



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 6, 2021 – 02:15 pm BST

PDB ID : 7B2H  
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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.22  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.22

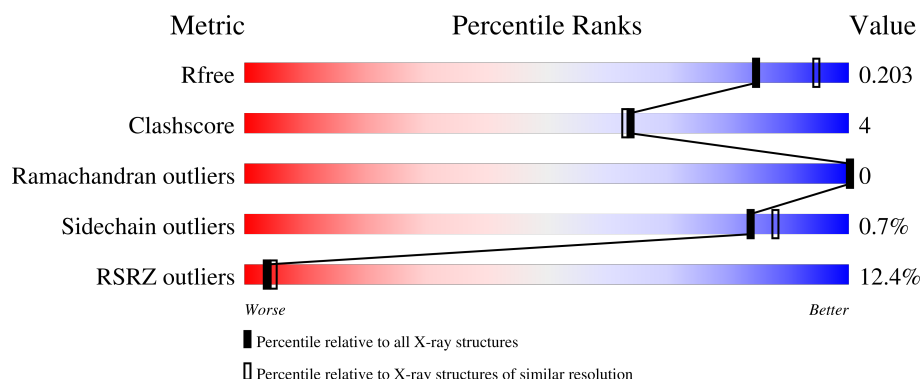
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (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	<div> <div>12%</div> <div>89%</div> <div>10%</div> </div>
1	D	550	<div> <div>7%</div> <div>90%</div> <div>9%</div> <div>..</div> </div>
2	B	443	<div> <div>10%</div> <div>91%</div> <div>8%</div> </div>
2	E	443	<div> <div>13%</div> <div>92%</div> <div>7%</div> </div>
3	C	249	<div> <div>20%</div> <div>94%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	249	

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
11	MG	A	611	-	-	-	X
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	-
7	PEG	B	503	-	-	-	X

## 2 Entry composition

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
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			

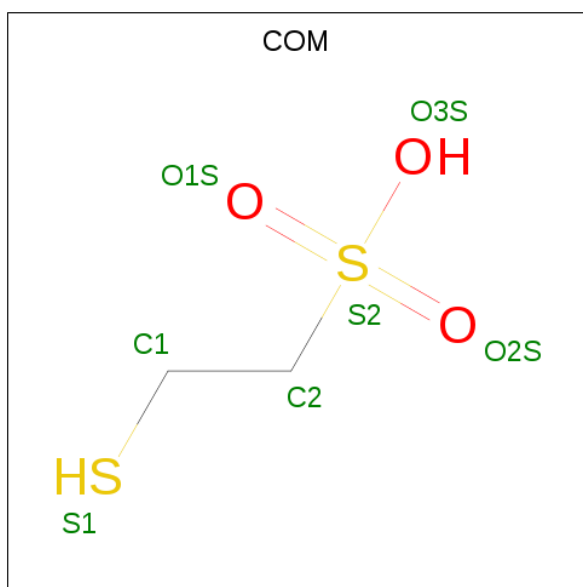
- Molecule 2 is a protein called Methyl-coenzyme M reductase I subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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.

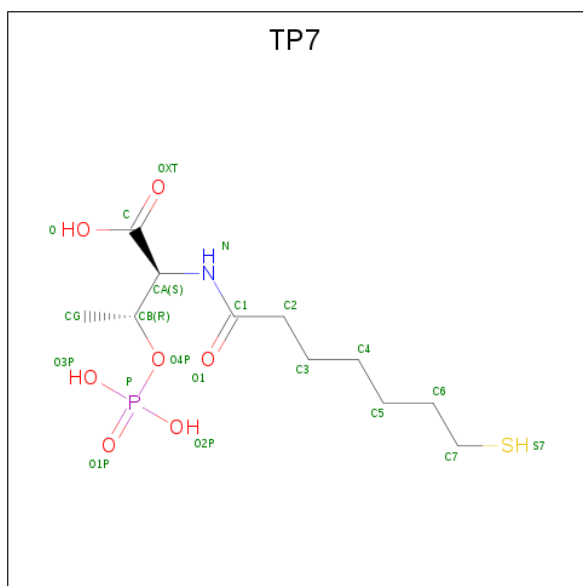
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	248	Total	C	N	O	S	0	2	0
			1983	1230	353	389	11			
3	F	239	Total	C	N	O	S	0	2	0
			1909	1188	344	367	10			

- Molecule 4 is 1-THIOETHANESULFONIC ACID (three-letter code: 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 (three-letter code: TP7) (formula:  $C_{11}H_{22}NO_7PS$ ).

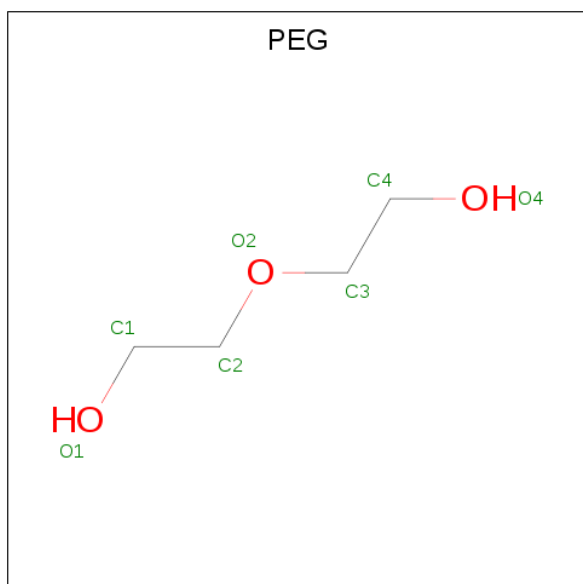


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
5	D	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		

- Molecule 6 is POTASSIUM ION (three-letter code: 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 (three-letter code: 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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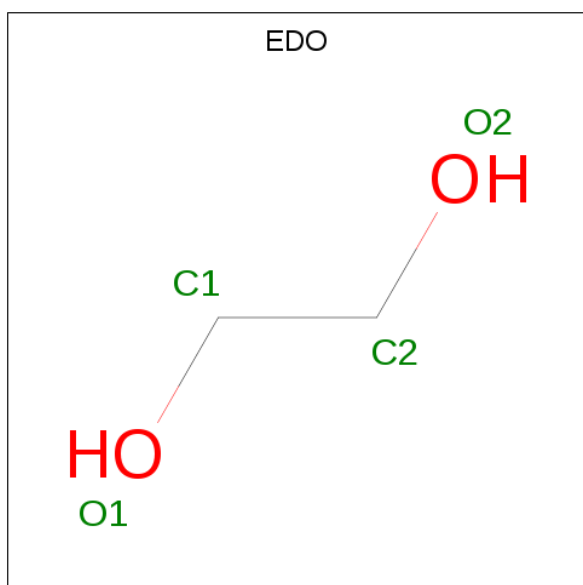
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			5	3	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



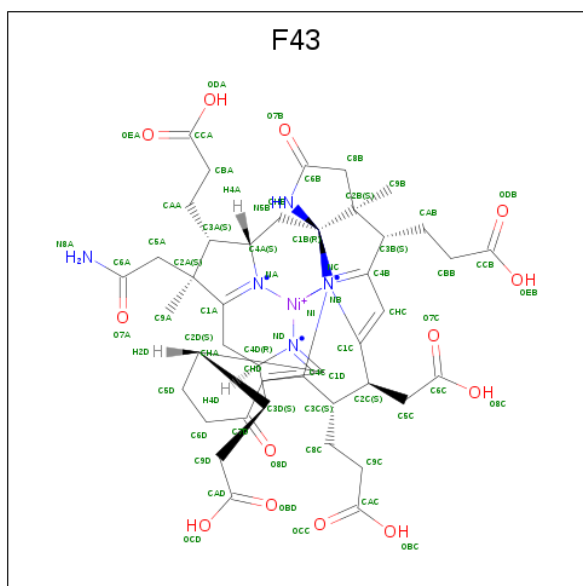
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 10 is FACTOR 430 (three-letter code: F43) (formula:  $C_{42}H_{51}N_6NiO_{13}$ ).



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

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

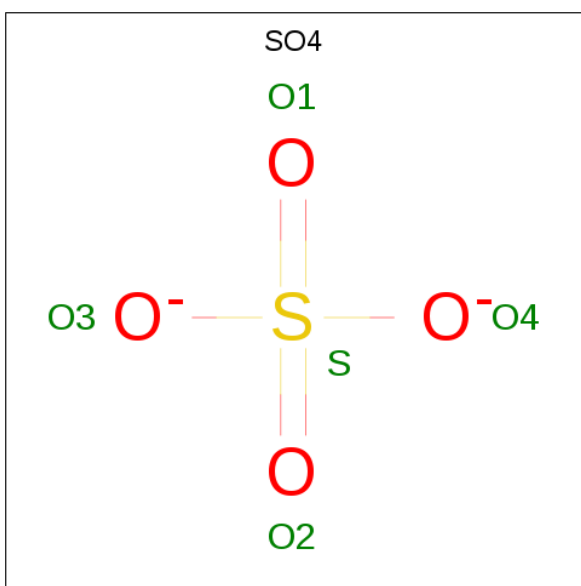
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	4	Total	Mg	0	0
			4	4		
11	B	4	Total	Mg	0	0
			4	4		
11	D	2	Total	Mg	0	0
			2	2		
11	E	4	Total	Mg	0	0
			4	4		
11	F	1	Total	Mg	0	0
			1	1		

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



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

- Molecule 13 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 14 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

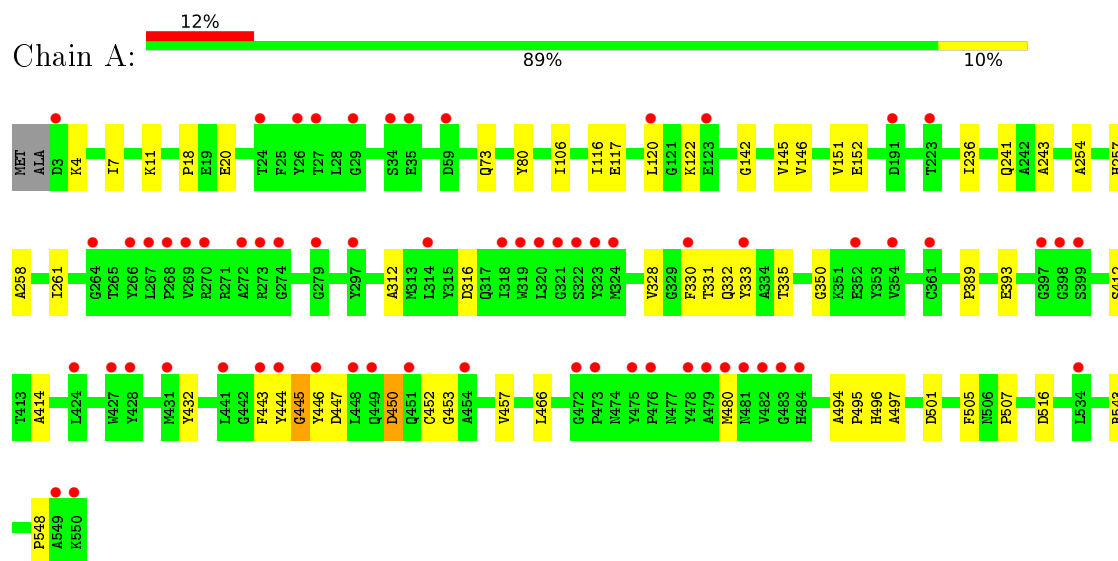
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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

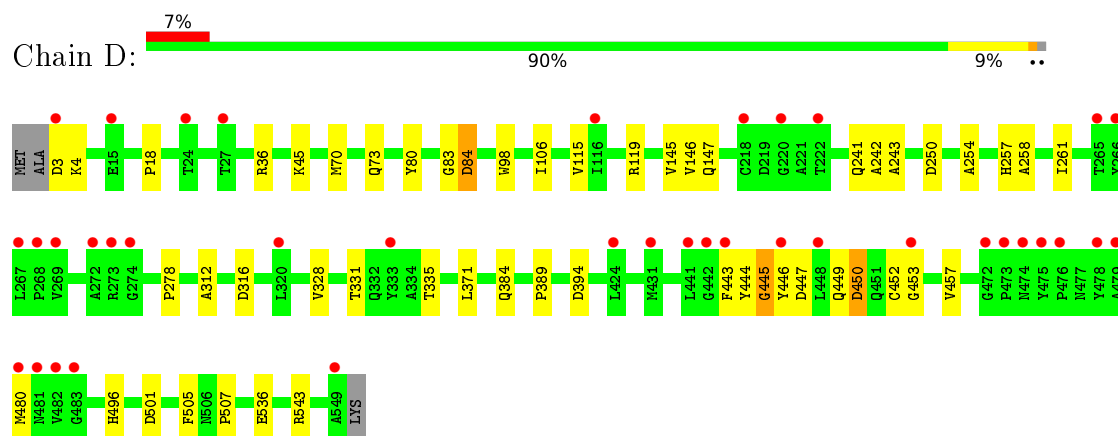
### 3 Residue-property plots [i](#)

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

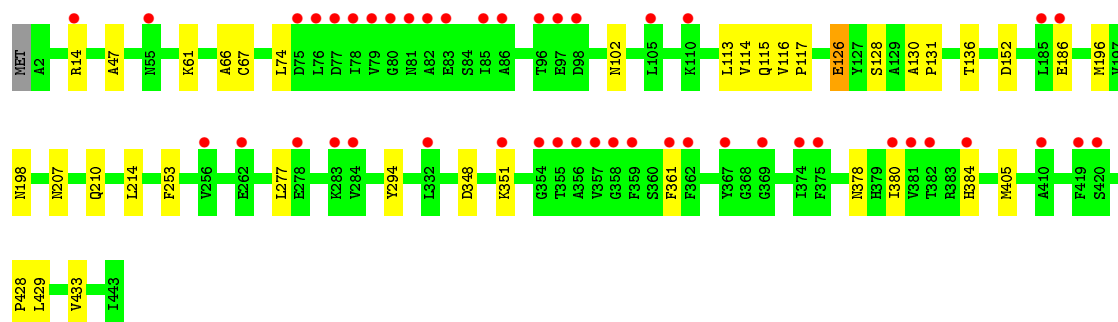


- Molecule 1: Methyl-coenzyme M reductase I subunit alpha

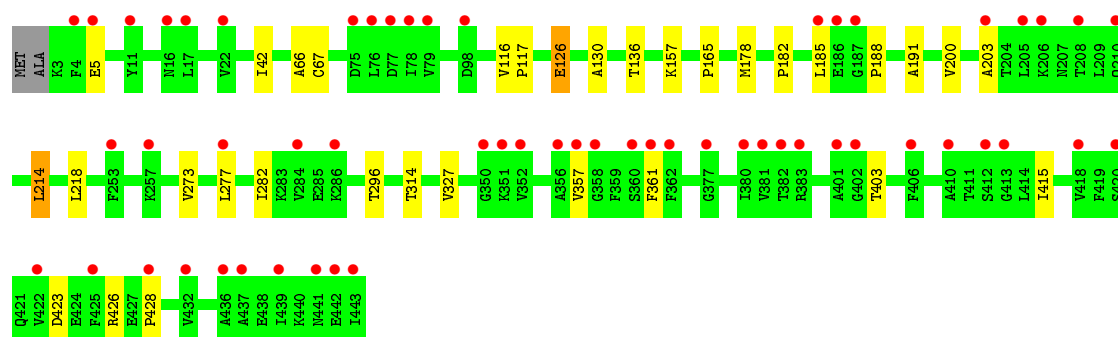
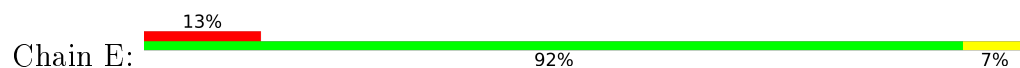


- Molecule 2: Methyl-coenzyme M reductase I subunit beta

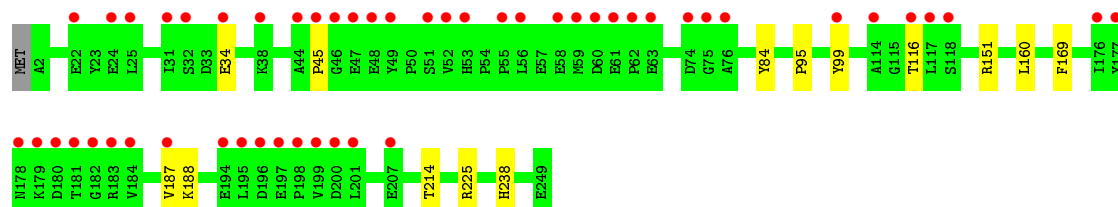




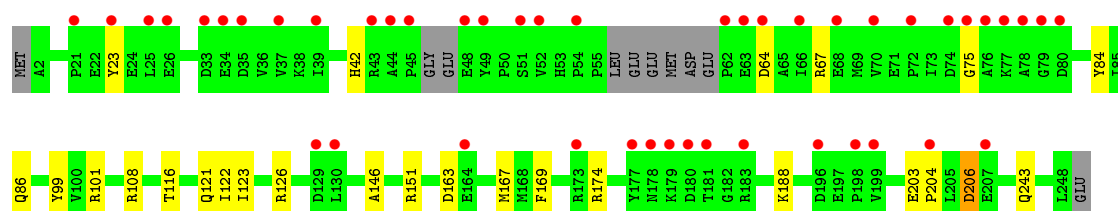
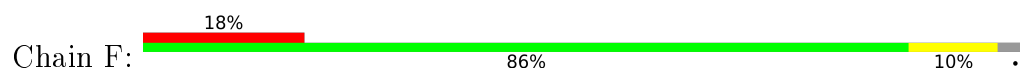
- Molecule 2: Methyl-coenzyme M reductase I subunit beta



- 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)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.177 , 0.204 0.176 , 0.203	Depositor DCC
$R_{free}$ test set	5810 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 60.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	20066	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage'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: GOL, PEG, GL3, MHS, TP7, MGN, K, AGM, EDO, XE, SMC, CL, MG, F43, COM, SO4, DYA

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	0.34	0/4322	0.49	0/5869
1	D	0.34	0/4309	0.50	0/5853
2	B	0.38	0/3365	0.53	0/4560
2	E	0.34	0/3347	0.51	0/4543
3	C	0.34	0/2026	0.52	0/2734
3	F	0.36	0/1949	0.53	0/2628
All	All	0.35	0/19318	0.51	0/26187

There are no bond length outliers.

There are no bond angle outliers.

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	40	0
1	D	4254	0	4062	34	0
2	B	3311	0	3297	37	0
2	E	3286	0	3239	32	0
3	C	1983	0	1900	9	0
3	F	1909	0	1841	16	0
4	A	7	0	6	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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	0	0
15	F	40	0	0	1	0
All	All	20066	0	18630	158	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 4.

The worst 5 of 158 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%)	434 (100%)	2 (0%)	88	92
1	D	434/434 (100%)	429 (99%)	5 (1%)	71	77
2	B	341/342 (100%)	340 (100%)	1 (0%)	92	95
2	E	337/342 (98%)	334 (99%)	3 (1%)	78	83
3	C	210/217 (97%)	210 (100%)	0	100	100
3	F	201/217 (93%)	199 (99%)	2 (1%)	76	81
All	All	1959/1986 (99%)	1946 (99%)	13 (1%)	84	88

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

Mol	Chain	Res	Type
1	D	543	ARG
2	E	126	GLU
3	F	206	ASP
2	E	403	THR
3	F	203	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	4,7,8	1.48	1 (25%)	1,8,10	4.86	1 (100%)
1	AGM	A	271	1	10,11,12	0.54	0	6,13,15	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	GL3	A	445	1	2,3,4	1.65	1 (50%)	1,2,4	0.89	0
1	MHS	D	257	1	7,11,12	0.76	0	6,14,16	1.37	1 (16%)
1	SMC	A	452	1	5,6,7	1.54	1 (20%)	2,6,8	3.10	1 (50%)
1	GL3	D	445	1	2,3,4	1.85	1 (50%)	1,2,4	1.01	0
1	MHS	A	257	1	7,11,12	0.74	0	6,14,16	1.46	1 (16%)
1	AGM	D	271	1	10,11,12	0.54	0	6,13,15	0.27	0
1	MGN	D	400	1	6,9,10	1.02	0	5,12,14	0.14	0
1	MGN	A	400	1	6,9,10	1.08	0	5,12,14	0.17	0
1	DYA	A	450	1	4,7,8	1.54	1 (25%)	1,8,10	4.97	1 (100%)
1	SMC	D	452	1	5,6,7	1.48	1 (20%)	2,6,8	3.09	1 (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	-	2/2/6/8	-
1	AGM	A	271	1	-	4/10/11/13	-
1	GL3	A	445	1	-	1/1/1/2	-
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1
1	SMC	A	452	1	-	1/3/5/7	-
1	GL3	D	445	1	-	1/1/1/2	-
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	MGN	A	400	1	-	0/7/9/12	-
1	DYA	A	450	1	-	2/2/6/8	-
1	SMC	D	452	1	-	1/3/5/7	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	452	SMC	CB-SG	-3.05	1.76	1.80
1	D	452	SMC	CB-SG	-2.92	1.76	1.80
1	D	445	GL3	C-S	-2.62	1.71	1.80
1	A	445	GL3	C-S	-2.33	1.72	1.80
1	D	450	DYA	CA-N	2.16	1.40	1.35

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	DYA	O-C-CA	-4.97	119.07	125.39
1	D	450	DYA	O-C-CA	-4.86	119.22	125.39
1	A	452	SMC	CS-SG-CB	4.37	109.33	101.30
1	D	452	SMC	CS-SG-CB	4.32	109.24	101.30
1	D	257	MHS	NE2-CE1-ND1	-2.31	108.82	112.26

There are no chirality outliers.

5 of 15 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.

4 monomers are involved in 5 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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
7	PEG	F	302	-	4,4,6	0.11	0	3,3,5	0.19	0
7	PEG	A	604	-	6,6,6	0.08	0	5,5,5	0.07	0
4	COM	D	602	-	6,6,6	0.38	0	7,8,8	1.08	1 (14%)
7	PEG	B	502	-	3,3,6	0.13	0	2,2,5	0.18	0
9	EDO	A	607	-	3,3,3	0.35	0	2,2,2	0.43	0
10	F43	A	608	1	46,71,71	2.28	6 (13%)	48,118,118	1.34	5 (10%)
7	PEG	D	607	-	6,6,6	0.10	0	5,5,5	0.01	0
7	PEG	D	605	-	6,6,6	0.08	0	5,5,5	0.04	0
13	SO4	A	614	-	4,4,4	0.14	0	6,6,6	0.05	0
7	PEG	B	503	-	4,4,6	0.20	0	3,3,5	0.20	0
4	COM	A	601	-	6,6,6	0.25	0	7,8,8	1.02	1 (14%)
8	GOL	A	606	-	5,5,5	0.13	0	5,5,5	0.22	0
7	PEG	D	606	-	6,6,6	0.08	0	5,5,5	0.06	0
10	F43	D	601	1	46,71,71	2.30	7 (15%)	48,118,118	1.31	5 (10%)
7	PEG	A	605	-	4,4,6	0.23	0	3,3,5	0.23	0
5	TP7	D	603	-	16,20,20	0.54	0	18,26,26	0.89	0
7	PEG	E	502	-	6,6,6	0.09	0	5,5,5	0.06	0
5	TP7	A	602	-	16,20,20	0.55	0	18,26,26	0.86	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
7	PEG	F	302	-	-	1/2/2/4	-
7	PEG	A	604	-	-	3/4/4/4	-
4	COM	D	602	-	-	3/4/4/4	-
7	PEG	B	502	-	-	0/1/1/4	-
9	EDO	A	607	-	-	1/1/1/1	-
10	F43	A	608	1	-	2/18/185/185	-
7	PEG	D	607	-	-	1/4/4/4	-
7	PEG	D	605	-	-	1/4/4/4	-
7	PEG	B	503	-	-	1/2/2/4	-
4	COM	A	601	-	-	3/4/4/4	-
8	GOL	A	606	-	-	3/4/4/4	-
7	PEG	D	606	-	-	3/4/4/4	-
10	F43	D	601	1	-	2/18/185/185	-
7	PEG	A	605	-	-	0/2/2/4	-
5	TP7	D	603	-	-	1/20/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PEG	E	502	-	-	0/4/4/4	-
5	TP7	A	602	-	-	2/20/24/24	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	608	F43	NI-NA	7.56	2.05	1.89
10	D	601	F43	NI-NA	7.44	2.05	1.89
10	A	608	F43	CHD-C1D	-7.16	1.34	1.43
10	D	601	F43	CHD-C1D	-7.07	1.34	1.43
10	D	601	F43	NI-NB	6.92	2.04	1.89

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	608	F43	CAB-C3B-C2B	-4.35	109.88	119.09
10	D	601	F43	CAB-C3B-C2B	-3.81	111.02	119.09
10	D	601	F43	O7B-C6B-C8B	-3.40	122.44	126.59
10	A	608	F43	O7B-C6B-C8B	-3.04	122.88	126.59
10	D	601	F43	C4D-ND-C1D	2.85	112.27	108.51

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	COM	C1-C2-S2-O1S
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 23 short contacts:

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

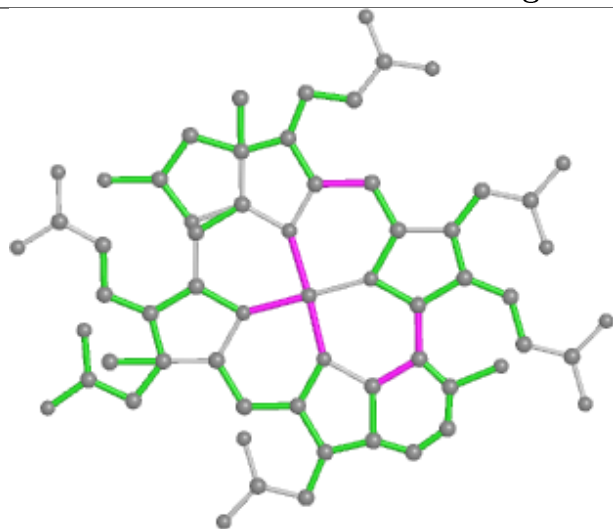
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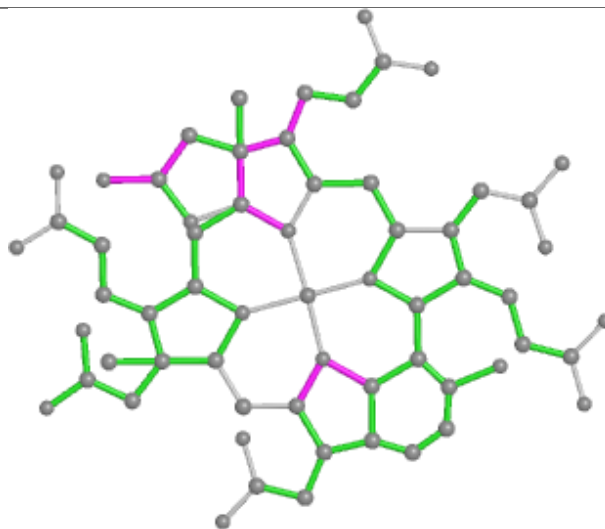
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	601	F43	5	0
5	D	603	TP7	1	0
5	A	602	TP7	1	0

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

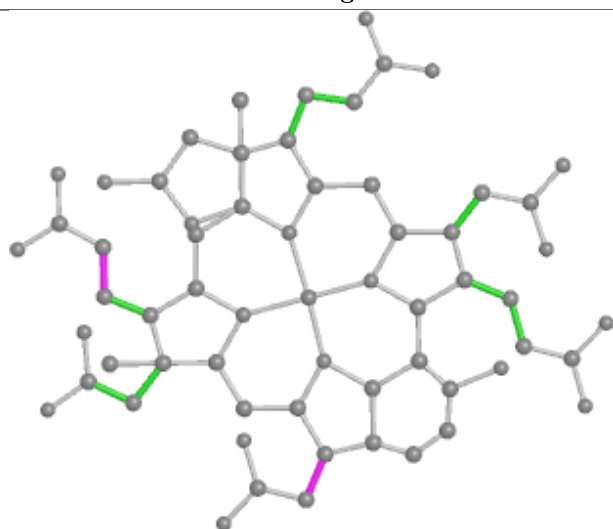
## Ligand F43 A 608



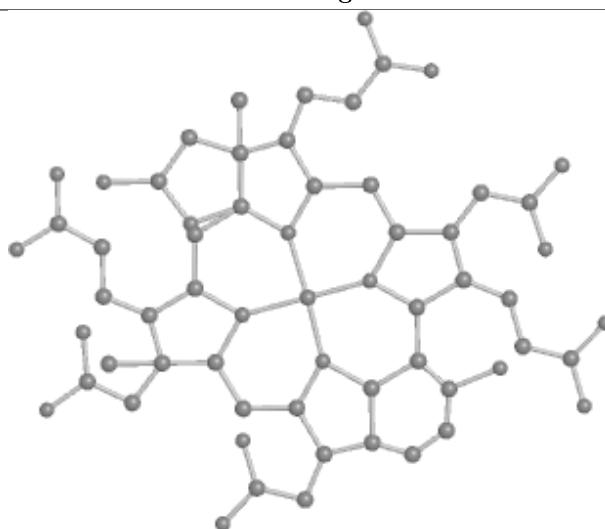
Bond lengths



Bond angles

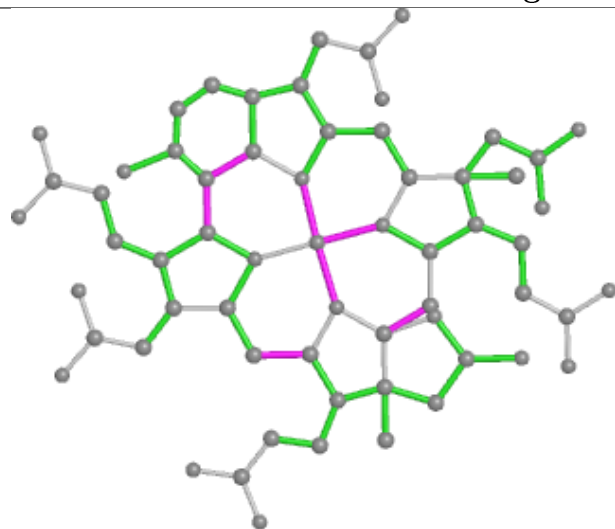


Torsions

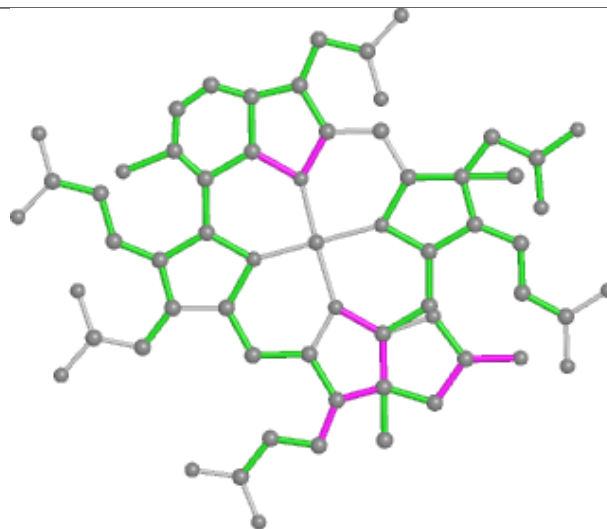


Rings

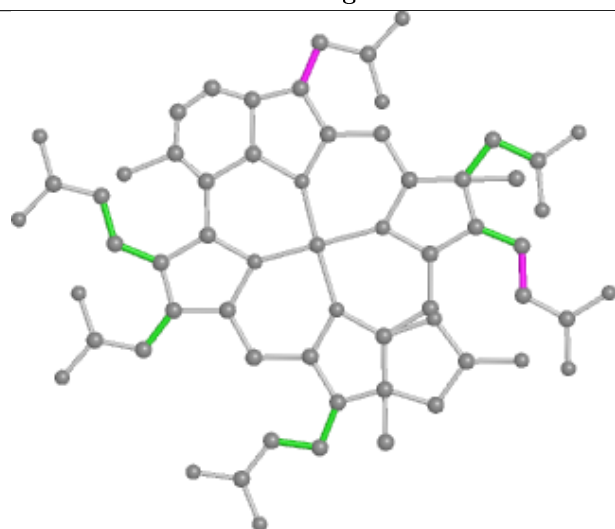
## Ligand F43 D 601



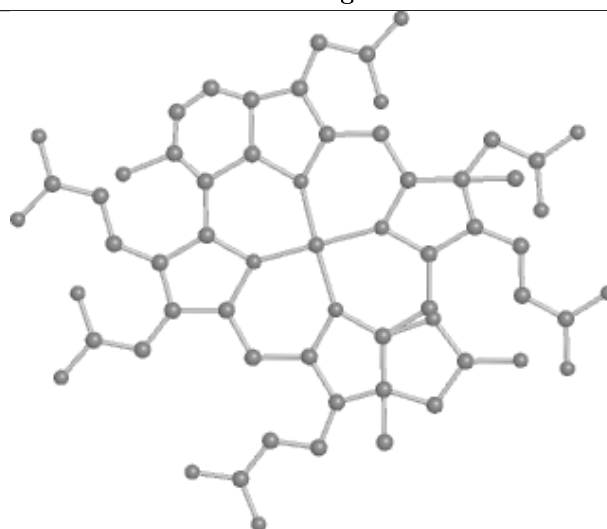
Bond lengths



Bond angles

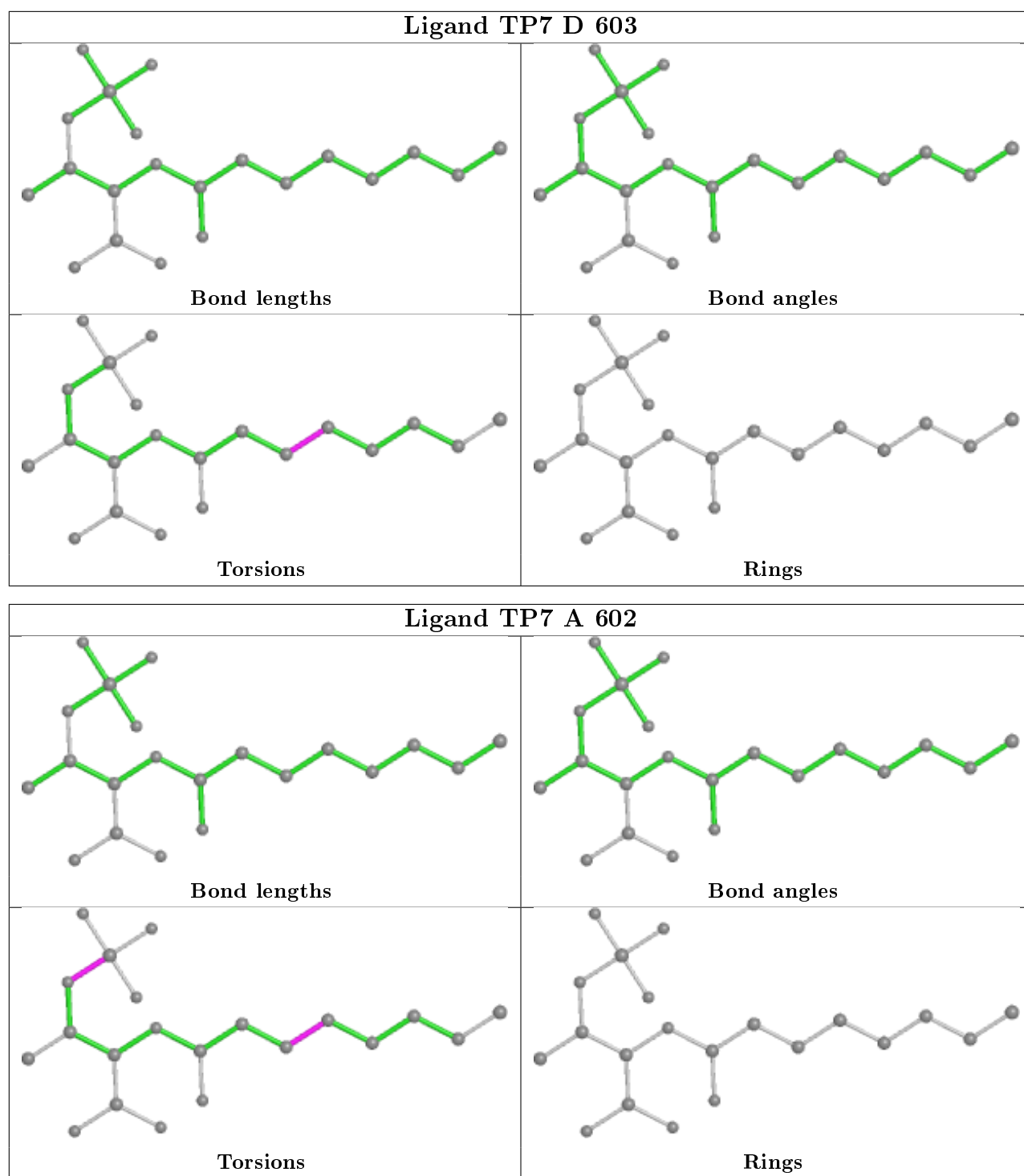


Torsions



Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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%)	0.55	65 (11%) 4 5	26, 42, 68, 122	1 (0%)
1	D	541/550 (98%)	0.34	38 (7%) 16 20	24, 39, 63, 97	0
2	B	442/443 (99%)	0.58	46 (10%) 6 8	28, 48, 73, 127	1 (0%)
2	E	441/443 (99%)	0.78	57 (12%) 3 4	27, 51, 84, 118	1 (0%)
3	C	248/249 (99%)	1.00	51 (20%) 1 1	38, 58, 88, 124	0
3	F	239/249 (95%)	1.06	46 (19%) 1 1	38, 65, 93, 138	0
All	All	2453/2484 (98%)	0.65	303 (12%) 4 5	24, 48, 80, 138	3 (0%)

The worst 5 of 303 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	402	GLY	6.7
3	C	44	ALA	5.7
1	A	267[A]	LEU	5.5
3	F	164	GLU	5.4
3	C	201	LEU	5.2

### 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	0.84	0.21	50,52,53,55	0
1	GL3	A	445	4/5	0.91	0.34	34,36,36,37	0
1	GL3	D	445	4/5	0.92	0.25	32,33,33,34	0
1	MHS	D	257	11/12	0.93	0.20	39,41,44,45	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	0.29	32,35,36,37	0
1	SMC	A	452	7/8	0.94	0.25	38,38,40,41	0
1	DYA	A	450	8/9	0.95	0.26	33,35,40,41	0
1	AGM	A	271	12/13	0.96	0.28	29,31,33,36	0
1	MGN	D	400	10/11	0.96	0.18	33,36,38,41	0
1	MGN	A	400	10/11	0.96	0.15	36,38,40,40	0
1	DYA	D	450	8/9	0.96	0.15	31,34,34,35	0
1	SMC	D	452	7/8	0.97	0.26	35,38,39,40	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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	B	501	1/1	0.55	0.13	80,80,80,80	0
11	MG	D	608	1/1	0.62	0.15	64,64,64,64	0
11	MG	E	505	1/1	0.67	0.09	89,89,89,89	0
7	PEG	B	503	5/7	0.68	0.41	55,56,57,57	5
11	MG	E	503	1/1	0.70	0.31	87,87,87,87	0
11	MG	B	504	1/1	0.70	0.10	76,76,76,76	0
11	MG	A	609	1/1	0.73	0.11	72,72,72,72	0
11	MG	A	610	1/1	0.73	0.18	99,99,99,99	0
11	MG	D	604	1/1	0.73	0.10	69,69,69,69	0
11	MG	B	506	1/1	0.74	0.19	86,86,86,86	0
11	MG	A	611	1/1	0.77	0.99	80,80,80,80	0
9	EDO	A	607	4/4	0.77	0.17	73,73,75,76	0
11	MG	B	505	1/1	0.78	0.23	103,103,103,103	0
7	PEG	A	605	5/7	0.78	0.18	80,80,81,82	0
7	PEG	B	502	4/7	0.81	0.16	51,52,52,54	0
12	XE	B	508	1/1	0.81	0.11	68,68,68,68	1
7	PEG	A	604	7/7	0.83	0.19	52,53,54,55	0
7	PEG	D	606	7/7	0.84	0.15	74,74,75,76	0
12	XE	B	511	1/1	0.84	0.24	47,47,47,47	1
11	MG	F	301	1/1	0.85	0.07	89,89,89,89	0

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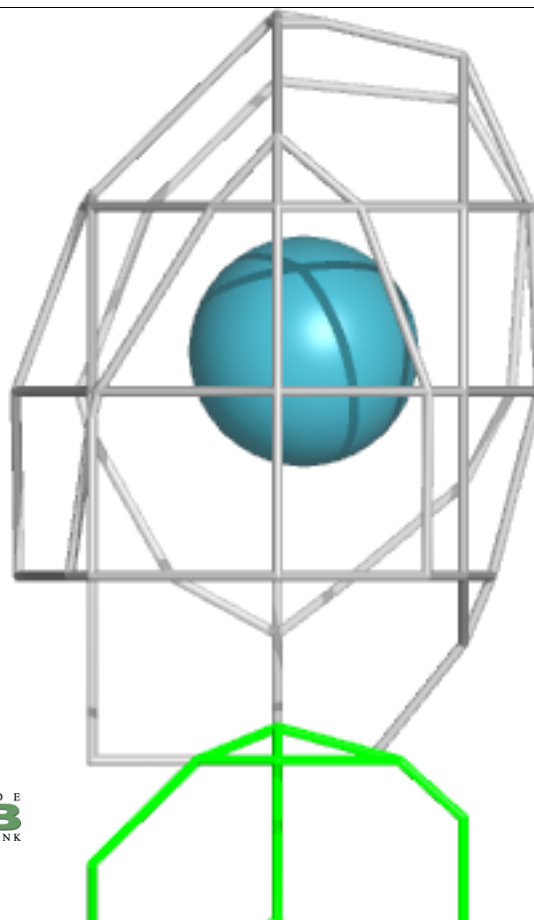
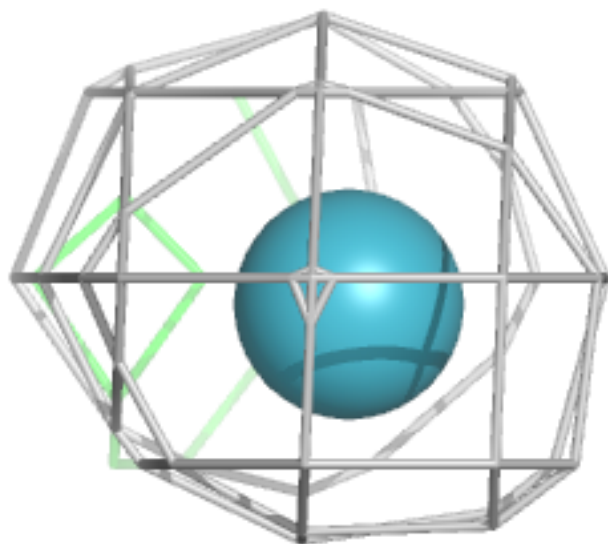
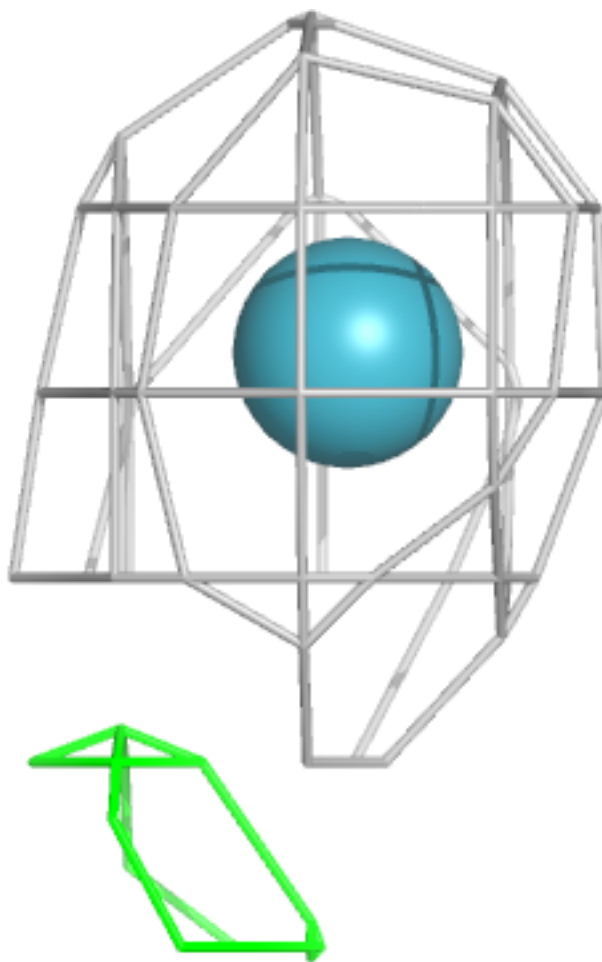
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	K	A	615	1/1	0.87	0.23	70,70,70,70	0
4	COM	D	602	7/7	0.87	0.21	54,57,62,62	0
7	PEG	E	502	7/7	0.87	0.11	88,89,92,92	0
8	GOL	A	606	6/6	0.88	0.14	86,86,87,87	0
7	PEG	D	605	7/7	0.89	0.16	70,72,74,74	0
7	PEG	F	302	5/7	0.89	0.52	50,50,52,52	5
6	K	D	610	1/1	0.89	0.09	82,82,82,82	0
12	XE	E	506[B]	1/1	0.90	0.20	62,62,62,62	1
13	SO4	A	614	5/5	0.90	0.14	128,128,129,130	0
4	COM	A	601	7/7	0.91	0.19	49,52,54,55	0
11	MG	A	612	1/1	0.91	0.31	97,97,97,97	0
7	PEG	D	607	7/7	0.91	0.23	48,49,50,52	7
11	MG	E	501	1/1	0.92	0.07	51,51,51,51	0
11	MG	E	504	1/1	0.92	0.12	103,103,103,103	0
14	CL	B	512	1/1	0.92	0.08	64,64,64,64	0
5	TP7	D	603	21/21	0.93	0.23	33,39,44,46	0
12	XE	B	510	1/1	0.94	0.07	100,100,100,100	1
12	XE	E	507	1/1	0.94	0.10	46,46,46,46	1
10	F43	A	608	62/62	0.95	0.16	35,38,43,45	0
10	F43	D	601	62/62	0.95	0.14	32,40,45,48	0
6	K	B	513	1/1	0.95	0.21	77,77,77,77	0
14	CL	E	510	1/1	0.95	0.08	65,65,65,65	0
12	XE	E	509	1/1	0.96	0.11	50,50,50,50	1
5	TP7	A	602	21/21	0.96	0.25	28,33,36,37	0
12	XE	B	509	1/1	0.96	0.09	71,71,71,71	1
12	XE	E	508[A]	1/1	0.96	0.04	65,65,65,65	1
12	XE	F	303	1/1	0.99	0.09	78,78,78,78	1
12	XE	B	507	1/1	0.99	0.06	71,71,71,71	1
12	XE	D	609	1/1	0.99	0.06	62,62,62,62	1
6	K	A	603	1/1	0.99	0.08	47,47,47,47	0
12	XE	A	613	1/1	1.00	0.05	64,64,64,64	1

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.

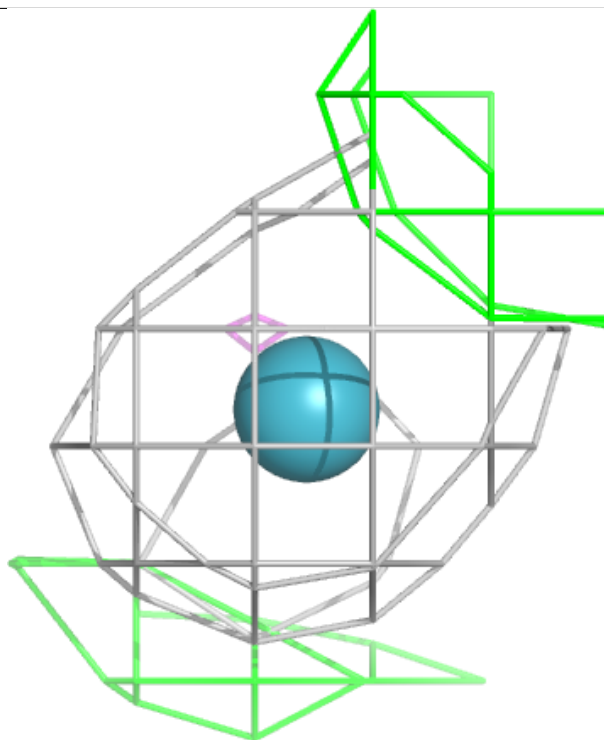
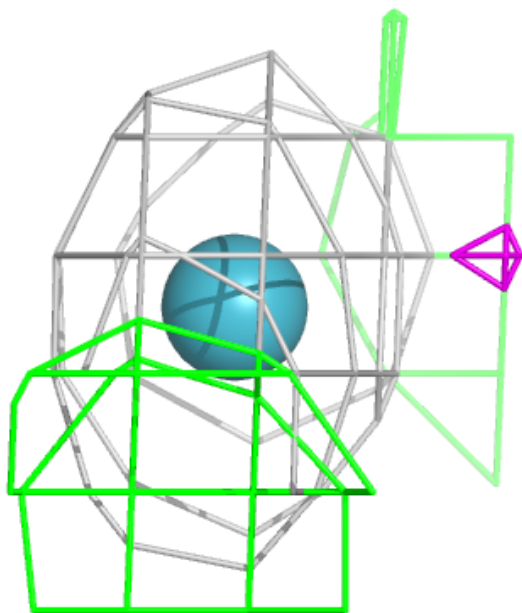
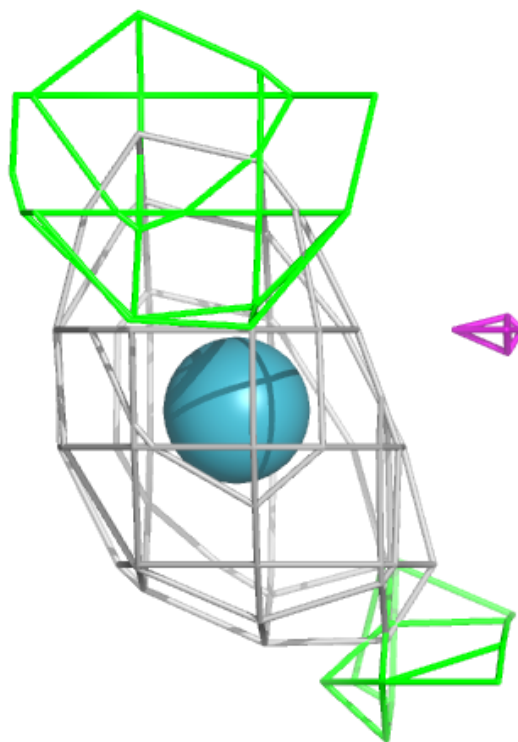
**Electron density around XE B 508:**

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



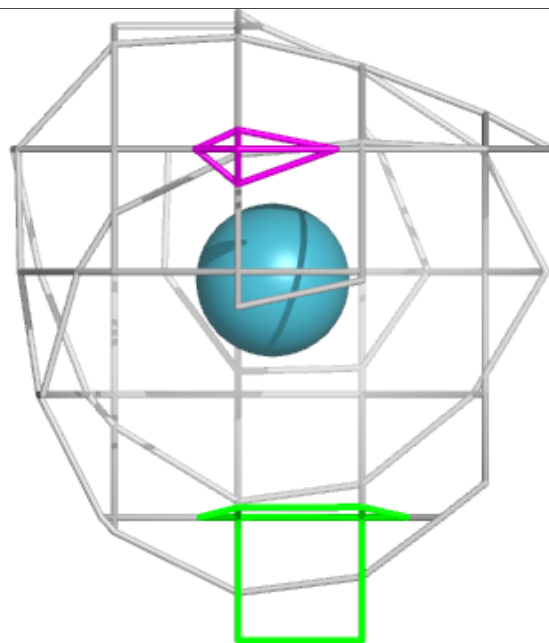
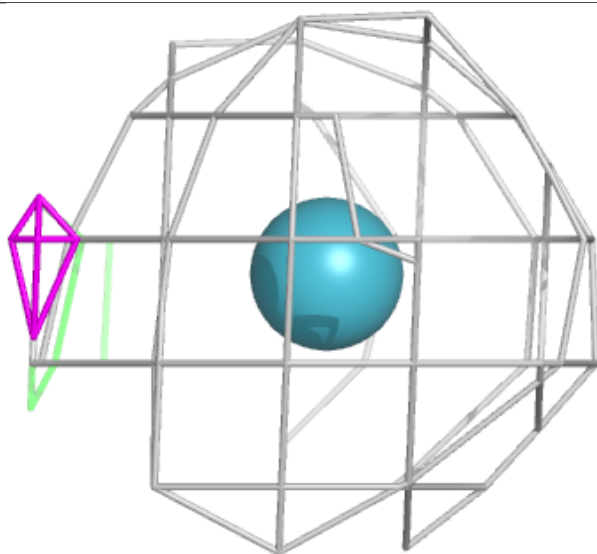
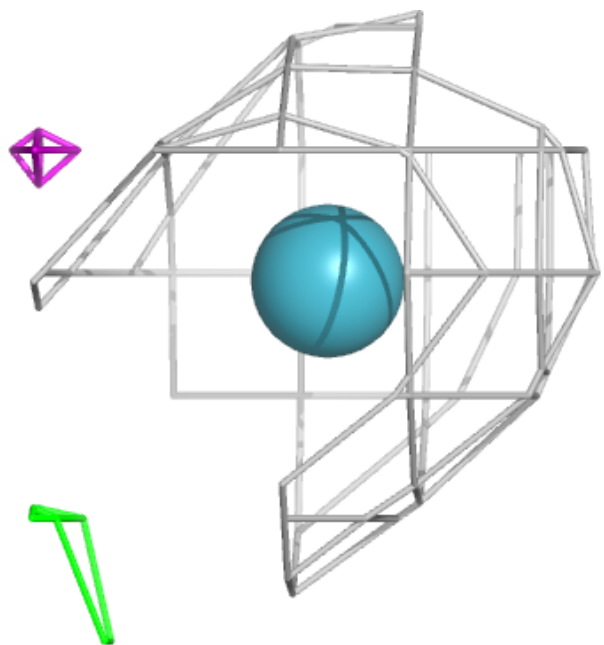
**Electron density around XE B 511:**

$2mF_o-DF_c$  (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:**

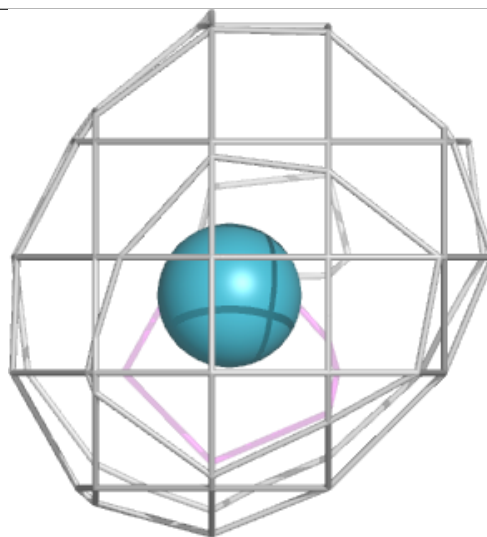
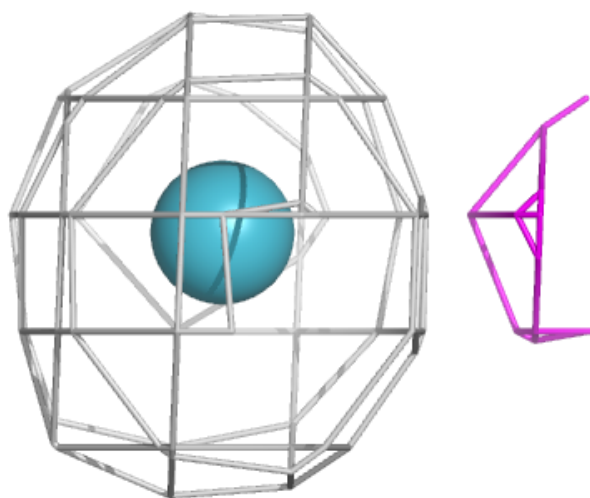
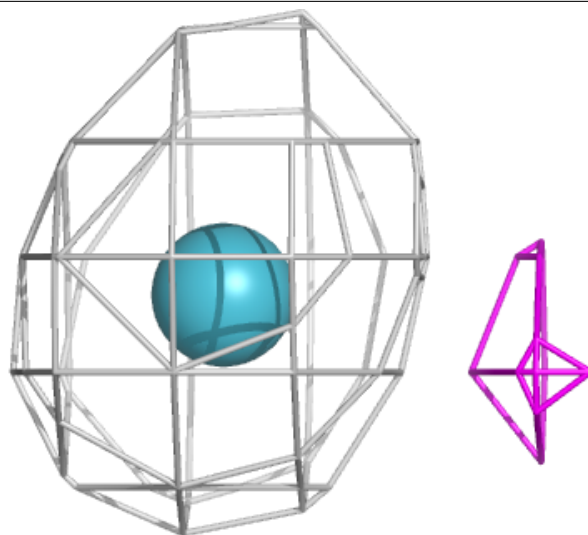
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





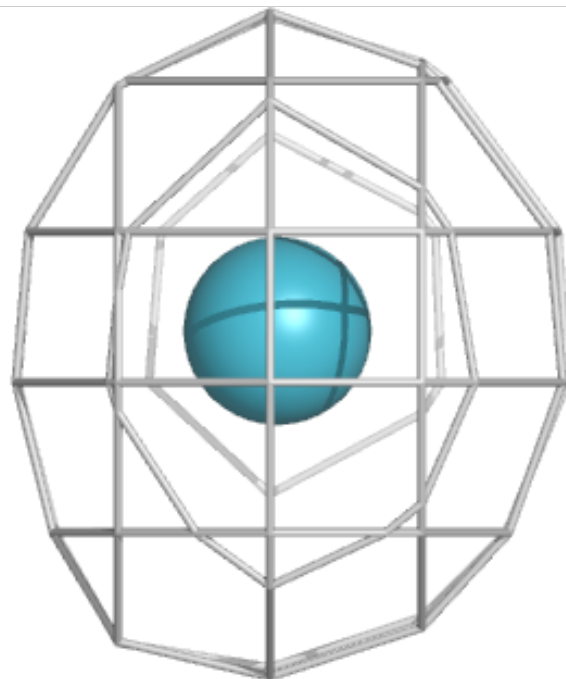
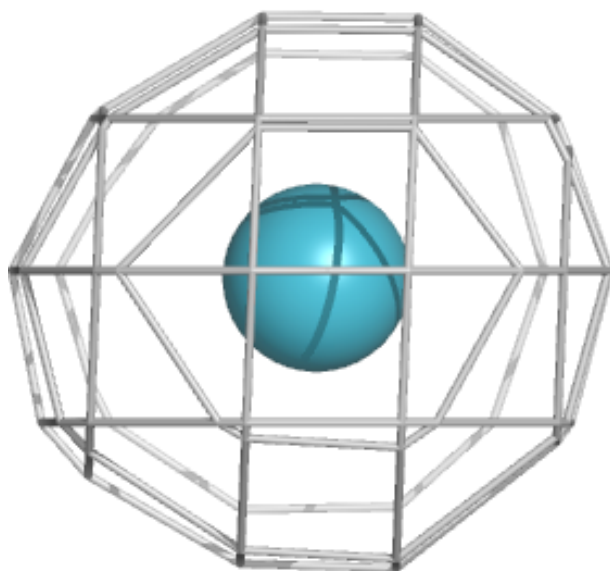
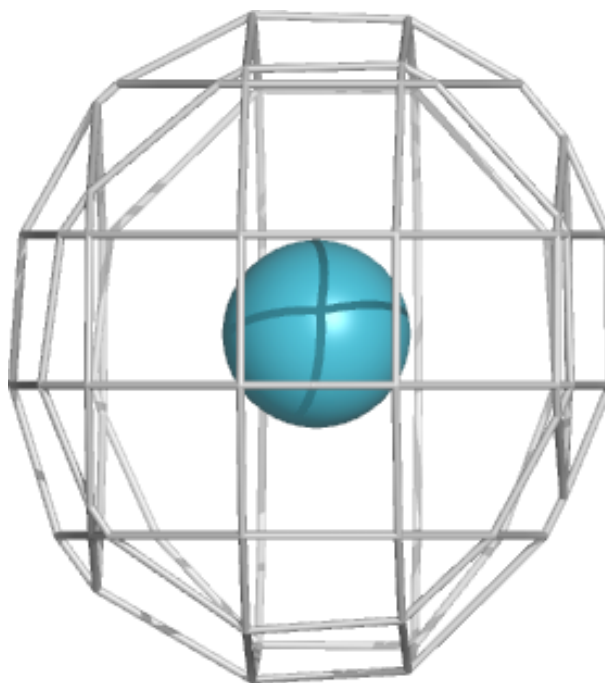
**Electron density around XE B 509:**

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



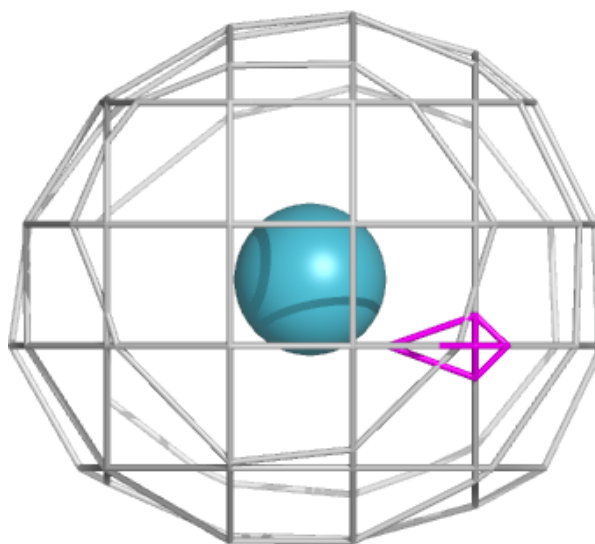
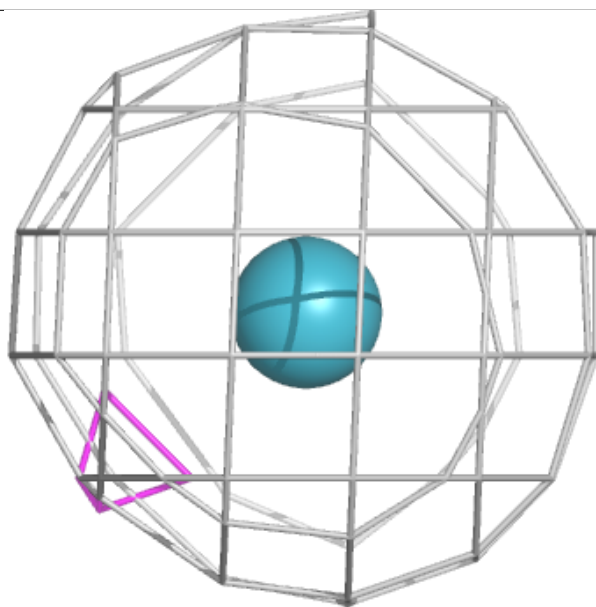
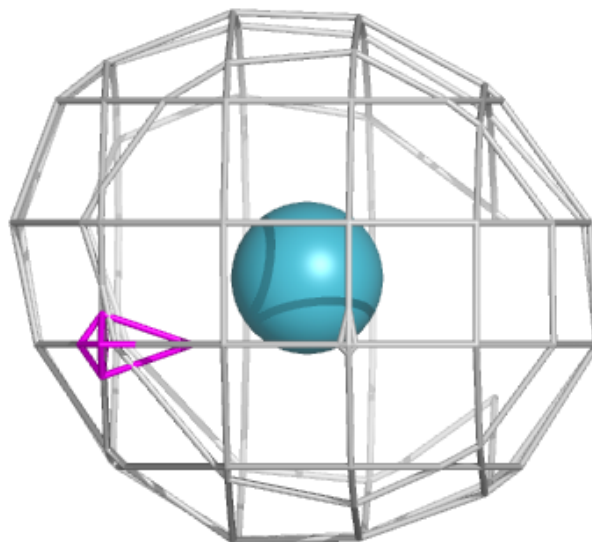
**Electron density around XE B 507:**

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



**Electron density around XE A 613:**

$2mF_o-DF_c$  (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.