wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 06:15 am GMT

PDB ID	:	1E6Y
Title	:	Methyl-coenzyme M reductase from Methanosarcina barkeri
Authors	:	Grabarse, W.; Ermler, U.
Deposited on	:	2000-08-23
Resolution	:	1.60 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

PERCENTILES INFOmissingINFO

1 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 21340 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 SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	568	4346	2735	737	846	28	0	4	0
1	D	568	4348	2738	740	842	28	0	3	0

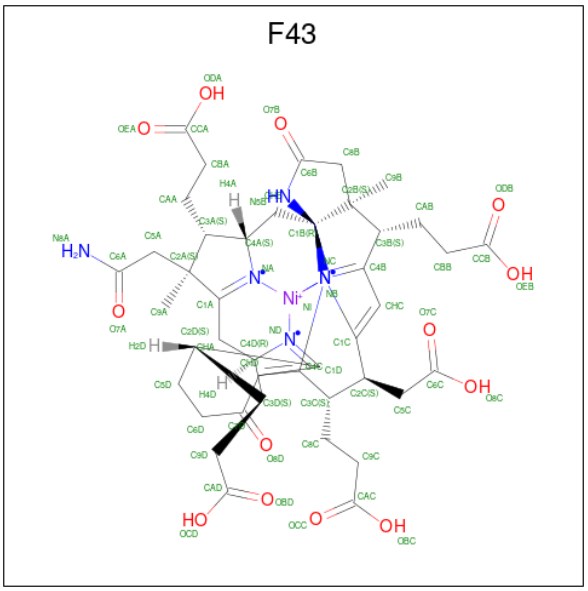
- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE I BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	432	3176	1987	549	621	19	0	4	0
2	E	433	3178	1990	550	620	18	0	1	0

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

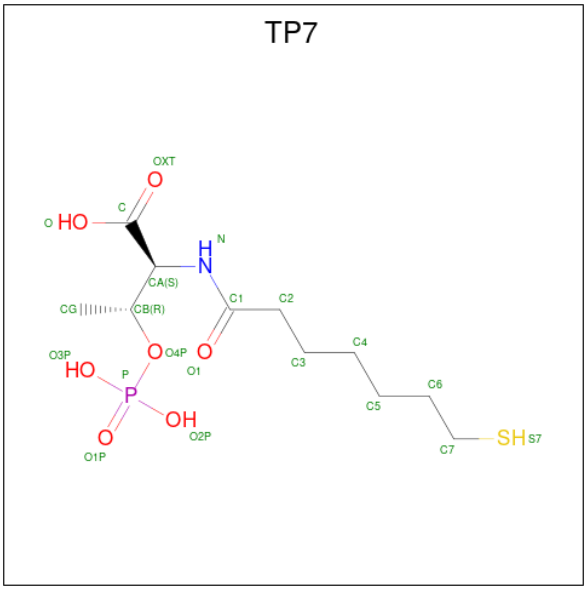
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	247	1947	1202	359	375	11	0	0	0
3	F	247	1950	1205	359	375	11	0	1	0

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



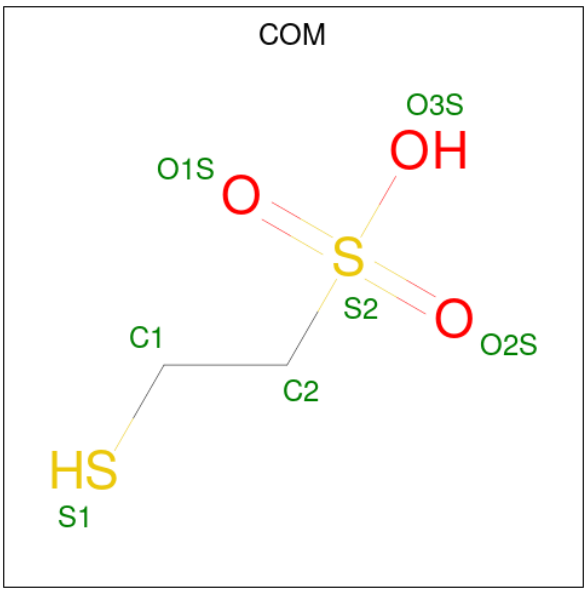
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	Ni	O		
4	A	1	62	42	6	1	13	0	0
4	D	1	62	42	6	1	13	0	0

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



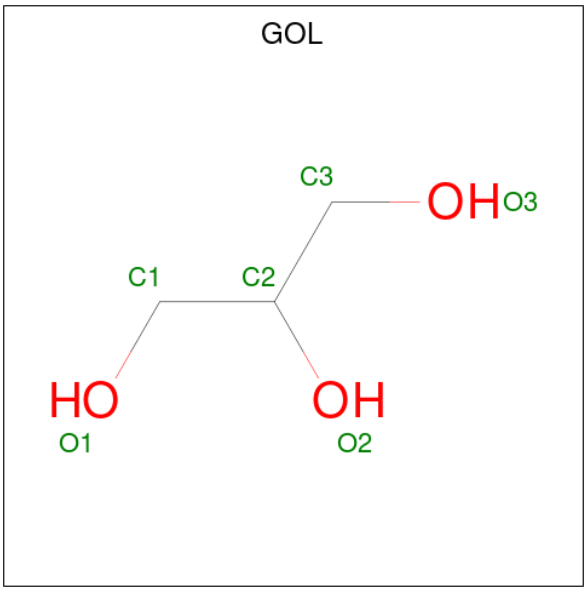
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
5	A	1	21	11	1	7	1	1	0	0
5	D	1	21	11	1	7	1	1	0	0

- Molecule 6 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: $C_2H_6O_3S_2$).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	489	489	489	0	0
			Total	O		
8	B	340	342	342	0	2
			Total	O		
8	C	241	241	241	0	0
			Total	O		
8	D	522	522	522	0	0
			Total	O		
8	E	339	339	339	0	0
			Total	O		
8	F	264	264	264	0	0

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.68Å 153.10Å 153.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60	Depositor
% Data completeness (in resolution range)	89.0 (30.00-1.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.98 (at 1.60Å)	Xtriage
Refinement program	CNS 0.3	Depositor
R, R_{free}	0.160 , 0.179	Depositor
Wilson B-factor (Å^2)	11.0	Xtriage
Anisotropy	0.817	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
Total number of atoms	21340	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2047e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

3 Model quality (i)

3.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: COM, AGM, F43, TP7, MHS, GOL, OCS, GL3, SMC

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	0.31	0/4423	0.68	9/5988 (0.2%)
1	D	0.64	6/4418 (0.1%)	1.95	26/5979 (0.4%)
2	B	0.29	0/3244	0.61	8/4390 (0.2%)
2	E	0.30	0/3231	0.65	8/4372 (0.2%)
3	C	0.31	0/1976	0.85	17/2666 (0.6%)
3	F	0.32	0/1983	1.85	15/2676 (0.6%)
All	All	0.41	6/19275 (0.0%)	1.24	83/26071 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	2
2	B	0	2
2	E	0	3
3	C	0	1
3	F	0	1
All	All	0	11

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4551[A]	ARG	CZ-NH2	22.62	1.62	1.33
1	D	4551[B]	ARG	CZ-NH2	22.62	1.62	1.33
1	D	4551[A]	ARG	NE-CZ	10.05	1.46	1.33
1	D	4551[B]	ARG	NE-CZ	10.05	1.46	1.33
1	D	4551[A]	ARG	CG-CD	-8.02	1.31	1.51

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	4551[A]	ARG	NH1-CZ-NH2	-85.30	25.57	119.40
1	D	4551[B]	ARG	NH1-CZ-NH2	-85.30	25.57	119.40
3	F	6040[A]	VAL	CG1-CB-CG2	-59.08	16.37	110.90
3	F	6040[B]	VAL	CG1-CB-CG2	-59.08	16.37	110.90
1	D	4551[A]	ARG	NE-CZ-NH2	-44.85	97.87	120.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1396[A]	GLU	Sidechain
1	A	1396[B]	GLU	Sidechain
2	B	2331	TYR	Sidechain
2	B	2347	TYR	Sidechain
3	C	3093	TYR	Sidechain

3.2 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	4346	0	4191	39	0
1	D	4348	0	4205	50	0
2	B	3176	0	3161	17	0
2	E	3178	0	3170	22	0
3	C	1947	0	1888	9	0
3	F	1950	0	1894	13	0
4	A	62	0	43	6	0
4	D	62	0	43	5	0
5	A	21	0	19	2	0
5	D	21	0	19	1	0
6	A	7	0	5	1	0
6	D	7	0	5	0	0
7	A	12	0	16	0	0
7	D	6	0	8	0	0
8	A	489	0	0	5	0
8	B	342	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	241	0	0	1	0
8	D	522	0	0	4	0
8	E	339	0	0	4	0
8	F	264	0	0	2	0
All	All	21340	0	18667	131	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 3.

The worst 5 of 131 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)
1:D:4551[B]:ARG:NH2	1:D:4551[B]:ARG:CZ	1.69	1.56
1:D:4551[B]:ARG:CD	1:D:4551[B]:ARG:CG	1.76	1.55
1:D:4551[B]:ARG:CG	1:D:4551[B]:ARG:NE	1.87	1.38
1:D:4551[B]:ARG:CD	1:D:4551[B]:ARG:CB	2.38	1.01
1:D:4551[B]:ARG:HE	1:D:4551[B]:ARG:HG2	1.24	1.01

There are no symmetry-related clashes.

3.3 Torsion angles (i)

3.3.1 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	566/569 (100%)	546 (96%)	19 (3%)	1 (0%)	47	26
1	D	565/569 (99%)	546 (97%)	18 (3%)	1 (0%)	47	26
2	B	434/433 (100%)	428 (99%)	6 (1%)	0	100	100
2	E	432/433 (100%)	426 (99%)	6 (1%)	0	100	100
3	C	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
3	F	245/247 (99%)	237 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2486/2498 (100%)	2422 (97%)	62 (2%)	2 (0%)	51 29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1525	VAL
1	D	4525	VAL

3.3.2 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	446/443 (101%)	436 (98%)	10 (2%)	52 27
1	D	445/443 (100%)	436 (98%)	9 (2%)	55 31
2	B	335/332 (101%)	333 (99%)	2 (1%)	86 77
2	E	333/332 (100%)	331 (99%)	2 (1%)	86 77
3	C	201/201 (100%)	197 (98%)	4 (2%)	55 31
3	F	202/201 (100%)	198 (98%)	4 (2%)	55 31
All	All	1962/1952 (100%)	1931 (98%)	31 (2%)	65 41

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	3178	LEU
3	F	6176	ARG
1	D	4131	GLU
3	F	6195	ASP
1	D	4551[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	3239	GLN
1	D	4019	GLN
3	F	6133	GLN
2	E	5402	GLN
2	B	2241	GLN

3.3.3 RNA (i)

There are no RNA molecules in this entry.

3.4 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	MHS	D	4271	1	7,11,12	1.81	1 (14%)	6,14,16	1.29	1 (16%)
3	OCS	F	6065	3	7,8,9	1.24	2 (28%)	6,11,13	1.68	3 (50%)
3	OCS	C	3065	3	7,8,9	1.34	2 (28%)	6,11,13	1.70	2 (33%)
1	MHS	A	1271	1	7,11,12	1.82	1 (14%)	6,14,16	1.35	1 (16%)
1	SMC	A	1472	1	5,6,7	0.61	0	2,6,8	0.53	0
1	AGM	A	1285	1	10,11,12	0.49	0	6,13,15	0.33	0
1	AGM	D	4285	1	10,11,12	0.46	0	6,13,15	0.25	0
1	SMC	D	4472	1	5,6,7	0.60	0	2,6,8	0.52	0
1	GL3	A	1465	1	2,3,4	3.52	1 (50%)	1,2,4	0.12	0
1	GL3	D	4465	1	2,3,4	3.47	1 (50%)	1,2,4	0.03	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	4271	1	-	0/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OCS	F	6065	3	-	0/4/7/9	-
3	OCS	C	3065	3	-	0/4/7/9	-
1	MHS	A	1271	1	-	0/5/6/8	0/1/1/1
1	SMC	A	1472	1	-	1/3/5/7	-
1	AGM	A	1285	1	-	0/10/11/13	-
1	AGM	D	4285	1	-	0/10/11/13	-
1	SMC	D	4472	1	-	1/3/5/7	-
1	GL3	A	1465	1	-	1/1/1/2	-
1	GL3	D	4465	1	-	1/1/1/2	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1465	GL3	C-S	-4.97	1.63	1.80
1	D	4465	GL3	C-S	-4.91	1.63	1.80
1	D	4271	MHS	CM-ND1	4.57	1.58	1.47
1	A	1271	MHS	CM-ND1	4.49	1.57	1.47
3	C	3065	OCS	OD1-SG	2.29	1.51	1.45

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3065	OCS	OD3-SG-CB	2.55	109.97	106.94
3	F	6065	OCS	OD2-SG-CB	2.43	109.61	105.74
3	C	3065	OCS	OD2-SG-CB	2.20	109.25	105.74
1	D	4271	MHS	NE2-CE1-ND1	-2.10	109.14	112.26
1	A	1271	MHS	NE2-CE1-ND1	-2.10	109.14	112.26

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1472	SMC	CA-CB-SG-CS
1	D	4472	SMC	CA-CB-SG-CS
1	A	1465	GL3	S-C-CA-N
1	D	4465	GL3	S-C-CA-N

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	4271	MHS	1	0
1	A	1271	MHS	1	0
1	A	1472	SMC	1	0
1	D	4472	SMC	1	0
1	A	1465	GL3	1	0
1	D	4465	GL3	1	0

3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

3.6 Ligand geometry (i)

9 ligands 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	$\#\|Z\| > 2$
5	TP7	D	5571	-	19,20,20	2.05	4 (21%)	24,26,26	1.23	2 (8%)
4	F43	A	2570	6,1	61,71,71	3.85	20 (32%)	64,118,118	2.11	15 (23%)
6	COM	D	5572	4	6,6,6	1.56	1 (16%)	7,8,8	1.39	1 (14%)
7	GOL	A	2573	-	5,5,5	1.02	0	5,5,5	0.49	0
7	GOL	A	2574	-	5,5,5	0.89	0	5,5,5	0.48	0
5	TP7	A	2571	-	19,20,20	2.03	5 (26%)	24,26,26	1.23	2 (8%)
6	COM	A	2572	4	6,6,6	1.66	2 (33%)	7,8,8	1.35	1 (14%)
7	GOL	D	5573	-	5,5,5	1.05	0	5,5,5	0.55	0
4	F43	D	5570	6,1	61,71,71	3.87	21 (34%)	64,118,118	2.10	16 (25%)

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	TP7	D	5571	-	-	2/24/24/24	-
4	F43	A	2570	6,1	-	10/28/185/185	-
6	COM	D	5572	4	-	2/4/4/4	-
7	GOL	A	2573	-	-	1/4/4/4	-
7	GOL	A	2574	-	-	0/4/4/4	-
5	TP7	A	2571	-	-	2/24/24/24	-
6	COM	A	2572	4	-	0/4/4/4	-
7	GOL	D	5573	-	-	0/4/4/4	-
4	F43	D	5570	6,1	-	10/28/185/185	-

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5570	F43	CHB-C1B	-18.14	1.41	1.53
4	A	2570	F43	CHB-C1B	-17.79	1.41	1.53
4	D	5570	F43	NI-NA	12.09	2.15	1.89
4	A	2570	F43	NI-NA	12.02	2.15	1.89
4	D	5570	F43	CHD-C1D	10.48	1.57	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2570	F43	C4D-ND-C1D	-5.83	100.85	108.51
4	D	5570	F43	C4D-ND-C1D	-5.71	101.00	108.51
4	A	2570	F43	CAB-C3B-C2B	-5.62	107.20	119.09
4	D	5570	F43	CAB-C3B-C2B	-5.60	107.24	119.09
4	A	2570	F43	C3B-C4B-CHC	-5.60	111.24	123.32

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2570	F43	C3A-CAA-CBA-CCA
4	D	5570	F43	C3A-CAA-CBA-CCA
5	D	5571	TP7	O1-C1-N-CA
5	A	2571	TP7	O1-C1-N-CA
5	D	5571	TP7	C2-C1-N-CA

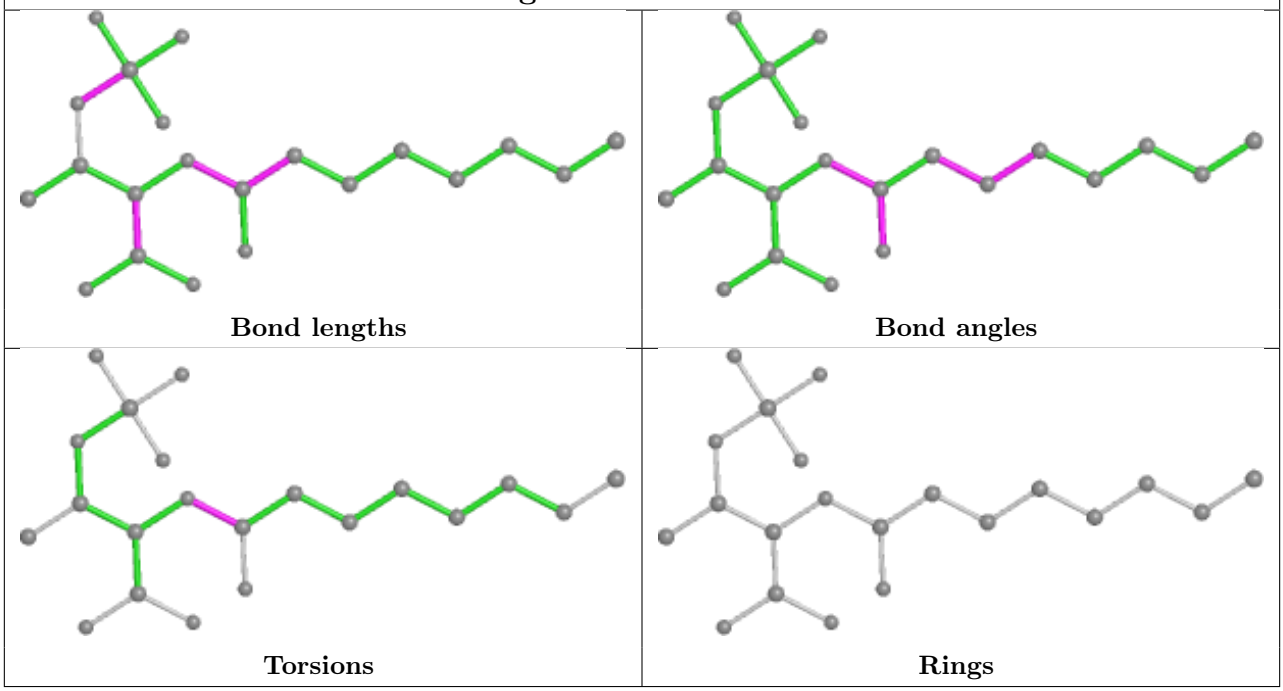
There are no ring outliers.

5 monomers are involved in 15 short contacts:

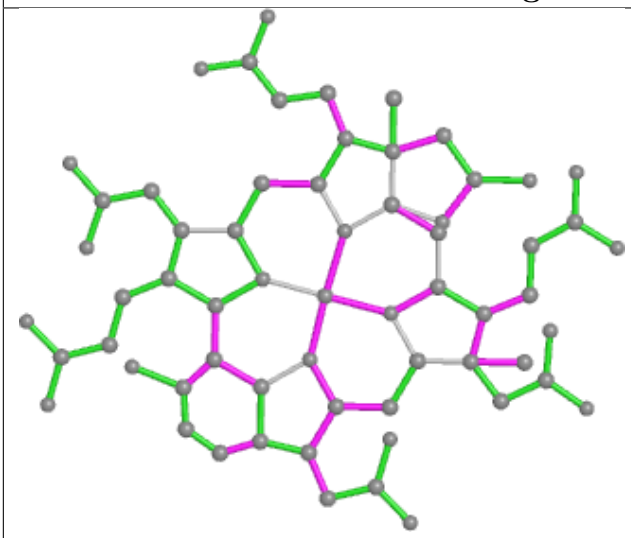
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	5571	TP7	1	0
4	A	2570	F43	6	0
5	A	2571	TP7	2	0
6	A	2572	COM	1	0
4	D	5570	F43	5	0

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 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.

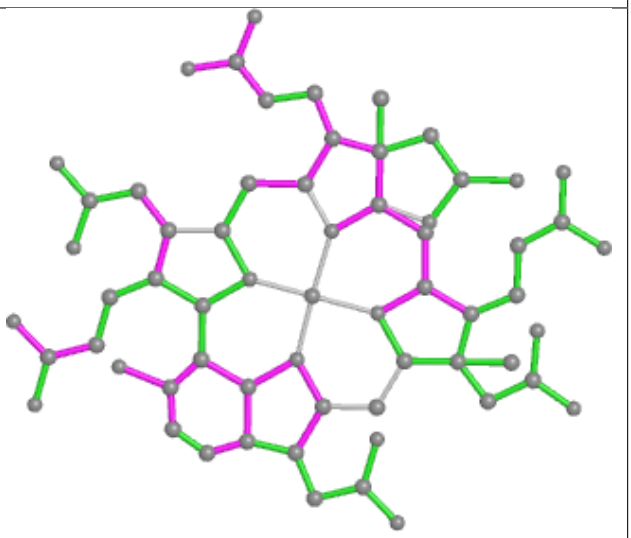
Ligand TP7 D 5571



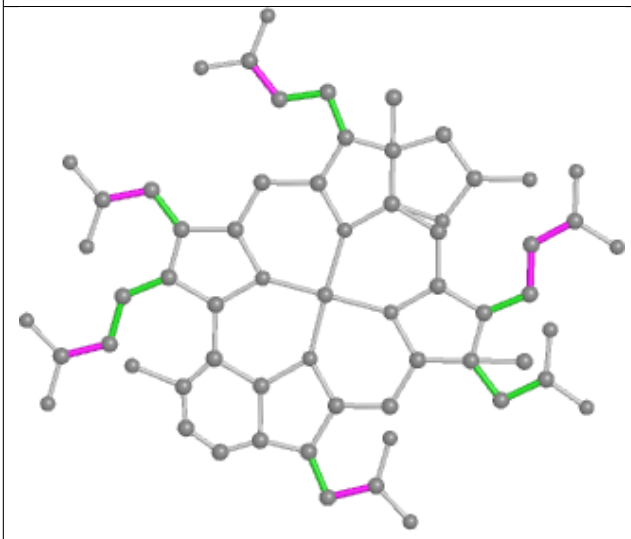
Ligand F43 A 2570



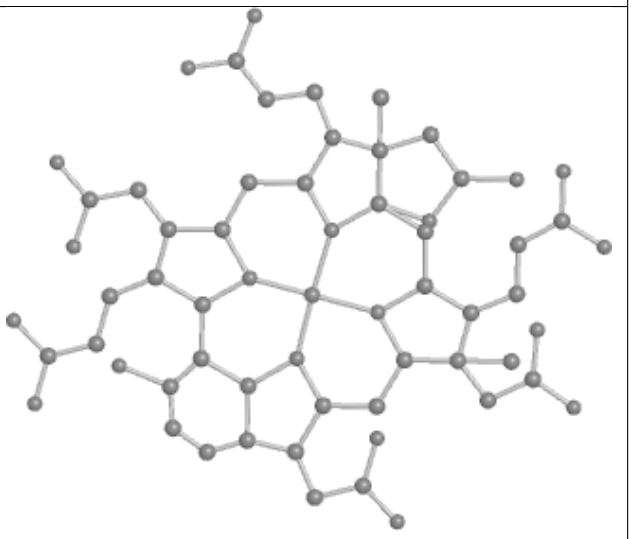
Bond lengths



Bond angles

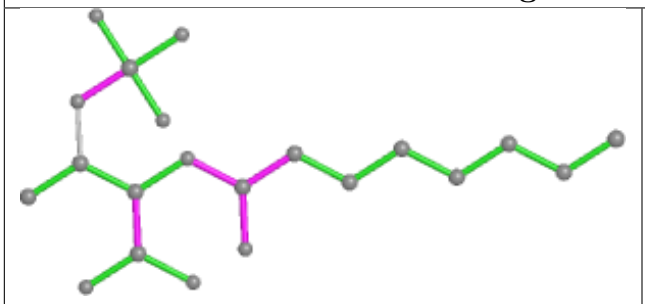


Torsions

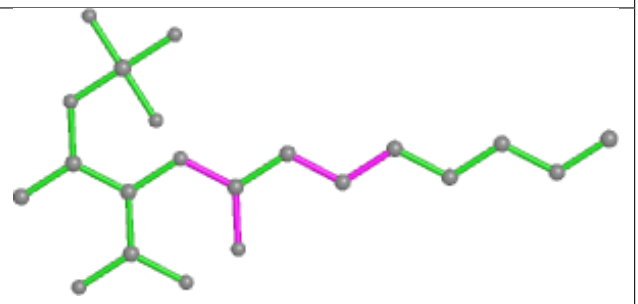


Rings

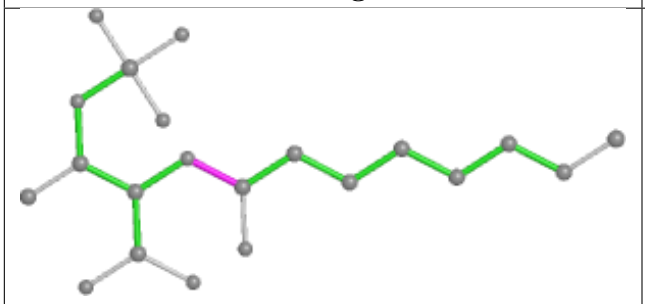
Ligand TP7 A 2571



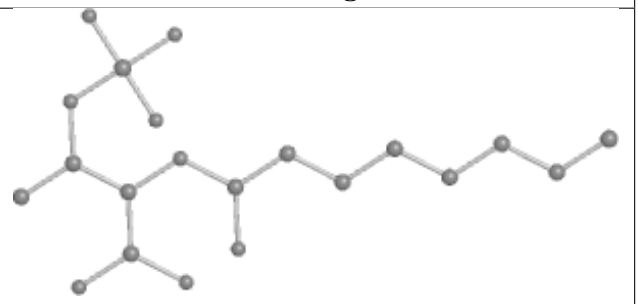
Bond lengths



Bond angles

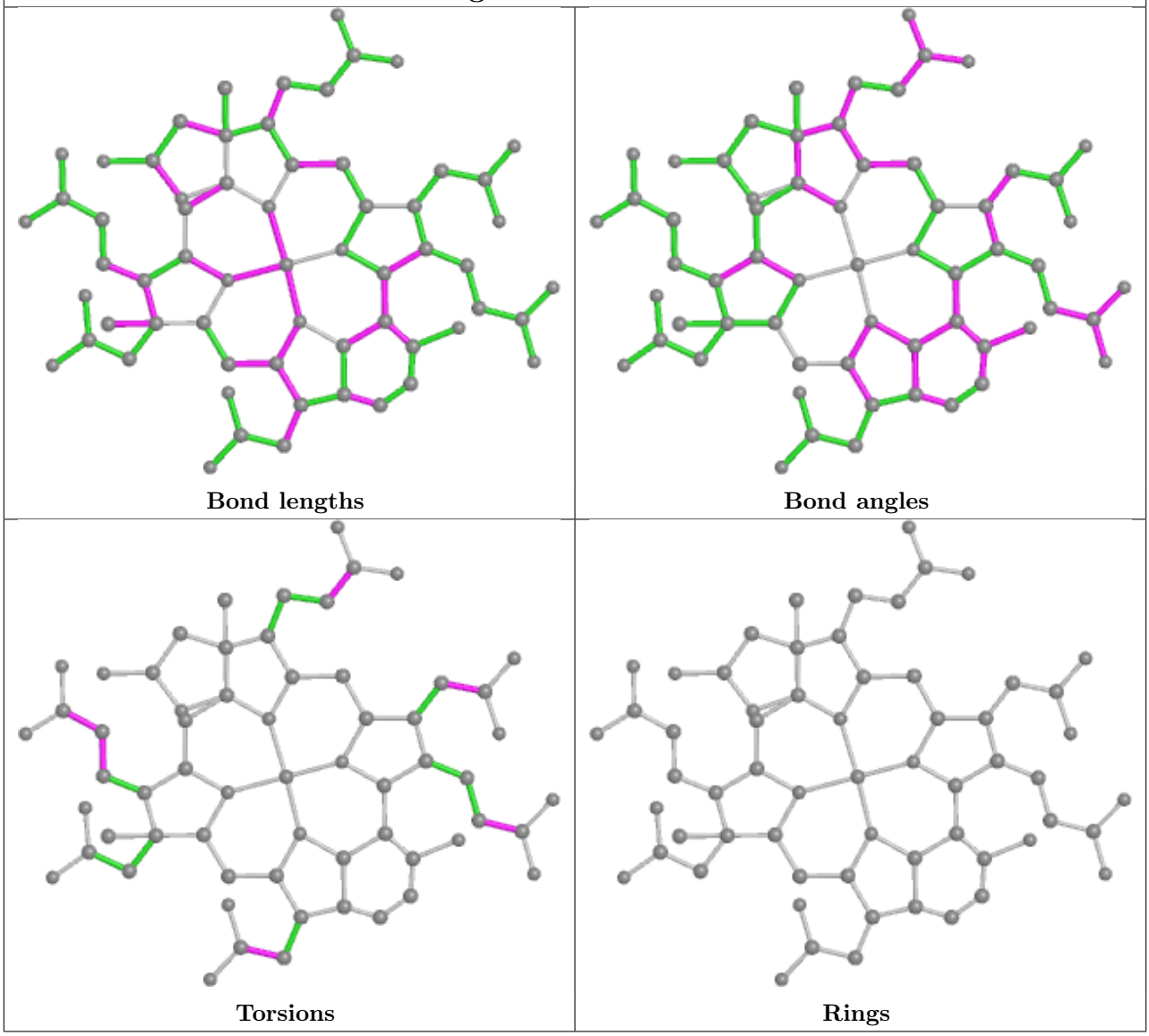


Torsions



Rings

Ligand F43 D 5570



3.7 Other polymers (i)

There are no such residues in this entry.

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

4 Fit of model and data (i)

4.1 Protein, DNA and RNA chains (i)

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

4.2 Non-standard residues in protein, DNA, RNA chains (i)

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

4.3 Carbohydrates (i)

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

4.4 Ligands (i)

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

4.5 Other polymers (i)

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