wwPDB X-ray Structure Validation Summary Report (i)

Dec 8, 2023 – 12:26 am GMT

PDB ID	:	1HBM
Title	:	METHYL-COENZYME M REDUCTASE ENZYME PRODUCT COMPLEX
Authors	:	Ermler, U.; Grabarse, W.
Deposited on	:	2001-04-20
Resolution	:	1.80 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:

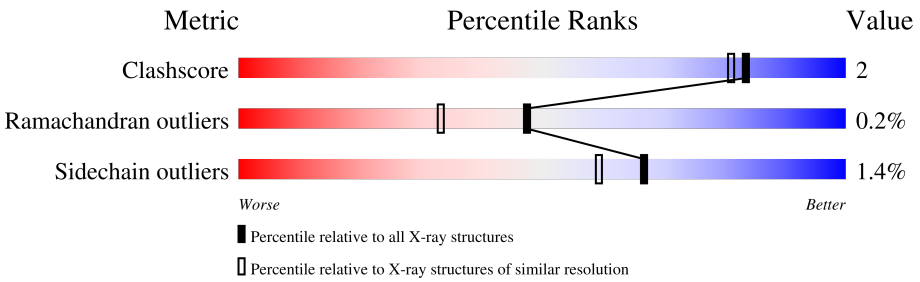
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	549	89% 9% •
1	D	549	91% 8% •
2	B	442	90% 9%
2	E	442	91% 7% •
3	C	248	91% 7% •
3	F	248	90% 7% •

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 21641 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
			Total	C	N	O	S			
1	A	548	4291	2712	723	836	20	23	13	0
1	D	548	4296	2717	721	838	20	23	16	0

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

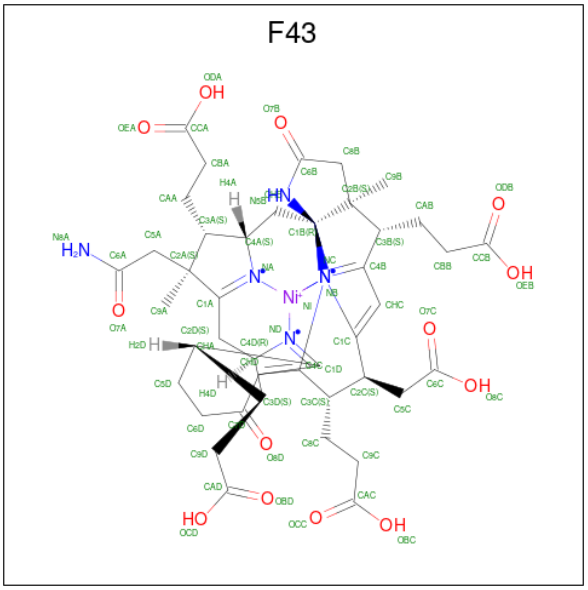
- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE I BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	442	3347	2115	557	653	22	26	15	0
2	E	442	3339	2115	551	652	21	41	12	0

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

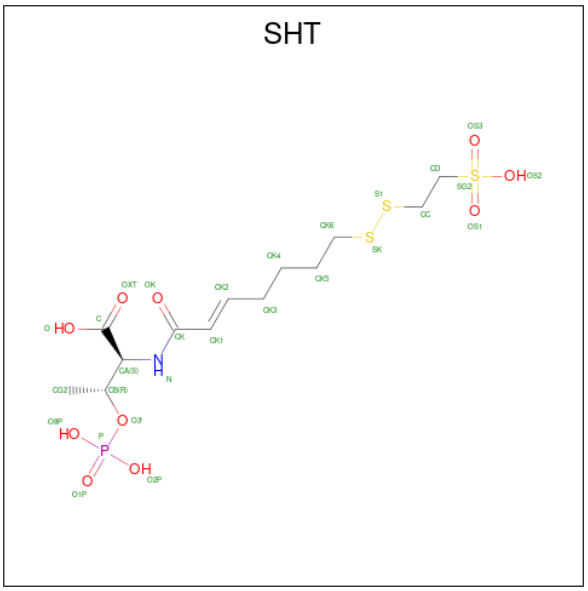
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	247	2007	1242	355	398	12	39	5	0
			Total	C	N	O	S			
3	F	247	2006	1242	354	398	12	44	5	0

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



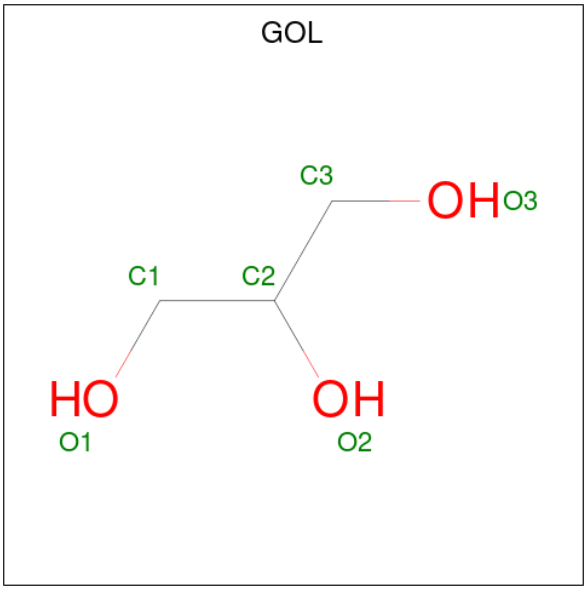
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	Ni	O		
4	A	1	62	42	6	1	13	0	0
			Total	C	N	Ni	O		
4	D	1	62	42	6	1	13	0	0

- Molecule 5 is O-PHOSPHONO-N-{(2E)-7-[(2-SULFOETHYL)DITHIO]HEPT-2-ENOYL}-L-THREONINE (three-letter code: SHT) (formula: $C_{13}H_{24}NO_{10}PS_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
5	A	1	28	13	1	10	1	3	0	0
5	D	1	28	13	1	10	1	3	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
9	F	4	4	4	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
10	D	1	1	1	0	1

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	427	427	427	0	0
			Total	O		
11	B	369	369	369	0	1
			Total	O		
11	C	257	257	257	0	0
			Total	O		
11	D	438	438	438	0	1
			Total	O		
11	E	353	353	353	0	0
			Total	O		
11	F	248	248	248	0	1

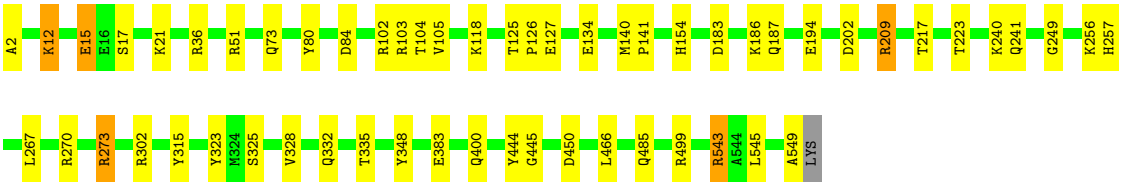
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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 was not executed.

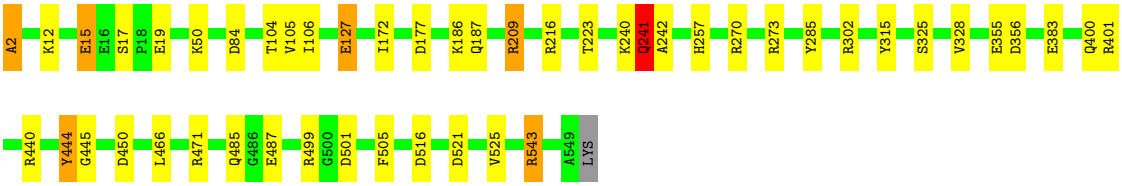
• Molecule 1: METHYL-COENZYME M REDUCTASE I ALPHA SUBUNIT

Chain A:



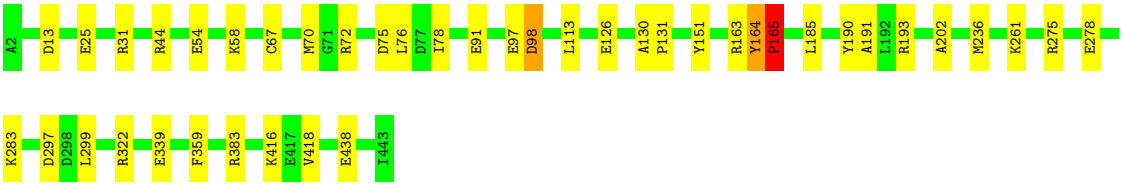
• Molecule 1: METHYL-COENZYME M REDUCTASE I ALPHA SUBUNIT

Chain D:



• Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT

Chain B:



• Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT

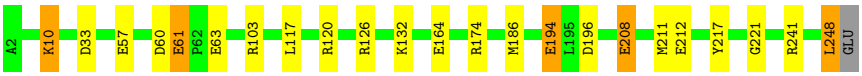
Chain E:

• Molecule 3: METHYL-COENZYME M REDUCTASE I GAMMA SUBUNIT

Chain C:

• Molecule 3: METHYL-COENZYME M REDUCTASE I GAMMA SUBUNIT

Chain F:



4 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	82.00Å 118.30Å 122.80Å 90.00° 92.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80	Depositor
% Data completeness (in resolution range)	91.8 (10.00-1.80)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.164 , 0.193	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21641	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

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: SMC, ZN, F43, AGM, GOL, MG, CL, GL3, SHT, MHS, NA, MGN

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	0.77	5/4411 (0.1%)	1.13	23/5986 (0.4%)
1	D	1.12	6/4432 (0.1%)	1.20	30/6015 (0.5%)
2	B	0.82	5/3492 (0.1%)	1.30	31/4724 (0.7%)
2	E	1.54	8/3458 (0.2%)	1.28	26/4682 (0.6%)
3	C	1.16	8/2072 (0.4%)	1.29	19/2790 (0.7%)
3	F	0.82	9/2070 (0.4%)	1.37	14/2789 (0.5%)
All	All	1.07	41/19935 (0.2%)	1.25	143/26986 (0.5%)

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	3
1	D	0	5
2	B	0	2
2	E	0	4
3	C	0	1
All	All	0	15

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	438	GLU	CG-CD	53.14	2.31	1.51
1	D	355	GLU	CG-CD	45.45	2.20	1.51
2	E	91[A]	GLU	CG-CD	38.62	2.09	1.51
2	E	91[B]	GLU	CG-CD	38.62	2.09	1.51
2	E	83	GLU	CG-CD	30.66	1.98	1.51

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	196	ASP	CB-CG-OD2	29.36	144.72	118.30
2	B	98	ASP	CB-CG-OD2	27.17	142.76	118.30
3	F	196	ASP	CB-CG-OD1	-25.80	95.08	118.30
2	B	98	ASP	CB-CG-OD1	-25.10	95.71	118.30
3	C	60	ASP	CB-CG-OD1	-22.84	97.74	118.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134[A]	GLU	Sidechain
1	A	134[B]	GLU	Sidechain
1	A	241	GLN	Peptide
2	B	164	TYR	Peptide,Mainchain
3	C	60	ASP	Sidechain

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	4291	0	4093	19	0
1	D	4296	0	4108	17	0
2	B	3347	0	3331	25	0
2	E	3339	0	3325	22	0
3	C	2007	0	1937	9	0
3	F	2006	0	1937	8	0
4	A	62	0	43	1	0
4	D	62	0	43	1	0
5	A	28	0	21	0	0
5	D	28	0	21	0	0
6	A	24	0	31	5	0
6	B	6	0	8	3	0
6	C	6	0	8	0	0
6	D	24	0	31	1	0
6	E	6	0	8	2	0
7	A	4	0	0	0	0
7	B	2	0	0	0	0
7	D	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	1	0	0	0	0
8	E	1	0	0	0	0
9	C	1	0	0	0	0
9	F	4	0	0	0	0
10	D	1	0	0	0	0
11	A	427	0	0	5	0
11	B	369	0	0	4	0
11	C	257	0	0	2	0
11	D	438	0	0	4	0
11	E	353	0	0	3	0
11	F	248	0	0	0	0
All	All	21641	0	18945	91	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 2.

The worst 5 of 91 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:236[C]:MET:SD	2:B:236[C]:MET:CE	2.04	1.45
2:B:185[B]:LEU:HD21	2:B:191:ALA:HA	1.62	0.80
2:E:349:PHE:HZ	3:F:248:LEU:HD21	1.57	0.70
2:E:246[A]:MET:CE	2:E:429:LEU:HD12	2.21	0.69
2:B:58[A]:LYS:HE3	2:B:75:ASP:OD1	1.94	0.68

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	554/549 (101%)	537 (97%)	16 (3%)	1 (0%)	47 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	557/549 (102%)	535 (96%)	21 (4%)	1 (0%)	47	33
2	B	456/442 (103%)	447 (98%)	8 (2%)	1 (0%)	47	33
2	E	452/442 (102%)	443 (98%)	8 (2%)	1 (0%)	47	33
3	C	250/248 (101%)	243 (97%)	7 (3%)	0	100	100
3	F	250/248 (101%)	245 (98%)	5 (2%)	0	100	100
All	All	2519/2478 (102%)	2450 (97%)	65 (3%)	4 (0%)	47	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	165	PRO
2	E	165	PRO
1	A	325	SER
1	D	325	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/434 (103%)	440 (99%)	6 (1%)	69	62
1	D	449/434 (104%)	443 (99%)	6 (1%)	69	62
2	B	357/341 (105%)	354 (99%)	3 (1%)	81	78
2	E	353/341 (104%)	348 (99%)	5 (1%)	67	59
3	C	220/216 (102%)	218 (99%)	2 (1%)	78	75
3	F	220/216 (102%)	215 (98%)	5 (2%)	50	37
All	All	2045/1982 (103%)	2018 (99%)	27 (1%)	67	62

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	444	TYR
2	E	5	GLU

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Mol	Chain	Res	Type
3	F	186	MET
1	D	543	ARG
2	E	98	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	187	GLN
1	D	365	ASN
2	E	40	GLN
1	D	485	GLN
1	D	111	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 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	A	257	1	7,11,12	1.85	1 (14%)	6,14,16	1.00	0
1	SMC	D	452	1	5,6,7	0.79	0	2,6,8	0.10	0
1	SMC	A	452	1	5,6,7	0.71	0	2,6,8	0.56	0
1	GL3	A	445	1	2,3,4	2.78	1 (50%)	1,2,4	0.18	0
1	MHS	D	257	1	7,11,12	1.88	1 (14%)	6,14,16	1.28	0
1	MGN	A	400	1	6,9,10	0.41	0	5,12,14	2.36	1 (20%)
1	AGM	D	271	1	10,11,12	0.64	0	6,13,15	0.58	0
1	MGN	D	400	1	6,9,10	0.82	0	5,12,14	2.19	1 (20%)
1	GL3	D	445	1	2,3,4	3.20	1 (50%)	1,2,4	0.16	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	0.86	0	6,13,15	1.11	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	257	1	-	0/5/6/8	0/1/1/1
1	SMC	D	452	1	-	1/3/5/7	-
1	SMC	A	452	1	-	1/3/5/7	-
1	GL3	A	445	1	-	1/1/1/2	-
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1
1	MGN	A	400	1	-	0/7/9/12	-
1	AGM	D	271	1	-	2/10/11/13	-
1	MGN	D	400	1	-	0/7/9/12	-
1	GL3	D	445	1	-	1/1/1/2	-
1	AGM	A	271	1	-	3/10/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	MHS	CM-ND1	4.60	1.58	1.47
1	D	445	GL3	C-S	-4.49	1.65	1.80
1	D	257	MHS	CM-ND1	4.11	1.57	1.47
1	A	445	GL3	C-S	-3.89	1.67	1.80

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	400	MGN	CB2-CA-CB1	-5.01	102.18	111.00
1	D	400	MGN	CB2-CA-CB1	-4.55	102.99	111.00

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	445	GL3	S-C-CA-N
1	D	445	GL3	S-C-CA-N

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Mol	Chain	Res	Type	Atoms
1	A	271	AGM	CE2-CD-NE1-CZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 17 are monoatomic - leaving 15 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	GOL	C	1249	-	5,5,5	0.60	0	5,5,5	0.57	0
6	GOL	B	1444	-	5,5,5	0.80	0	5,5,5	1.30	0
6	GOL	D	1552	-	5,5,5	0.71	0	5,5,5	0.30	0
5	SHT	D	1551	4	26,27,27	2.23	9 (34%)	30,36,36	1.19	2 (6%)
4	F43	A	1550	1,5	61,71,71	3.21	18 (29%)	64,118,118	2.33	25 (39%)
6	GOL	D	1555	-	5,5,5	0.67	0	5,5,5	0.91	0
5	SHT	A	1551	4	26,27,27	2.15	9 (34%)	30,36,36	1.49	4 (13%)
6	GOL	A	1555	-	5,5,5	0.72	0	5,5,5	0.79	0
6	GOL	D	1554	-	5,5,5	0.68	0	5,5,5	0.94	0
6	GOL	E	1444	-	5,5,5	0.84	0	5,5,5	1.38	0
6	GOL	A	1552	7	5,5,5	0.63	0	5,5,5	1.47	1 (20%)
6	GOL	D	1553	7	5,5,5	0.65	0	5,5,5	0.82	0
4	F43	D	1550	1,5	61,71,71	3.45	18 (29%)	64,118,118	2.40	26 (40%)
6	GOL	A	1553	-	5,5,5	0.55	0	5,5,5	1.04	0
6	GOL	A	1554	-	5,5,5	0.69	0	5,5,5	0.82	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
6	GOL	C	1249	-	-	2/4/4/4	-
6	GOL	B	1444	-	-	4/4/4/4	-
6	GOL	D	1552	-	-	0/4/4/4	-
5	SHT	D	1551	4	-	3/31/31/31	-
4	F43	A	1550	1,5	-	6/28/185/185	-
6	GOL	D	1555	-	-	2/4/4/4	-
5	SHT	A	1551	4	-	4/31/31/31	-
6	GOL	A	1555	-	-	2/4/4/4	-
6	GOL	D	1554	-	-	0/4/4/4	-
6	GOL	E	1444	-	-	4/4/4/4	-
6	GOL	A	1552	7	-	2/4/4/4	-
6	GOL	D	1553	7	-	0/4/4/4	-
4	F43	D	1550	1,5	-	6/28/185/185	-
6	GOL	A	1553	-	-	2/4/4/4	-
6	GOL	A	1554	-	-	2/4/4/4	-

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1550	F43	NI-NA	17.33	2.26	1.89
4	D	1550	F43	NI-NA	15.88	2.23	1.89
4	D	1550	F43	NI-NB	12.13	2.15	1.89
4	D	1550	F43	NI-ND	7.98	2.06	1.89
4	A	1550	F43	NI-ND	7.37	2.05	1.89

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1550	F43	O7B-C6B-C8B	-6.81	118.28	126.59
4	A	1550	F43	C4A-NA-C1A	6.69	117.07	108.97
4	D	1550	F43	CAB-C3B-C2B	-6.04	106.31	119.09
4	A	1550	F43	CAB-C3B-C2B	-5.85	106.71	119.09
4	D	1550	F43	O8D-C7D-C6D	-5.50	111.84	120.86

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1551	SHT	S1-CC-CD-SG2
5	A	1551	SHT	CK5-CK6-SK-S1
5	A	1551	SHT	CK-CK1-CK2-CK3
5	D	1551	SHT	CK5-CK6-SK-S1
6	A	1554	GOL	O1-C1-C2-C3

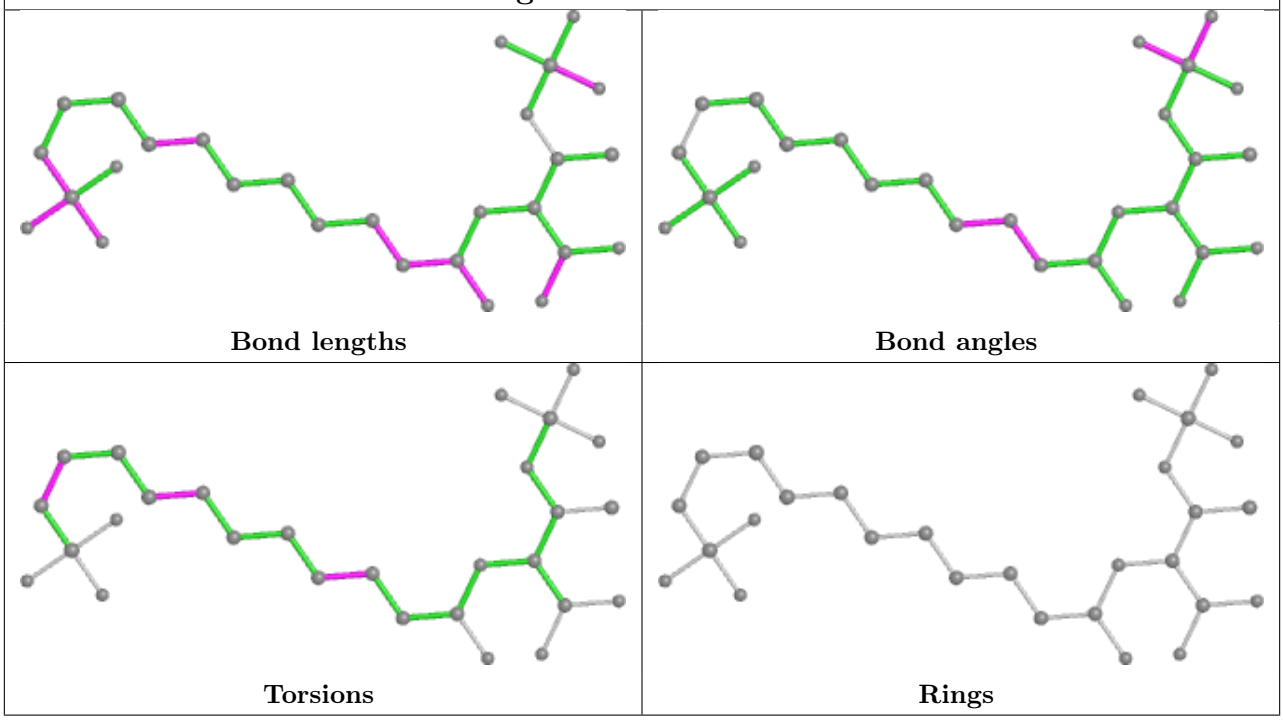
There are no ring outliers.

8 monomers are involved in 13 short contacts:

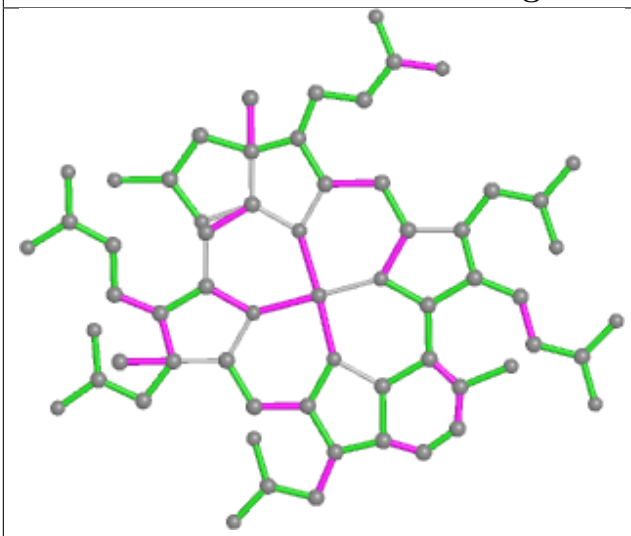
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1444	GOL	3	0
4	A	1550	F43	1	0
6	A	1555	GOL	3	0
6	D	1554	GOL	1	0
6	E	1444	GOL	2	0
6	A	1552	GOL	1	0
4	D	1550	F43	1	0
6	A	1554	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

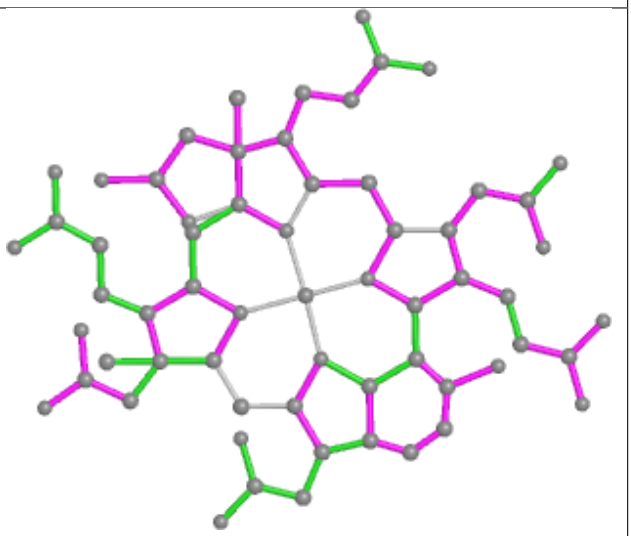
Ligand SHT D 1551



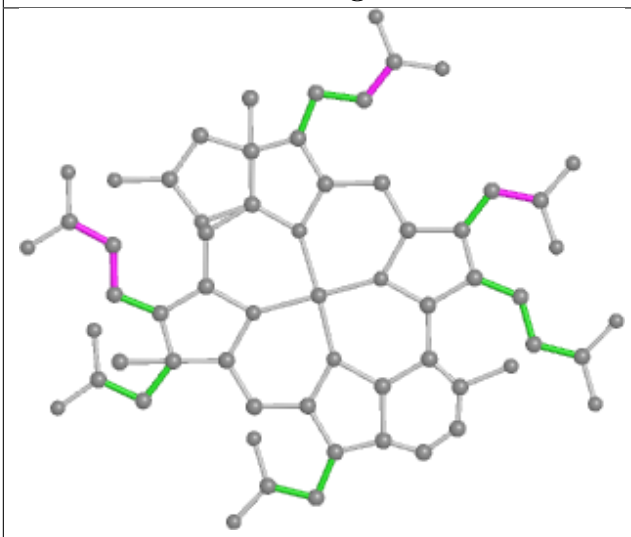
Ligand F43 A 1550



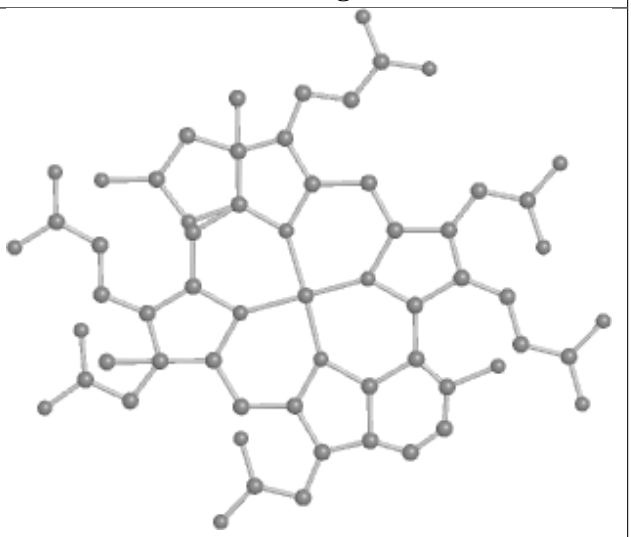
Bond lengths



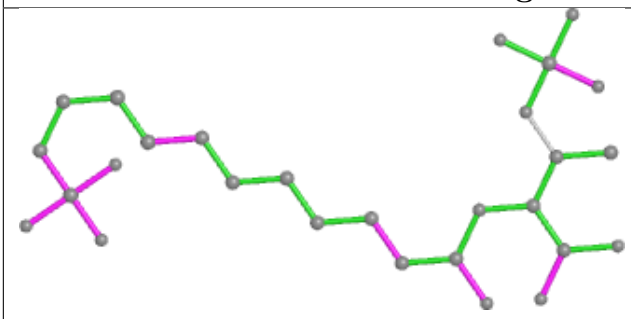
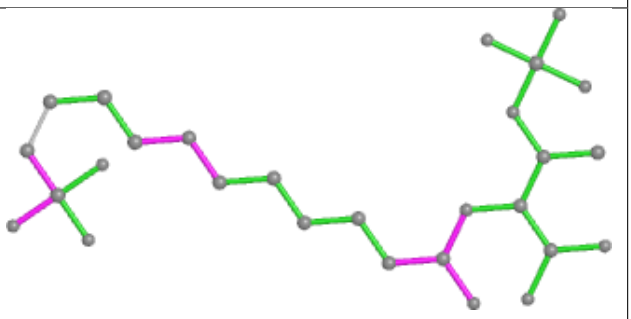
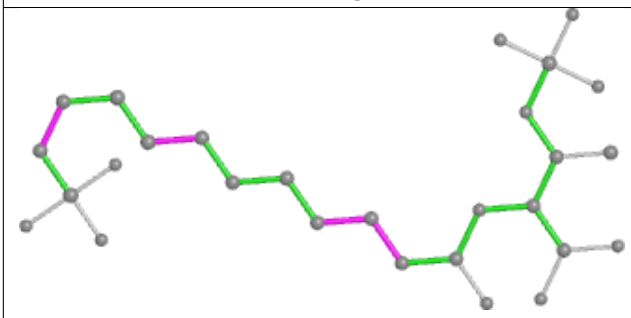
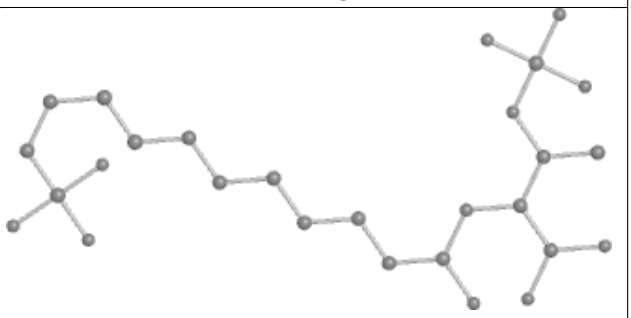
Bond angles



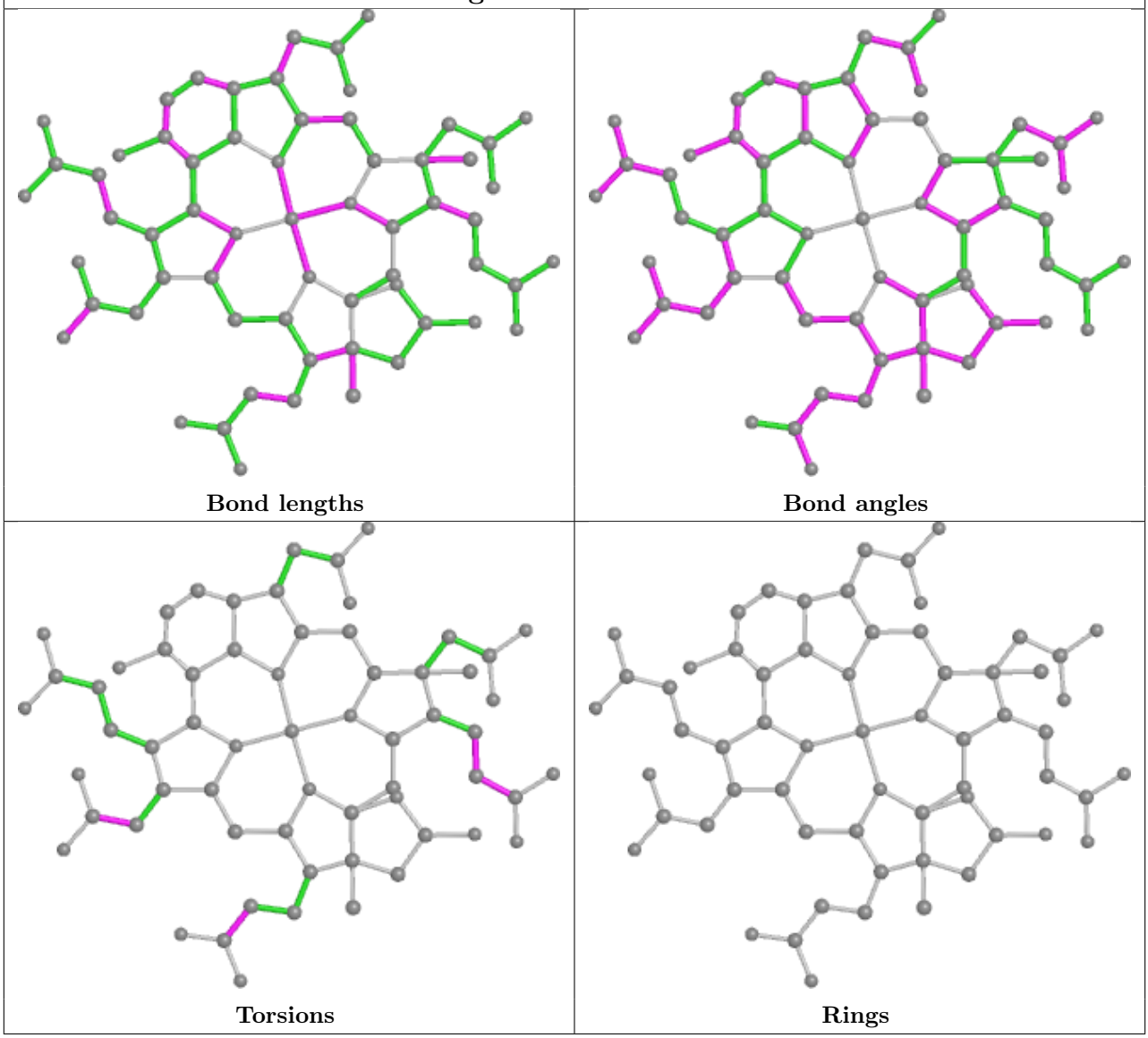
Torsions



Rings

Ligand SHT A 1551	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand F43 D 1550



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.