



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 11:27 AM UTC

PDB ID : 1HBU / pdb_00001hbu
Title : METHYL-COENZYME M REDUCTASE IN THE MCR-RED1-SILENT
STATE IN COMPLEX with COENZYME M
Authors : Ermler, U.; Grabarse, W.
Deposited on : 2001-04-20
Resolution : 1.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly; EDS was not executed - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21670 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 ALPHA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	24	10	0
			4284	2708	723	833	20			
1	D	548	Total	C	N	O	S	23	13	0
			4289	2710	721	838	20			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	MHS	HIS	modified residue	UNP P11558
A	271	AGM	ARG	modified residue	UNP P11558
A	400	MGN	GLN	modified residue	UNP P11558
A	445	GL3	GLY	modified residue	UNP P11558
A	452	SMC	CYS	modified residue	UNP P11558
D	257	MHS	HIS	modified residue	UNP P11558
D	271	AGM	ARG	modified residue	UNP P11558
D	400	MGN	GLN	modified residue	UNP P11558
D	445	GL3	GLY	modified residue	UNP P11558
D	452	SMC	CYS	modified residue	UNP P11558

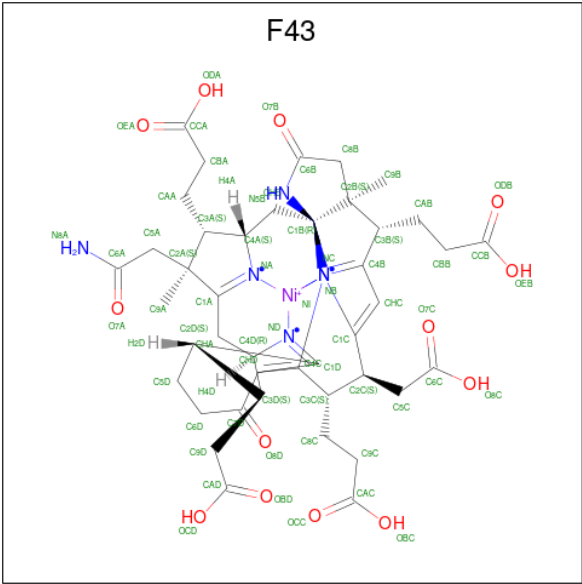
- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE I BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	26	13	0
			3344	2113	556	654	21			
2	E	442	Total	C	N	O	S	41	11	0
			3333	2108	551	653	21			

- Molecule 3 is a protein called METHYL-COENZYME M REDUCTASE I GAMMA SUB-UNIT.

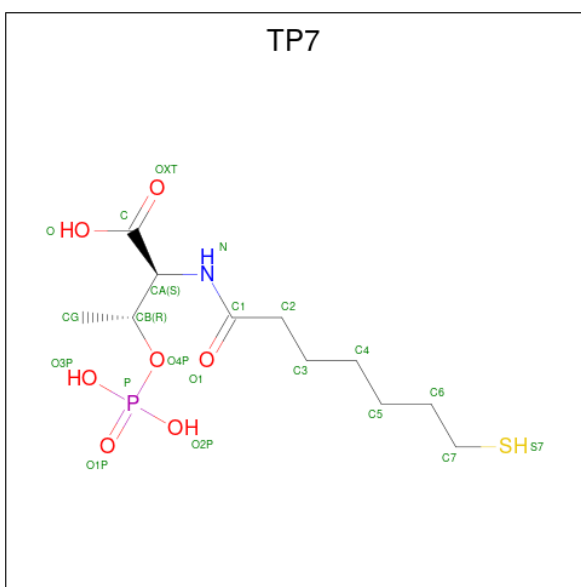
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total	C	N	O	S	39	5	0
			2007	1242	355	398	12			
3	F	247	Total	C	N	O	S	44	5	0
			2006	1242	354	398	12			

- Molecule 4 is FACTOR 430 (CCD ID: F43) (formula: C₄₂H₅₁N₆NiO₁₃).



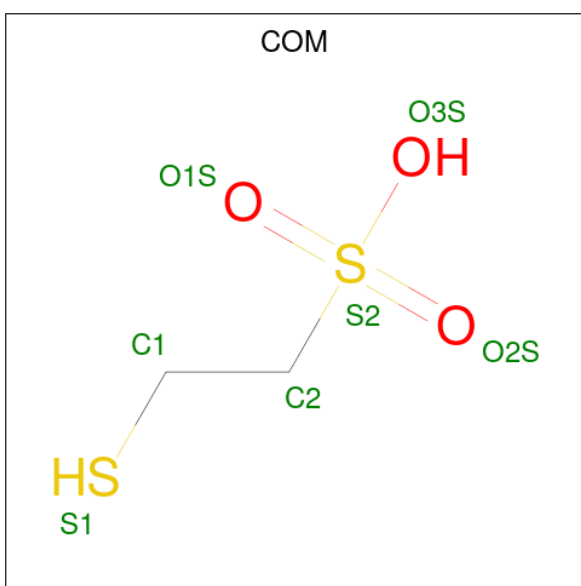
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
4	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 5 is Coenzyme B (CCD ID: TP7) (formula: C₁₁H₂₂NO₇PS).



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 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $C_2H_6O_3S_2$).



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

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



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

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Zn	0	1
			1	1		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	5	Total	Mg	0	0
			5	5		
9	B	2	Total	Mg	0	0
			2	2		
9	C	1	Total	Mg	0	0
			1	1		
9	D	1	Total	Mg	0	0
			1	1		
9	E	3	Total	Mg	0	0
			3	3		
9	F	1	Total	Mg	0	0
			1	1		

- Molecule 10 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	4	Total	Na	0	0
			4	4		
10	B	2	Total	Na	0	0
			2	2		
10	D	3	Total	Na	0	0
			3	3		

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	444	Total	O	0	27
			444	444		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	385	Total 385	O 385	0	23
12	C	254	Total 254	O 254	0	23
12	D	440	Total 440	O 440	0	32
12	E	360	Total 360	O 360	0	23
12	F	253	Total 253	O 253	0	13

MolProbity failed to run properly; EDS was not executed - this section is therefore empty.

3 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.10Å 116.50Å 121.80Å 90.00° 91.80° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90	Depositor
% Data completeness (in resolution range)	94.3 (10.00-1.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.162 , 0.211	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21670	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

10 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	AGM	A	271	1	10,11,12	0.91	0	7,13,15	1.97	3 (42%)
1	MGN	D	400	1	6,9,10	1.02	0	7,12,14	2.19	1 (14%)
1	MGN	A	400	1	6,9,10	1.08	1 (16%)	7,12,14	2.35	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MHS	D	257	1	10,11,12	1.78	1 (10%)	5,14,16	2.28	2 (40%)
1	GL3	A	445	1	2,3,4	2.78	1 (50%)	1,2,4	0.42	0
1	MHS	A	257	1	10,11,12	1.79	1 (10%)	5,14,16	3.10	2 (40%)
1	AGM	D	271	1	10,11,12	0.80	0	7,13,15	0.52	0
1	SMC	D	452	1	5,6,7	0.75	0	3,6,8	0.78	0
1	GL3	D	445	1	2,3,4	2.67	1 (50%)	1,2,4	0.49	0
1	SMC	A	452	1	5,6,7	0.94	0	3,6,8	1.53	1 (33%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	MHS	CM-ND1	5.39	1.57	1.46
1	D	257	MHS	CM-ND1	5.04	1.56	1.46
1	A	445	GL3	C-S	-3.91	1.64	1.80
1	D	445	GL3	C-S	-3.76	1.65	1.80
1	A	400	MGN	CB1-CA	2.21	1.57	1.55

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	MHS	ND1-CE1-NE2	-5.77	109.51	112.94
1	D	400	MGN	CB2-CA-CB1	-5.33	102.20	110.97
1	A	400	MGN	CB2-CA-CB1	-5.30	102.24	110.97
1	D	257	MHS	ND1-CE1-NE2	-4.00	110.56	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	MHS	CD2-NE2-CE1	3.35	109.62	105.24
1	A	271	AGM	NE1-CZ-NH2	-3.04	115.36	120.58
1	A	271	AGM	NH1-CZ-NE1	2.61	125.33	119.58
1	A	452	SMC	CA-CB-SG	-2.43	110.12	114.04
1	A	271	AGM	CG-CD-NE1	-2.35	106.38	110.42
1	A	400	MGN	CB1-CG-CD	-2.12	107.90	112.13
1	D	257	MHS	CD2-NE2-CE1	2.06	107.93	105.24

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	452	SMC	CA-CB-SG-CS
1	D	452	SMC	CA-CB-SG-CS
1	D	271	AGM	CE2-CD-NE1-CZ
1	A	445	GL3	S-C-CA-N
1	D	445	GL3	S-C-CA-N
1	A	271	AGM	CE2-CD-NE1-CZ
1	D	271	AGM	NE1-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 25 are monoatomic - leaving 17 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	GOL	A	1553	10	5,5,5	0.70	0	5,5,5	1.35	0
7	GOL	D	1556	-	5,5,5	0.74	0	5,5,5	0.94	0
7	GOL	E	1444	-	5,5,5	0.64	0	5,5,5	0.95	0
5	TP7	A	1551	-	19,20,20	2.52	7 (36%)	24,26,26	2.19	9 (37%)
7	GOL	D	1553	-	5,5,5	0.91	0	5,5,5	0.79	0
7	GOL	D	1555	-	5,5,5	0.69	0	5,5,5	0.75	0
4	F43	A	1550	6,1	63,71,71	2.92	20 (31%)	73,118,118	2.39	30 (41%)
7	GOL	A	1556	-	5,5,5	0.65	0	5,5,5	1.00	0
6	COM	D	1552	4	6,6,6	1.62	1 (16%)	8,8,8	1.73	1 (12%)
7	GOL	C	1249	-	5,5,5	0.64	0	5,5,5	0.51	0
6	COM	A	1552	4	6,6,6	1.72	1 (16%)	8,8,8	1.26	1 (12%)
7	GOL	B	1444	-	5,5,5	0.84	0	5,5,5	1.41	1 (20%)
7	GOL	A	1555	-	5,5,5	0.79	0	5,5,5	1.00	0
7	GOL	D	1554	10	5,5,5	0.53	0	5,5,5	1.31	1 (20%)
5	TP7	D	1551	-	19,20,20	2.25	6 (31%)	24,26,26	2.13	9 (37%)
7	GOL	A	1554	-	5,5,5	0.66	0	5,5,5	1.10	0
4	F43	D	1550	6,1	63,71,71	3.02	19 (30%)	73,118,118	2.11	29 (39%)

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	GOL	A	1553	10	-	2/4/4/4	-
7	GOL	D	1556	-	-	4/4/4/4	-
7	GOL	E	1444	-	-	3/4/4/4	-
5	TP7	A	1551	-	-	5/24/24/24	-
7	GOL	D	1553	-	-	0/4/4/4	-
7	GOL	D	1555	-	-	4/4/4/4	-
4	F43	A	1550	6,1	-	7/28/185/185	-
7	GOL	A	1556	-	-	2/4/4/4	-
6	COM	D	1552	4	-	1/4/4/4	-
7	GOL	C	1249	-	-	0/4/4/4	-
6	COM	A	1552	4	-	0/4/4/4	-
7	GOL	B	1444	-	-	2/4/4/4	-
7	GOL	A	1555	-	-	2/4/4/4	-
7	GOL	D	1554	10	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TP7	D	1551	-	-	4/24/24/24	-
7	GOL	A	1554	-	-	0/4/4/4	-
4	F43	D	1550	6,1	-	6/28/185/185	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1550	F43	NI-NA	15.13	2.25	1.89
4	D	1550	F43	NI-NB	11.10	2.16	1.89
4	D	1550	F43	NI-NA	7.97	2.08	1.89
4	D	1550	F43	NI-ND	7.76	2.08	1.89
5	A	1551	TP7	CA-C	6.59	1.63	1.52
4	A	1550	F43	C4A-NA	-6.36	1.39	1.49
4	A	1550	F43	CHB-C4A	6.24	1.60	1.51
4	D	1550	F43	C4A-NA	-6.06	1.40	1.49
4	D	1550	F43	CHA-C4D	5.76	1.58	1.53
5	A	1551	TP7	C2-C1	-5.39	1.40	1.51
4	D	1550	F43	CHB-C4A	5.28	1.59	1.51
4	A	1550	F43	NI-ND	5.15	2.01	1.89
4	D	1550	F43	C9B-C2B	-5.12	1.44	1.54
4	D	1550	F43	C6D-C7D	5.06	1.57	1.50
4	A	1550	F43	C6D-C7D	4.89	1.57	1.50
4	D	1550	F43	C1C-NC	4.83	1.48	1.37
5	D	1551	TP7	C2-C1	-4.77	1.41	1.51
5	D	1551	TP7	CA-C	4.60	1.59	1.52
4	A	1550	F43	CAA-C3A	4.44	1.61	1.53
4	D	1550	F43	C5D-C2D	-4.30	1.45	1.53
4	D	1550	F43	C9D-C3D	-4.07	1.46	1.53
4	A	1550	F43	CHB-C1B	4.01	1.56	1.53
6	A	1552	COM	C2-S2	3.70	1.82	1.77
4	A	1550	F43	C9D-C3D	-3.58	1.47	1.53
5	D	1551	TP7	P-O4P	3.50	1.65	1.59
5	A	1551	TP7	P-O4P	3.36	1.65	1.59
6	D	1552	COM	C2-S2	3.35	1.82	1.77
4	D	1550	F43	C9A-C2A	3.33	1.60	1.54
4	D	1550	F43	CAA-C3A	3.24	1.59	1.53
4	A	1550	F43	C1C-NC	3.09	1.44	1.37
5	A	1551	TP7	C1-N	2.97	1.40	1.34
5	D	1551	TP7	C1-N	2.89	1.40	1.34
4	A	1550	F43	C5D-C2D	-2.84	1.48	1.53
4	A	1550	F43	C3D-C4D	-2.79	1.48	1.53
5	D	1551	TP7	CB-CA	-2.75	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1550	F43	C5C-C2C	2.75	1.57	1.53
4	A	1550	F43	OEB-CCB	-2.64	1.22	1.30
5	A	1551	TP7	CB-CA	-2.61	1.48	1.53
4	D	1550	F43	C2B-C3B	2.61	1.64	1.57
4	D	1550	F43	C4D-ND	-2.51	1.45	1.49
4	A	1550	F43	C9B-C2B	-2.49	1.49	1.54
4	A	1550	F43	NI-NB	2.40	1.95	1.89
4	A	1550	F43	C5A-C2A	-2.39	1.48	1.56
4	D	1550	F43	C8C-C9C	2.35	1.59	1.52
5	D	1551	TP7	CA-N	-2.35	1.41	1.45
4	D	1550	F43	CHB-C1B	2.32	1.54	1.53
4	D	1550	F43	O7A-C6A	2.21	1.30	1.23
4	A	1550	F43	C6A-N8A	-2.19	1.25	1.32
5	A	1551	TP7	CA-N	-2.14	1.41	1.45
4	D	1550	F43	CAB-CBB	2.14	1.59	1.52
4	A	1550	F43	C8C-C9C	2.13	1.59	1.52
4	A	1550	F43	CHC-C4B	2.13	1.45	1.39
4	A	1550	F43	C2B-C3B	2.08	1.63	1.57
5	A	1551	TP7	P-O3P	-2.01	1.47	1.54

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1550	F43	C2B-C1B-NB	5.63	110.22	101.86
4	A	1550	F43	C5D-C2D-C1D	5.46	117.55	110.43
4	A	1550	F43	C3D-C4D-ND	5.14	110.32	102.34
4	D	1550	F43	O8D-C7D-C6D	-5.05	112.59	120.87
4	D	1550	F43	C4B-CHC-C1C	5.04	134.00	125.84
4	A	1550	F43	CAB-C3B-C4B	4.96	119.84	111.19
5	A	1551	TP7	CB-CA-C	-4.80	100.30	110.80
4	A	1550	F43	C4A-NA-C1A	4.69	115.45	109.08
4	A	1550	F43	C3B-C4B-CHC	-4.57	113.61	123.33
4	A	1550	F43	CAB-C3B-C2B	-4.44	109.21	119.00
5	D	1551	TP7	CG-CB-CA	4.23	121.56	113.26
4	D	1550	F43	C5D-C2D-C1D	4.07	115.74	110.43
4	A	1550	F43	CHC-C1C-NC	3.89	130.67	124.39
5	D	1551	TP7	C5-C6-C7	-3.88	106.19	113.09
5	A	1551	TP7	CG-CB-CA	3.79	120.70	113.26
4	A	1550	F43	C5C-C2C-C3C	-3.70	105.91	115.05
4	D	1550	F43	C3A-C2A-C1A	-3.66	96.31	99.97
4	D	1550	F43	CAB-C3B-C2B	-3.65	110.94	119.00
6	D	1552	COM	C2-C1-S1	-3.65	103.85	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1551	TP7	CA-N-C1	3.62	128.95	121.80
4	D	1550	F43	C5D-C2D-C3D	3.62	124.85	118.26
4	A	1550	F43	C9A-C2A-C5A	3.58	116.83	110.74
5	D	1551	TP7	CB-CA-C	-3.45	103.24	110.80
4	D	1550	F43	C5C-C2C-C3C	-3.41	106.64	115.05
4	D	1550	F43	CAB-C3B-C4B	3.37	117.06	111.19
5	A	1551	TP7	O1-C1-N	-3.31	117.35	122.95
4	A	1550	F43	O7A-C6A-C5A	-3.29	111.80	121.98
4	A	1550	F43	C6D-C7D-CHD	3.24	122.91	116.94
5	A	1551	TP7	P-O4P-CB	-3.18	114.68	123.33
4	A	1550	F43	C3A-C2A-C1A	-3.16	96.81	99.97
5	A	1551	TP7	C5-C6-C7	-3.10	107.56	113.09
4	D	1550	F43	OBC-CAC-OCC	-3.06	115.46	123.33
4	D	1550	F43	C3D-C4D-ND	3.04	107.07	102.34
4	D	1550	F43	C5A-C6A-N8A	3.01	125.83	116.49
4	D	1550	F43	O7A-C6A-N8A	-2.95	114.66	122.53
4	D	1550	F43	O7C-C6C-C5C	-2.94	113.83	122.84
4	D	1550	F43	C6D-C5D-C2D	2.93	117.28	111.45
4	A	1550	F43	C2A-C3A-C4A	-2.91	97.95	102.36
4	A	1550	F43	OCC-CAC-C9C	-2.91	113.85	123.09
5	D	1551	TP7	O-C-OXT	-2.89	117.53	124.08
4	A	1550	F43	O8D-C7D-C6D	-2.85	116.20	120.87
4	D	1550	F43	OCC-CAC-C9C	-2.84	114.10	123.09
5	D	1551	TP7	O1-C1-N	-2.77	118.26	122.95
4	D	1550	F43	OBC-CAC-C9C	2.75	122.69	114.00
4	A	1550	F43	O8C-C6C-C5C	2.73	122.49	114.00
4	D	1550	F43	ODB-CCB-CBB	-2.72	114.47	123.09
4	A	1550	F43	O8D-C7D-CHD	-2.71	118.36	122.77
5	A	1551	TP7	OXT-C-CA	-2.65	113.06	121.86
4	D	1550	F43	C6D-C7D-CHD	2.65	121.82	116.94
4	A	1550	F43	OBC-CAC-OCC	-2.61	116.62	123.33
4	D	1550	F43	CHA-C4D-C3D	-2.58	110.61	117.90
4	D	1550	F43	OCD-CAD-C9D	2.57	122.00	114.00
4	A	1550	F43	C9C-C8C-C3C	-2.56	106.19	113.79
4	A	1550	F43	C2B-C3B-C4B	-2.54	98.80	101.64
4	D	1550	F43	CBB-CAB-C3B	-2.54	107.45	114.65
4	A	1550	F43	ODB-CCB-CBB	-2.48	115.22	123.09
4	D	1550	F43	C3B-C4B-CHC	-2.47	118.07	123.33
4	A	1550	F43	CHA-C4D-C3D	-2.46	110.96	117.90
4	A	1550	F43	OCD-CAD-C9D	2.43	121.56	114.00
4	D	1550	F43	C9A-C2A-C1A	2.43	113.36	107.54
4	A	1550	F43	C4D-ND-C1D	-2.39	104.88	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1551	TP7	O4P-P-O1P	-2.36	100.93	109.33
5	D	1551	TP7	C4-C3-C2	2.31	121.60	113.13
4	D	1550	F43	C3A-C4A-NA	2.29	105.78	102.30
4	A	1550	F43	O7C-C6C-C5C	-2.28	115.84	122.84
5	D	1551	TP7	O-C-CA	2.28	122.06	114.15
4	D	1550	F43	C2A-C3A-C4A	-2.28	98.91	102.36
4	D	1550	F43	C2C-C5C-C6C	-2.26	109.72	113.95
4	D	1550	F43	C9B-C2B-C3B	2.26	118.64	112.91
5	A	1551	TP7	O-C-OXT	-2.22	119.03	124.08
6	A	1552	COM	O2S-S2-O1S	2.20	120.99	113.82
4	A	1550	F43	C9B-C2B-C3B	2.19	118.47	112.91
7	D	1554	GOL	O3-C3-C2	-2.18	100.54	110.38
4	A	1550	F43	C8C-C3C-C4C	-2.17	105.04	112.19
7	B	1444	GOL	C3-C2-C1	-2.17	103.85	111.80
4	A	1550	F43	C9B-C2B-C8B	-2.15	105.21	110.61
5	A	1551	TP7	C4-C3-C2	2.14	120.97	113.13
4	D	1550	F43	C4D-ND-C1D	2.11	111.61	108.46
5	A	1551	TP7	C6-C7-S7	2.06	119.39	113.10
4	A	1550	F43	C2D-C1D-ND	2.05	115.40	110.54
4	D	1550	F43	OEB-CCB-ODB	-2.00	118.18	123.33

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1553	GOL	C1-C2-C3-O3
7	A	1555	GOL	O1-C1-C2-C3
7	A	1556	GOL	C1-C2-C3-O3
7	A	1556	GOL	O2-C2-C3-O3
7	B	1444	GOL	O1-C1-C2-C3
7	D	1554	GOL	O2-C2-C3-O3
7	D	1555	GOL	O1-C1-C2-C3
7	D	1555	GOL	C1-C2-C3-O3
7	D	1556	GOL	O1-C1-C2-C3
7	D	1556	GOL	C1-C2-C3-O3
7	D	1556	GOL	O2-C2-C3-O3
5	D	1551	TP7	C2-C3-C4-C5
7	A	1555	GOL	O1-C1-C2-O2
4	D	1550	F43	C3A-CAA-CBA-CCA
4	A	1550	F43	C3A-CAA-CBA-CCA
7	D	1554	GOL	C1-C2-C3-O3
7	B	1444	GOL	O1-C1-C2-O2

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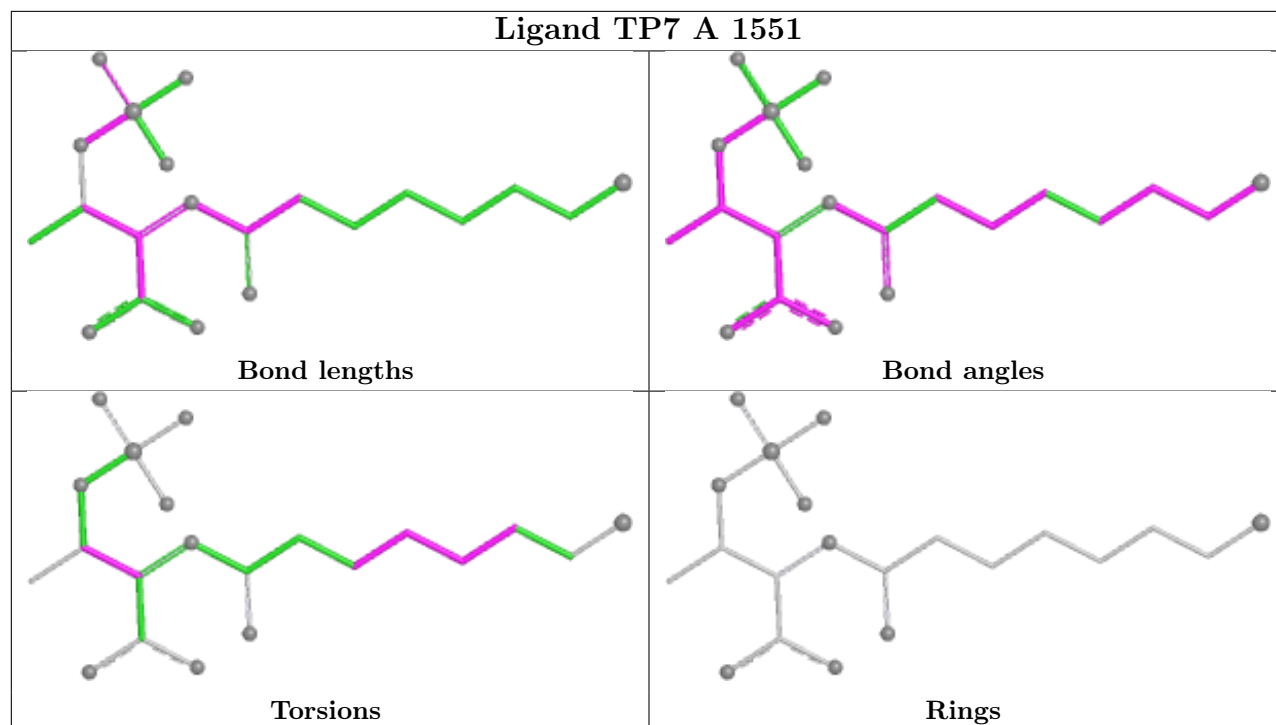
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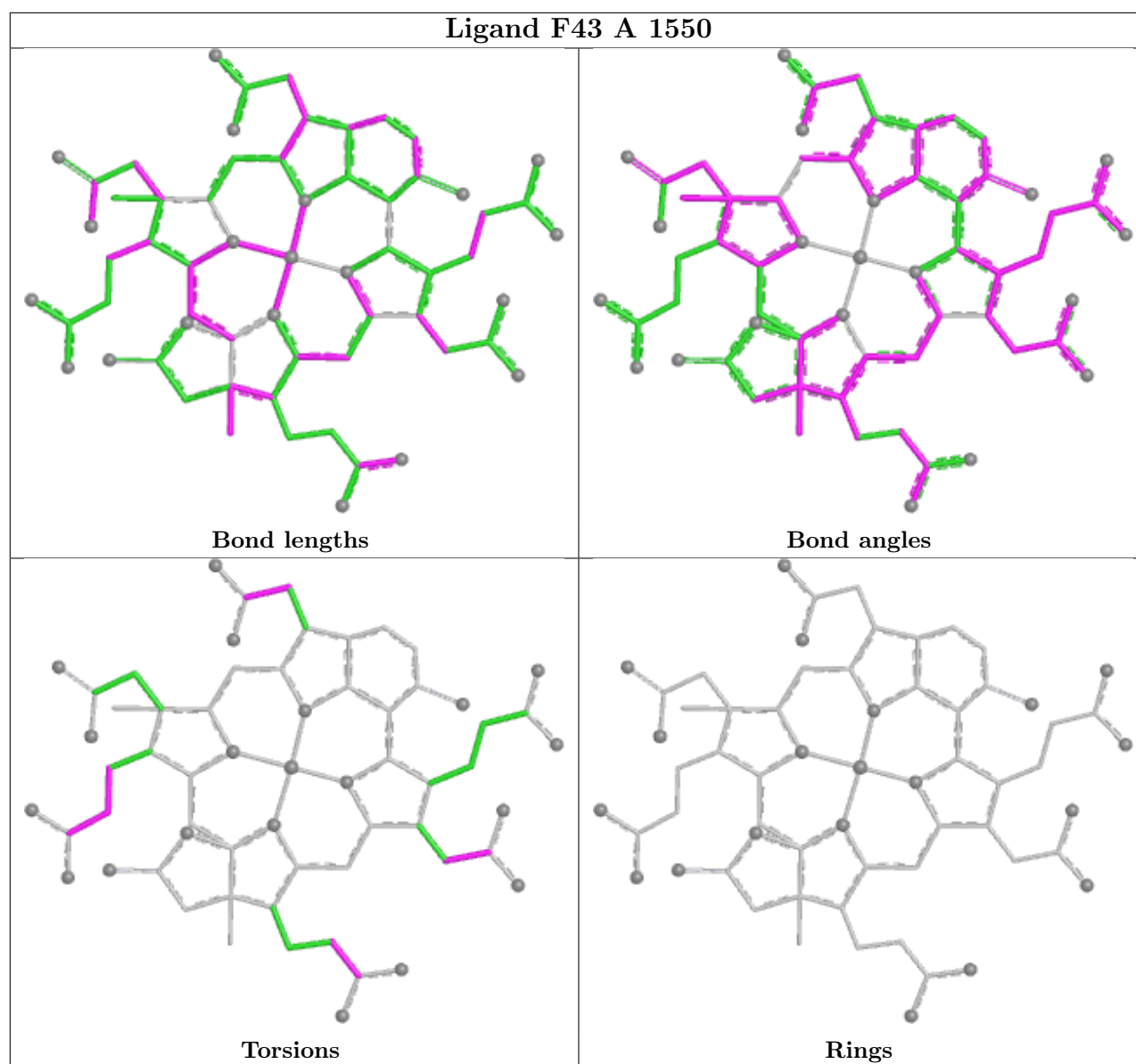
Mol	Chain	Res	Type	Atoms
7	D	1555	GOL	O1-C1-C2-O2
7	D	1555	GOL	O2-C2-C3-O3
7	E	1444	GOL	O2-C2-C3-O3
5	D	1551	TP7	O1-C1-N-CA
5	A	1551	TP7	C2-C3-C4-C5
5	D	1551	TP7	C3-C4-C5-C6
7	A	1553	GOL	O2-C2-C3-O3
7	D	1556	GOL	O1-C1-C2-O2
5	A	1551	TP7	C3-C4-C5-C6
5	A	1551	TP7	C-CA-CB-O4P
4	A	1550	F43	C2C-C5C-C6C-O8C
6	D	1552	COM	C1-C2-S2-O2S
4	A	1550	F43	CAA-CBA-CCA-OEA
7	E	1444	GOL	O1-C1-C2-C3
7	E	1444	GOL	C1-C2-C3-O3
5	A	1551	TP7	C4-C5-C6-C7
5	D	1551	TP7	C4-C5-C6-C7
4	D	1550	F43	C2C-C5C-C6C-O7C
4	D	1550	F43	CAB-CBB-CCB-OEB
4	D	1550	F43	CAA-CBA-CCA-OEA
5	A	1551	TP7	C-CA-CB-CG
4	D	1550	F43	CAA-CBA-CCA-ODA
4	A	1550	F43	CAB-CBB-CCB-ODB
4	A	1550	F43	C3D-C9D-CAD- OCD
4	A	1550	F43	CAA-CBA-CCA-ODA
4	A	1550	F43	C3D-C9D-CAD- OBD
4	D	1550	F43	C3D-C9D-CAD- OCD

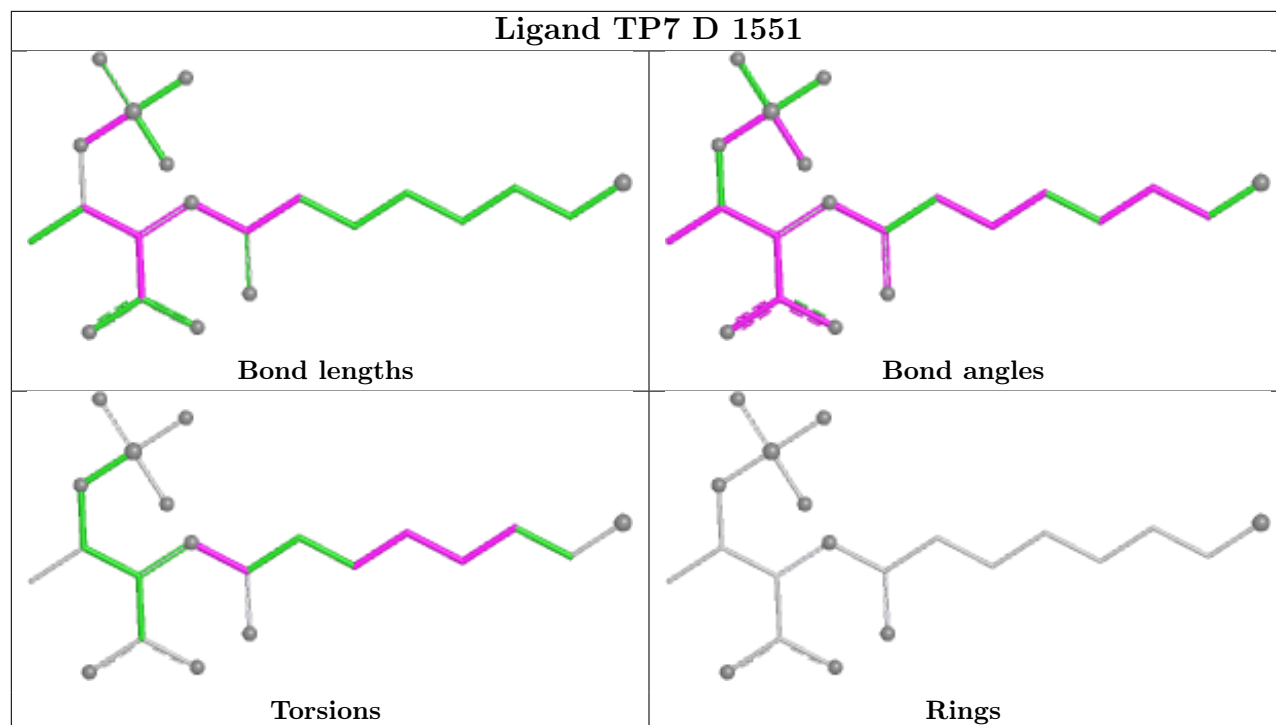
There are no ring outliers.

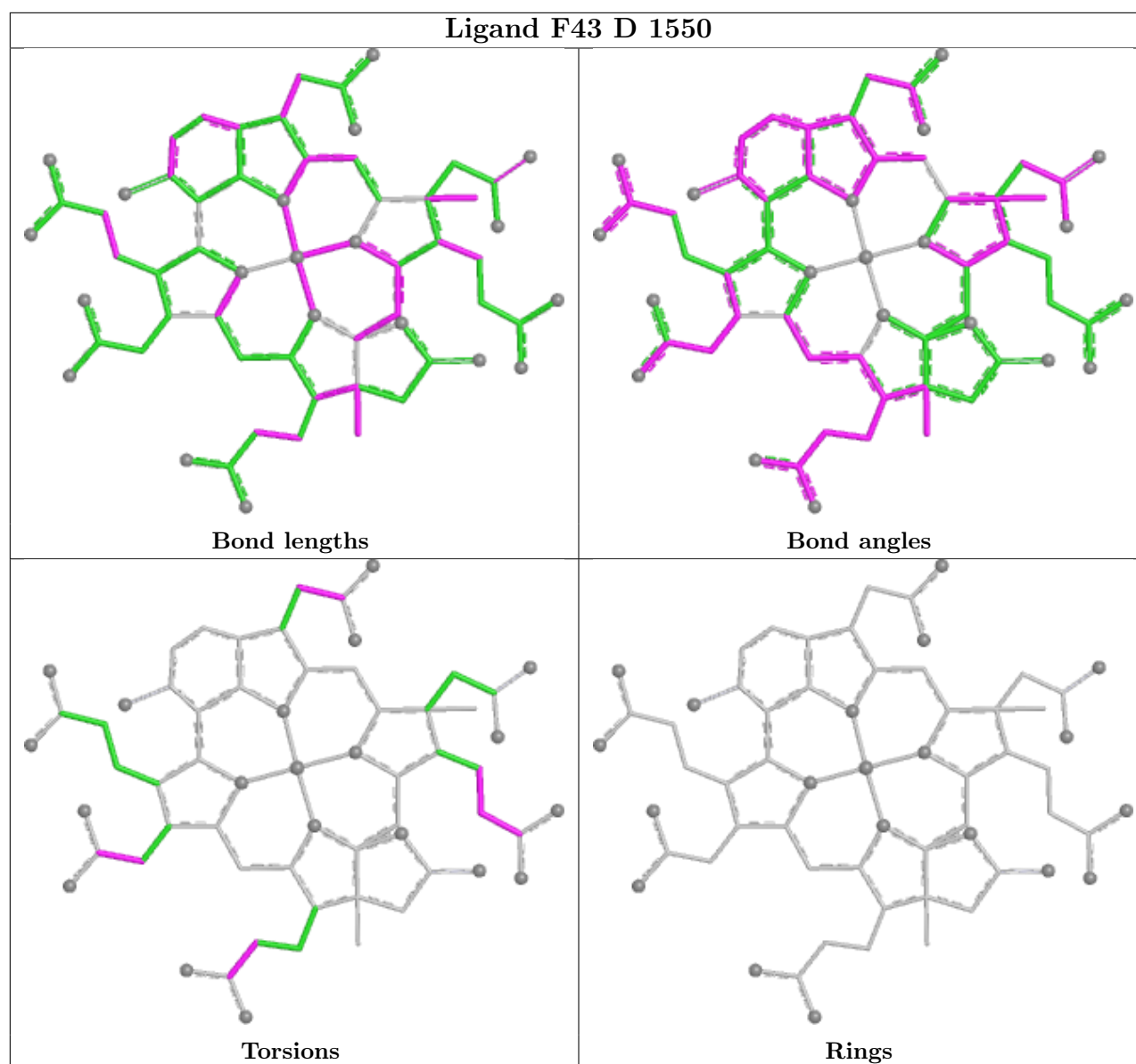
No monomer is involved in short contacts.

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.









4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates

EDS was not executed - this section is therefore empty.

5.4 Ligands

EDS was not executed - this section is therefore empty.

5.5 Other polymers

EDS was not executed - this section is therefore empty.