



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 01:53 AM EDT

PDB ID : 9N46 / pdb_00009n46
Title : Methyl-coenzyme M Reductase red1/red1-silent ensemble
Authors : Ohmer, C.J.; Ragsdale, S.W.
Deposited on : 2025-02-02
Resolution : 1.55 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

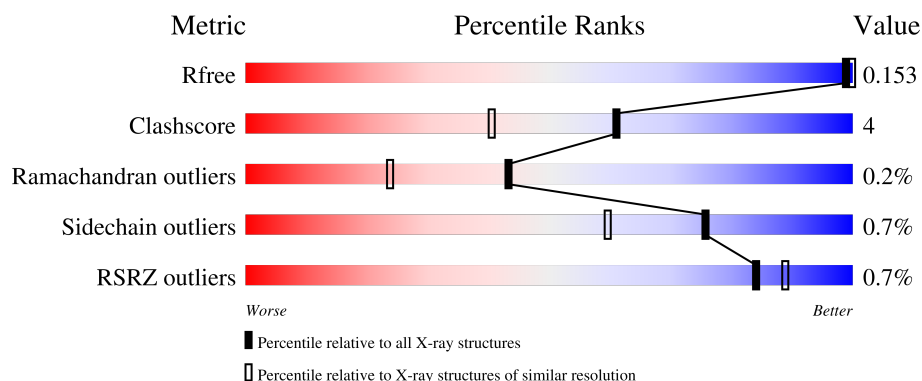
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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))
R_{free}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	550	2% 83% 17%
1	a	550	82% 17%
2	B	443	84% 16%
2	b	443	84% 15%
3	C	249	2% 85% 13%

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Mol	Chain	Length	Quality of chain
3	c	249	

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
1	DYA	A	450[A]	-	X	-	-
1	DYA	a	450[A]	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 77395 atoms, of which 37380 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 subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	548	Total	C	H	N	O	S	0	548	0
			16619	5382	8117	1428	1652	40			
1	a	548	Total	C	H	N	O	S	0	548	0
			16622	5382	8120	1428	1652	40			

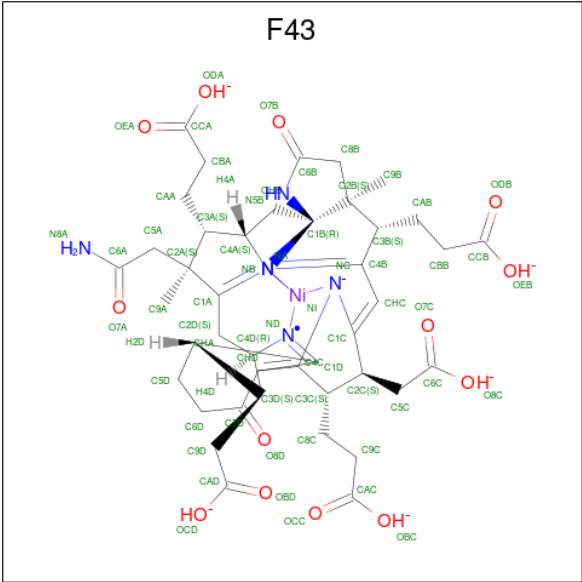
- Molecule 2 is a protein called Methyl-coenzyme M reductase I subunit beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	442	Total	C	H	N	O	S	0	442	0
			13202	4184	6588	1098	1296	36			
2	b	442	Total	C	H	N	O	S	0	442	0
			13191	4184	6577	1098	1296	36			

- Molecule 3 is a protein called Methyl-coenzyme M reductase I subunit gamma.

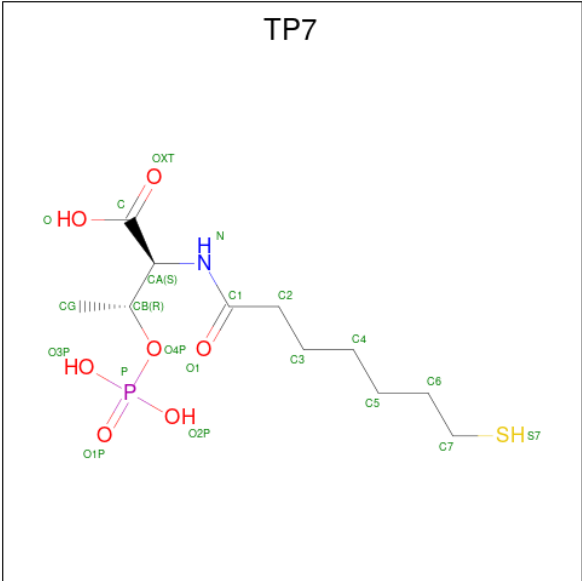
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	248	Total	C	H	N	O	S	0	248	0
			7887	2486	3869	710	800	22			
3	c	248	Total	C	H	N	O	S	0	248	0
			7883	2486	3865	710	800	22			

- Molecule 4 is FACTOR 430 (CCD ID: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	Ni	O	0	1
			219	84	95	12	2	26		
4	A	1	Total	C	H	N	Ni	O	0	1
			217	84	93	12	2	26		

- Molecule 5 is Coenzyme B (CCD ID: TP7) (formula: C₁₁H₂₂NO₇PS) (labeled as "Ligand of Interest" by depositor).



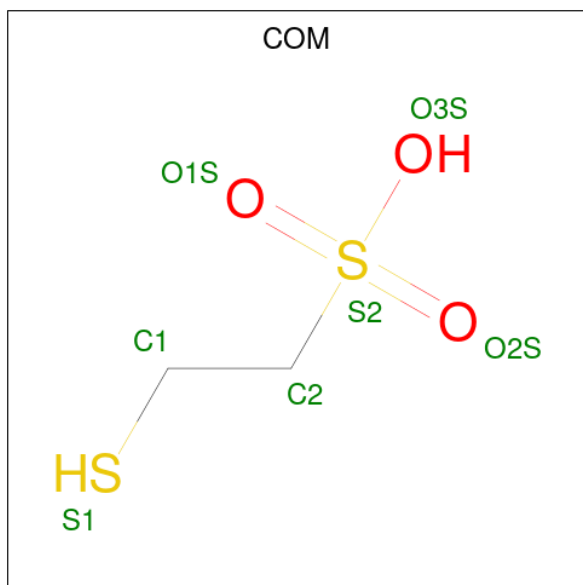
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	S	0	1
			40	11	19	1	7	1	1		

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	a	1	Total	C	H	N	O	P	S	0	1
			40	11	19	1	7	1	1		

- Molecule 6 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $C_2H_6O_3S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	O	S	0	1
			23	4	9	6	4		
6	a	1	Total	C	H	O	S	0	1
			23	4	9	6	4		

- Molecule 7 is TITANIUM ION (CCD ID: 4TI) (formula: Ti).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ti	0	0
			1	1		

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	a	1	Total	Na	0	0
			1	1		

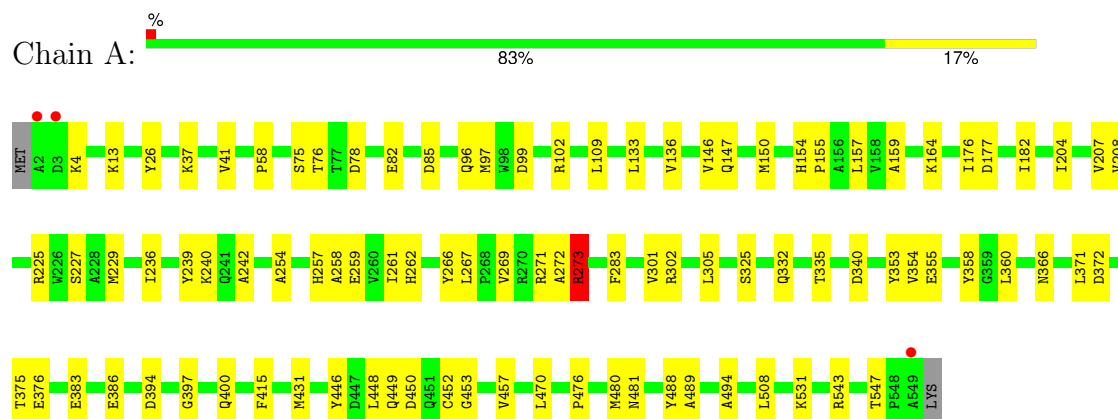
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	347	Total 372	O 372	0	82
9	B	205	Total 243	O 243	0	70
9	C	104	Total 129	O 129	0	44
9	a	332	Total 365	O 365	0	73
9	b	176	Total 203	O 203	0	67
9	c	93	Total 115	O 115	0	46

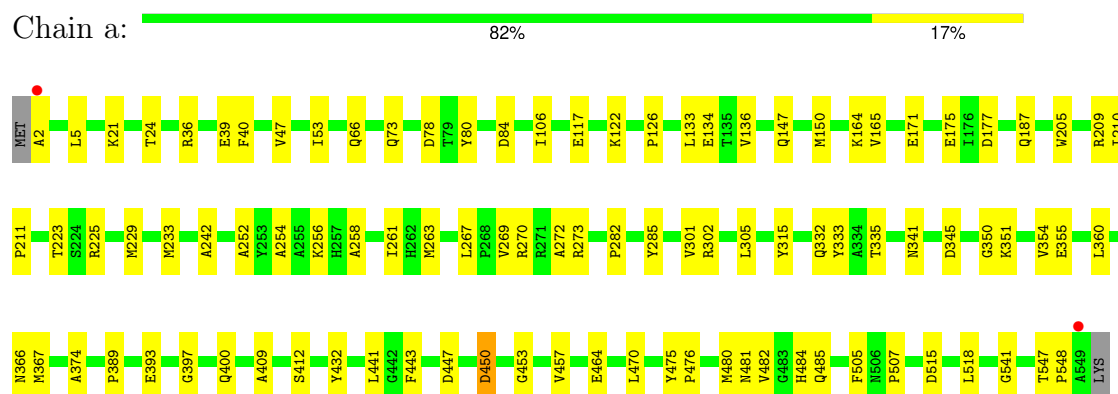
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

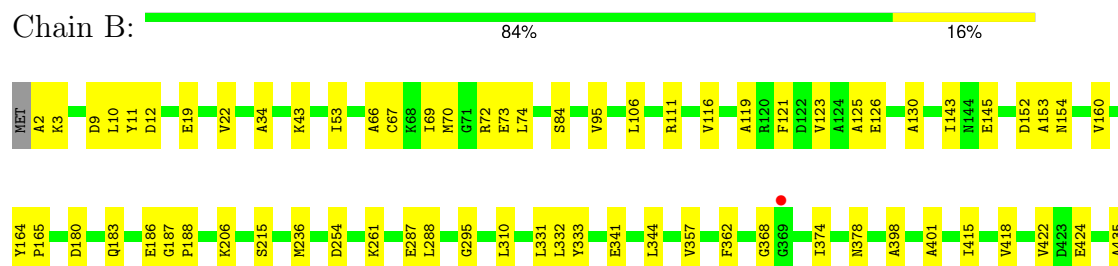
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha

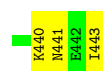


- Molecule 1: Methyl-coenzyme M reductase I subunit alpha



- Molecule 2: Methyl-coenzyme M reductase I subunit beta





• Molecule 2: Methyl-coenzyme M reductase I subunit beta

Chain b: 84% 15%



• Molecule 3: Methyl-coenzyme M reductase I subunit gamma

Chain C: 2% 85% 13%



• Molecule 3: Methyl-coenzyme M reductase I subunit gamma

Chain c: 2% 78% 21%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.32Å 117.89Å 125.03Å 90.00° 92.70° 90.00°	Depositor
Resolution (Å)	20.49 – 1.55 20.49 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.49-1.55) 99.8 (20.49-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 1.55Å)	Xtriage
Refinement program	PHENIX 2.0_5936	Depositor
R, R_{free}	0.123 , 0.153 0.124 , 0.153	Depositor DCC
R_{free} test set	2014 reflections (0.58%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	77395	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: COM, AGM, DYA, F43, MGN, GL3, TP7, MHS, NA, SMC, 4TI

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	0.25	0/8586	0.40	0/11652
1	a	0.25	0/8586	0.40	0/11652
2	B	0.20	0/6716	0.35	0/9100
2	b	0.20	0/6716	0.33	0/9100
3	C	0.19	0/4090	0.37	0/5508
3	c	0.18	0/4090	0.36	0/5508
All	All	0.22	0/38784	0.37	0/52520

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	a	0	1
2	b	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273[A]	ARG	Sidechain
1	a	480[W]	MET	Peptide
2	b	72[A]	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	8502	8117	8110	83	0
1	a	8502	8120	8113	79	0
2	B	6614	6588	6586	57	0
2	b	6614	6577	6584	52	0
3	C	4018	3869	3868	36	0
3	c	4018	3865	3867	52	0
4	A	248	188	170	10	0
5	A	21	19	19	2	0
5	a	21	19	19	3	0
6	A	14	9	9	1	0
6	a	14	9	9	2	0
7	A	1	0	0	0	0
8	a	1	0	0	0	0
9	A	372	0	0	24	0
9	B	243	0	0	19	0
9	C	129	0	0	7	0
9	a	365	0	0	9	0
9	b	203	0	0	4	0
9	c	115	0	0	5	0
All	All	40015	37380	37354	319	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 4.

The worst 5 of 319 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)
6:A:603[A]:COM:O2S	9:A:702:HOH:O	1.82	0.96
1:a:171[W]:GLU:OE2	9:a:702:HOH:O	1.85	0.94
2:b:305[W]:TYR:OH	9:b:501[W]:HOH:O	1.87	0.93
1:a:66[W]:GLN:NE2	3:c:171[W]:MET:O	2.07	0.86
1:A:82[A]:GLU:OE2	9:A:704[A]:HOH:O	2.02	0.77

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1080/550 (196%)	1036 (96%)	44 (4%)	0	100	100
1	a	1080/550 (196%)	1042 (96%)	38 (4%)	0	100	100
2	B	880/443 (199%)	842 (96%)	38 (4%)	0	100	100
2	b	880/443 (199%)	856 (97%)	22 (2%)	2 (0%)	43	24
3	C	492/249 (198%)	474 (96%)	16 (3%)	2 (0%)	30	13
3	c	492/249 (198%)	468 (95%)	18 (4%)	6 (1%)	10	2
All	All	4904/2484 (197%)	4718 (96%)	176 (4%)	10 (0%)	43	24

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	287[A]	GLU
2	b	287[W]	GLU
3	c	156[A]	HIS
3	c	156[W]	HIS
3	C	63[A]	GLU

5.3.2 Protein sidechains ⓘ

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	864/434 (199%)	862 (100%)	2 (0%)	87	79
1	a	864/434 (199%)	862 (100%)	2 (0%)	87	79
2	B	682/342 (199%)	676 (99%)	6 (1%)	70	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	682/342 (199%)	678 (99%)	4 (1%)	78	64
3	C	432/217 (199%)	426 (99%)	6 (1%)	59	33
3	c	432/217 (199%)	426 (99%)	6 (1%)	59	33
All	All	3956/1986 (199%)	3930 (99%)	26 (1%)	76	59

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	78[A]	ASP
2	b	126[W]	GLU
3	c	186[A]	MET
2	b	126[A]	GLU
2	b	382[A]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

24 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	DYA	a	450[W]	1	6,7,8	2.20	1 (16%)	6,8,10	3.38	2 (33%)
1	SMC	a	452[A]	1	5,6,7	0.90	0	3,6,8	1.34	0
1	AGM	A	271[A]	1	10,11,12	0.60	0	7,13,15	1.13	0
1	SMC	A	452[A]	1	5,6,7	1.13	0	3,6,8	2.29	1 (33%)
1	MHS	a	257[W]	1	10,11,12	0.54	0	5,14,16	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	DYA	A	450[W]	1	6,7,8	2.27	2 (33%)	6,8,10	2.30	1 (16%)
1	MGN	A	400[W]	1	6,9,10	0.52	0	7,12,14	0.94	0
1	MHS	A	257[A]	1	10,11,12	0.70	0	5,14,16	0.67	0
1	AGM	a	271[W]	1	10,11,12	0.52	0	7,13,15	0.78	0
1	SMC	a	452[W]	1	5,6,7	1.00	0	3,6,8	1.31	0
1	AGM	A	271[W]	1	10,11,12	0.58	0	7,13,15	0.69	0
1	GL3	A	445[A]	1	2,3,4	0.78	0	1,2,4	0.39	0
1	SMC	A	452[W]	1	5,6,7	0.91	0	3,6,8	1.13	0
1	MHS	A	257[W]	1	10,11,12	0.59	0	5,14,16	0.69	0
1	MGN	a	400[A]	1	6,9,10	0.69	0	7,12,14	0.50	0
1	GL3	a	445[A]	1	2,3,4	0.58	0	1,2,4	0.06	0
1	DYA	a	450[A]	1	6,7,8	2.09	1 (16%)	6,8,10	3.39	5 (83%)
1	GL3	A	445[W]	1	2,3,4	0.64	0	1,2,4	0.11	0
1	MHS	a	257[A]	1	10,11,12	0.62	0	5,14,16	0.63	0
1	DYA	A	450[A]	1	6,7,8	2.11	1 (16%)	6,8,10	3.41	4 (66%)
1	MGN	A	400[A]	1	6,9,10	0.70	0	7,12,14	0.65	0
1	AGM	a	271[A]	1	10,11,12	0.61	0	7,13,15	0.89	0
1	MGN	a	400[W]	1	6,9,10	0.64	0	7,12,14	0.38	0
1	GL3	a	445[W]	1	2,3,4	0.41	0	1,2,4	0.35	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	DYA	a	450[W]	1	-	4/4/6/8	-
1	SMC	a	452[A]	1	-	1/3/5/7	-
1	AGM	A	271[A]	1	-	3/10/11/13	-
1	SMC	A	452[A]	1	-	1/3/5/7	-
1	MHS	a	257[W]	1	-	0/5/6/8	0/1/1/1
1	DYA	A	450[W]	1	-	3/4/6/8	-
1	MGN	A	400[W]	1	-	0/7/9/12	-
1	MHS	A	257[A]	1	-	0/5/6/8	0/1/1/1
1	AGM	a	271[W]	1	-	2/10/11/13	-
1	SMC	a	452[W]	1	-	1/3/5/7	-
1	AGM	A	271[W]	1	-	1/10/11/13	-
1	GL3	A	445[A]	1	-	1/1/1/2	-
1	SMC	A	452[W]	1	-	1/3/5/7	-
1	MHS	A	257[W]	1	-	0/5/6/8	0/1/1/1
1	MGN	a	400[A]	1	-	1/7/9/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GL3	a	445[A]	1	-	0/1/1/2	-
1	DYA	a	450[A]	1	-	4/4/6/8	-
1	GL3	A	445[W]	1	-	0/1/1/2	-
1	MHS	a	257[A]	1	-	0/5/6/8	0/1/1/1
1	DYA	A	450[A]	1	-	4/4/6/8	-
1	MGN	A	400[A]	1	-	2/7/9/12	-
1	AGM	a	271[A]	1	-	4/10/11/13	-
1	MGN	a	400[W]	1	-	0/7/9/12	-
1	GL3	a	445[W]	1	-	1/1/1/2	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	450[W]	DYA	C-CA	4.88	1.53	1.45
1	A	450[W]	DYA	C-CA	4.84	1.53	1.45
1	A	450[A]	DYA	C-CA	4.41	1.52	1.45
1	a	450[A]	DYA	C-CA	4.35	1.52	1.45
1	A	450[W]	DYA	OD1-CG	-2.11	1.25	1.30

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	450[W]	DYA	O-C-CA	-7.28	116.26	125.39
1	A	450[A]	DYA	O-C-CA	-6.47	117.28	125.39
1	a	450[A]	DYA	O-C-CA	-6.29	117.51	125.39
1	A	450[W]	DYA	O-C-CA	-5.11	118.98	125.39
1	A	452[A]	SMC	CA-CB-SG	-3.91	107.72	114.04

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	271[A]	AGM	CE2-CD-CG-CB
1	A	271[A]	AGM	NE1-CD-CG-CB
1	A	450[A]	DYA	N-CA-CB-CG
1	A	450[A]	DYA	O-C-CA-CB
1	A	450[W]	DYA	O-C-CA-CB

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	271[A]	AGM	1	0
1	A	400[W]	MGN	1	0
1	A	257[W]	MHS	1	0
1	a	400[A]	MGN	1	0
1	a	450[A]	DYA	1	0
1	A	400[A]	MGN	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	A	602[W]	-	19,20,20	1.51	2 (10%)	24,26,26	1.01	0
4	F43	A	604[A]	9	63,71,71	1.75	3 (4%)	73,118,118	1.24	10 (13%)
4	F43	A	601[W]	1,6	63,71,71	1.91	4 (6%)	73,118,118	1.84	17 (23%)
6	COM	A	603[W]	4	6,6,6	1.24	1 (16%)	8,8,8	0.60	0
6	COM	a	602[A]	-	6,6,6	1.10	1 (16%)	8,8,8	0.94	0
4	F43	A	604[W]	1,6	63,71,71	1.88	4 (6%)	73,118,118	1.73	20 (27%)
6	COM	A	603[A]	-	6,6,6	1.03	1 (16%)	8,8,8	0.80	0
6	COM	a	602[W]	4	6,6,6	1.75	1 (16%)	8,8,8	1.08	0
5	TP7	a	601[W]	-	19,20,20	1.98	2 (10%)	24,26,26	1.27	3 (12%)
4	F43	A	601[A]	9	63,71,71	1.70	3 (4%)	73,118,118	1.29	12 (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
5	TP7	A	602[W]	-	-	0/24/24/24	-
4	F43	A	604[A]	9	-	9/28/185/185	-
4	F43	A	601[W]	1,6	-	9/28/185/185	-
6	COM	A	603[W]	4	-	0/4/4/4	-
6	COM	a	602[A]	-	-	0/4/4/4	-
4	F43	A	604[W]	1,6	-	7/28/185/185	-
6	COM	A	603[A]	-	-	0/4/4/4	-
6	COM	a	602[W]	4	-	0/4/4/4	-
5	TP7	a	601[W]	-	-	0/24/24/24	-
4	F43	A	601[A]	9	-	10/28/185/185	-

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601[W]	F43	NI-NA	9.19	2.11	1.89
4	A	604[A]	F43	NI-NB	9.07	2.11	1.89
4	A	604[W]	F43	NI-NB	8.73	2.10	1.89
4	A	604[A]	F43	NI-NA	8.56	2.10	1.89
4	A	604[W]	F43	NI-NA	8.48	2.09	1.89

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601[W]	F43	CAB-C3B-C4B	-6.60	99.67	111.19
4	A	604[W]	F43	CAB-C3B-C4B	-4.53	103.28	111.19
4	A	604[W]	F43	C4B-CHC-C1C	4.51	133.13	125.84
4	A	601[W]	F43	C3A-C4A-NA	4.33	108.89	102.30
4	A	604[W]	F43	CAB-C3B-C2B	-4.16	109.82	119.00

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

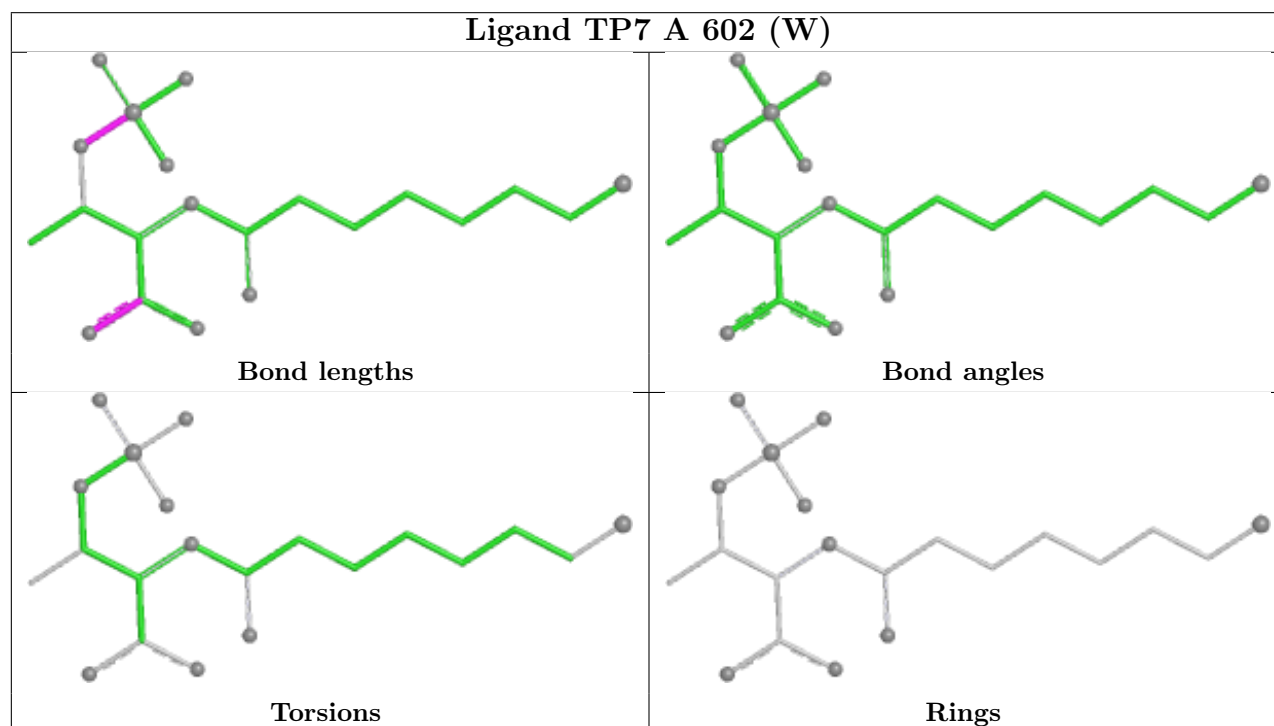
Mol	Chain	Res	Type	Atoms
4	A	601[A]	F43	C3A-CAA-CBA-CCA
4	A	601[W]	F43	C3A-CAA-CBA-CCA
4	A	604[W]	F43	C3A-CAA-CBA-CCA
4	A	604[A]	F43	C3A-CAA-CBA-CCA
4	A	604[A]	F43	C2C-C5C-C6C-O8C

There are no ring outliers.

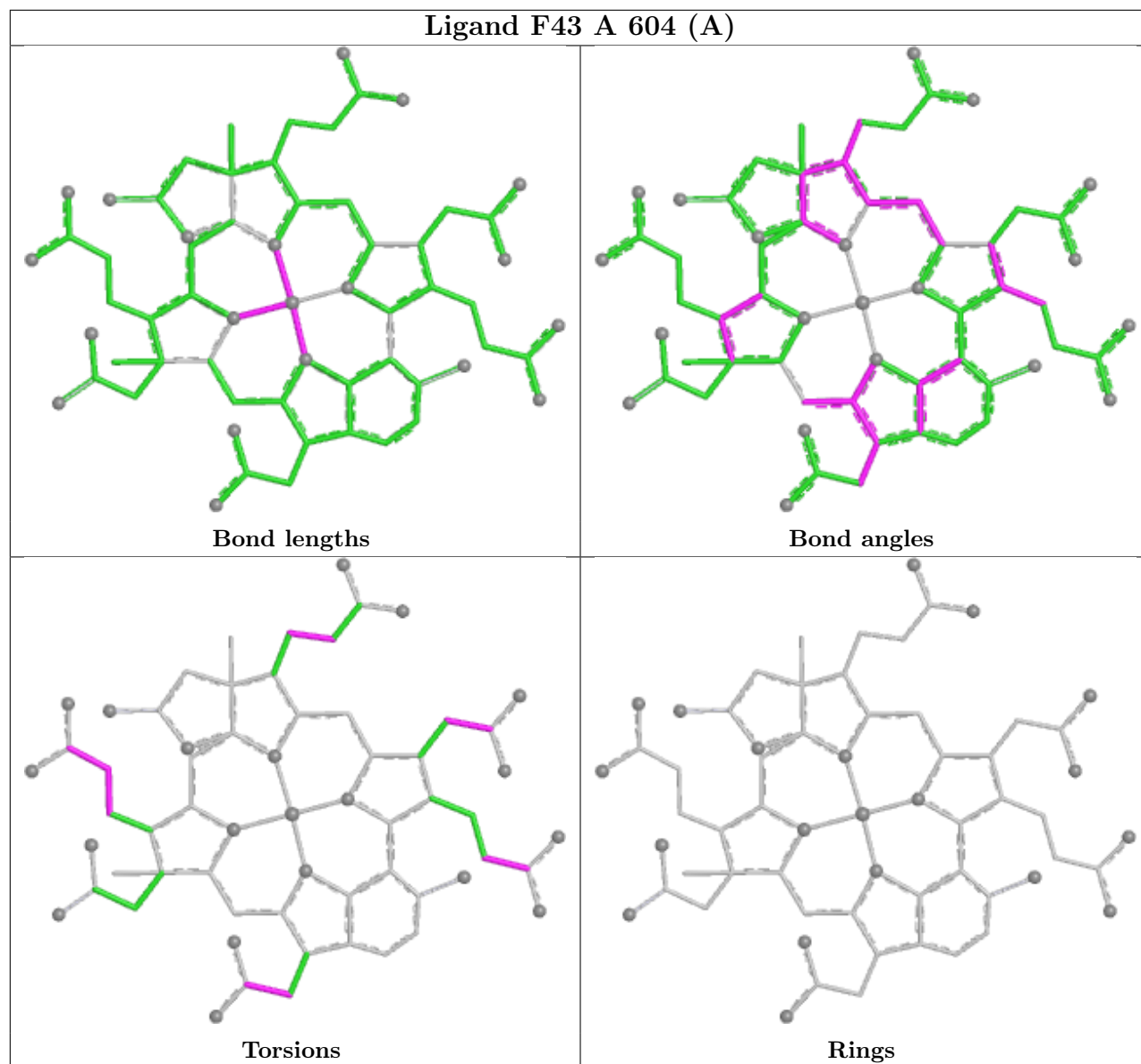
7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602[W]	TP7	2	0
4	A	604[A]	F43	1	0
6	a	602[A]	COM	2	0
4	A	604[W]	F43	5	0
6	A	603[A]	COM	1	0
5	a	601[W]	TP7	3	0
4	A	601[A]	F43	4	0

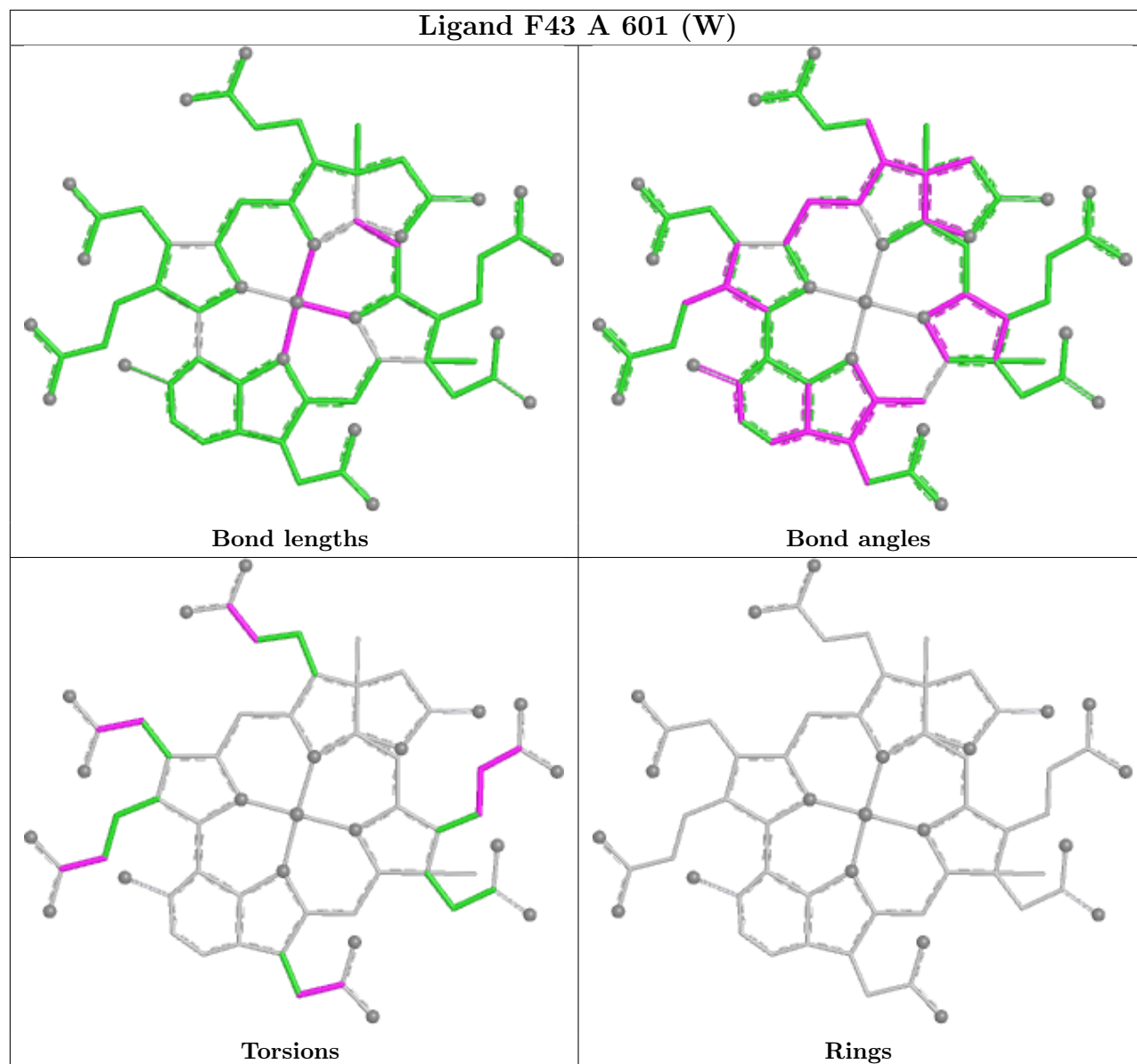
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



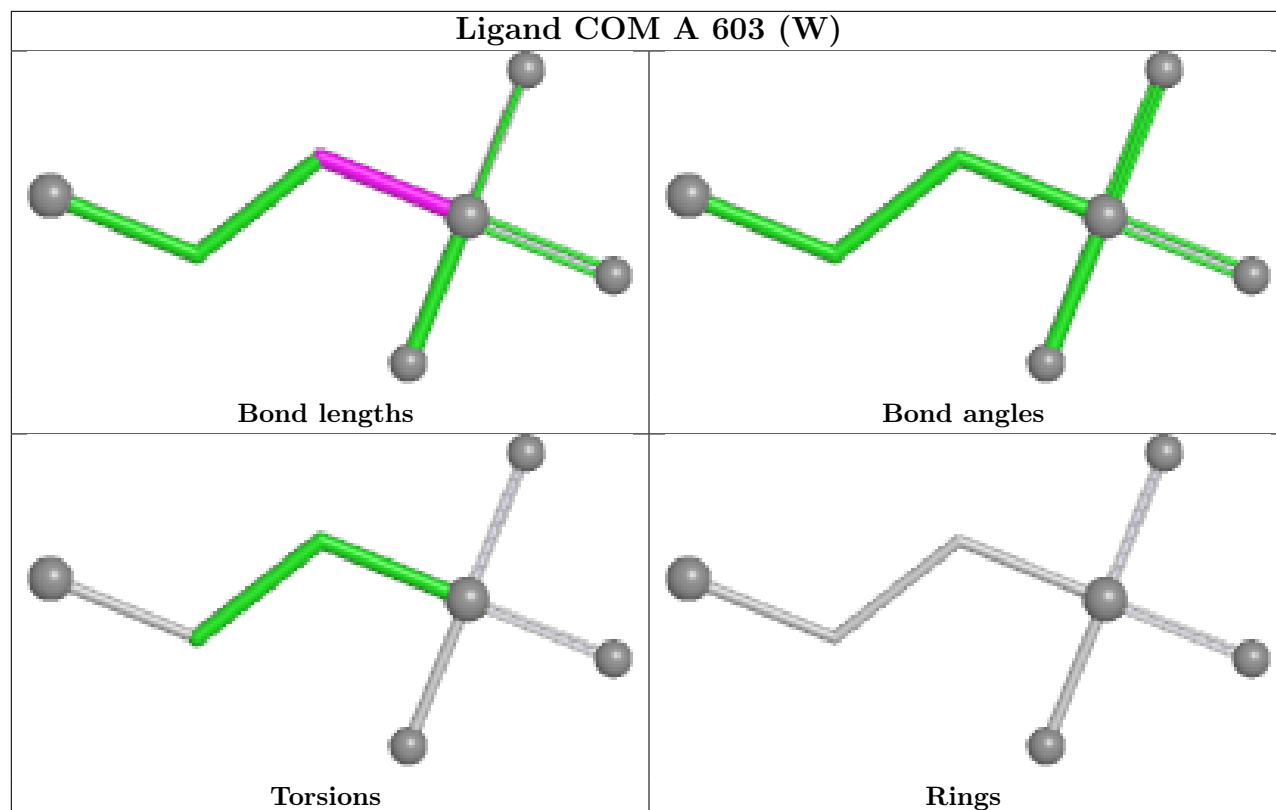
Ligand F43 A 604 (A)



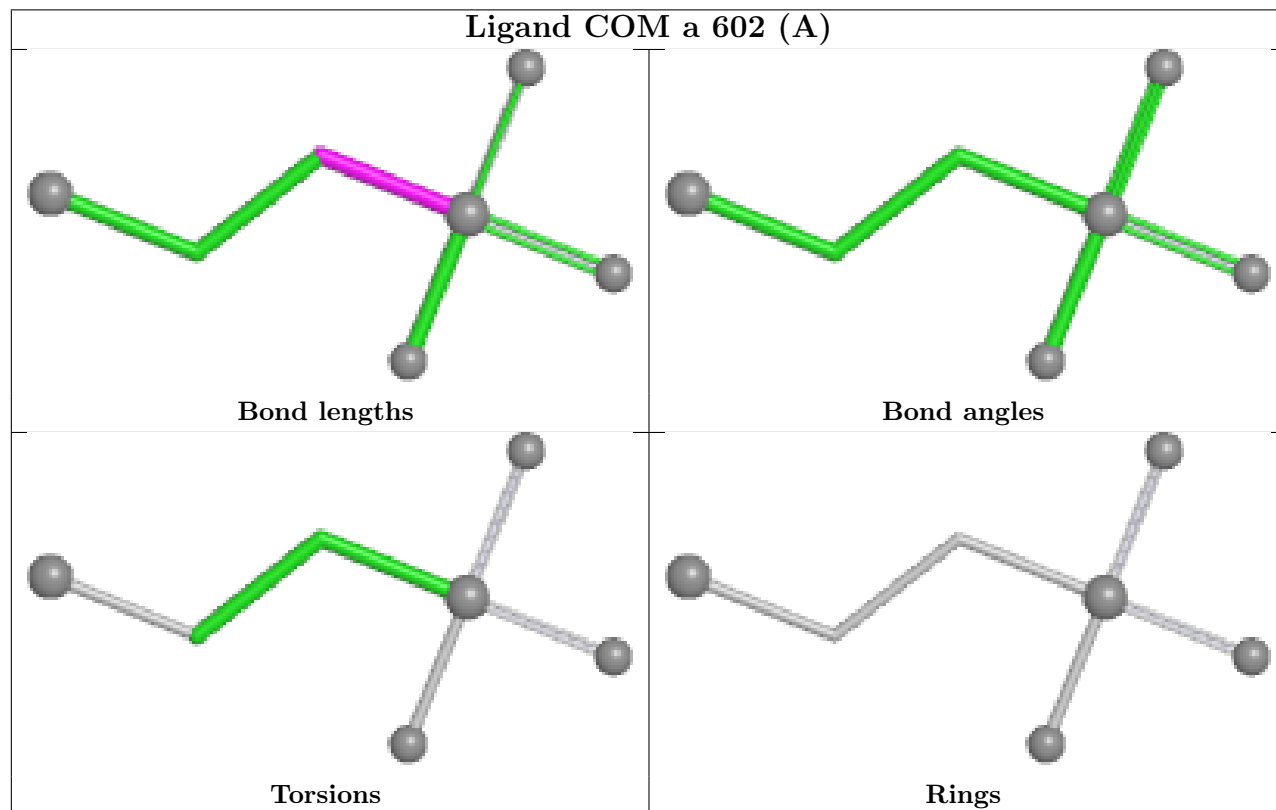
Ligand F43 A 601 (W)



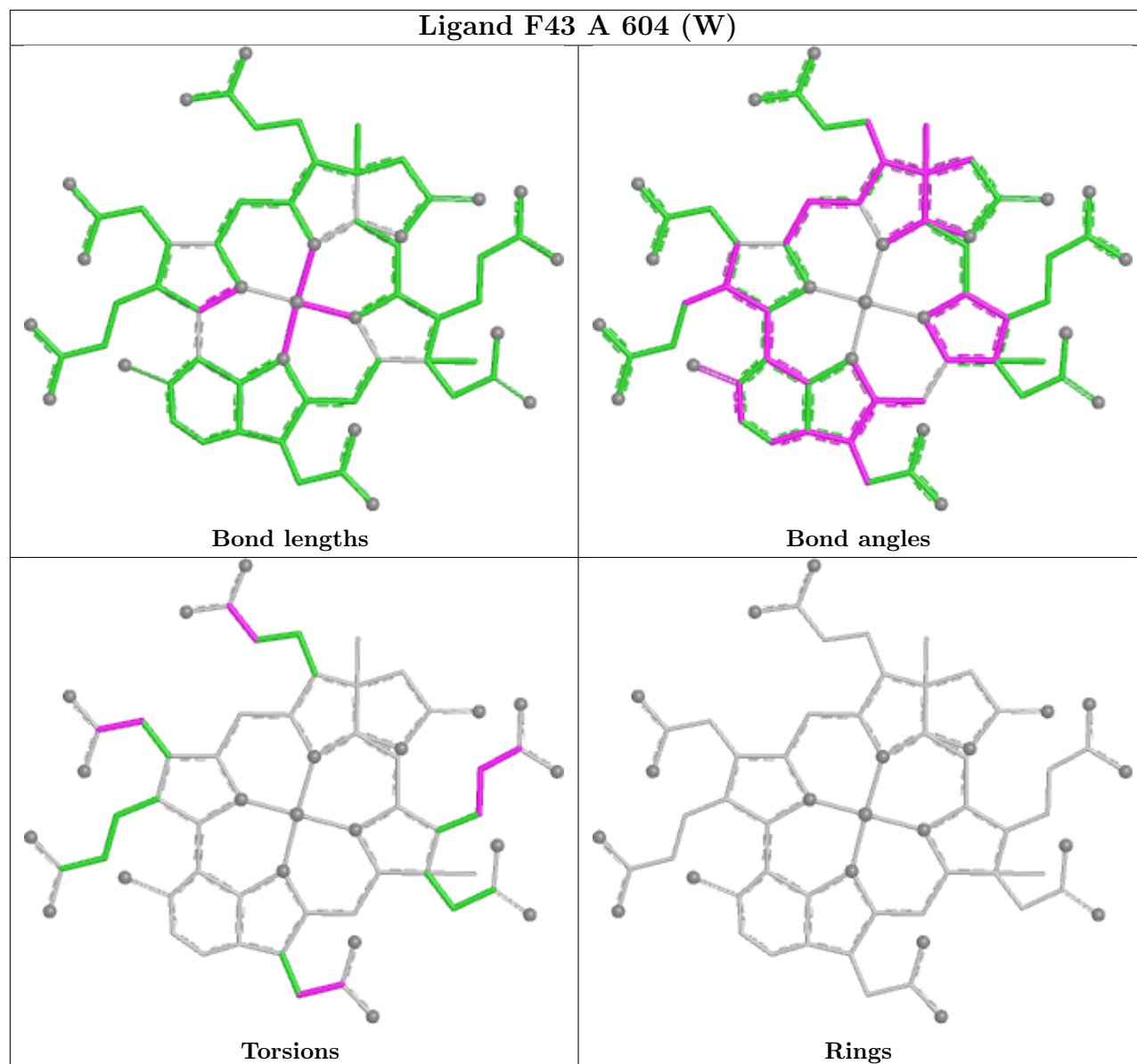
Ligand COM A 603 (W)

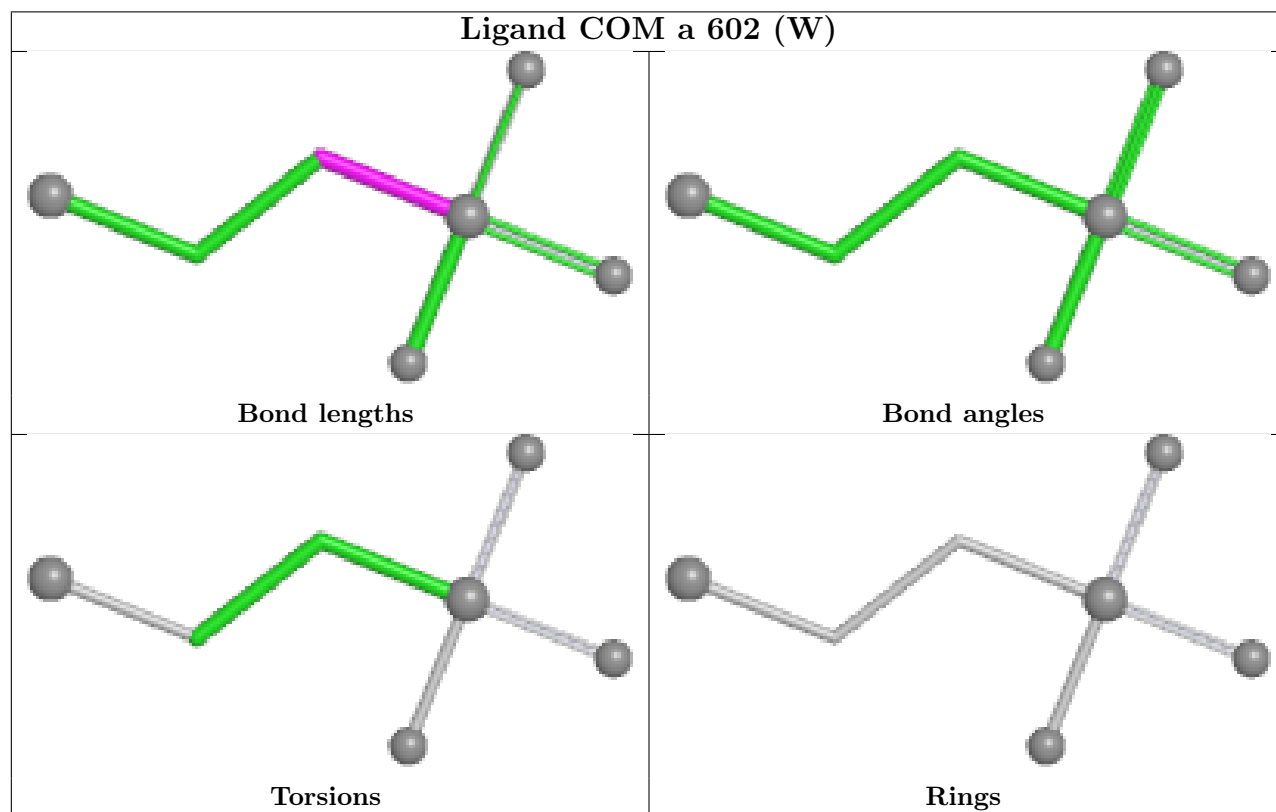
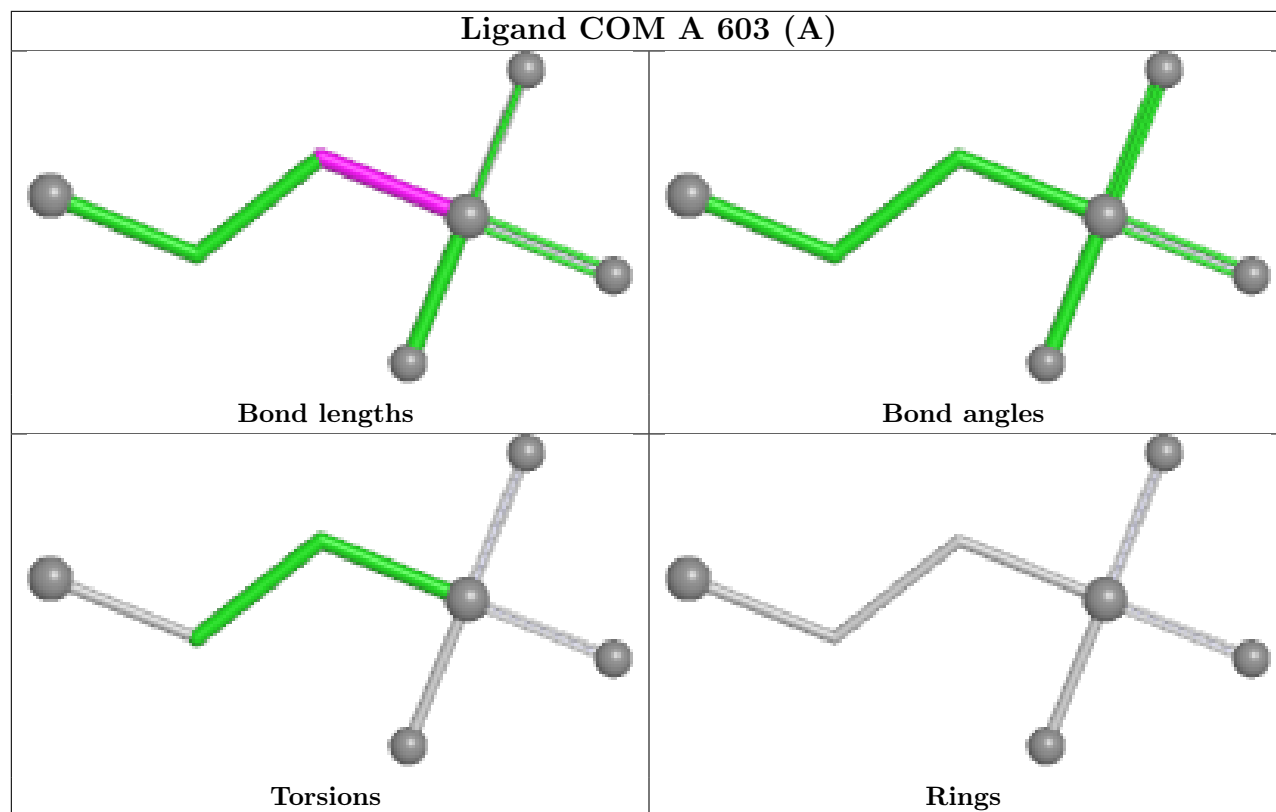


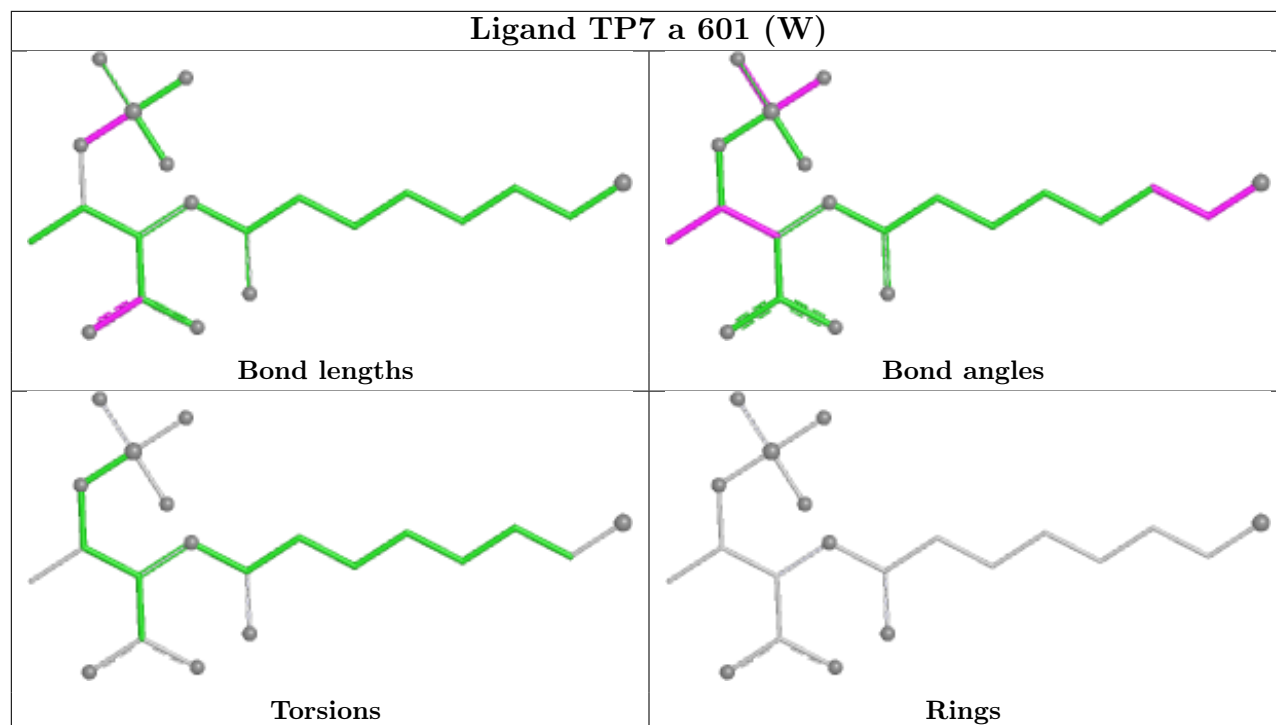
Ligand COM a 602 (A)

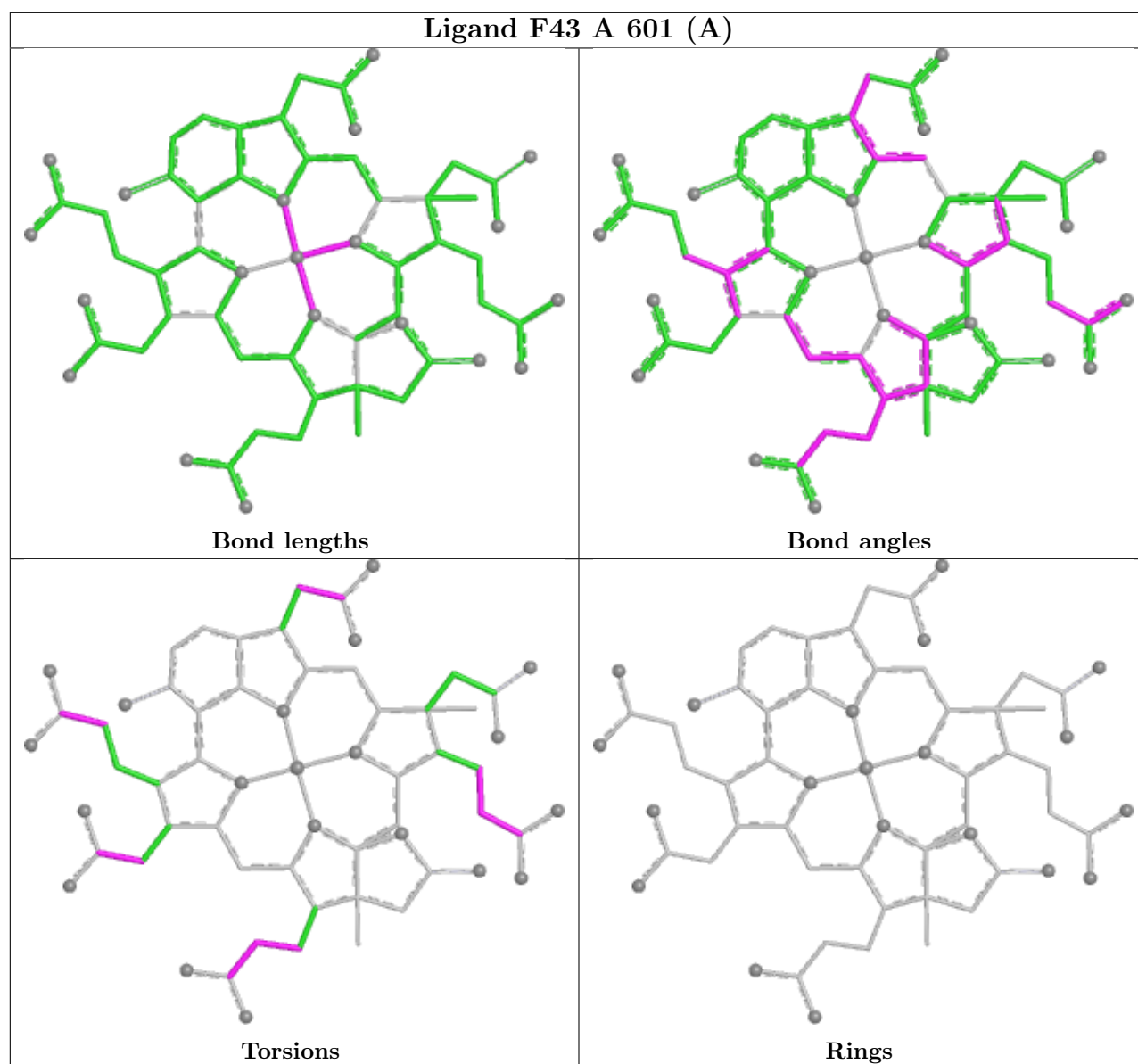


Ligand F43 A 604 (W)









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](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	542/550 (98%)	-0.78	3 (0%) 85 89	8, 14, 22, 41	542 (100%)
1	a	542/550 (98%)	-0.81	2 (0%) 88 92	8, 13, 22, 36	542 (100%)
2	B	442/443 (99%)	-0.53	1 (0%) 91 94	10, 16, 26, 35	442 (100%)
2	b	442/443 (99%)	-0.36	2 (0%) 87 90	10, 17, 27, 49	442 (100%)
3	C	248/249 (99%)	-0.18	5 (2%) 65 73	12, 19, 32, 41	248 (100%)
3	c	248/249 (99%)	-0.14	4 (1%) 70 78	12, 20, 32, 47	248 (100%)
All	All	2464/2484 (99%)	-0.54	17 (0%) 84 89	8, 16, 27, 49	2464 (100%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	549[A]	ALA	4.3
1	a	549[A]	ALA	3.9
2	b	2[A]	ALA	3.3
3	c	248[A]	LEU	3.3
1	A	2[A]	ALA	3.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	MHS	A	257[A]	11/12	0.96	0.07	20,27,41,41	19
1	MHS	A	257[W]	11/12	0.96	0.07	18,28,38,38	19
1	AGM	A	271[A]	12/13	0.97	0.04	19,23,27,28	25
1	AGM	A	271[W]	12/13	0.97	0.04	14,17,23,23	26

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MHS	a	257[A]	11/12	0.97	0.05	23,28,34,34	19
1	MHS	a	257[W]	11/12	0.97	0.05	21,25,33,33	19
1	MGN	a	400[A]	10/11	0.98	0.04	18,22,27,27	20
1	MGN	a	400[W]	10/11	0.98	0.04	19,23,27,27	20
1	DYA	a	450[A]	8/9	0.98	0.05	20,22,24,27	10
1	DYA	a	450[W]	8/9	0.98	0.05	19,22,24,26	9
1	SMC	A	452[A]	7/8	0.99	0.03	18,22,27,27	14
1	SMC	A	452[W]	7/8	0.99	0.03	19,23,27,27	14
1	MGN	A	400[A]	10/11	0.99	0.03	17,21,25,27	20
1	MGN	A	400[W]	10/11	0.99	0.03	19,23,25,25	20
1	AGM	a	271[A]	12/13	0.99	0.03	14,22,26,26	26
1	AGM	a	271[W]	12/13	0.99	0.03	14,20,22,24	26
1	GL3	A	445[A]	4/5	0.99	0.04	17,19,23,23	7
1	GL3	A	445[W]	4/5	0.99	0.04	16,19,22,22	7
1	DYA	A	450[A]	8/9	0.99	0.04	17,21,23,25	10
1	DYA	A	450[W]	8/9	0.99	0.04	15,20,22,24	9
1	GL3	a	445[A]	4/5	1.00	0.03	19,20,24,24	7
1	GL3	a	445[W]	4/5	1.00	0.03	16,21,22,26	7
1	SMC	a	452[A]	7/8	1.00	0.03	20,24,29,29	14
1	SMC	a	452[W]	7/8	1.00	0.03	21,25,28,28	14

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NA	a	603	1/1	0.93	0.15	41,41,41,41	0
5	TP7	a	601[W]	21/21	0.96	0.07	15,23,30,34	40
5	TP7	A	602[W]	21/21	0.97	0.06	16,21,33,35	40
6	COM	A	603[W]	7/7	0.98	0.07	13,17,21,21	11
6	COM	a	602[A]	7/7	0.98	0.06	17,21,31,38	12
6	COM	a	602[W]	7/7	0.98	0.06	19,21,24,24	11
6	COM	A	603[A]	7/7	0.98	0.07	16,24,30,37	12
4	F43	A	604[W]	62/62	0.99	0.04	12,18,22,26	108

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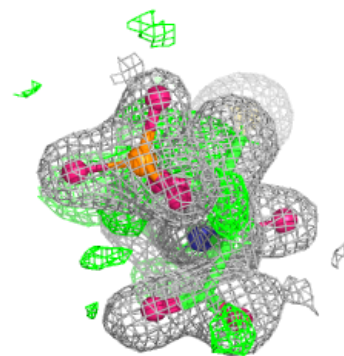
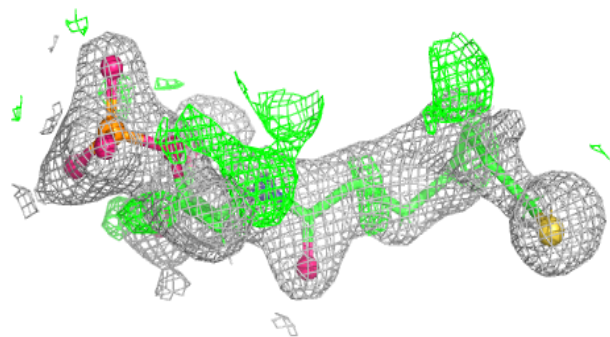
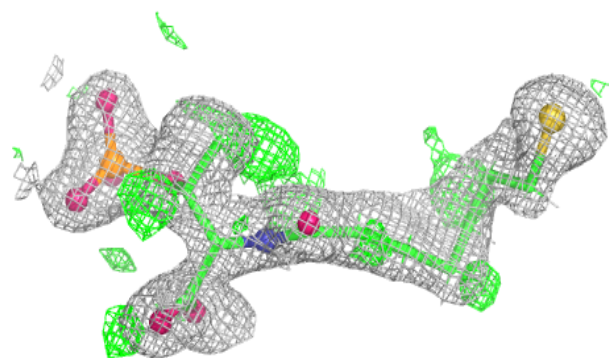
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	F43	A	601[A]	62/62	0.99	0.05	14,20,27,41	110
4	F43	A	601[W]	62/62	0.99	0.05	10,20,25,28	109
7	4TI	A	605	1/1	0.99	0.08	29,29,29,29	0
4	F43	A	604[A]	62/62	0.99	0.04	13,19,24,27	109

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

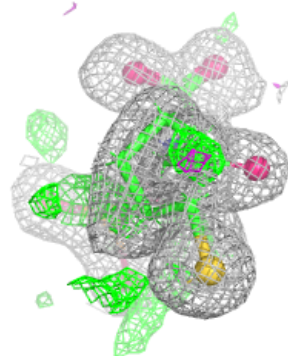
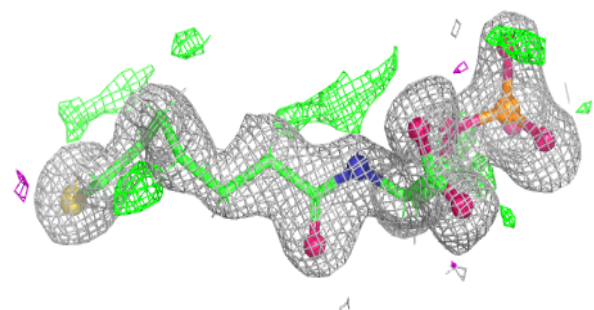
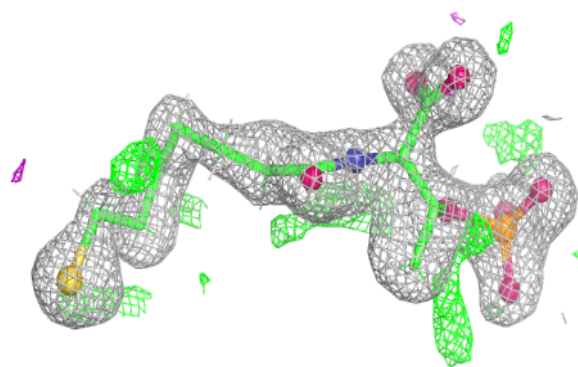
Electron density around TP7 a 601 (W):

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

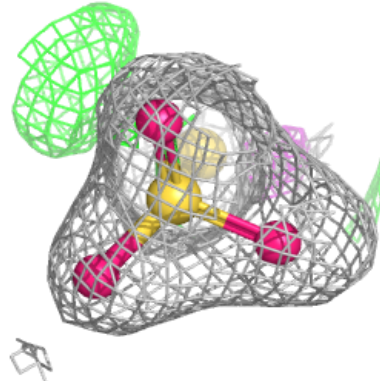
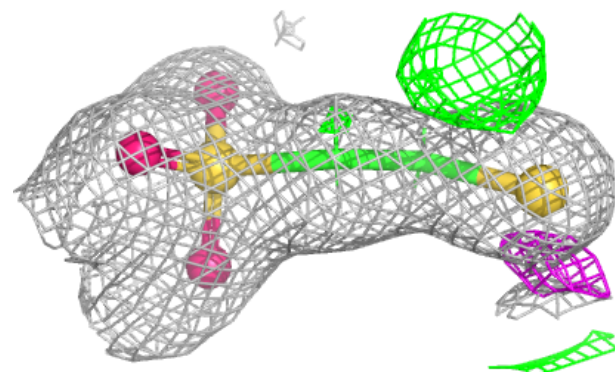
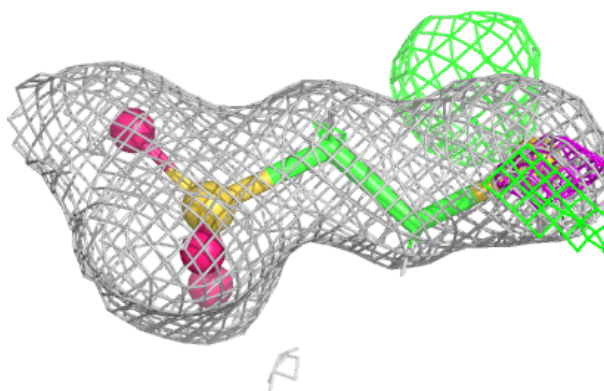


Electron density around TP7 A 602 (W):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

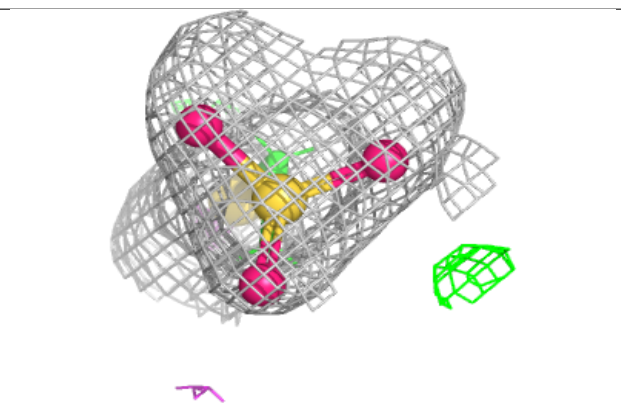
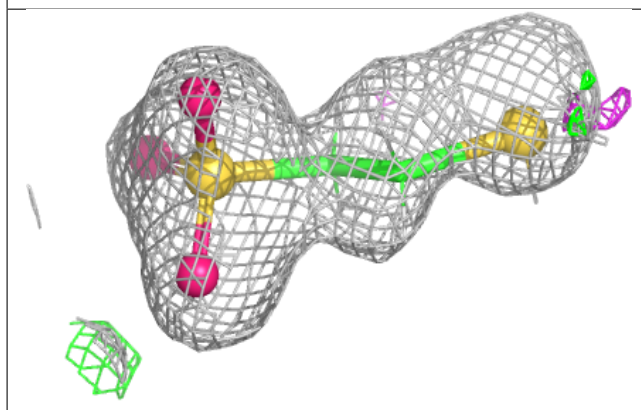
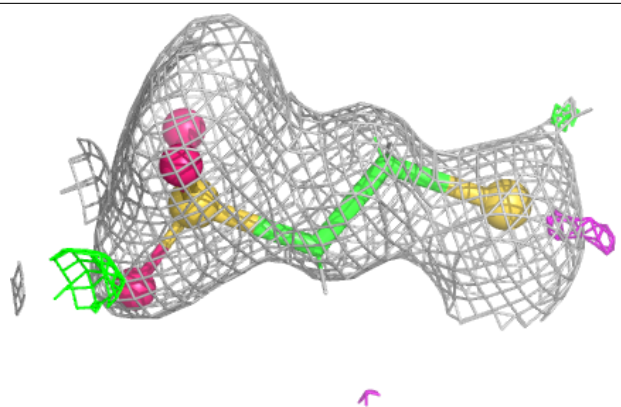
**Electron density around COM A 603 (W):**

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and green (positive)

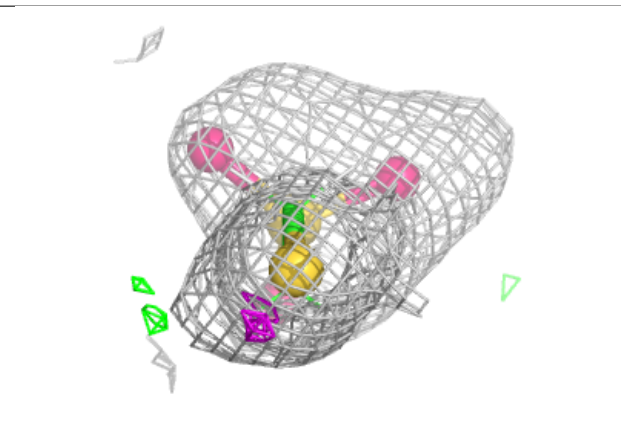
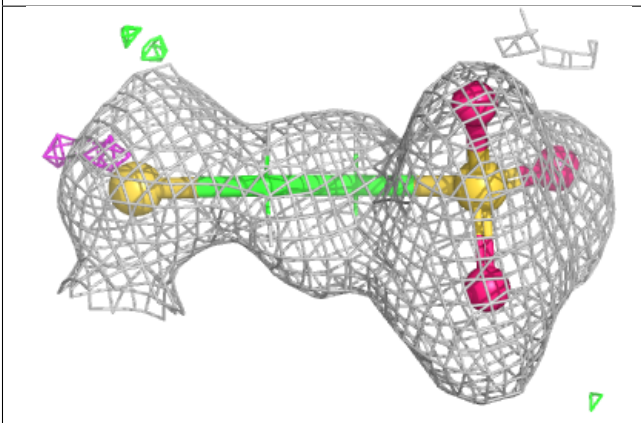
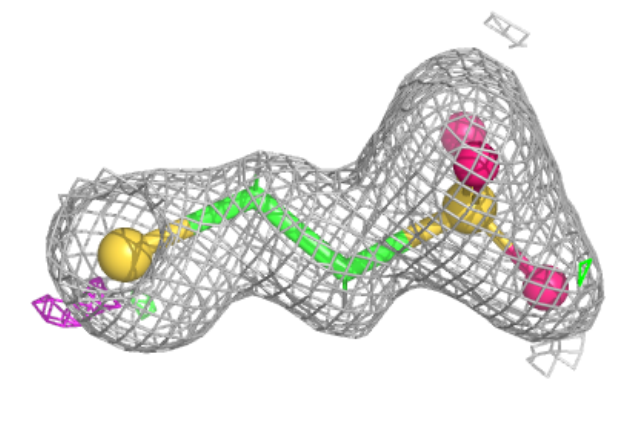


Electron density around COM a 602 (A):

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and green (positive)

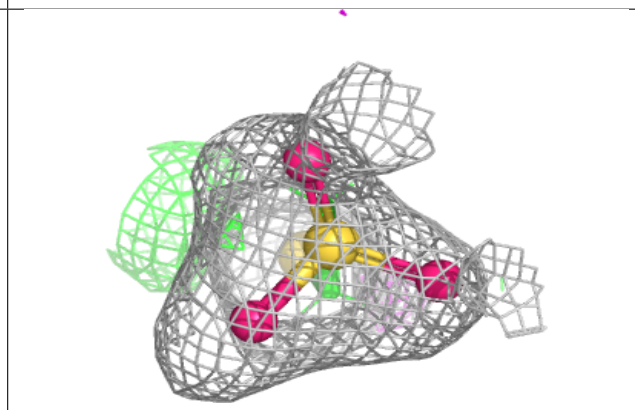
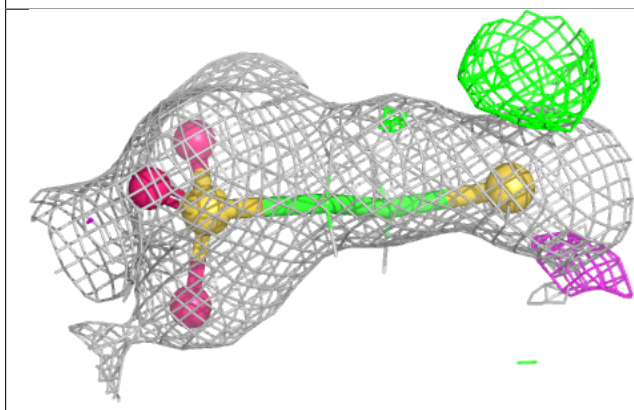
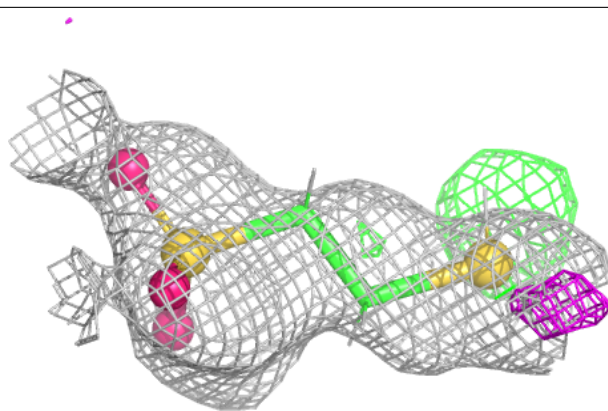
**Electron density around COM a 602 (W):**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



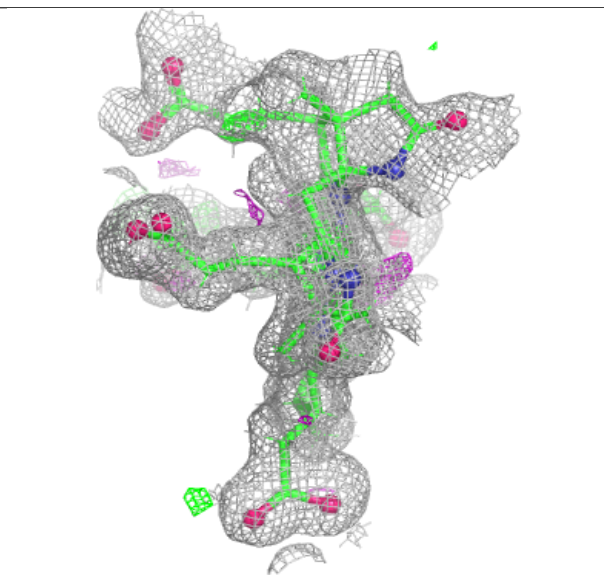
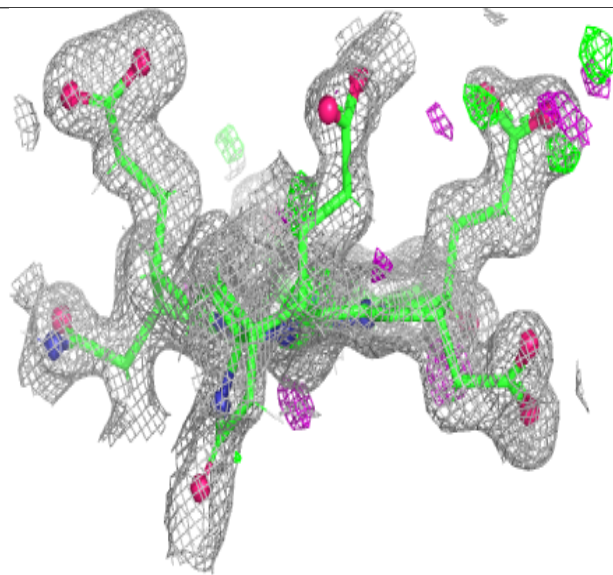
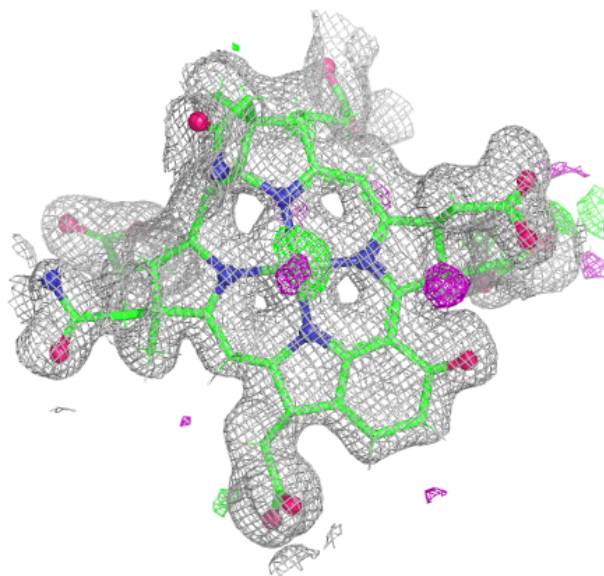
Electron density around COM A 603 (A):

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and green (positive)



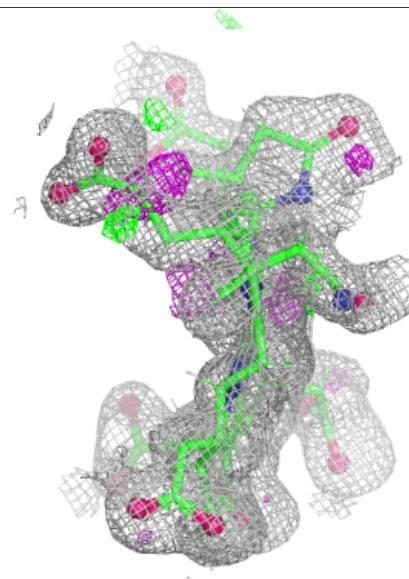
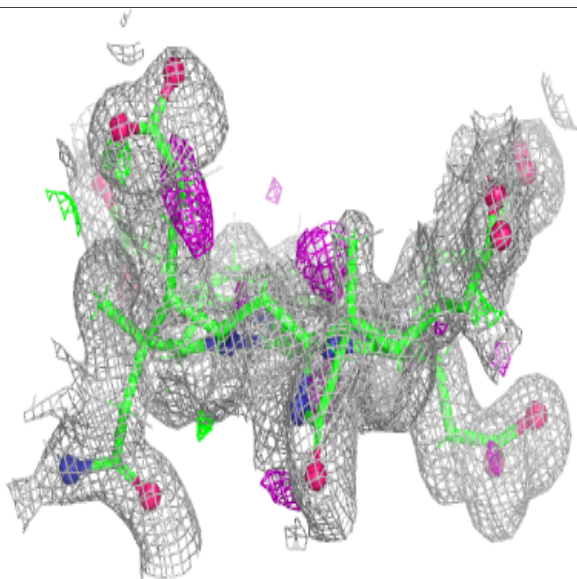
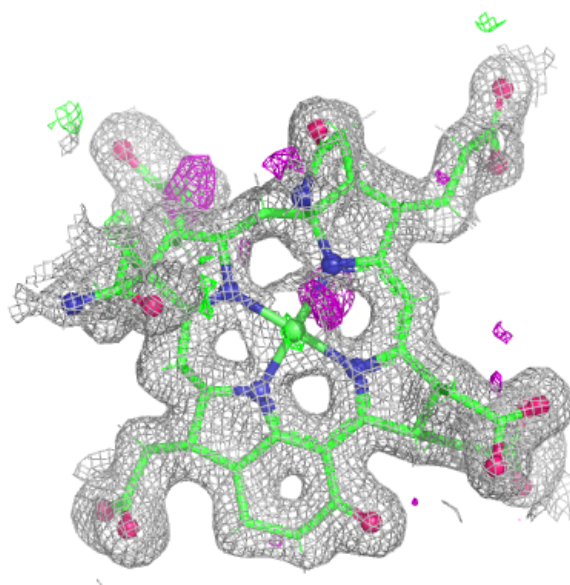
Electron density around F43 A 604 (W):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



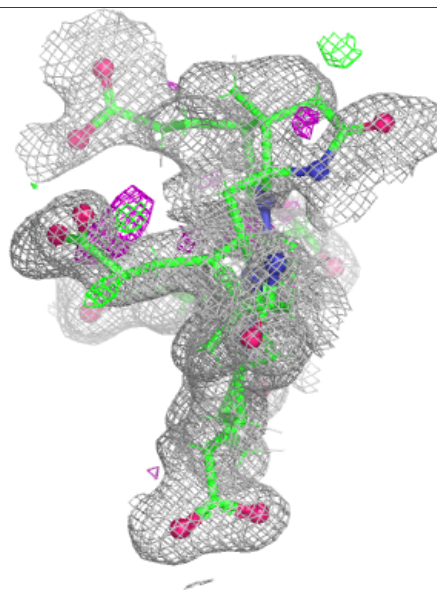
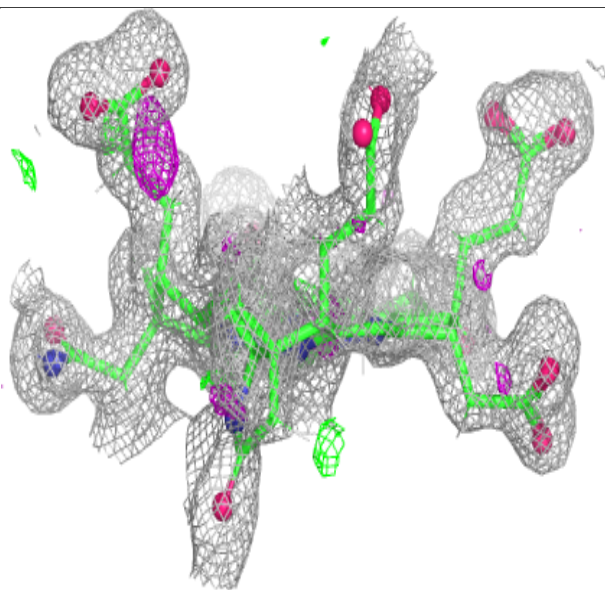
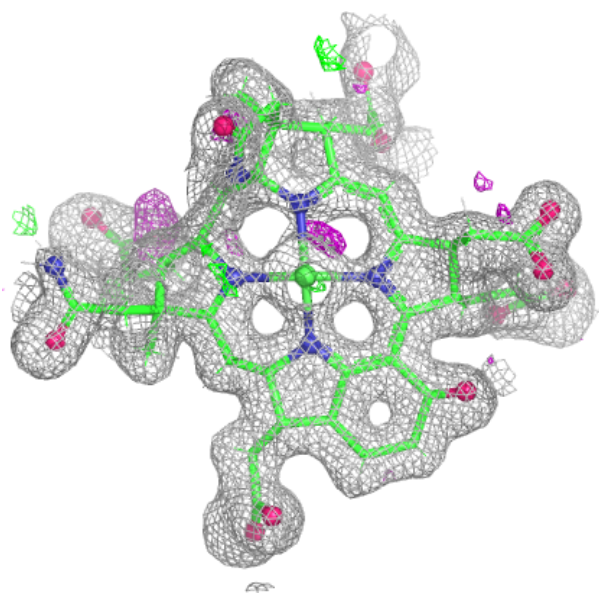
Electron density around F43 A 601 (A):

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



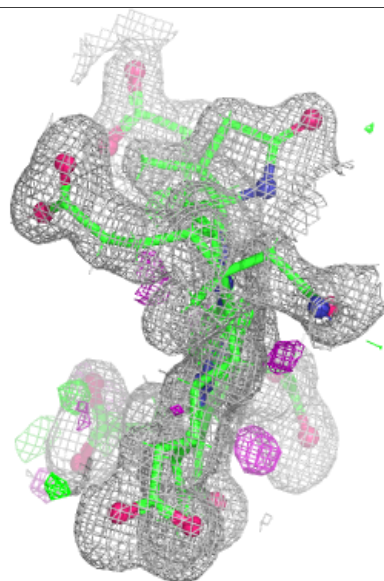
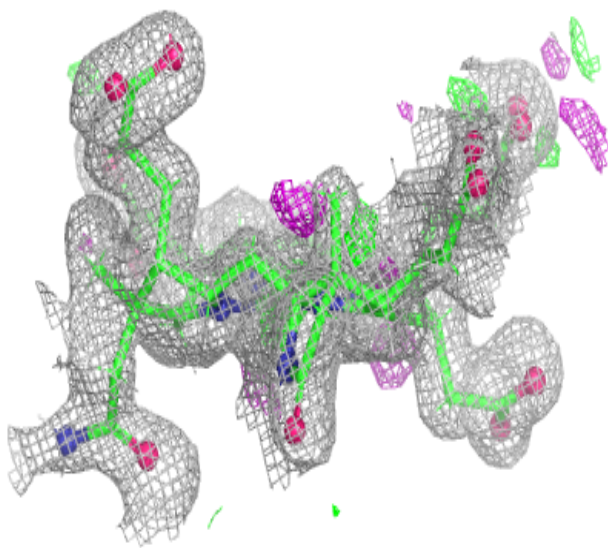
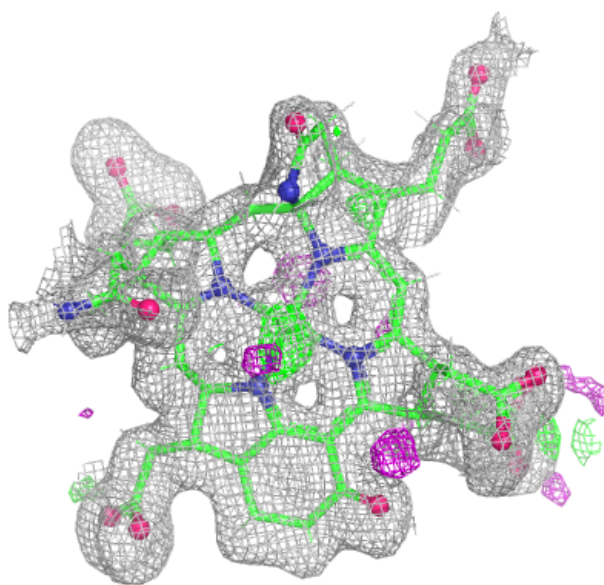
Electron density around F43 A 601 (W):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around F43 A 604 (A):

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.