



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 9, 2023 – 03:52 pm GMT

PDB ID : 1HBU
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 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 ⓘ 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (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

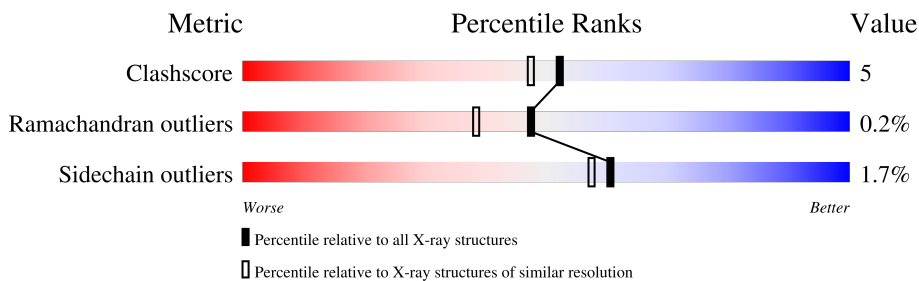
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	549	
1	D	549	
2	B	442	
2	E	442	
3	C	248	
3	F	248	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GOL	B	1444	-	-	X	-

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
			Total	C	N	O	S			
1	A	548	4284	2708	723	833	20	24	10	0
1	D	548	4289	2710	721	838	20	23	13	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

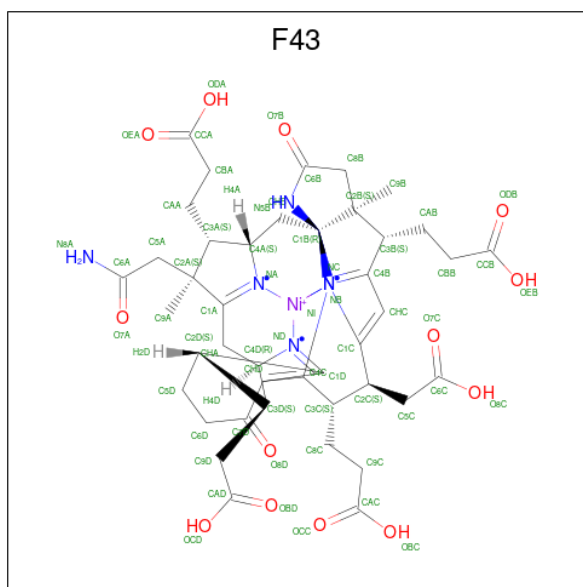
- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE I BETA SUBUNIT.

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

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

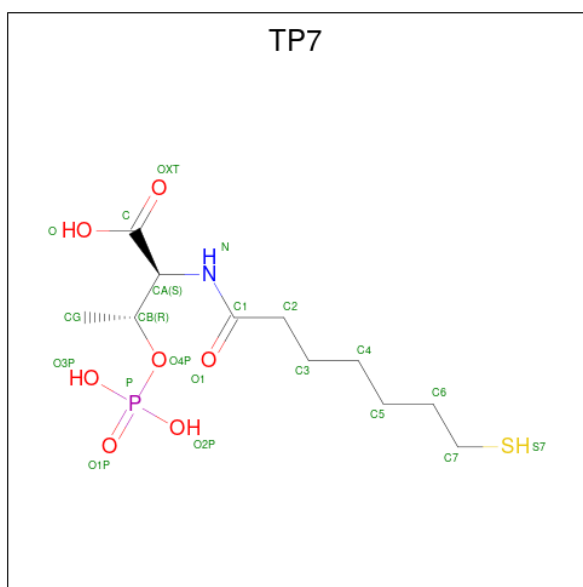
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	247	Total 2007	1242	355	398	12	39	5	0
3	F	247	Total 2006	1242	354	398	12	44	5	0

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



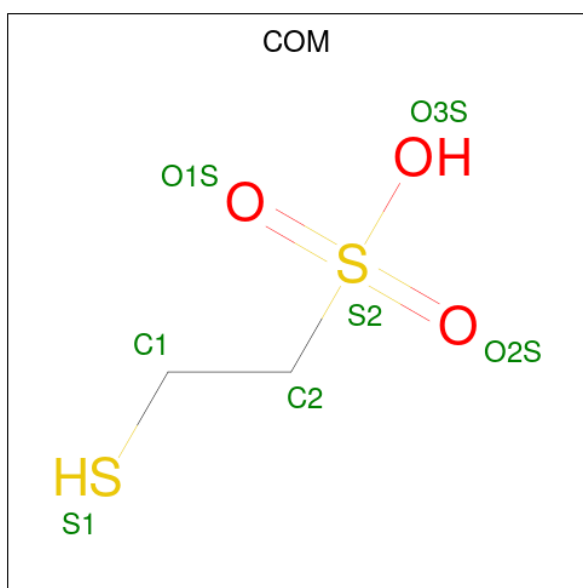
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	Ni	O		
4	A	1	Total 62	42	6	1	13	0	0
4	D	1	Total 62	42	6	1	13	0	0

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



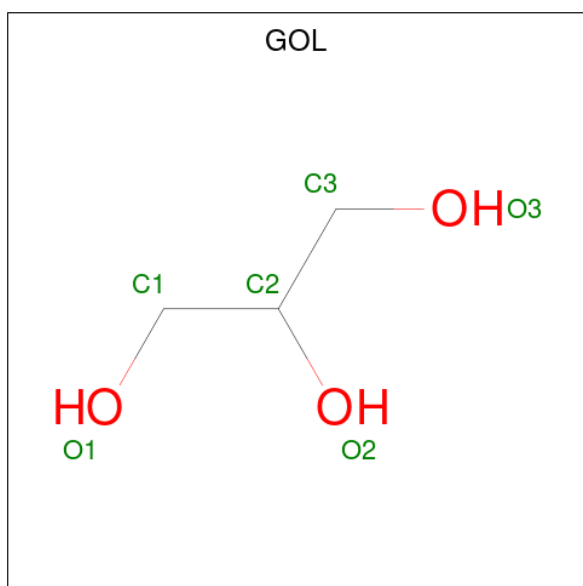
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
5	A	1	21	11	1	7	1	1	0	0
5	D	1	21	11	1	7	1	1	0	0

- 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
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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 9 is MAGNESIUM ION (three-letter code: 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	1	Total Mg 1 1	0	0
9	D	1	Total Mg 1 1	0	0
9	E	3	Total Mg 3 3	0	0
9	F	1	Total Mg 1 1	0	0

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	4	Total Na 4 4	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 (three-letter code: 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	444	Total O 444 444	0	27

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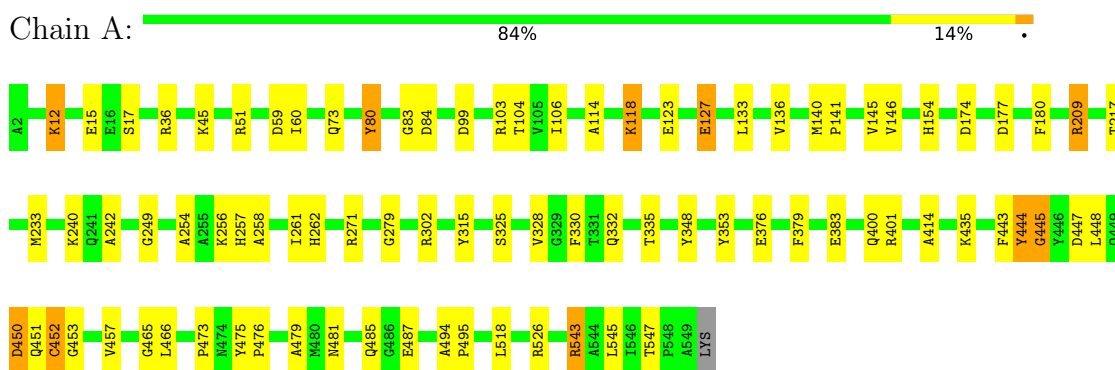
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	385	Total 385	O 385	0	23
12	C	254	Total 254	O 254	0	23
12	D	440	Total 440	O 440	0	32
12	E	360	Total 360	O 360	0	23
12	F	253	Total 253	O 253	0	13

3 Residue-property plots [i](#)

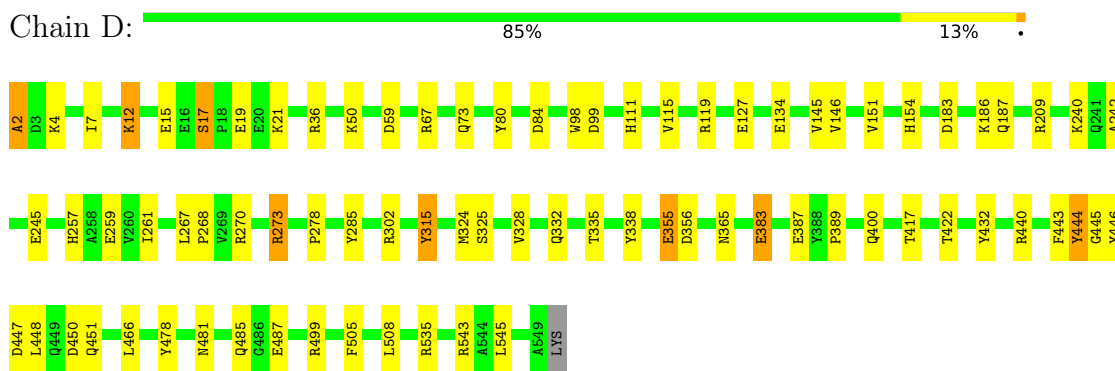
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

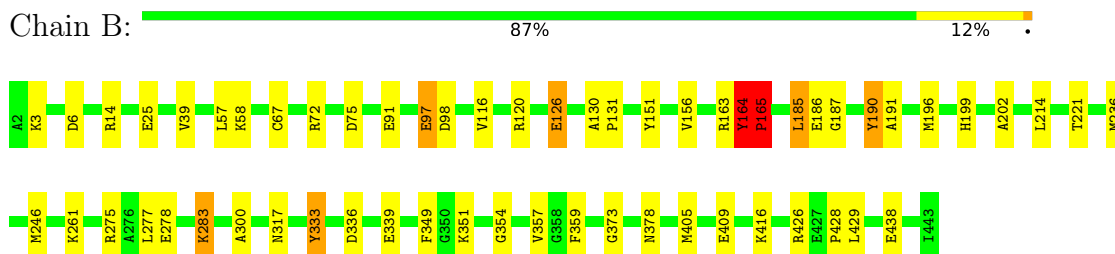
- Molecule 1: METHYL-COENZYME M REDUCTASE I ALPHA SUBUNIT




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

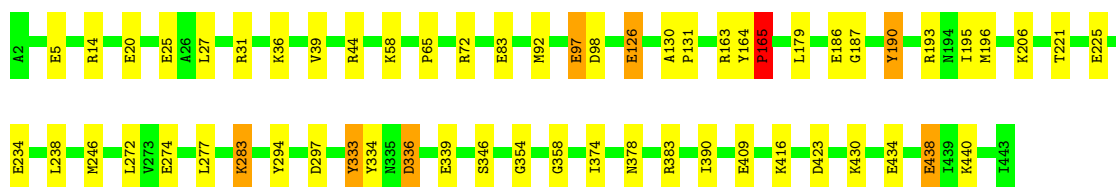


- Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT




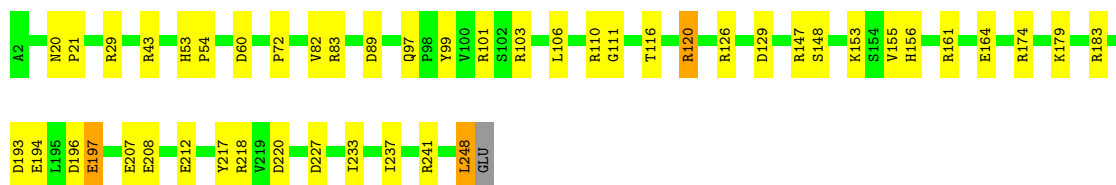
- Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT

Chain E:  87% 12%




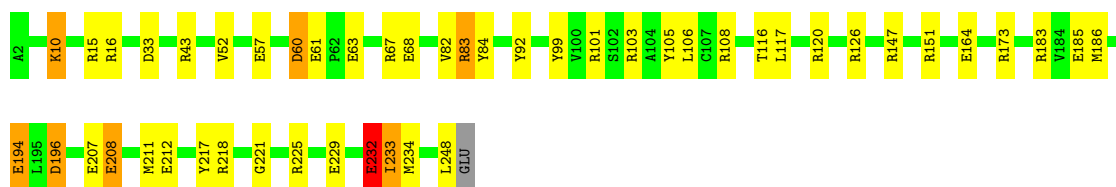
• Molecule 3: METHYL-COENZYME M REDUCTASE I GAMMA SUBUNIT

Chain C:  81% 18%



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

Chain F:  80% 16%



4 Data and refinement statistics

Xtrriage (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.	Xtrriage
Total number of atoms	21670	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: MGN, AGM, F43, SMC, COM, TP7, GL3, GOL, MG, NA, ZN, CL, MHS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.04	6/4389 (0.1%)	1.25	22/5956 (0.4%)
1	D	1.15	8/4410 (0.2%)	1.37	44/5984 (0.7%)
2	B	1.00	6/3476 (0.2%)	1.27	28/4703 (0.6%)
2	E	2.03	8/3447 (0.2%)	1.30	29/4666 (0.6%)
3	C	1.43	4/2072 (0.2%)	1.37	32/2790 (1.1%)
3	F	2.38	11/2070 (0.5%)	1.58	45/2789 (1.6%)
All	All	1.49	43/19864 (0.2%)	1.34	200/26888 (0.7%)

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	1
1	D	0	5
2	B	0	2
2	E	0	3
3	C	0	1
All	All	0	12

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	438	GLU	CG-CD	90.76	2.88	1.51
3	F	207	GLU	CG-CD	53.45	2.32	1.51
1	A	127	GLU	CG-CD	49.49	2.26	1.51
3	F	164	GLU	CB-CG	45.51	2.38	1.52
3	F	194	GLU	CB-CG	42.64	2.33	1.52

The worst 5 of 200 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	438	GLU	CB-CG-CD	-22.34	53.90	114.20
3	F	10	LYS	CB-CG-CD	17.37	156.75	111.60
3	F	232	GLU	O-C-N	16.81	149.60	122.70
1	D	15	GLU	CA-CB-CG	16.76	150.27	113.40
3	F	196	ASP	CB-CG-OD1	15.76	132.48	118.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	547	THR	Mainchain
2	B	164	TYR	Mainchain,Peptide
3	C	197	GLU	Sidechain
1	D	2	ALA	Mainchain,Peptide
1	D	355	GLU	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	4284	0	4085	52	0
1	D	4289	0	4091	40	0
2	B	3344	0	3329	62	0
2	E	3333	0	3320	34	0
3	C	2007	0	1937	23	0
3	F	2006	0	1937	23	0
4	A	62	0	43	4	0
4	D	62	0	43	2	0
5	A	21	0	19	4	0
5	D	21	0	19	6	0
6	A	7	0	5	3	0
6	D	7	0	5	1	0
7	A	24	0	31	5	0
7	B	6	0	8	6	0
7	C	6	0	8	0	0
7	D	24	0	31	1	0
7	E	6	0	8	1	0
8	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	5	0	0	0	0
9	B	2	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	3	0	0	0	0
9	F	1	0	0	0	0
10	A	4	0	0	0	0
10	B	2	0	0	0	0
10	D	3	0	0	0	0
11	B	1	0	0	0	0
11	E	1	0	0	0	0
12	A	444	0	0	5	0
12	B	385	0	0	6	0
12	C	254	0	0	2	0
12	D	440	0	0	7	0
12	E	360	0	0	6	0
12	F	253	0	0	5	0
All	All	21670	0	18919	209	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 5.

The worst 5 of 209 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:185[B]:LEU:HD22	2:B:190:TYR:CB	1.26	1.62
2:B:185[B]:LEU:CD2	2:B:190:TYR:CB	2.02	1.36
2:B:236[B]:MET:CE	2:B:236[B]:MET:SD	2.14	1.36
2:B:185[B]:LEU:HD21	2:B:190:TYR:C	1.48	1.33
3:F:232:GLU:CA	12:F:2241:HOH:O	1.75	1.27

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	551/549 (100%)	532 (97%)	18 (3%)	1 (0%)	47	38
1	D	554/549 (101%)	530 (96%)	23 (4%)	1 (0%)	47	38
2	B	454/442 (103%)	441 (97%)	12 (3%)	1 (0%)	47	38
2	E	451/442 (102%)	438 (97%)	12 (3%)	1 (0%)	47	38
3	C	250/248 (101%)	242 (97%)	8 (3%)	0	100	100
3	F	250/248 (101%)	240 (96%)	9 (4%)	1 (0%)	34	24
All	All	2510/2478 (101%)	2423 (96%)	82 (3%)	5 (0%)	47	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	165	PRO
2	B	165	PRO
3	F	232	GLU
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	443/434 (102%)	436 (98%)	7 (2%)	62	60
1	D	446/434 (103%)	440 (99%)	6 (1%)	69	68
2	B	355/341 (104%)	350 (99%)	5 (1%)	67	65
2	E	352/341 (103%)	347 (99%)	5 (1%)	67	65
3	C	220/216 (102%)	214 (97%)	6 (3%)	44	38
3	F	220/216 (102%)	213 (97%)	7 (3%)	39	30
All	All	2036/1982 (103%)	2000 (98%)	36 (2%)	60	55

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	438	GLU
3	F	232	GLU
3	F	10	LYS
3	F	194	GLU
3	C	72	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	235	GLN
2	E	40	GLN
1	D	365	ASN
1	D	187	GLN
1	D	485	GLN

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	SMC	D	452	1	5,6,7	0.78	0	2,6,8	0.88	0
1	MGN	D	400	1	6,9,10	1.00	0	5,12,14	2.48	1 (20%)
1	MGN	A	400	1	6,9,10	1.08	1 (16%)	5,12,14	2.51	1 (20%)
1	GL3	A	445	1	2,3,4	3.31	1 (50%)	1,2,4	0.44	0
1	AGM	D	271	1	10,11,12	0.79	0	6,13,15	0.52	0
1	AGM	A	271	1	10,11,12	0.89	0	6,13,15	1.99	3 (50%)
1	SMC	A	452	1	5,6,7	1.26	1 (20%)	2,6,8	1.73	1 (50%)
1	MHS	A	257	1	7,11,12	1.78	1 (14%)	6,14,16	1.56	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GL3	D	445	1	2,3,4	3.18	1 (50%)	1,2,4	0.44	0
1	MHS	D	257	1	7,11,12	1.72	1 (14%)	6,14,16	1.16	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SMC	D	452	1	-	1/3/5/7	-
1	MGN	D	400	1	-	0/7/9/12	-
1	MGN	A	400	1	-	0/7/9/12	-
1	GL3	A	445	1	-	1/1/1/2	-
1	AGM	D	271	1	-	2/10/11/13	-
1	AGM	A	271	1	-	2/10/11/13	-
1	SMC	A	452	1	-	1/3/5/7	-
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1
1	GL3	D	445	1	-	1/1/1/2	-
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	445	GL3	C-S	-4.66	1.64	1.80
1	D	445	GL3	C-S	-4.49	1.65	1.80
1	A	257	MHS	CM-ND1	4.25	1.57	1.47
1	D	257	MHS	CM-ND1	3.95	1.56	1.47
1	A	452	SMC	CB-SG	-2.37	1.77	1.80

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	400	MGN	CB2-CA-CB1	-5.00	102.20	111.00
1	A	400	MGN	CB2-CA-CB1	-4.97	102.24	111.00
1	A	271	AGM	NE1-CZ-NH2	-2.99	115.36	120.59
1	A	271	AGM	NH1-CZ-NE1	2.59	125.33	119.55
1	A	257	MHS	CD2-NE2-CE1	2.46	109.62	105.78

There are no chirality outliers.

5 of 8 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
1	D	271	AGM	CE2-CD-NE1-CZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	445	GL3	1	0
1	A	452	SMC	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 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
5	TP7	D	1551	-	19,20,20	2.25	6 (31%)	24,26,26	2.11	9 (37%)
4	F43	D	1550	1,6	61,71,71	3.13	19 (31%)	64,118,118	2.14	28 (43%)
7	GOL	A	1556	-	5,5,5	0.63	0	5,5,5	0.92	0
7	GOL	A	1554	-	5,5,5	0.64	0	5,5,5	1.01	0
7	GOL	A	1555	-	5,5,5	0.77	0	5,5,5	0.91	0
6	COM	D	1552	4	6,6,6	1.61	1 (16%)	7,8,8	1.86	1 (14%)
5	TP7	A	1551	-	19,20,20	2.54	6 (31%)	24,26,26	2.14	10 (41%)
7	GOL	B	1444	-	5,5,5	0.81	0	5,5,5	1.30	1 (20%)
7	GOL	D	1556	-	5,5,5	0.72	0	5,5,5	0.86	0
7	GOL	C	1249	-	5,5,5	0.61	0	5,5,5	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	F43	A	1550	6,1	61,71,71	3.02	18 (29%)	64,118,118	2.43	27 (42%)
6	COM	A	1552	4	6,6,6	1.72	1 (16%)	7,8,8	1.34	1 (14%)
7	GOL	D	1554	10	5,5,5	0.52	0	5,5,5	1.21	1 (20%)
7	GOL	D	1555	-	5,5,5	0.65	0	5,5,5	0.70	0
7	GOL	E	1444	-	5,5,5	0.62	0	5,5,5	0.87	0
7	GOL	D	1553	-	5,5,5	0.86	0	5,5,5	0.73	0
7	GOL	A	1553	10	5,5,5	0.68	0	5,5,5	1.25	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
5	TP7	D	1551	-	-	5/24/24/24	-
4	F43	D	1550	1,6	-	5/28/185/185	-
7	GOL	A	1556	-	-	2/4/4/4	-
7	GOL	A	1554	-	-	0/4/4/4	-
7	GOL	A	1555	-	-	2/4/4/4	-
6	COM	D	1552	4	-	1/4/4/4	-
5	TP7	A	1551	-	-	6/24/24/24	-
7	GOL	B	1444	-	-	2/4/4/4	-
7	GOL	D	1556	-	-	4/4/4/4	-
7	GOL	C	1249	-	-	0/4/4/4	-
4	F43	A	1550	6,1	-	6/28/185/185	-
6	COM	A	1552	4	-	0/4/4/4	-
7	GOL	D	1554	10	-	2/4/4/4	-
7	GOL	D	1555	-	-	4/4/4/4	-
7	GOL	E	1444	-	-	3/4/4/4	-
7	GOL	D	1553	-	-	0/4/4/4	-
7	GOL	A	1553	10	-	2/4/4/4	-

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1550	F43	NI-NA	16.80	2.25	1.89
4	D	1550	F43	NI-NB	12.35	2.16	1.89
4	D	1550	F43	NI-NA	8.88	2.08	1.89
4	D	1550	F43	NI-ND	8.65	2.08	1.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1551	TP7	CA-C	6.68	1.63	1.52

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1550	F43	C2B-C1B-NB	5.60	110.22	101.84
4	A	1550	F43	C4A-NA-C1A	5.35	115.45	108.97
4	A	1550	F43	C5D-C2D-C1D	5.28	117.55	110.45
4	A	1550	F43	C3D-C4D-ND	5.13	110.32	102.34
4	D	1550	F43	O8D-C7D-C6D	-5.05	112.59	120.86

There are no chirality outliers.

5 of 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

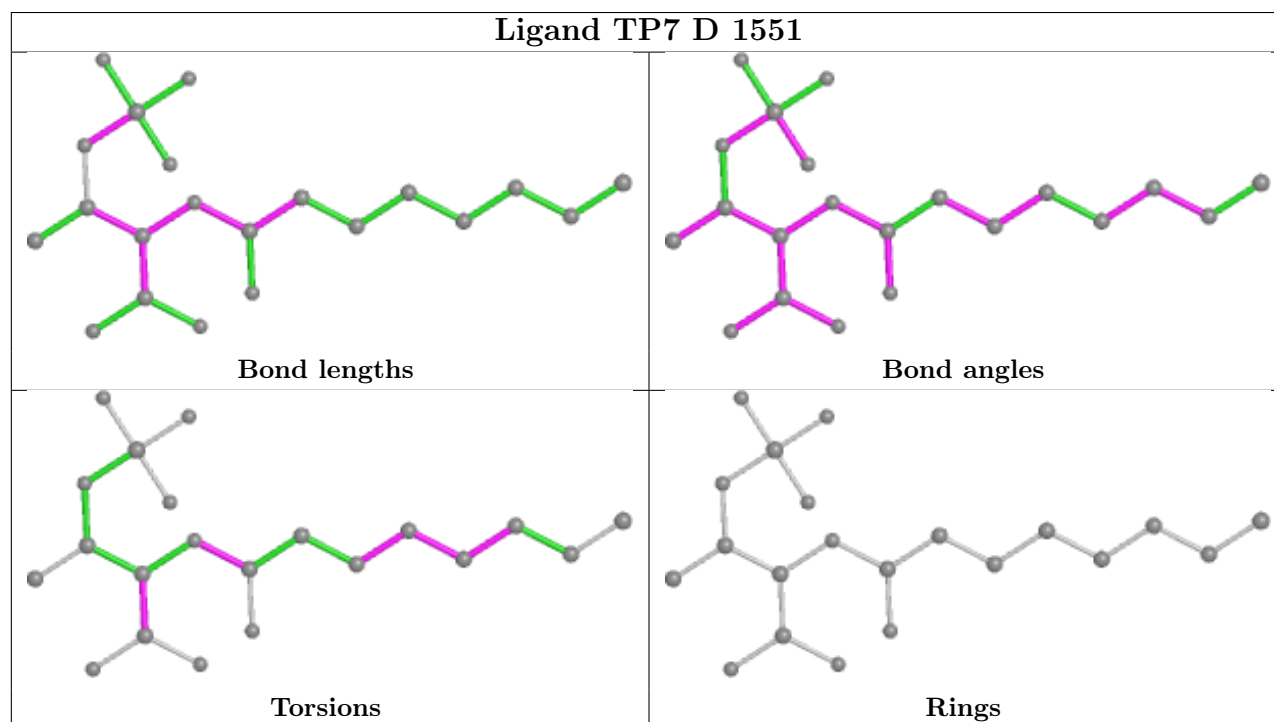
There are no ring outliers.

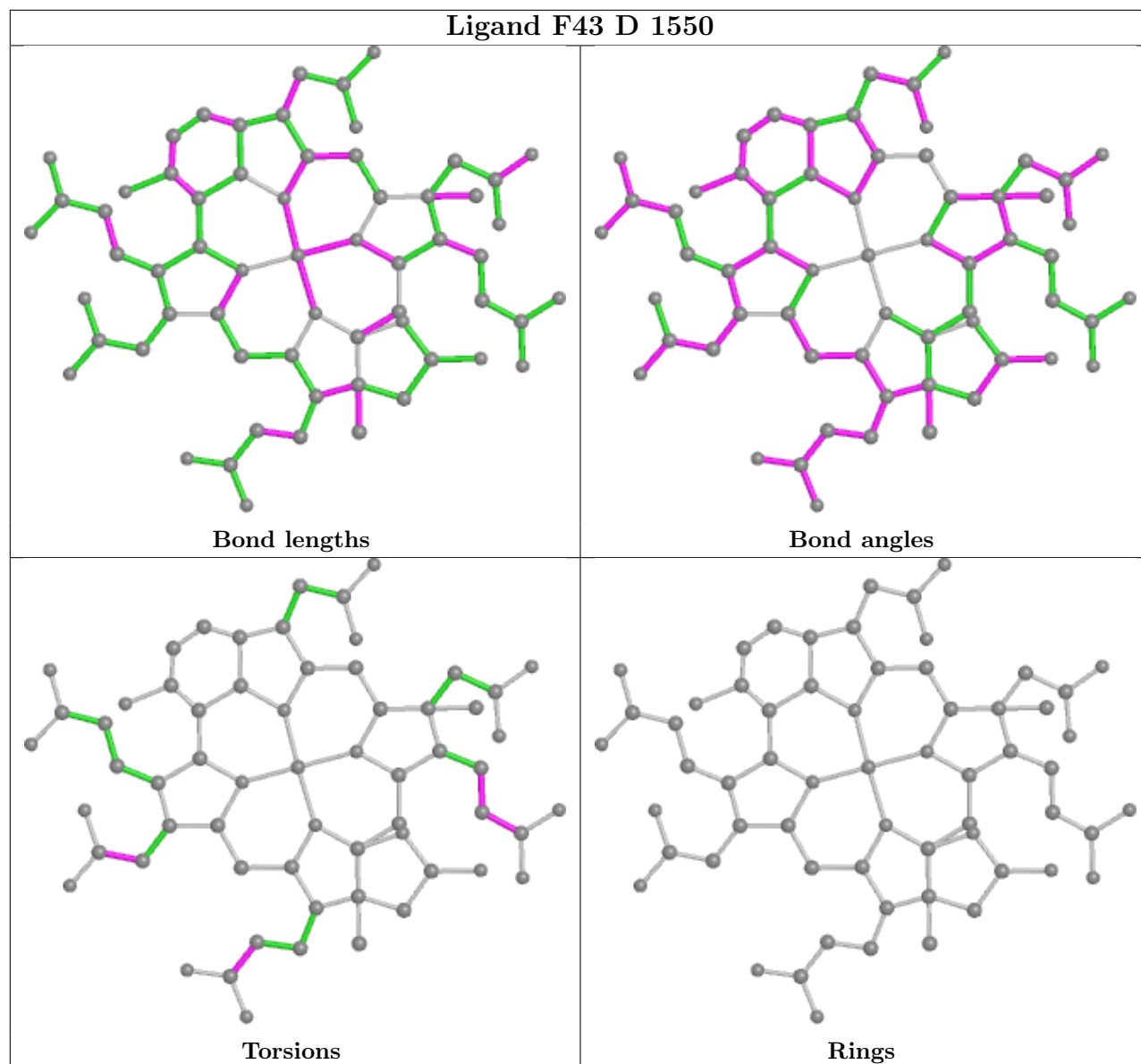
12 monomers are involved in 31 short contacts:

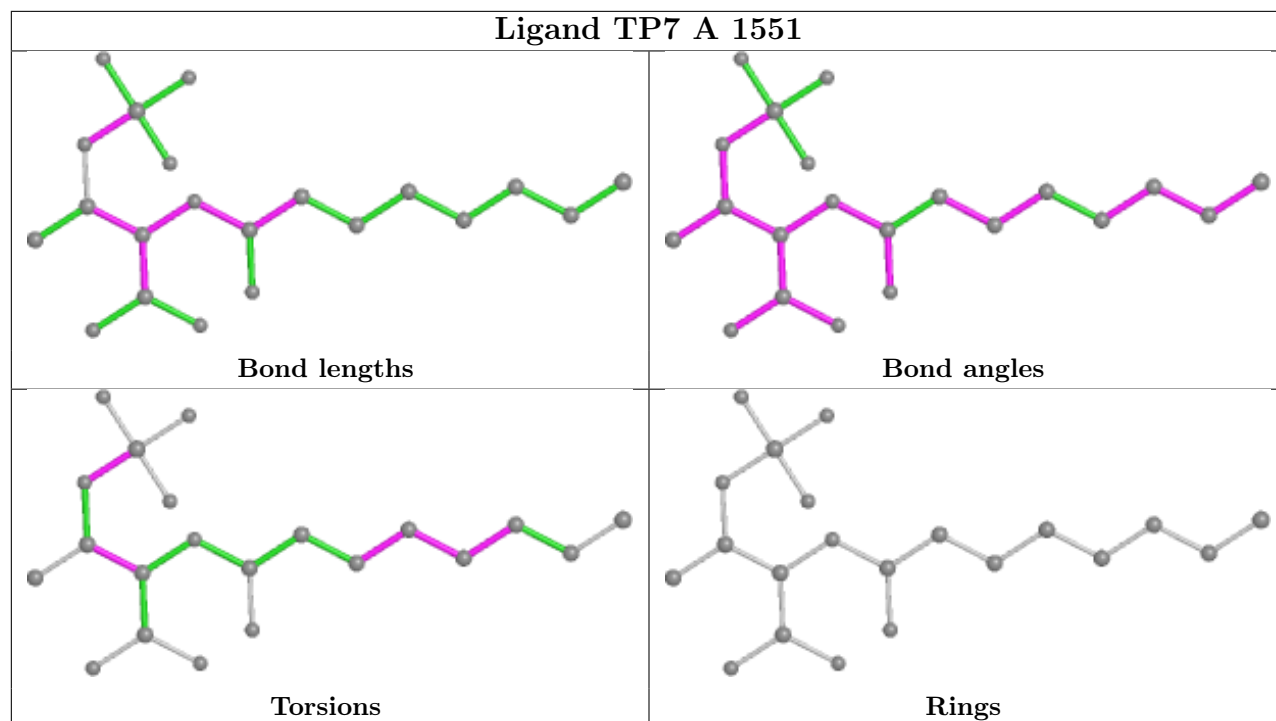
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1551	TP7	6	0
4	D	1550	F43	2	0
7	A	1556	GOL	3	0
7	A	1555	GOL	1	0
6	D	1552	COM	1	0
5	A	1551	TP7	4	0
7	B	1444	GOL	6	0
7	D	1556	GOL	1	0
4	A	1550	F43	4	0
6	A	1552	COM	3	0
7	E	1444	GOL	1	0
7	A	1553	GOL	1	0

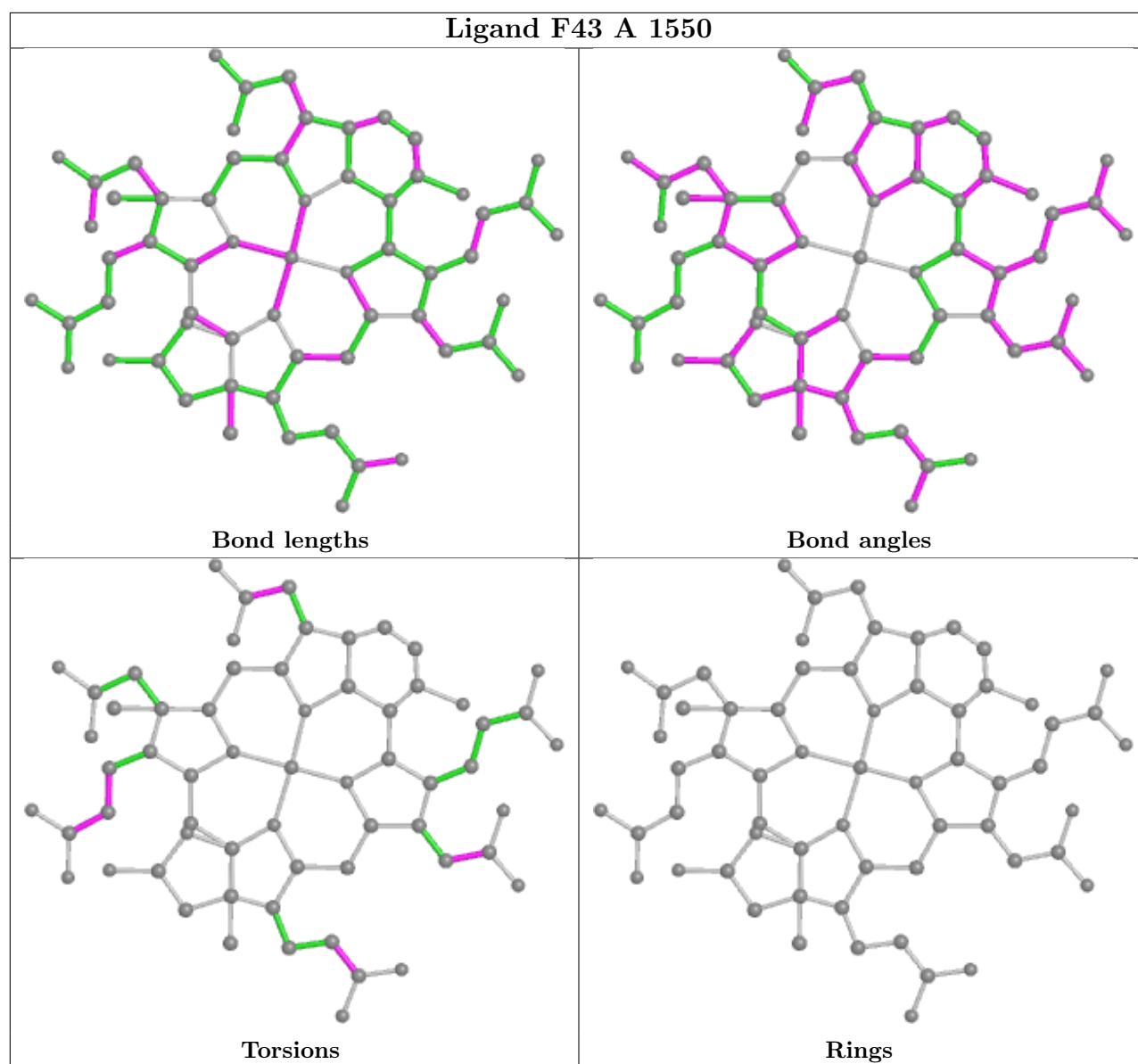
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.