wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2026 – 04:23 am BST

PDB ID	:	1HBN / pdb_00001hbn
Title	:	METHYL-COENZYME M REDUCTASE
Authors	:	Ermler, U.; Grabarse, W.
Deposited on	:	2001-04-20
Resolution	:	1.16 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
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)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.16 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.

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
7	GOL	D	1556	-	X	-	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 21958 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 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	23	13	0
			4291	2712	723	836	20			
1	D	548	Total	C	N	O	S	23	16	0
			4296	2717	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

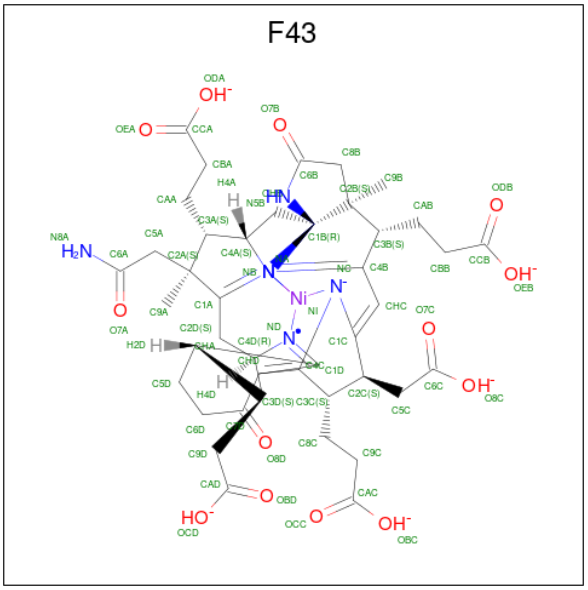
- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE I BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	26	15	0
			3348	2115	557	654	22			
2	E	442	Total	C	N	O	S	41	12	0
			3340	2115	551	653	21			

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

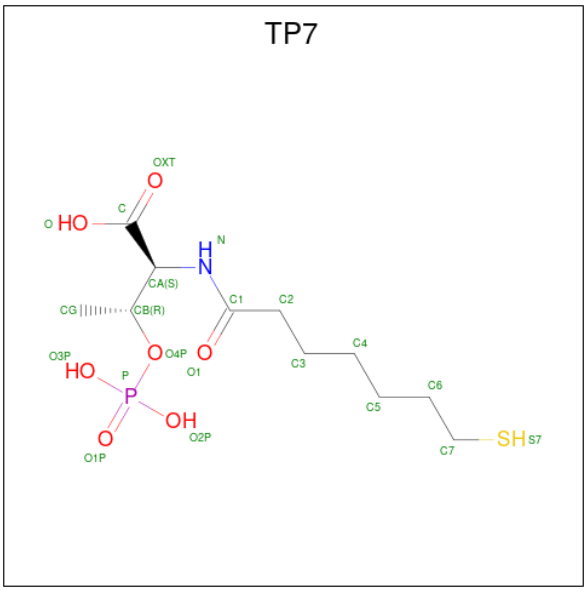
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total	C	N	O	S	39	5	0
			2007	1242	355	398	12			
3	F	247	Total	C	N	O	S	44	5	0
			2006	1242	354	398	12			

- Molecule 4 is FACTOR 430 (CCD ID: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$).



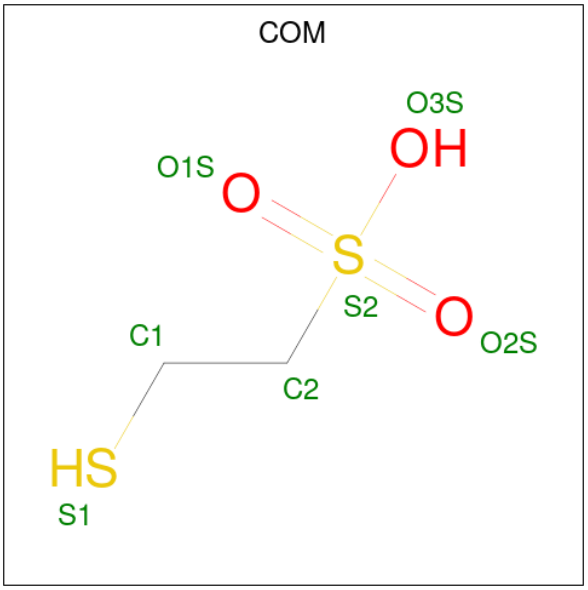
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
4	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

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



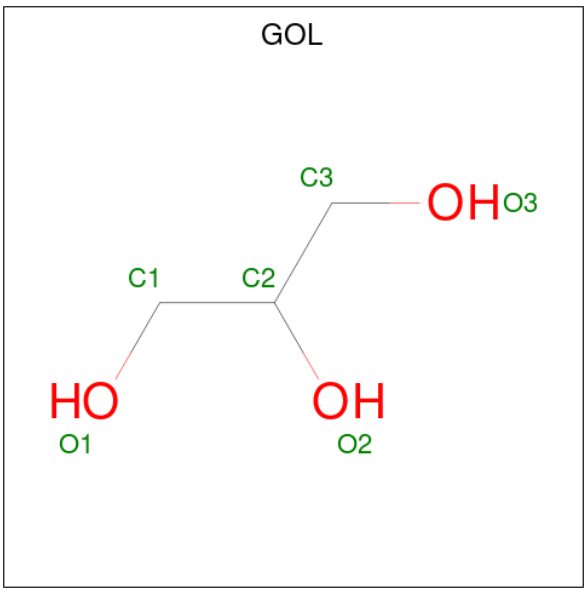
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
5	D	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		

- Molecule 6 is 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 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	C	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0
7	E	1	Total C O 6 3 3	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	5	Total Na 5 5	0	0
10	B	2	Total Na 2 2	0	0
10	D	3	Total Na 3 3	0	0

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

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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	489	Total O 489 489	0	29

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	423	Total O 423 423	0	31
12	C	294	Total O 294 294	0	25
12	D	510	Total O 510 510	0	37
12	E	402	Total O 402 402	0	33
12	F	275	Total O 275 275	0	15

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

3 Data and refinement statistics (i)

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	81.72Å 116.88Å 122.58Å 90.00° 92.02° 90.00°	Depositor
Resolution (Å)	30.00 – 1.16	Depositor
% Data completeness (in resolution range)	93.1 (30.00-1.16)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.124 , 0.190	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21958	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

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

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	MHS	D	257	1	10,11,12	1.52	1 (10%)	6,14,16	4.35	2 (33%)
1	GL3	D	445	1	2,3,4	3.10	1 (50%)	1,2,4	0.21	0
1	SMC	D	452	1	5,6,7	0.95	0	2,6,8	1.41	0
1	AGM	D	271	1	10,11,12	0.90	0	6,13,15	0.94	0

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	0.77	0	6,13,15	1.00	0
1	MHS	A	257	1	10,11,12	1.66	1 (10%)	6,14,16	2.46	2 (33%)
1	MGN	D	400	1	6,9,10	1.21	1 (16%)	5,12,14	0.72	0
1	GL3	A	445	1	2,3,4	2.45	1 (50%)	1,2,4	0.03	0
1	SMC	A	452	1	5,6,7	0.63	0	2,6,8	0.96	0
1	MGN	A	400	1	6,9,10	0.72	0	5,12,14	0.80	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	D	257	1	-	0/5/6/8	0/1/1/1
1	GL3	D	445	1	-	0/1/1/2	-
1	SMC	D	452	1	-	1/3/5/7	-
1	AGM	D	271	1	-	3/10/11/13	-
1	AGM	A	271	1	-	3/10/11/13	-
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1
1	MGN	D	400	1	-	0/7/9/12	-
1	GL3	A	445	1	-	1/1/1/2	-
1	SMC	A	452	1	-	1/3/5/7	-
1	MGN	A	400	1	-	0/7/9/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	MHS	CM-ND1	4.39	1.55	1.46
1	D	445	GL3	C-S	-4.38	1.65	1.80
1	D	257	MHS	CM-ND1	3.99	1.54	1.46
1	A	445	GL3	C-S	-3.43	1.68	1.80
1	D	400	MGN	CB1-CA	-2.29	1.52	1.55

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	257	MHS	ND1-CE1-NE2	-9.62	107.30	112.93
1	A	257	MHS	ND1-CE1-NE2	-4.82	110.11	112.93
1	D	257	MHS	CD2-NE2-CE1	4.25	110.40	105.22
1	A	257	MHS	CD2-NE2-CE1	3.04	108.93	105.22

There are no chirality outliers.

5 of 9 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	A	271	AGM	CE2-CD-NE1-CZ
1	D	271	AGM	CE2-CD-NE1-CZ
1	A	445	GL3	S-C-CA-N

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 48 ligands modelled in this entry, 31 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	$\#\|Z\| > 2$
6	COM	D	1552	4	6,6,6	1.35	1 (16%)	7,8,8	0.56	0
7	GOL	D	1555	-	5,5,5	0.66	0	5,5,5	0.99	0
7	GOL	A	1553	10	5,5,5	0.35	0	5,5,5	1.96	2 (40%)
4	F43	A	1550	6,1	61,71,71	2.34	12 (19%)	64,118,118	1.63	11 (17%)
7	GOL	A	1555	-	5,5,5	0.88	0	5,5,5	0.98	0
7	GOL	C	1249	-	5,5,5	0.50	0	5,5,5	0.37	0
7	GOL	D	1556	-	5,5,5	1.07	1 (20%)	5,5,5	1.68	2 (40%)
7	GOL	D	1553	-	5,5,5	0.77	0	5,5,5	0.85	0
7	GOL	E	1444	-	5,5,5	0.81	0	5,5,5	0.84	0
7	GOL	D	1554	10	5,5,5	0.55	0	5,5,5	0.58	0
5	TP7	A	1551	-	19,20,20	1.57	3 (15%)	24,26,26	1.11	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	GOL	A	1556	-	5,5,5	1.05	0	5,5,5	1.00	1 (20%)
6	COM	A	1552	4	6,6,6	1.43	2 (33%)	7,8,8	1.23	1 (14%)
4	F43	D	1550	6,1	61,71,71	2.77	11 (18%)	64,118,118	1.50	15 (23%)
7	GOL	B	1444	-	5,5,5	1.21	1 (20%)	5,5,5	1.24	0
7	GOL	A	1554	-	5,5,5	0.62	0	5,5,5	1.28	1 (20%)
5	TP7	D	1551	-	19,20,20	1.84	5 (26%)	24,26,26	1.10	2 (8%)

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
6	COM	D	1552	4	-	0/4/4/4	-
7	GOL	D	1555	-	-	0/4/4/4	-
7	GOL	A	1553	10	-	2/4/4/4	-
4	F43	A	1550	6,1	-	9/28/185/185	-
7	GOL	A	1555	-	-	2/4/4/4	-
7	GOL	C	1249	-	-	0/4/4/4	-
7	GOL	D	1556	-	-	4/4/4/4	-
7	GOL	D	1553	-	-	0/4/4/4	-
7	GOL	E	1444	-	-	0/4/4/4	-
7	GOL	D	1554	10	-	0/4/4/4	-
5	TP7	A	1551	-	-	0/24/24/24	-
7	GOL	A	1556	-	-	0/4/4/4	-
6	COM	A	1552	4	-	0/4/4/4	-
4	F43	D	1550	6,1	-	9/28/185/185	-
7	GOL	B	1444	-	-	2/4/4/4	-
7	GOL	A	1554	-	-	0/4/4/4	-
5	TP7	D	1551	-	-	0/24/24/24	-

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1550	F43	NI-NA	12.74	2.17	1.89
4	D	1550	F43	NI-NB	11.20	2.13	1.89
4	A	1550	F43	NI-NA	9.86	2.10	1.89
4	A	1550	F43	NI-NB	8.52	2.07	1.89
4	D	1550	F43	NI-ND	7.29	2.05	1.89

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1550	F43	C3D-C4D-ND	5.02	110.16	102.34
4	A	1550	F43	C5D-C2D-C1D	4.78	116.88	110.45
4	A	1550	F43	CAB-C3B-C2B	-3.99	110.64	119.09
4	D	1550	F43	CAB-C3B-C2B	-3.79	111.08	119.09
4	D	1550	F43	C3B-C4B-CHC	-3.52	115.72	123.32

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

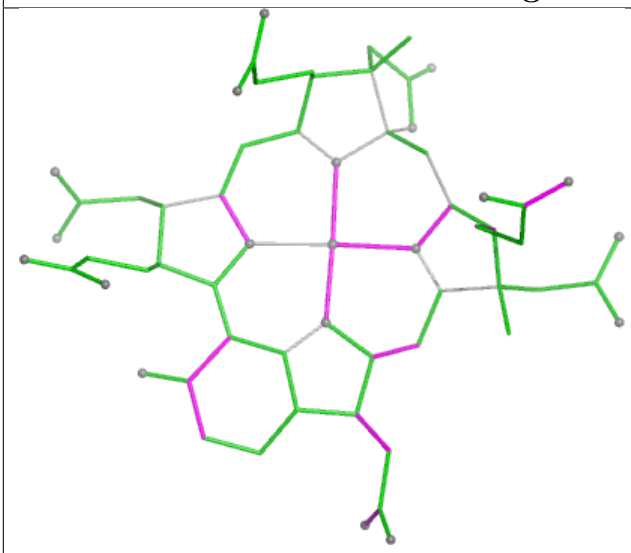
Mol	Chain	Res	Type	Atoms
7	A	1553	GOL	C1-C2-C3-O3
7	B	1444	GOL	C1-C2-C3-O3
7	D	1556	GOL	O1-C1-C2-C3
7	D	1556	GOL	C1-C2-C3-O3
7	D	1556	GOL	O2-C2-C3-O3

There are no ring outliers.

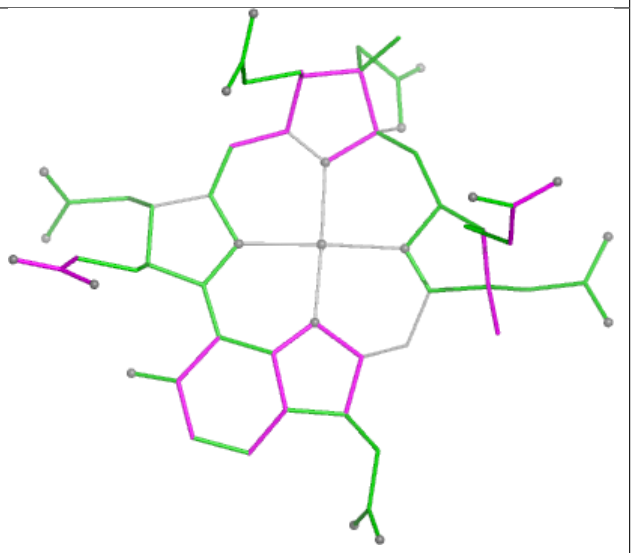
No monomer is involved in short contacts.

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 then 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.

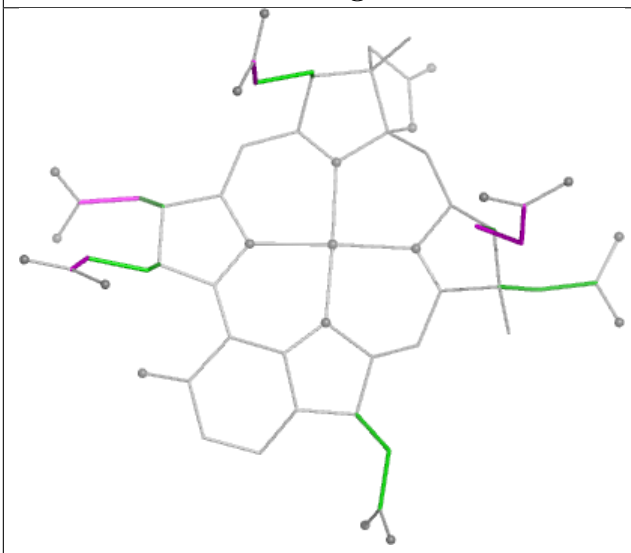
Ligand F43 A 1550



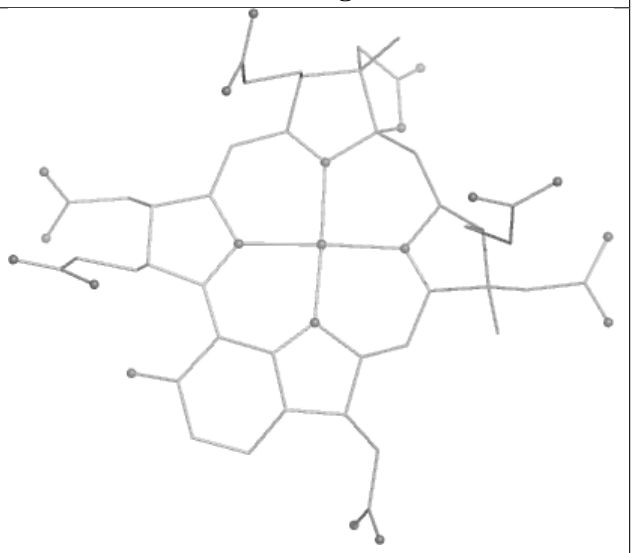
Bond lengths



Bond angles

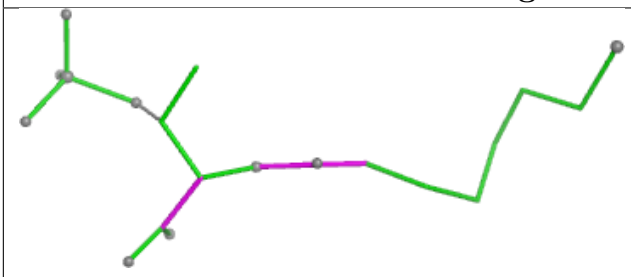


Torsions

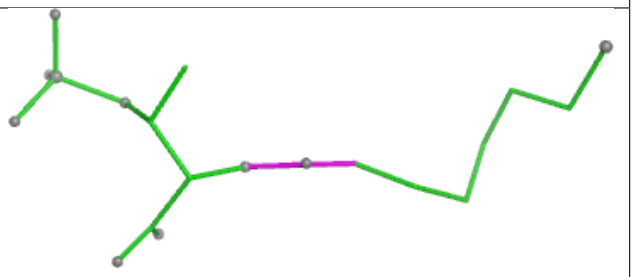


Rings

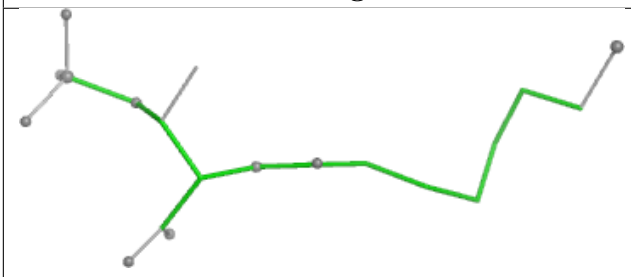
Ligand TP7 A 1551



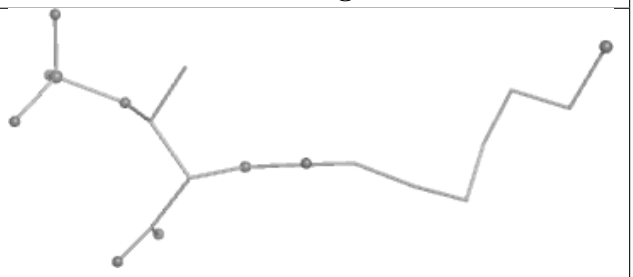
Bond lengths



Bond angles

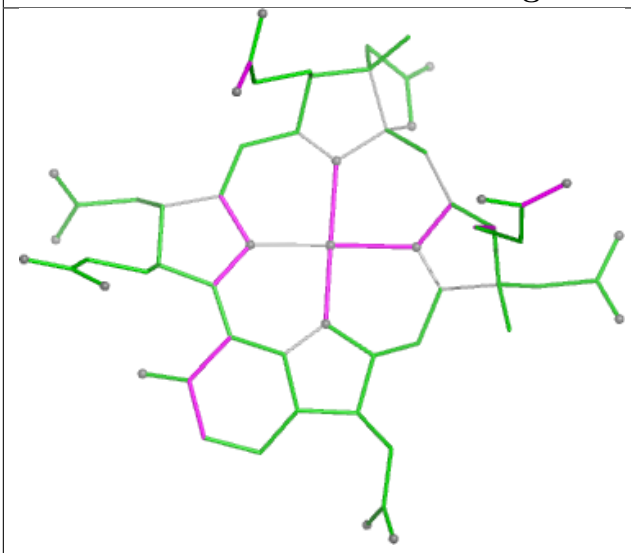


Torsions

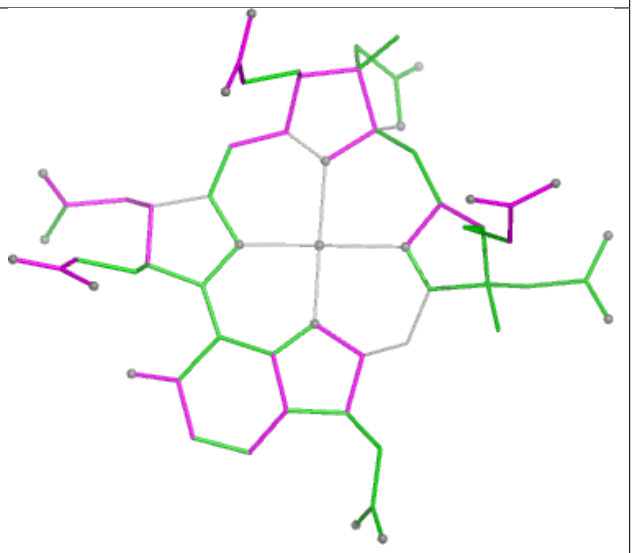


Rings

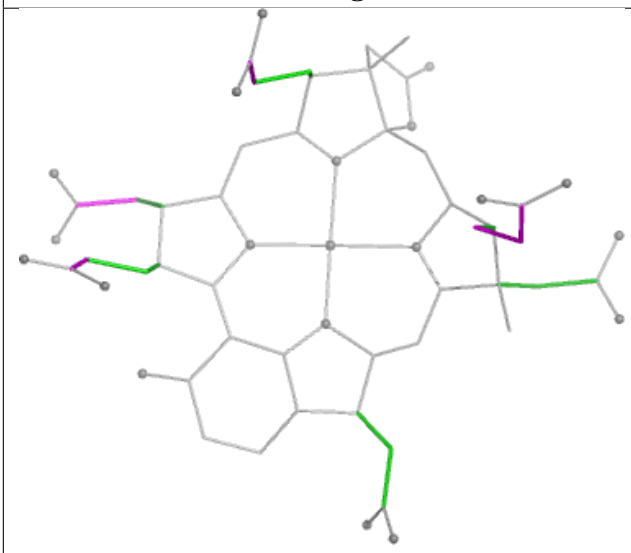
Ligand F43 D 1550



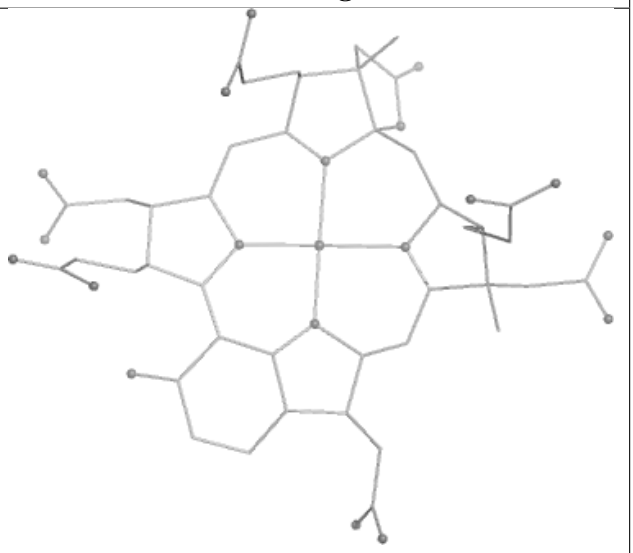
Bond lengths



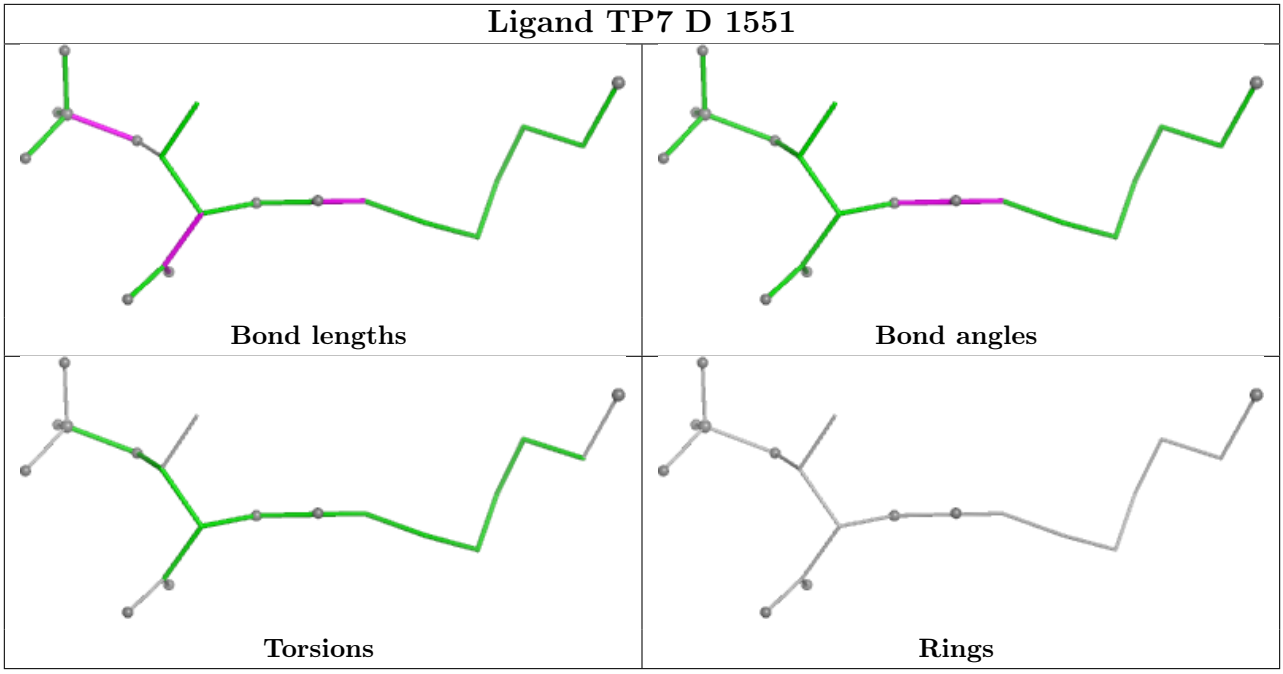
Bond angles



Torsions



Rings



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.