



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:26 PM UTC

PDB ID : 8RTL / pdb\_00008rtl  
Title : Af Aio C65F-C80G  
Authors : Engrola, F.; Romao, M.J.; Correia, M.; Santos-Silva, T.  
Deposited on : 2024-01-26  
Resolution : 1.89 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](mailto: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>.

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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

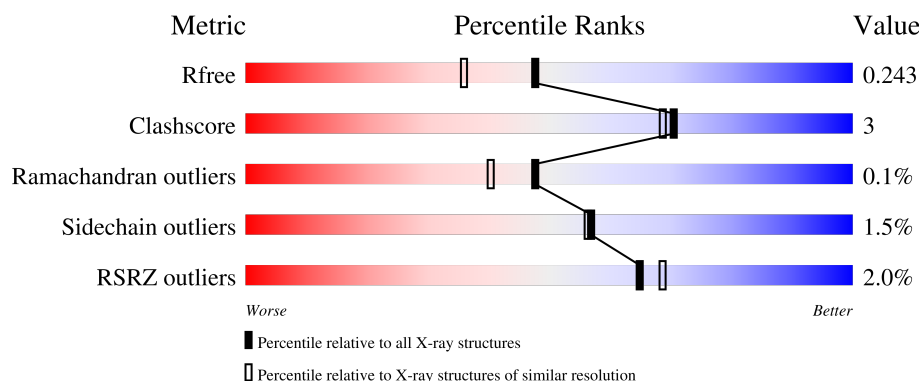
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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  $\geq 3$ , 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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>%</span> <span>91%</span> <span>9%</span> <span>.</span> </div> </div>
1	C	822	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>3%</span> <span>91%</span> <span>8%</span> <span>.</span> </div> </div>
2	B	134	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>%</span> <span>93%</span> <span>7%</span> <span>.</span> </div> </div>
3	D	135	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>4%</span> <span>88%</span> <span>10%</span> <span>..</span> </div> </div>
3	F	135	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>2%</span> <span>95%</span> <span>5%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
3	H	135	 90% 7%
4	E	824	 91% 8%
5	G	823	 90% 9%

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
14	O	E	912	-	-	X	-
17	P4G	C	905	-	-	X	-
18	PG0	D	2203	-	-	X	-
9	PEG	A	911	-	-	X	-
9	PEG	E	909	-	-	X	-
9	PEG	H	203	-	-	X	-

## 2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 32670 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	4	0
			6495	4086	1150	1218	41			
1	C	822	Total	C	N	O	S	0	4	0
			6498	4086	1150	1221	41			

- 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	0	0
			1003	632	168	197	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	LEU	-	expression tag	UNP Q7SIF3
B	65	PHE	CYS	conflict	UNP Q7SIF3
B	80	GLY	CYS	conflict	UNP Q7SIF3

- Molecule 3 is a protein called Arsenite oxidase subunit AioB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	135	Total	C	N	O	S	0	0	0
			1004	631	169	198	6			
3	F	135	Total	C	N	O	S	0	0	0
			1004	631	169	198	6			
3	H	135	Total	C	N	O	S	0	0	0
			1004	631	169	198	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	65	PHE	CYS	conflict	UNP Q7SIF3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	80	GLY	CYS	conflict	UNP Q7SIF3
F	65	PHE	CYS	conflict	UNP Q7SIF3
F	80	GLY	CYS	conflict	UNP Q7SIF3
H	65	PHE	CYS	conflict	UNP Q7SIF3
H	80	GLY	CYS	conflict	UNP Q7SIF3

- Molecule 4 is a protein called Arsenite oxidase subunit AioA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	824	Total	C	N	O	S	0	4	0
			6507	4094	1152	1219	42			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	2	ALA	-	expression tag	UNP Q7SIF4
E	3	ALA	-	expression tag	UNP Q7SIF4

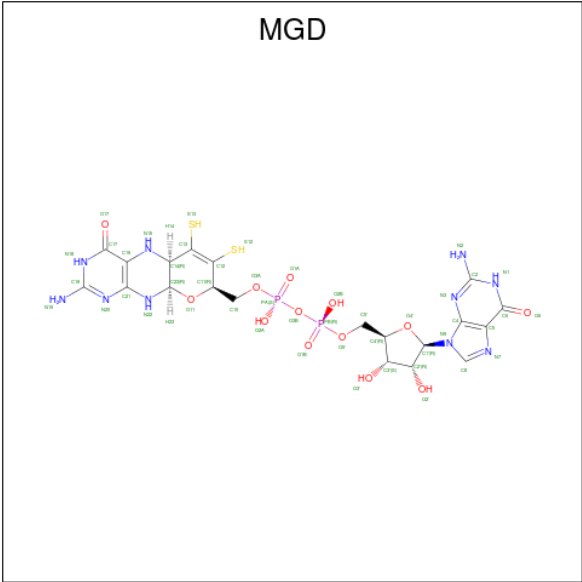
- Molecule 5 is a protein called Arsenite oxidase subunit AioA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	823	Total	C	N	O	S	0	5	0
			6511	4094	1153	1223	41			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	3	ALA	-	expression tag	UNP Q7SIF4

- Molecule 6 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: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is MOLYBDENUM(IV) ION (CCD ID: 4MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

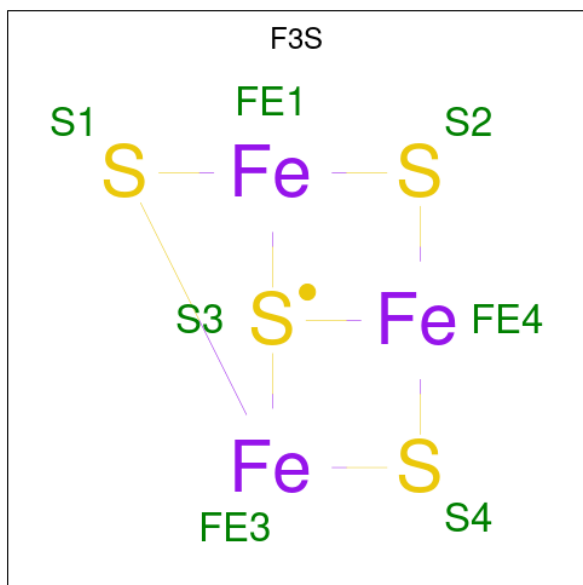
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mo	0	0
			1	1		
7	C	1	Total	Mo	0	0
			1	1		
7	E	1	Total	Mo	0	0
			1	1		

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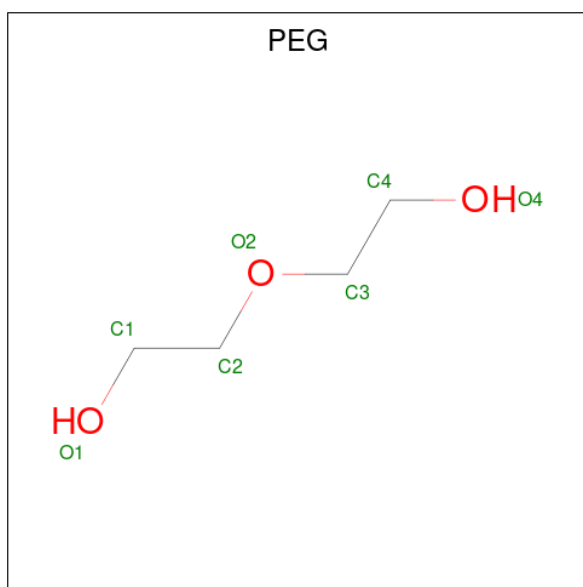
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Mo	0	0
			1	1		

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $\text{C}_4\text{H}_{10}\text{O}_3$ ).



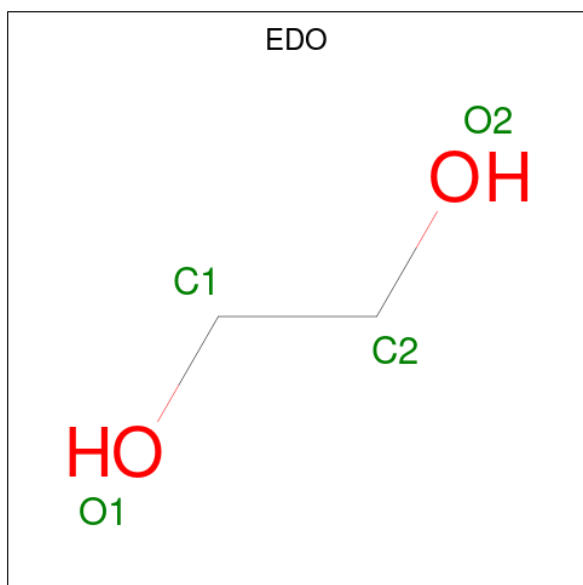
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	C	1	Total	C	O	0	0
			7	4	3		
9	C	1	Total	C	O	0	0
			7	4	3		
9	E	1	Total	C	O	0	0
			7	4	3		
9	E	1	Total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

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

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



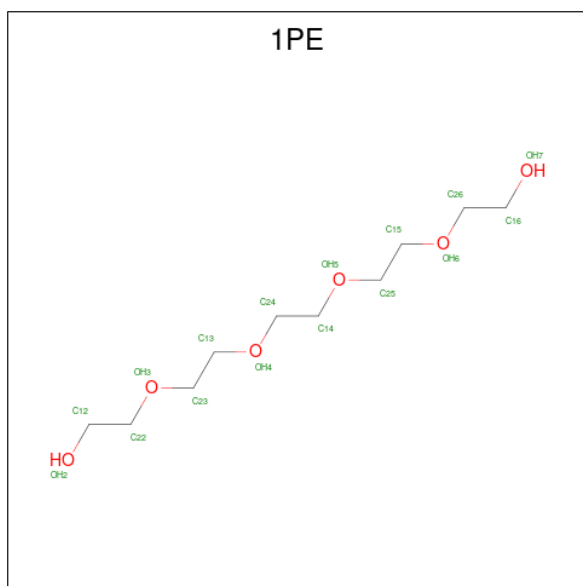
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	C	1	Total	C	O	0	0
			4	2	2		
10	D	1	Total	C	O	0	0
			4	2	2		
10	D	1	Total	C	O	0	0
			4	2	2		
10	E	1	Total	C	O	0	0
			4	2	2		
10	E	1	Total	C	O	0	0
			4	2	2		
10	E	1	Total	C	O	0	0
			4	2	2		

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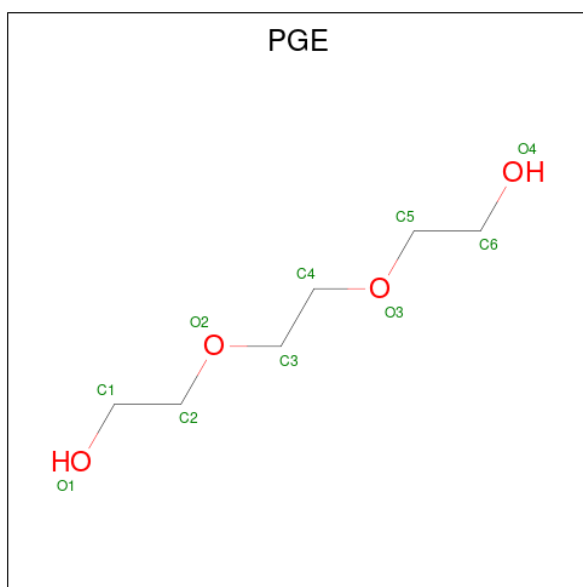
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	E	1	Total	C	O	0	0
			4	2	2		
10	G	1	Total	C	O	0	0
			4	2	2		
10	G	1	Total	C	O	0	0
			4	2	2		
10	G	1	Total	C	O	0	0
			4	2	2		
10	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



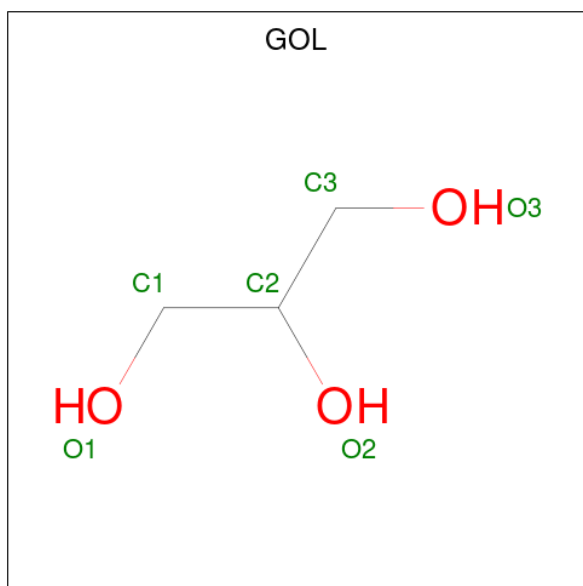
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			16	10	6		
11	C	1	Total	C	O	0	0
			16	10	6		
11	C	1	Total	C	O	0	0
			16	10	6		
11	G	1	Total	C	O	0	0
			16	10	6		

- Molecule 12 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



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

- Molecule 13 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

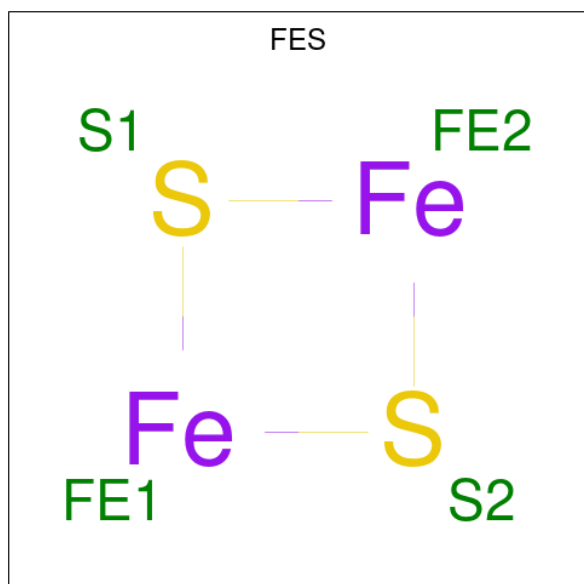
- Molecule 14 is OXYGEN ATOM (CCD ID: O) (formula: O) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 15 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total Na 1 1	0	0
15	C	1	Total Na 1 1	0	0
15	E	1	Total Na 1 1	0	0
15	G	1	Total Na 1 1	0	0

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



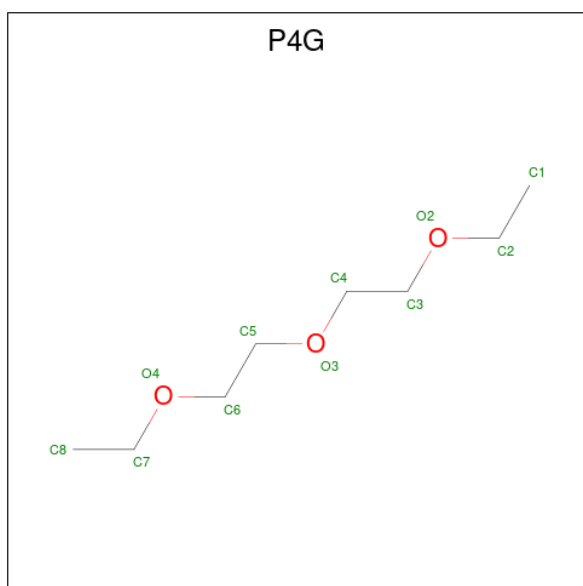
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total Fe S 4 2 2	0	0

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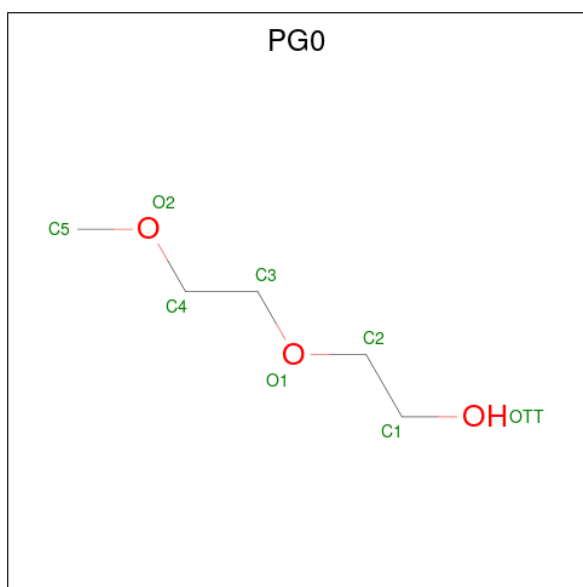
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	D	1	Total	Fe	S	0	0
			4	2	2		
16	F	1	Total	Fe	S	0	0
			4	2	2		
16	H	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 17 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (CCD ID: P4G) (formula:  $C_8H_{18}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			11	8	3		

- Molecule 18 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula:  $C_5H_{12}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	D	1	Total	C	O	0	0
			8	5	3		

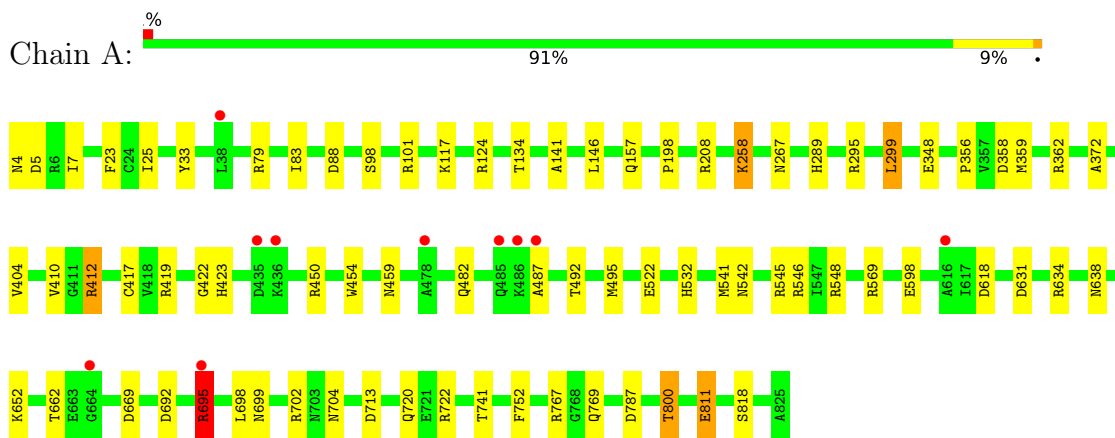
- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	410	Total	O	0	0
			410	410		
19	B	76	Total	O	0	0
			76	76		
19	C	416	Total	O	0	0
			416	416		
19	D	78	Total	O	0	0
			78	78		
19	E	391	Total	O	0	0
			391	391		
19	F	71	Total	O	0	0
			71	71		
19	G	426	Total	O	0	0
			426	426		
19	H	73	Total	O	0	0
			73	73		

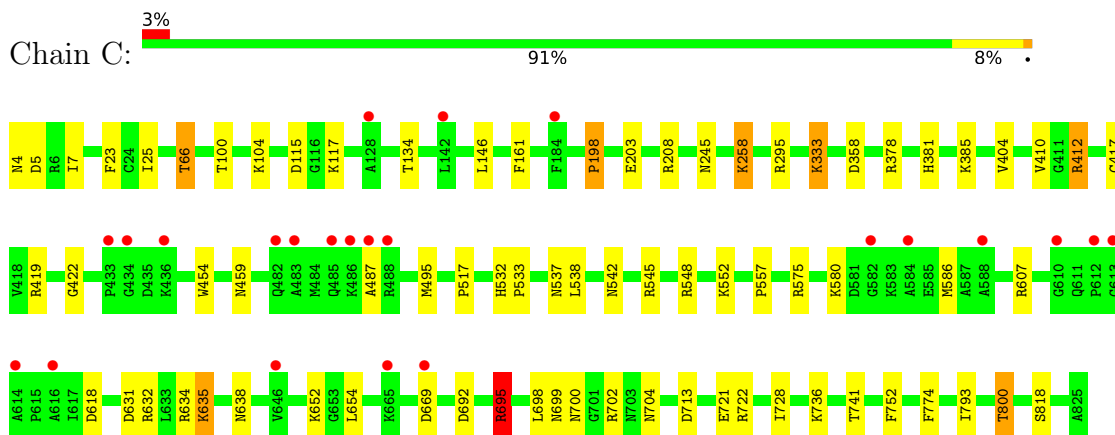
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

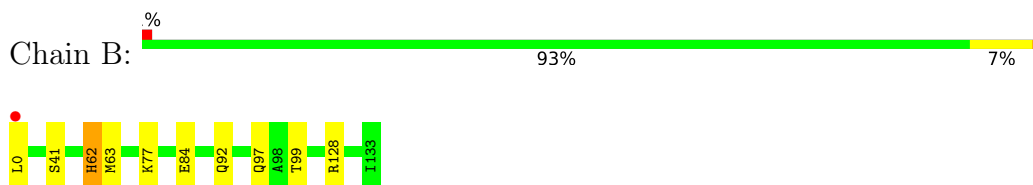
- Molecule 1: Arsenite oxidase subunit AioA



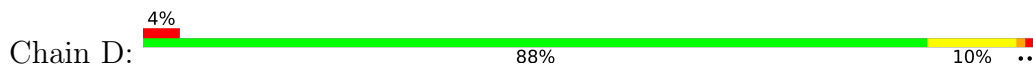
- Molecule 1: Arsenite oxidase subunit AioA



- Molecule 2: Arsenite oxidase subunit AioB



- Molecule 3: Arsenite oxidase subunit AioB





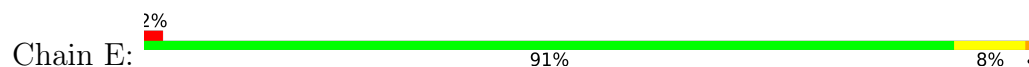
- Molecule 3: Arsenite oxidase subunit AioB



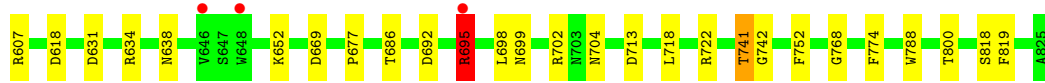
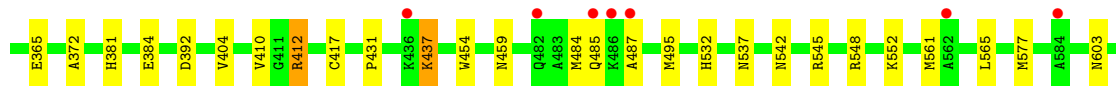
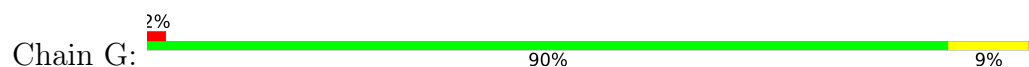
- Molecule 3: Arsenite oxidase subunit AioB



- Molecule 4: Arsenite oxidase subunit AioA



- Molecule 5: Arsenite oxidase subunit AioA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.16Å 108.80Å 117.11Å 97.58° 90.04° 96.18°	Depositor
Resolution (Å)	116.07 – 1.89 116.07 – 1.89	Depositor EDS
% Data completeness (in resolution range)	92.9 (116.07-1.89) 92.9 (116.07-1.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.200 , 0.235 0.211 , 0.243	Depositor DCC
$R_{free}$ test set	16419 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 38.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32670	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 1PE, F3S, EDO, 4MO, GOL, P4G, FES, PG0, PEG, PGE, MGD, O, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.98	1/6656 (0.0%)	1.33	31/9018 (0.3%)
1	C	0.97	1/6659 (0.0%)	1.31	27/9022 (0.3%)
2	B	0.99	0/1025	1.29	0/1396
3	D	1.04	0/1026	1.31	2/1397 (0.1%)
3	F	1.04	1/1026 (0.1%)	1.30	0/1397
3	H	1.01	0/1026	1.31	4/1397 (0.3%)
4	E	0.98	1/6668 (0.0%)	1.31	26/9034 (0.3%)
5	G	0.99	3/6672 (0.0%)	1.31	26/9043 (0.3%)
All	All	0.98	7/30758 (0.0%)	1.31	116/41704 (0.3%)

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	7
1	C	0	8
2	B	0	1
3	D	0	2
3	F	0	1
3	H	0	1
4	E	0	11
5	G	0	4
All	All	0	35

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	81	HIS	CE1-NE2	6.42	1.39	1.32
5	G	677	PRO	CA-CB	6.24	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	208	ARG	NE-CZ	6.14	1.39	1.33
1	A	695	ARG	NE-CZ	5.77	1.39	1.33
1	C	695	ARG	NE-CZ	5.51	1.39	1.33
5	G	166	HIS	ND1-CE1	5.27	1.37	1.32
5	G	268	PHE	C-O	-5.08	1.20	1.24

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	100	GLU	CB-CG-CD	11.88	132.80	112.60
5	G	695	ARG	NE-CZ-NH2	10.22	128.40	119.20
5	G	652	LYS	CB-CA-C	-9.08	93.35	109.24
1	A	652	LYS	CB-CA-C	-8.86	93.74	109.24
1	A	811	GLU	CB-CG-CD	8.20	126.54	112.60
1	C	652	LYS	CB-CA-C	-8.18	93.23	109.67
4	E	652	LYS	CB-CA-C	-7.92	93.75	109.67
1	A	5	ASP	CA-CB-CG	7.83	120.43	112.60
1	C	741	THR	CA-CB-OG1	-7.77	97.95	109.60
4	E	695	ARG	CB-CG-CD	7.55	128.66	111.30
1	A	695	ARG	NE-CZ-NH2	7.54	125.98	119.20
5	G	741	THR	CA-CB-OG1	-7.52	98.32	109.60
1	A	741	THR	CA-CB-OG1	-7.39	98.52	109.60
1	C	713	ASP	CA-CB-CG	7.29	119.89	112.60
4	E	695	ARG	CD-NE-CZ	7.24	134.54	124.40
1	C	695	ARG	CB-CG-CD	7.21	127.89	111.30
1	A	695	ARG	CB-CG-CD	7.20	127.87	111.30
1	A	569	ARG	NH1-CZ-NH2	7.19	128.65	119.30
4	E	800	THR	CA-CB-OG1	-7.12	98.92	109.60
1	A	412	ARG	CD-NE-CZ	7.07	134.29	124.40
1	C	5	ASP	CA-CB-CG	7.06	119.66	112.60
1	A	295	ARG	CD-NE-CZ	6.97	134.16	124.40
5	G	348	GLU	CG-CD-OE1	-6.97	102.36	118.40
1	C	695	ARG	NE-CZ-NH2	6.87	125.38	119.20
1	C	258	LYS	CB-CA-C	6.84	121.71	110.90
4	E	5	ASP	CA-CB-CG	6.82	119.42	112.60
5	G	412	ARG	CD-NE-CZ	6.77	133.88	124.40
1	C	412	ARG	CD-NE-CZ	6.75	133.85	124.40
4	E	741	THR	CA-CB-OG1	-6.72	99.52	109.60
5	G	695	ARG	NH1-CZ-NH2	-6.62	110.69	119.30
4	E	586	MET	CG-SD-CE	6.57	115.35	100.90
4	E	258	LYS	CB-CA-C	6.55	121.99	110.85
5	G	695	ARG	CB-CG-CD	6.52	126.30	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	669	ASP	CA-CB-CG	6.43	119.03	112.60
5	G	532	HIS	CB-CA-C	6.42	118.85	109.48
5	G	295	ARG	CD-NE-CZ	6.30	133.22	124.40
1	C	586	MET	CG-SD-CE	6.25	114.66	100.90
1	A	258	LYS	CB-CA-C	6.23	121.45	110.85
4	E	295	ARG	CD-NE-CZ	6.22	133.11	124.40
1	C	117	LYS	CA-CB-CG	6.22	126.53	114.10
1	A	289	HIS	CA-CB-CG	-6.20	107.60	113.80
1	C	295	ARG	CD-NE-CZ	6.13	132.99	124.40
4	E	692	ASP	CA-CB-CG	6.09	118.69	112.60
5	G	692	ASP	CA-CB-CG	6.09	118.69	112.60
5	G	5	ASP	CA-CB-CG	6.06	118.66	112.60
5	G	23	PHE	CB-CA-C	6.06	122.47	110.42
1	A	713	ASP	CA-CB-CG	6.04	118.64	112.60
1	C	358	ASP	CA-CB-CG	6.01	118.61	112.60
5	G	752	PHE	CA-CB-CG	-6.00	107.80	113.80
1	A	800	THR	CA-CB-OG1	-5.99	100.61	109.60
1	C	800	THR	CA-CB-OG1	-5.96	100.66	109.60
4	E	4	ASN	CB-CA-C	-5.95	97.47	109.55
5	G	669	ASP	CA-CB-CG	5.93	118.53	112.60
3	D	82	PHE	CA-CB-CG	-5.91	107.89	113.80
1	C	66	THR	CA-CB-OG1	-5.90	100.74	109.60
5	G	348	GLU	CG-CD-OE2	5.89	131.95	118.40
4	E	358	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	767	ARG	NE-CZ-NH2	5.86	124.47	119.20
1	A	532	HIS	CB-CA-C	5.84	118.00	109.48
1	A	618	ASP	CA-CB-CG	5.84	118.44	112.60
5	G	713	ASP	CA-CB-CG	5.82	118.42	112.60
4	E	662	THR	CA-CB-OG1	-5.75	100.98	109.60
1	C	23	PHE	CB-CA-C	5.74	121.85	110.42
4	E	134	THR	CA-CB-OG1	-5.72	101.01	109.60
1	A	198	PRO	N-CA-CB	-5.71	97.26	103.25
5	G	485	GLN	N-CA-CB	-5.71	101.43	110.22
5	G	258	LYS	CB-CA-C	5.71	121.14	110.70
1	A	669	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	134	THR	CA-CB-OG1	-5.62	101.18	109.60
1	C	557	PRO	N-CA-CB	5.61	108.30	103.31
5	G	484	MET	CA-C-N	5.61	128.36	120.28
5	G	484	MET	C-N-CA	5.61	128.36	120.28
4	E	166	HIS	CB-CG-CD2	-5.52	124.03	131.20
1	C	728	ILE	CB-CA-C	5.51	117.28	110.73
1	A	695	ARG	CD-NE-CZ	5.50	132.10	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	PHE	CB-CA-C	5.49	121.35	110.42
1	A	598	GLU	CB-CG-CD	5.49	121.93	112.60
1	A	692	ASP	CA-CB-CG	5.49	118.08	112.60
1	A	787	ASP	CA-CB-CG	5.48	118.08	112.60
1	C	669	ASP	CA-CB-CG	5.47	118.07	112.60
4	E	412	ARG	CD-NE-CZ	5.45	132.02	124.40
1	A	811	GLU	CG-CD-OE1	5.43	130.90	118.40
4	E	718	LEU	N-CA-CB	5.40	117.84	110.01
3	H	28	PRO	N-CA-CB	-5.39	96.67	102.60
1	A	752	PHE	CA-CB-CG	-5.36	108.44	113.80
4	E	713	ASP	CA-CB-CG	5.33	117.94	112.60
5	G	88	ASP	CA-CB-CG	5.32	117.92	112.60
4	E	23	PHE	N-CA-CB	-5.32	101.50	110.49
1	A	358	ASP	CA-CB-CG	5.31	117.91	112.60
1	C	134	THR	CA-CB-OG1	-5.29	101.67	109.60
3	H	122	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	115	ASP	CA-CB-CG	5.27	117.87	112.60
5	G	134	THR	CA-CB-OG1	-5.27	101.70	109.60
4	E	198	PRO	N-CA-C	5.26	123.32	112.47
4	E	198	PRO	N-CA-CB	-5.24	97.75	103.25
1	C	752	PHE	CA-CB-CG	-5.24	108.56	113.80
5	G	23	PHE	N-CA-CB	-5.23	101.65	110.49
3	H	123	GLY	CA-C-O	-5.22	118.69	122.45
3	H	100	GLU	CB-CG-CD	5.21	121.46	112.60
4	E	340	LYS	N-CA-CB	5.20	117.60	110.07
5	G	819	PHE	CA-CB-CG	-5.18	108.62	113.80
4	E	415	THR	CA-CB-OG1	5.18	117.37	109.60
1	C	692	ASP	CA-CB-CG	5.17	117.77	112.60
1	C	695	ARG	NH1-CZ-NH2	-5.17	112.57	119.30
1	C	532	HIS	CA-CB-CG	5.17	118.97	113.80
1	C	695	ARG	CD-NE-CZ	5.17	131.63	124.40
1	A	348	GLU	CG-CD-OE2	-5.14	106.57	118.40
1	C	198	PRO	N-CA-C	5.14	123.07	112.47
1	C	618	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	88	ASP	CA-CB-CG	5.10	117.70	112.60
4	E	208	ARG	N-CA-CB	5.09	117.39	110.01
4	E	590	PHE	CA-CB-CG	-5.08	108.72	113.80
5	G	384	GLU	CB-CA-C	5.05	120.47	110.42
5	G	358	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	569	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	A	662	THR	CA-CB-OG1	-5.01	102.09	109.60

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	ASN	Peptide
1	A	412	ARG	Sidechain
1	A	450	ARG	Sidechain
1	A	545	ARG	Sidechain
1	A	702	ARG	Sidechain
1	A	722	ARG	Sidechain
1	A	79	ARG	Sidechain
2	B	128	ARG	Sidechain
1	C	161	PHE	Peptide
1	C	378	ARG	Sidechain
1	C	4	ASN	Peptide
1	C	412	ARG	Sidechain
1	C	545	ARG	Sidechain
1	C	607	ARG	Sidechain
1	C	702	ARG	Sidechain
1	C	722	ARG	Sidechain
3	D	1	ARG	Sidechain
3	D	128	ARG	Sidechain
4	E	124	ARG	Sidechain
4	E	161	PHE	Peptide
4	E	378	ARG	Sidechain
4	E	450	ARG	Sidechain
4	E	488	ARG	Sidechain
4	E	545	ARG	Sidechain
4	E	55	ARG	Sidechain
4	E	569	ARG	Sidechain
4	E	695	ARG	Sidechain
4	E	702	ARG	Sidechain
4	E	722	ARG	Sidechain
3	F	128	ARG	Sidechain
5	G	412	ARG	Sidechain
5	G	545	ARG	Sidechain
5	G	702	ARG	Sidechain
5	G	722	ARG	Sidechain
3	H	128	ARG	Sidechain

## 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	6495	0	6279	46	0
1	C	6498	0	6273	39	0
2	B	1003	0	989	8	0
3	D	1004	0	986	20	0
3	F	1004	0	986	3	0
3	H	1004	0	986	10	0
4	E	6507	0	6293	26	0
5	G	6511	0	6287	49	0
6	A	94	0	44	3	0
6	C	94	0	44	5	0
6	E	94	0	44	3	0
6	G	94	0	44	1	0
7	A	1	0	0	1	0
7	C	1	0	0	1	0
7	E	1	0	0	0	0
7	G	1	0	0	1	0
8	A	7	0	0	0	0
8	C	7	0	0	0	0
8	E	7	0	0	0	0
8	G	7	0	0	0	0
9	A	28	0	40	13	0
9	B	7	0	10	1	0
9	C	14	0	20	2	0
9	E	21	0	30	7	0
9	G	28	0	40	5	0
9	H	14	0	20	7	0
10	A	12	0	18	4	0
10	C	4	0	6	0	0
10	D	8	0	12	3	0
10	E	16	0	24	0	0
10	G	20	0	30	0	0
11	A	16	0	22	1	0
11	C	32	0	44	9	0
11	G	16	0	22	3	0
12	A	10	0	14	3	0
13	A	6	0	8	0	0
14	A	1	0	0	1	0
14	C	1	0	0	1	0
14	E	1	0	0	2	0
14	G	1	0	0	1	0
15	A	1	0	0	0	0
15	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	E	1	0	0	0	0
15	G	1	0	0	0	0
16	B	4	0	0	0	0
16	D	4	0	0	0	0
16	F	4	0	0	0	0
16	H	4	0	0	0	0
17	C	11	0	18	7	0
18	D	8	0	12	13	0
19	A	410	0	0	3	0
19	B	76	0	0	0	0
19	C	416	0	0	4	0
19	D	78	0	0	2	0
19	E	391	0	0	0	0
19	F	71	0	0	0	0
19	G	426	0	0	9	0
19	H	73	0	0	0	0
All	All	32670	0	29645	206	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (206) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ARG:HH22	9:A:911:PEG:C2	1.74	0.98
1:A:419:ARG:HH22	9:A:911:PEG:H21	1.26	0.95
5:G:299[A]:LEU:HD22	5:G:299[A]:LEU:N	1.84	0.90
9:E:909:PEG:H11	14:E:912:O:O	1.73	0.89
1:A:419:ARG:NH2	9:A:911:PEG:H21	1.87	0.88
7:G:901:4MO:MO	14:G:915:O:O	1.47	0.85
1:A:299[A]:LEU:HD22	1:A:299[A]:LEU:N	1.90	0.84
4:E:128:ALA:HB1	4:E:485:GLN:HB3	1.58	0.83
5:G:299[A]:LEU:N	5:G:299[A]:LEU:CD2	2.44	0.80
7:A:903:4MO:MO	14:A:915:O:O	1.53	0.80
5:G:603:ASN:HD22	5:G:607:ARG:HD3	1.47	0.80
1:A:704:ASN:HD21	2:B:97:GLN:HE22	1.30	0.80
1:A:522:GLU:OE2	11:C:908:1PE:H262	1.82	0.79
5:G:359[B]:MET:HE1	5:G:362:ARG:HH12	1.50	0.77
3:D:128:ARG:O	18:D:2203:PG0:H51	1.83	0.77
1:A:299[A]:LEU:N	1:A:299[A]:LEU:CD2	2.48	0.76
17:C:905:P4G:H13	3:D:101:ASN:HD21	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:125:ILE:O	18:D:2203:PG0:H52	1.85	0.76
3:H:104:ARG:HH22	9:H:203:PEG:H31	1.50	0.76
9:E:909:PEG:C1	14:E:912:O:O	2.34	0.75
4:E:88:ASP:OD1	9:E:911:PEG:H41	1.86	0.75
1:C:419:ARG:HH12	11:C:909:1PE:H162	1.50	0.75
1:A:359[B]:MET:SD	1:A:362:ARG:NH1	2.62	0.73
5:G:343:ARG:NH1	19:G:1001:HOH:O	2.20	0.72
1:A:419:ARG:HH22	9:A:911:PEG:H22	1.55	0.71
5:G:686:THR:HG21	5:G:788:TRP:HB2	1.74	0.70
1:A:419:ARG:HH12	9:A:911:PEG:H21	1.55	0.70
1:A:419:ARG:NH1	9:A:911:PEG:H21	2.07	0.69
4:E:700:ASN:ND2	6:E:903:MGD:H18	1.91	0.69
1:C:736:LYS:NZ	19:C:1001:HOH:O	2.25	0.69
1:A:419:ARG:CZ	9:A:911:PEG:H21	2.23	0.68
5:G:631[B]:ASP:OD1	5:G:634:ARG:NH1	2.27	0.67
3:D:13:VAL:HG13	9:G:907:PEG:H12	1.76	0.67
1:A:208:ARG:HH12	12:A:912:PGE:C4	2.08	0.66
1:C:632:ARG:O	1:C:635:LYS:HG3	1.96	0.66
1:C:700:ASN:ND2	6:C:901:MGD:H18	1.93	0.65
1:C:245:ASN:O	9:C:907:PEG:H22	1.95	0.65
5:G:121:LYS:HD2	19:G:1095:HOH:O	1.96	0.65
5:G:359[B]:MET:HE1	5:G:362:ARG:NH1	2.10	0.65
4:E:166:HIS:HD2	4:E:167:GLY:O	1.80	0.64
5:G:289:HIS:HD2	19:G:1096:HOH:O	1.80	0.64
9:C:907:PEG:H21	19:C:1364:HOH:O	1.98	0.64
1:C:635:LYS:HE2	19:C:1190:HOH:O	1.99	0.63
4:E:128:ALA:HB1	4:E:485:GLN:CB	2.26	0.62
1:C:203:GLU:OE2	11:C:909:1PE:H161	1.98	0.62
3:D:124:LEU:O	18:D:2203:PG0:H12	1.99	0.62
17:C:905:P4G:H52	17:C:905:P4G:H82	1.81	0.61
1:C:721:GLU:HB3	17:C:905:P4G:H22	1.81	0.61
1:A:208:ARG:HH12	12:A:912:PGE:H4	1.66	0.61
7:C:903:4MO:MO	14:C:911:O:O	1.70	0.61
3:D:100:GLU:HG2	18:D:2203:PG0:C2	2.32	0.60
10:A:910:EDO:H12	19:A:1315:HOH:O	2.00	0.60
1:A:704:ASN:ND2	2:B:97:GLN:HE22	1.99	0.58
4:E:190:PRO:HG2	4:E:191:MET:HE2	1.85	0.58
1:A:359[B]:MET:HE1	10:A:907:EDO:O1	2.04	0.58
3:D:128:ARG:H	18:D:2203:PG0:C5	2.17	0.57
1:A:124:ARG:NH1	9:A:914:PEG:H41	2.20	0.57
4:E:698:LEU:HB2	4:E:800:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:419:ARG:HH12	9:E:909:PEG:C3	2.17	0.56
1:A:404:VAL:HG11	1:A:417:CYS:HB2	1.87	0.56
1:C:721:GLU:OE1	17:C:905:P4G:H11	2.06	0.56
4:E:404:VAL:HG11	4:E:417:CYS:HB2	1.86	0.56
5:G:299[A]:LEU:CD2	5:G:299[A]:LEU:H	2.17	0.56
1:A:720:GLN:HE21	9:A:905:PEG:H22	1.72	0.55
3:H:123:GLY:HA2	9:H:203:PEG:H11	1.88	0.55
4:E:423:HIS:ND1	9:E:909:PEG:O1	2.32	0.55
1:A:818:SER:H	2:B:92:GLN:HE22	1.55	0.55
1:A:208:ARG:NH1	12:A:912:PGE:H4	2.23	0.54
5:G:267:ASN:ND2	5:G:372:ALA:HB3	2.23	0.54
1:A:299[A]:LEU:CD2	1:A:299[A]:LEU:H	2.20	0.54
1:C:699:ASN:OD1	6:C:902:MGD:H8	2.08	0.53
3:H:101:ASN:O	9:H:203:PEG:H21	2.07	0.53
1:C:698:LEU:HB2	1:C:800:THR:HG23	1.89	0.53
1:A:487:ALA:HB3	1:A:495:MET:HE1	1.89	0.53
4:E:695:ARG:NH1	4:E:737:GLN:OE1	2.43	0.52
5:G:603:ASN:ND2	5:G:607:ARG:HD3	2.21	0.52
1:C:208:ARG:HH22	11:C:909:1PE:H242	1.75	0.52
4:E:88:ASP:OD1	9:E:911:PEG:C4	2.56	0.52
4:E:166:HIS:CD2	4:E:167:GLY:O	2.62	0.52
9:E:906:PEG:H12	3:F:93:MET:HB3	1.90	0.52
2:B:62:HIS:CD2	2:B:63:MET:HG3	2.45	0.51
3:D:104:ARG:HH12	10:D:2204:EDO:C2	2.23	0.51
5:G:618:ASP:OD2	9:G:914:PEG:H21	2.10	0.51
5:G:698:LEU:HB2	5:G:800:THR:HG23	1.91	0.51
5:G:487:ALA:CB	5:G:495:MET:HE1	2.40	0.50
3:H:99:THR:HA	9:H:201:PEG:H11	1.93	0.50
1:C:404:VAL:HG11	1:C:417:CYS:HB2	1.93	0.50
3:D:127:GLY:H	18:D:2203:PG0:H53	1.76	0.50
5:G:818:SER:H	3:H:92:GLN:HE22	1.58	0.50
1:A:423:HIS:HB2	9:A:911:PEG:H42	1.93	0.49
3:D:127:GLY:N	18:D:2203:PG0:H53	2.27	0.49
1:A:25:ILE:O	1:A:542:ASN:HB2	2.12	0.49
5:G:50:LEU:HD22	9:G:908:PEG:H42	1.95	0.49
1:C:631[A]:ASP:OD1	1:C:634:ARG:NH1	2.45	0.49
5:G:695:ARG:HH12	5:G:768:GLY:HA2	1.78	0.49
1:C:208:ARG:HH22	11:C:909:1PE:C24	2.26	0.49
18:D:2203:PG0:H41	19:D:2330:HOH:O	2.12	0.49
5:G:404:VAL:HG11	5:G:417:CYS:HB2	1.96	0.48
5:G:695:ARG:NH1	5:G:768:GLY:HA2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:912:1PE:C13	19:G:1235:HOH:O	2.61	0.48
1:A:720:GLN:HE21	9:A:905:PEG:C2	2.27	0.48
2:B:99:THR:HA	9:B:201:PEG:H21	1.94	0.48
1:C:66:THR:HG22	18:D:2203:PG0:H32	1.96	0.48
1:C:333:LYS:HA	1:C:333:LYS:HE2	1.96	0.48
3:D:100:GLU:HB3	18:D:2203:PG0:H11	1.96	0.48
11:G:912:1PE:H131	19:G:1235:HOH:O	2.14	0.48
1:A:267:ASN:ND2	1:A:372:ALA:HB3	2.30	0.47
3:D:100:GLU:HG2	18:D:2203:PG0:H21	1.96	0.47
5:G:25:ILE:O	5:G:542:ASN:HB2	2.15	0.47
3:H:99:THR:O	9:H:201:PEG:C1	2.63	0.47
4:E:700:ASN:HD22	6:E:903:MGD:H18	1.63	0.47
5:G:362:ARG:HA	5:G:365:GLU:HG2	1.96	0.47
5:G:299[A]:LEU:H	5:G:299[A]:LEU:HD23	1.80	0.46
4:E:818:SER:H	3:F:92:GLN:HE22	1.64	0.46
5:G:165:ASP:OD2	11:G:912:1PE:H241	2.14	0.46
1:A:522:GLU:OE2	11:C:908:1PE:C26	2.59	0.46
5:G:66:THR:HB	3:H:100:GLU:CG	2.46	0.46
10:A:910:EDO:C1	19:A:1315:HOH:O	2.61	0.46
1:A:454:TRP:HE1	1:A:459:ASN:HD22	1.64	0.46
4:E:333:LYS:HA	4:E:333:LYS:HE2	1.97	0.46
1:A:699:ASN:OD1	6:A:901:MGD:H8	2.17	0.46
1:C:487:ALA:HB3	1:C:495:MET:HE1	1.97	0.46
5:G:686:THR:CG2	5:G:788:TRP:HB2	2.45	0.46
5:G:548:ARG:HD2	5:G:638:ASN:O	2.16	0.45
3:H:70:ASP:HB2	3:H:77:LYS:HE2	1.98	0.45
3:D:124:LEU:O	18:D:2203:PG0:O1	2.35	0.45
1:C:104:LYS:NZ	17:C:905:P4G:H83	2.32	0.45
5:G:618:ASP:OD1	9:G:914:PEG:H32	2.17	0.45
1:C:381:HIS:O	1:C:417:CYS:HA	2.17	0.45
4:E:25:ILE:O	4:E:542:ASN:HB2	2.16	0.45
1:A:769:GLN:HE21	10:A:908:EDO:C2	2.29	0.45
11:A:909:1PE:OH4	11:A:909:1PE:C25	2.64	0.45
3:F:70:ASP:HB2	3:F:77:LYS:HE2	1.99	0.45
1:A:698:LEU:HB2	1:A:800:THR:HG23	1.97	0.45
4:E:810[B]:MET:HB2	4:E:810[B]:MET:HE2	1.56	0.45
5:G:454:TRP:HE1	5:G:459:ASN:HD22	1.64	0.44
1:A:141:ALA:CB	1:A:492:THR:HG21	2.48	0.44
17:C:905:P4G:H13	3:D:101:ASN:ND2	2.28	0.44
19:G:1109:HOH:O	9:H:203:PEG:H11	2.17	0.44
9:A:911:PEG:C1	9:A:911:PEG:C4	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:SER:H	2:B:92:GLN:NE2	2.16	0.44
5:G:431:PRO:HB3	9:G:914:PEG:H12	1.98	0.44
1:C:632:ARG:O	1:C:635:LYS:HE3	2.18	0.44
4:E:699:ASN:OD1	6:E:902:MGD:H8	2.18	0.44
1:C:25:ILE:O	1:C:542:ASN:HB2	2.17	0.44
1:A:422:GLY:HA2	6:A:901:MGD:C12	2.48	0.44
5:G:561:MET:HG2	5:G:565:LEU:HB2	2.00	0.44
1:C:100:THR:OG1	3:D:98:ALA:O	2.35	0.43
1:C:695:ARG:HG3	1:C:695:ARG:HH11	1.83	0.43
1:C:700:ASN:HD22	6:C:901:MGD:H18	1.63	0.43
1:A:299[A]:LEU:H	1:A:299[A]:LEU:HD23	1.83	0.43
1:C:66:THR:HA	18:D:2203:PG0:H32	1.99	0.43
5:G:603:ASN:ND2	5:G:607:ARG:HH11	2.15	0.43
5:G:345:SER:OG	5:G:348:GLU:HG3	2.19	0.43
1:A:98:SER:O	2:B:62:HIS:HE1	2.02	0.43
1:A:101:ARG:HD3	6:A:901:MGD:N19	2.34	0.43
5:G:537:ASN:ND2	5:G:552:LYS:H	2.17	0.42
5:G:699:ASN:OD1	6:G:903:MGD:H8	2.19	0.42
1:A:117:LYS:CE	19:A:1064:HOH:O	2.66	0.42
1:C:533:PRO:HG3	1:C:538:LEU:HD13	2.00	0.42
1:C:537:ASN:ND2	1:C:552:LYS:H	2.17	0.42
1:C:419:ARG:NH1	11:C:909:1PE:H162	2.28	0.42
3:D:104:ARG:HH22	10:D:2204:EDO:C2	2.32	0.42
5:G:267:ASN:HD21	5:G:372:ALA:HB3	1.82	0.42
4:E:299[A]:LEU:CD1	4:E:299[A]:LEU:N	2.82	0.42
5:G:718:LEU:HB3	9:H:201:PEG:H21	2.02	0.42
2:B:77:LYS:HE2	2:B:84:GLU:OE2	2.20	0.42
4:E:548:ARG:HD2	4:E:638:ASN:O	2.18	0.42
1:C:385:LYS:HE2	6:C:901:MGD:S13	2.59	0.42
1:C:704:ASN:ND2	3:D:96:GLY:O	2.53	0.42
3:D:104:ARG:HH12	10:D:2204:EDO:H22	1.85	0.42
5:G:148:LYS:HD3	5:G:577:MET:HE2	2.02	0.42
3:D:70:ASP:HB2	3:D:77:LYS:HE2	2.01	0.42
4:E:537:ASN:ND2	4:E:552:LYS:H	2.18	0.42
17:C:905:P4G:C1	19:D:2340:HOH:O	2.68	0.41
1:C:422:GLY:HA2	6:C:902:MGD:C12	2.49	0.41
1:C:454:TRP:HE1	1:C:459:ASN:HD22	1.68	0.41
5:G:359[B]:MET:CE	5:G:362:ARG:NH1	2.83	0.41
1:C:575:ARG:HD3	19:C:1300:HOH:O	2.20	0.41
1:A:356:PRO:HG2	1:A:359[B]:MET:HG2	2.03	0.41
5:G:48:ASN:HD22	5:G:50:LEU:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:MET:HA	1:A:546:ARG:O	2.20	0.41
4:E:631:ASP:OD1	4:E:634:ARG:NH1	2.54	0.41
9:A:911:PEG:H22	9:A:911:PEG:H41	1.76	0.41
1:C:548:ARG:HD2	1:C:638:ASN:O	2.20	0.41
1:C:818:SER:H	3:D:92:GLN:HE22	1.69	0.41
5:G:741:THR:OG1	5:G:742:GLY:N	2.54	0.41
1:A:141:ALA:HB1	1:A:492:THR:HG21	2.02	0.41
1:C:635:LYS:HZ3	1:C:654:LEU:H	1.69	0.41
1:A:695:ARG:HH11	1:A:695:ARG:HG3	1.85	0.41
4:E:33:TYR:CE2	4:E:49:ALA:HB1	2.56	0.41
5:G:437:LYS:HG2	19:G:1343:HOH:O	2.21	0.41
4:E:381:HIS:O	4:E:417:CYS:HA	2.21	0.40
5:G:289:HIS:CD2	19:G:1096:HOH:O	2.64	0.40
5:G:704:ASN:ND2	3:H:96:GLY:O	2.54	0.40
19:G:1111:HOH:O	3:H:44:PRO:HG3	2.20	0.40
1:A:631:ASP:OD1	1:A:634:ARG:NH1	2.52	0.40
5:G:381:HIS:O	5:G:417:CYS:HA	2.20	0.40
5:G:45:PRO:O	5:G:51:GLY:HA2	2.21	0.40
1:A:548:ARG:HD2	1:A:638:ASN:O	2.21	0.40
1:C:517:PRO:HG3	11:C:908:1PE:C13	2.51	0.40
5:G:121:LYS:HE3	5:G:121:LYS:HB3	1.80	0.40
1:A:33:TYR:O	1:A:83:ILE:HA	2.22	0.40
1:C:419:ARG:HH22	11:C:909:1PE:C16	2.34	0.40
4:E:33:TYR:O	4:E:83:ILE:HA	2.21	0.40
5:G:65:LEU:HD11	5:G:84:MET:HE2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	823/822 (100%)	789 (96%)	34 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	823/822 (100%)	797 (97%)	26 (3%)	0	100	100
2	B	132/134 (98%)	129 (98%)	2 (2%)	1 (1%)	16	8
3	D	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
3	F	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
3	H	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
4	E	825/824 (100%)	794 (96%)	31 (4%)	0	100	100
5	G	826/823 (100%)	795 (96%)	30 (4%)	1 (0%)	48	40
All	All	3828/3830 (100%)	3687 (96%)	139 (4%)	2 (0%)	48	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G	392	ASP
2	B	62	HIS

### 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	678/675 (100%)	668 (98%)	10 (2%)	57	56
1	C	678/675 (100%)	667 (98%)	11 (2%)	55	54
2	B	111/111 (100%)	109 (98%)	2 (2%)	51	50
3	D	110/110 (100%)	108 (98%)	2 (2%)	51	50
3	F	110/110 (100%)	109 (99%)	1 (1%)	70	73
3	H	110/110 (100%)	109 (99%)	1 (1%)	70	73
4	E	678/675 (100%)	666 (98%)	12 (2%)	51	50
5	G	680/675 (101%)	668 (98%)	12 (2%)	51	50
All	All	3155/3141 (100%)	3104 (98%)	51 (2%)	57	54

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	146	LEU
1	A	157	GLN
1	A	258	LYS
1	A	299[A]	LEU
1	A	299[B]	LEU
1	A	410	VAL
1	A	482	GLN
1	A	695	ARG
1	A	811	GLU
2	B	0	LEU
2	B	41	SER
1	C	7	ILE
1	C	146	LEU
1	C	198	PRO
1	C	258	LYS
1	C	333	LYS
1	C	410	VAL
1	C	580	LYS
1	C	635	LYS
1	C	695	ARG
1	C	774	PHE
1	C	793	ILE
3	D	100	GLU
3	D	111	GLU
4	E	7	ILE
4	E	146	LEU
4	E	157	GLN
4	E	249	PRO
4	E	258	LYS
4	E	299[A]	LEU
4	E	299[B]	LEU
4	E	410	VAL
4	E	437	LYS
4	E	485	GLN
4	E	635	LYS
4	E	774	PHE
3	F	100	GLU
5	G	4	ASN
5	G	7	ILE
5	G	121	LYS
5	G	146	LEU
5	G	258	LYS

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Mol	Chain	Res	Type
5	G	299[A]	LEU
5	G	299[B]	LEU
5	G	333	LYS
5	G	410	VAL
5	G	437	LYS
5	G	695	ARG
5	G	774	PHE
3	H	28	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	13	ASN
1	A	48	ASN
1	A	138	HIS
1	A	157	GLN
1	A	216	ASN
1	A	270	GLN
1	A	459	ASN
1	A	475	GLN
1	A	537	ASN
1	A	572	ASN
1	A	611	GLN
1	A	626	HIS
1	A	638	ASN
1	A	688	GLN
1	A	690	GLN
1	A	704	ASN
1	A	720	GLN
1	A	769	GLN
2	B	10	GLN
2	B	62	HIS
2	B	92	GLN
1	C	4	ASN
1	C	13	ASN
1	C	138	HIS
1	C	216	ASN
1	C	442	GLN
1	C	459	ASN
1	C	537	ASN
1	C	572	ASN

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Mol	Chain	Res	Type
1	C	638	ASN
1	C	642	GLN
1	C	700	ASN
1	C	720	GLN
4	E	13	ASN
4	E	138	HIS
4	E	157	GLN
4	E	166	HIS
4	E	216	ASN
4	E	233	ASN
4	E	442	GLN
4	E	459	ASN
4	E	537	ASN
4	E	572	ASN
4	E	579	GLN
4	E	611	GLN
4	E	638	ASN
4	E	642	GLN
4	E	700	ASN
4	E	720	GLN
4	E	792	ASN
3	F	10	GLN
3	F	92	GLN
5	G	4	ASN
5	G	13	ASN
5	G	48	ASN
5	G	82	ASN
5	G	138	HIS
5	G	216	ASN
5	G	233	ASN
5	G	267	ASN
5	G	289	HIS
5	G	459	ASN
5	G	485	GLN
5	G	537	ASN
5	G	572	ASN
5	G	603	ASN
5	G	611	GLN
5	G	638	ASN
5	G	681	ASN
5	G	720	GLN
5	G	769	GLN

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Mol	Chain	Res	Type
5	G	792	ASN
3	H	92	GLN

### 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 67 ligands modelled in this entry, 12 are monoatomic - leaving 55 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
16	FES	F	201	3	0,4,4	-	-	-		
11	1PE	C	908	-	15,15,15	0.99	0	14,14,14	0.77	0
9	PEG	B	201	-	6,6,6	0.42	0	5,5,5	0.22	0
13	GOL	A	913	-	5,5,5	0.25	0	5,5,5	0.48	0
10	EDO	E	908	-	3,3,3	0.31	0	2,2,2	0.52	0
9	PEG	G	908	-	6,6,6	0.46	0	5,5,5	0.53	0
10	EDO	A	908	-	3,3,3	0.53	0	2,2,2	0.81	0
10	EDO	D	2204	-	3,3,3	0.94	0	2,2,2	0.40	0
6	MGD	E	903	7	47,52,52	1.07	4 (8%)	58,81,81	1.63	9 (15%)
11	1PE	C	909	-	15,15,15	0.62	0	14,14,14	0.65	0
6	MGD	C	901	7	47,52,52	1.37	4 (8%)	58,81,81	1.28	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	EDO	E	910	-	3,3,3	0.55	0	2,2,2	0.18	0
6	MGD	A	901	7	47,52,52	1.04	4 (8%)	58,81,81	1.44	12 (20%)
10	EDO	C	910	-	3,3,3	0.28	0	2,2,2	0.12	0
18	PG0	D	2203	-	7,7,7	0.98	0	6,6,6	0.66	0
9	PEG	A	914	-	6,6,6	0.90	0	5,5,5	0.51	0
9	PEG	G	914	-	6,6,6	0.41	0	5,5,5	0.69	0
10	EDO	A	907	-	3,3,3	0.51	0	2,2,2	0.60	0
8	F3S	G	904	5	0,9,9	-	-	-	-	-
9	PEG	G	906	-	6,6,6	0.76	0	5,5,5	0.83	0
10	EDO	G	905	-	3,3,3	1.13	0	2,2,2	0.52	0
8	F3S	A	904	1	0,9,9	-	-	-	-	-
9	PEG	E	909	-	6,6,6	0.43	0	5,5,5	0.44	0
10	EDO	D	2201	-	3,3,3	0.97	0	2,2,2	0.65	0
9	PEG	H	203	-	6,6,6	1.38	1 (16%)	5,5,5	1.11	0
11	1PE	A	909	-	15,15,15	0.52	0	14,14,14	0.68	0
9	PEG	H	201	-	6,6,6	0.68	0	5,5,5	0.38	0
10	EDO	A	910	-	3,3,3	0.87	0	2,2,2	0.48	0
9	PEG	A	911	-	6,6,6	0.40	0	5,5,5	1.18	1 (20%)
9	PEG	A	906	-	6,6,6	0.76	0	5,5,5	0.60	0
11	1PE	G	912	-	15,15,15	0.46	0	14,14,14	0.51	0
9	PEG	A	905	-	6,6,6	0.41	0	5,5,5	0.23	0
12	PGE	A	912	-	9,9,9	0.58	0	8,8,8	0.69	0
10	EDO	G	911	-	3,3,3	1.15	0	2,2,2	0.63	0
10	EDO	E	905	-	3,3,3	0.95	0	2,2,2	1.14	0
16	FES	H	202	3	0,4,4	-	-	-	-	-
6	MGD	C	902	7	47,52,52	1.59	3 (6%)	58,81,81	1.32	6 (10%)
8	F3S	C	904	1	0,9,9	-	-	-	-	-
9	PEG	E	911	-	6,6,6	0.95	0	5,5,5	0.80	0
10	EDO	G	913	-	3,3,3	0.93	0	2,2,2	0.51	0
8	F3S	E	901	4	0,9,9	-	-	-	-	-
10	EDO	E	907	-	3,3,3	0.13	0	2,2,2	0.47	0
9	PEG	C	906	-	6,6,6	0.88	0	5,5,5	0.60	0
6	MGD	E	902	7	47,52,52	1.87	3 (6%)	58,81,81	1.59	14 (24%)
16	FES	D	2202	3	0,4,4	-	-	-	-	-
9	PEG	C	907	-	6,6,6	0.64	0	5,5,5	0.72	0
6	MGD	A	902	7	47,52,52	0.94	2 (4%)	58,81,81	1.48	6 (10%)
6	MGD	G	903	7	47,52,52	1.15	4 (8%)	58,81,81	1.46	10 (17%)
10	EDO	G	910	-	3,3,3	0.49	0	2,2,2	0.64	0
6	MGD	G	902	7	47,52,52	1.34	2 (4%)	58,81,81	1.59	9 (15%)
17	P4G	C	905	-	10,10,10	0.59	0	9,9,9	1.01	0
9	PEG	G	907	-	6,6,6	0.97	0	5,5,5	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	FES	B	202	2	0,4,4	-	-	-		
9	PEG	E	906	-	6,6,6	1.07	0	5,5,5	0.58	0
10	EDO	G	909	-	3,3,3	0.88	0	2,2,2	0.41	0

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
16	FES	F	201	3	-	-	0/1/1/1
11	1PE	C	908	-	-	6/13/13/13	-
9	PEG	B	201	-	-	1/4/4/4	-
13	GOL	A	913	-	-	1/4/4/4	-
10	EDO	E	908	-	-	0/1/1/1	-
9	PEG	G	908	-	-	2/4/4/4	-
10	EDO	A	908	-	-	1/1/1/1	-
10	EDO	D	2204	-	-	1/1/1/1	-
6	MGD	E	903	7	-	6/22/66/66	0/6/6/6
11	1PE	C	909	-	-	8/13/13/13	-
6	MGD	C	901	7	-	6/22/66/66	0/6/6/6
10	EDO	E	910	-	-	1/1/1/1	-
6	MGD	A	901	7	-	4/22/66/66	0/6/6/6
10	EDO	C	910	-	-	1/1/1/1	-
18	PG0	D	2203	-	-	2/5/5/5	-
9	PEG	A	914	-	-	1/4/4/4	-
9	PEG	G	914	-	-	1/4/4/4	-
10	EDO	A	907	-	-	1/1/1/1	-
9	PEG	G	906	-	-	2/4/4/4	-
10	EDO	G	905	-	-	1/1/1/1	-
8	F3S	G	904	5	-	-	0/3/3/3
9	PEG	E	909	-	-	4/4/4/4	-
8	F3S	A	904	1	-	-	0/3/3/3
10	EDO	D	2201	-	-	1/1/1/1	-
9	PEG	H	203	-	-	1/4/4/4	-
11	1PE	A	909	-	-	9/13/13/13	-
9	PEG	H	201	-	-	1/4/4/4	-
10	EDO	A	910	-	-	1/1/1/1	-
9	PEG	A	911	-	-	4/4/4/4	-
9	PEG	A	906	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	1PE	G	912	-	-	6/13/13/13	-
9	PEG	A	905	-	-	3/4/4/4	-
12	PGE	A	912	-	-	4/7/7/7	-
10	EDO	G	911	-	-	1/1/1/1	-
10	EDO	E	905	-	-	1/1/1/1	-
16	FES	H	202	3	-	-	0/1/1/1
6	MGD	C	902	7	-	5/22/66/66	0/6/6/6
9	PEG	E	911	-	-	3/4/4/4	-
10	EDO	G	913	-	-	1/1/1/1	-
8	F3S	C	904	1	-	-	0/3/3/3
10	EDO	E	907	-	-	0/1/1/1	-
8	F3S	E	901	4	-	-	0/3/3/3
9	PEG	C	906	-	-	3/4/4/4	-
6	MGD	E	902	7	-	3/22/66/66	0/6/6/6
16	FES	D	2202	3	-	-	0/1/1/1
9	PEG	C	907	-	-	1/4/4/4	-
6	MGD	A	902	7	-	4/22/66/66	0/6/6/6
6	MGD	G	903	7	-	4/22/66/66	0/6/6/6
10	EDO	G	910	-	-	1/1/1/1	-
6	MGD	G	902	7	-	4/22/66/66	0/6/6/6
17	P4G	C	905	-	-	8/8/8/8	-
9	PEG	G	907	-	-	4/4/4/4	-
16	FES	B	202	2	-	-	0/1/1/1
9	PEG	E	906	-	-	1/4/4/4	-
10	EDO	G	909	-	-	1/1/1/1	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	902	MGD	PA-O3B	8.35	1.68	1.59
6	C	902	MGD	PA-O3B	6.64	1.66	1.59
6	E	902	MGD	PB-O3B	6.38	1.66	1.59
6	C	902	MGD	PB-O3B	6.16	1.66	1.59
6	C	901	MGD	C23-C14	5.61	1.58	1.53
6	G	902	MGD	C10-C11	-5.55	1.44	1.51
6	G	902	MGD	C23-C14	-5.49	1.49	1.53
6	G	903	MGD	PA-O3B	4.84	1.64	1.59
6	E	902	MGD	C23-C14	-4.32	1.50	1.53
6	C	901	MGD	PA-O3B	-4.13	1.55	1.59
6	A	901	MGD	C23-C14	-3.35	1.51	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	902	MGD	C23-C14	-3.03	1.51	1.53
6	C	901	MGD	C16-N15	-2.93	1.31	1.37
6	G	903	MGD	C21-N22	-2.79	1.32	1.35
6	E	903	MGD	C23-C14	2.75	1.55	1.53
6	A	901	MGD	C16-N15	2.64	1.44	1.37
6	E	903	MGD	C21-N22	2.64	1.38	1.35
6	E	903	MGD	PB-O3B	2.52	1.62	1.59
6	A	901	MGD	PB-O3B	-2.41	1.56	1.59
6	E	903	MGD	PA-O3B	-2.36	1.57	1.59
6	G	903	MGD	PB-O5'	2.35	1.68	1.59
6	A	902	MGD	O11-C23	-2.35	1.40	1.43
6	A	902	MGD	C23-C14	2.32	1.55	1.53
6	A	901	MGD	O11-C23	-2.31	1.40	1.43
9	H	203	PEG	C2-C1	2.29	1.61	1.49
6	G	903	MGD	C23-C14	-2.29	1.51	1.53
6	C	901	MGD	C23-N22	-2.07	1.41	1.45

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	902	MGD	C23-C14-N15	6.82	114.57	107.87
6	G	902	MGD	C23-C14-N15	6.44	114.19	107.87
6	E	903	MGD	O2B-PB-O3B	5.41	121.90	107.27
6	E	903	MGD	C23-C14-N15	4.84	112.63	107.87
6	G	902	MGD	O11-C23-C14	4.80	112.16	108.96
6	E	903	MGD	O11-C23-C14	4.39	111.89	108.96
6	G	903	MGD	O2B-PB-O3B	4.34	119.00	107.27
6	A	901	MGD	O11-C23-N22	-4.19	104.81	108.61
6	E	902	MGD	C19-N20-C21	4.14	120.66	113.36
6	G	903	MGD	O11-C23-N22	-3.84	105.12	108.61
6	A	902	MGD	O2A-PA-O1A	3.61	129.26	112.44
6	A	902	MGD	O2B-PB-O3B	3.59	116.99	107.27
6	E	902	MGD	O11-C23-N22	-3.59	105.35	108.61
6	E	903	MGD	C19-N20-C21	3.57	119.65	113.36
6	C	902	MGD	O2A-PA-O1A	3.55	128.94	112.44
6	G	902	MGD	O11-C23-N22	-3.53	105.40	108.61
6	E	903	MGD	O11-C23-N22	-3.44	105.48	108.61
6	A	901	MGD	O2A-PA-O3A	-3.43	92.00	107.57
6	G	902	MGD	O2B-PB-O3B	3.21	115.95	107.27
6	C	901	MGD	C23-C14-N15	3.20	111.01	107.87
6	E	902	MGD	O2A-PA-O1A	3.15	127.11	112.44
6	G	902	MGD	C19-N20-C21	3.14	118.90	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	902	MGD	C23-C14-N15	3.09	110.90	107.87
6	G	903	MGD	O2A-PA-O3B	3.06	115.53	107.27
6	C	902	MGD	C19-N20-C21	3.05	118.74	113.36
6	A	901	MGD	O3'-C3'-C2'	3.03	121.54	111.82
6	G	903	MGD	C19-N20-C21	2.90	118.47	113.36
6	A	902	MGD	O2B-PB-O1B	2.90	125.91	112.44
6	C	901	MGD	O3B-PB-O1B	-2.83	102.20	110.70
6	G	903	MGD	O3B-PA-O1A	-2.82	102.22	110.70
6	C	902	MGD	C2'-C1'-N9	2.74	120.88	113.25
6	G	903	MGD	O2A-PA-O1A	2.74	125.18	112.44
6	E	903	MGD	O2A-PA-O3A	-2.70	95.35	107.57
6	C	901	MGD	C19-N20-C21	2.67	118.07	113.36
6	G	903	MGD	C4'-O4'-C1'	-2.64	103.63	109.47
6	E	903	MGD	O3B-PA-O1A	2.63	118.62	110.70
6	C	901	MGD	O3'-C3'-C2'	2.63	120.23	111.82
6	A	901	MGD	O2A-PA-O1A	2.57	124.41	112.44
6	E	902	MGD	C19-N18-C17	-2.53	120.51	125.11
6	A	901	MGD	C19-N20-C21	2.51	117.78	113.36
6	E	902	MGD	O2A-PA-O3A	-2.49	96.26	107.57
6	G	902	MGD	O2A-PA-O1A	2.48	124.00	112.44
6	G	903	MGD	O3'-C3'-C2'	2.48	119.77	111.82
6	A	901	MGD	O2B-PB-O3B	2.47	113.95	107.27
6	C	901	MGD	O3'-C3'-C4'	-2.44	104.08	111.08
6	G	902	MGD	O3'-C3'-C2'	2.44	119.63	111.82
6	E	902	MGD	C23-C14-N15	2.43	110.26	107.87
6	E	902	MGD	O2'-C2'-C1'	2.43	118.48	110.10
6	E	902	MGD	C4'-O4'-C1'	-2.39	104.18	109.47
6	A	901	MGD	O2A-PA-O3B	2.37	113.69	107.27
6	A	901	MGD	C17-C16-N15	2.34	122.65	116.27
6	C	902	MGD	O2B-PB-O3B	2.31	113.53	107.27
9	A	911	PEG	O2-C2-C1	2.26	120.05	110.11
6	A	901	MGD	C4'-O4'-C1'	-2.25	104.51	109.47
6	G	903	MGD	O2'-C2'-C1'	2.24	117.82	110.10
6	E	902	MGD	O11-C23-C14	-2.23	107.48	108.96
6	G	903	MGD	C17-C16-N15	2.22	122.33	116.27
6	C	901	MGD	N19-C19-N18	2.22	121.44	116.76
6	E	902	MGD	C2'-C1'-N9	2.18	119.31	113.25
6	A	902	MGD	O3A-C10-C11	-2.18	103.21	108.58
6	E	902	MGD	O3'-C3'-C2'	2.16	118.74	111.82
6	E	902	MGD	O6-C6-C5	2.16	132.22	126.53
6	E	902	MGD	C16-C17-N18	2.15	118.03	112.13
6	E	902	MGD	O2'-C2'-C3'	-2.13	104.98	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	903	MGD	O2A-PA-O3B	2.13	113.02	107.27
6	A	901	MGD	C19-N18-C17	-2.13	121.25	125.11
6	E	903	MGD	O2B-PB-O1B	2.11	122.26	112.44
6	A	902	MGD	O3B-PB-O1B	-2.10	104.38	110.70
6	C	901	MGD	N18-C19-N20	-2.10	119.48	123.32
6	G	902	MGD	C17-C16-N15	2.05	121.86	116.27
6	A	901	MGD	O4'-C1'-N9	2.05	113.00	108.36
6	C	902	MGD	O3'-C3'-C2'	2.05	118.37	111.82
6	A	901	MGD	O3A-PA-O1A	2.03	116.98	108.94
6	G	902	MGD	O3A-C10-C11	2.02	113.57	108.58
6	C	901	MGD	O2A-PA-O3B	2.01	112.71	107.27

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	901	MGD	C5'-O5'-PB-O1B
6	A	901	MGD	C5'-O5'-PB-O3B
6	A	902	MGD	C5'-O5'-PB-O1B
6	C	901	MGD	PA-O3B-PB-O5'
6	C	901	MGD	C5'-O5'-PB-O1B
6	C	902	MGD	C5'-O5'-PB-O1B
6	E	903	MGD	C5'-O5'-PB-O1B
6	G	902	MGD	C5'-O5'-PB-O1B
6	G	903	MGD	PA-O3B-PB-O5'
6	G	903	MGD	C5'-O5'-PB-O1B
9	H	203	PEG	C1-C2-O2-C3
17	C	905	P4G	C3-C4-O3-C5
9	A	911	PEG	C4-C3-O2-C2
11	C	908	1PE	OH6-C15-C25-OH5
9	G	908	PEG	O2-C3-C4-O4
18	D	2203	PG0	O1-C3-C4-O2
17	C	905	P4G	O2-C3-C4-O3
12	A	912	PGE	O2-C3-C4-O3
9	E	909	PEG	O2-C3-C4-O4
11	A	909	1PE	OH2-C12-C22-OH3
11	G	912	1PE	OH7-C16-C26-OH6
11	A	909	1PE	OH6-C15-C25-OH5
9	A	911	PEG	O2-C3-C4-O4
9	G	906	PEG	O2-C3-C4-O4
9	G	907	PEG	O1-C1-C2-O2
9	A	911	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
13	A	913	GOL	C1-C2-C3-O3
9	A	905	PEG	O2-C3-C4-O4
9	A	906	PEG	O2-C3-C4-O4
12	A	912	PGE	O3-C5-C6-O4
18	D	2203	PG0	OTT-C1-C2-O1
11	A	909	1PE	OH4-C13-C23-OH3
6	C	901	MGD	O4'-C4'-C5'-O5'
9	A	911	PEG	O1-C1-C2-O2
9	B	201	PEG	O1-C1-C2-O2
9	E	906	PEG	O1-C1-C2-O2
9	E	909	PEG	O1-C1-C2-O2
10	A	908	EDO	O1-C1-C2-O2
10	E	910	EDO	O1-C1-C2-O2
11	C	909	1PE	OH7-C16-C26-OH6
6	C	901	MGD	C3'-C4'-C5'-O5'
6	E	903	MGD	O4'-C4'-C5'-O5'
11	C	909	1PE	OH4-C13-C23-OH3
9	C	906	PEG	O1-C1-C2-O2
9	G	907	PEG	O2-C3-C4-O4
9	G	908	PEG	O1-C1-C2-O2
11	A	909	1PE	OH5-C14-C24-OH4
17	C	905	P4G	O3-C5-C6-O4
6	A	902	MGD	O4'-C4'-C5'-O5'
6	G	902	MGD	O4'-C4'-C5'-O5'
9	A	905	PEG	O1-C1-C2-O2
10	C	910	EDO	O1-C1-C2-O2
10	G	910	EDO	O1-C1-C2-O2
11	G	912	1PE	OH4-C13-C23-OH3
9	H	201	PEG	O1-C1-C2-O2
17	C	905	P4G	C1-C2-O2-C3
6	A	902	MGD	C3'-C4'-C5'-O5'
17	C	905	P4G	C8-C7-O4-C6
10	G	913	EDO	O1-C1-C2-O2
9	E	911	PEG	O2-C3-C4-O4
6	A	901	MGD	PA-O3B-PB-O5'
6	C	902	MGD	PA-O3B-PB-O5'
6	E	902	MGD	PA-O3B-PB-O5'
6	G	902	MGD	PA-O3B-PB-O5'
11	C	909	1PE	C13-C23-OH3-C22
11	C	908	1PE	C15-C25-OH5-C14
11	G	912	1PE	C15-C25-OH5-C14
9	E	909	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
11	A	909	1PE	C23-C13-OH4-C24
6	E	903	MGD	C3'-C4'-C5'-O5'
9	A	905	PEG	C1-C2-O2-C3
11	C	909	1PE	C23-C13-OH4-C24
9	E	911	PEG	O1-C1-C2-O2
9	G	914	PEG	C1-C2-O2-C3
9	E	911	PEG	C4-C3-O2-C2
11	C	909	1PE	C12-C22-OH3-C23
17	C	905	P4G	C6-C5-O3-C4
12	A	912	PGE	C1-C2-O2-C3
6	E	903	MGD	PB-O3B-PA-O1A
11	A	909	1PE	C15-C25-OH5-C14
17	C	905	P4G	C4-C3-O2-C2
9	G	907	PEG	C4-C3-O2-C2
11	C	908	1PE	OH4-C13-C23-OH3
9	C	906	PEG	O2-C3-C4-O4
10	A	910	EDO	O1-C1-C2-O2
6	C	901	MGD	C10-O3A-PA-O1A
6	C	902	MGD	C5'-O5'-PB-O2B
6	C	902	MGD	C5'-O5'-PB-O3B
6	E	902	MGD	C5'-O5'-PB-O1B
6	E	903	MGD	C10-O3A-PA-O1A
6	G	903	MGD	C5'-O5'-PB-O3B
9	C	907	PEG	O2-C3-C4-O4
11	A	909	1PE	C16-C26-OH6-C15
11	C	908	1PE	OH2-C12-C22-OH3
11	G	912	1PE	C16-C26-OH6-C15
10	D	2201	EDO	O1-C1-C2-O2
11	C	909	1PE	C16-C26-OH6-C15
11	G	912	1PE	OH5-C14-C24-OH4
11	C	908	1PE	OH7-C16-C26-OH6
11	G	912	1PE	C24-C14-OH5-C25
12	A	912	PGE	O1-C1-C2-O2
10	E	905	EDO	O1-C1-C2-O2
10	G	911	EDO	O1-C1-C2-O2
9	G	907	PEG	C1-C2-O2-C3
11	A	909	1PE	C14-C24-OH4-C13
9	A	914	PEG	C1-C2-O2-C3
11	A	909	1PE	C12-C22-OH3-C23
10	A	907	EDO	O1-C1-C2-O2
10	D	2204	EDO	O1-C1-C2-O2
10	G	909	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	A	902	MGD	PB-O3B-PA-O2A
6	E	903	MGD	PB-O3B-PA-O2A
11	C	909	1PE	OH5-C14-C24-OH4
11	C	908	1PE	C25-C15-OH6-C26
9	G	906	PEG	C1-C2-O2-C3
9	E	909	PEG	C4-C3-O2-C2
9	C	906	PEG	C1-C2-O2-C3
17	C	905	P4G	C5-C6-O4-C7
10	G	905	EDO	O1-C1-C2-O2
11	C	909	1PE	OH2-C12-C22-OH3
6	A	901	MGD	PB-O3B-PA-O2A
6	C	901	MGD	PB-O3B-PA-O2A
6	C	902	MGD	PB-O3B-PA-O2A
6	E	902	MGD	PB-O3B-PA-O2A
6	G	902	MGD	PB-O3B-PA-O2A
6	G	903	MGD	PB-O3B-PA-O2A

There are no ring outliers.

30 monomers are involved in 90 short contacts:

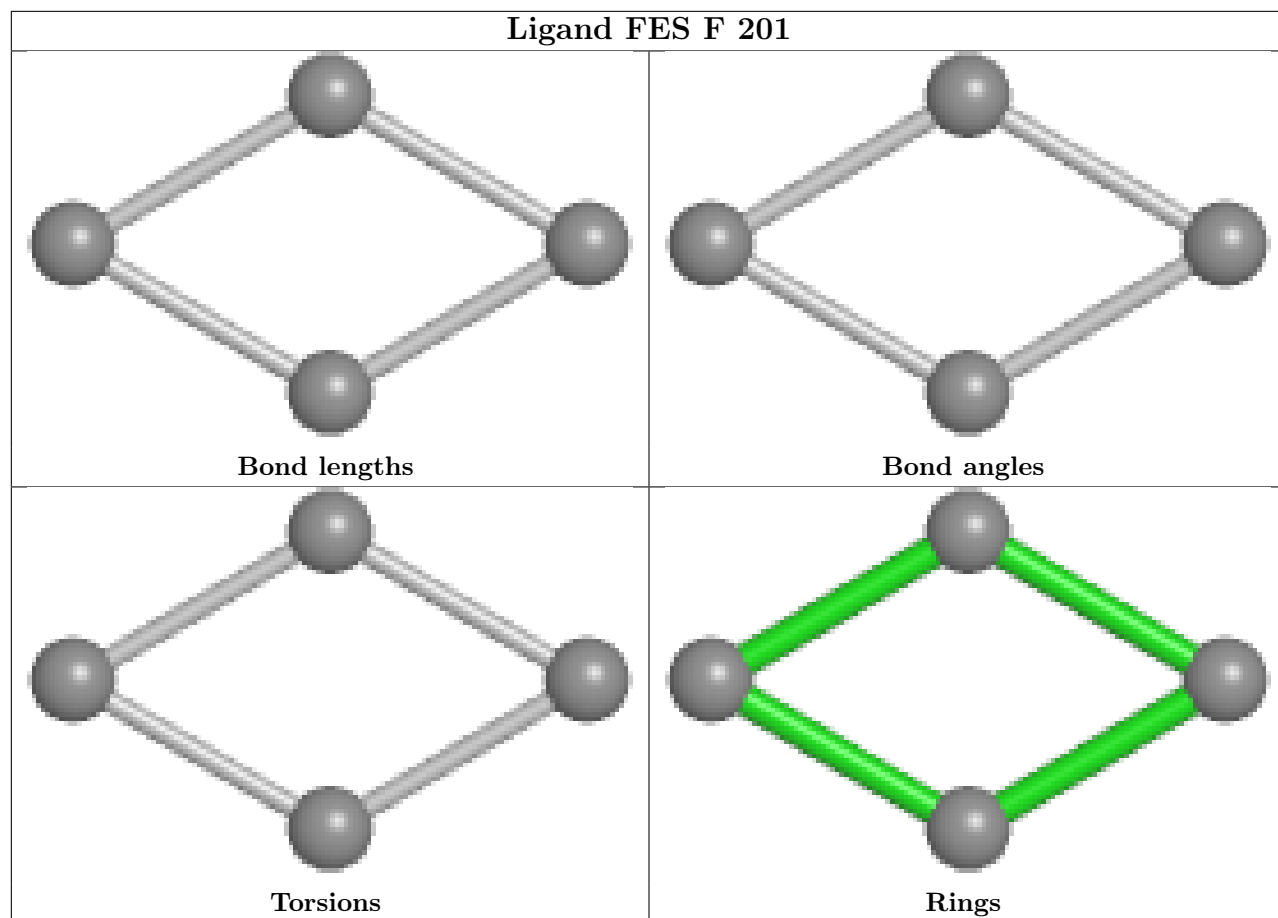
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	908	1PE	3	0
9	B	201	PEG	1	0
9	G	908	PEG	1	0
10	A	908	EDO	1	0
10	D	2204	EDO	3	0
6	E	903	MGD	2	0
11	C	909	1PE	6	0
6	C	901	MGD	3	0
6	A	901	MGD	3	0
18	D	2203	PG0	13	0
9	A	914	PEG	1	0
9	G	914	PEG	3	0
10	A	907	EDO	1	0
9	E	909	PEG	4	0
9	H	203	PEG	4	0
11	A	909	1PE	1	0
9	H	201	PEG	3	0
10	A	910	EDO	2	0
9	A	911	PEG	10	0
11	G	912	1PE	3	0
9	A	905	PEG	2	0

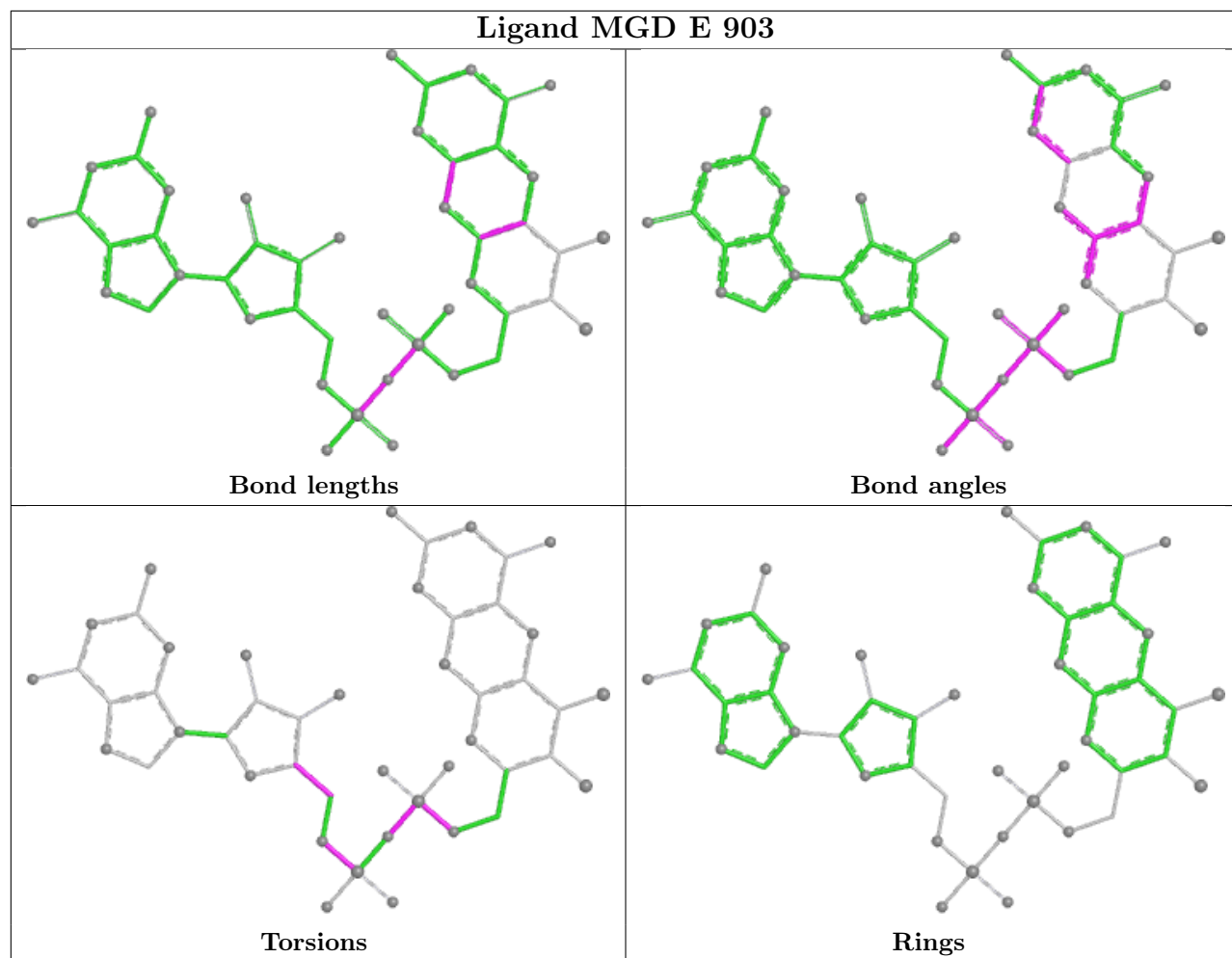
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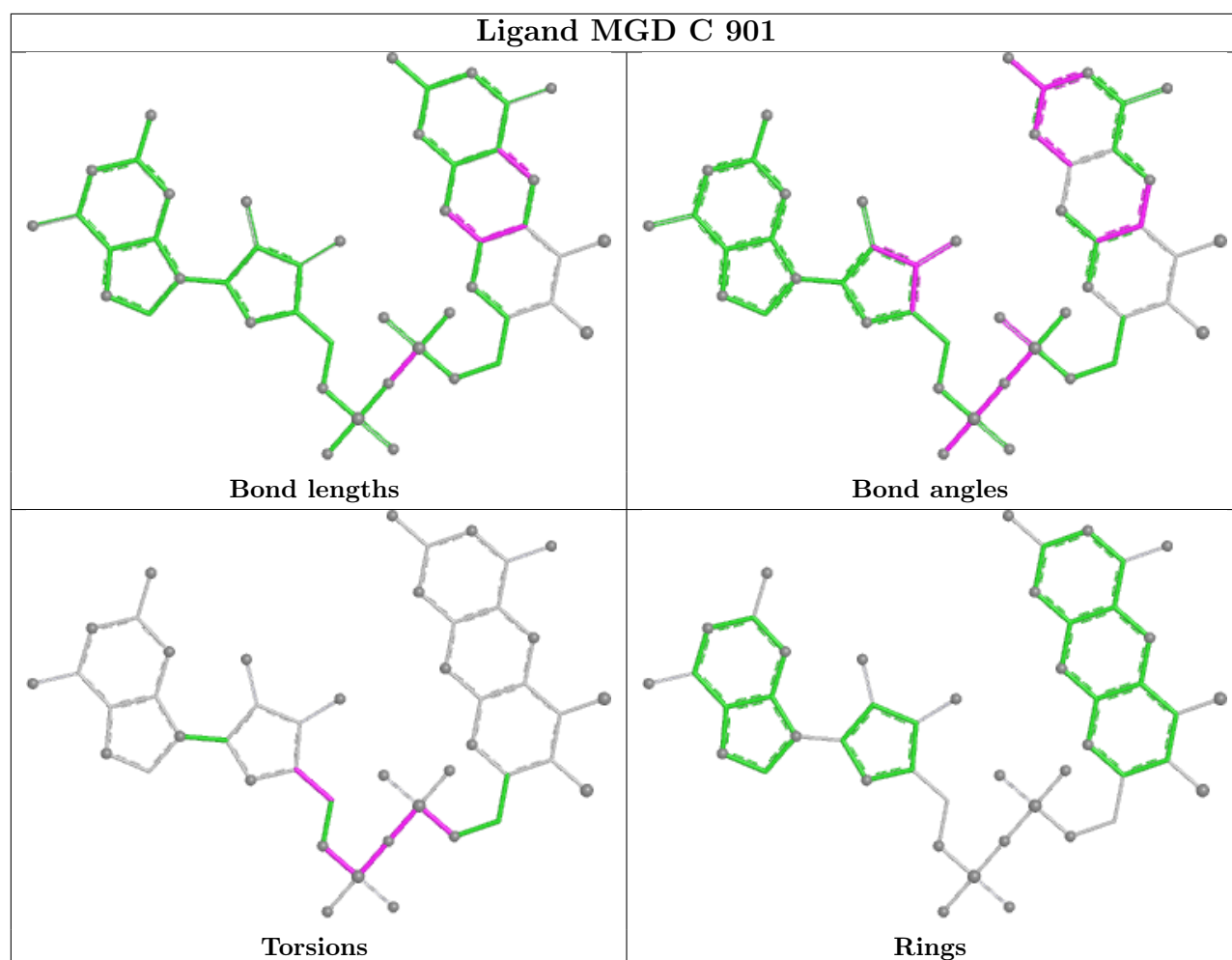
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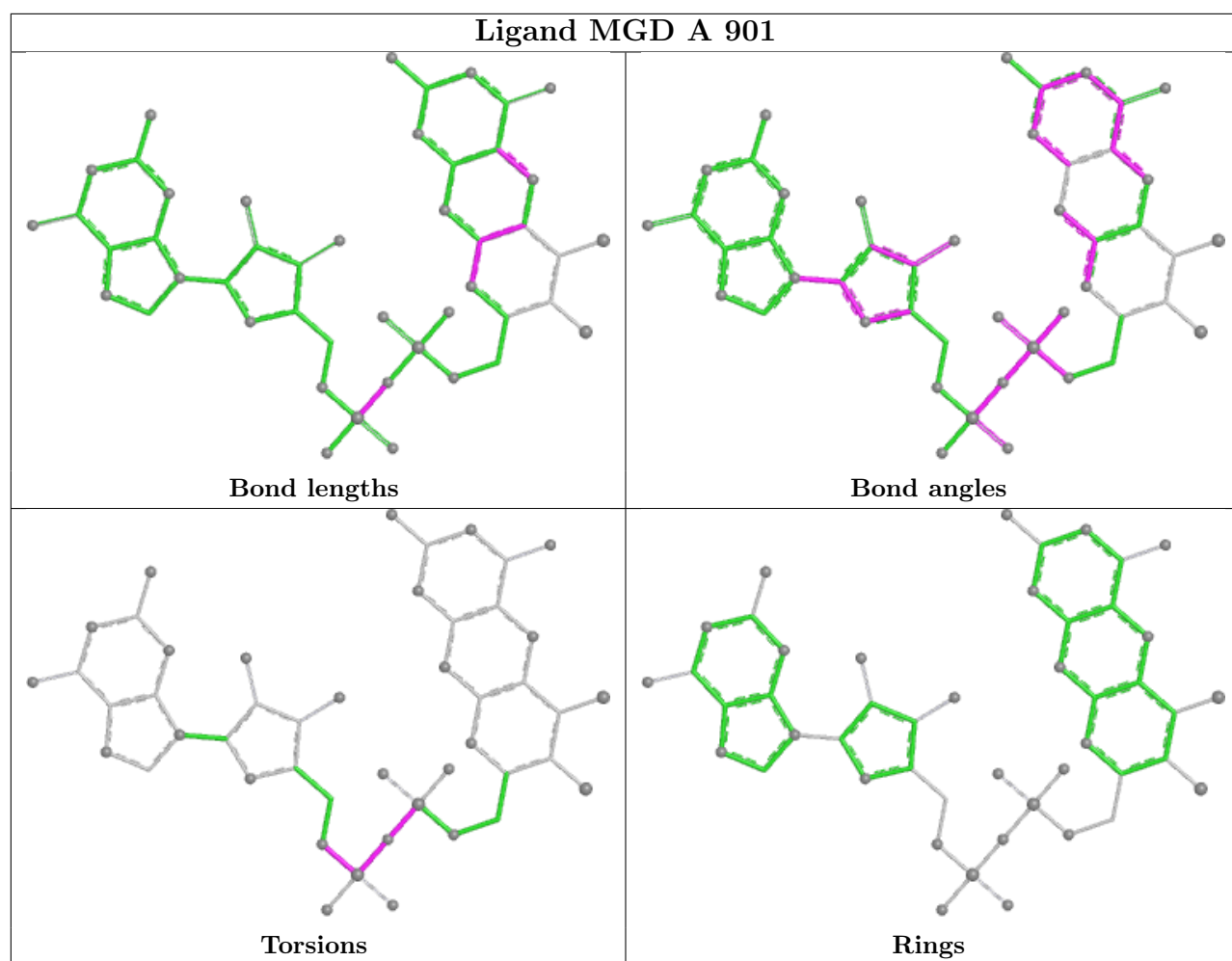
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	912	PGE	3	0
6	C	902	MGD	2	0
9	E	911	PEG	2	0
6	E	902	MGD	1	0
9	C	907	PEG	2	0
6	G	903	MGD	1	0
17	C	905	P4G	7	0
9	G	907	PEG	1	0
9	E	906	PEG	1	0

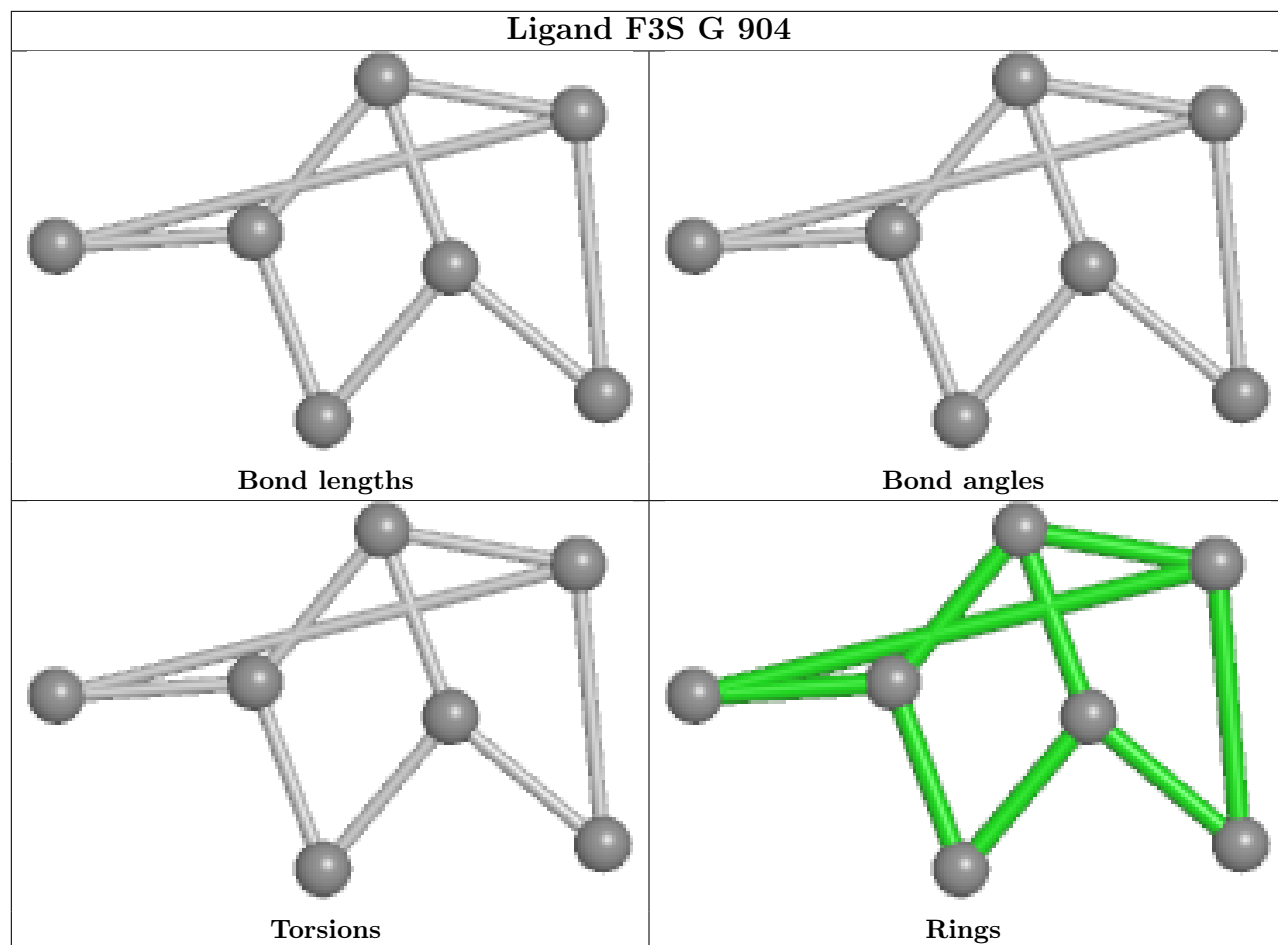
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

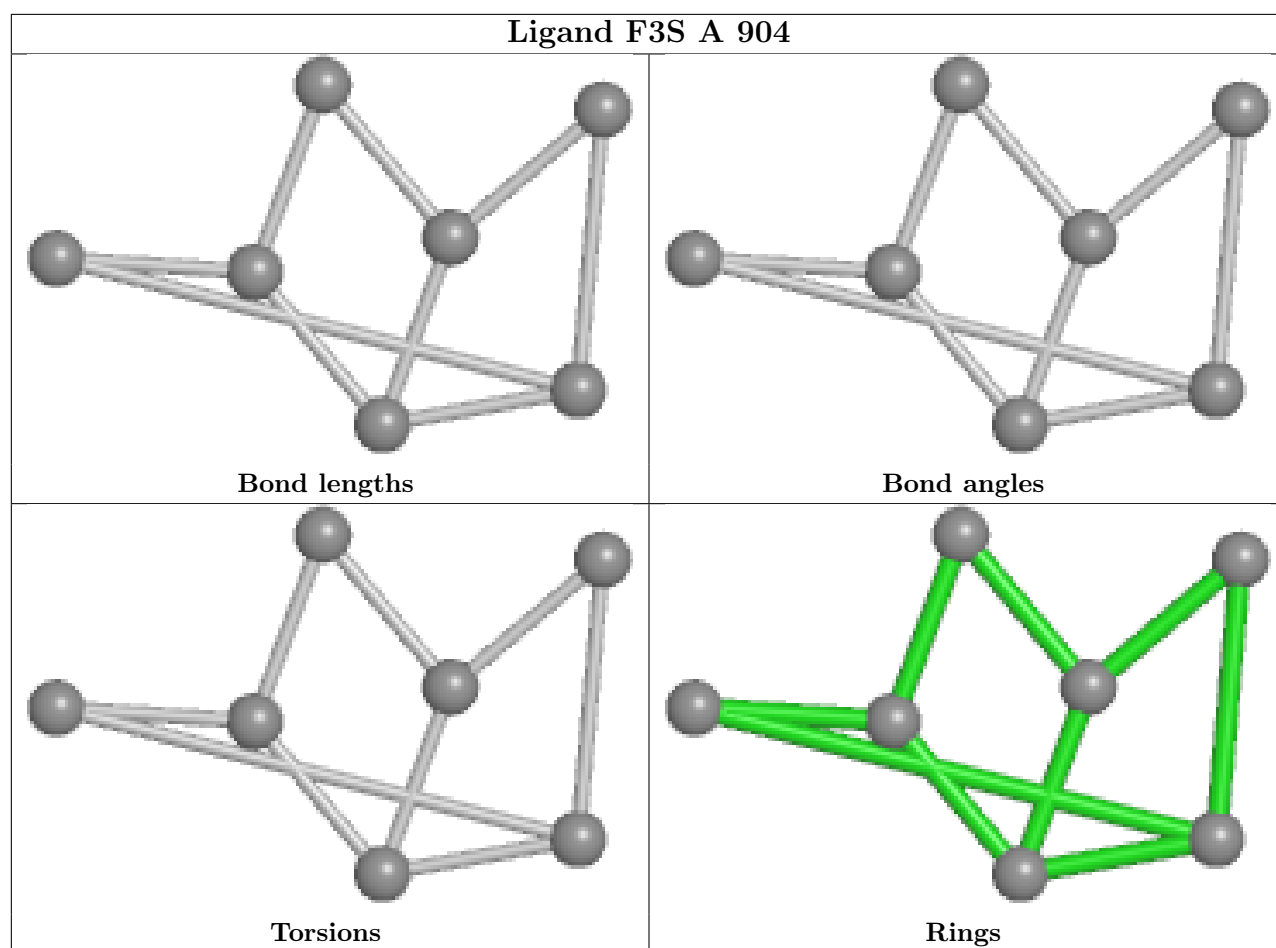


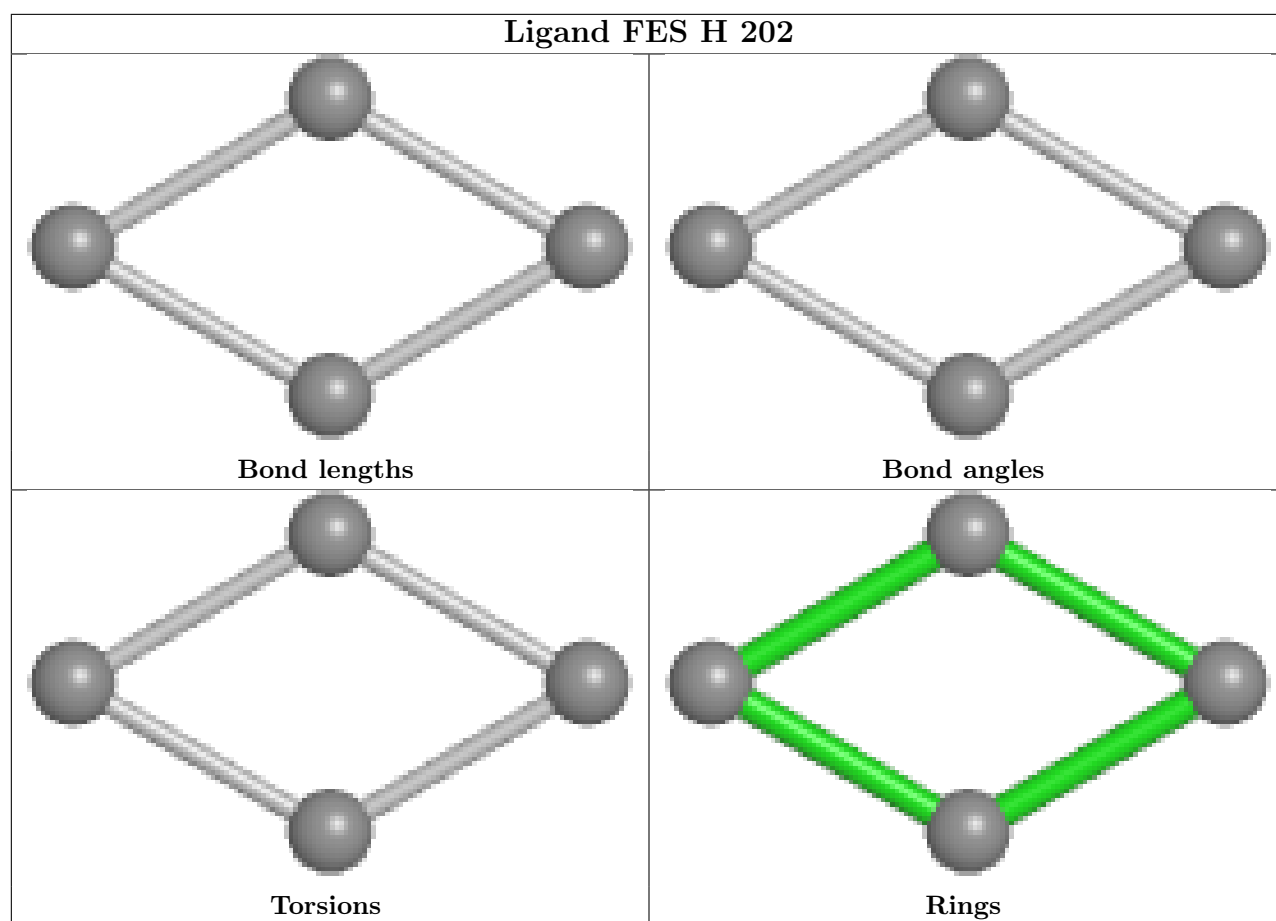


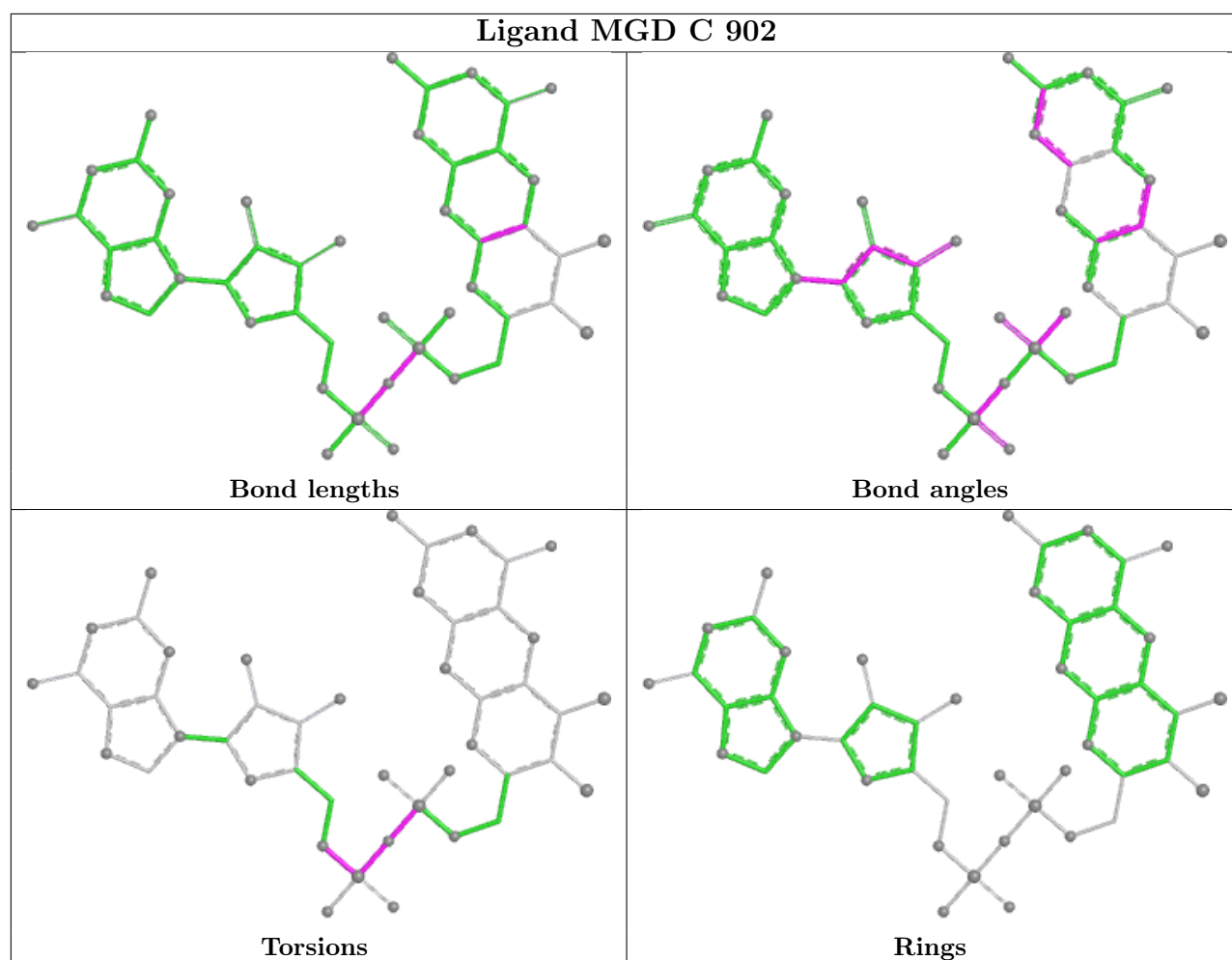


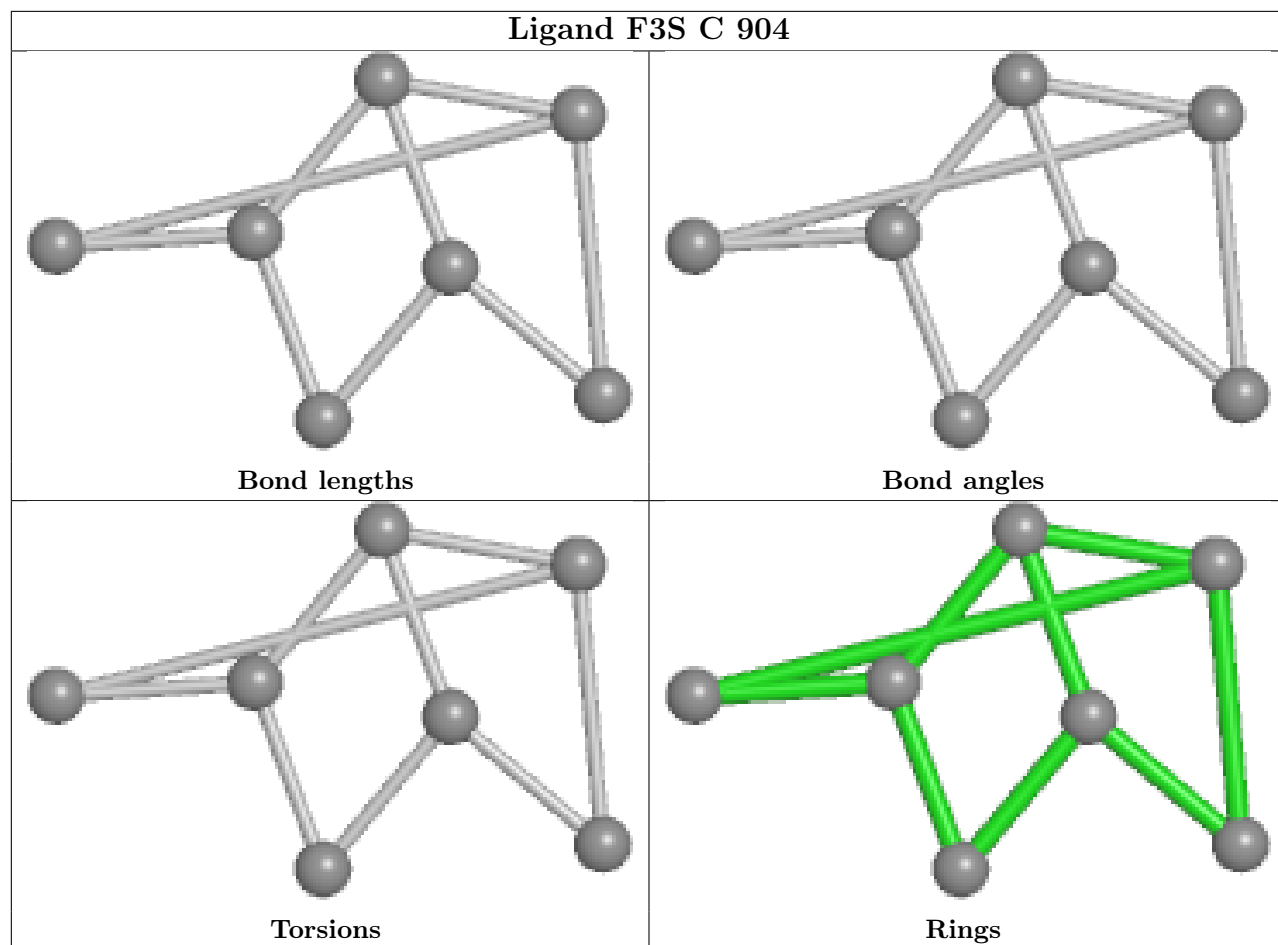


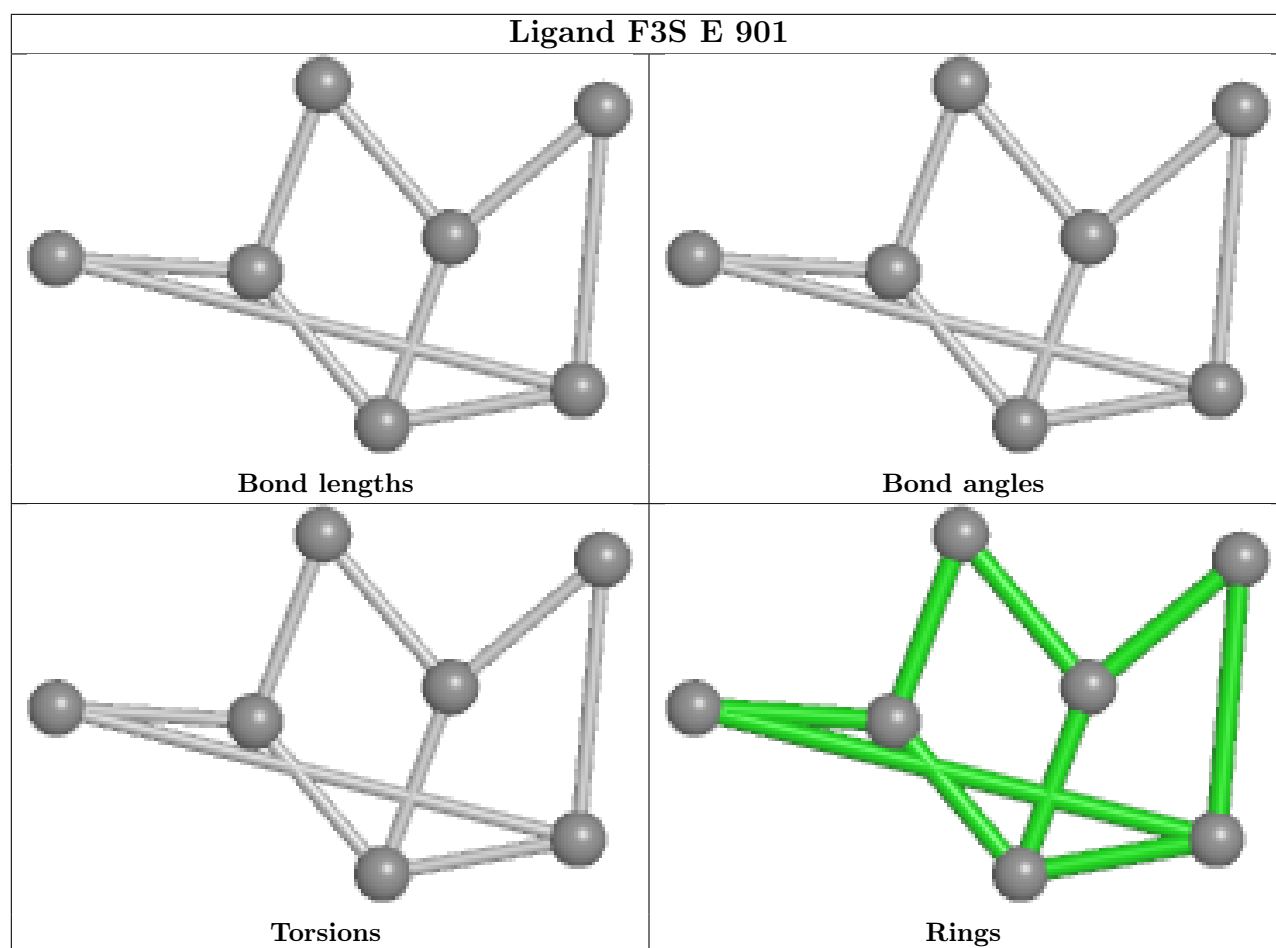


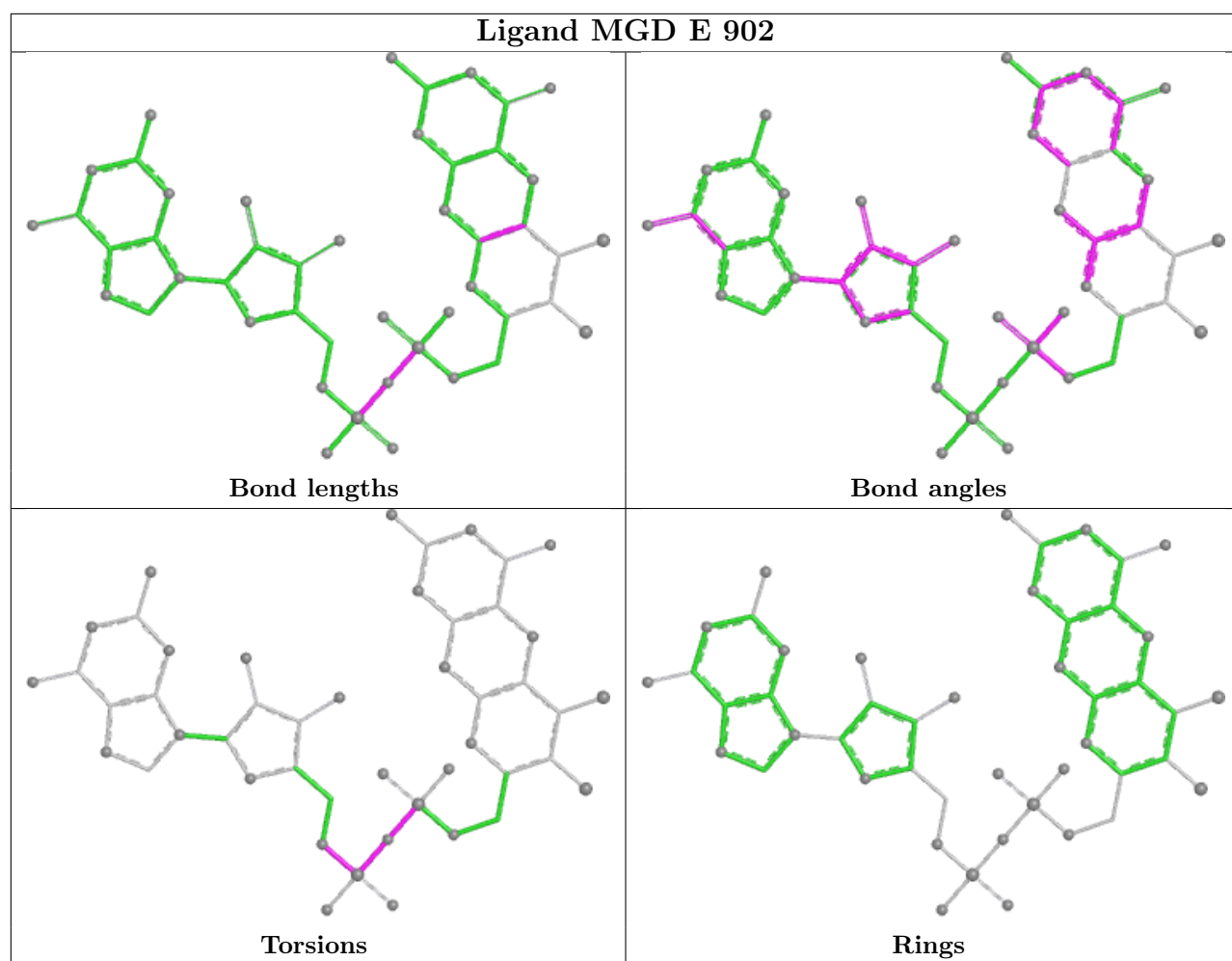


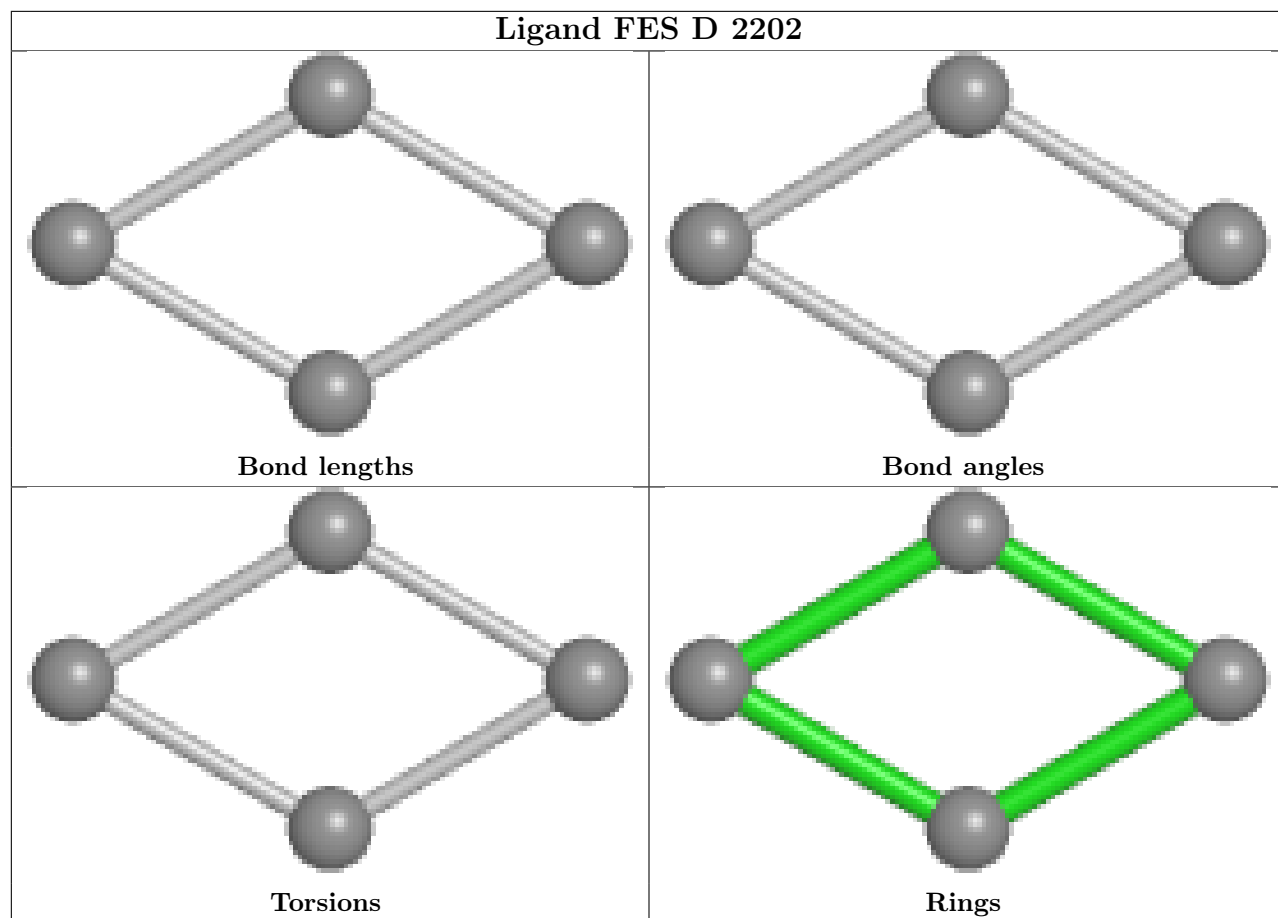


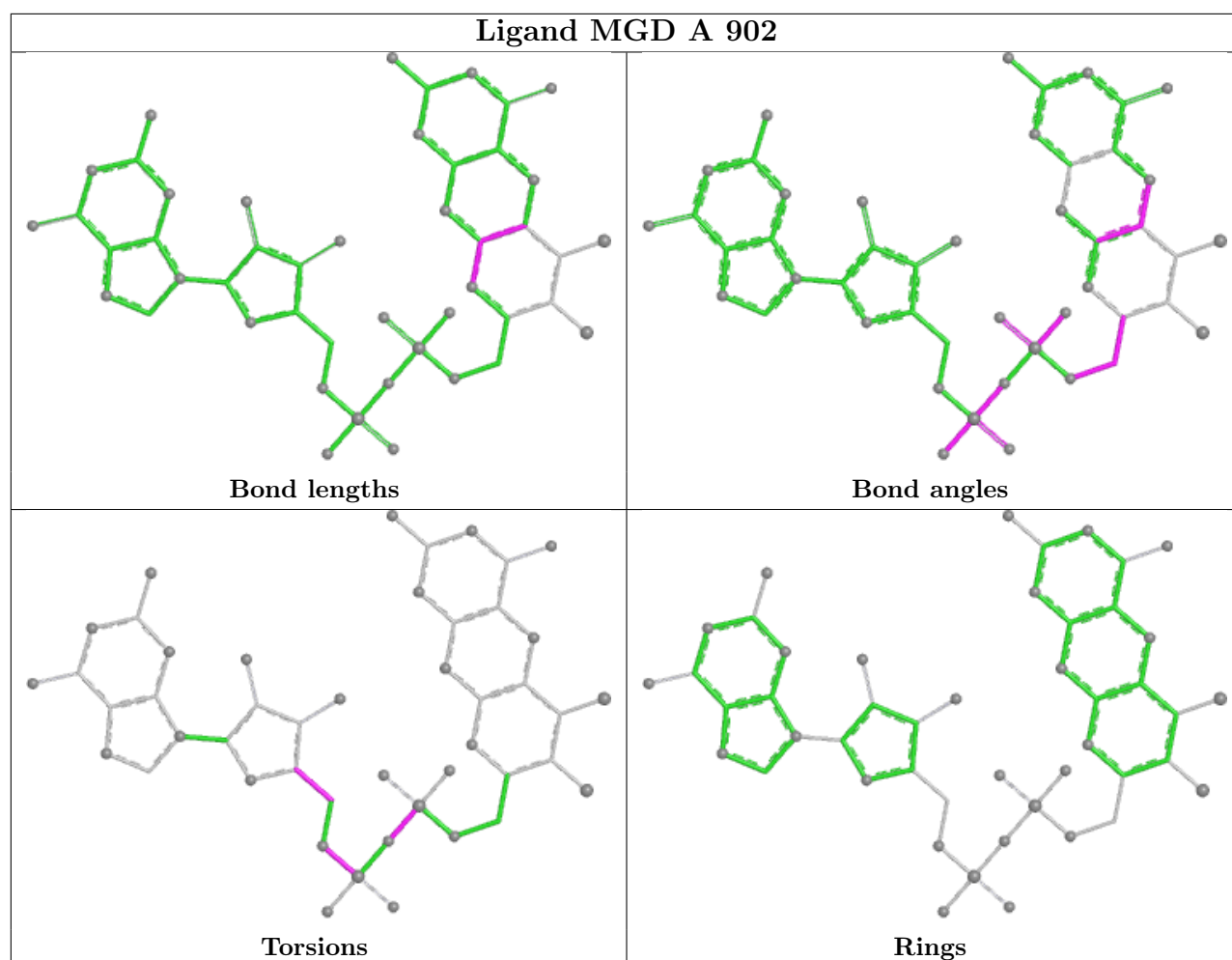


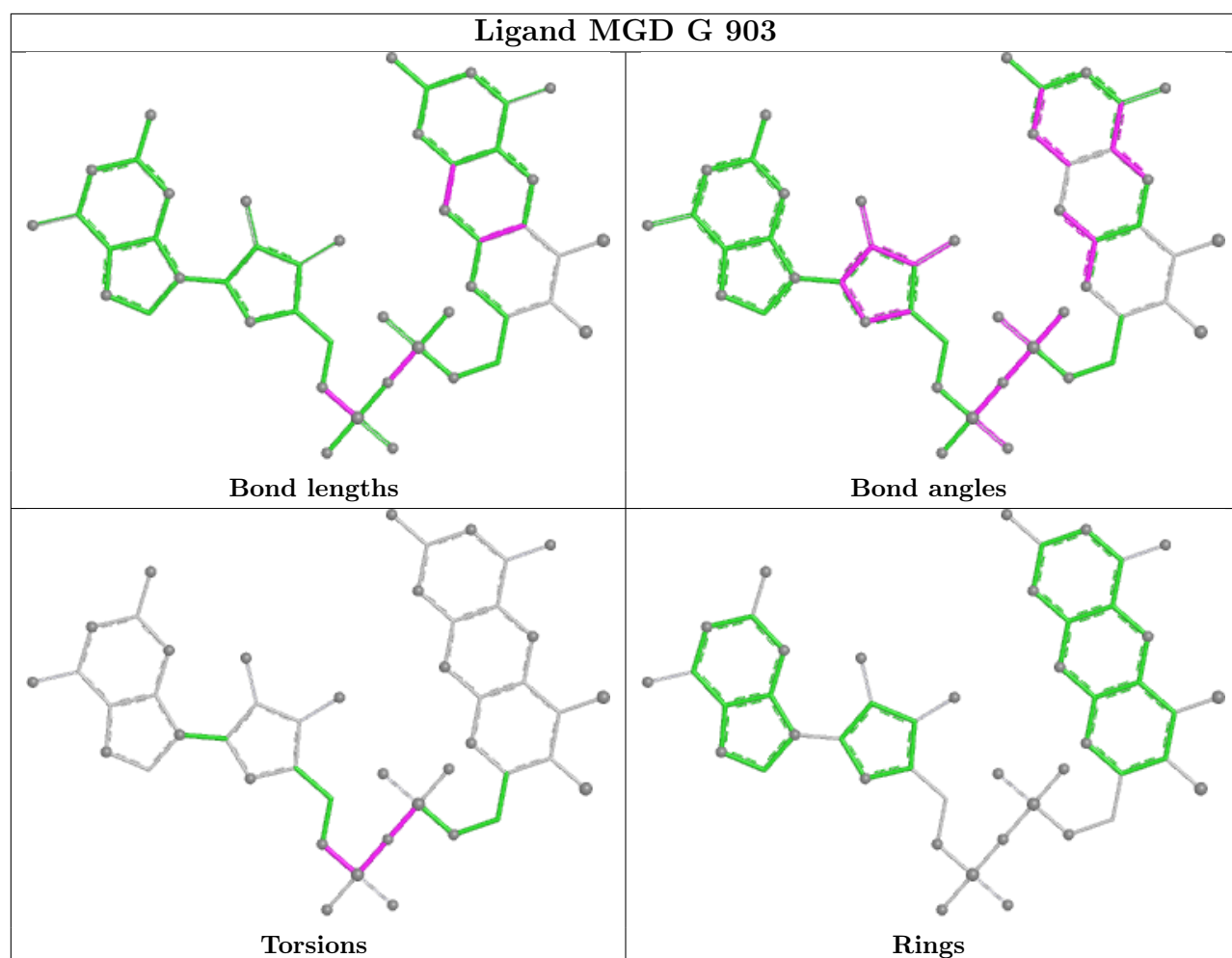


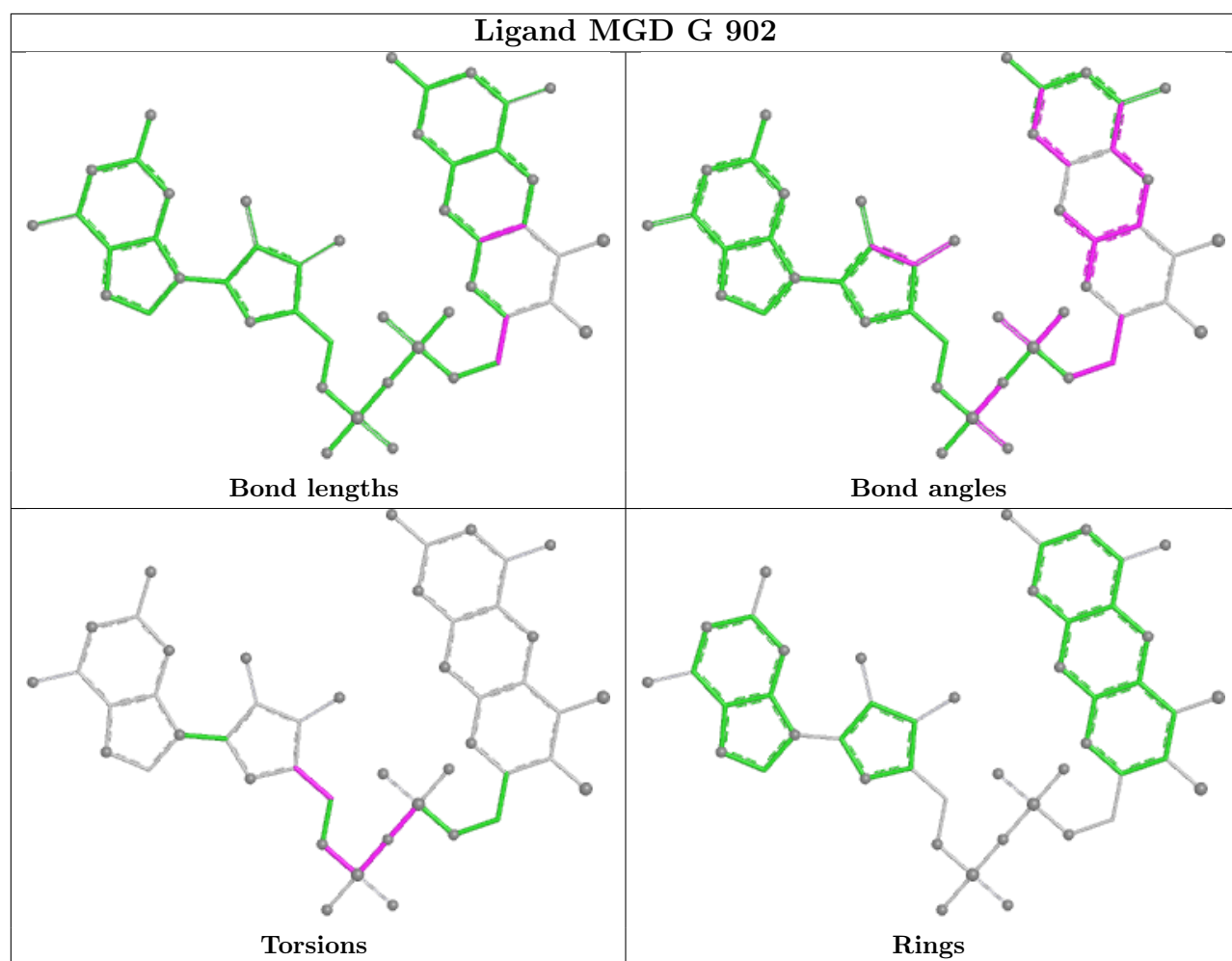


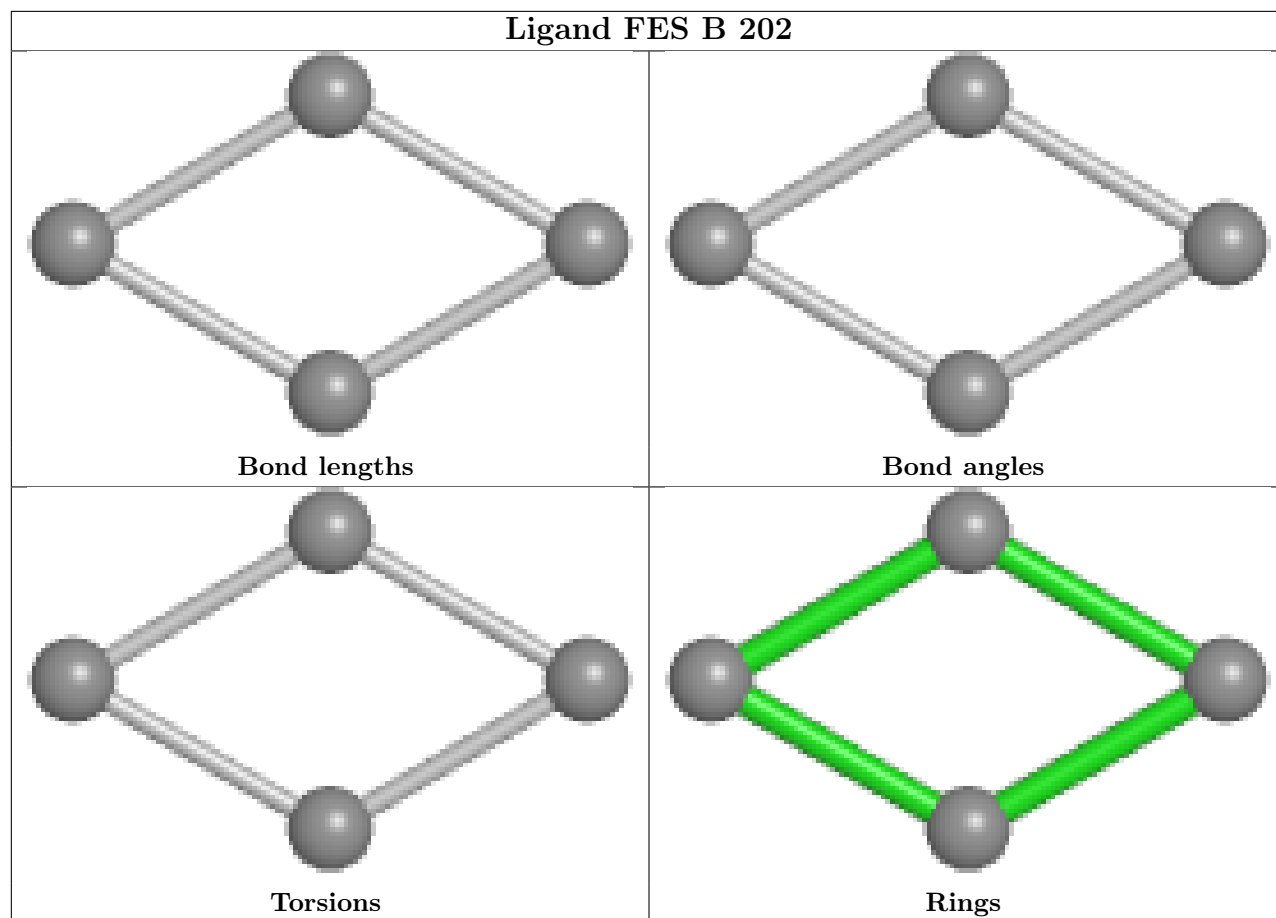












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	822/822 (100%)	0.30	10 (1%) 76 79	12, 25, 41, 74	4 (0%)
1	C	822/822 (100%)	0.39	23 (2%) 55 59	14, 26, 42, 76	4 (0%)
2	B	134/134 (100%)	0.39	1 (0%) 84 86	18, 25, 37, 54	0
3	D	135/135 (100%)	0.45	5 (3%) 45 48	17, 25, 40, 59	0
3	F	135/135 (100%)	0.34	3 (2%) 62 66	18, 25, 38, 64	0
3	H	135/135 (100%)	0.41	2 (1%) 72 75	18, 25, 38, 75	0
4	E	824/824 (100%)	0.36	18 (2%) 62 66	12, 25, 41, 67	4 (0%)
5	G	823/823 (100%)	0.23	13 (1%) 70 74	11, 24, 39, 62	5 (0%)
All	All	3830/3830 (100%)	0.33	75 (1%) 65 69	11, 25, 41, 76	17 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	-1	ALA	7.7
4	E	2	ALA	5.9
5	G	3	ALA	5.6
2	B	0	LEU	5.3
4	E	3	ALA	4.7
3	D	-1	ALA	4.6
3	H	0	GLY	4.6
3	F	-1	ALA	4.3
1	A	485	GLN	4.1
1	A	487	ALA	4.0
4	E	487	ALA	3.5
5	G	487	ALA	3.5
3	F	0	GLY	3.5
1	C	487	ALA	3.4
1	C	482	GLN	3.4
1	C	485	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
4	E	38	LEU	3.1
1	C	612	PRO	3.1
1	A	616	ALA	3.1
4	E	486	LYS	2.9
4	E	588	ALA	2.8
3	D	0	GLY	2.8
4	E	613	GLY	2.8
4	E	584	ALA	2.8
1	C	142	LEU	2.7
3	D	10	GLN	2.7
5	G	38	LEU	2.7
1	C	665	LYS	2.6
1	A	436	LYS	2.6
1	C	436	LYS	2.6
1	A	486	LYS	2.5
1	C	584	ALA	2.5
4	E	483	ALA	2.5
5	G	485	GLN	2.5
1	C	434	GLY	2.5
1	A	695	ARG	2.5
3	D	41	SER	2.5
1	C	646	VAL	2.5
4	E	646	VAL	2.5
1	C	610	GLY	2.5
4	E	669	ASP	2.5
5	G	7	ILE	2.4
1	C	669	ASP	2.4
1	A	664	GLY	2.4
1	A	38	LEU	2.3
1	C	588	ALA	2.3
1	A	435	ASP	2.3
5	G	436	LYS	2.3
1	C	128	ALA	2.3
4	E	651	SER	2.2
4	E	485	GLN	2.2
5	G	482	GLN	2.2
5	G	646	VAL	2.2
1	C	486	LYS	2.2
4	E	580	LYS	2.2
4	E	695	ARG	2.2
1	C	613	GLY	2.2
3	F	12	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	614	ALA	2.2
5	G	584	ALA	2.2
1	C	184	PHE	2.1
5	G	486	LYS	2.1
4	E	503	THR	2.1
4	E	482	GLN	2.1
1	C	433	PRO	2.1
1	A	478	ALA	2.1
4	E	614	ALA	2.1
5	G	562	ALA	2.1
1	C	488	ARG	2.1
5	G	695	ARG	2.1
1	C	582	GLY	2.0
5	G	648	TRP	2.0
1	C	483	ALA	2.0
1	C	616	ALA	2.0
3	D	43	VAL	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, 95<sup>th</sup> 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
9	PEG	G	906	7/7	0.71	0.26	41,50,60,63	0
9	PEG	E	911	7/7	0.73	0.18	30,43,50,52	0
10	EDO	D	2204	4/4	0.73	0.23	31,46,46,46	0
11	1PE	C	908	16/16	0.76	0.19	36,42,45,52	0
9	PEG	G	908	7/7	0.77	0.18	45,47,48,53	0
9	PEG	C	907	7/7	0.78	0.20	34,41,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	PEG	H	203	7/7	0.78	0.19	24,32,37,38	0
10	EDO	A	910	4/4	0.79	0.15	33,34,35,37	0
9	PEG	C	906	7/7	0.79	0.18	28,41,44,52	0
10	EDO	E	905	4/4	0.79	0.18	34,35,37,38	0
10	EDO	G	913	4/4	0.79	0.19	33,39,42,42	0
9	PEG	A	905	7/7	0.79	0.17	40,46,52,55	0
11	1PE	C	909	16/16	0.79	0.21	44,49,61,62	0
13	GOL	A	913	6/6	0.79	0.15	36,41,42,43	0
17	P4G	C	905	11/11	0.79	0.18	25,35,45,47	0
9	PEG	E	906	7/7	0.81	0.17	29,37,43,51	0
9	PEG	A	914	7/7	0.81	0.21	35,40,50,54	0
9	PEG	H	201	7/7	0.81	0.19	30,46,54,61	0
18	PG0	D	2203	8/8	0.81	0.17	25,41,44,44	0
9	PEG	G	914	7/7	0.82	0.21	51,53,65,65	0
10	EDO	E	907	4/4	0.82	0.16	34,36,40,44	0
10	EDO	E	910	4/4	0.82	0.19	37,42,46,48	0
10	EDO	A	907	4/4	0.82	0.20	47,47,50,52	0
11	1PE	A	909	16/16	0.82	0.19	37,49,59,62	0
11	1PE	G	912	16/16	0.83	0.19	47,58,65,65	0
10	EDO	A	908	4/4	0.83	0.17	37,40,42,43	0
9	PEG	G	907	7/7	0.84	0.17	28,35,48,48	0
9	PEG	A	911	7/7	0.85	0.18	33,42,52,56	0
10	EDO	C	910	4/4	0.85	0.15	39,42,44,46	0
10	EDO	E	908	4/4	0.85	0.18	32,39,40,47	0
9	PEG	A	906	7/7	0.85	0.18	39,48,52,55	0
12	PGE	A	912	10/10	0.86	0.18	49,52,57,60	0
10	EDO	G	909	4/4	0.87	0.17	28,32,34,42	0
10	EDO	G	910	4/4	0.87	0.14	38,41,42,47	0
10	EDO	G	911	4/4	0.87	0.13	35,37,41,41	0
10	EDO	G	905	4/4	0.88	0.14	24,29,30,30	0
9	PEG	B	201	7/7	0.90	0.12	39,41,47,49	0
9	PEG	E	909	7/7	0.91	0.14	38,40,43,51	0
10	EDO	D	2201	4/4	0.92	0.09	29,31,31,33	0
15	NA	G	916	1/1	0.96	0.05	25,25,25,25	0
6	MGD	E	903	47/47	0.97	0.06	15,21,25,26	0
6	MGD	G	903	47/47	0.97	0.06	16,19,22,22	0
6	MGD	A	901	47/47	0.97	0.06	16,19,22,24	0
14	O	C	911	1/1	0.97	0.06	11,11,11,11	0
15	NA	C	912	1/1	0.97	0.04	19,19,19,19	0
6	MGD	C	901	47/47	0.97	0.06	16,21,26,27	0
6	MGD	C	902	47/47	0.97	0.06	18,20,23,24	0
6	MGD	E	902	47/47	0.97	0.06	15,21,23,25	0

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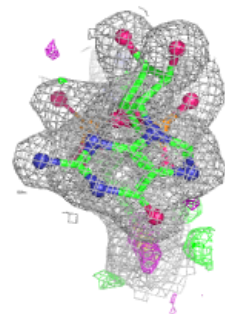
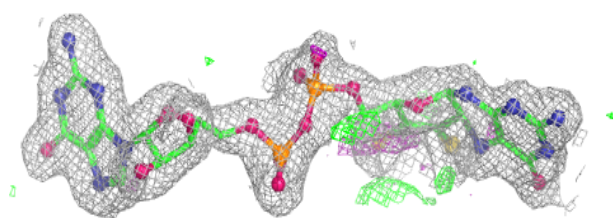
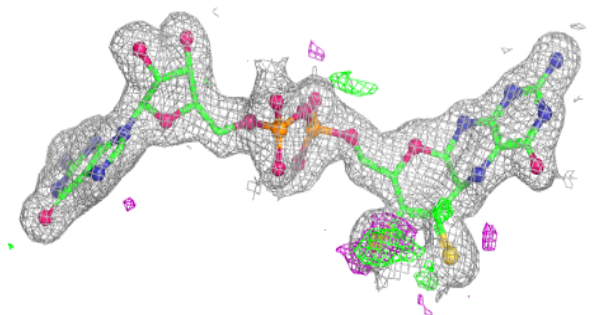
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	O	G	915	1/1	0.98	0.07	21,21,21,21	0
6	MGD	G	902	47/47	0.98	0.06	16,20,22,24	0
15	NA	E	913	1/1	0.98	0.04	22,22,22,22	0
14	O	A	915	1/1	0.98	0.08	22,22,22,22	0
6	MGD	A	902	47/47	0.98	0.05	18,20,24,29	0
14	O	E	912	1/1	0.98	0.05	14,14,14,14	0
8	F3S	C	904	7/7	0.99	0.04	18,18,22,22	0
8	F3S	E	901	7/7	0.99	0.03	14,17,19,19	0
8	F3S	G	904	7/7	0.99	0.04	18,21,21,21	0
16	FES	B	202	4/4	0.99	0.03	15,16,19,19	0
16	FES	D	2202	4/4	0.99	0.03	20,21,21,22	0
16	FES	H	202	4/4	0.99	0.02	18,19,21,21	0
8	F3S	A	904	7/7	0.99	0.03	16,17,18,20	0
15	NA	A	916	1/1	0.99	0.04	23,23,23,23	0
7	4MO	E	904	1/1	1.00	0.02	20,20,20,20	0
16	FES	F	201	4/4	1.00	0.02	19,21,22,23	0
7	4MO	G	901	1/1	1.00	0.01	21,21,21,21	0
7	4MO	A	903	1/1	1.00	0.03	21,21,21,21	0
7	4MO	C	903	1/1	1.00	0.03	23,23,23,23	0

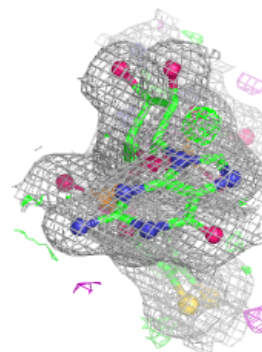
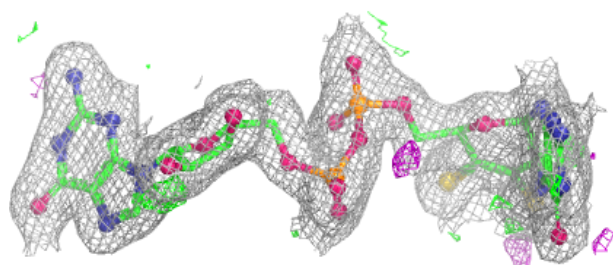
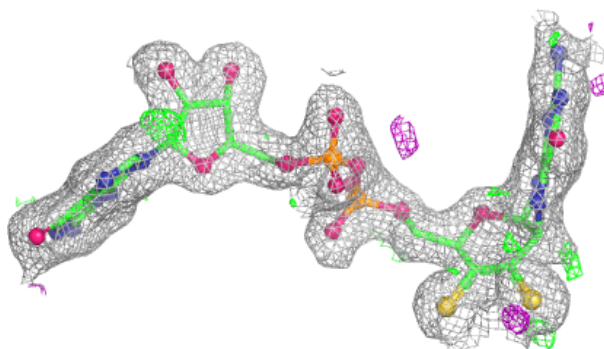
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 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)

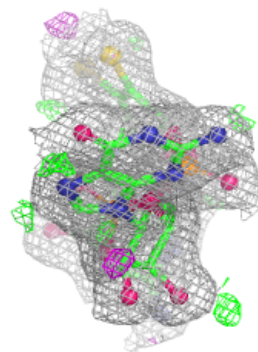
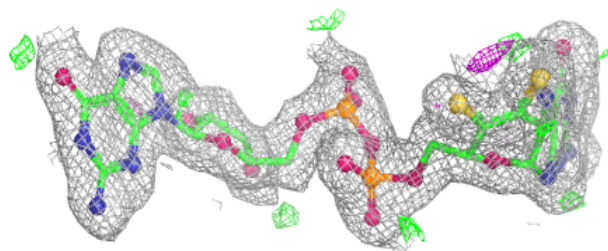
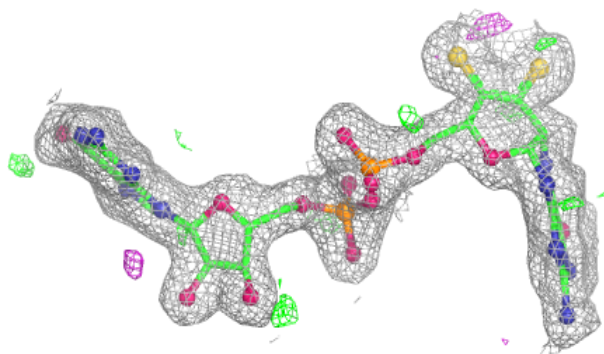
**Electron density around MGD G 903:**

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



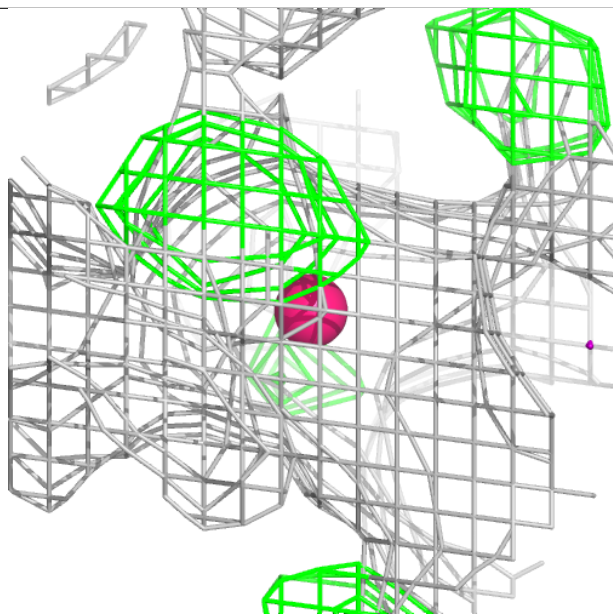
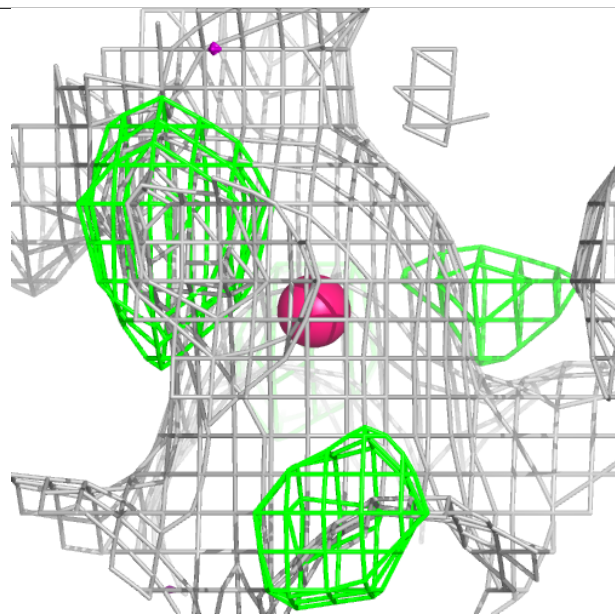
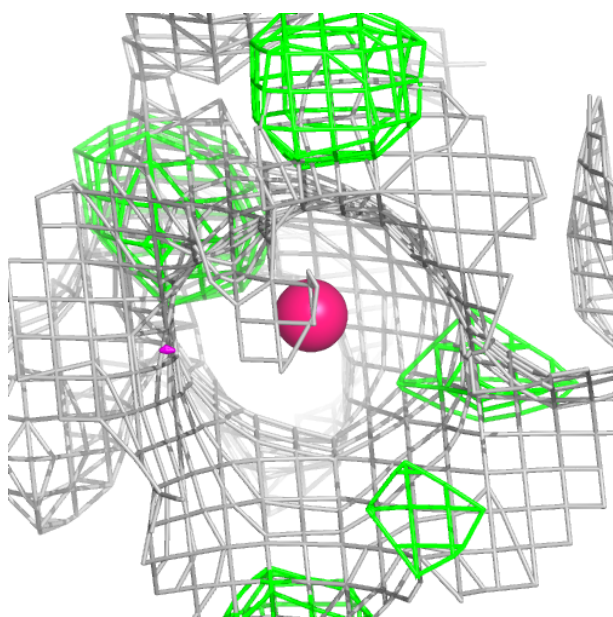
**Electron density around MGD A 901:**

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



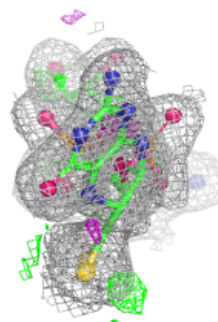
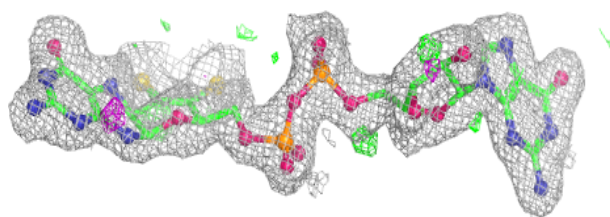
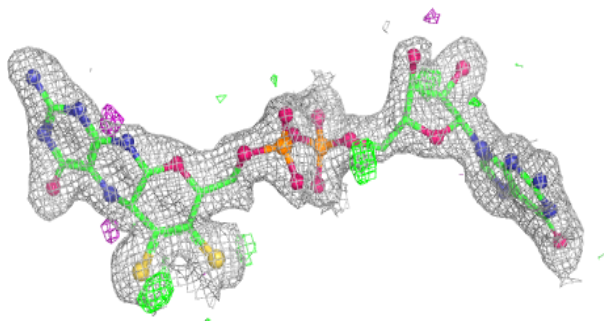
**Electron density around O C 911:**

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

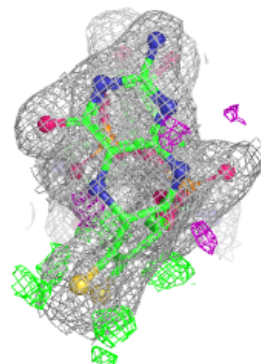
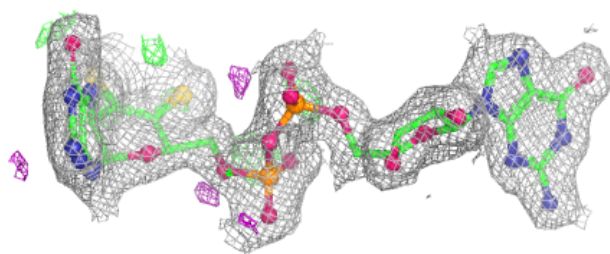
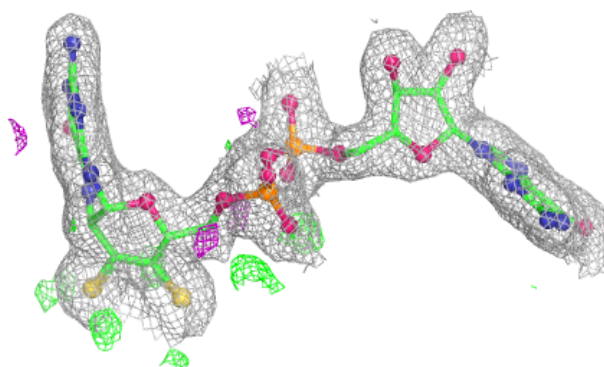


**Electron density around MGD C 901:**

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

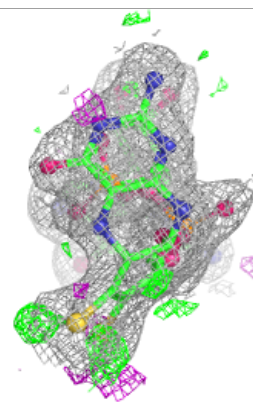
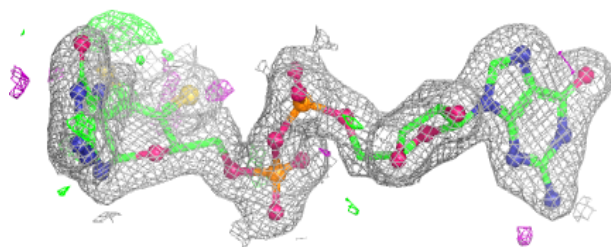
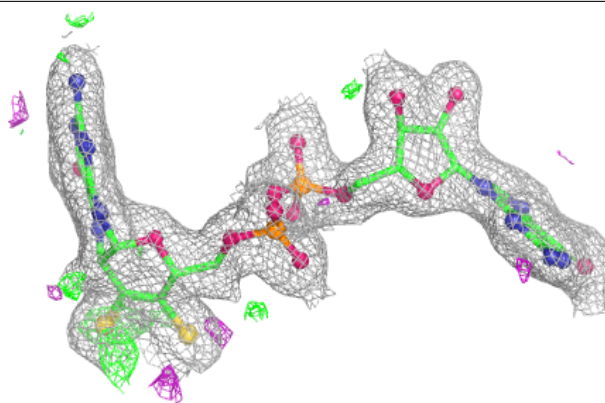
**Electron density around MGD C 902:**

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



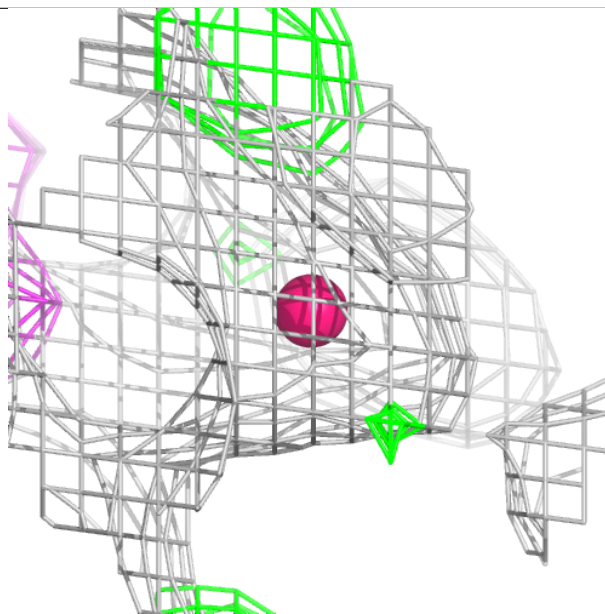
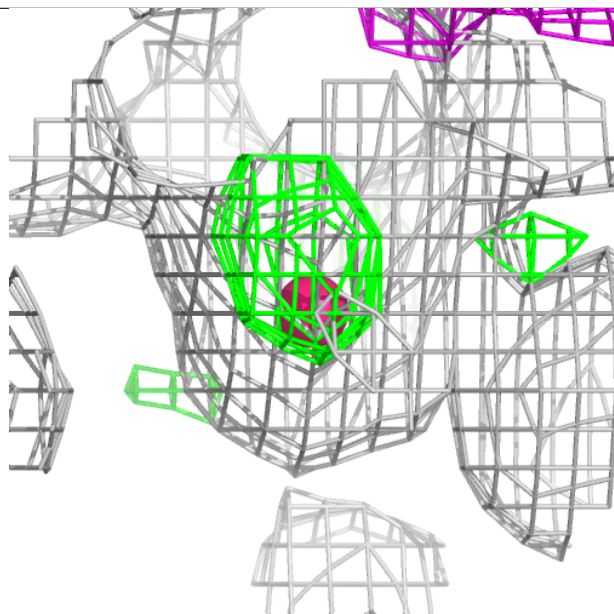
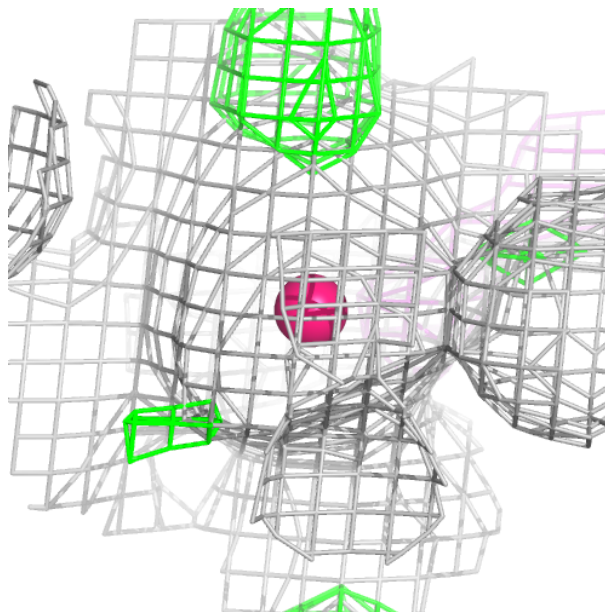
**Electron density around MGD E 902:**

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



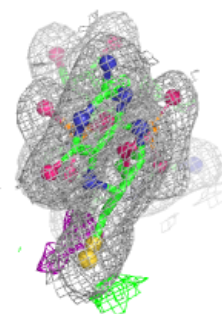
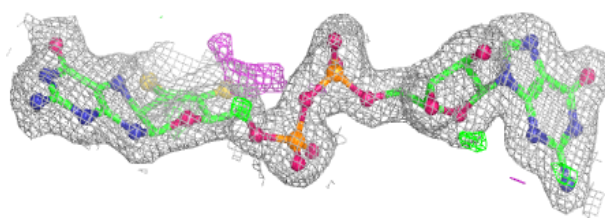
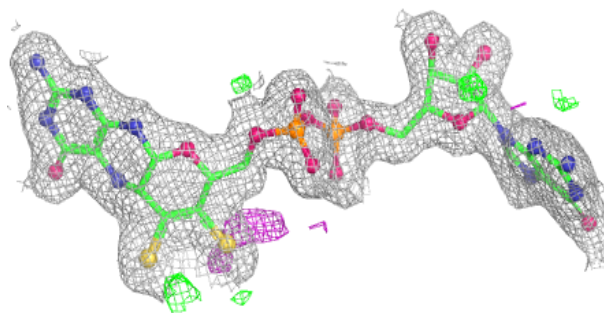
**Electron density around O G 915:**

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



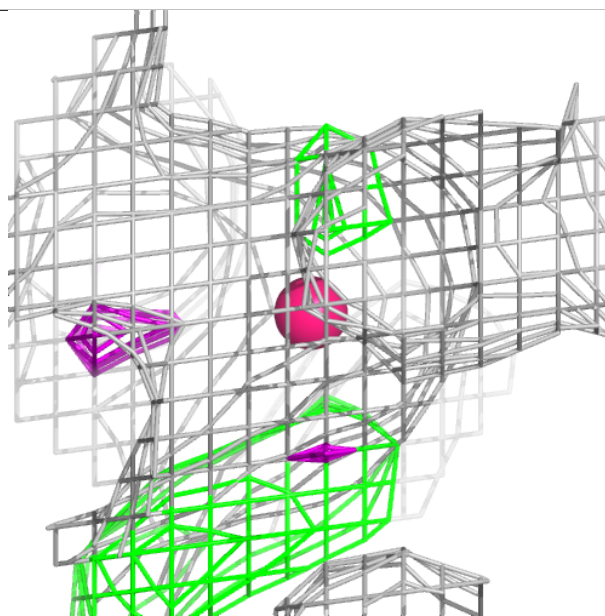
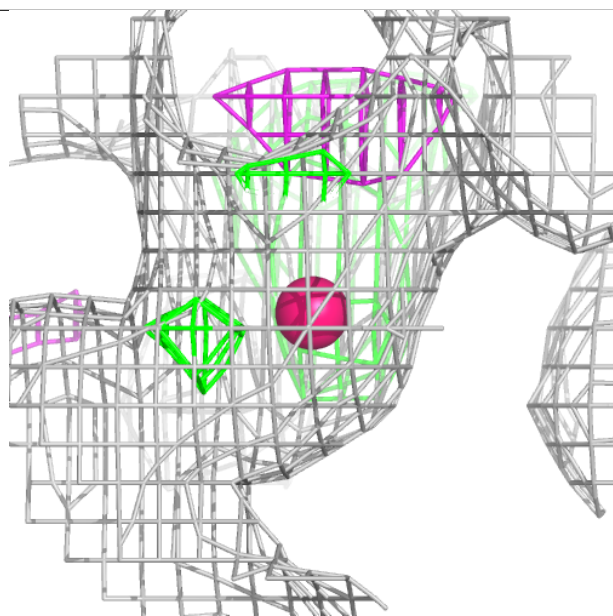
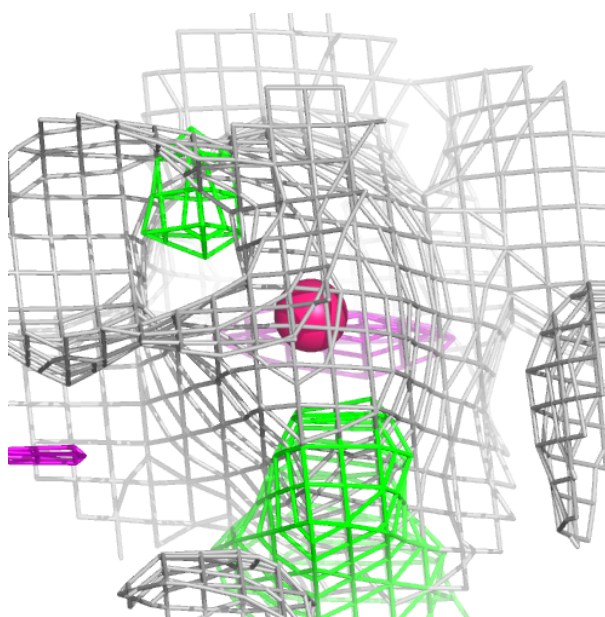
**Electron density around MGD G 902:**

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



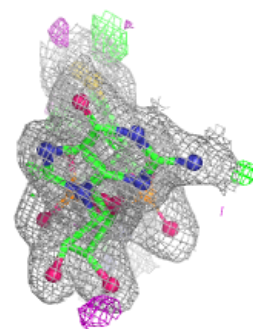
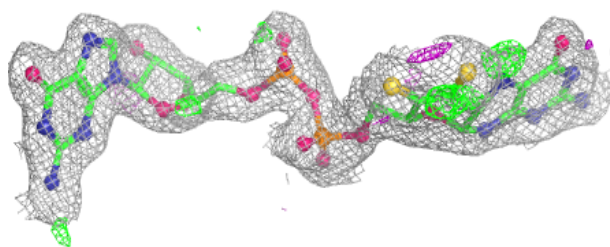
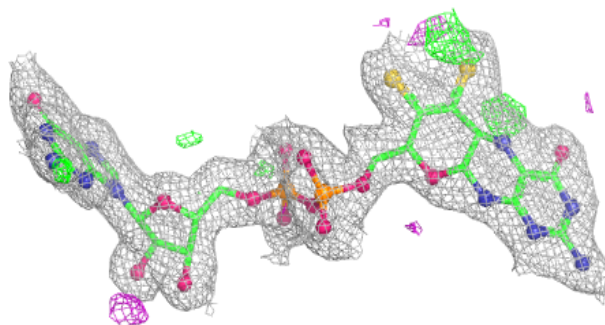
**Electron density around O A 915:**

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



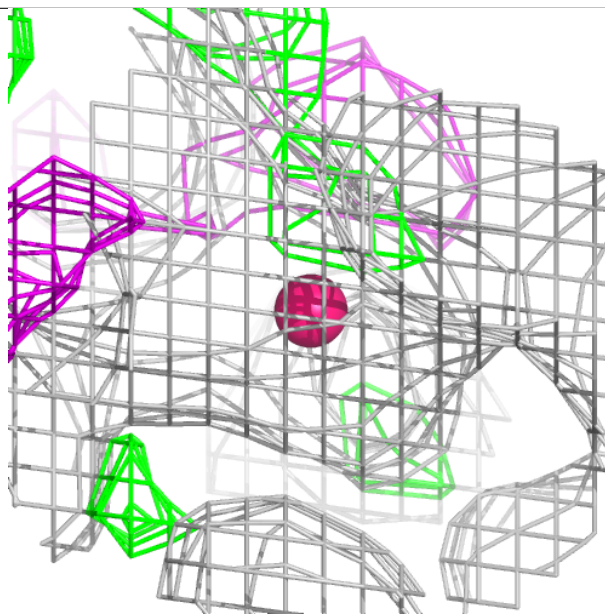
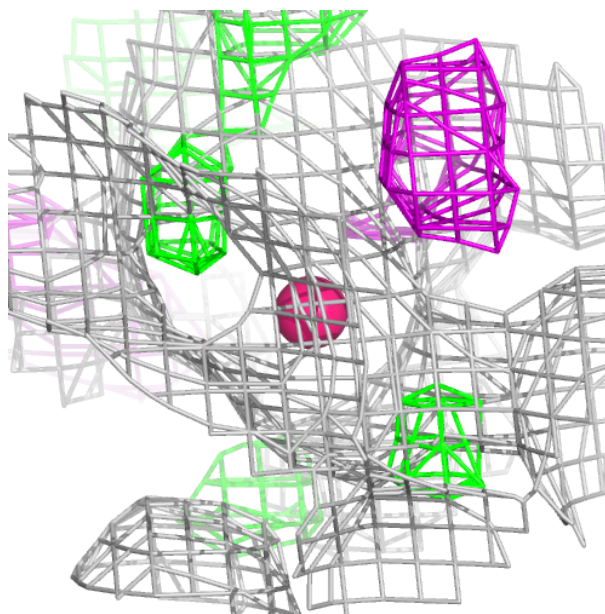
**Electron density around MGD A 902:**

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



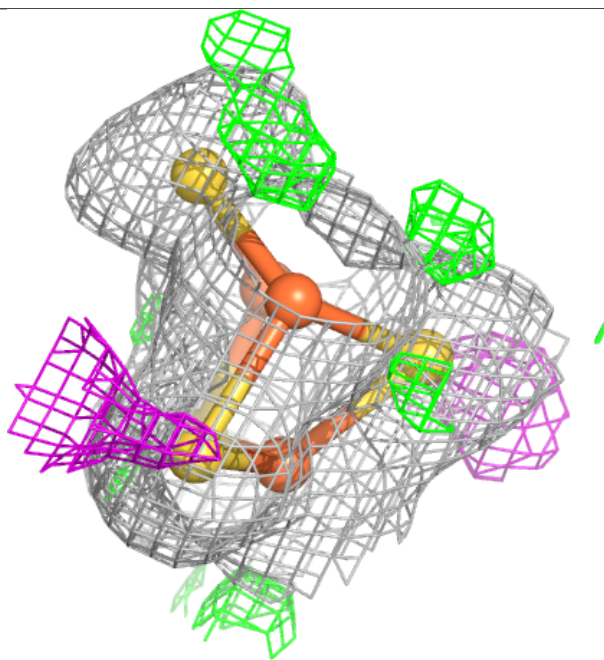
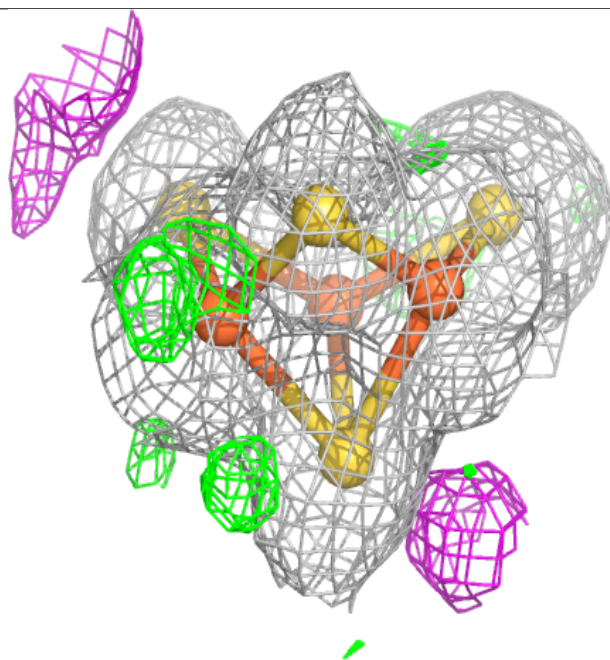
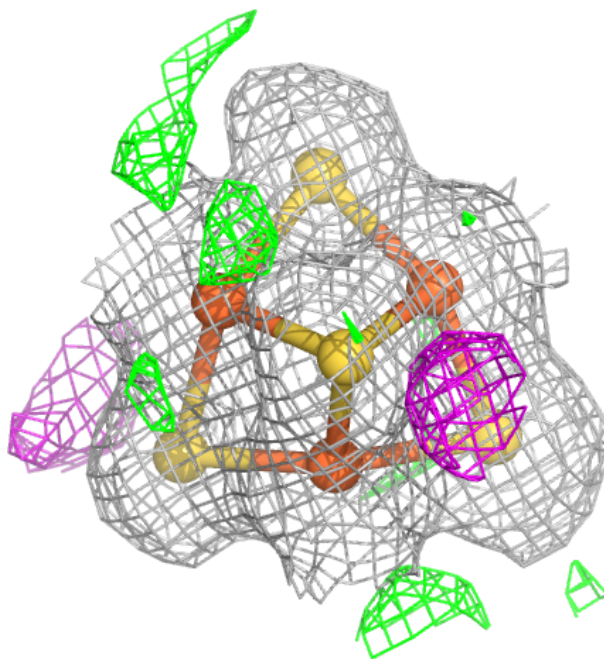
**Electron density around O E 912:**

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



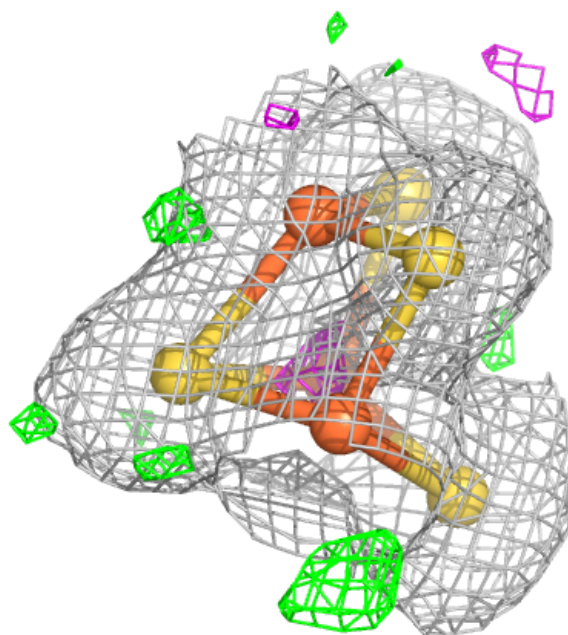
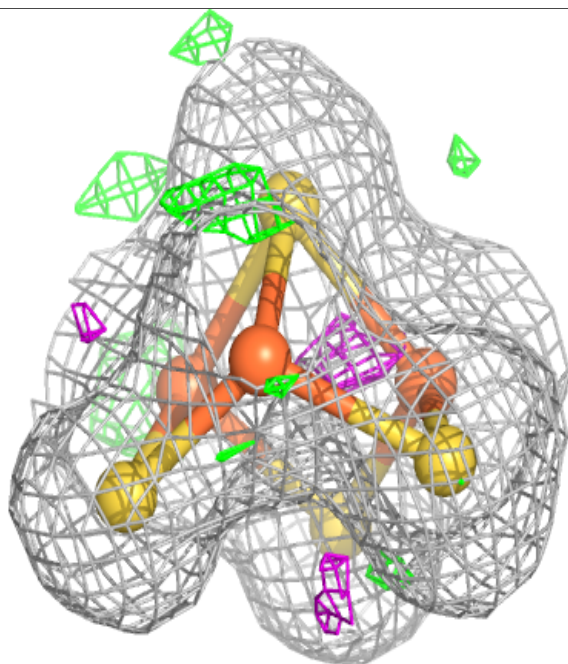
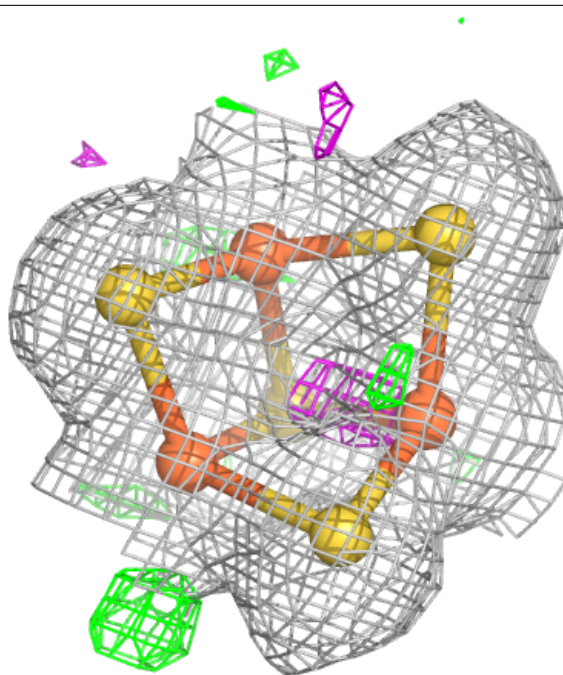
**Electron density around F3S C 904:**

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



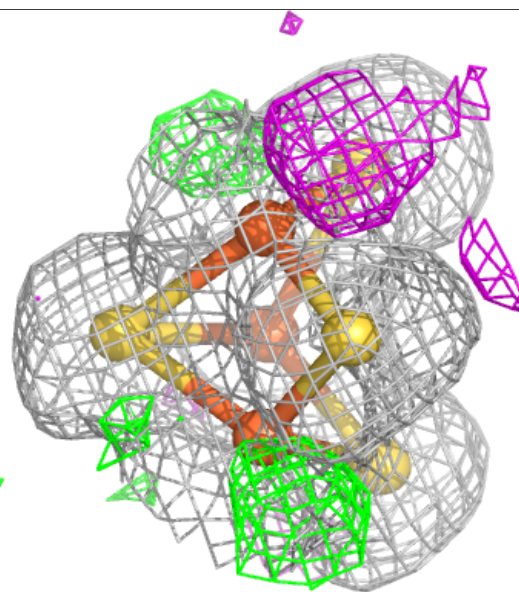
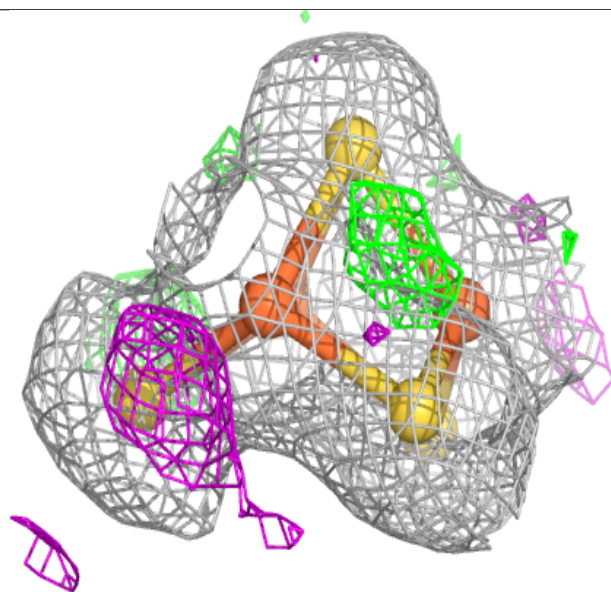
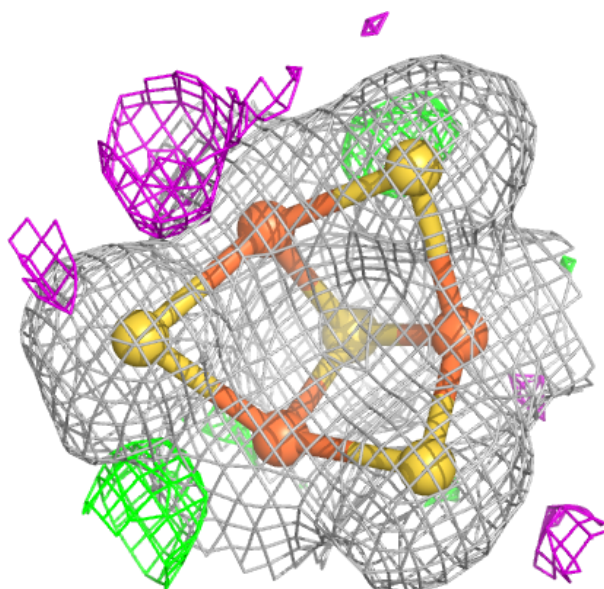
**Electron density around F3S E 901:**

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



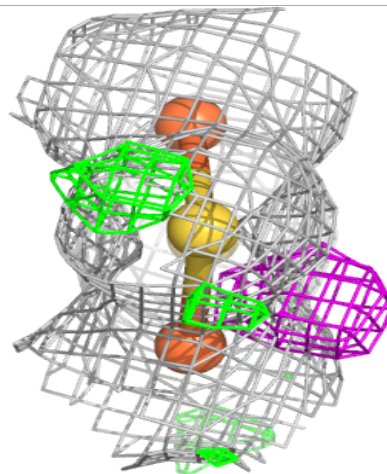
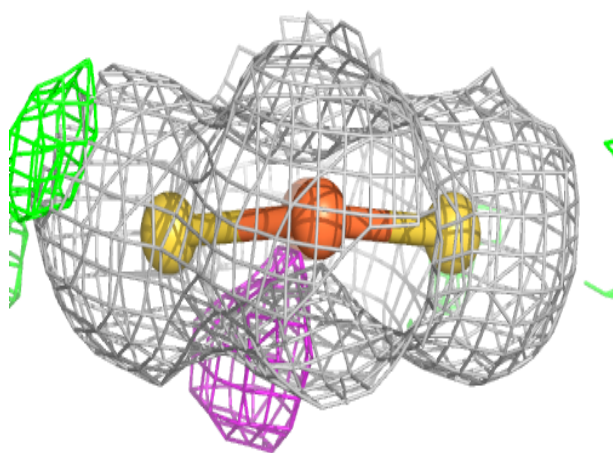
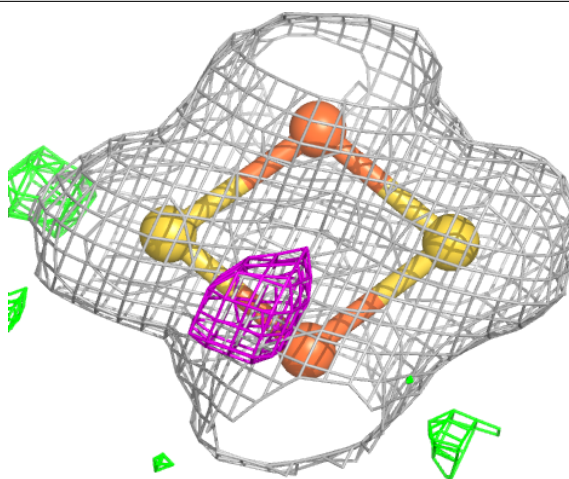
**Electron density around F3S G 904:**

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



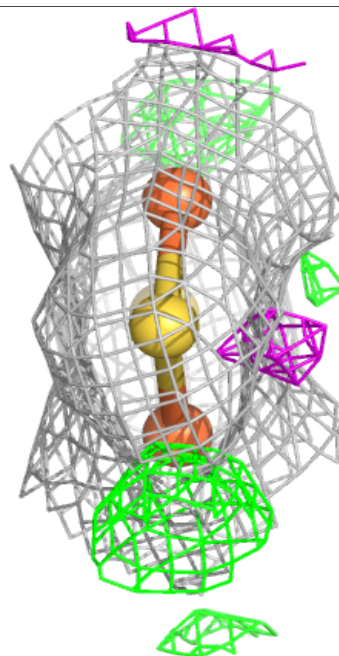
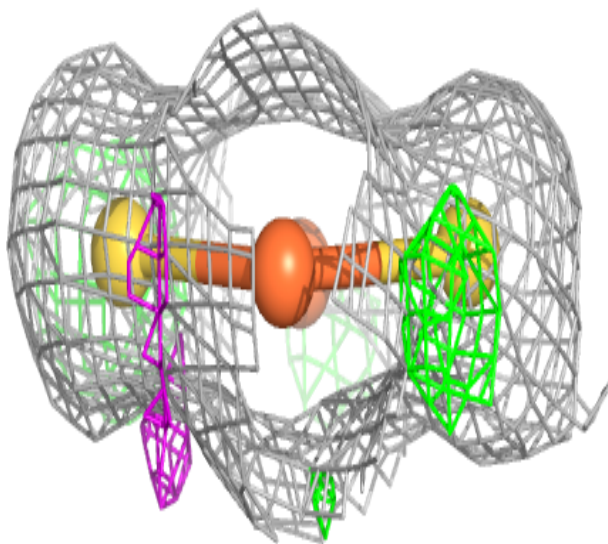
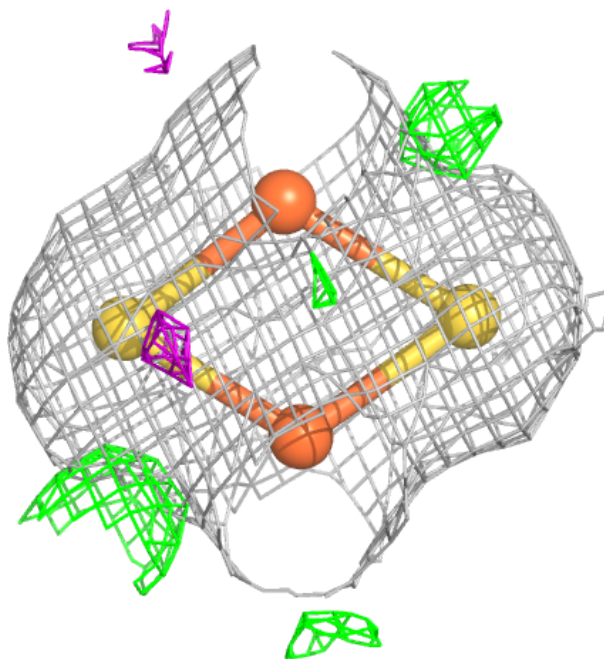
**Electron density around FES B 202:**

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



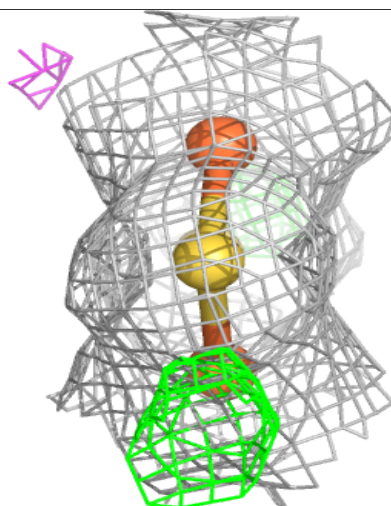
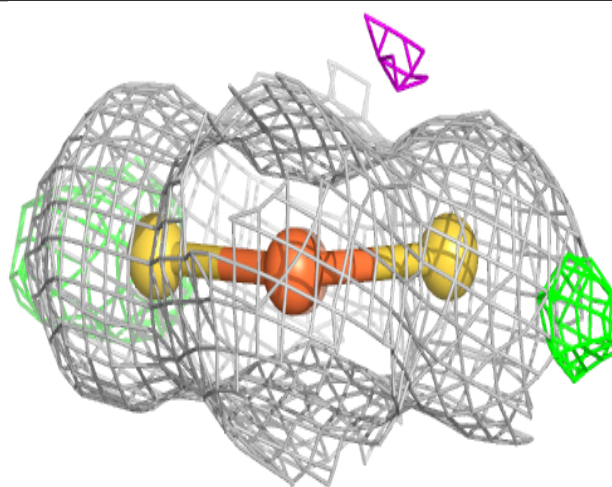
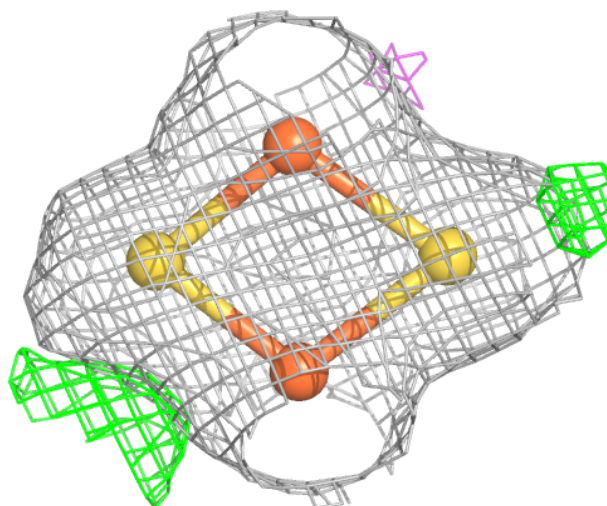
**Electron density around FES D 2202:**

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



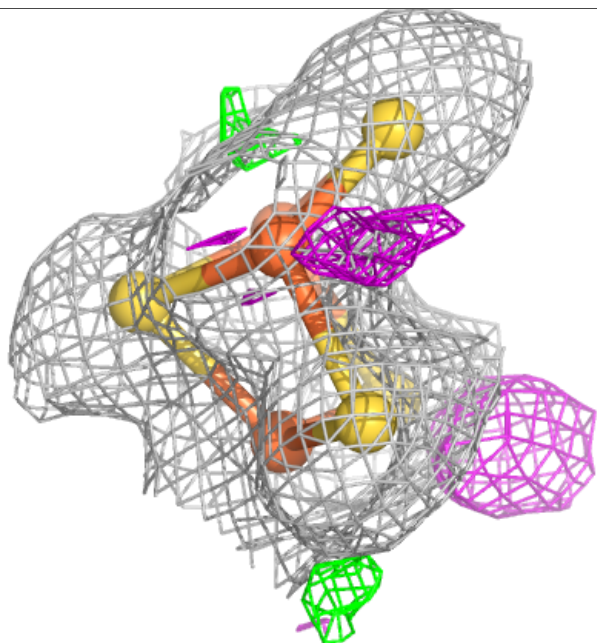
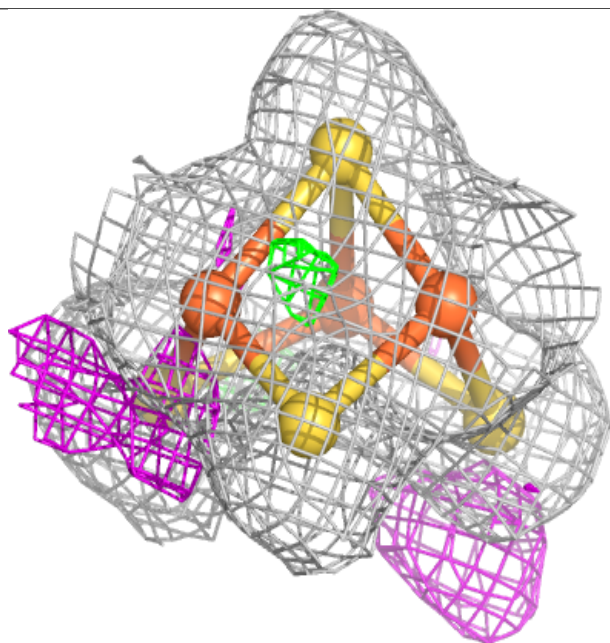
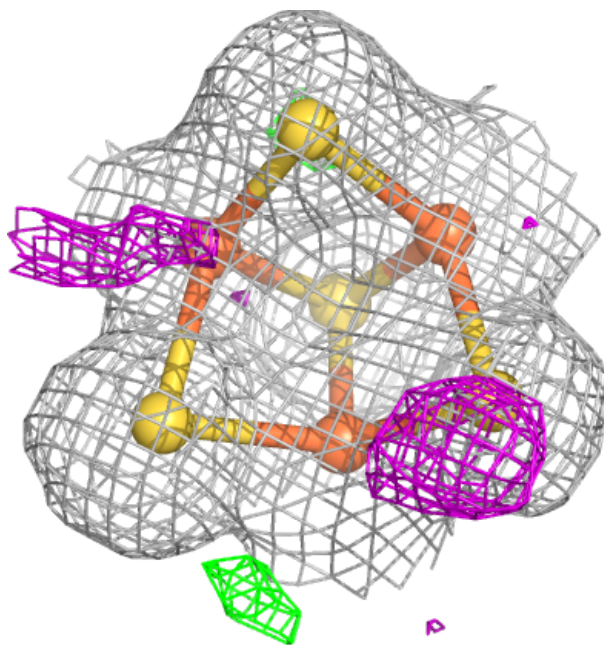
**Electron density around FES H 202:**

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



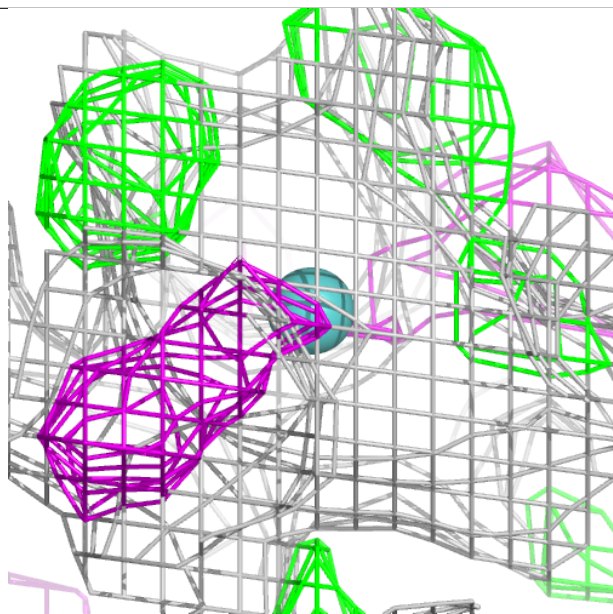
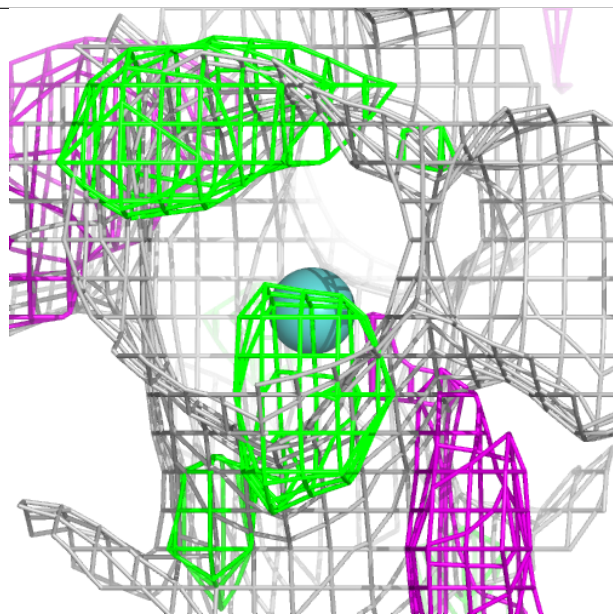
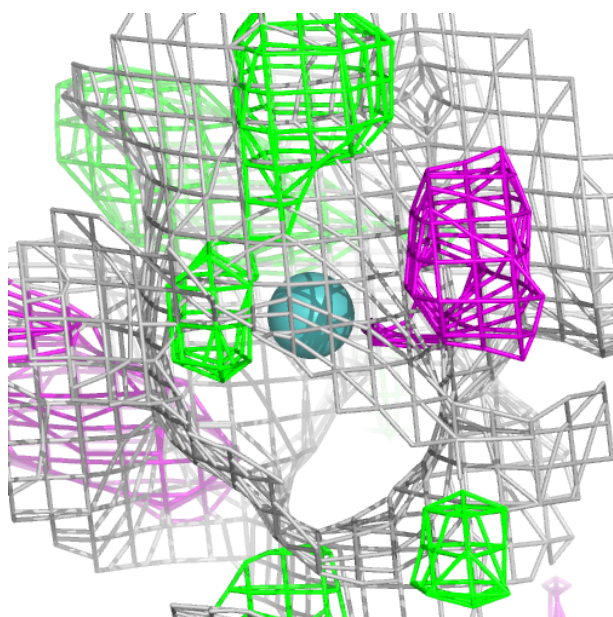
**Electron density around F3S A 904:**

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



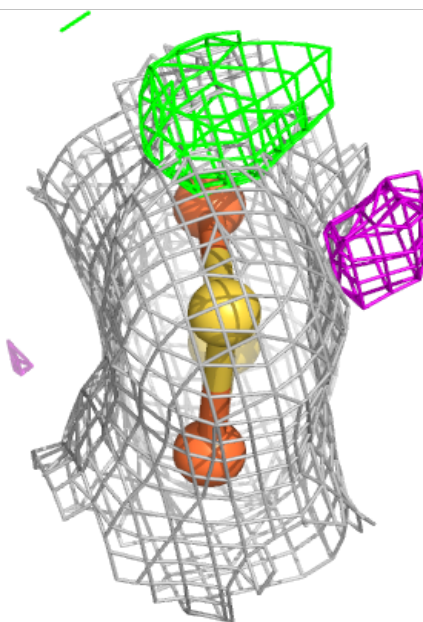
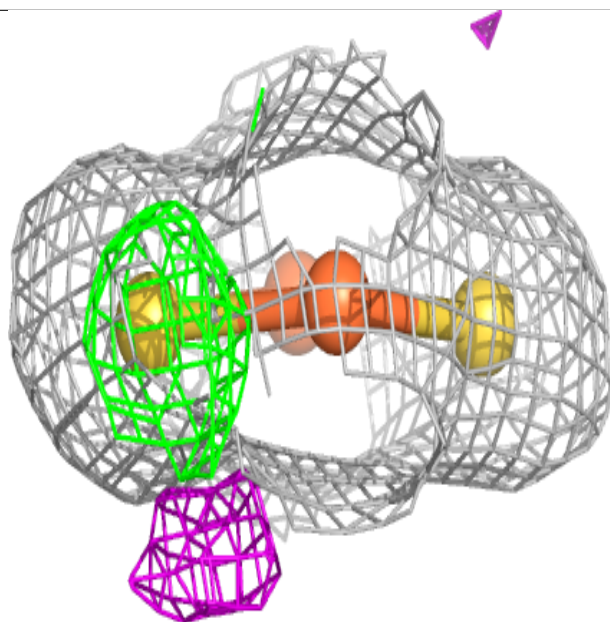
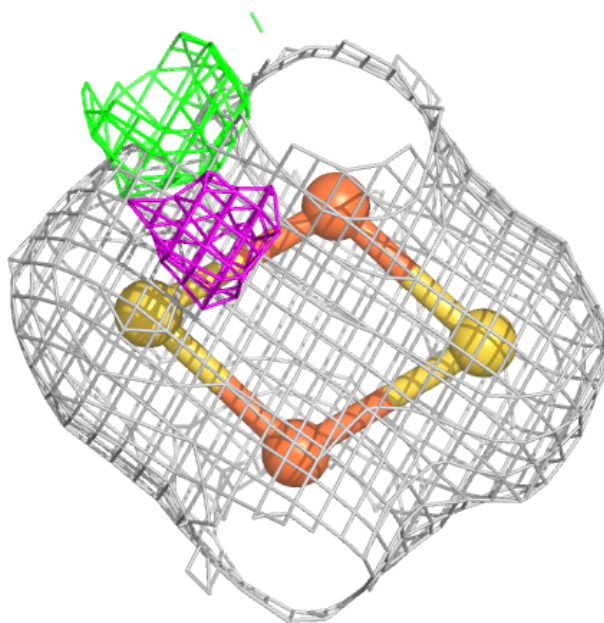
**Electron density around 4MO E 904:**

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



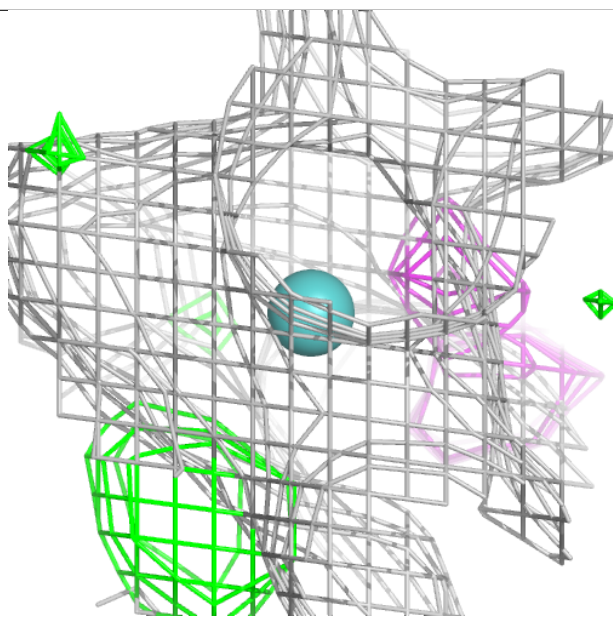
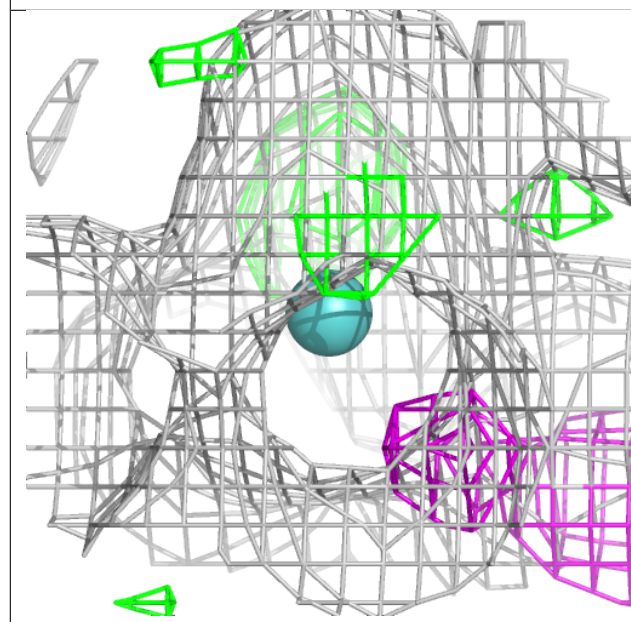
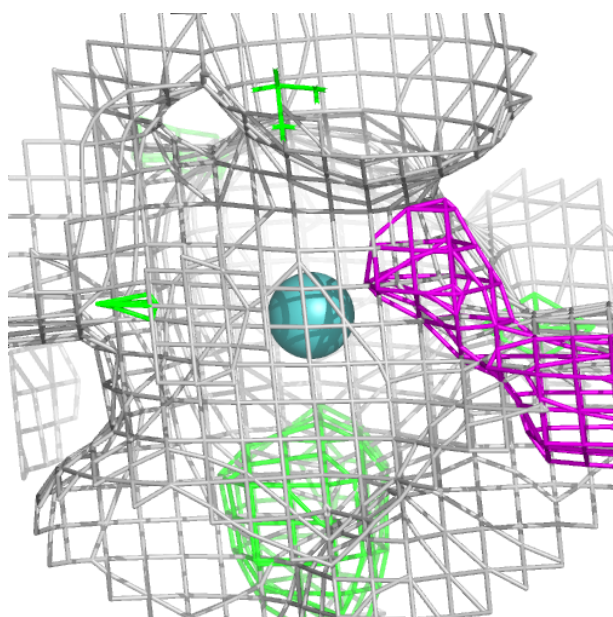
**Electron density around FES F 201:**

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



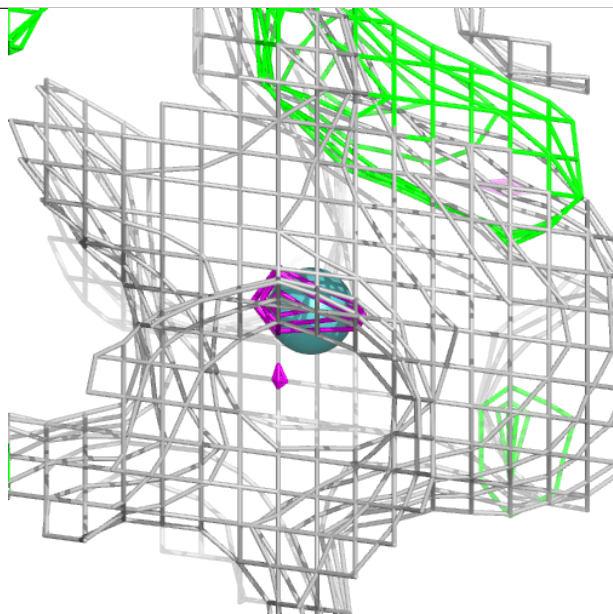
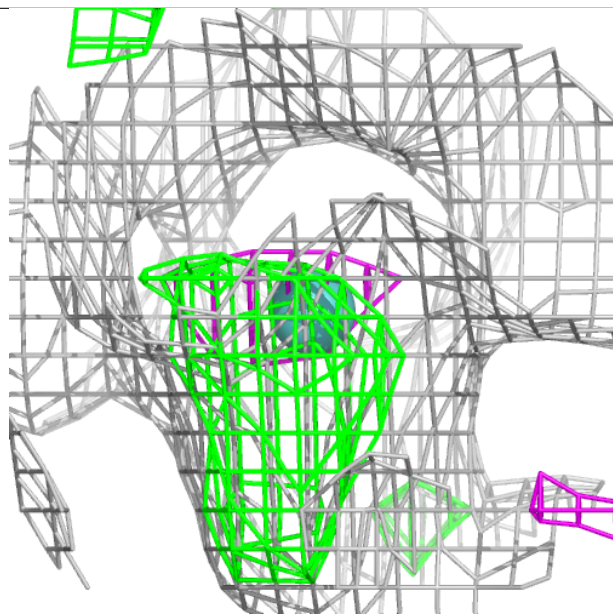
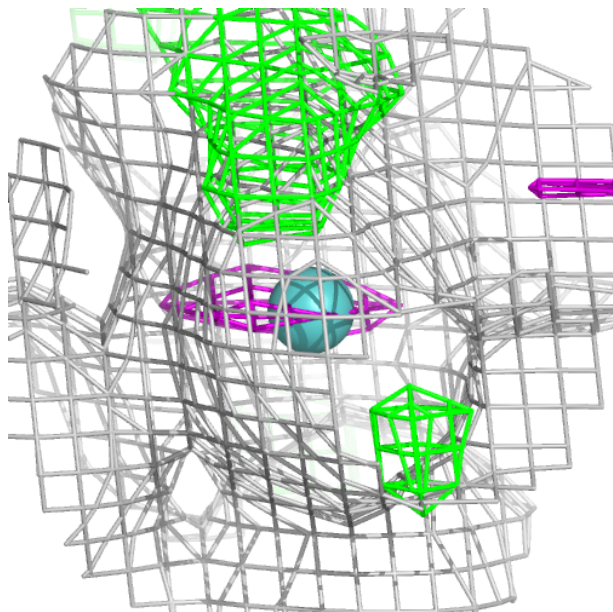
**Electron density around 4MO G 901:**

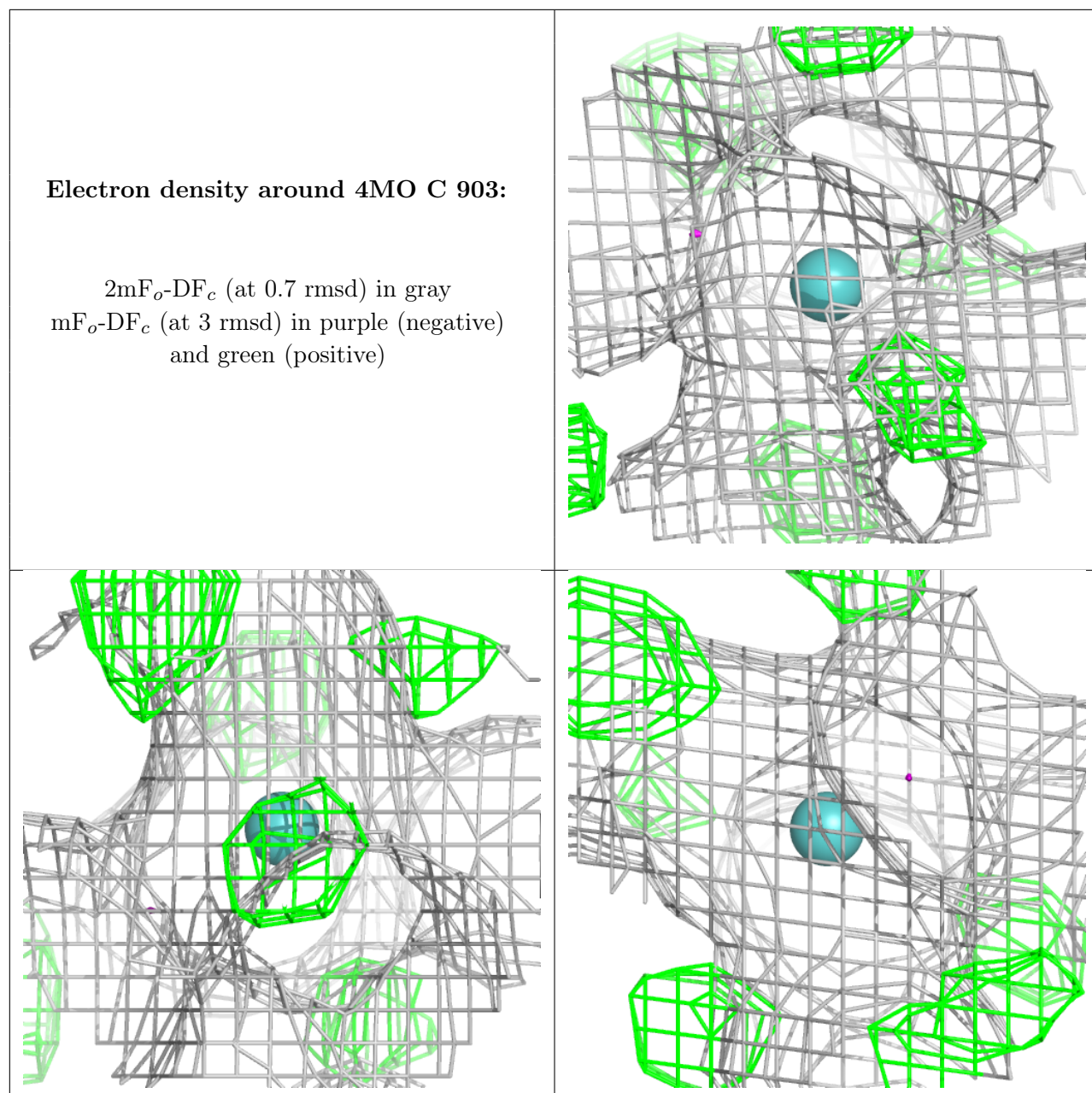
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 4MO 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)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.