



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 22, 2025 – 06:18 PM EDT

PDB ID : 3SQG  
Title : Crystal structure of a methyl-coenzyme M reductase purified from Black Sea mats  
Authors : Shima, S.; Krueger, M.; Weinert, T.; Demmer, U.; Thauer, R.K.; Ermler, U.  
Deposited on : 2011-07-05  
Resolution : 2.10 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	<b>FAILED</b>
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

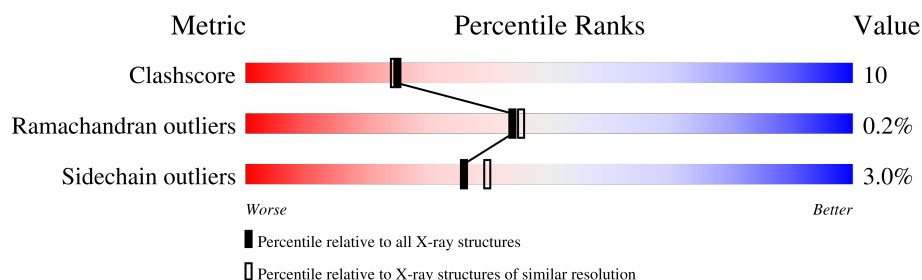
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)


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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	579	83% 15% .
1	D	579	83% 16% .
1	G	579	86% 12% .
2	B	433	81% 18% .
2	E	433	77% 22% .
2	H	433	80% 18% .
3	C	279	88% 11% .
3	F	279	80% 19% .

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Mol	Chain	Length	Quality of chain
3	I	279	 <div>85% 14%</div>

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
1	GL3	A	464	-	-	X	-
10	CL	A	586	-	-	X	-
12	P6G	B	434	-	-	X	-
5	COM	A	1003	-	X	X	-
6	M43	D	1001	X	-	-	-
6	M43	G	1001	X	-	-	-
7	1PE	D	580	-	-	X	-
7	1PE	G	580	-	-	X	-

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 32144 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, alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4467	2814	761	855	37			
1	D	578	Total	C	N	O	S	0	1	0
			4475	2819	764	855	37			
1	G	578	Total	C	N	O	S	0	0	0
			4467	2814	761	855	37			

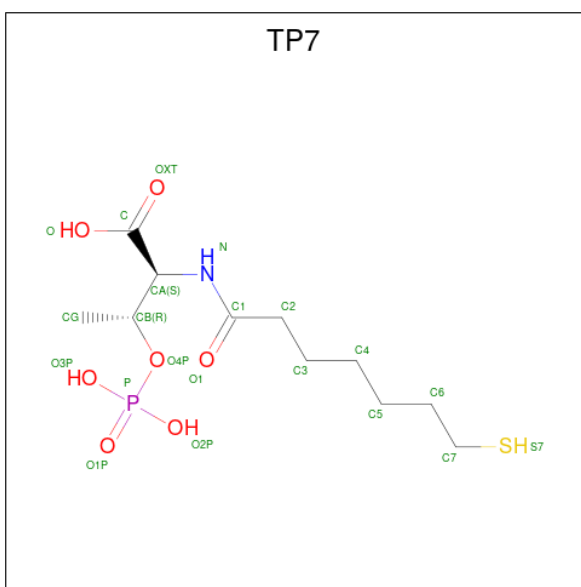
- Molecule 2 is a protein called Methyl-coenzyme M reductase, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	431	Total	C	N	O	S	0	0	0
			3197	2013	552	600	32			
2	E	431	Total	C	N	O	S	0	0	0
			3197	2013	552	600	32			
2	H	431	Total	C	N	O	S	0	1	0
			3205	2018	555	600	32			

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

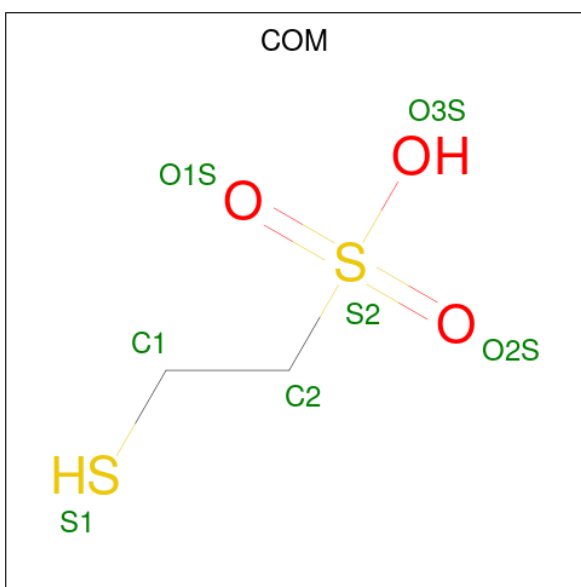
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	278	Total	C	N	O	S	0	0	0
			2205	1379	400	414	12			
3	F	278	Total	C	N	O	S	0	1	0
			2210	1382	401	415	12			
3	I	278	Total	C	N	O	S	0	0	0
			2205	1379	400	414	12			

- Molecule 4 is Coenzyme B (three-letter code: TP7) (formula: C<sub>11</sub>H<sub>22</sub>NO<sub>7</sub>PS).



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

- Molecule 5 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula:  $C_2H_6O_3S_2$ ).



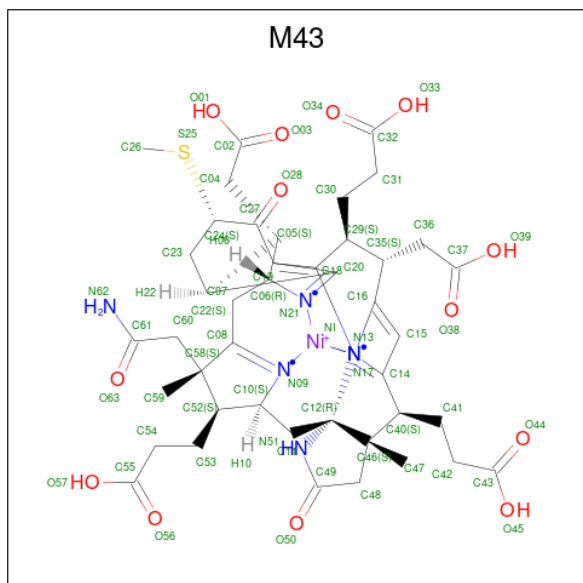
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			7	2	3	2		

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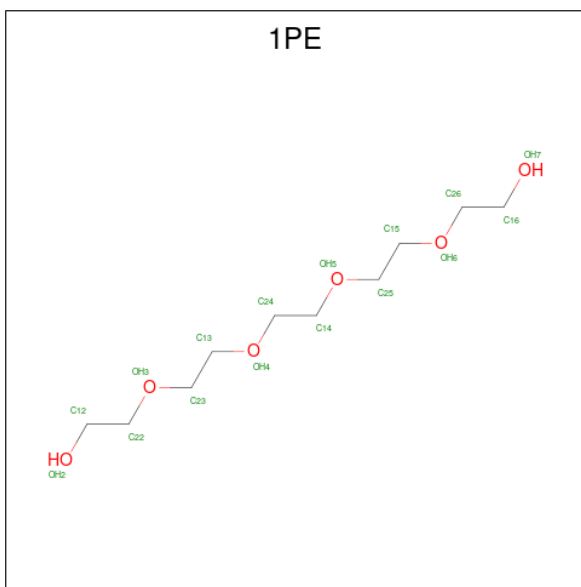
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	O	S	0	0
			7	2	3	2		
5	G	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 6 is (17[2]S)-17[2]-methylthio-coenzyme F43 (three-letter code: M43) (formula:  $C_{43}H_{53}N_6NiO_{13}S$ ).



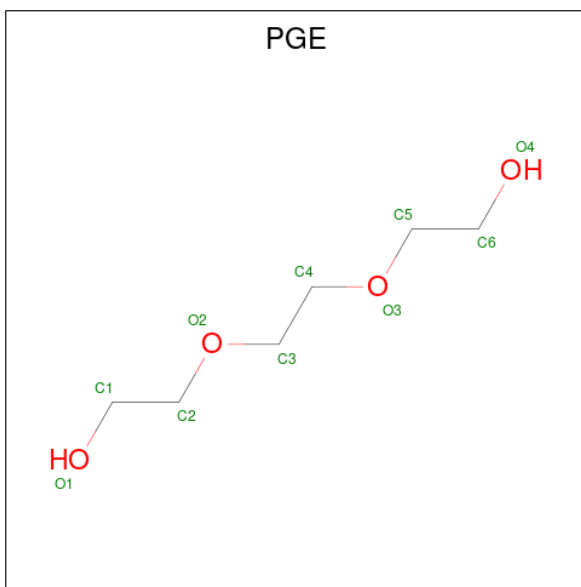
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	Ni	O	S	0	0
			64	43	6	1	13	1		
6	D	1	Total	C	N	Ni	O	S	0	0
			64	43	6	1	13	1		
6	G	1	Total	C	N	Ni	O	S	0	0
			64	43	6	1	13	1		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			16	10	6		
7	D	1	Total	C	O	0	0
			16	10	6		
7	E	1	Total	C	O	0	0
			16	10	6		
7	F	1	Total	C	O	0	0
			16	10	6		
7	G	1	Total	C	O	0	0
			16	10	6		
7	H	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



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

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	H	1	Total	O	S	0	0
			5	4	1		
9	I	1	Total	O	S	0	0
			5	4	1		

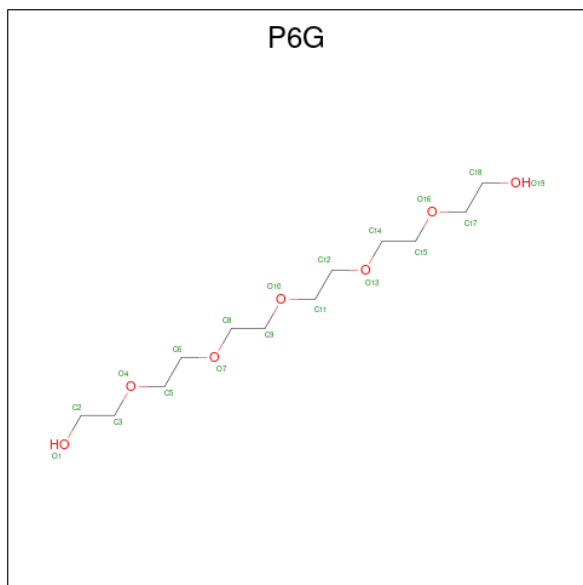
- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Cl	0	0
			1	1		

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

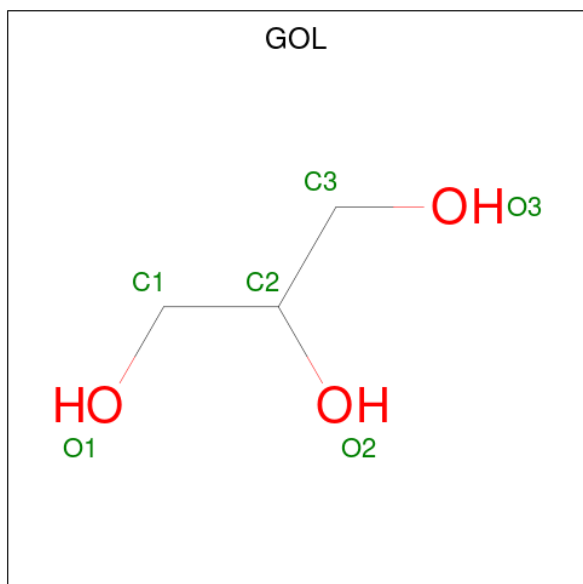
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Ca	0	0
			1	1		
11	G	1	Total	Ca	0	0
			1	1		

- Molecule 12 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 13 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 14 is water.

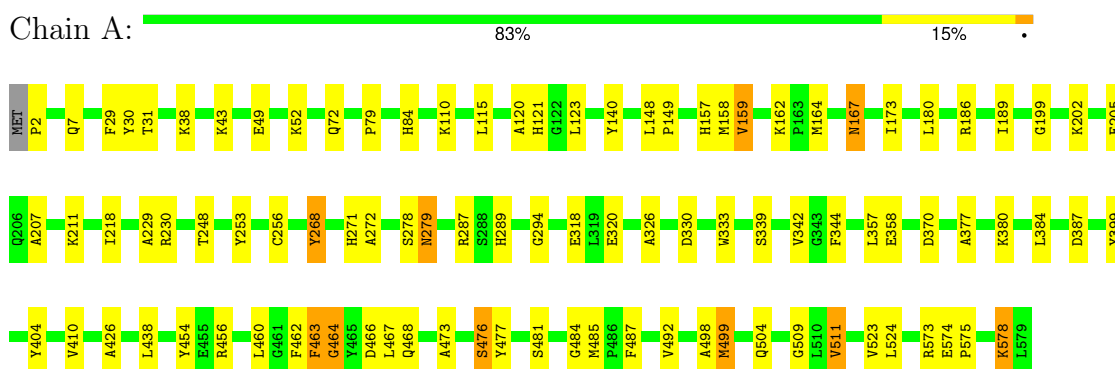
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	391	Total	O	0	0
			391	391		
14	B	173	Total	O	0	0
			173	173		
14	C	178	Total	O	0	0
			178	178		
14	D	341	Total	O	0	0
			341	341		
14	E	142	Total	O	0	0
			142	142		
14	F	120	Total	O	0	0
			120	120		
14	G	364	Total	O	0	0
			364	364		
14	H	140	Total	O	0	0
			140	140		
14	I	156	Total	O	0	0
			156	156		

### 3 Residue-property plots

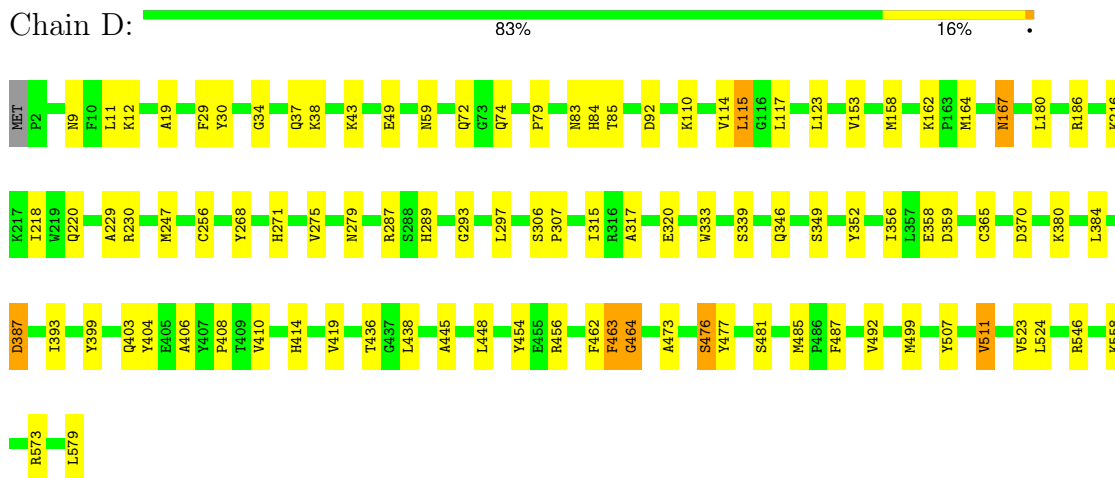
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

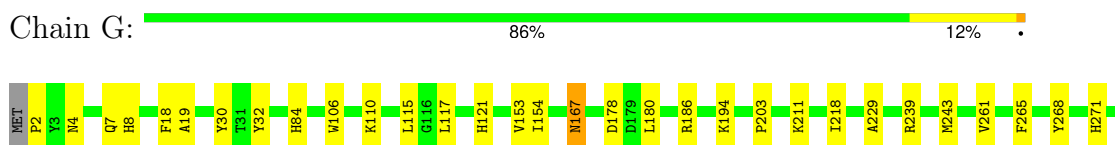
- Molecule 1: Methyl coenzyme M reductase, alpha subunit

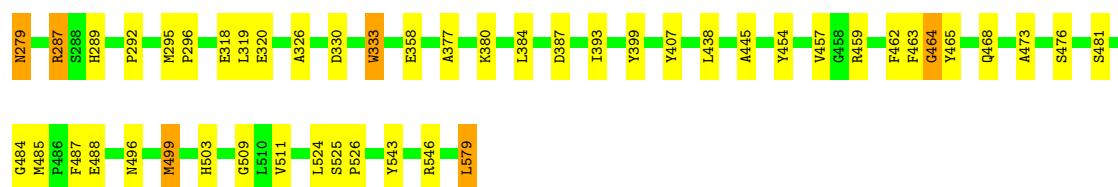


- Molecule 1: Methyl coenzyme M reductase, alpha subunit



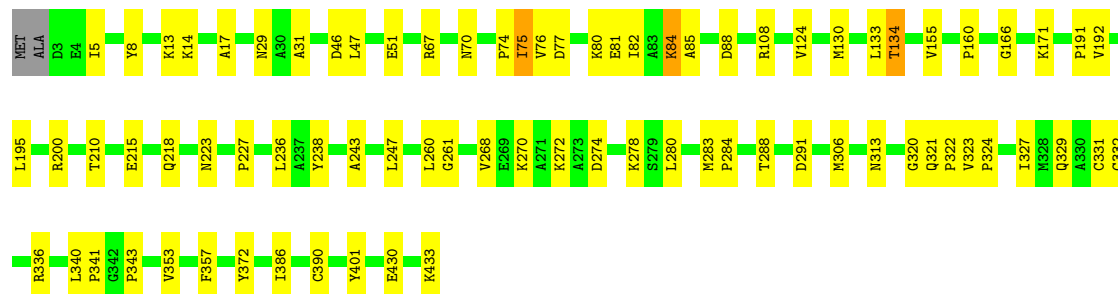
- Molecule 1: Methyl coenzyme M reductase, alpha subunit





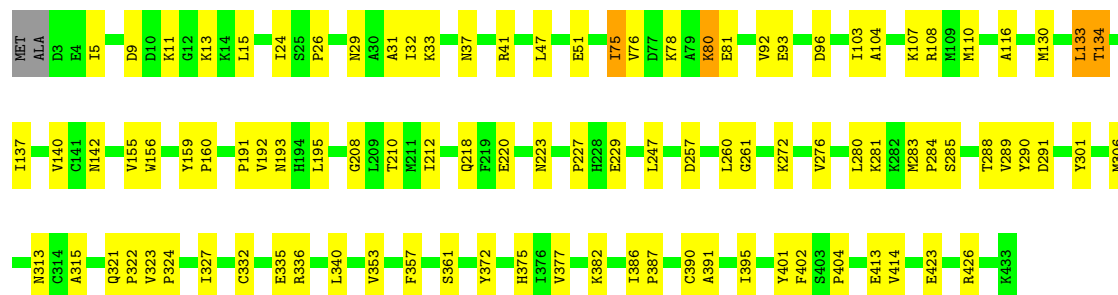
- Molecule 2: Methyl-coenzyme M reductase, beta subunit

Chain B: 81% 18%



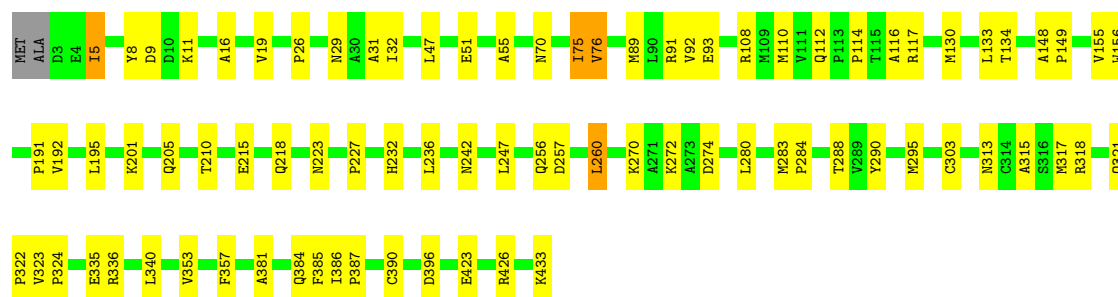
- Molecule 2: Methyl-coenzyme M reductase, beta subunit

Chain E: 77% 22%



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

Chain H: 80% 18%



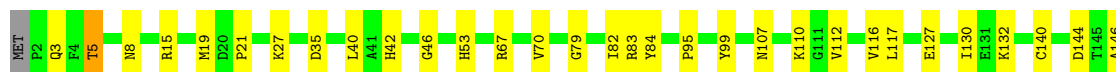
- Molecule 3: Methyl-coenzyme M reductase, gamma subunit

Chain C: 88% 11%



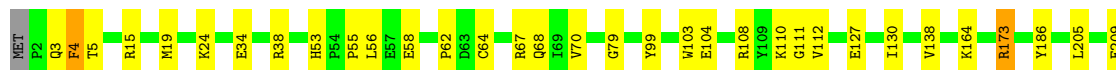
- Molecule 3: Methyl-coenzyme M reductase, gamma subunit

Chain F: 80% 19%



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

Chain I: 85% 14%



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.86Å 412.49Å 165.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.58 – 2.10	Depositor
% Data completeness (in resolution range)	95.2 (47.58-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.161 , 0.206	Depositor
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.724	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32144	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: MHO, TP7, P6G, CA, GOL, SO4, CL, GL3, 1PE, 0AF, PGE, COM, M43, MHS

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	0.44	0/4528	0.55	0/6126
1	D	0.41	0/4539	0.53	0/6140
1	G	0.41	0/4528	0.54	0/6126
2	B	0.35	0/3258	0.49	0/4410
2	E	0.32	0/3258	0.49	0/4410
2	H	0.34	0/3269	0.50	0/4424
3	C	0.40	0/2251	0.55	0/3034
3	F	0.31	0/2259	0.49	0/3045
3	I	0.38	0/2251	0.52	0/3034
All	All	0.38	0/30141	0.52	0/40749

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	4467	0	4266	89	0
1	D	4475	0	4279	101	0
1	G	4467	0	4266	72	0
2	B	3197	0	3195	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3197	0	3195	96	0
2	H	3205	0	3208	92	0
3	C	2205	0	2187	35	0
3	F	2210	0	2193	55	0
3	I	2205	0	2187	42	0
4	A	42	0	38	1	0
4	G	21	0	19	1	0
5	A	7	0	5	4	0
5	D	7	0	5	3	0
5	G	7	0	5	3	0
6	A	64	0	48	3	0
6	D	64	0	48	1	0
6	G	64	0	48	3	0
7	A	16	0	22	5	0
7	D	16	0	22	8	0
7	E	16	0	22	2	0
7	F	16	0	22	4	0
7	G	16	0	22	9	0
7	H	16	0	22	5	0
8	A	20	0	28	5	0
8	D	20	0	28	5	0
8	G	20	0	28	1	0
9	A	10	0	0	0	0
9	B	10	0	0	0	0
9	C	5	0	0	0	0
9	D	10	0	0	0	0
9	H	5	0	0	0	0
9	I	5	0	0	0	0
10	A	1	0	0	3	0
11	A	1	0	0	0	0
11	G	1	0	0	0	0
12	B	19	0	26	11	0
13	C	6	0	8	0	0
13	E	6	0	8	0	0
14	A	391	0	0	5	0
14	B	173	0	0	7	0
14	C	178	0	0	4	0
14	D	341	0	0	8	0
14	E	142	0	0	8	0
14	F	120	0	0	4	0
14	G	364	0	0	2	0
14	H	140	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	I	156	0	0	1	0
All	All	32144	0	29450	572	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 10.

The worst 5 of 572 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:B:51:GLU:HB2	2:B:75:ILE:CD1	1.77	1.15
1:D:186:ARG:HH12	7:G:580:1PE:H221	1.16	1.10
2:B:14:LYS:CE	2:B:17:ALA:HB2	1.86	1.06
1:A:186:ARG:HH12	7:A:581:1PE:H121	1.20	1.03
7:D:580:1PE:H141	1:G:186:ARG:HH11	1.25	1.02

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	572/579 (99%)	547 (96%)	23 (4%)	2 (0%)	37	37
1	D	573/579 (99%)	545 (95%)	26 (4%)	2 (0%)	37	37
1	G	572/579 (99%)	547 (96%)	24 (4%)	1 (0%)	44	45
2	B	429/433 (99%)	421 (98%)	8 (2%)	0	100	100
2	E	429/433 (99%)	418 (97%)	11 (3%)	0	100	100
2	H	430/433 (99%)	417 (97%)	13 (3%)	0	100	100
3	C	276/279 (99%)	267 (97%)	8 (3%)	1 (0%)	30	29
3	F	277/279 (99%)	269 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	276/279 (99%)	267 (97%)	8 (3%)	1 (0%)	30	29
All	All	3834/3873 (99%)	3698 (96%)	129 (3%)	7 (0%)	44	45

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	481	SER
1	A	481	SER
1	D	481	SER
3	I	4	PHE
1	A	339	SER

### 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	453/454 (100%)	435 (96%)	18 (4%)	27	28
1	D	454/454 (100%)	437 (96%)	17 (4%)	29	31
1	G	453/454 (100%)	438 (97%)	15 (3%)	33	36
2	B	331/332 (100%)	320 (97%)	11 (3%)	33	36
2	E	331/332 (100%)	323 (98%)	8 (2%)	44	49
2	H	332/332 (100%)	324 (98%)	8 (2%)	44	49
3	C	231/232 (100%)	226 (98%)	5 (2%)	47	53
3	F	232/232 (100%)	228 (98%)	4 (2%)	56	63
3	I	231/232 (100%)	226 (98%)	5 (2%)	47	53
All	All	3048/3054 (100%)	2957 (97%)	91 (3%)	36	40

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	195	LEU
1	G	387	ASP

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Mol	Chain	Res	Type
3	F	5	THR
1	G	117	LEU
1	G	487	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	4	ASN
1	G	279	ASN
1	G	72	GLN
1	G	121	HIS
1	G	480	GLN

### 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	MHS	A	271	1	7,11,12	0.51	0	7,14,16	1.75	3 (42%)
1	OAF	A	333	1	13,16,17	1.17	2 (15%)	9,22,24	1.28	0
1	GL3	A	464	1	2,3,4	2.98	1 (50%)	1,2,4	0.47	0
1	MHS	G	271	1	7,11,12	0.72	0	7,14,16	1.08	1 (14%)
1	OAF	D	333	1	13,16,17	1.26	1 (7%)	9,22,24	1.28	0
1	MHS	D	271	1	7,11,12	0.77	0	7,14,16	1.14	1 (14%)
1	MHO	A	499	1	6,8,9	0.63	0	3,9,11	1.64	1 (33%)
1	GL3	D	464	1	2,3,4	2.80	1 (50%)	1,2,4	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MHO	D	499	1	6,8,9	0.74	0	3,9,11	1.69	1 (33%)
1	GL3	G	464	1	2,3,4	2.60	1 (50%)	1,2,4	0.25	0
1	MHO	G	499	1	6,8,9	0.76	0	3,9,11	2.38	2 (66%)
1	0AF	G	333	1	13,16,17	1.23	2 (15%)	9,22,24	1.07	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
1	MHS	A	271	1	-	0/5/6/8	0/1/1/1
1	0AF	A	333	1	-	0/4/6/8	0/2/2/2
1	GL3	A	464	1	-	0/1/1/2	-
1	MHS	G	271	1	-	0/5/6/8	0/1/1/1
1	0AF	D	333	1	-	0/4/6/8	0/2/2/2
1	MHS	D	271	1	-	0/5/6/8	0/1/1/1
1	MHO	A	499	1	-	3/6/7/9	-
1	GL3	D	464	1	-	1/1/1/2	-
1	MHO	D	499	1	-	3/6/7/9	-
1	GL3	G	464	1	-	1/1/1/2	-
1	MHO	G	499	1	-	3/6/7/9	-
1	0AF	G	333	1	-	0/4/6/8	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	464	GL3	C-S	-4.17	1.63	1.80
1	D	464	GL3	C-S	-3.89	1.64	1.80
1	G	464	GL3	C-S	-3.57	1.66	1.80
1	D	333	0AF	CD1-NE1	2.35	1.41	1.36
1	G	333	0AF	O-C	2.23	1.28	1.20

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	499	MHO	CE-SD-CG	-2.97	90.04	97.45
1	G	499	MHO	OD1-SD-CG	2.86	113.41	105.89
1	A	271	MHS	NE2-CE1-ND1	-2.73	108.20	112.26
1	A	499	MHO	CE-SD-CG	-2.64	90.85	97.45
1	D	499	MHO	CE-SD-CG	-2.29	91.72	97.45

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	499	MHO	O-C-CA-CB
1	A	499	MHO	CB-CG-SD-CE
1	D	499	MHO	O-C-CA-CB
1	G	499	MHO	O-C-CA-CB
1	A	499	MHO	CB-CG-SD-OD1

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	464	GL3	4	0
1	A	499	MHO	1	0
1	D	464	GL3	3	0
1	G	464	GL3	3	0
1	G	499	MHO	1	0
1	G	333	0AF	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 3 are monoatomic - leaving 33 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	$\# Z  > 2$
5	COM	D	1003	6	6,6,6	2.86	1 (16%)	8,8,8	2.01	2 (25%)
9	SO4	A	584	-	4,4,4	0.24	0	6,6,6	0.15	0
7	1PE	E	434	-	15,15,15	0.69	0	14,14,14	1.49	2 (14%)
9	SO4	A	585	-	4,4,4	0.25	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	M43	D	1001	5,1	64,73,73	3.67	26 (40%)	71,121,121	2.21	13 (18%)
8	PGE	G	581	-	9,9,9	0.51	0	8,8,8	0.21	0
7	1PE	H	434	-	15,15,15	0.68	0	14,14,14	1.58	3 (21%)
8	PGE	A	582	-	9,9,9	0.41	0	8,8,8	0.43	0
9	SO4	C	282	-	4,4,4	0.24	0	6,6,6	0.20	0
7	1PE	A	581	-	15,15,15	0.65	0	14,14,14	1.52	0
13	GOL	E	435	-	5,5,5	0.41	0	5,5,5	0.23	0
9	SO4	D	584	-	4,4,4	0.24	0	6,6,6	0.10	0
4	TP7	A	580	-	19,20,20	2.73	2 (10%)	24,26,26	2.38	5 (20%)
5	COM	A	1003	6	6,6,6	2.80	1 (16%)	8,8,8	3.12	3 (37%)
4	TP7	G	1002	-	19,20,20	2.79	2 (10%)	24,26,26	2.32	5 (20%)
6	M43	A	1001	5,1	64,73,73	3.51	25 (39%)	71,121,121	2.38	15 (21%)
9	SO4	B	435	-	4,4,4	0.24	0	6,6,6	0.09	0
7	1PE	D	580	-	15,15,15	0.67	0	14,14,14	1.55	2 (14%)
9	SO4	H	435	-	4,4,4	0.23	0	6,6,6	0.10	0
9	SO4	B	436	-	4,4,4	0.24	0	6,6,6	0.23	0
9	SO4	D	583	-	4,4,4	0.24	0	6,6,6	0.12	0
12	P6G	B	434	-	18,18,18	0.71	0	17,17,17	1.52	0
8	PGE	D	582	-	9,9,9	0.54	0	8,8,8	0.25	0
8	PGE	A	583	-	9,9,9	0.54	0	8,8,8	0.36	0
13	GOL	C	281	-	5,5,5	0.44	0	5,5,5	0.50	0
7	1PE	F	281	-	15,15,15	0.65	0	14,14,14	1.58	3 (21%)
5	COM	G	1003	6	6,6,6	3.06	1 (16%)	8,8,8	1.59	2 (25%)
9	SO4	I	281	-	4,4,4	0.22	0	6,6,6	0.10	0
7	1PE	G	580	-	15,15,15	0.58	0	14,14,14	1.65	3 (21%)
8	PGE	G	582	-	9,9,9	0.51	0	8,8,8	0.18	0
8	PGE	D	581	-	9,9,9	0.53	0	8,8,8	0.28	0
4	TP7	A	1002	-	19,20,20	2.68	2 (10%)	24,26,26	2.38	2 (8%)
6	M43	G	1001	5	64,73,73	3.37	25 (39%)	71,121,121	2.18	12 (16%)

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
5	COM	D	1003	6	-	3/4/4/4	-
7	1PE	E	434	-	-	8/13/13/13	-
6	M43	D	1001	5,1	1/1/31/33	10/28/190/190	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PGE	G	581	-	-	3/7/7/7	-
7	1PE	H	434	-	-	7/13/13/13	-
8	PGE	A	582	-	-	4/7/7/7	-
7	1PE	A	581	-	-	9/13/13/13	-
13	GOL	E	435	-	-	3/4/4/4	-
4	TP7	A	580	-	-	2/24/24/24	-
5	COM	A	1003	6	-	4/4/4/4	-
4	TP7	G	1002	-	-	3/24/24/24	-
6	M43	A	1001	5,1	-	9/28/190/190	-
7	1PE	D	580	-	-	5/13/13/13	-
12	P6G	B	434	-	-	8/16/16/16	-
8	PGE	D	582	-	-	2/7/7/7	-
8	PGE	A	583	-	-	6/7/7/7	-
13	GOL	C	281	-	-	0/4/4/4	-
7	1PE	F	281	-	-	5/13/13/13	-
5	COM	G	1003	6	-	3/4/4/4	-
7	1PE	G	580	-	-	9/13/13/13	-
8	PGE	G	582	-	-	1/7/7/7	-
8	PGE	D	581	-	-	2/7/7/7	-
4	TP7	A	1002	-	-	3/24/24/24	-
6	M43	G	1001	5	1/1/31/33	7/28/190/190	-

The worst 5 of 85 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1001	M43	NI-N13	13.23	2.21	1.89
6	A	1001	M43	NI-N13	12.78	2.20	1.89
6	D	1001	M43	NI-N21	11.42	2.16	1.89
6	G	1001	M43	NI-N21	11.32	2.16	1.89
4	G	1002	TP7	O1-C1	10.50	1.44	1.23

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1001	M43	C59-C58-C60	13.84	134.26	110.74
6	G	1001	M43	C59-C58-C60	11.20	129.77	110.74
6	D	1001	M43	C59-C58-C60	9.80	127.39	110.74
4	A	580	TP7	O1-C1-N	-8.89	107.90	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	TP7	O1-C1-N	-8.71	108.21	122.95

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	D	1001	M43	N17
6	G	1001	M43	N17

5 of 116 torsion outliers are listed below:

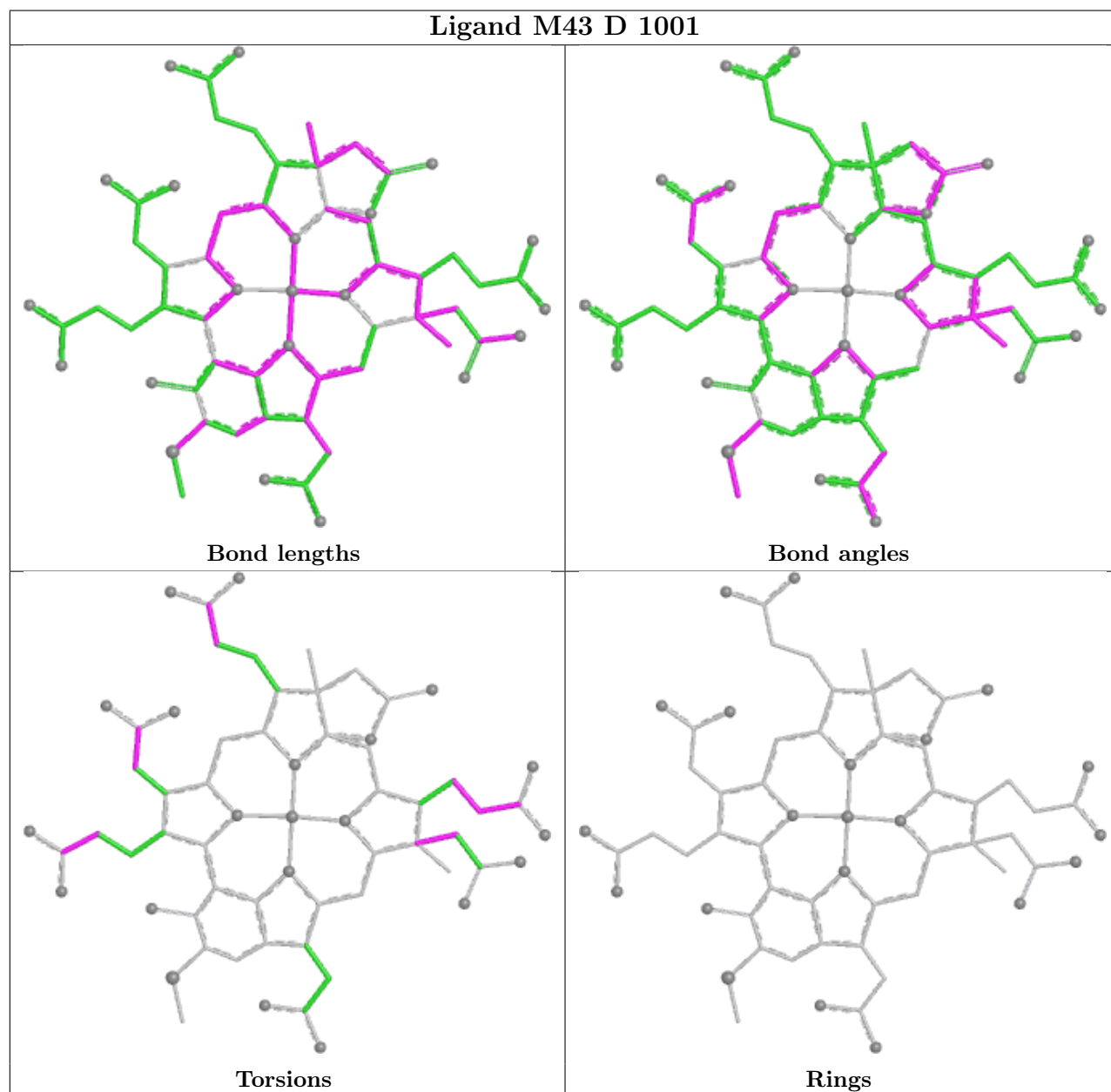
Mol	Chain	Res	Type	Atoms
4	A	1002	TP7	O1-C1-N-CA
4	A	580	TP7	O1-C1-N-CA
4	G	1002	TP7	O1-C1-N-CA
5	A	1003	COM	C1-C2-S2-O1S
5	A	1003	COM	C1-C2-S2-O2S

There are no ring outliers.

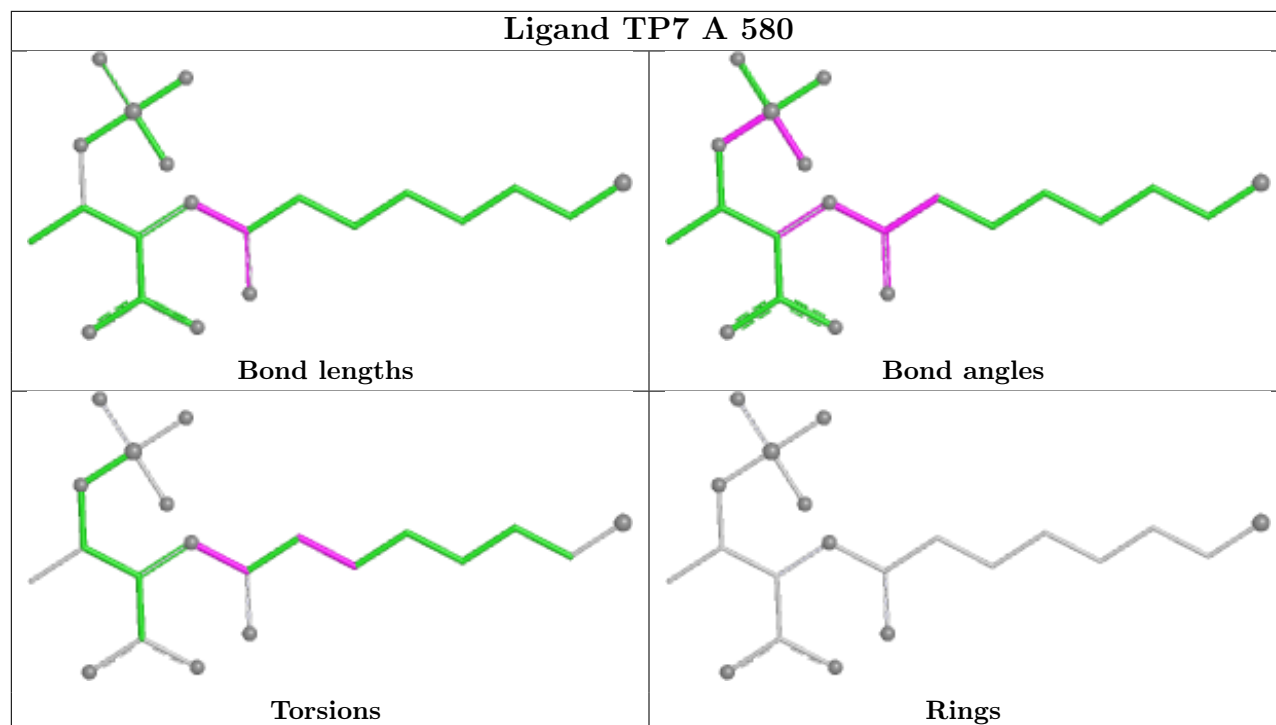
20 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1003	COM	3	0
7	E	434	1PE	2	0
6	D	1001	M43	1	0
7	H	434	1PE	5	0
8	A	582	PGE	1	0
7	A	581	1PE	5	0
5	A	1003	COM	4	0
4	G	1002	TP7	1	0
6	A	1001	M43	3	0
7	D	580	1PE	8	0
12	B	434	P6G	11	0
8	D	582	PGE	2	0
8	A	583	PGE	4	0
7	F	281	1PE	4	0
5	G	1003	COM	3	0
7	G	580	1PE	9	0
8	G	582	PGE	1	0
8	D	581	PGE	3	0
4	A	1002	TP7	1	0
6	G	1001	M43	3	0

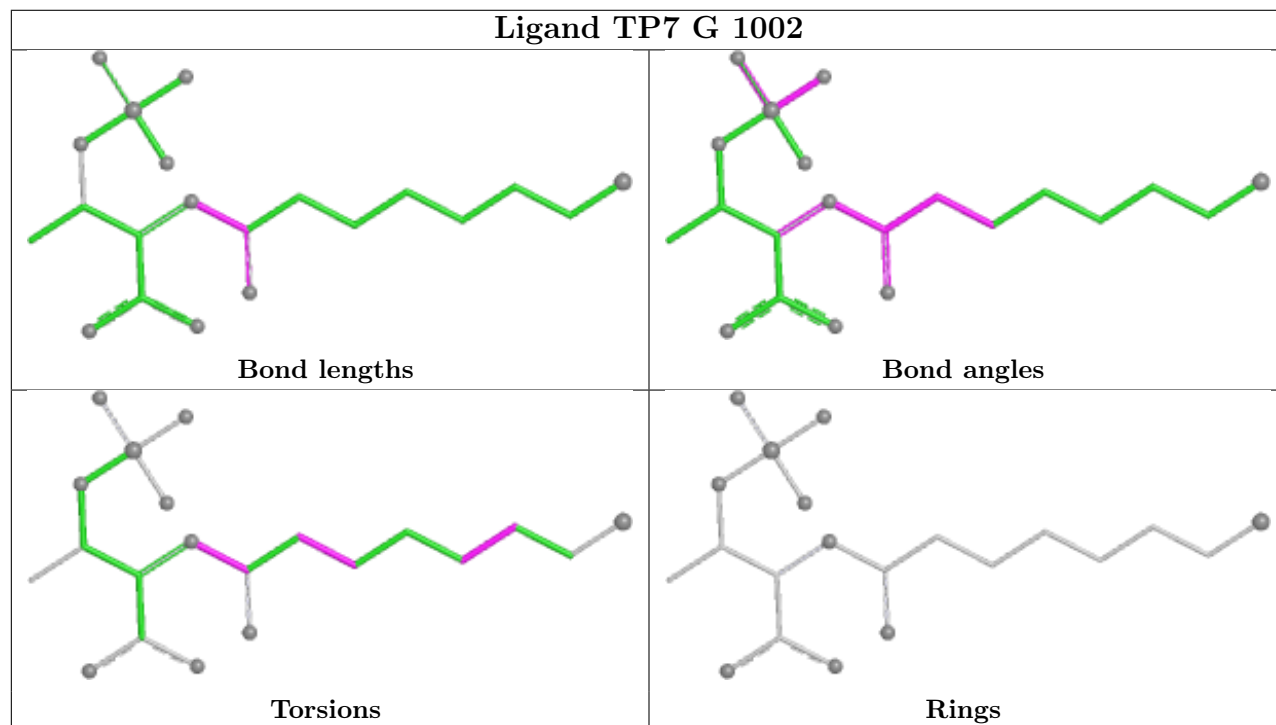
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

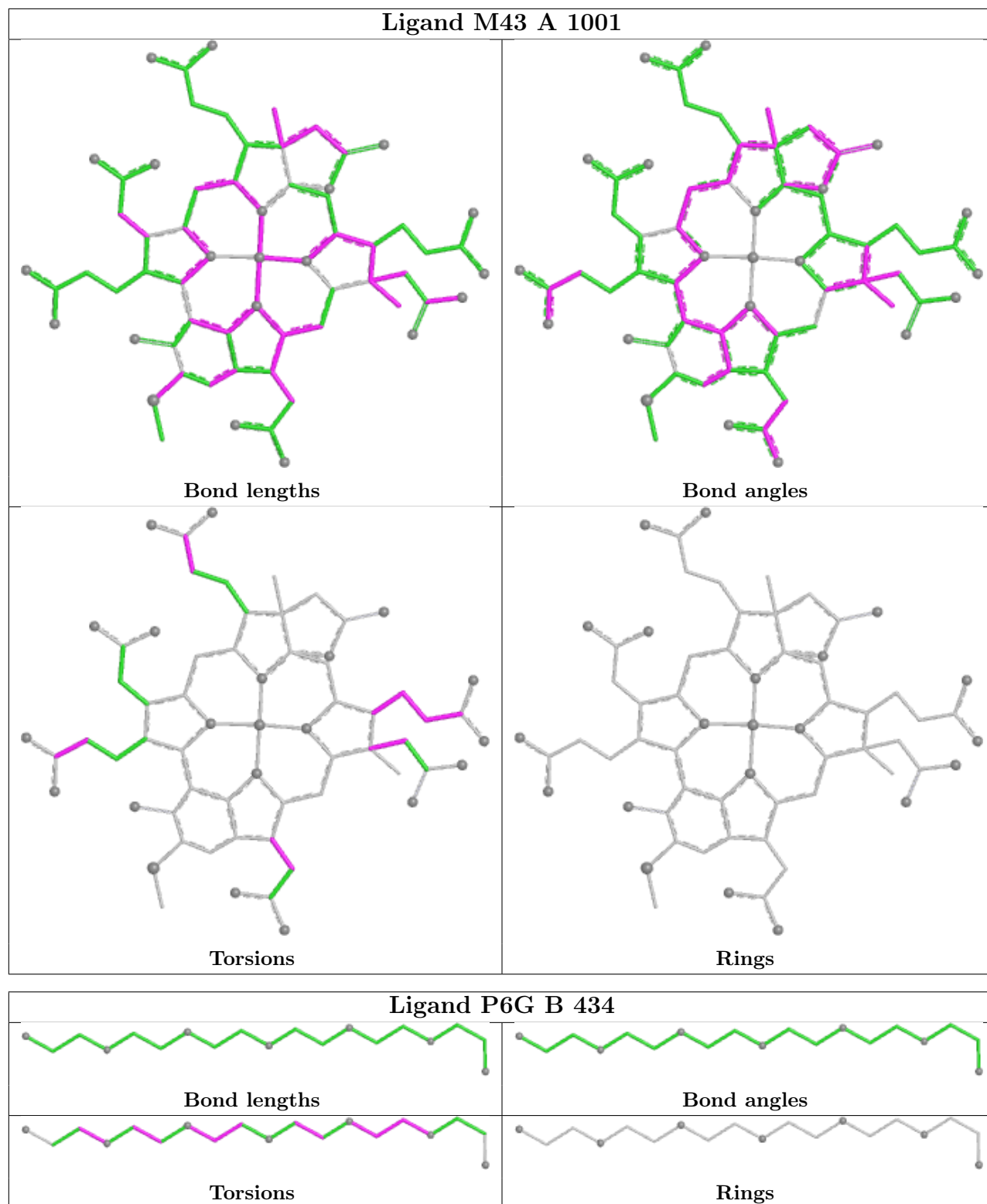


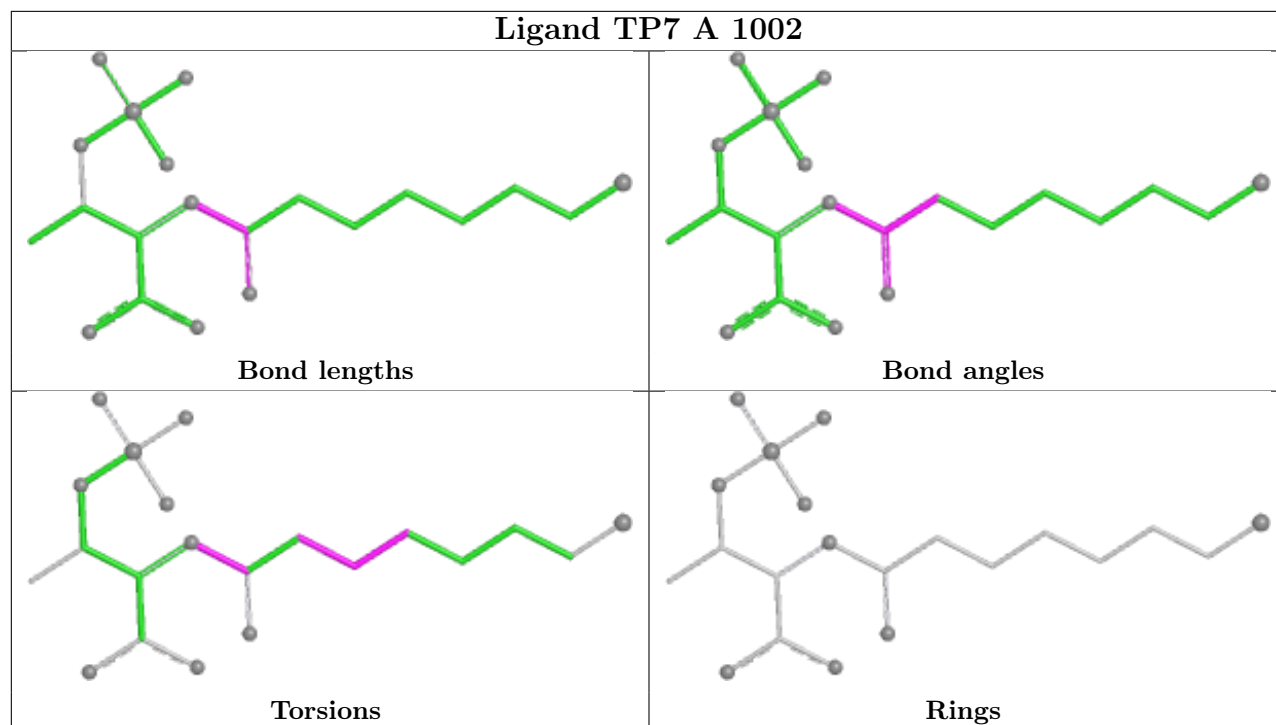
## Ligand TP7 A 580

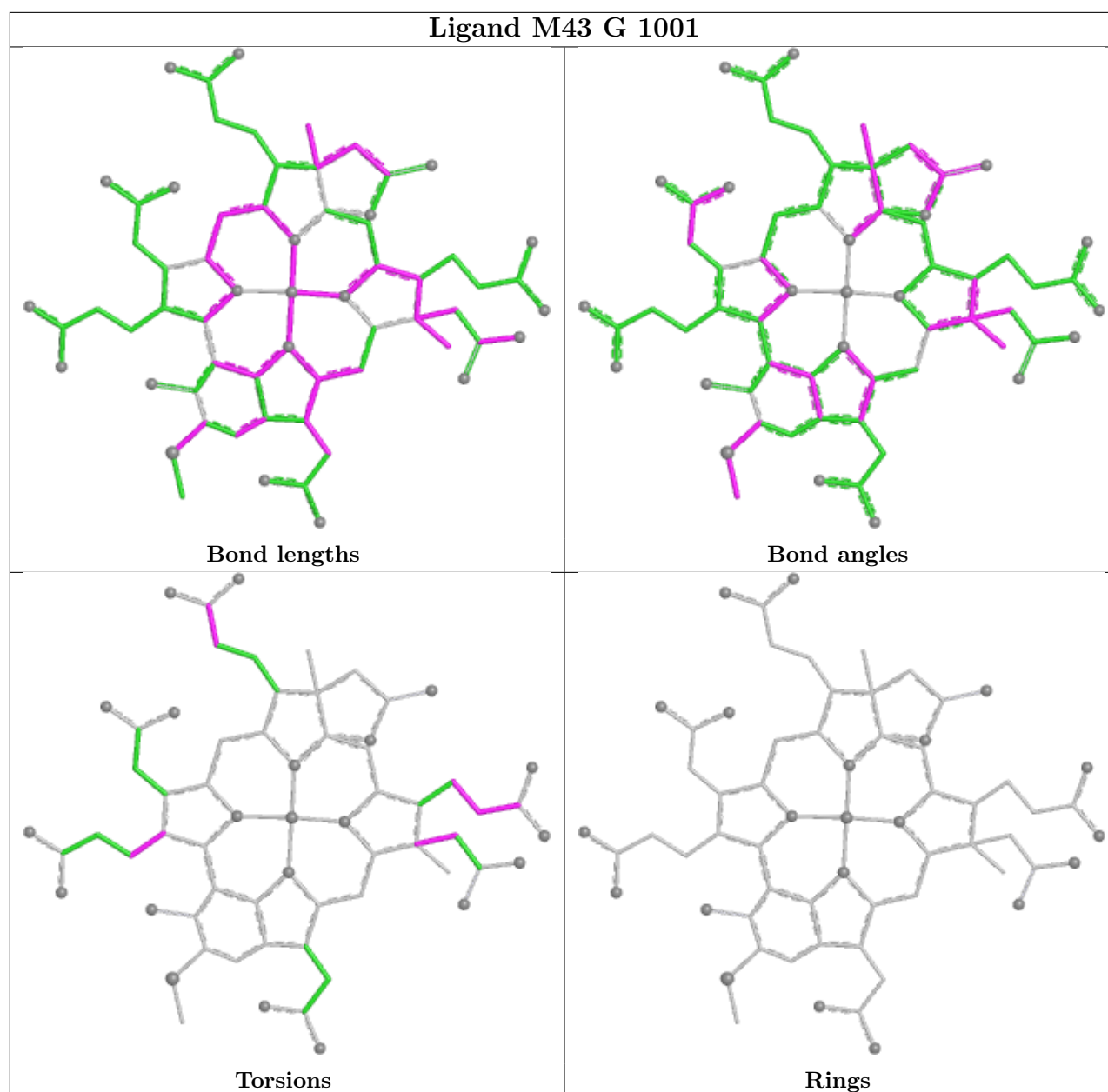


## Ligand TP7 G 1002









## 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

EDS failed to run properly - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.