



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 08:52 PM UTC

PDB ID : 7B2H / pdb\_00007b2h  
Title : Crystal structure of the methyl-coenzyme M reductase from Methanothermobacter Marburgensis derivatized with xenon  
Authors : Wagner, T.; Lemaire, O.N.; Engilberge, S.  
Deposited on : 2020-11-27  
Resolution : 2.12 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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)  
Xtrriage (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

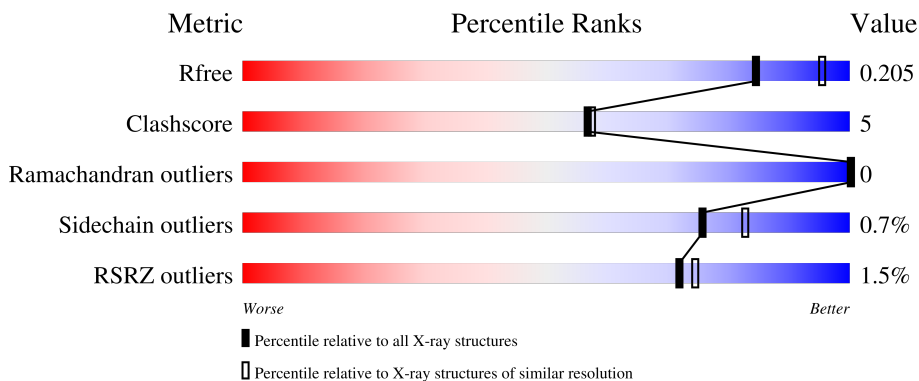
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	550	 88% 11%
1	D	550	 90% 9% ..
2	B	443	 91% 9%
2	E	443	 90% 9%
3	C	249	 94% 6%

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Mol	Chain	Length	Quality of chain
3	F	249	 3% 85% 10%

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
12	XE	B	511	-	-	X	-
12	XE	E	507	-	-	X	-
12	XE	E	508[A]	-	-	X	-
12	XE	E	509	-	-	X	-
7	PEG	B	502	-	-	X	-

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 20066 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 Methyl-coenzyme M reductase I subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	548	Total	C	N	O	S	0	5	1
			4266	2702	714	830	20			
1	D	547	Total	C	N	O	S	0	4	0
			4254	2697	711	826	20			

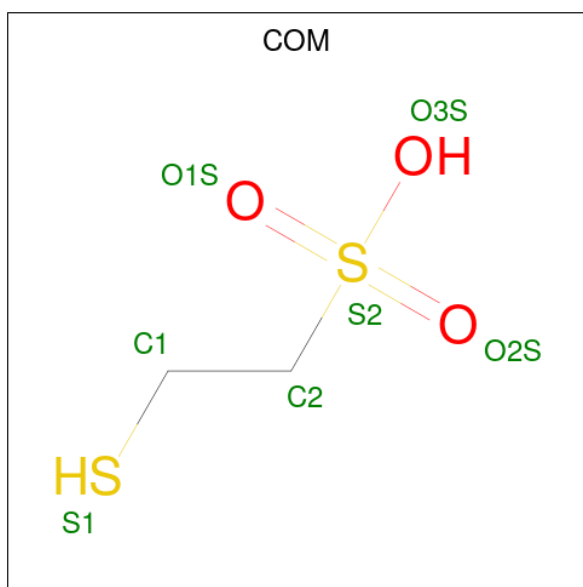
- Molecule 2 is a protein called Methyl-coenzyme M reductase I subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	442	Total	C	N	O	S	0	1	0
			3311	2094	551	648	18			
2	E	441	Total	C	N	O	S	0	5	0
			3286	2079	543	646	18			

- Molecule 3 is a protein called Methyl-coenzyme M reductase I subunit gamma.

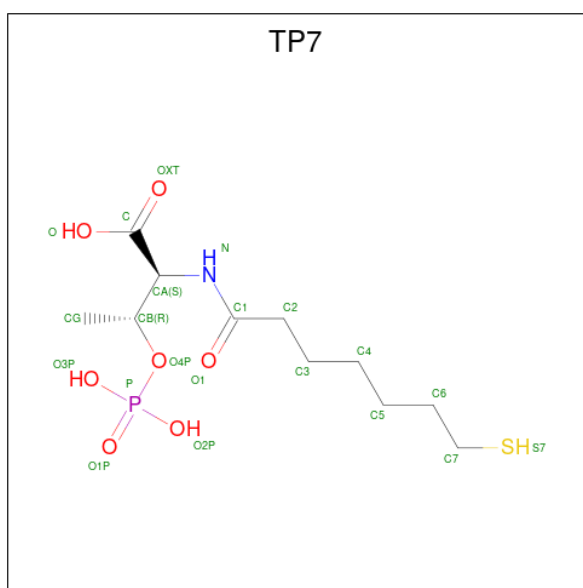
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	248	Total	C	N	O	S	0	2	0
			1983	1230	353	389	11			
3	F	239	Total	C	N	O	S	0	2	0
			1909	1188	344	367	10			

- Molecule 4 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>3</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			7	2	3	2		
4	D	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 5 is Coenzyme B (CCD ID: TP7) (formula:  $C_{11}H_{22}NO_7PS$ ).

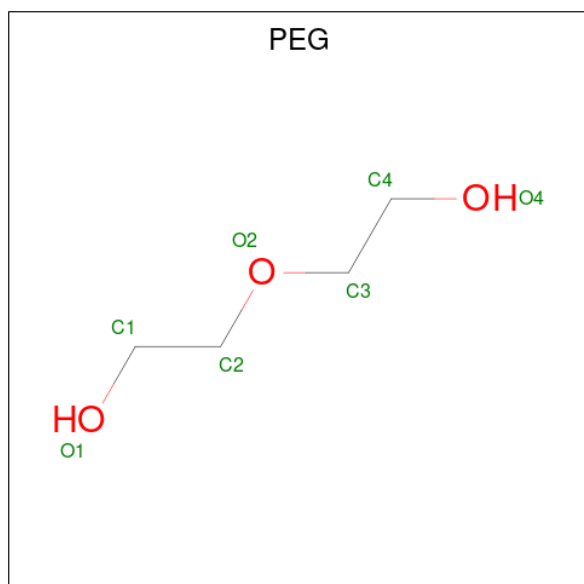


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
5	D	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total K 2 2	0	0
6	B	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



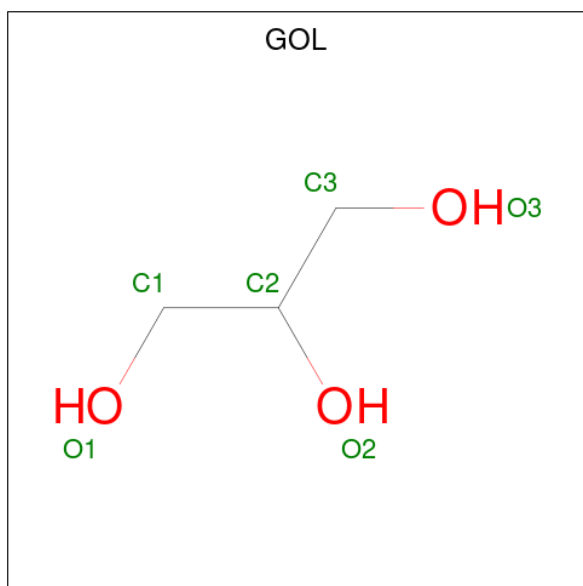
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 7 4 3	0	0
7	A	1	Total C O 5 3 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 5 3 2	0	0
7	D	1	Total C O 7 4 3	0	0
7	D	1	Total C O 7 4 3	0	0
7	D	1	Total C O 7 4 3	0	0
7	E	1	Total C O 7 4 3	0	0

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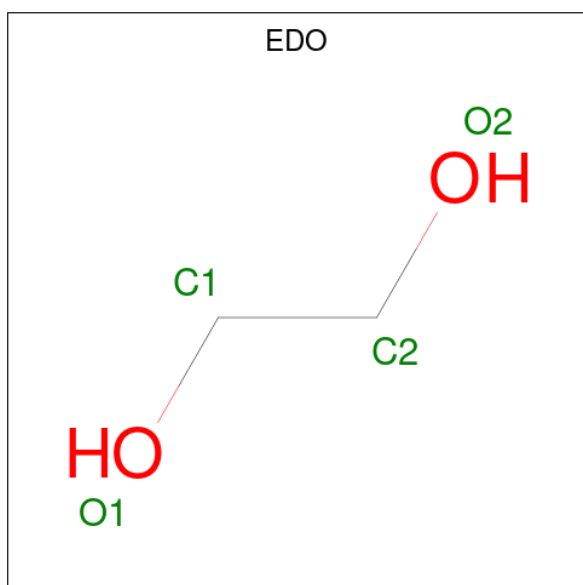
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	F	1	5	3	2	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



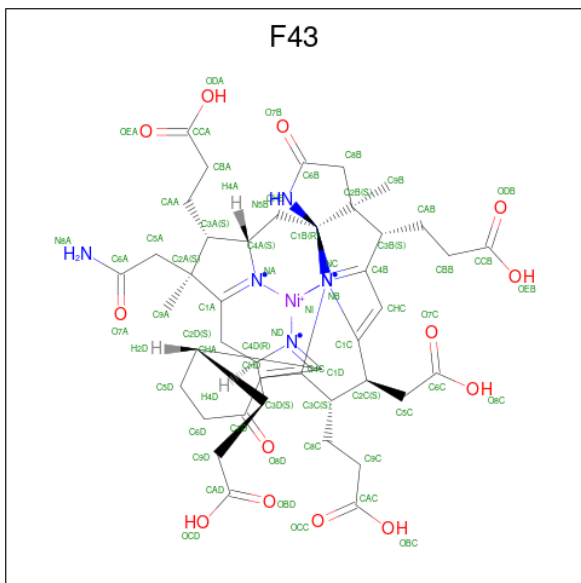
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	6	3	3	0	0

- 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 4 2 2	0	0

- Molecule 10 is FACTOR 430 (CCD ID: F43) (formula: C<sub>42</sub>H<sub>51</sub>N<sub>6</sub>NiO<sub>13</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N Ni O 62 42 6 1 13	0	0
10	D	1	Total C N Ni O 62 42 6 1 13	0	0

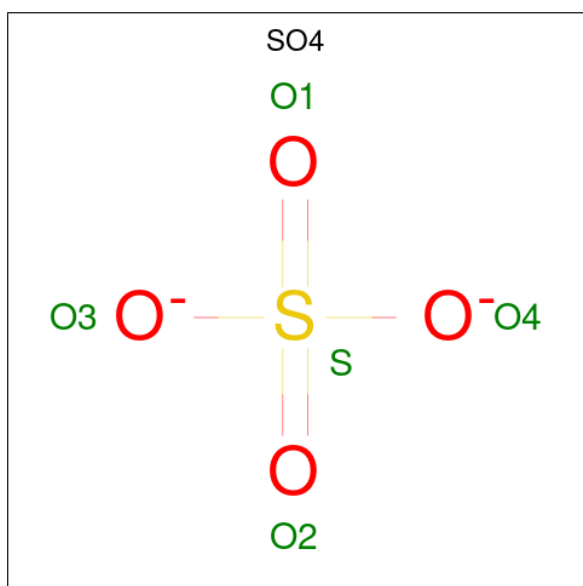
- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	4	Total Mg 4 4	0	0
11	B	4	Total Mg 4 4	0	0
11	D	2	Total Mg 2 2	0	0
11	E	4	Total Mg 4 4	0	0
11	F	1	Total Mg 1 1	0	0

- Molecule 12 is XENON (CCD ID: XE) (formula: Xe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total Xe 1 1	0	0
12	B	5	Total Xe 5 5	0	0
12	D	1	Total Xe 1 1	0	0
12	E	4	Total Xe 4 4	0	2
12	F	1	Total Xe 1 1	0	0

- Molecule 13 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total O S 5 4 1	0	0

- Molecule 14 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total Cl 1 1	0	0
14	E	1	Total Cl 1 1	0	0

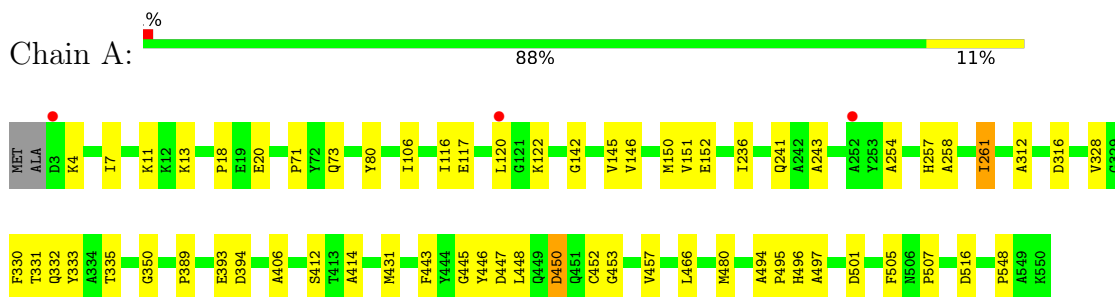
- Molecule 15 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
15	A	204	Total 207	O 207	0	3
15	B	148	Total 148	O 148	0	0
15	C	54	Total 54	O 54	0	0
15	D	208	Total 208	O 208	0	1
15	E	118	Total 118	O 118	0	0
15	F	40	Total 40	O 40	0	0

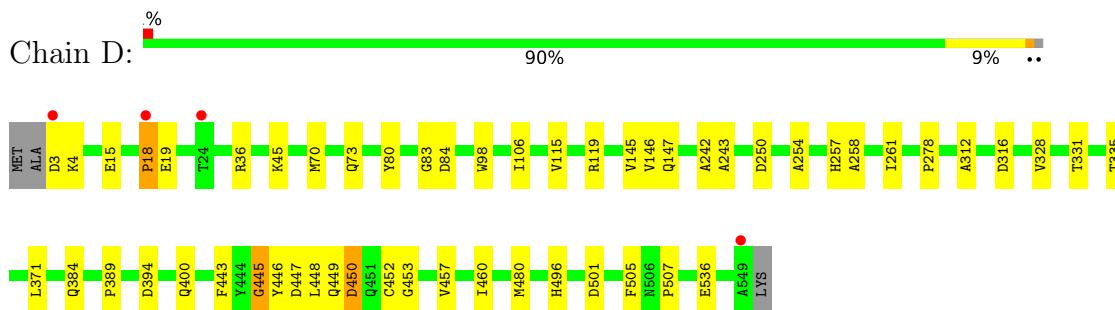
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

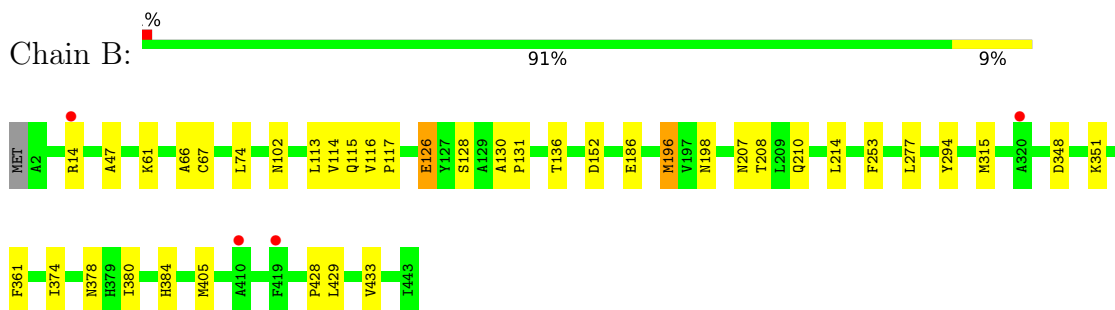
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha



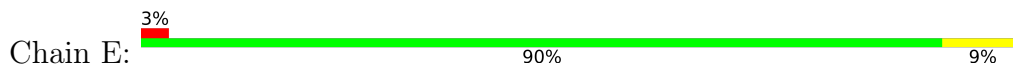
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha

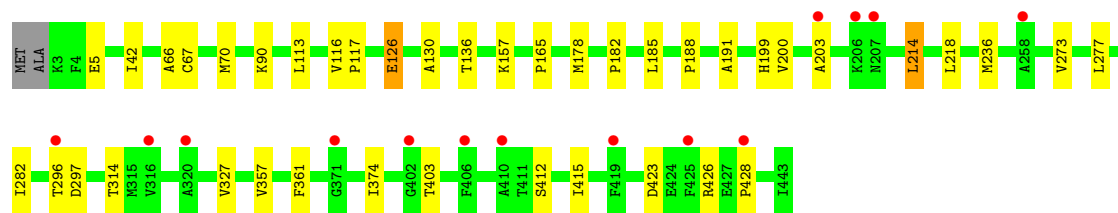


- Molecule 2: Methyl-coenzyme M reductase I subunit beta



- Molecule 2: Methyl-coenzyme M reductase I subunit beta

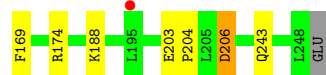
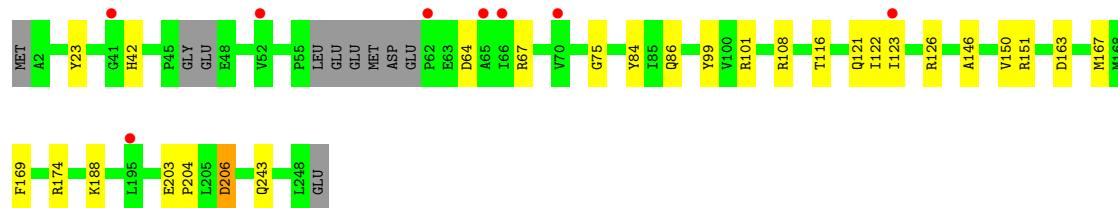
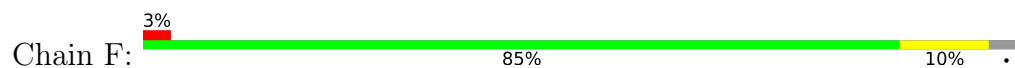




- Molecule 3: Methyl-coenzyme M reductase I subunit gamma



- Molecule 3: Methyl-coenzyme M reductase I subunit gamma



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.72Å 116.39Å 123.07Å 90.00° 92.36° 90.00°	Depositor
Resolution (Å)	48.17 – 2.12 48.17 – 2.12	Depositor EDS
% Data completeness (in resolution range)	88.1 (48.17-2.12) 89.4 (48.17-2.12)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.12Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.177 , 0.204 0.178 , 0.205	Depositor DCC
$R_{free}$ test set	5810 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtrriage
Anisotropy	0.298	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 59.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20066	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MHS, SMC, AGM, GOL, MG, XE, COM, GL3, SO4, EDO, MGN, CL, K, DYA, PEG, F43, TP7

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	0.39	0/4322	0.56	0/5869
1	D	0.35	0/4309	0.55	2/5853 (0.0%)
2	B	0.47	0/3365	0.66	0/4560
2	E	0.37	2/3347 (0.1%)	0.54	2/4543 (0.0%)
3	C	0.41	0/2026	0.59	0/2734
3	F	0.44	0/1949	0.63	0/2628
All	All	0.40	2/19318 (0.0%)	0.58	4/26187 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	297[A]	ASP	C-O	5.60	1.31	1.24
2	E	297[B]	ASP	C-O	5.60	1.31	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	297[A]	ASP	N-CA-C	7.86	122.71	113.20
2	E	297[B]	ASP	N-CA-C	7.86	122.71	113.20
1	D	19	GLU	N-CA-C	-7.00	105.00	113.97
1	D	18	PRO	CB-CA-C	-6.43	100.21	111.21

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4266	0	4071	46	0
1	D	4254	0	4063	37	0
2	B	3311	0	3297	39	0
2	E	3286	0	3239	39	0
3	C	1983	0	1900	8	0
3	F	1909	0	1841	16	0
4	A	7	0	6	3	0
4	D	7	0	6	3	0
5	A	21	0	19	1	0
5	D	21	0	19	1	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	12	0	15	0	0
7	B	9	0	10	5	0
7	D	21	0	30	2	0
7	E	7	0	10	0	0
7	F	5	0	5	0	0
8	A	6	0	8	0	0
9	A	4	0	6	0	0
10	A	62	0	43	7	0
10	D	62	0	43	5	0
11	A	4	0	0	0	0
11	B	4	0	0	0	0
11	D	2	0	0	0	0
11	E	4	0	0	0	0
11	F	1	0	0	0	0
12	A	1	0	0	1	0
12	B	5	0	0	6	0
12	D	1	0	0	0	0
12	E	4	0	0	10	0
12	F	1	0	0	0	0
13	A	5	0	0	0	0
14	B	1	0	0	0	0
14	E	1	0	0	0	0
15	A	207	0	0	0	0
15	B	148	0	0	0	0
15	C	54	0	0	1	0
15	D	208	0	0	0	0
15	E	118	0	0	2	0
15	F	40	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20066	0	18631	174	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 5.

The worst 5 of 174 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:203:ALA:HB3	12:E:507:XE:XE	2.32	1.08
2:E:203:ALA:CB	12:E:507:XE:XE	2.91	0.97
1:A:254:ALA:HA	1:A:258:ALA:HB3	1.61	0.81
1:A:151:VAL:HG11	1:D:83:GLY:HA3	1.64	0.79
2:E:178:MET:SD	12:E:507:XE:XE	3.20	0.78

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	545/550 (99%)	517 (95%)	28 (5%)	0	100	100
1	D	543/550 (99%)	517 (95%)	26 (5%)	0	100	100
2	B	441/443 (100%)	432 (98%)	9 (2%)	0	100	100
2	E	442/443 (100%)	436 (99%)	6 (1%)	0	100	100
3	C	248/249 (100%)	242 (98%)	6 (2%)	0	100	100
3	F	235/249 (94%)	228 (97%)	7 (3%)	0	100	100
All	All	2454/2484 (99%)	2372 (97%)	82 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	436/434 (100%)	435 (100%)	1 (0%)	87	92
1	D	434/434 (100%)	432 (100%)	2 (0%)	81	87
2	B	341/342 (100%)	339 (99%)	2 (1%)	78	85
2	E	337/342 (98%)	333 (99%)	4 (1%)	63	71
3	C	210/217 (97%)	209 (100%)	1 (0%)	81	87
3	F	201/217 (93%)	198 (98%)	3 (2%)	57	65
All	All	1959/1986 (99%)	1946 (99%)	13 (1%)	76	83

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	214	LEU
2	E	236	MET
3	F	206	ASP
3	F	150	VAL
3	F	203	GLU

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

Mol	Chain	Res	Type
2	E	21	GLN
2	E	174	ASN
2	E	441	ASN
2	B	21	GLN
2	B	115	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	DYA	D	450	1	6,7,8	1.20	0	6,8,10	3.05	2 (33%)
1	GL3	A	445	1	2,3,4	1.35	0	1,2,4	0.96	0
1	MGN	A	400	1	6,9,10	1.10	0	7,12,14	0.79	0
1	SMC	A	452	1	5,6,7	1.13	0	3,6,8	1.07	0
1	MHS	D	257	1	10,11,12	1.22	0	5,14,16	3.29	2 (40%)
1	AGM	A	271	1	10,11,12	0.56	0	7,13,15	0.57	0
1	MHS	A	257	1	10,11,12	1.29	1 (10%)	5,14,16	3.24	2 (40%)
1	AGM	D	271	1	10,11,12	0.55	0	7,13,15	0.47	0
1	MGN	D	400	1	6,9,10	1.05	0	7,12,14	0.83	1 (14%)
1	GL3	D	445	1	2,3,4	1.52	1 (50%)	1,2,4	1.09	0
1	SMC	D	452	1	5,6,7	1.08	0	3,6,8	1.08	0
1	DYA	A	450	1	6,7,8	1.31	1 (16%)	6,8,10	3.34	3 (50%)

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
1	DYA	D	450	1	-	4/4/6/8	-
1	GL3	A	445	1	-	1/1/1/2	-
1	MGN	A	400	1	-	0/7/9/12	-
1	SMC	A	452	1	-	1/3/5/7	-
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1
1	AGM	A	271	1	-	3/10/11/13	-
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1
1	AGM	D	271	1	-	3/10/11/13	-
1	MGN	D	400	1	-	0/7/9/12	-
1	GL3	D	445	1	-	1/1/1/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SMC	D	452	1	-	1/3/5/7	-
1	DYA	A	450	1	-	4/4/6/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	MHS	CG-ND1	-2.26	1.34	1.38
1	D	445	GL3	C-S	-2.15	1.71	1.80
1	A	450	DYA	OD1-CG	-2.03	1.25	1.30

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	MHS	ND1-CE1-NE2	-6.92	108.82	112.94
1	A	257	MHS	ND1-CE1-NE2	-6.81	108.89	112.94
1	A	450	DYA	CB-CA-N	-5.41	113.42	123.25
1	A	450	DYA	O-C-CA	-5.04	119.07	125.39
1	D	450	DYA	CB-CA-N	-4.94	114.27	123.25

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	450	DYA	N-CA-CB-CG
1	A	450	DYA	O-C-CA-CB
1	A	452	SMC	CA-CB-SG-CS
1	D	450	DYA	N-CA-CB-CG
1	D	450	DYA	O-C-CA-CB

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	450	DYA	1	0
1	A	445	GL3	1	0
1	A	452	SMC	1	0
1	D	445	GL3	2	0
1	D	452	SMC	1	0
1	A	450	DYA	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 33 are monoatomic - leaving 18 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
10	F43	A	608	1	63,71,71	1.83	5 (7%)	73,118,118	1.22	8 (10%)
7	PEG	A	605	-	4,4,6	0.22	0	3,3,5	0.23	0
7	PEG	A	604	-	6,6,6	0.09	0	5,5,5	0.07	0
7	PEG	B	502	-	3,3,6	0.12	0	2,2,5	0.22	0
7	PEG	D	605	-	6,6,6	0.08	0	5,5,5	0.04	0
7	PEG	E	502	-	6,6,6	0.09	0	5,5,5	0.07	0
5	TP7	A	602	-	19,20,20	0.72	0	24,26,26	0.83	0
7	PEG	D	606	-	6,6,6	0.08	0	5,5,5	0.06	0
13	SO4	A	614	-	4,4,4	0.24	0	6,6,6	0.08	0
8	GOL	A	606	-	5,5,5	0.14	0	5,5,5	0.21	0
5	TP7	D	603	-	19,20,20	0.73	0	24,26,26	0.86	0
7	PEG	B	503	-	4,4,6	0.20	0	3,3,5	0.19	0
7	PEG	F	302	-	4,4,6	0.11	0	3,3,5	0.19	0
10	F43	D	601	1	63,71,71	1.86	7 (11%)	73,118,118	1.19	7 (9%)
4	COM	D	602	-	6,6,6	0.44	0	8,8,8	1.01	1 (12%)
4	COM	A	601	-	6,6,6	0.30	0	8,8,8	1.01	1 (12%)
9	EDO	A	607	-	3,3,3	0.35	0	2,2,2	0.35	0
7	PEG	D	607	-	6,6,6	0.10	0	5,5,5	0.02	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
10	F43	A	608	1	-	5/28/185/185	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PEG	A	605	-	-	0/2/2/4	-
7	PEG	A	604	-	-	3/4/4/4	-
7	PEG	B	502	-	-	0/1/1/4	-
7	PEG	D	605	-	-	1/4/4/4	-
7	PEG	E	502	-	-	0/4/4/4	-
5	TP7	A	602	-	-	2/24/24/24	-
7	PEG	D	606	-	-	3/4/4/4	-
8	GOL	A	606	-	-	3/4/4/4	-
5	TP7	D	603	-	-	1/24/24/24	-
7	PEG	B	503	-	-	1/2/2/4	-
7	PEG	F	302	-	-	1/2/2/4	-
10	F43	D	601	1	-	5/28/185/185	-
4	COM	D	602	-	-	3/4/4/4	-
4	COM	A	601	-	-	3/4/4/4	-
9	EDO	A	607	-	-	1/1/1/1	-
7	PEG	D	607	-	-	1/4/4/4	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	608	F43	NI-NA	6.77	2.05	1.89
10	D	601	F43	NI-NA	6.67	2.05	1.89
10	D	601	F43	NI-NB	6.20	2.04	1.89
10	A	608	F43	NI-NB	5.93	2.03	1.89
10	D	601	F43	NI-ND	5.91	2.03	1.89

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	608	F43	CAB-C3B-C2B	-4.14	109.88	119.00
10	D	601	F43	CAB-C3B-C2B	-3.62	111.02	119.00
4	D	602	COM	C2-C1-S1	-2.74	106.14	113.10
4	A	601	COM	C2-C1-S1	-2.66	106.36	113.10
10	D	601	F43	C4D-ND-C1D	2.54	112.27	108.46

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	COM	C1-C2-S2-O1S

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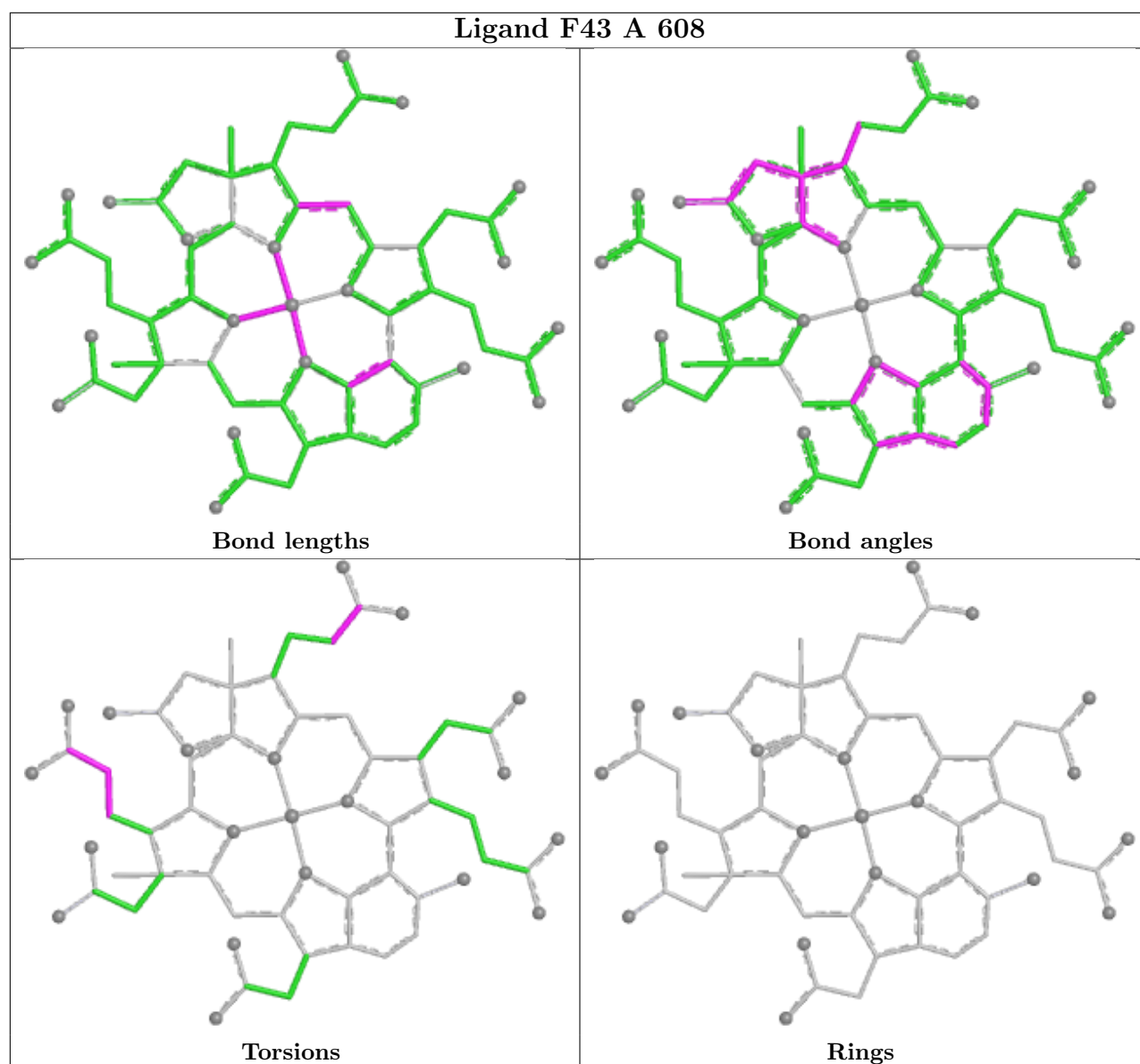
Mol	Chain	Res	Type	Atoms
4	A	601	COM	C1-C2-S2-O2S
4	A	601	COM	C1-C2-S2-O3S
4	D	602	COM	C1-C2-S2-O1S
4	D	602	COM	C1-C2-S2-O2S

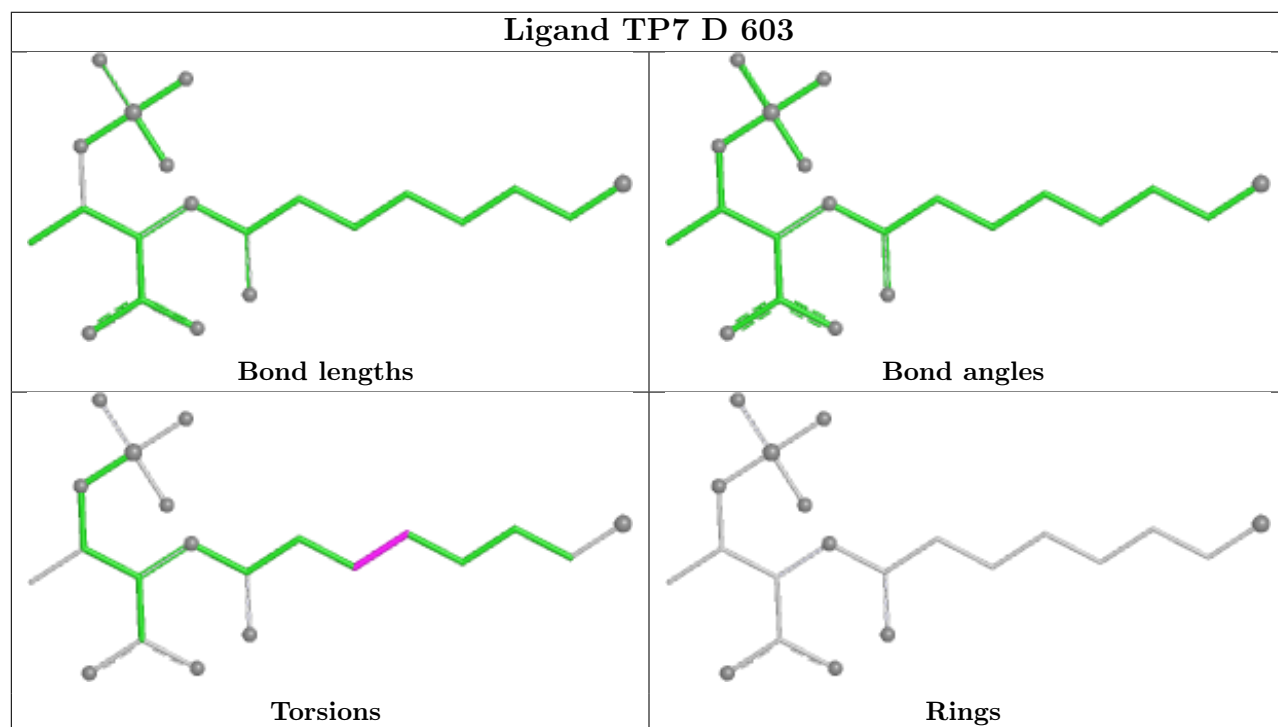
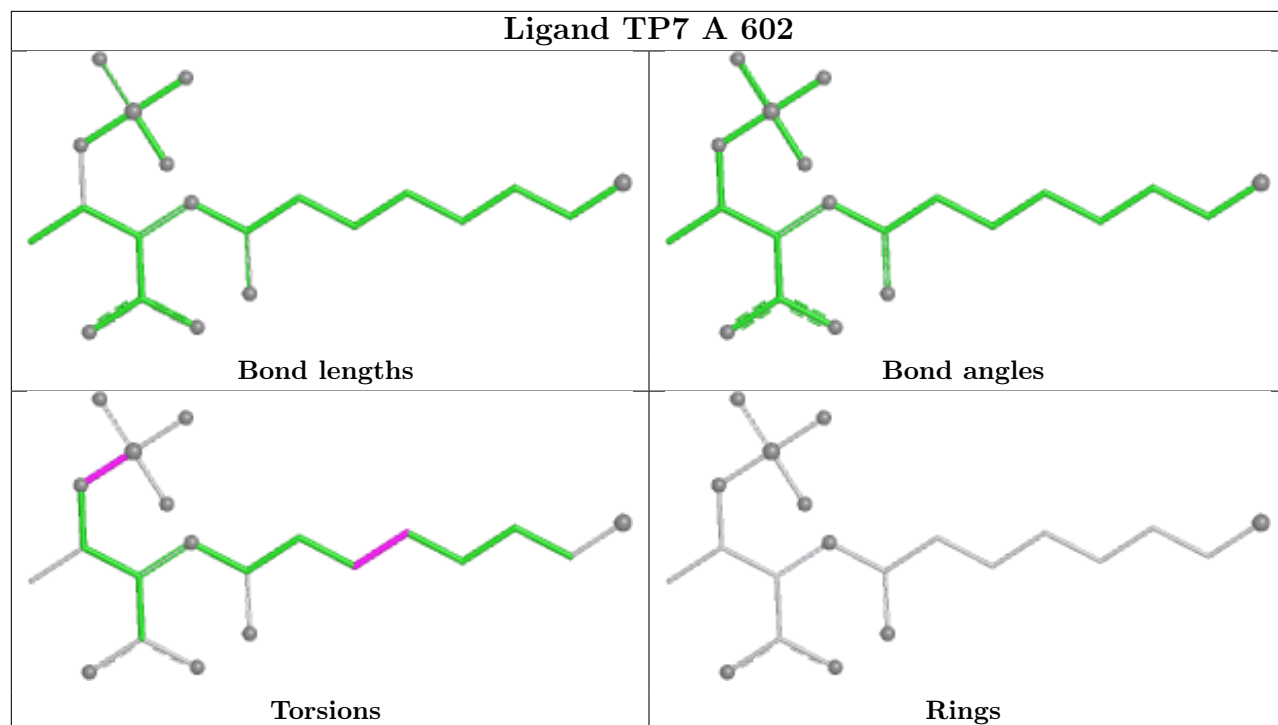
There are no ring outliers.

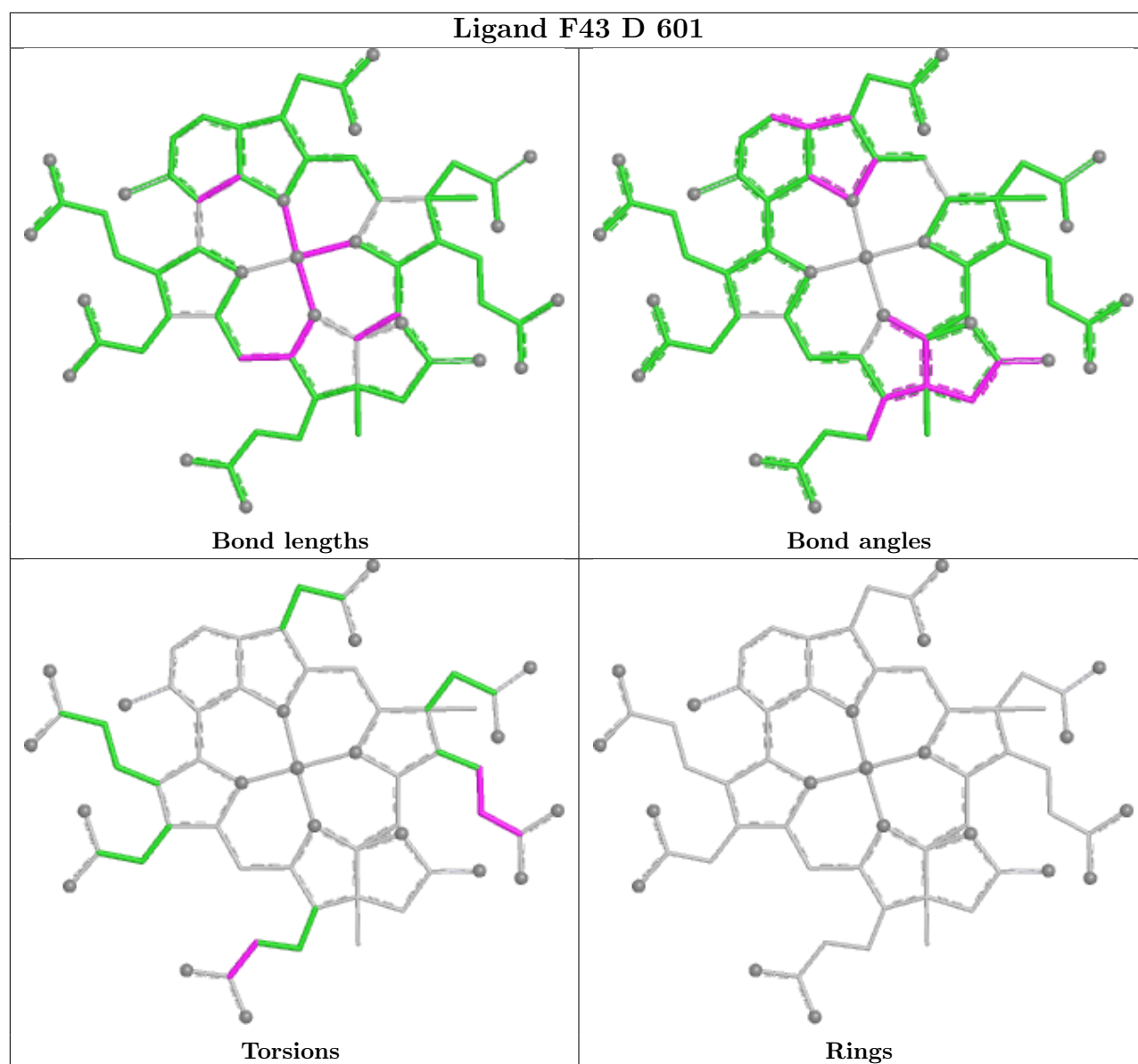
9 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	608	F43	7	0
7	B	502	PEG	4	0
7	D	605	PEG	2	0
5	A	602	TP7	1	0
5	D	603	TP7	1	0
7	B	503	PEG	1	0
10	D	601	F43	5	0
4	D	602	COM	3	0
4	A	601	COM	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.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	542/550 (98%)	-0.07	3 (0%) 85 87	18, 42, 68, 122	6 (1%)
1	D	541/550 (98%)	-0.13	4 (0%) 84 86	17, 39, 63, 97	4 (0%)
2	B	442/443 (99%)	0.10	4 (0%) 81 83	28, 48, 73, 127	2 (0%)
2	E	441/443 (99%)	0.32	14 (3%) 50 53	23, 51, 84, 118	4 (0%)
3	C	248/249 (99%)	0.40	3 (1%) 76 79	38, 58, 88, 124	2 (0%)
3	F	239/249 (95%)	0.70	8 (3%) 49 52	27, 65, 93, 138	2 (0%)
All	All	2453/2484 (98%)	0.14	36 (1%) 72 74	17, 47, 80, 138	20 (0%)

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	549	ALA	4.6
2	B	410	ALA	4.0
2	B	419	PHE	3.7
2	E	425	PHE	3.1
2	E	419[B]	PHE	3.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	MHS	A	257	11/12	0.89	0.10	50,52,53,55	0
1	MHS	D	257	11/12	0.93	0.09	39,41,44,45	0
1	GL3	A	445	4/5	0.94	0.09	34,36,36,37	0
1	AGM	A	271	12/13	0.94	0.08	29,31,33,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	AGM	D	271	12/13	0.94	0.07	32,35,36,37	0
1	GL3	D	445	4/5	0.94	0.09	32,33,33,34	0
1	DYA	D	450	8/9	0.94	0.07	31,34,34,35	0
1	DYA	A	450	8/9	0.95	0.07	33,35,40,41	0
1	MGN	D	400	10/11	0.95	0.07	33,36,38,41	0
1	SMC	A	452	7/8	0.97	0.06	38,38,40,41	0
1	MGN	A	400	10/11	0.97	0.06	36,38,40,40	0
1	SMC	D	452	7/8	0.98	0.06	35,38,39,40	0

### 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
11	MG	F	301	1/1	0.65	0.13	89,89,89,89	0
11	MG	B	505	1/1	0.67	0.17	103,103,103,103	0
8	GOL	A	606	6/6	0.72	0.14	86,86,87,87	0
11	MG	E	505	1/1	0.73	0.15	89,89,89,89	0
11	MG	E	503	1/1	0.73	0.23	87,87,87,87	0
7	PEG	B	503	5/7	0.74	0.29	55,56,57,57	5
11	MG	A	612	1/1	0.77	0.24	97,97,97,97	0
11	MG	B	501	1/1	0.77	0.09	80,80,80,80	0
7	PEG	F	302	5/7	0.77	0.32	50,50,52,52	5
11	MG	A	610	1/1	0.79	0.17	99,99,99,99	0
11	MG	E	504	1/1	0.79	0.09	103,103,103,103	0
7	PEG	E	502	7/7	0.80	0.14	88,89,92,92	0
6	K	D	610	1/1	0.80	0.14	82,82,82,82	0
11	MG	A	611	1/1	0.80	0.18	80,80,80,80	0
11	MG	B	506	1/1	0.80	0.22	86,86,86,86	0
9	EDO	A	607	4/4	0.81	0.13	73,73,75,76	0
11	MG	B	504	1/1	0.81	0.20	76,76,76,76	0
7	PEG	A	605	5/7	0.82	0.20	80,80,81,82	0
6	K	A	615	1/1	0.86	0.15	70,70,70,70	0
12	XE	B	511	1/1	0.86	0.14	47,47,47,47	1

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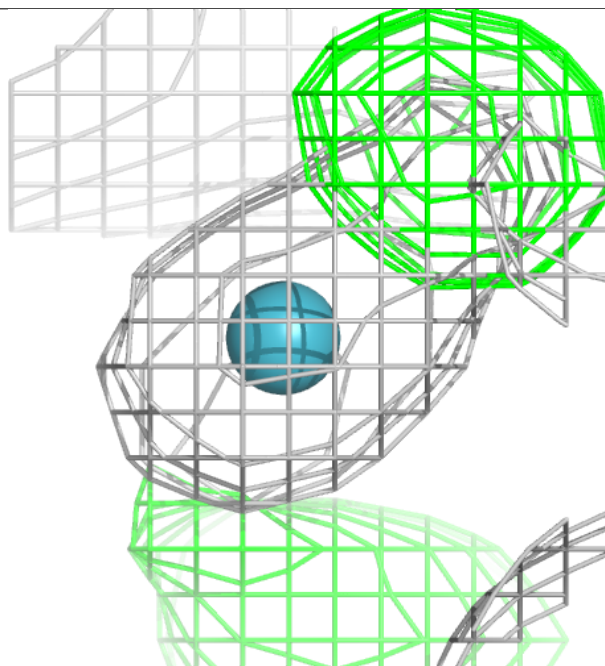
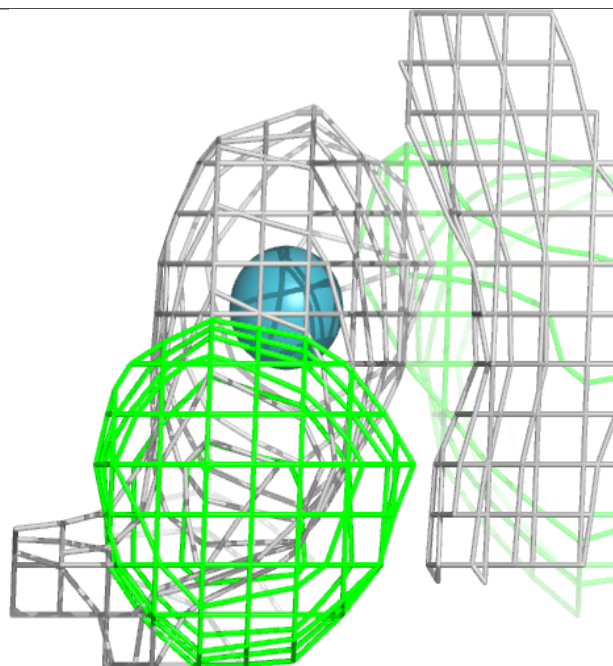
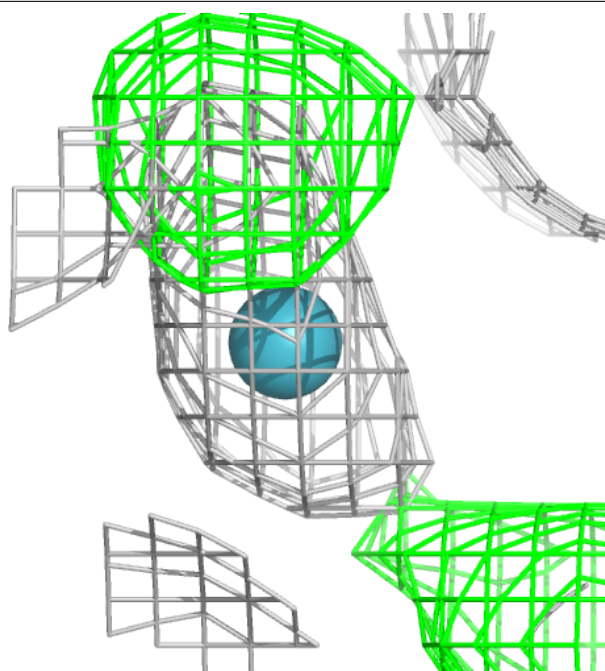
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	PEG	D	606	7/7	0.87	0.13	74,74,75,76	0
7	PEG	D	607	7/7	0.87	0.18	48,49,50,52	7
7	PEG	B	502	4/7	0.87	0.11	51,52,52,54	0
12	XE	B	508	1/1	0.88	0.11	68,68,68,68	1
4	COM	D	602	7/7	0.88	0.14	54,57,62,62	0
13	SO4	A	614	5/5	0.88	0.09	128,128,129,130	0
7	PEG	A	604	7/7	0.89	0.14	52,53,54,55	0
11	MG	A	609	1/1	0.89	0.09	72,72,72,72	0
14	CL	E	510	1/1	0.89	0.16	65,65,65,65	0
11	MG	D	608	1/1	0.90	0.07	64,64,64,64	0
12	XE	E	509	1/1	0.90	0.12	50,50,50,50	1
7	PEG	D	605	7/7	0.91	0.12	70,72,74,74	0
11	MG	D	604	1/1	0.91	0.09	69,69,69,69	0
4	COM	A	601	7/7	0.91	0.12	49,52,54,55	0
12	XE	E	506[B]	1/1	0.92	0.20	62,62,62,62	1
12	XE	B	510	1/1	0.93	0.12	100,100,100,100	1
11	MG	E	501	1/1	0.95	0.07	51,51,51,51	0
5	TP7	D	603	21/21	0.95	0.08	33,39,44,46	0
14	CL	B	512	1/1	0.95	0.12	64,64,64,64	0
6	K	B	513	1/1	0.95	0.31	77,77,77,77	0
10	F43	A	608	62/62	0.96	0.07	35,38,43,45	0
12	XE	B	507	1/1	0.96	0.07	71,71,71,71	1
10	F43	D	601	62/62	0.96	0.07	32,40,45,48	0
12	XE	E	507	1/1	0.96	0.09	46,46,46,46	1
12	XE	B	509	1/1	0.97	0.07	71,71,71,71	1
12	XE	E	508[A]	1/1	0.97	0.10	65,65,65,65	1
12	XE	F	303	1/1	0.98	0.10	78,78,78,78	1
5	TP7	A	602	21/21	0.98	0.05	28,33,36,37	0
12	XE	D	609	1/1	0.99	0.04	62,62,62,62	1
12	XE	A	613	1/1	0.99	0.03	64,64,64,64	1
6	K	A	603	1/1	0.99	0.17	47,47,47,47	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.

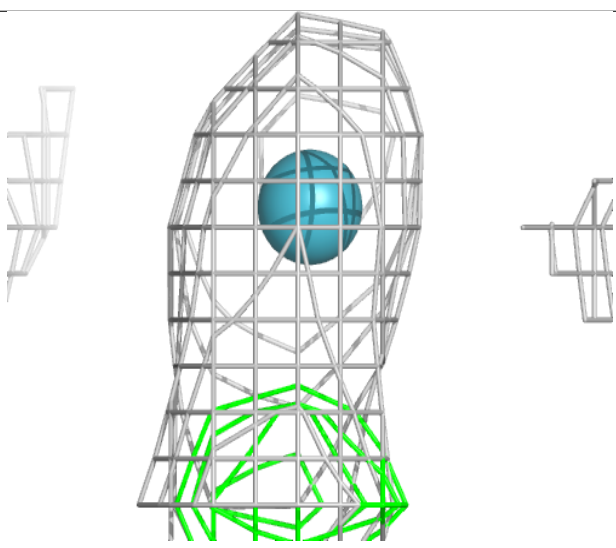
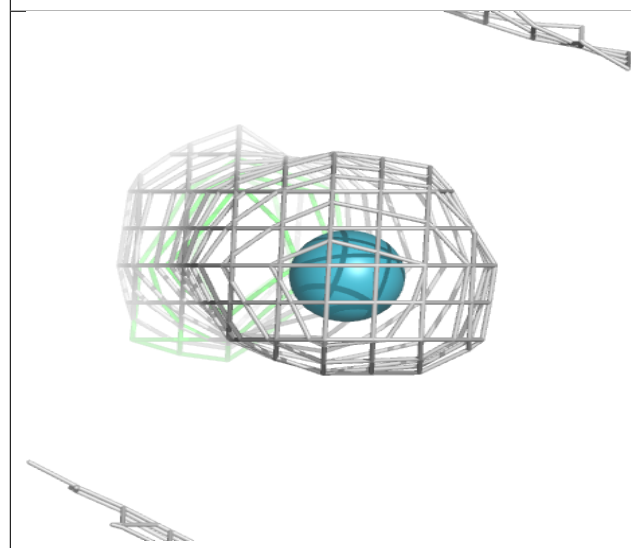
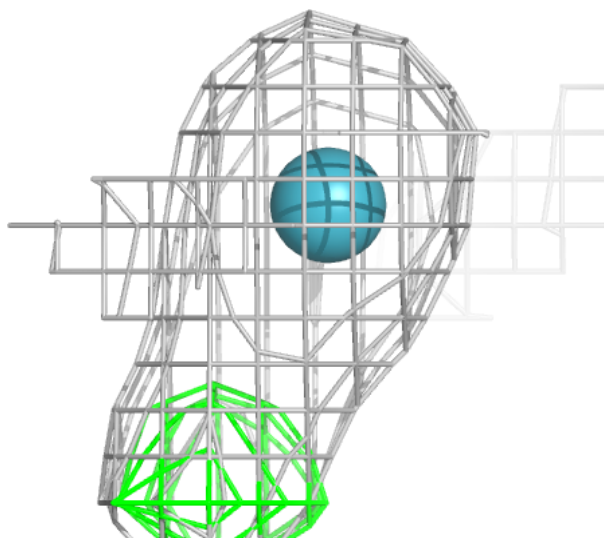
**Electron density around XE B 511:**

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



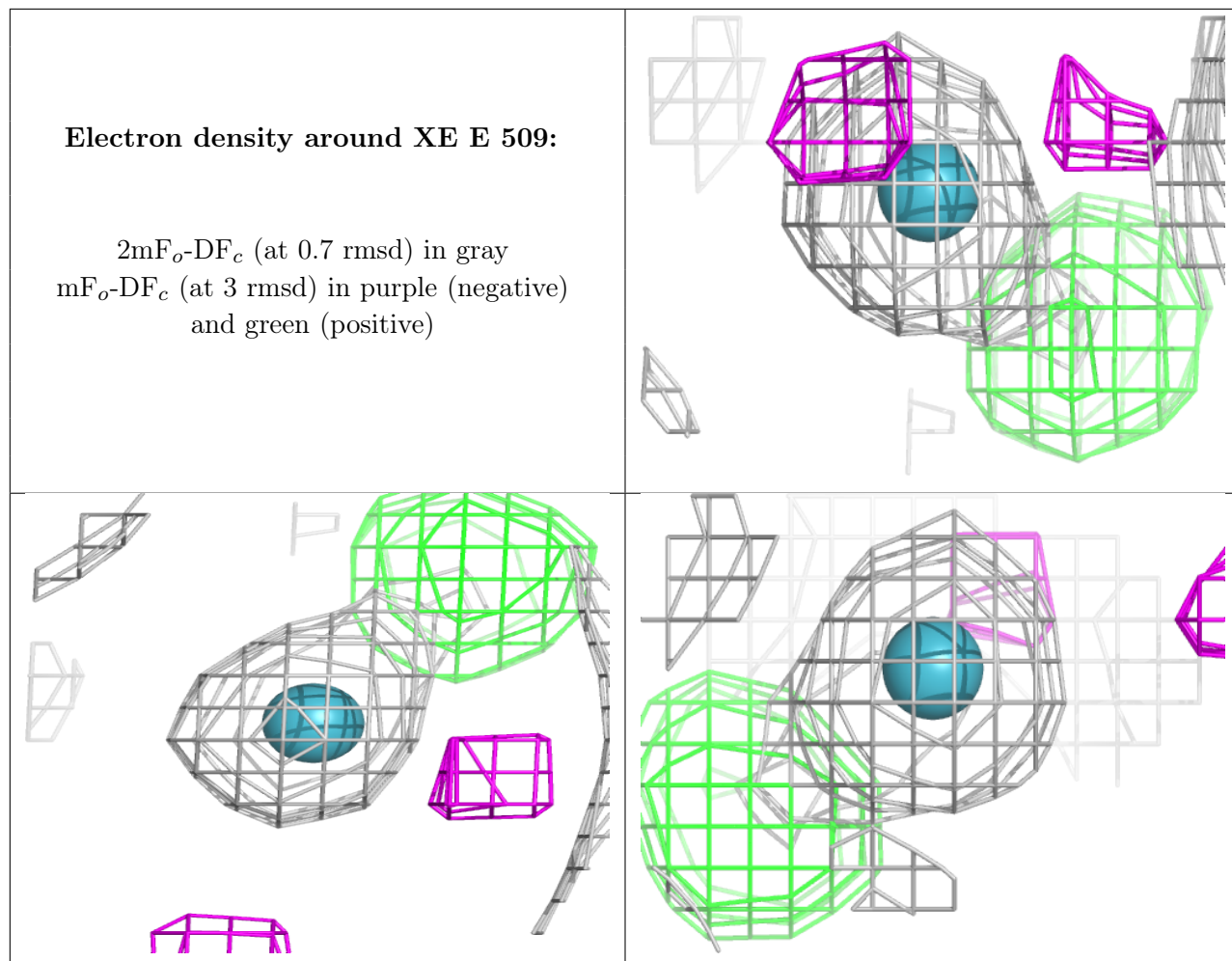
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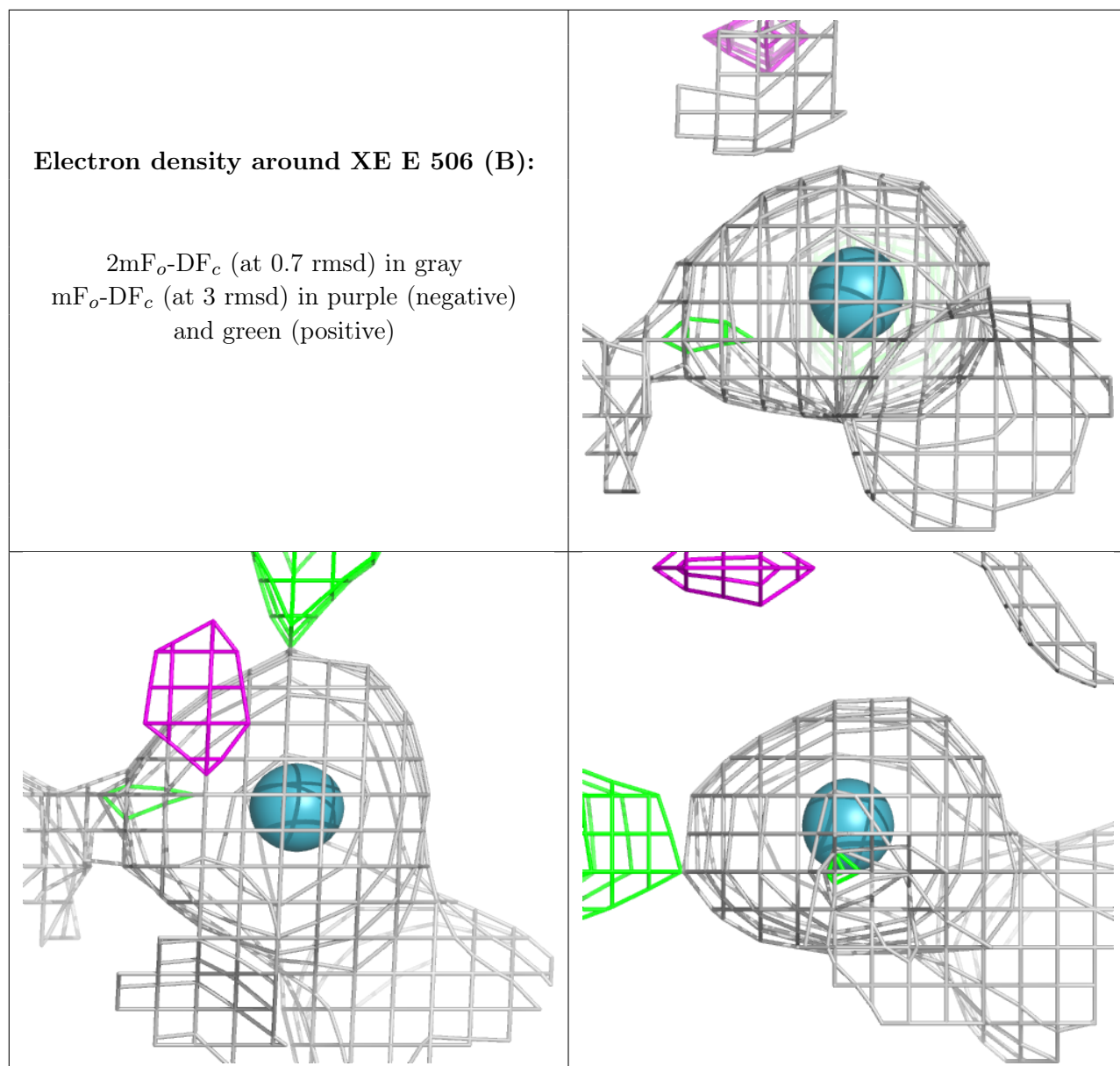
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around XE E 509:**

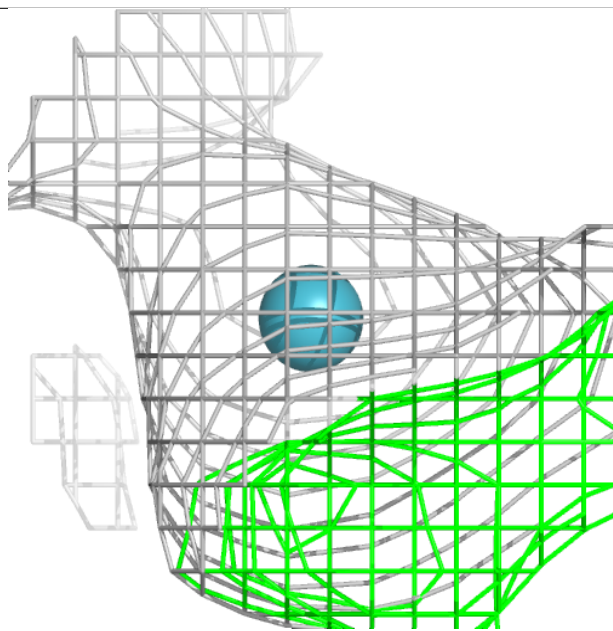
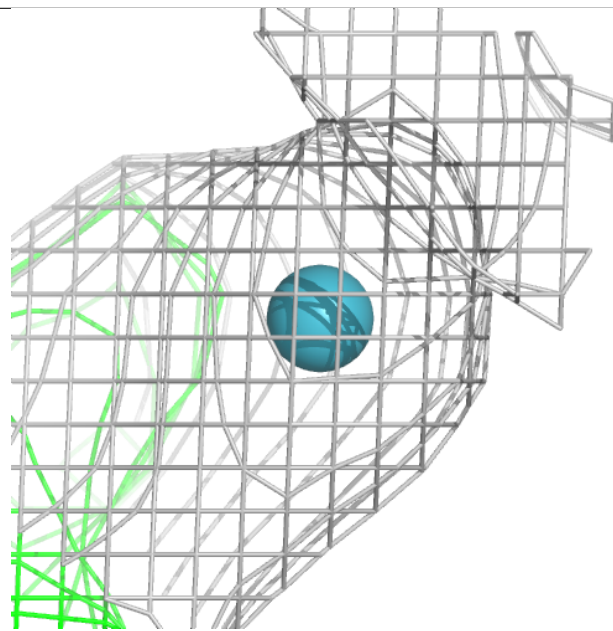
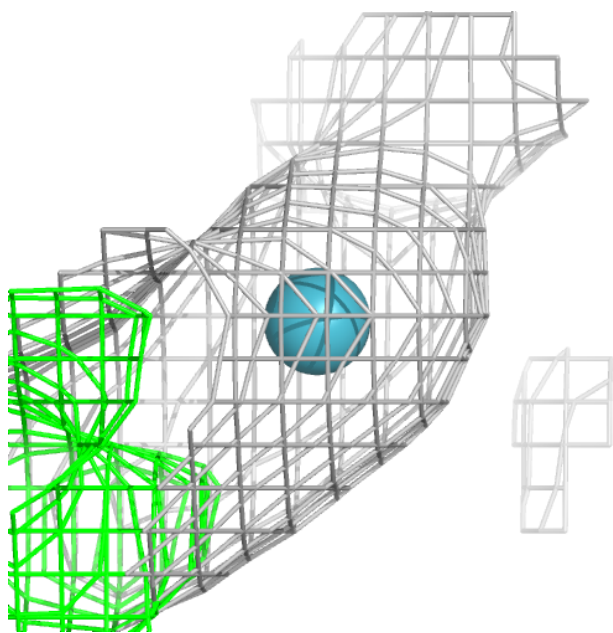
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





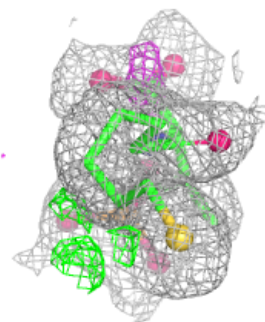
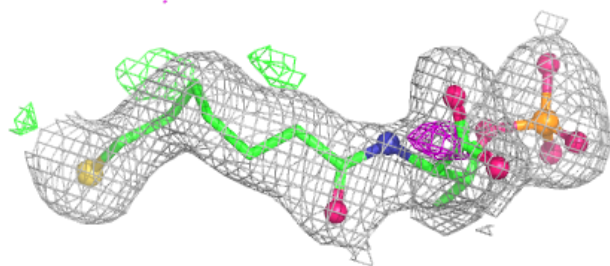
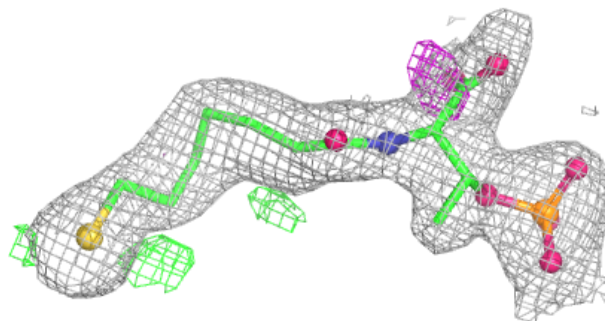
**Electron density around XE B 510:**

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



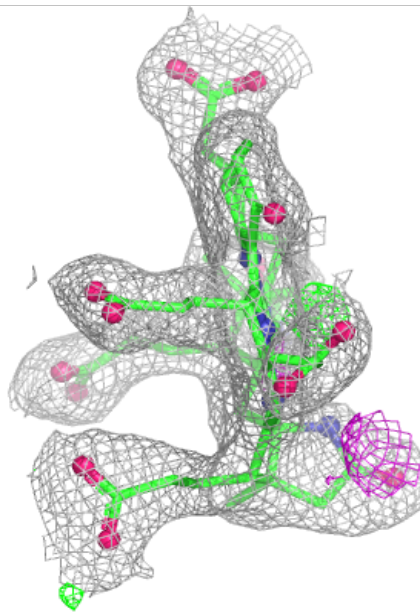
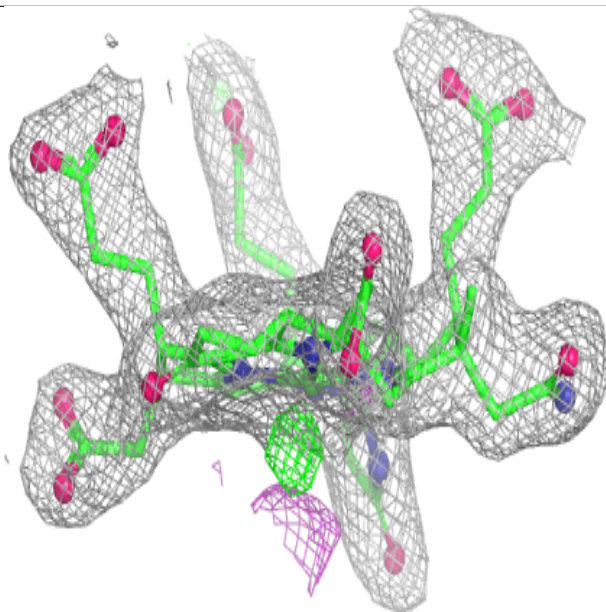
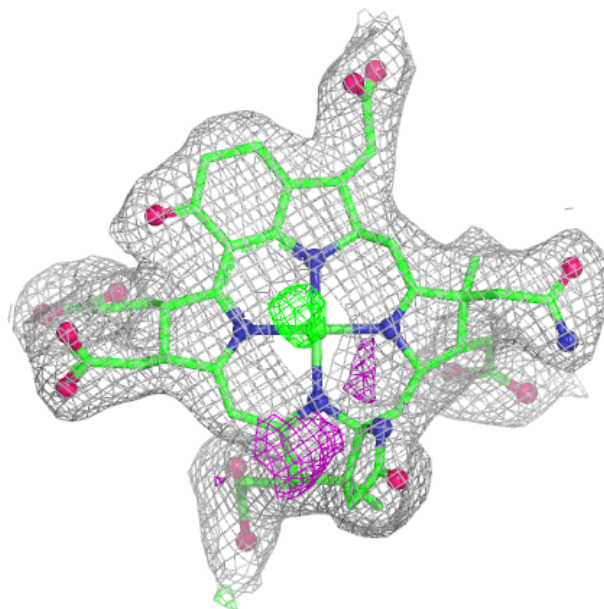
**Electron density around TP7 D 603:**

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



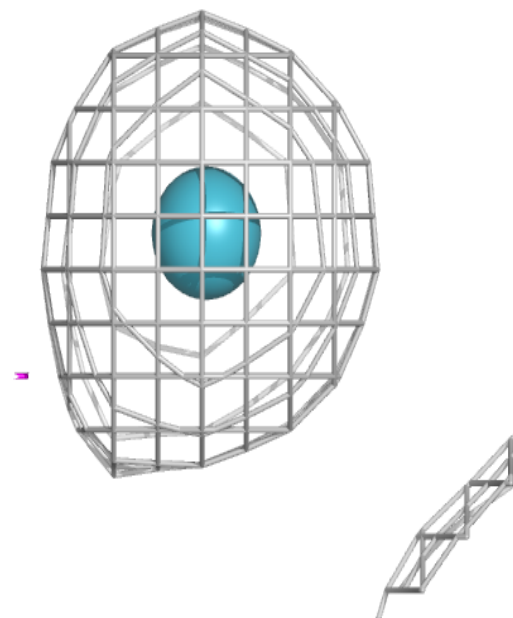
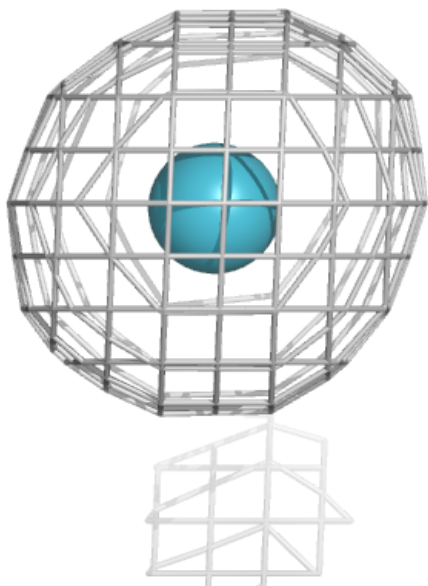
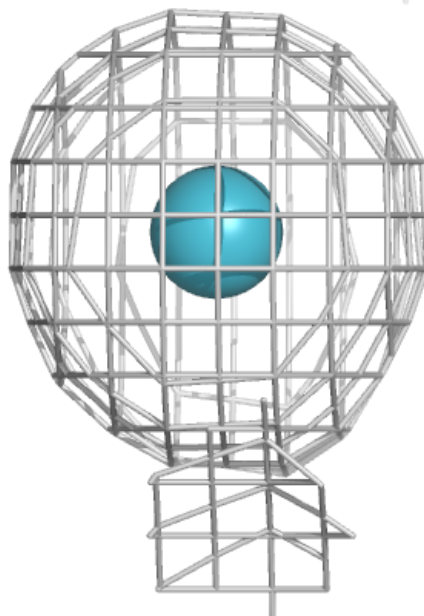
**Electron density around F43 A 608:**

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



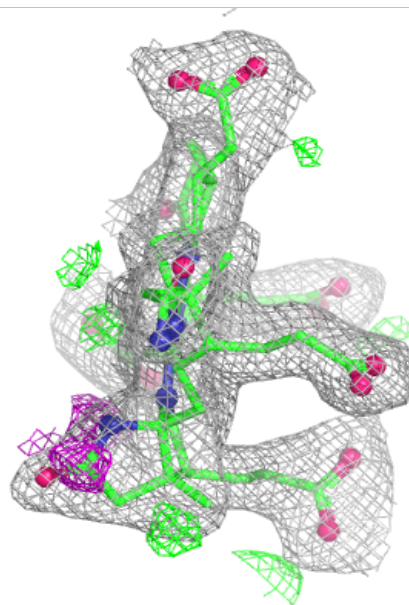
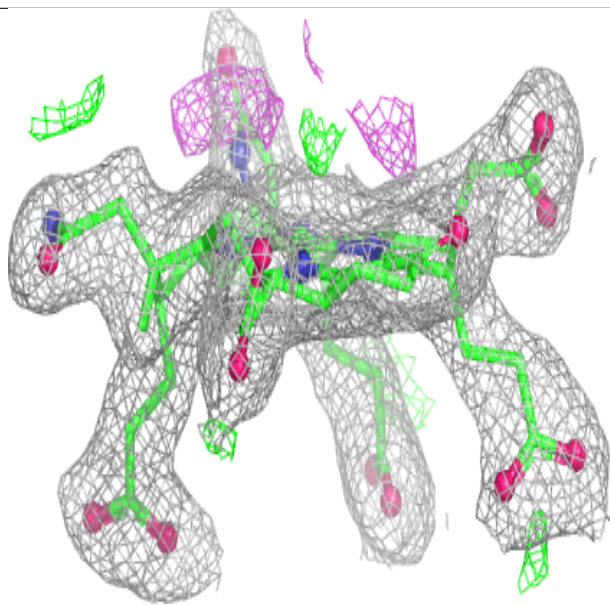
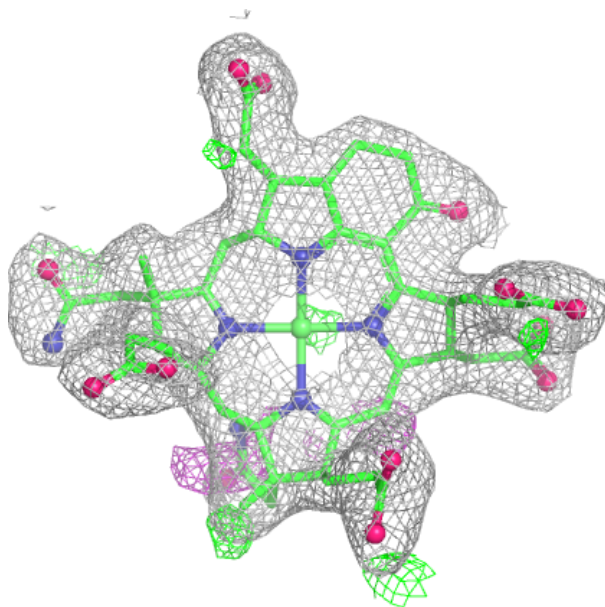
**Electron density around XE B 507:**

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



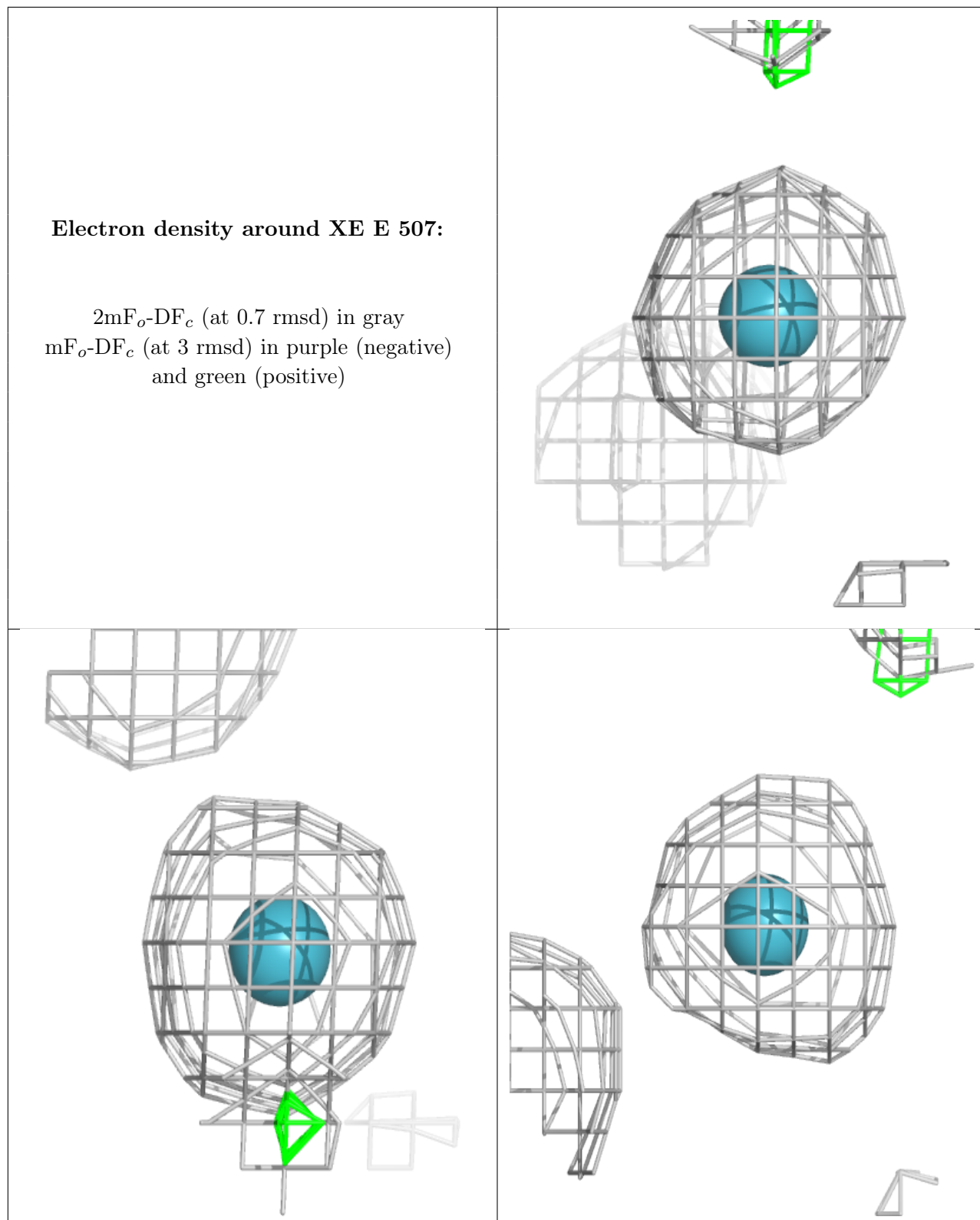
**Electron density around F43 D 601:**

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



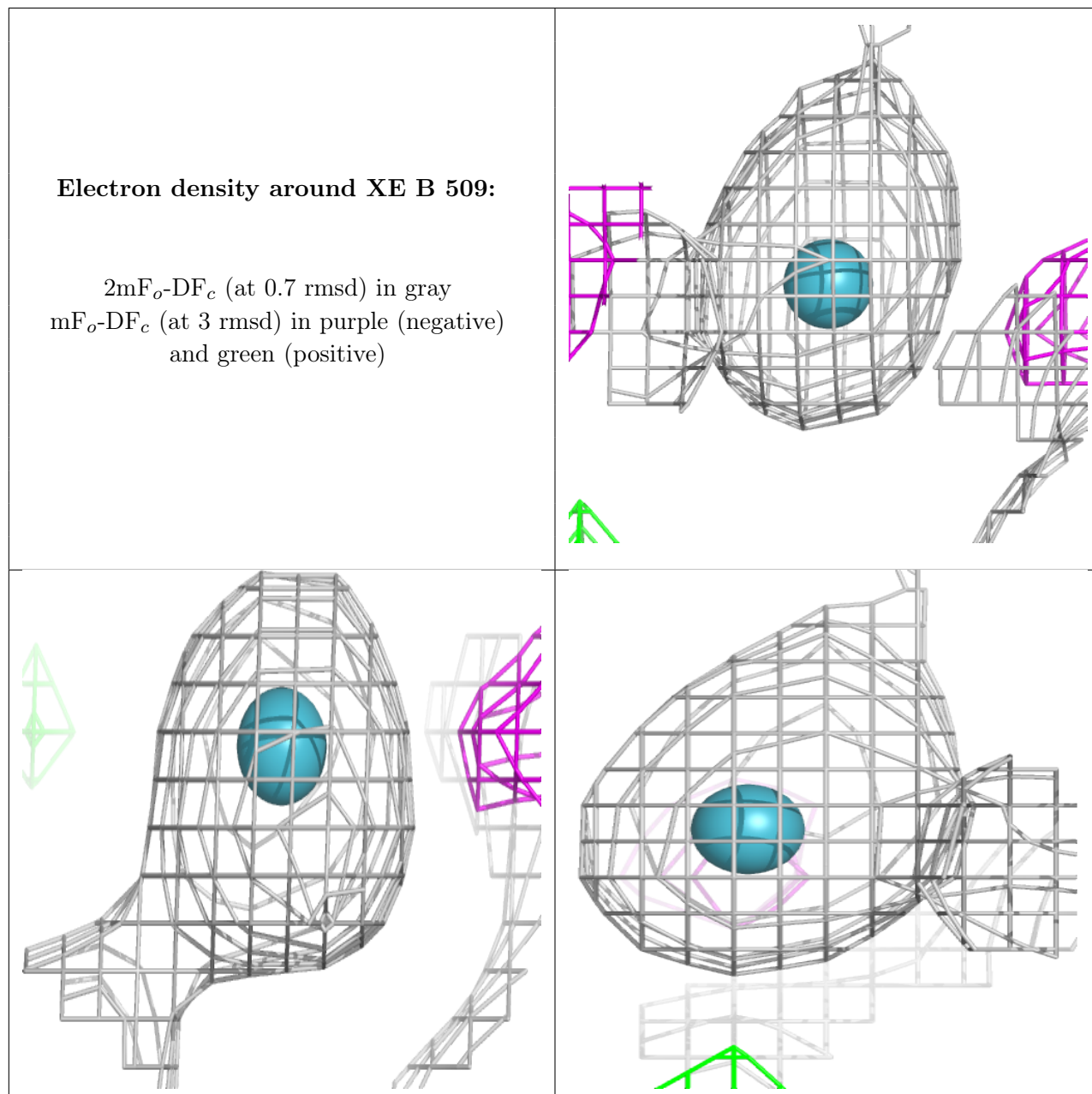
**Electron density around XE E 507:**

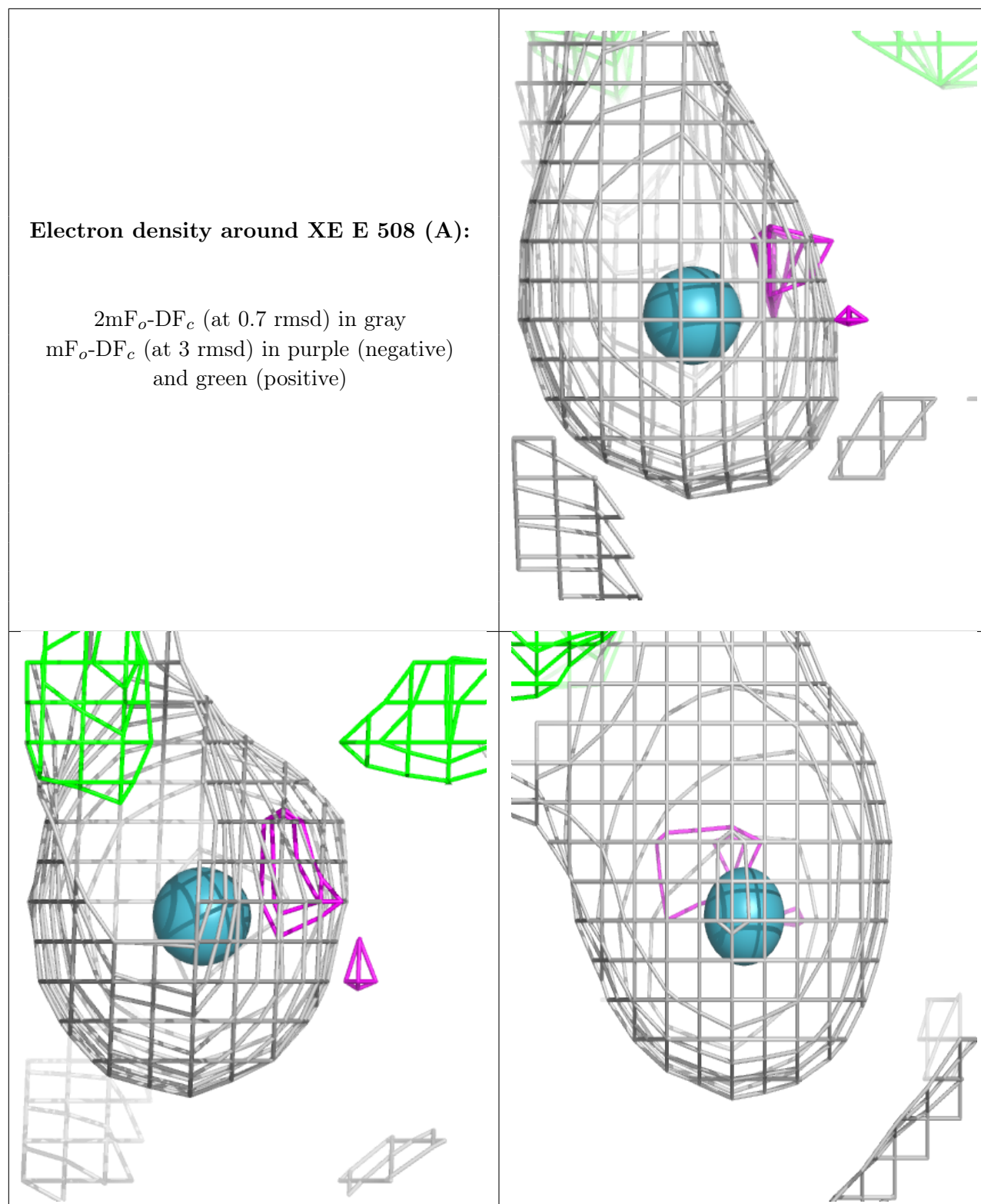
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around XE B 509:**

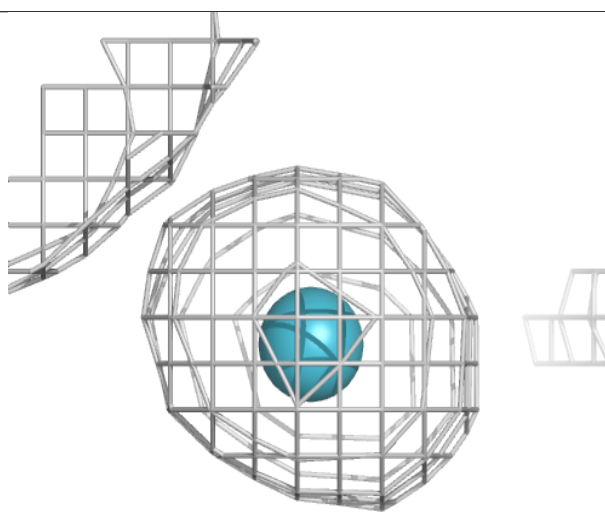
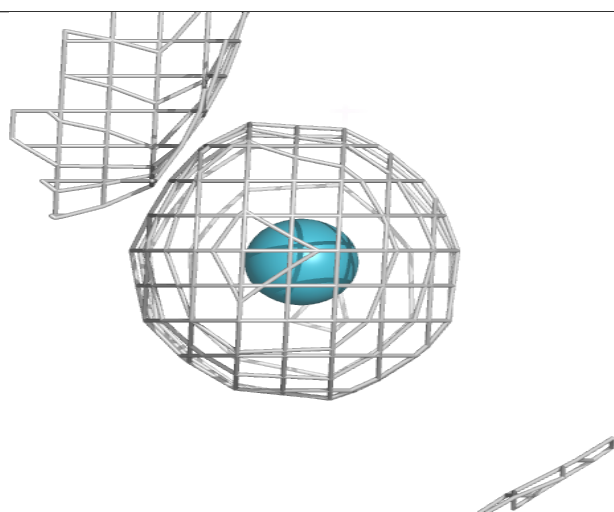
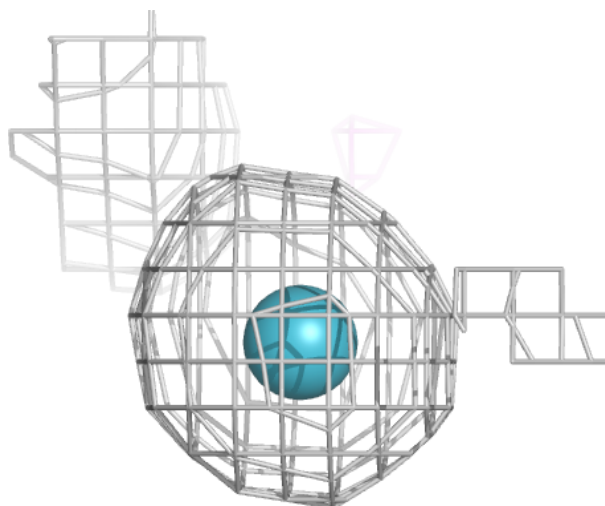
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





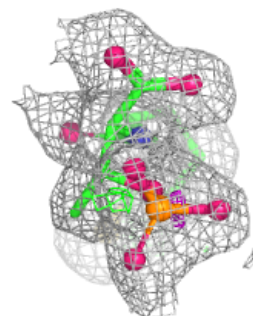
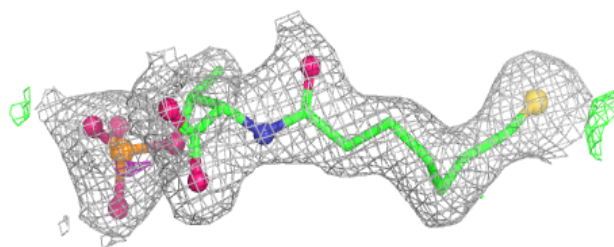
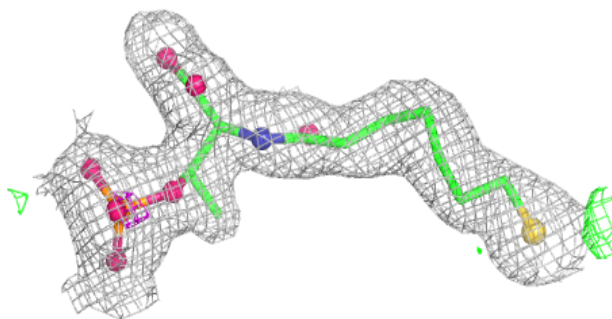
**Electron density around XE F 303:**

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



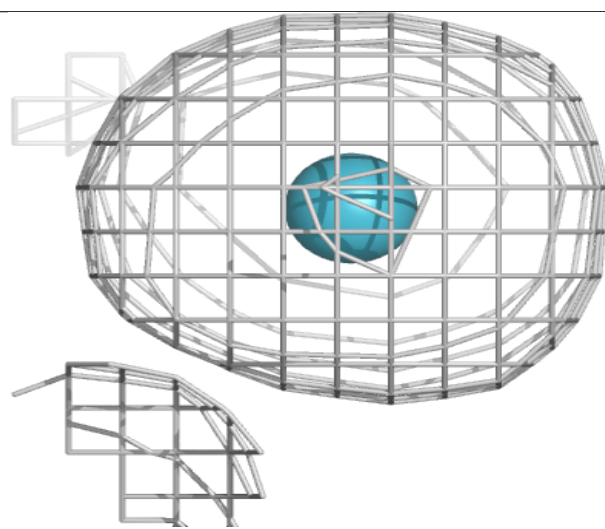
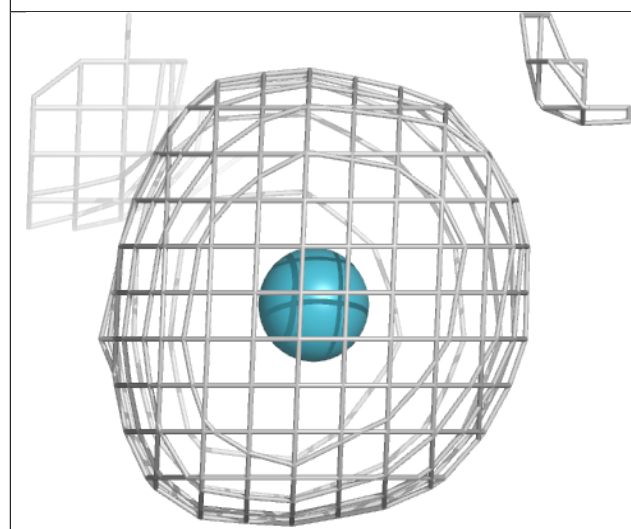
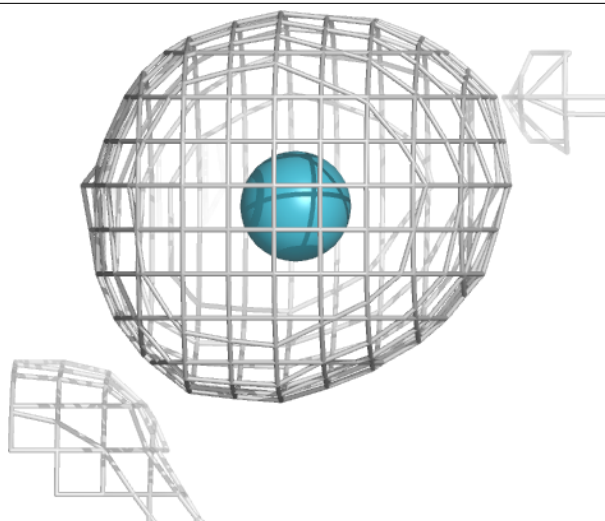
**Electron density around TP7 A 602:**

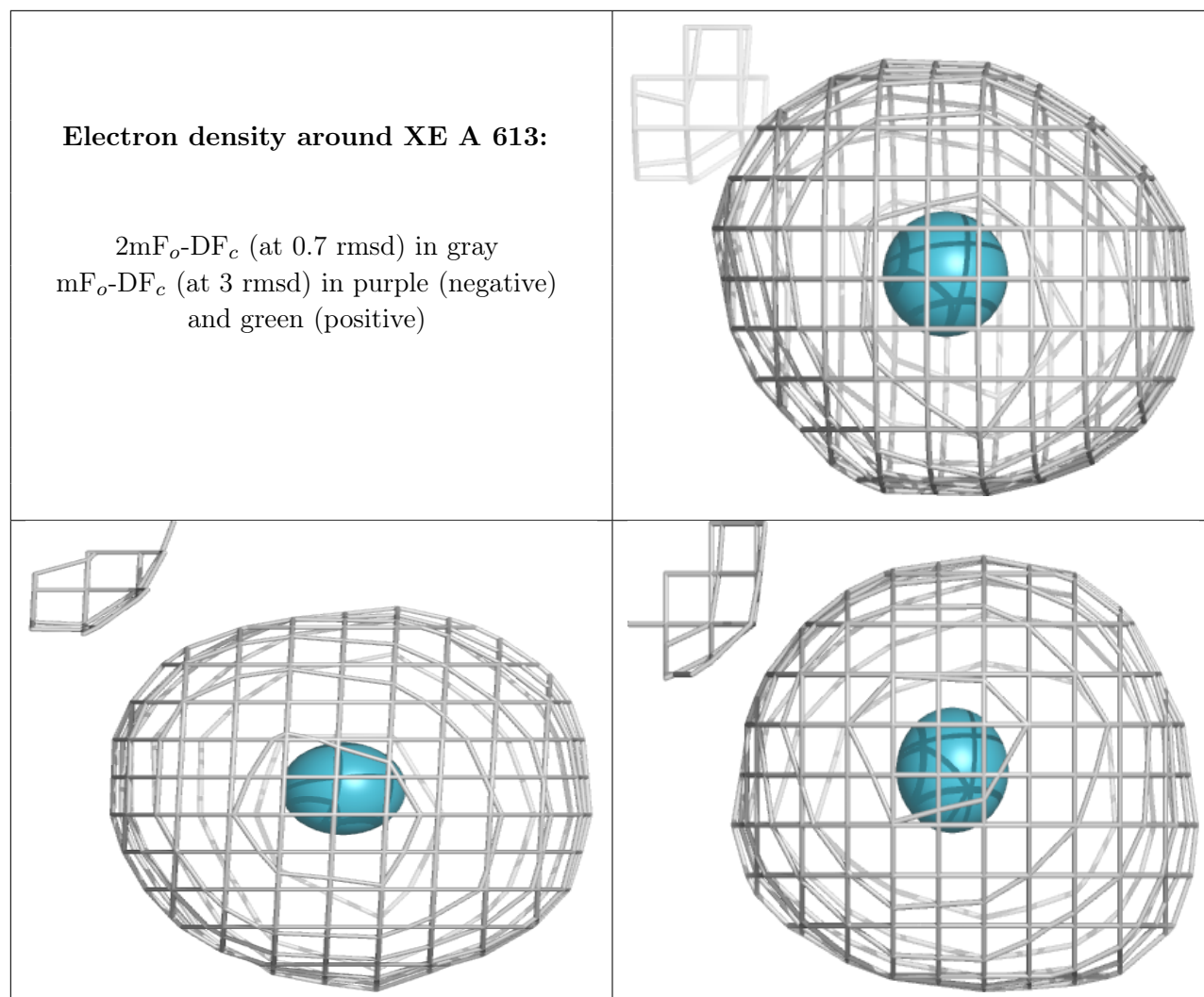
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around XE D 609:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.