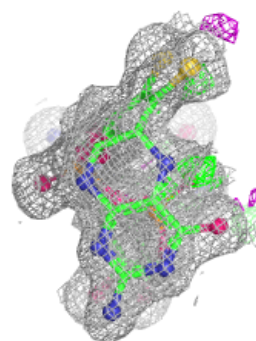
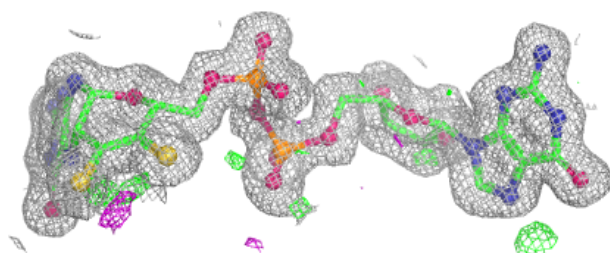
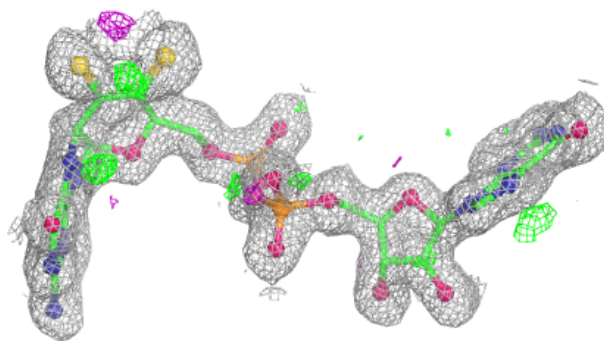
Electron density around AST C 905:

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

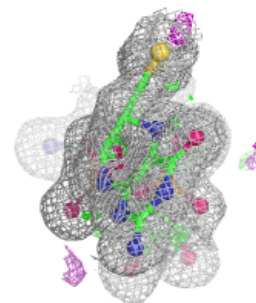
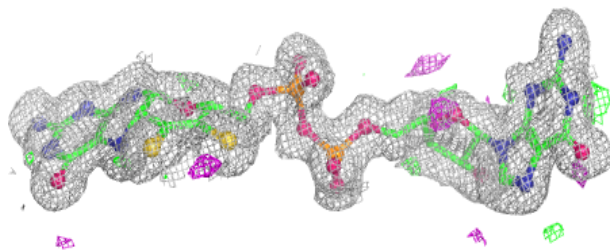
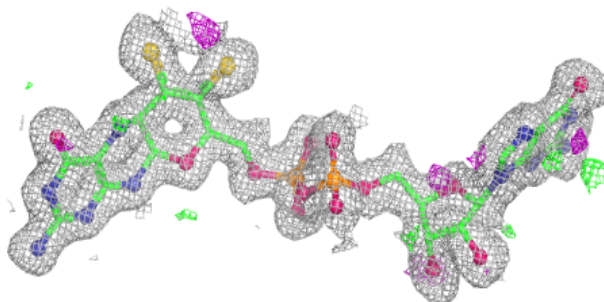


Electron density around MGD C 902:

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

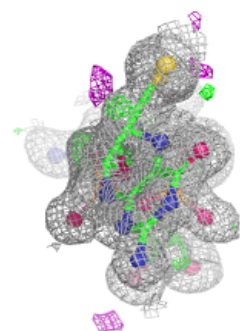
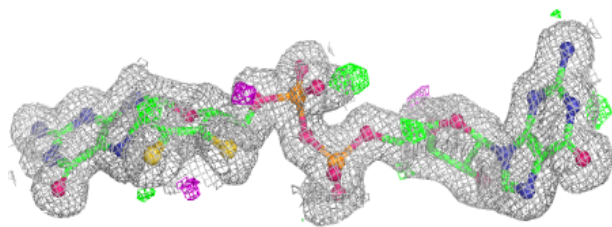
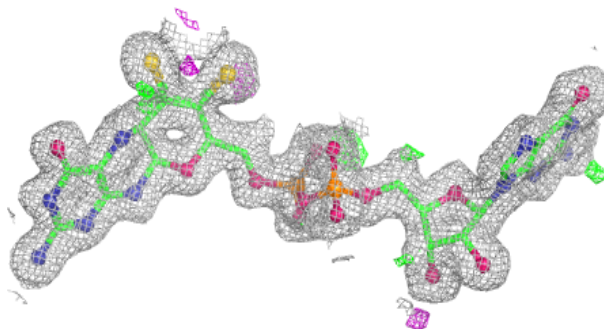
**Electron density around MGD C 903:**

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

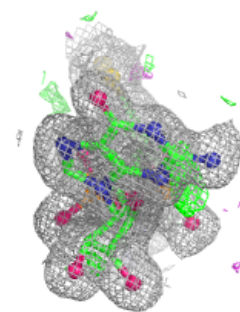
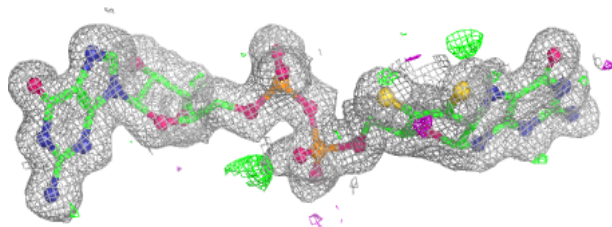
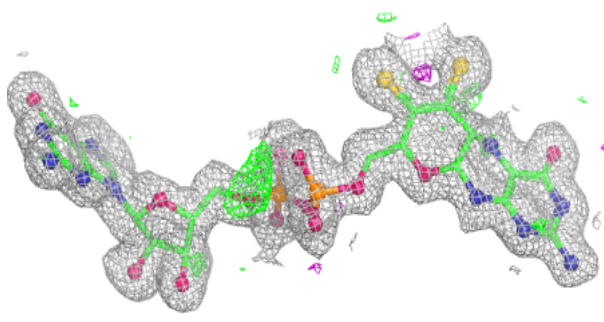


Electron density around MGD E 901:

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

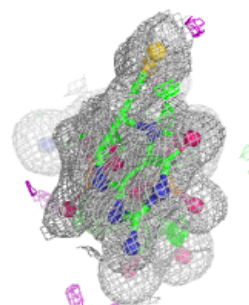
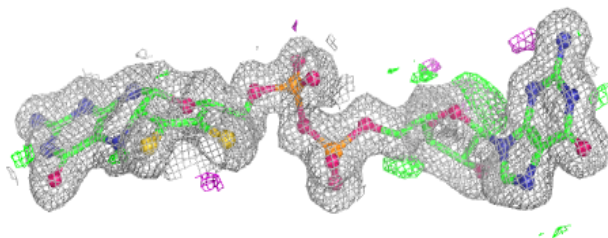
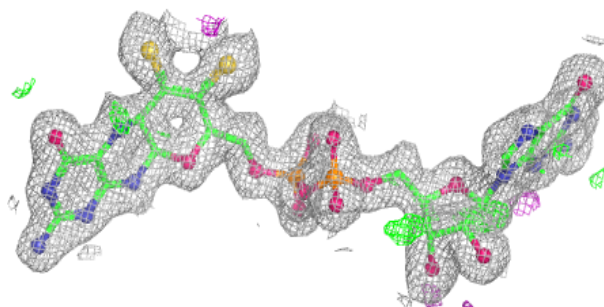
**Electron density around MGD G 902:**

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

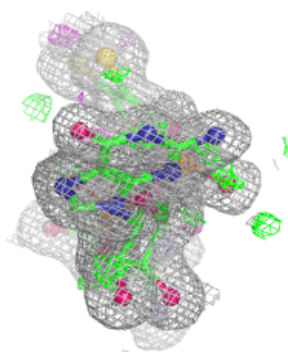
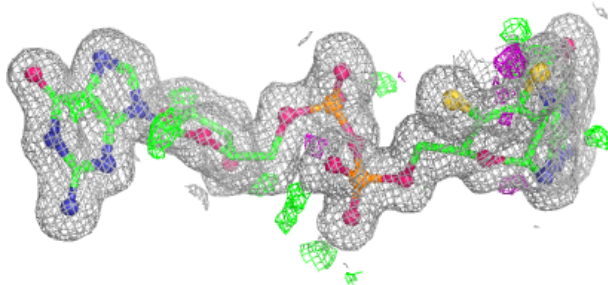
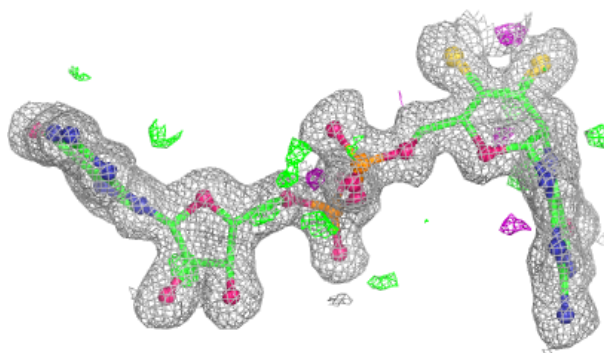


Electron density around MGD A 901:

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

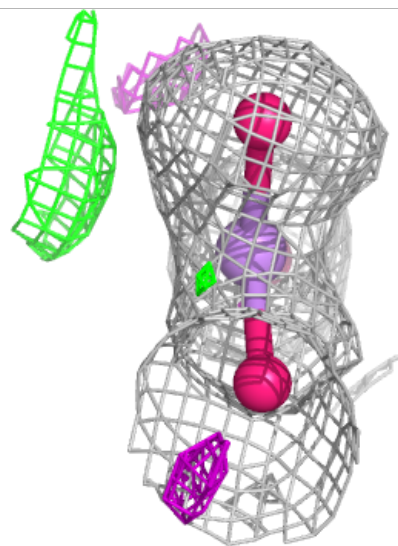
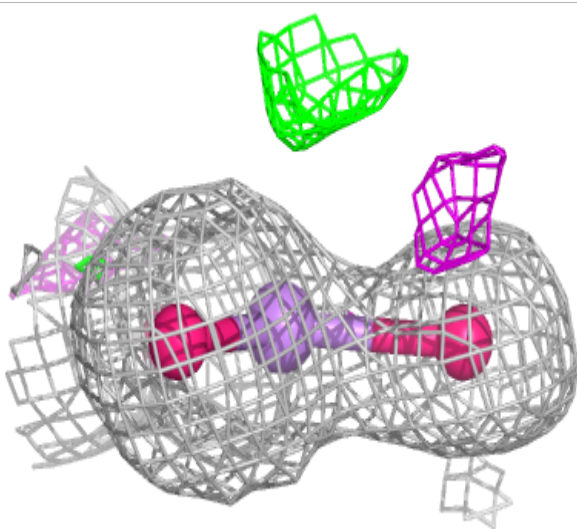
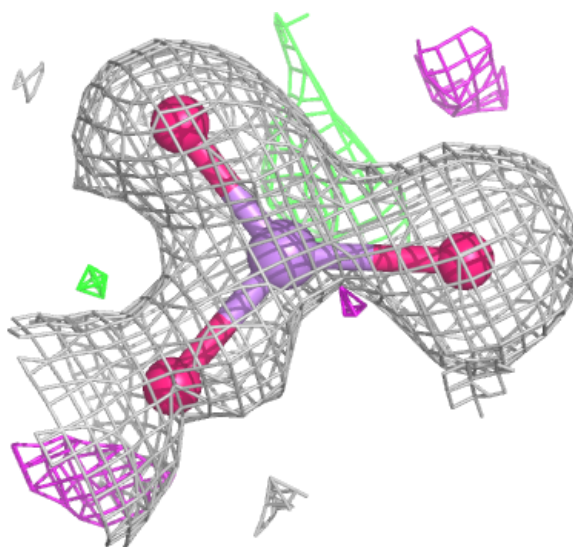
**Electron density around MGD A 902:**

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



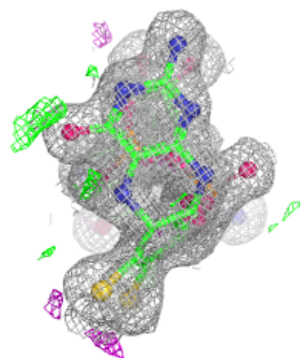
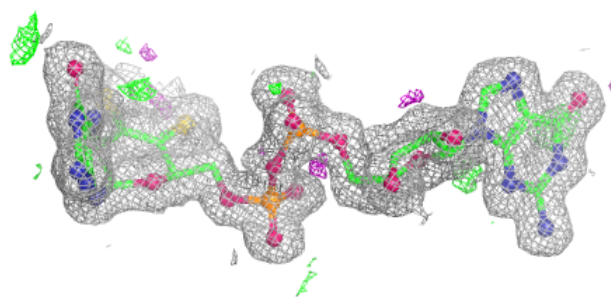
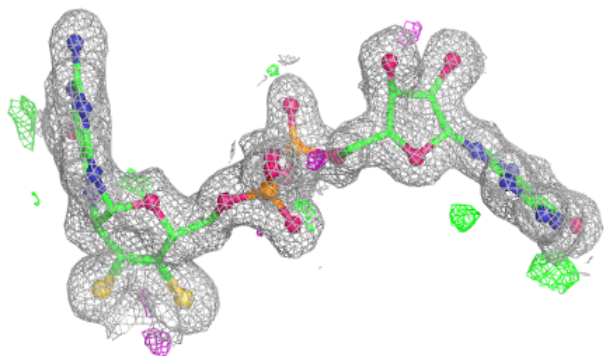
Electron density around AST E 906:

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

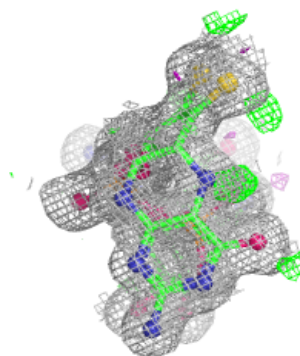
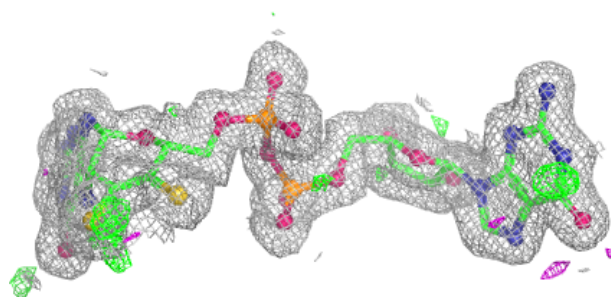
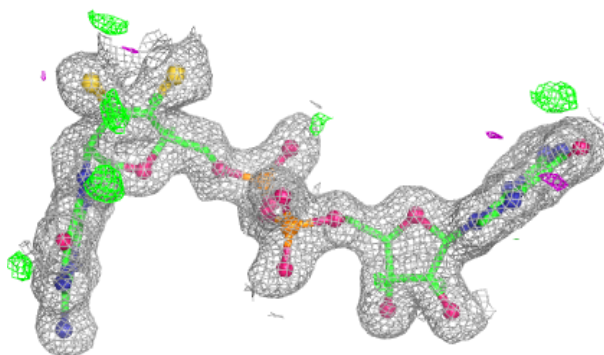


Electron density around MGD E 903:

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

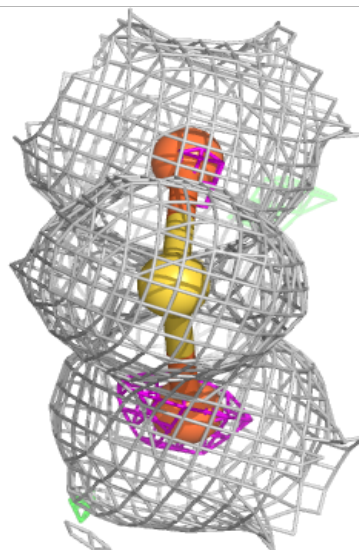
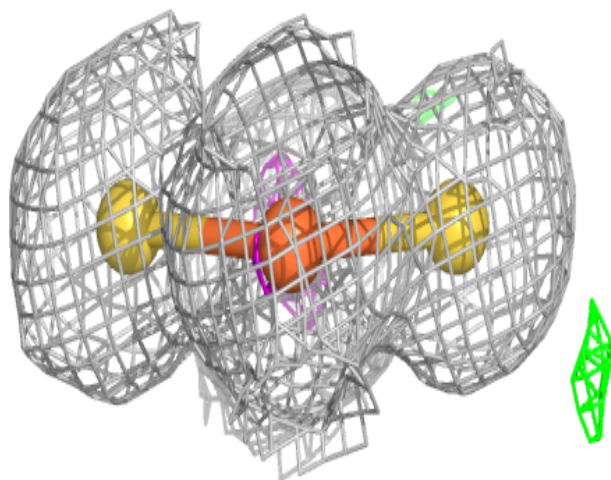
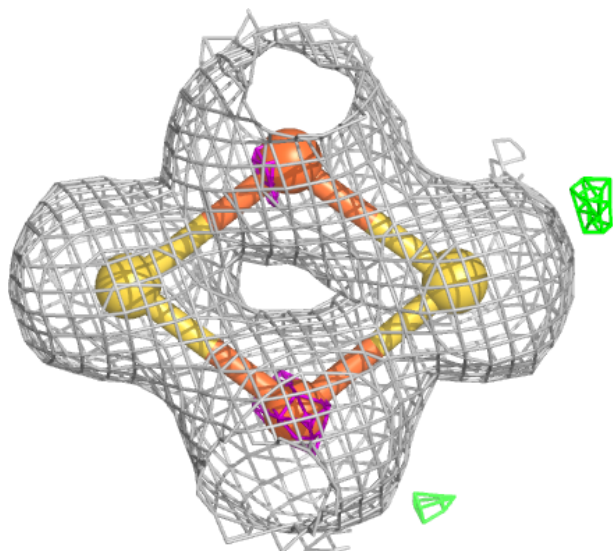
**Electron density around MGD G 903:**

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



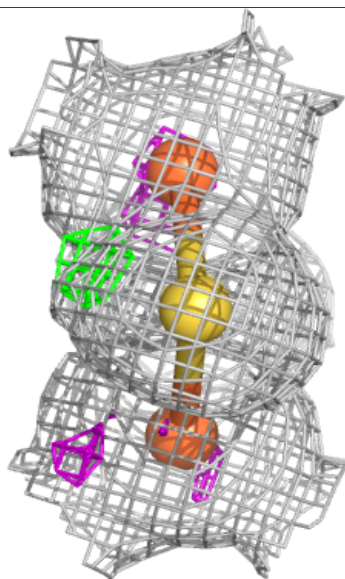
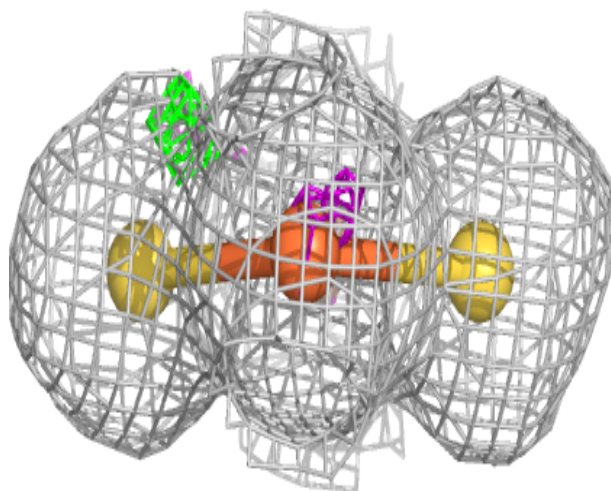
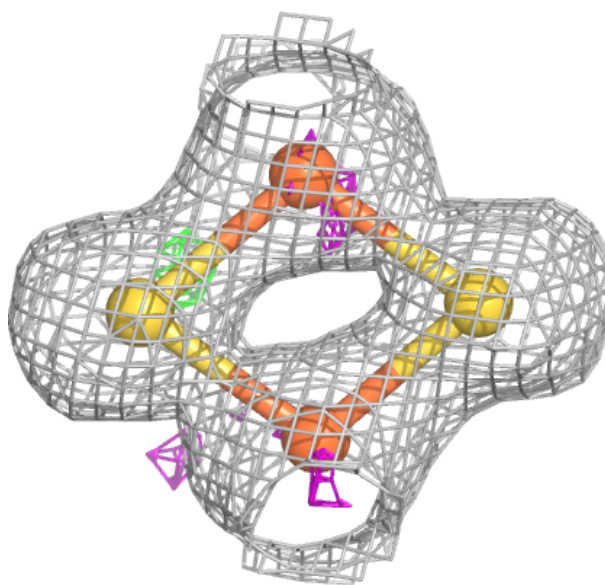
Electron density around FES B 2302:

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



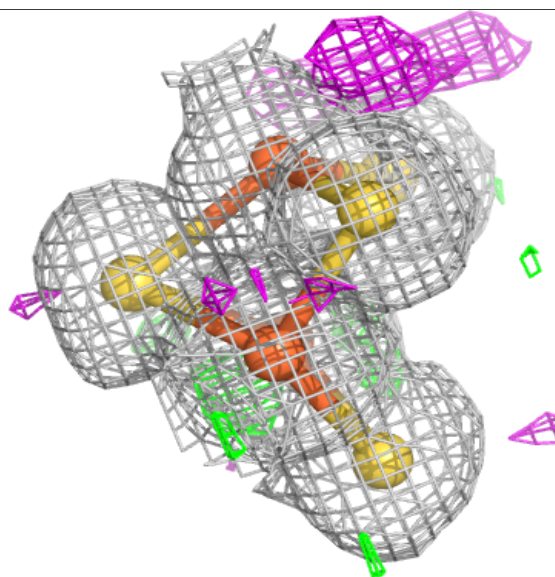
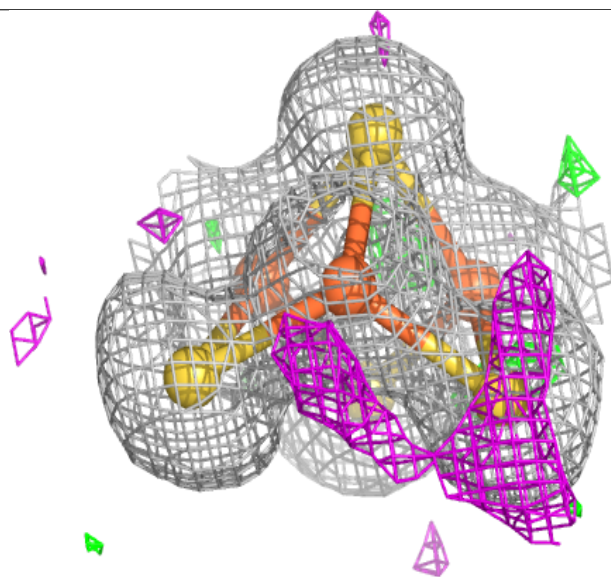
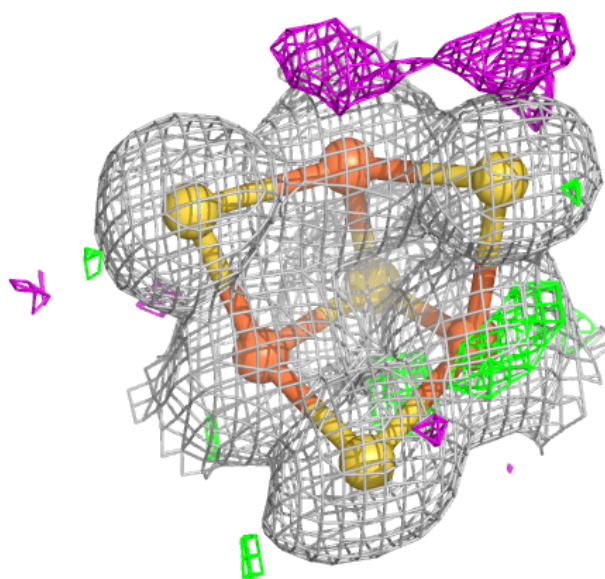
Electron density around FES H 201:

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



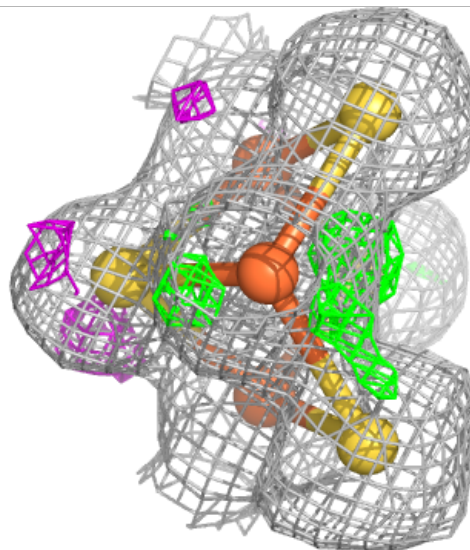
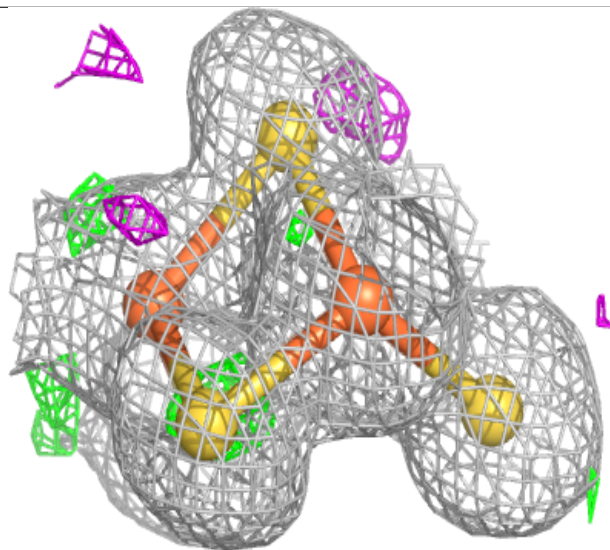
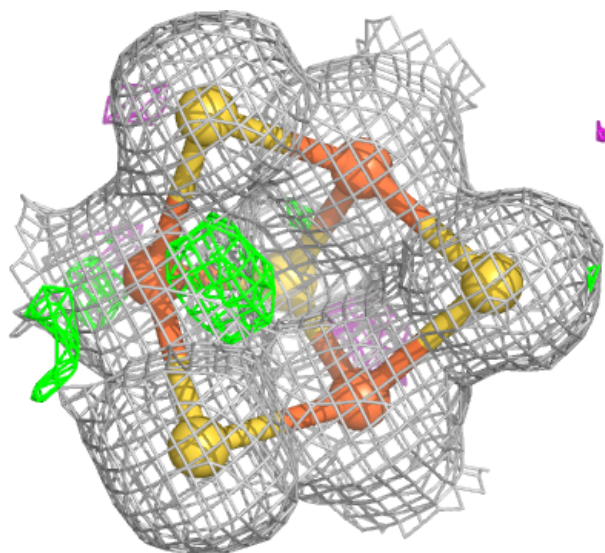
Electron density around F3S A 904:

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



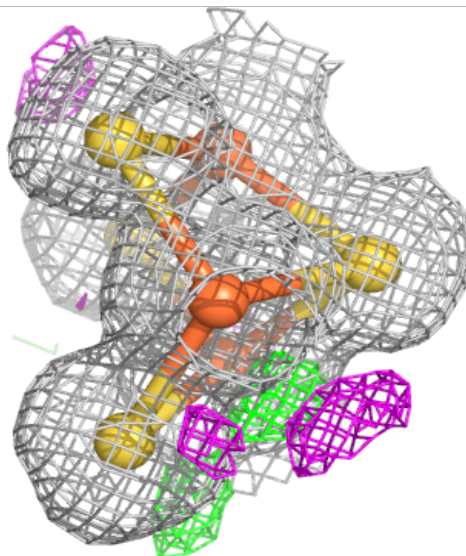
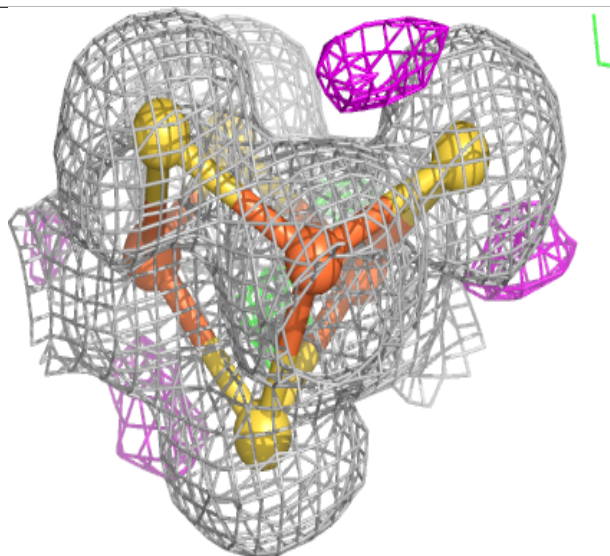
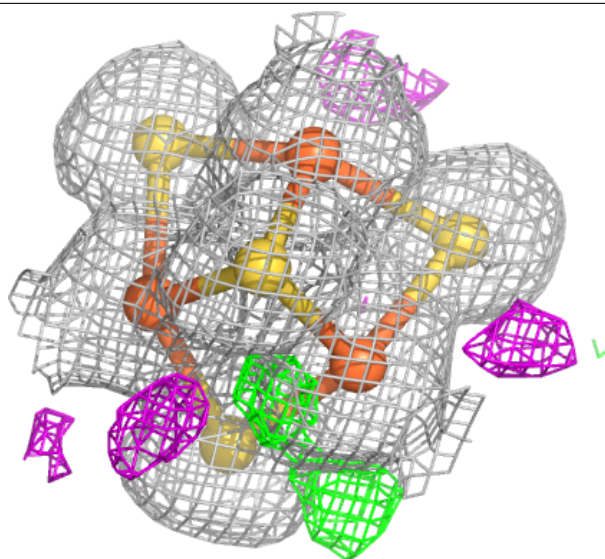
Electron density around F3S C 904:

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



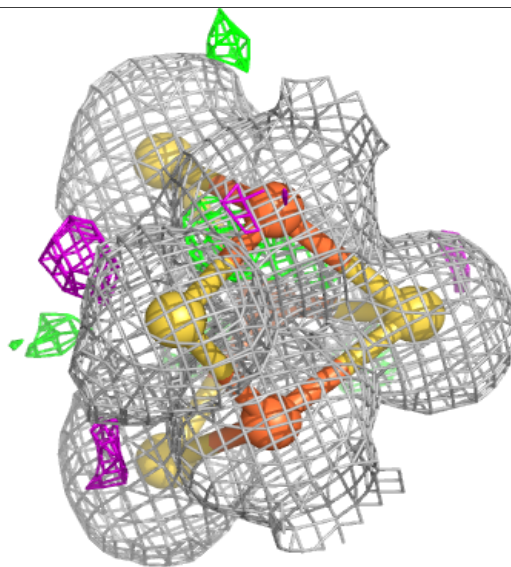
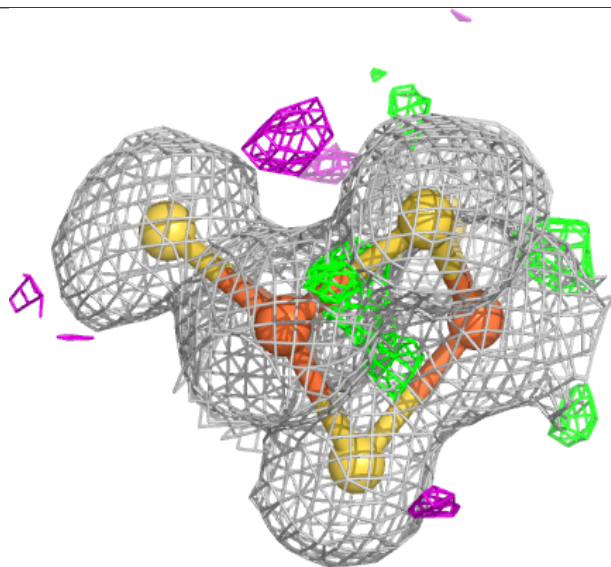
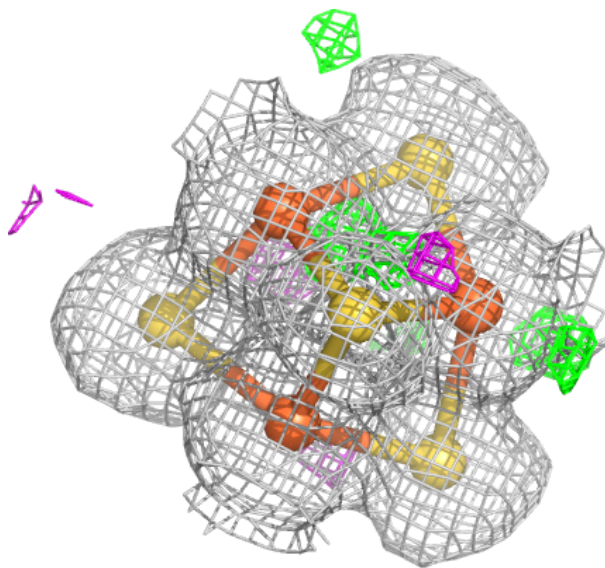
Electron density around F3S E 904:

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



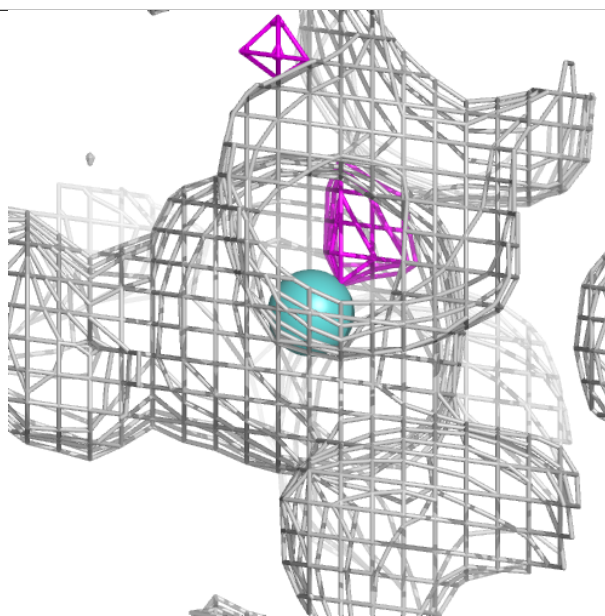
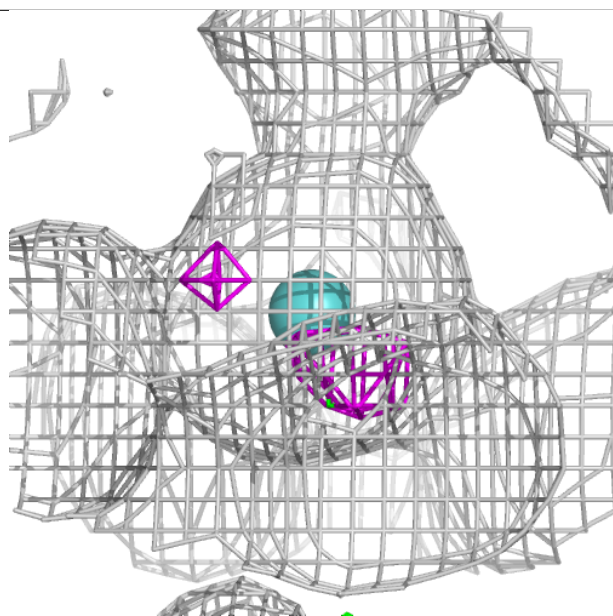
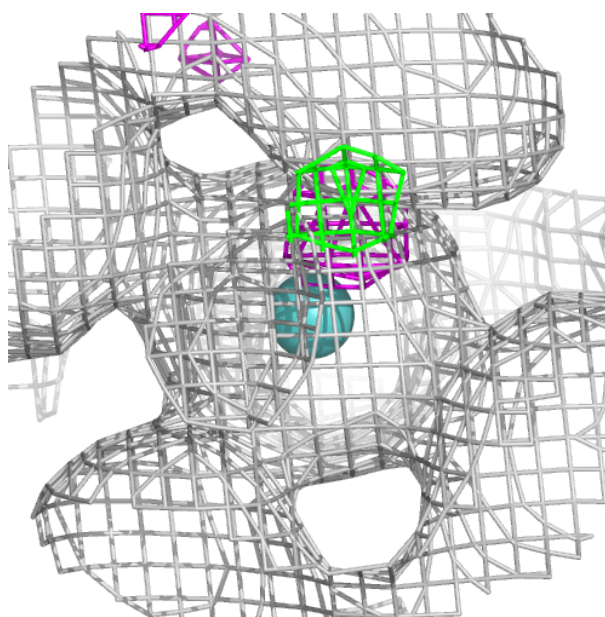
Electron density around F3S G 904:

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



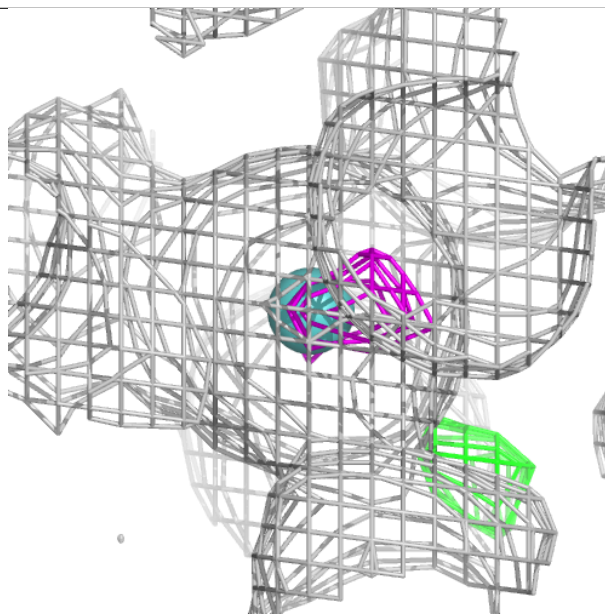
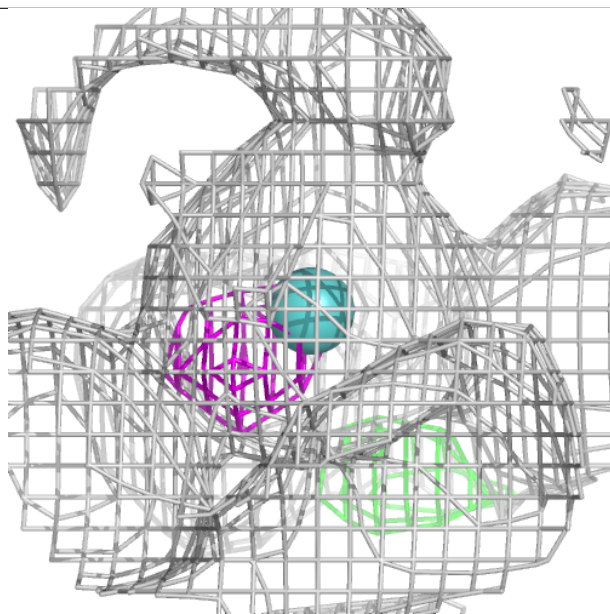
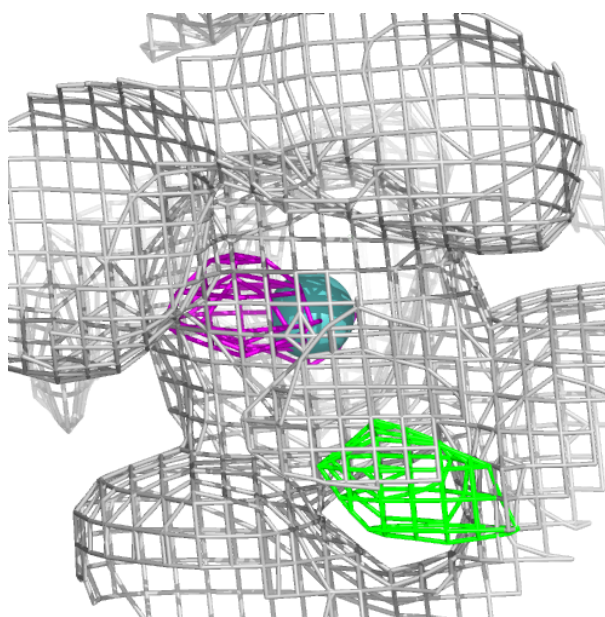
Electron density around MO A 903:

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



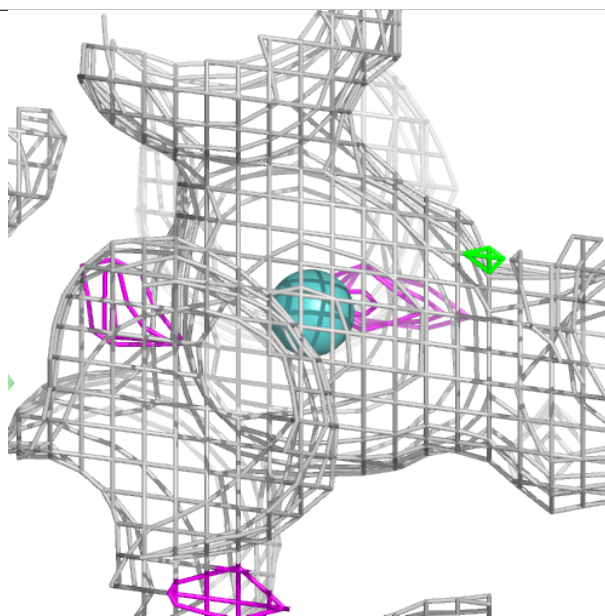
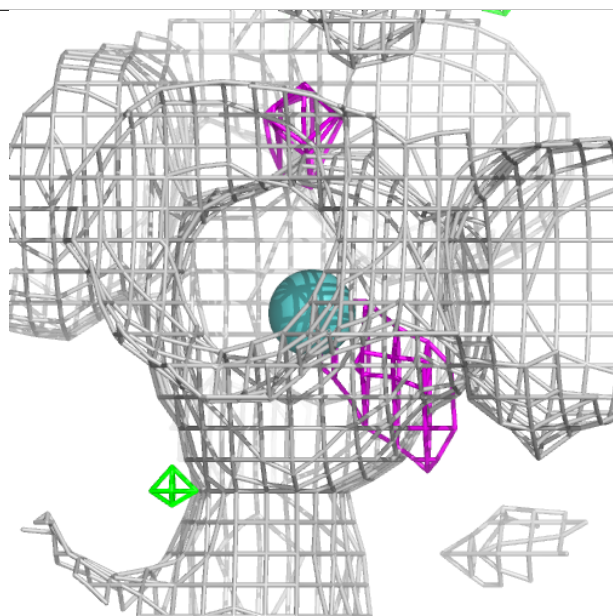
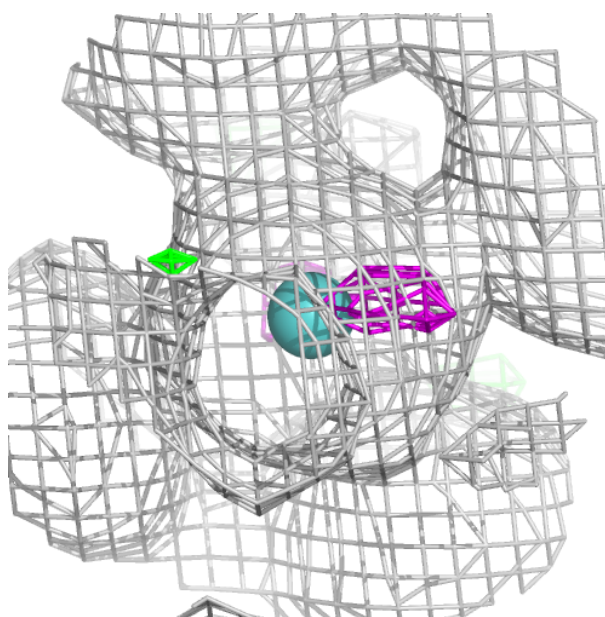
Electron density around MO C 901:

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



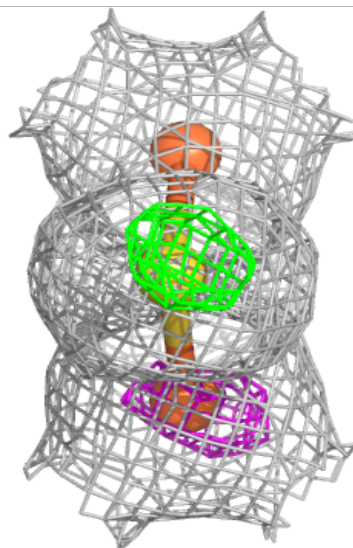
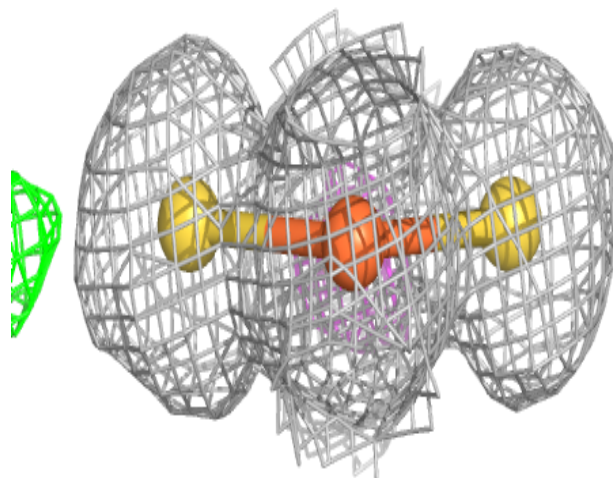
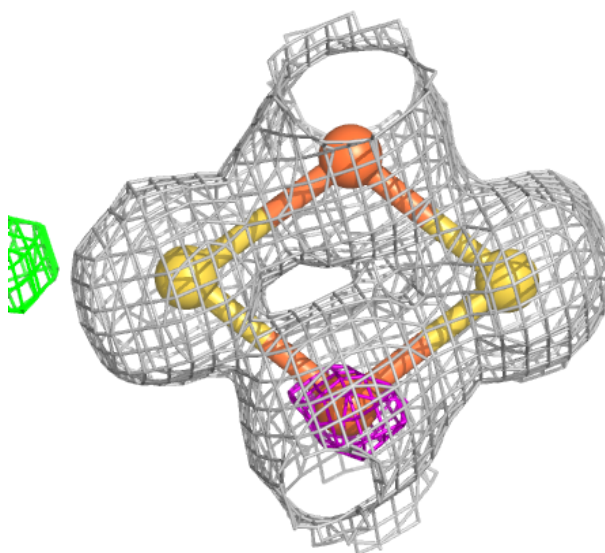
Electron density around MO E 902:

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



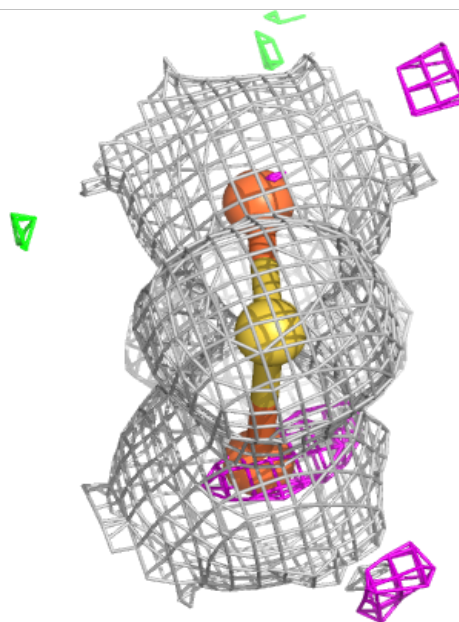
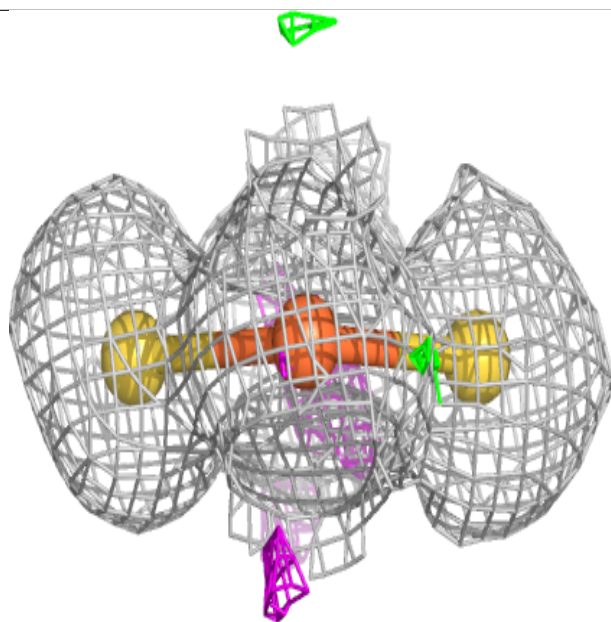
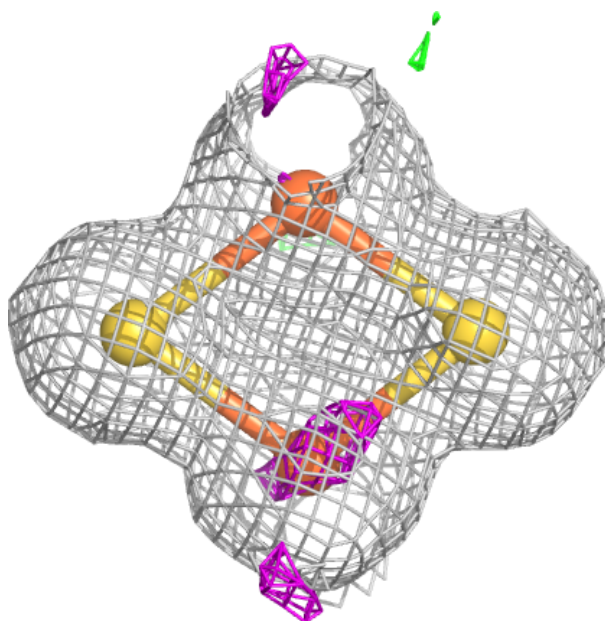
Electron density around FES D 201:

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



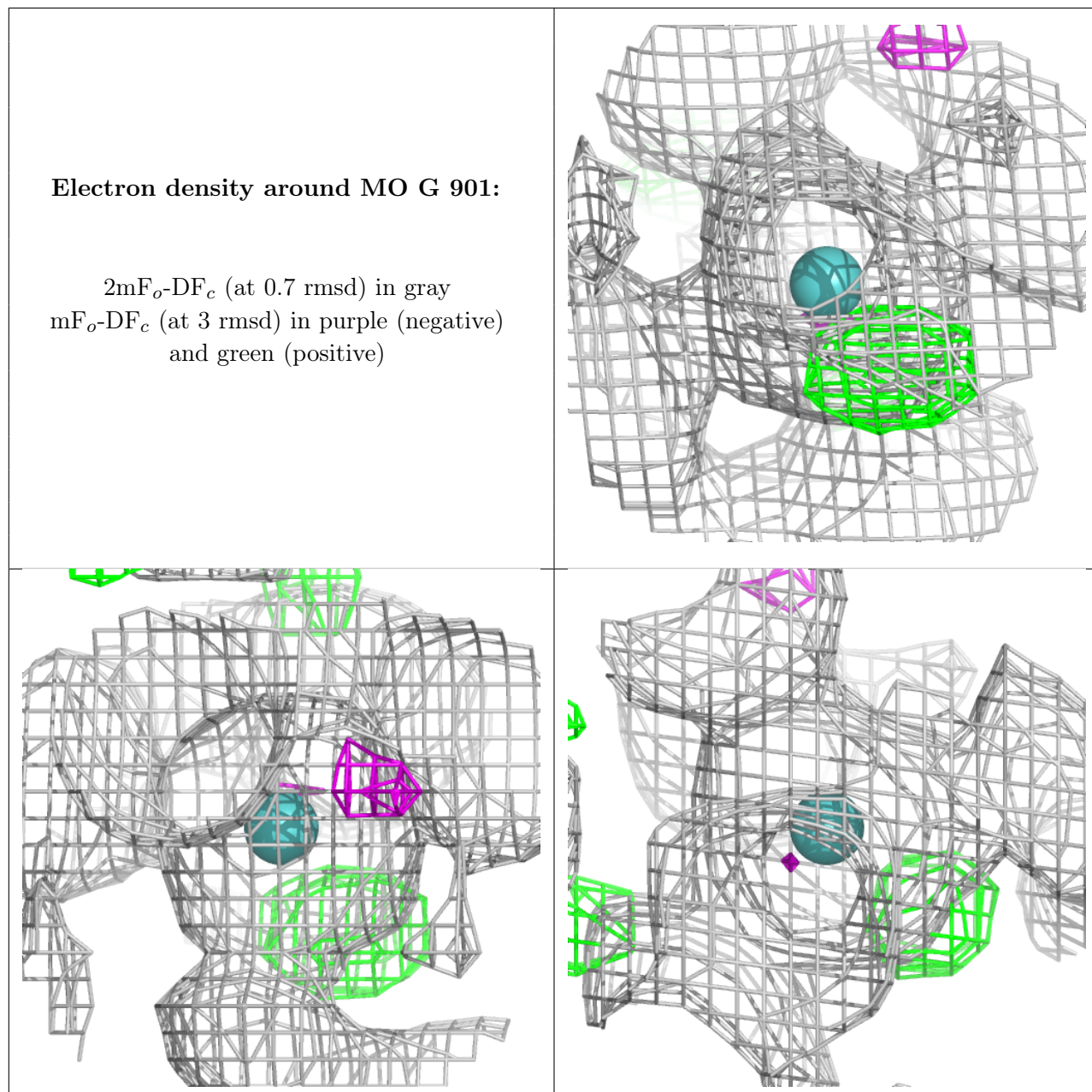
Electron density around FES F 201:

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



Electron density around MO G 901:

$2mF_o-DF_c$ (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.