



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 9, 2025 – 02:40 pm BST

PDB ID : 9QR3 / pdb\_00009qr3  
Title : Methyl-coenzyme M reductase of an ANME-2c from a microbial enrichment  
Authors : Mueller, M.-C.; Wagner, T.  
Deposited on : 2025-04-02  
Resolution : 1.34 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

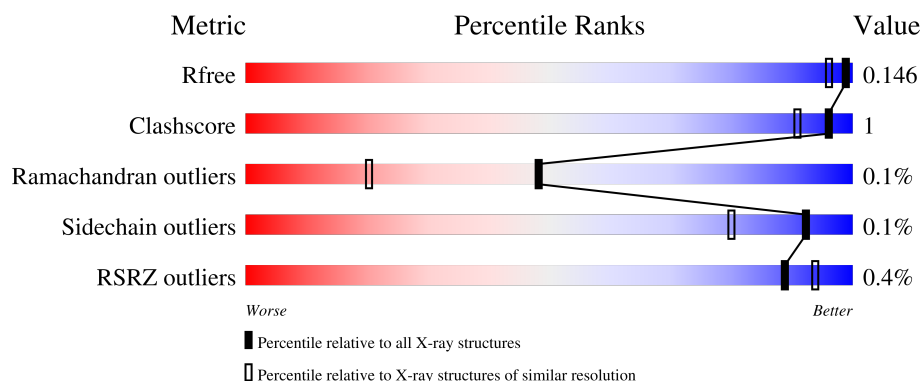
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.34 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.



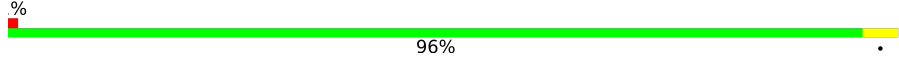
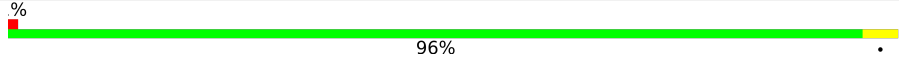
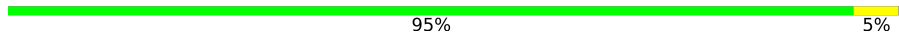
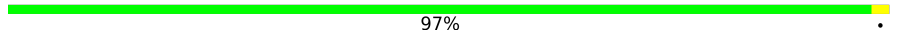
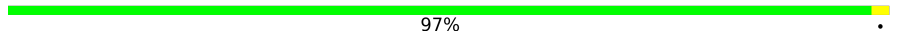
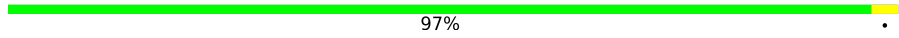
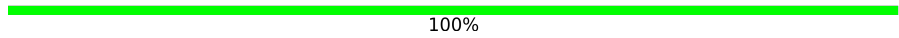
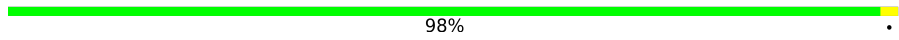
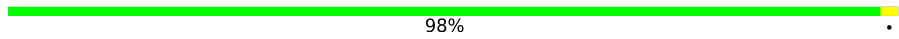
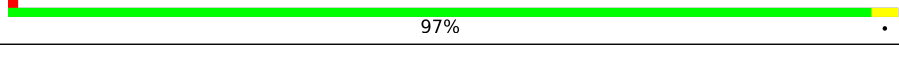
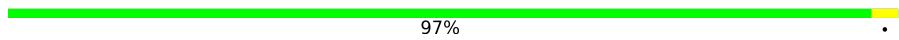
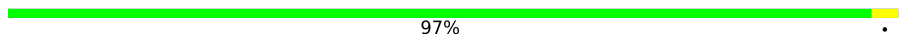
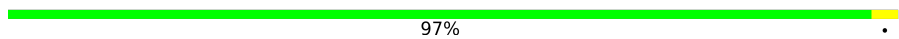
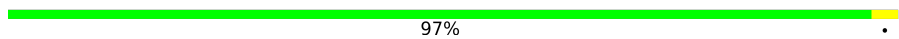
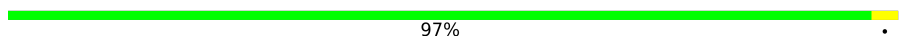
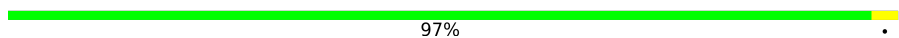
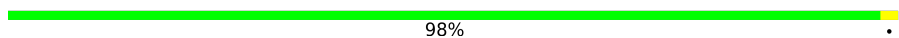
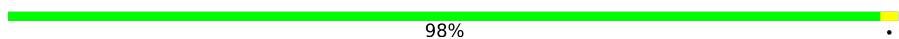
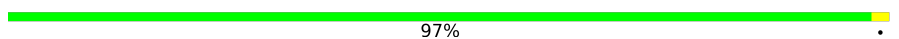
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1904 (1.36-1.32)
Clashscore	180529	2038 (1.36-1.32)
Ramachandran outliers	177936	2016 (1.36-1.32)
Sidechain outliers	177891	2016 (1.36-1.32)
RSRZ outliers	164620	1903 (1.36-1.32)

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  $\geq 3$ , 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	561	<div> <div style="width: 96%;"></div> <div>96%</div> </div>
1	D	561	<div> <div style="width: 97%;"></div> <div>97%</div> </div>
1	G	561	<div> <div style="width: 95%;"></div> <div>95%</div> </div>
1	J	561	<div> <div style="width: 95%;"></div> <div>95%</div> </div>
1	M	561	<div> <div style="width: 95%;"></div> <div>95%</div> </div>

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Mol	Chain	Length	Quality of chain
1	P	561	 96% .
1	S	561	 96% .
1	V	561	 95% 5% .
2	B	434	 97% .
2	E	434	 97% .
2	H	434	 97% .
2	K	434	 100% .
2	N	434	 98% .
2	Q	434	 98% .
2	T	434	 97% .
2	W	434	 97% .
3	C	265	 97% .
3	F	265	 97% .
3	I	265	 97% .
3	L	265	 97% .
3	O	265	 97% .
3	R	265	 98% .
3	U	265	 98% .
3	X	265	 97% .

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
10	GOL	F	302	-	X	-	-

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 163698 atoms, of which 75381 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 Alpha subunit of the Methyl-coenzyme M reductase from ANME-2c.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	560	Total	C	H	N	O	S	0	7	0
			8467	2738	4116	735	838	40			
1	D	560	Total	C	H	N	O	S	0	13	0
			8513	2752	4136	738	847	40			
1	G	560	Total	C	H	N	O	S	0	8	0
			8470	2739	4116	735	840	40			
1	J	558	Total	C	H	N	O	S	0	8	0
			8439	2730	4097	733	839	40			
1	M	560	Total	C	H	N	O	S	0	6	0
			8447	2733	4102	733	839	40			
1	P	560	Total	C	H	N	O	S	0	10	0
			8480	2743	4117	736	844	40			
1	S	560	Total	C	H	N	O	S	0	4	0
			8419	2726	4086	729	838	40			
1	V	558	Total	C	H	N	O	S	0	6	0
			8417	2725	4085	729	838	40			

- Molecule 2 is a protein called Beta subunit of the Methyl-coenzyme M reductase from ANME-2c.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	433	Total	C	H	N	O	S	0	11	0
			6547	2048	3278	556	633	32			
2	E	433	Total	C	H	N	O	S	0	19	0
			6618	2067	3315	563	640	33			
2	H	433	Total	C	H	N	O	S	0	8	0
			6508	2035	3256	557	629	31			
2	K	433	Total	C	H	N	O	S	0	13	0
			6549	2048	3274	559	637	31			
2	N	433	Total	C	H	N	O	S	0	9	0
			6512	2036	3257	558	630	31			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	Q	433	Total	C	H	N	O	S	0	13	0
			6554	2049	3279	559	635	32			
2	T	433	Total	C	H	N	O	S	0	8	0
			6511	2037	3258	556	629	31			
2	W	433	Total	C	H	N	O	S	0	7	0
			6489	2030	3243	556	629	31			

- Molecule 3 is a protein called Gamma subunit of the Methyl-coenzyme M reductase from ANME-2c.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	264	Total	C	H	N	O	S	0	7	0
			4085	1282	2007	378	403	15			
3	F	264	Total	C	H	N	O	S	0	13	0
			4151	1299	2046	385	406	15			
3	I	264	Total	C	H	N	O	S	0	2	0
			4046	1272	1986	374	399	15			
3	L	264	Total	C	H	N	O	S	0	6	0
			4074	1279	2000	378	402	15			
3	O	264	Total	C	H	N	O	S	0	3	0
			4057	1274	1994	376	398	15			
3	R	264	Total	C	H	N	O	S	0	6	0
			4073	1279	1999	378	402	15			
3	U	264	Total	C	H	N	O	S	0	3	0
			4050	1273	1987	375	400	15			
3	X	264	Total	C	H	N	O	S	0	6	0
			4082	1282	2005	377	403	15			

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	G	1	Total	K	0	0
			1	1		
4	M	1	Total	K	0	0
			1	1		
4	S	1	Total	K	0	0
			1	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0
5	H	1	Total Na 1 1	0	0
5	P	1	Total Na 1 1	0	0
5	V	1	Total Na 1 1	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

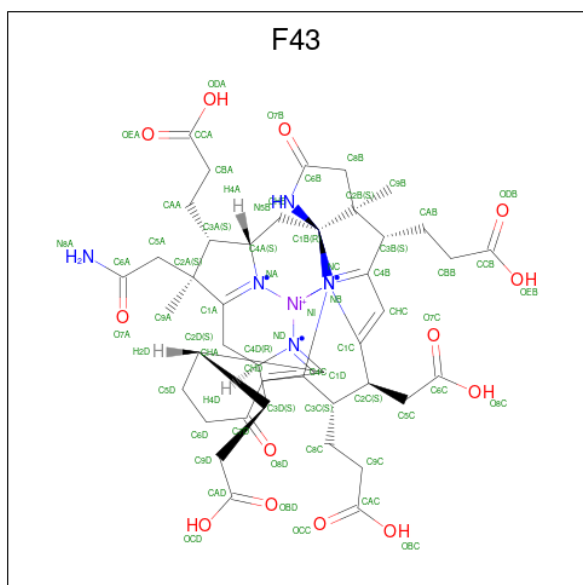
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	B	1	Total Cl 1 1	0	0
6	C	1	Total Cl 1 1	0	0
6	D	1	Total Cl 1 1	0	0
6	E	1	Total Cl 1 1	0	0
6	F	1	Total Cl 1 1	0	0
6	G	1	Total Cl 1 1	0	0
6	H	1	Total Cl 1 1	0	0
6	I	1	Total Cl 1 1	0	0
6	J	1	Total Cl 1 1	0	0
6	K	2	Total Cl 2 2	0	0
6	L	1	Total Cl 1 1	0	0
6	M	1	Total Cl 1 1	0	0
6	N	1	Total Cl 1 1	0	0
6	O	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	1	Total	Cl	0	0
			1	1		
6	Q	1	Total	Cl	0	0
			1	1		
6	R	1	Total	Cl	0	0
			1	1		
6	S	1	Total	Cl	0	0
			1	1		
6	T	1	Total	Cl	0	0
			1	1		
6	U	1	Total	Cl	0	0
			1	1		
6	V	1	Total	Cl	0	0
			1	1		
6	W	1	Total	Cl	0	0
			1	1		
6	X	1	Total	Cl	0	0
			1	1		

- Molecule 7 is FACTOR 430 (CCD ID: F43) (formula:  $C_{42}H_{51}N_6NiO_{13}$ ) (labeled as "Ligand of Interest" by depositor).



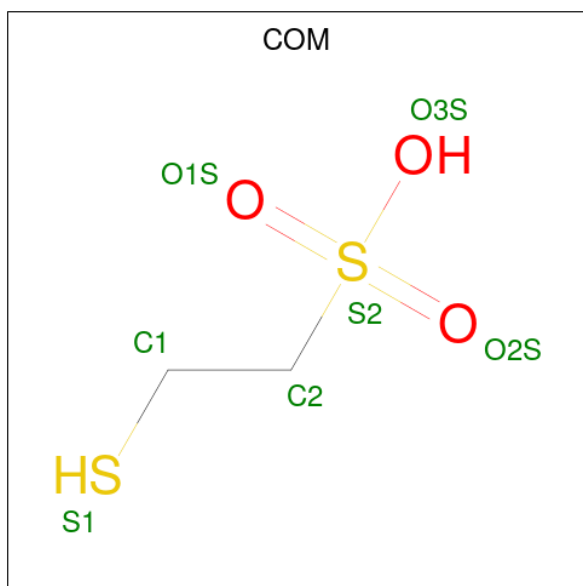
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
7	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	G	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
7	G	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
7	M	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
7	P	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
7	S	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
7	S	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 8 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
8	A	1	Total	C	O	S	0	0
			7	2	3	2		
8	D	1	Total	C	O	S	0	0
			7	2	3	2		
8	G	1	Total	C	O	S	0	0
			7	2	3	2		
8	J	1	Total	C	O	S	0	0
			7	2	3	2		
8	M	1	Total	C	O	S	0	0
			7	2	3	2		

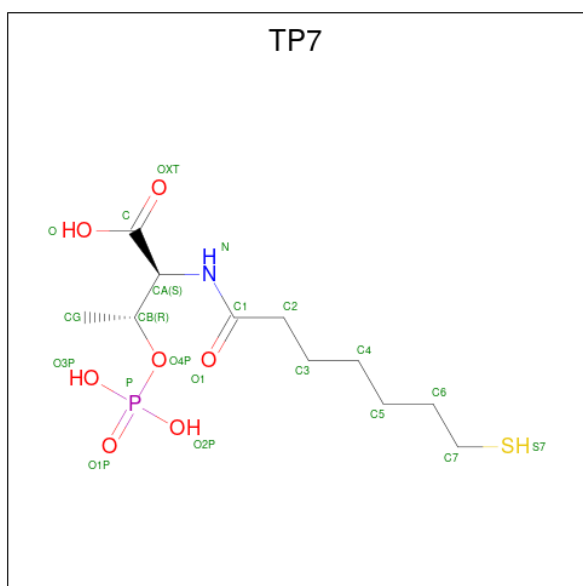
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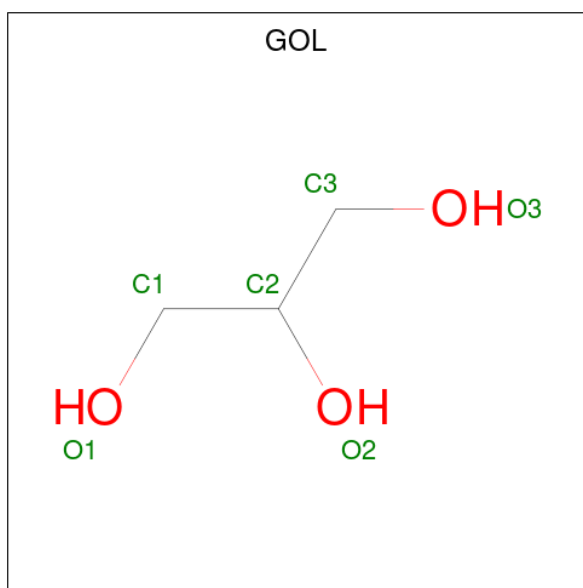
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	P	1	Total	C	O	S	0	0
			7	2	3	2		
8	S	1	Total	C	O	S	0	0
			7	2	3	2		
8	V	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 9 is Coenzyme B (CCD ID: TP7) (formula:  $C_{11}H_{22}NO_7PS$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	A	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0
9	D	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0
9	G	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0
9	J	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0
9	M	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0
9	P	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0
9	S	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0
9	V	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



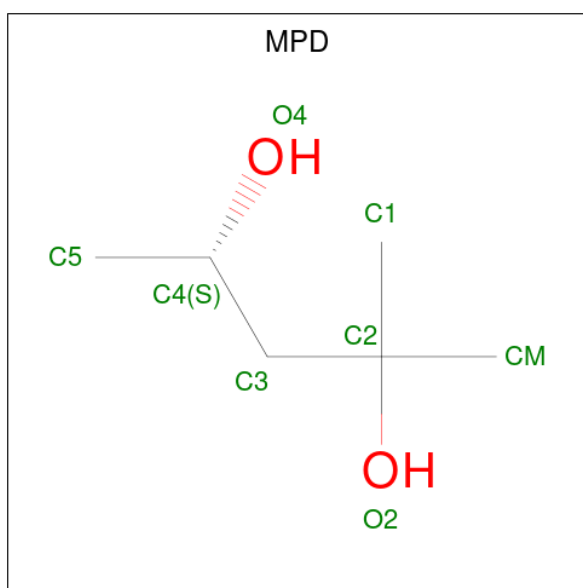
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			12	3	6	3		
10	A	1	Total	C	H	O	0	0
			14	3	8	3		
10	A	1	Total	C	H	O	0	0
			14	3	8	3		
10	D	1	Total	C	H	O	0	0
			14	3	8	3		
10	D	1	Total	C	H	O	0	0
			14	3	8	3		
10	F	1	Total	C	H	O	0	0
			13	3	7	3		
10	G	1	Total	C	H	O	0	0
			12	3	6	3		
10	G	1	Total	C	H	O	0	0
			14	3	8	3		
10	J	1	Total	C	H	O	0	0
			13	3	7	3		
10	L	1	Total	C	H	O	0	0
			13	3	7	3		
10	M	1	Total	C	H	O	0	0
			14	3	8	3		
10	M	1	Total	C	H	O	0	0
			14	3	8	3		
10	O	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	P	1	Total	C	H	O	0	0
			13	3	7	3		
10	Q	1	Total	C	H	O	0	0
			14	3	8	3		
10	R	1	Total	C	H	O	0	0
			14	3	8	3		
10	S	1	Total	C	H	O	0	0
			13	3	7	3		
10	V	1	Total	C	H	O	0	0
			13	3	7	3		

- Molecule 11 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



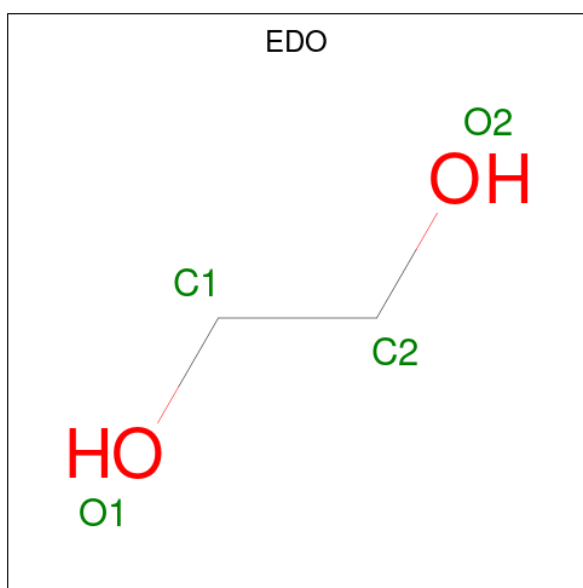
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			22	6	14	2		
11	B	1	Total	C	H	O	0	0
			22	6	14	2		
11	D	1	Total	C	H	O	0	0
			22	6	14	2		
11	H	1	Total	C	H	O	0	0
			22	6	14	2		
11	J	1	Total	C	H	O	0	0
			22	6	14	2		
11	J	1	Total	C	H	O	0	0
			22	6	14	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	K	1	Total	C	H	O	0	0
			22	6	14	2		
11	K	1	Total	C	H	O	0	1
			22	6	14	2		
11	N	1	Total	C	H	O	0	0
			22	6	14	2		
11	P	1	Total	C	H	O	0	0
			22	6	14	2		
11	V	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 12 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	H	O	0	0
			10	2	6	2		
12	A	1	Total	C	H	O	0	0
			10	2	6	2		
12	D	1	Total	C	H	O	0	0
			10	2	6	2		
12	F	1	Total	C	H	O	0	0
			10	2	6	2		
12	G	1	Total	C	H	O	0	0
			10	2	6	2		
12	N	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	P	1	Total	C	H	O	0	0
			10	2	6	2		
12	S	1	Total	C	H	O	0	0
			10	2	6	2		
12	V	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	579	Total	O	0	31
			579	579		
13	B	451	Total	O	0	42
			451	451		
13	C	373	Total	O	0	12
			373	373		
13	D	597	Total	O	0	29
			597	597		
13	E	469	Total	O	0	42
			469	469		
13	F	371	Total	O	0	18
			371	371		
13	G	592	Total	O	0	33
			592	592		
13	H	400	Total	O	0	36
			400	400		
13	I	374	Total	O	0	13
			374	374		
13	J	564	Total	O	0	30
			564	564		
13	K	382	Total	O	0	24
			382	382		
13	L	334	Total	O	0	12
			334	334		
13	M	528	Total	O	0	30
			528	528		
13	N	316	Total	O	0	20
			316	316		
13	O	289	Total	O	0	10
			289	289		
13	P	526	Total	O	0	16
			526	526		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	Q	359	Total 359	O 359	0	22
13	R	336	Total 336	O 336	0	15
13	S	477	Total 477	O 477	0	8
13	T	237	Total 237	O 237	0	4
13	U	239	Total 239	O 239	0	2
13	V	483	Total 483	O 483	0	16
13	W	260	Total 260	O 260	0	6
13	X	276	Total 276	O 276	0	9

### 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 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: Alpha subunit of the Methyl-coenzyme M reductase from ANME-2c



- Molecule 1: Alpha subunit of the Methyl-coenzyme M reductase from ANME-2c



- Molecule 1: Alpha subunit of the Methyl-coenzyme M reductase from ANME-2c



- Molecule 1: Alpha subunit of the Methyl-coenzyme M reductase from ANME-2c



- Molecule 1: Alpha subunit of the Methyl-coenzyme M reductase from ANME-2c



- Molecule 1: Alpha subunit of the Methyl-coenzyme M reductase from ANME-2c



- Molecule 1: Alpha subunit of the Methyl-coenzyme M reductase from ANME-2c



- Molecule 1: Alpha subunit of the Methyl-coenzyme M reductase from ANME-2c



- Molecule 2: Beta subunit of the Methyl-coenzyme M reductase from ANME-2c



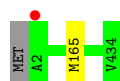
- Molecule 2: Beta subunit of the Methyl-coenzyme M reductase from ANME-2c



- Molecule 2: Beta subunit of the Methyl-coenzyme M reductase from ANME-2c



- Molecule 2: Beta subunit of the Methyl-coenzyme M reductase from ANME-2c





- Molecule 2: Beta subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain N:  98%



- Molecule 2: Beta subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain Q:  98%



- Molecule 2: Beta subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain T:  97%



- Molecule 2: Beta subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain W:  97%



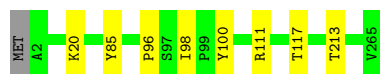
- Molecule 3: Gamma subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain C:  97%



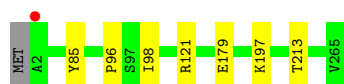
- Molecule 3: Gamma subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain F:  97%



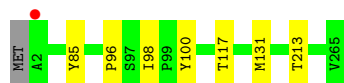
- Molecule 3: Gamma subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain I:  97%



- Molecule 3: Gamma subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain L: 97%



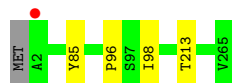
- Molecule 3: Gamma subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain O: 97%



- Molecule 3: Gamma subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain R: 98%



- Molecule 3: Gamma subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain U: 98%



- Molecule 3: Gamma subunit of the Methyl-coenzyme M reductase from ANME-2c

Chain X: 97%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.87Å 157.46Å 215.42Å 90.00° 90.34° 90.00°	Depositor
Resolution (Å)	98.93 – 1.34 98.93 – 1.34	Depositor EDS
% Data completeness (in resolution range)	66.2 (98.93-1.34) 66.3 (98.93-1.34)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.34Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, $R_{free}$	0.112 , 0.147 0.114 , 0.146	Depositor DCC
$R_{free}$ test set	115798 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.0	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l 0.000 for k,h,-l 0.019 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	163698	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EDO, DYA, AGM, NA, SMC, COM, TP7, MHS, K, MPD, GL3, MGN, GOL, CL, TRX, F43

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	0.56	0/4398	0.76	2/5949 (0.0%)
1	D	0.60	1/4451 (0.0%)	0.76	2/6020 (0.0%)
1	G	0.56	0/4409	0.75	2/5963 (0.0%)
1	J	0.53	0/4394	0.73	1/5945 (0.0%)
1	M	0.50	0/4389	0.71	2/5938 (0.0%)
1	P	0.52	0/4421	0.72	2/5981 (0.0%)
1	S	0.46	1/4372 (0.0%)	0.67	1/5916 (0.0%)
1	V	0.47	0/4379	0.69	2/5925 (0.0%)
2	B	0.54	1/3351 (0.0%)	0.71	0/4538
2	E	0.56	2/3420 (0.1%)	0.71	2/4629 (0.0%)
2	H	0.48	0/3325	0.66	1/4502 (0.0%)
2	K	0.50	0/3363	0.67	0/4554
2	N	0.46	1/3333 (0.0%)	0.64	0/4514
2	Q	0.47	0/3367	0.67	2/4558 (0.0%)
2	T	0.36	0/3329	0.57	1/4509 (0.0%)
2	W	0.38	0/3319	0.58	1/4496 (0.0%)
3	C	0.48	0/2150	0.69	2/2913 (0.1%)
3	F	0.50	0/2203	0.68	0/2982
3	I	0.48	0/2114	0.68	0/2865
3	L	0.42	0/2143	0.63	0/2904
3	O	0.39	0/2123	0.62	0/2876
3	R	0.41	0/2143	0.65	0/2904
3	U	0.35	0/2123	0.56	0/2877
3	X	0.40	0/2143	0.62	0/2904
All	All	0.49	6/79162 (0.0%)	0.68	23/107162 (0.0%)

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	1
1	G	0	3
1	J	0	2
1	M	0	2
1	P	0	2
1	S	0	1
1	V	0	2
3	I	0	1
3	O	0	1
All	All	0	16

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	227	CYS	C-O	-7.18	1.15	1.24
2	E	130[A]	CYS	C-O	5.95	1.31	1.24
2	E	130[B]	CYS	C-O	5.95	1.31	1.24
2	N	202	GLN	C-N	5.66	1.41	1.33
2	B	313	MET	C-O	-5.44	1.17	1.24

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	501	PHE	CA-CB-CG	6.00	119.80	113.80
2	W	141	GLU	CB-CA-C	-6.00	100.66	110.85
1	S	501	PHE	CA-CB-CG	5.99	119.79	113.80
1	P	502	THR	N-CA-C	-5.84	105.00	111.36
1	A	502	THR	N-CA-C	-5.61	105.06	111.07

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	33[A]	ARG	Sidechain
1	D	33[A]	ARG	Sidechain
1	G	33[A]	ARG	Mainchain,Sidechain
1	G	33[B]	ARG	Mainchain
3	I	121	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	4351	4116	4148	13	0
1	D	4377	4136	4129	9	0
1	G	4354	4116	4133	15	0
1	J	4342	4097	4116	14	0
1	M	4345	4102	4133	15	0
1	P	4363	4117	4131	13	0
1	S	4333	4086	4123	12	0
1	V	4332	4085	4110	12	0
2	B	3269	3278	3265	6	0
2	E	3303	3315	3262	7	0
2	H	3252	3256	3240	8	0
2	K	3275	3274	3244	1	0
2	N	3255	3257	3231	6	0
2	Q	3275	3279	3248	6	0
2	T	3253	3258	3238	6	0
2	W	3246	3243	3223	8	0
3	C	2078	2007	1985	6	0
3	F	2105	2046	1995	7	0
3	I	2060	1986	1985	4	0
3	L	2074	2000	1976	6	0
3	O	2063	1994	1986	6	0
3	R	2074	1999	1976	4	0
3	U	2063	1987	1979	3	0
3	X	2077	2005	1988	6	0
4	A	1	0	0	0	0
4	G	1	0	0	0	0
4	M	1	0	0	0	0
4	S	1	0	0	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	H	1	0	0	0	0
5	P	1	0	0	0	0
5	V	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	2	0	0	0	0
6	L	1	0	0	0	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
6	P	1	0	0	0	0
6	Q	1	0	0	0	0
6	R	1	0	0	0	0
6	S	1	0	0	0	0
6	T	1	0	0	0	0
6	U	1	0	0	0	0
6	V	1	0	0	0	0
6	W	1	0	0	0	0
6	X	1	0	0	0	0
7	A	124	0	86	3	0
7	G	124	0	86	3	0
7	M	62	0	43	1	0
7	P	62	0	43	2	0
7	S	124	0	86	4	0
8	A	7	0	5	0	0
8	D	7	0	4	1	0
8	G	7	0	5	1	0
8	J	7	0	5	0	0
8	M	7	0	5	0	0
8	P	7	0	5	0	0
8	S	7	0	5	2	0
8	V	7	0	4	0	0
9	A	21	0	19	0	0
9	D	21	0	19	0	0
9	G	21	0	19	0	0
9	J	21	0	19	0	0
9	M	21	0	19	0	0
9	P	21	0	19	0	0
9	S	21	0	19	0	0
9	V	21	0	19	0	0
10	A	18	22	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	12	16	16	0	0
10	F	6	7	7	0	0
10	G	12	14	14	0	0
10	J	6	7	7	0	0
10	L	6	7	7	0	0
10	M	12	16	16	1	0
10	O	6	8	8	0	0
10	P	6	7	7	1	0
10	Q	6	8	8	0	0
10	R	6	8	8	0	0
10	S	6	7	7	0	0
10	V	6	7	7	0	0
11	A	8	14	14	0	0
11	B	8	14	14	0	0
11	D	8	14	14	0	0
11	H	8	14	14	0	0
11	J	16	28	28	1	0
11	K	16	28	28	0	0
11	N	8	14	14	0	0
11	P	8	14	14	0	0
11	V	8	14	14	0	0
12	A	8	12	12	0	0
12	D	4	6	6	0	0
12	F	4	6	6	0	0
12	G	4	6	6	0	0
12	N	4	6	6	0	0
12	P	4	6	6	0	0
12	S	4	6	6	0	0
12	V	4	6	6	0	0
13	A	579	0	0	0	0
13	B	451	0	0	0	0
13	C	373	0	0	0	0
13	D	597	0	0	0	0
13	E	469	0	0	0	0
13	F	371	0	0	1	0
13	G	592	0	0	0	0
13	H	400	0	0	0	0
13	I	374	0	0	0	0
13	J	564	0	0	0	0
13	K	382	0	0	0	0
13	L	334	0	0	0	0
13	M	528	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	N	316	0	0	0	0
13	O	289	0	0	0	0
13	P	526	0	0	0	0
13	Q	359	0	0	1	0
13	R	336	0	0	0	0
13	S	477	0	0	0	0
13	T	237	0	0	0	0
13	U	239	0	0	0	0
13	V	483	0	0	0	0
13	W	260	0	0	0	0
13	X	276	0	0	0	0
All	All	88317	75381	75720	158	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 1.

The worst 5 of 158 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:M:251:CYS:HB2	3:R:85:TYR:CE1	2.36	0.60
1:S:251:CYS:HB2	3:X:85:TYR:CE1	2.40	0.56
1:A:251:CYS:HB2	3:F:85:TYR:CE1	2.39	0.56
1:D:449:GLY:HA3	3:F:98:ILE:HD12	1.88	0.56
1:M:449:GLY:HA3	3:O:98:ILE:HD12	1.86	0.56

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	558/561 (100%)	539 (97%)	18 (3%)	1 (0%)	44 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	564/561 (100%)	545 (97%)	18 (3%)	1 (0%)	44	19
1	G	559/561 (100%)	540 (97%)	18 (3%)	1 (0%)	44	19
1	J	557/561 (99%)	540 (97%)	17 (3%)	0	100	100
1	M	557/561 (99%)	538 (97%)	18 (3%)	1 (0%)	44	19
1	P	561/561 (100%)	541 (96%)	19 (3%)	1 (0%)	44	19
1	S	555/561 (99%)	535 (96%)	19 (3%)	1 (0%)	44	19
1	V	555/561 (99%)	536 (97%)	18 (3%)	1 (0%)	44	19
2	B	442/434 (102%)	435 (98%)	7 (2%)	0	100	100
2	E	450/434 (104%)	443 (98%)	7 (2%)	0	100	100
2	H	439/434 (101%)	431 (98%)	8 (2%)	0	100	100
2	K	444/434 (102%)	437 (98%)	7 (2%)	0	100	100
2	N	440/434 (101%)	433 (98%)	7 (2%)	0	100	100
2	Q	444/434 (102%)	437 (98%)	7 (2%)	0	100	100
2	T	439/434 (101%)	432 (98%)	7 (2%)	0	100	100
2	W	438/434 (101%)	432 (99%)	6 (1%)	0	100	100
3	C	269/265 (102%)	261 (97%)	8 (3%)	0	100	100
3	F	275/265 (104%)	270 (98%)	5 (2%)	0	100	100
3	I	264/265 (100%)	257 (97%)	7 (3%)	0	100	100
3	L	268/265 (101%)	260 (97%)	8 (3%)	0	100	100
3	O	265/265 (100%)	260 (98%)	5 (2%)	0	100	100
3	R	268/265 (101%)	262 (98%)	6 (2%)	0	100	100
3	U	265/265 (100%)	257 (97%)	8 (3%)	0	100	100
3	X	268/265 (101%)	260 (97%)	8 (3%)	0	100	100
All	All	10144/10080 (101%)	9881 (97%)	256 (2%)	7 (0%)	48	20

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	334	SER
1	A	334	SER
1	D	334	SER
1	M	334	SER
1	P	334	SER

### 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	442/437 (101%)	439 (99%)	3 (1%)	81	59
1	D	448/437 (102%)	447 (100%)	1 (0%)	92	80
1	G	443/437 (101%)	443 (100%)	0	100	100
1	J	442/437 (101%)	442 (100%)	0	100	100
1	M	441/437 (101%)	441 (100%)	0	100	100
1	P	445/437 (102%)	445 (100%)	0	100	100
1	S	440/437 (101%)	440 (100%)	0	100	100
1	V	441/437 (101%)	440 (100%)	1 (0%)	92	80
2	B	349/340 (103%)	347 (99%)	2 (1%)	84	64
2	E	356/340 (105%)	356 (100%)	0	100	100
2	H	345/340 (102%)	345 (100%)	0	100	100
2	K	349/340 (103%)	349 (100%)	0	100	100
2	N	346/340 (102%)	346 (100%)	0	100	100
2	Q	350/340 (103%)	350 (100%)	0	100	100
2	T	346/340 (102%)	346 (100%)	0	100	100
2	W	345/340 (102%)	345 (100%)	0	100	100
3	C	223/218 (102%)	223 (100%)	0	100	100
3	F	228/218 (105%)	228 (100%)	0	100	100
3	I	219/218 (100%)	219 (100%)	0	100	100
3	L	222/218 (102%)	222 (100%)	0	100	100
3	O	220/218 (101%)	220 (100%)	0	100	100
3	R	222/218 (102%)	222 (100%)	0	100	100
3	U	220/218 (101%)	220 (100%)	0	100	100
3	X	222/218 (102%)	222 (100%)	0	100	100
All	All	8104/7960 (102%)	8097 (100%)	7 (0%)	92	80

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	173[A]	LEU
2	B	173[B]	LEU
1	V	231	ASN
1	D	561	VAL
1	A	282	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
2	Q	234	GLN
1	V	231	ASN
1	S	231	ASN
2	T	217	HIS
1	V	459	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

56 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	TRX	M	437	1	14,16,17	0.72	0	15,22,24	0.66	0
1	TRX	G	437	1	14,16,17	0.78	0	15,22,24	0.79	0
1	DYA	V	460	1	7,7,8	1.69	2 (28%)	5,8,10	2.07	1 (20%)
1	TRX	J	437	1	14,16,17	0.72	0	15,22,24	0.74	0
1	GL3	V	455	1	2,3,4	3.34	1 (50%)	1,2,4	0.17	0
1	MGN	G	410	1	6,9,10	1.14	1 (16%)	5,12,14	0.32	0
1	AGM	A	280	1	10,11,12	0.42	0	6,13,15	0.27	0
1	AGM	D	280	1	10,11,12	1.18	1 (10%)	6,13,15	1.20	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MGN	J	410	1	6,9,10	0.64	0	5,12,14	0.47	0
1	MGN	M	410	1	6,9,10	0.69	0	5,12,14	0.49	0
1	GL3	P	455	1	2,3,4	2.90	1 (50%)	1,2,4	0.12	0
1	GL3	S	455	1	2,3,4	3.80	1 (50%)	1,2,4	0.08	0
1	GL3	J	455	1	2,3,4	3.82	1 (50%)	1,2,4	0.18	0
1	GL3	M	455	1	2,3,4	3.95	1 (50%)	1,2,4	0.33	0
1	MHS	M	266	1	7,11,12	1.18	0	6,14,16	1.23	1 (16%)
1	MHS	S	266	1	7,11,12	1.28	0	6,14,16	1.58	2 (33%)
1	TRX	D	437	1	14,16,17	0.75	0	15,22,24	0.84	0
1	MGN	S	410	1	6,9,10	0.65	0	5,12,14	0.34	0
1	MHS	J	266	1	7,11,12	1.15	0	6,14,16	1.03	1 (16%)
1	DYA	S	460	1	7,7,8	1.68	2 (28%)	5,8,10	2.27	1 (20%)
1	DYA	J	460	1	7,7,8	1.93	2 (28%)	5,8,10	2.09	1 (20%)
1	MGN	P	410	1	6,9,10	0.52	0	5,12,14	0.40	0
1	SMC	G	462	1	5,6,7	0.82	0	2,6,8	0.81	0
1	AGM	M	280	1	10,11,12	1.38	2 (20%)	6,13,15	0.57	0
1	GL3	D	455	1	2,3,4	3.93	1 (50%)	1,2,4	0.35	0
1	SMC	A	462	1	5,6,7	0.62	0	2,6,8	0.89	0
1	MGN	V	410	1	6,9,10	0.56	0	5,12,14	0.21	0
1	SMC	S	462	1	5,6,7	0.63	0	2,6,8	0.64	0
1	SMC	P	462	1	5,6,7	0.61	0	2,6,8	0.96	0
1	GL3	G	455	1	2,3,4	3.96	1 (50%)	1,2,4	0.06	0
1	SMC	V	462	1	5,6,7	0.54	0	2,6,8	0.62	0
1	DYA	D	460	1	7,7,8	2.08	2 (28%)	5,8,10	1.96	1 (20%)
1	AGM	G	280	1	10,11,12	0.42	0	6,13,15	0.23	0
1	TRX	A	437	1	14,16,17	0.71	0	15,22,24	0.78	0
1	MHS	G	266	1	7,11,12	1.14	0	6,14,16	1.51	2 (33%)
1	MHS	V	266	1	7,11,12	1.16	0	6,14,16	1.23	1 (16%)
1	SMC	D	462	1	5,6,7	0.74	0	2,6,8	0.26	0
1	DYA	G	460	1	7,7,8	1.89	2 (28%)	5,8,10	2.10	1 (20%)
1	MGN	D	410	1	6,9,10	0.70	0	5,12,14	0.47	0
1	DYA	M	460	1	7,7,8	1.78	2 (28%)	5,8,10	2.30	1 (20%)
1	MGN	A	410	1	6,9,10	0.77	0	5,12,14	0.39	0
1	TRX	S	437	1	14,16,17	0.66	0	15,22,24	0.83	0
1	MHS	P	266	1	7,11,12	1.25	0	6,14,16	0.84	0
1	DYA	A	460	1	7,7,8	1.99	2 (28%)	5,8,10	2.13	1 (20%)
1	AGM	J	280	1	10,11,12	1.25	1 (10%)	6,13,15	0.94	0
1	TRX	V	437	1	14,16,17	0.65	0	15,22,24	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	AGM	S	280	1	10,11,12	1.14	0	6,13,15	0.60	0
1	GL3	A	455	1	2,3,4	4.11	1 (50%)	1,2,4	0.19	0
1	DYA	P	460	1	7,7,8	1.84	2 (28%)	5,8,10	2.18	1 (20%)
1	AGM	V	280	1	10,11,12	1.27	1 (10%)	6,13,15	0.93	0
1	MHS	A	266	1	7,11,12	1.19	0	6,14,16	1.24	1 (16%)
1	AGM	P	280	1	10,11,12	1.34	1 (10%)	6,13,15	1.17	0
1	SMC	M	462	1	5,6,7	0.61	0	2,6,8	0.65	0
1	SMC	J	462	1	5,6,7	0.56	0	2,6,8	0.43	0
1	MHS	D	266	1	7,11,12	1.13	0	6,14,16	1.23	0
1	TRX	P	437	1	14,16,17	0.71	0	15,22,24	0.76	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	TRX	M	437	1	-	0/4/6/8	0/2/2/2
1	TRX	G	437	1	-	0/4/6/8	0/2/2/2
1	DYA	V	460	1	-	3/4/6/8	-
1	TRX	J	437	1	-	0/4/6/8	0/2/2/2
1	GL3	V	455	1	-	1/1/1/2	-
1	MGN	G	410	1	-	0/7/9/12	-
1	AGM	A	280	1	-	2/10/11/13	-
1	AGM	D	280	1	-	1/10/11/13	-
1	MGN	J	410	1	-	0/7/9/12	-
1	MGN	M	410	1	-	0/7/9/12	-
1	GL3	P	455	1	-	1/1/1/2	-
1	GL3	S	455	1	-	1/1/1/2	-
1	GL3	J	455	1	-	1/1/1/2	-
1	GL3	M	455	1	-	1/1/1/2	-
1	MHS	M	266	1	-	0/5/6/8	0/1/1/1
1	MHS	S	266	1	-	0/5/6/8	0/1/1/1
1	TRX	D	437	1	-	0/4/6/8	0/2/2/2
1	MGN	S	410	1	-	0/7/9/12	-
1	MHS	J	266	1	-	0/5/6/8	0/1/1/1
1	DYA	S	460	1	-	3/4/6/8	-
1	DYA	J	460	1	-	3/4/6/8	-
1	MGN	P	410	1	-	0/7/9/12	-
1	SMC	G	462	1	-	1/3/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AGM	M	280	1	-	2/10/11/13	-
1	GL3	D	455	1	-	1/1/1/2	-
1	SMC	A	462	1	-	1/3/5/7	-
1	MGN	V	410	1	-	0/7/9/12	-
1	SMC	S	462	1	-	1/3/5/7	-
1	SMC	P	462	1	-	1/3/5/7	-
1	GL3	G	455	1	-	1/1/1/2	-
1	SMC	V	462	1	-	1/3/5/7	-
1	DYA	D	460	1	-	3/4/6/8	-
1	AGM	G	280	1	-	2/10/11/13	-
1	TRX	A	437	1	-	0/4/6/8	0/2/2/2
1	MHS	G	266	1	-	0/5/6/8	0/1/1/1
1	MHS	V	266	1	-	0/5/6/8	0/1/1/1
1	SMC	D	462	1	-	1/3/5/7	-
1	DYA	G	460	1	-	3/4/6/8	-
1	MGN	D	410	1	-	0/7/9/12	-
1	DYA	M	460	1	-	3/4/6/8	-
1	MGN	A	410	1	-	0/7/9/12	-
1	TRX	S	437	1	-	0/4/6/8	0/2/2/2
1	MHS	P	266	1	-	0/5/6/8	0/1/1/1
1	DYA	A	460	1	-	3/4/6/8	-
1	AGM	J	280	1	-	2/10/11/13	-
1	TRX	V	437	1	-	0/4/6/8	0/2/2/2
1	AGM	S	280	1	-	2/10/11/13	-
1	GL3	A	455	1	-	1/1/1/2	-
1	DYA	P	460	1	-	3/4/6/8	-
1	AGM	V	280	1	-	2/10/11/13	-
1	MHS	A	266	1	-	0/5/6/8	0/1/1/1
1	AGM	P	280	1	-	2/10/11/13	-
1	SMC	M	462	1	-	1/3/5/7	-
1	SMC	J	462	1	-	1/3/5/7	-
1	MHS	D	266	1	-	0/5/6/8	0/1/1/1
1	TRX	P	437	1	-	0/4/6/8	0/2/2/2

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	455	GL3	C-S	-5.81	1.60	1.80
1	G	455	GL3	C-S	-5.60	1.61	1.80
1	M	455	GL3	C-S	-5.59	1.61	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	455	GL3	C-S	-5.56	1.61	1.80
1	J	455	GL3	C-S	-5.41	1.62	1.80

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	460	DYA	O-C-CA	-4.45	119.73	125.39
1	S	460	DYA	O-C-CA	-4.29	119.93	125.39
1	P	460	DYA	O-C-CA	-4.06	120.22	125.39
1	G	460	DYA	O-C-CA	-3.94	120.38	125.39
1	A	460	DYA	O-C-CA	-3.85	120.49	125.39

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	460	DYA	O-C-CA-CB
1	D	460	DYA	O-C-CA-CB
1	G	460	DYA	O-C-CA-CB
1	G	460	DYA	CA-CB-CG-OD2
1	J	460	DYA	O-C-CA-CB

There are no ring outliers.

10 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	437	TRX	1	0
1	G	437	TRX	1	0
1	J	437	TRX	1	0
1	P	455	GL3	1	0
1	D	437	TRX	1	0
1	G	455	GL3	1	0
1	A	437	TRX	1	0
1	S	437	TRX	1	0
1	V	437	TRX	1	0
1	P	437	TRX	1	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.



## 5.6 Ligand geometry

Of 96 ligands modelled in this entry, 34 are monoatomic - leaving 62 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
8	COM	D	604	7	6,6,6	1.35	1 (16%)	7,8,8	1.25	0
10	GOL	Q	502	-	5,5,5	0.08	0	5,5,5	0.29	0
11	MPD	H	503	-	7,7,7	0.14	0	9,10,10	0.45	0
11	MPD	V	606	-	7,7,7	0.14	0	9,10,10	0.42	0
12	EDO	N	503	-	3,3,3	0.11	0	2,2,2	0.15	0
7	F43	G	609	8,1	61,71,71	2.42	12 (19%)	64,118,118	1.41	10 (15%)
9	TP7	M	605	-	19,20,20	0.88	0	24,26,26	0.97	1 (4%)
8	COM	G	604	7	6,6,6	0.92	0	7,8,8	0.74	0
10	GOL	A	608	-	5,5,5	0.79	0	5,5,5	0.96	0
12	EDO	G	608	-	3,3,3	0.12	0	2,2,2	0.17	0
8	COM	M	604	7	6,6,6	0.88	0	7,8,8	0.94	0
12	EDO	S	607	-	3,3,3	0.08	0	2,2,2	0.18	0
11	MPD	K	503	-	7,7,7	0.14	0	9,10,10	0.44	0
9	TP7	S	605	-	19,20,20	0.83	1 (5%)	24,26,26	0.78	1 (4%)
9	TP7	G	605	-	19,20,20	0.84	1 (5%)	24,26,26	0.75	1 (4%)
10	GOL	D	605	-	5,5,5	1.11	0	5,5,5	1.23	0
10	GOL	F	302	-	5,5,5	1.41	1 (20%)	5,5,5	1.15	1 (20%)
11	MPD	B	502	-	7,7,7	0.12	0	9,10,10	0.45	0
10	GOL	A	610	-	5,5,5	0.08	0	5,5,5	0.31	0
10	GOL	P	606	-	5,5,5	1.13	0	5,5,5	1.24	0
8	COM	P	605	7	6,6,6	1.10	0	7,8,8	1.10	0
7	F43	S	603	8,1	61,71,71	2.09	9 (14%)	64,118,118	1.29	7 (10%)
8	COM	V	604	7	6,6,6	0.96	0	7,8,8	1.67	2 (28%)
7	F43	M	603	8,1	61,71,71	2.45	12 (19%)	64,118,118	1.52	12 (18%)
11	MPD	J	605	-	7,7,7	0.15	0	9,10,10	0.23	0
11	MPD	N	502	-	7,7,7	0.15	0	9,10,10	0.35	0
12	EDO	F	303	-	3,3,3	0.09	0	2,2,2	0.04	0
12	EDO	P	608	-	3,3,3	0.13	0	2,2,2	0.04	0
9	TP7	V	603	-	19,20,20	0.81	1 (5%)	24,26,26	0.78	1 (4%)
10	GOL	D	607	-	5,5,5	0.53	0	5,5,5	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	COM	A	605	7	6,6,6	0.87	0	7,8,8	0.89	0
7	F43	S	608	8,1	61,71,71	2.23	7 (11%)	64,118,118	1.23	8 (12%)
10	GOL	R	302	-	5,5,5	0.08	0	5,5,5	0.34	0
8	COM	J	603	7	6,6,6	1.16	0	7,8,8	1.16	0
11	MPD	D	606	-	7,7,7	0.20	0	9,10,10	0.28	0
10	GOL	L	302	-	5,5,5	1.18	0	5,5,5	0.60	0
10	GOL	O	302	-	5,5,5	1.11	0	5,5,5	0.78	0
11	MPD	K	504[A]	-	7,7,7	0.13	0	9,10,10	0.37	0
12	EDO	A	611	-	3,3,3	0.10	0	2,2,2	0.10	0
10	GOL	J	604	-	5,5,5	0.99	0	5,5,5	1.34	1 (20%)
9	TP7	D	603	-	19,20,20	0.89	1 (5%)	24,26,26	0.98	1 (4%)
9	TP7	J	602	-	19,20,20	0.93	1 (5%)	24,26,26	0.99	1 (4%)
9	TP7	A	606	-	19,20,20	0.98	1 (5%)	24,26,26	0.89	1 (4%)
7	F43	A	604	8,1	61,71,71	2.27	9 (14%)	64,118,118	1.34	9 (14%)
12	EDO	D	608	-	3,3,3	0.11	0	2,2,2	0.17	0
10	GOL	M	607	-	5,5,5	0.74	0	5,5,5	1.02	0
10	GOL	V	605	-	5,5,5	1.10	0	5,5,5	1.28	0
11	MPD	A	609	-	7,7,7	0.20	0	9,10,10	0.33	0
10	GOL	A	607	-	5,5,5	1.14	0	5,5,5	1.38	1 (20%)
9	TP7	P	603	-	19,20,20	0.80	0	24,26,26	0.81	1 (4%)
12	EDO	V	607	-	3,3,3	0.10	0	2,2,2	0.19	0
8	COM	S	604	7	6,6,6	0.93	0	7,8,8	1.50	2 (28%)
7	F43	G	603	8,1	61,71,71	2.37	11 (18%)	64,118,118	1.43	11 (17%)
7	F43	A	613	8,1	61,71,71	2.31	13 (21%)	64,118,118	1.36	6 (9%)
10	GOL	G	607	-	5,5,5	0.80	0	5,5,5	0.96	0
7	F43	P	604	8,1	61,71,71	2.23	6 (9%)	64,118,118	1.33	7 (10%)
10	GOL	S	606	-	5,5,5	0.91	0	5,5,5	1.12	0
10	GOL	M	606	-	5,5,5	0.09	0	5,5,5	0.40	0
10	GOL	G	606	-	5,5,5	1.28	0	5,5,5	1.15	0
11	MPD	J	606	-	7,7,7	0.10	0	9,10,10	0.33	0
11	MPD	P	607	-	7,7,7	0.16	0	9,10,10	0.28	0
12	EDO	A	612	-	3,3,3	0.08	0	2,2,2	0.12	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
8	COM	D	604	7	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	Q	502	-	-	2/4/4/4	-
11	MPD	H	503	-	-	0/5/5/5	-
11	MPD	V	606	-	-	0/5/5/5	-
12	EDO	N	503	-	-	1/1/1/1	-
7	F43	G	609	8,1	-	6/28/185/185	-
9	TP7	M	605	-	-	0/24/24/24	-
8	COM	G	604	7	-	0/4/4/4	-
10	GOL	A	608	-	-	3/4/4/4	-
12	EDO	G	608	-	-	1/1/1/1	-
8	COM	M	604	7	-	0/4/4/4	-
12	EDO	S	607	-	-	1/1/1/1	-
11	MPD	K	503	-	-	0/5/5/5	-
9	TP7	S	605	-	-	1/24/24/24	-
9	TP7	G	605	-	-	0/24/24/24	-
10	GOL	D	605	-	-	0/4/4/4	-
10	GOL	F	302	-	-	4/4/4/4	-
11	MPD	B	502	-	-	0/5/5/5	-
10	GOL	A	610	-	-	3/4/4/4	-
10	GOL	P	606	-	-	2/4/4/4	-
8	COM	P	605	7	-	0/4/4/4	-
7	F43	S	603	8,1	-	6/28/185/185	-
8	COM	V	604	7	-	0/4/4/4	-
7	F43	M	603	8,1	-	8/28/185/185	-
11	MPD	J	605	-	-	0/5/5/5	-
11	MPD	N	502	-	-	0/5/5/5	-
12	EDO	F	303	-	-	1/1/1/1	-
12	EDO	P	608	-	-	0/1/1/1	-
9	TP7	V	603	-	-	0/24/24/24	-
10	GOL	D	607	-	-	4/4/4/4	-
8	COM	A	605	7	-	0/4/4/4	-
7	F43	S	608	8,1	-	7/28/185/185	-
10	GOL	R	302	-	-	4/4/4/4	-
8	COM	J	603	7	-	0/4/4/4	-
11	MPD	D	606	-	-	0/5/5/5	-
10	GOL	L	302	-	-	2/4/4/4	-
10	GOL	O	302	-	-	2/4/4/4	-
11	MPD	K	504[A]	-	-	1/5/5/5	-
12	EDO	A	611	-	-	1/1/1/1	-
10	GOL	J	604	-	-	1/4/4/4	-

*Continued on next page...*

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	TP7	D	603	-	-	0/24/24/24	-
9	TP7	J	602	-	-	1/24/24/24	-
9	TP7	A	606	-	-	2/24/24/24	-
7	F43	A	604	8,1	-	5/28/185/185	-
12	EDO	D	608	-	-	1/1/1/1	-
10	GOL	M	607	-	-	1/4/4/4	-
10	GOL	V	605	-	-	1/4/4/4	-
11	MPD	A	609	-	-	0/5/5/5	-
10	GOL	A	607	-	-	1/4/4/4	-
9	TP7	P	603	-	-	0/24/24/24	-
12	EDO	V	607	-	-	1/1/1/1	-
8	COM	S	604	7	-	0/4/4/4	-
7	F43	G	603	8,1	-	5/28/185/185	-
7	F43	A	613	8,1	-	8/28/185/185	-
10	GOL	G	607	-	-	0/4/4/4	-
7	F43	P	604	8,1	-	7/28/185/185	-
10	GOL	S	606	-	-	1/4/4/4	-
10	GOL	M	606	-	-	1/4/4/4	-
10	GOL	G	606	-	-	2/4/4/4	-
11	MPD	J	606	-	-	3/5/5/5	-
11	MPD	P	607	-	-	0/5/5/5	-
12	EDO	A	612	-	-	1/1/1/1	-

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	603	F43	NI-NA	9.72	2.10	1.89
7	G	609	F43	NI-NA	9.60	2.10	1.89
7	M	603	F43	NI-NB	9.21	2.09	1.89
7	P	604	F43	NI-NB	9.15	2.09	1.89
7	A	604	F43	NI-NB	9.13	2.09	1.89

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	613	F43	O7B-C6B-C8B	-4.68	120.87	126.59
7	G	603	F43	O8D-C7D-C6D	-4.61	113.31	120.86
7	G	609	F43	O8D-C7D-C6D	-4.57	113.36	120.86
7	G	603	F43	O7B-C6B-C8B	-4.38	121.24	126.59
7	M	603	F43	O7B-C6B-C8B	-4.38	121.24	126.59

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

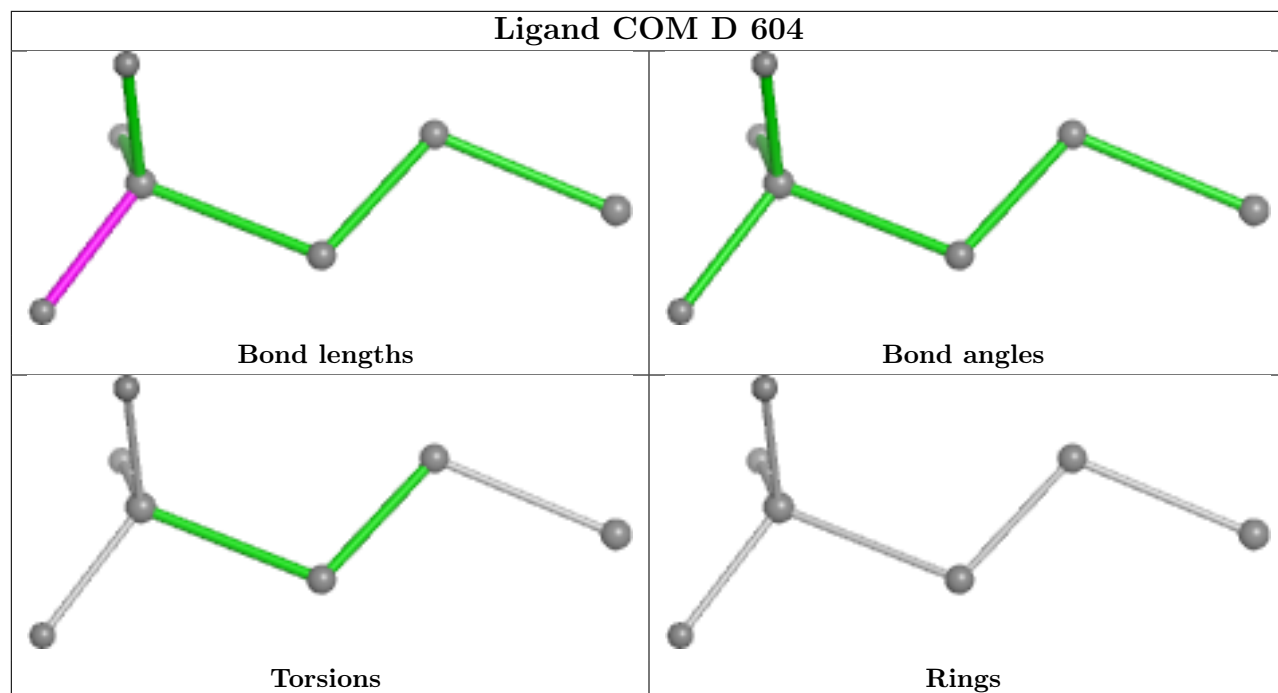
Mol	Chain	Res	Type	Atoms
10	A	608	GOL	O1-C1-C2-C3
10	D	607	GOL	C1-C2-C3-O3
10	F	302	GOL	O1-C1-C2-C3
10	F	302	GOL	C1-C2-C3-O3
10	G	606	GOL	C1-C2-C3-O3

There are no ring outliers.

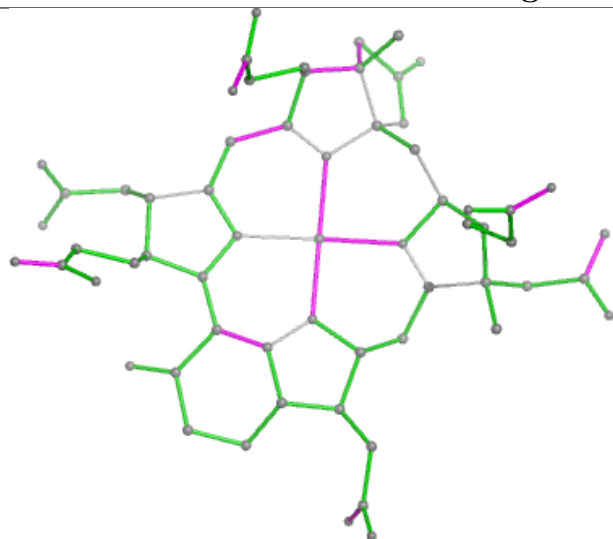
14 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	604	COM	1	0
7	G	609	F43	1	0
8	G	604	COM	1	0
10	P	606	GOL	1	0
7	S	603	F43	3	0
7	M	603	F43	1	0
7	S	608	F43	1	0
7	A	604	F43	1	0
8	S	604	COM	2	0
7	G	603	F43	2	0
7	A	613	F43	2	0
7	P	604	F43	2	0
10	M	606	GOL	1	0
11	J	606	MPD	1	0

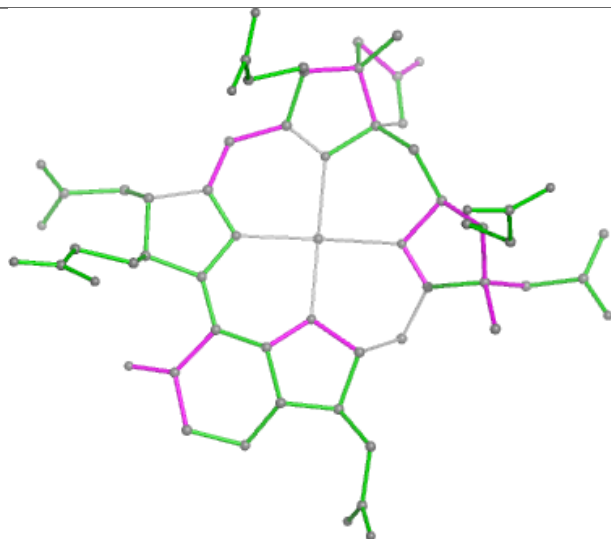
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



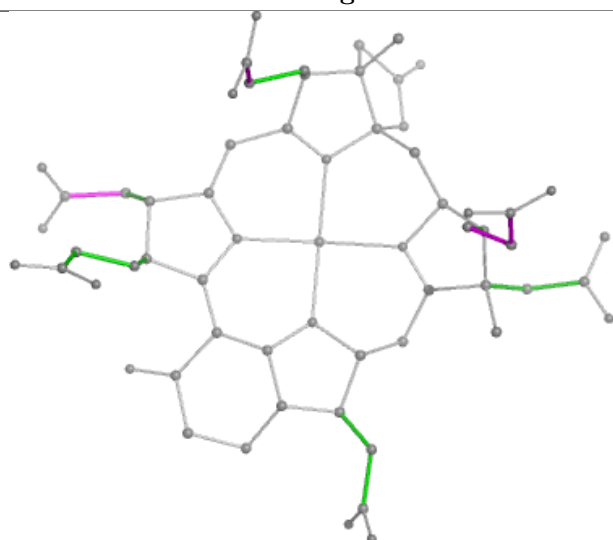
## Ligand F43 G 609



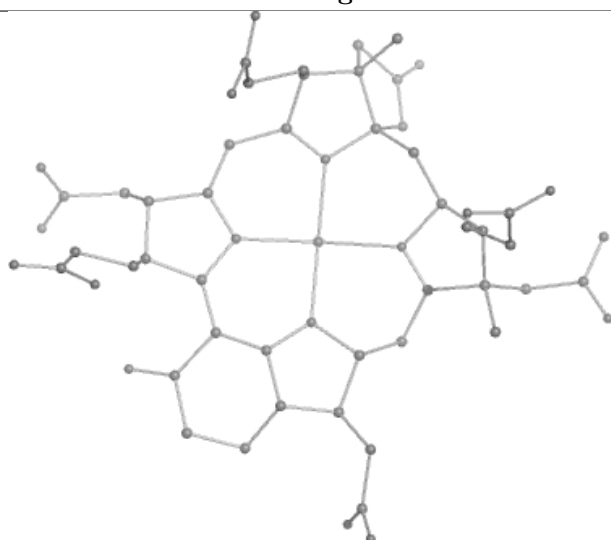
Bond lengths



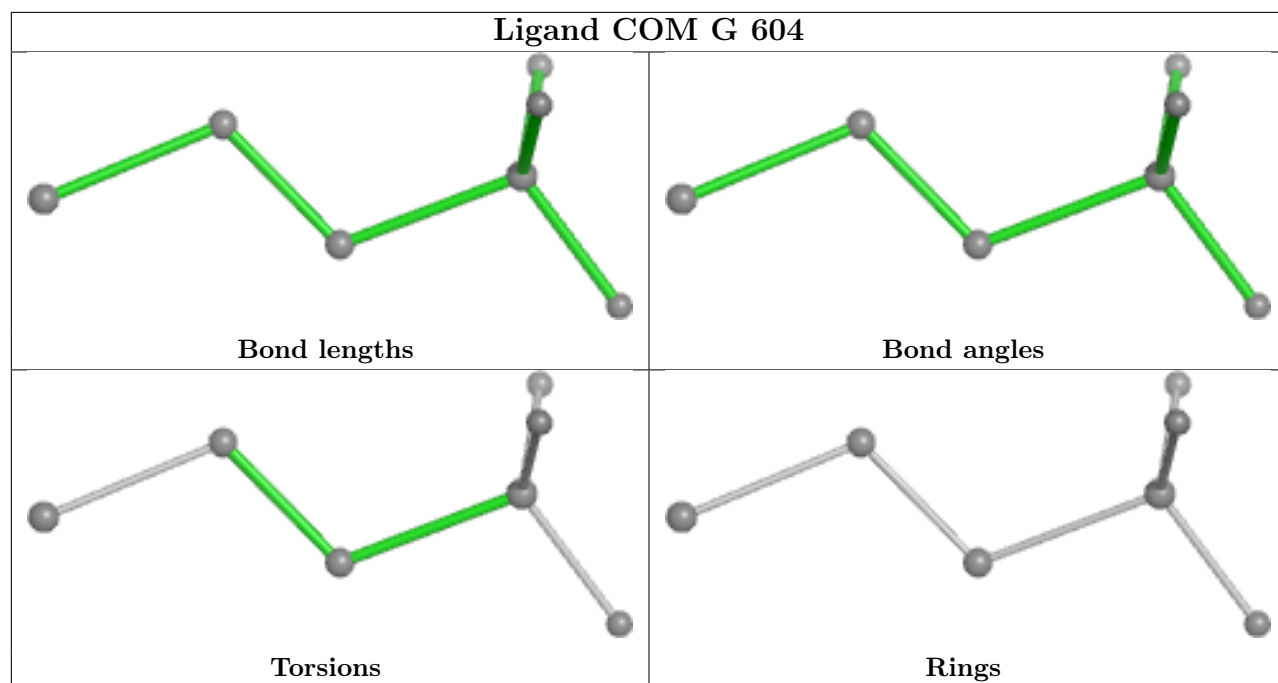
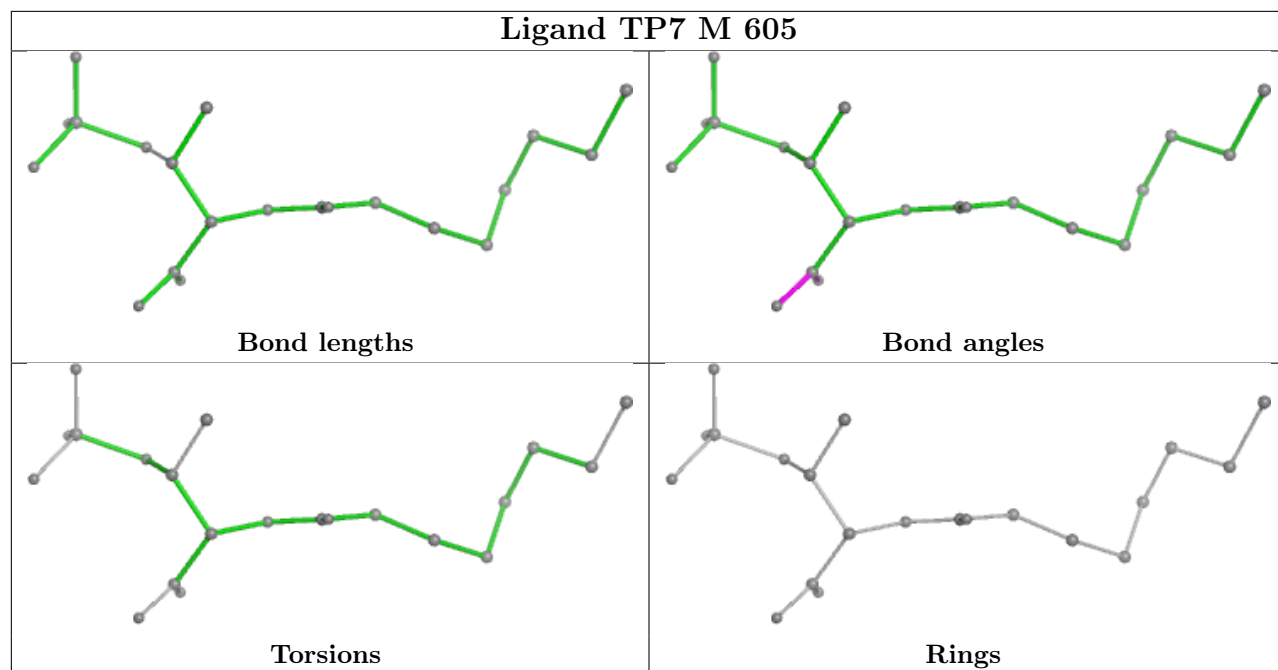
Bond angles



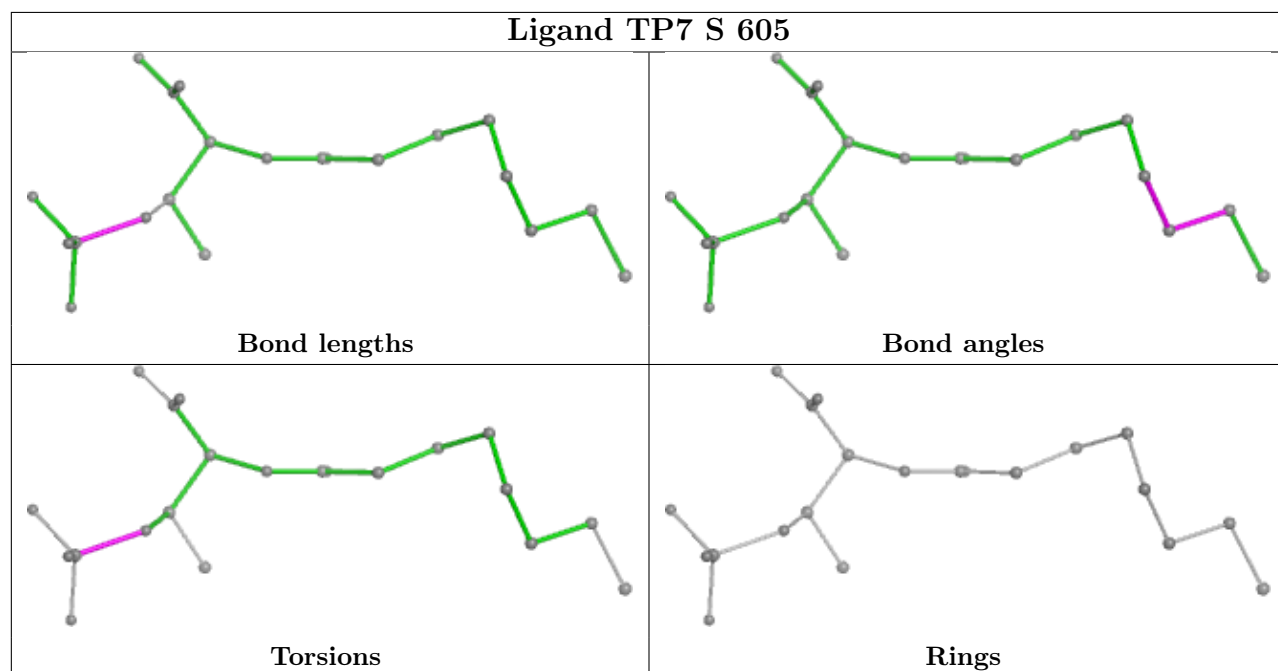
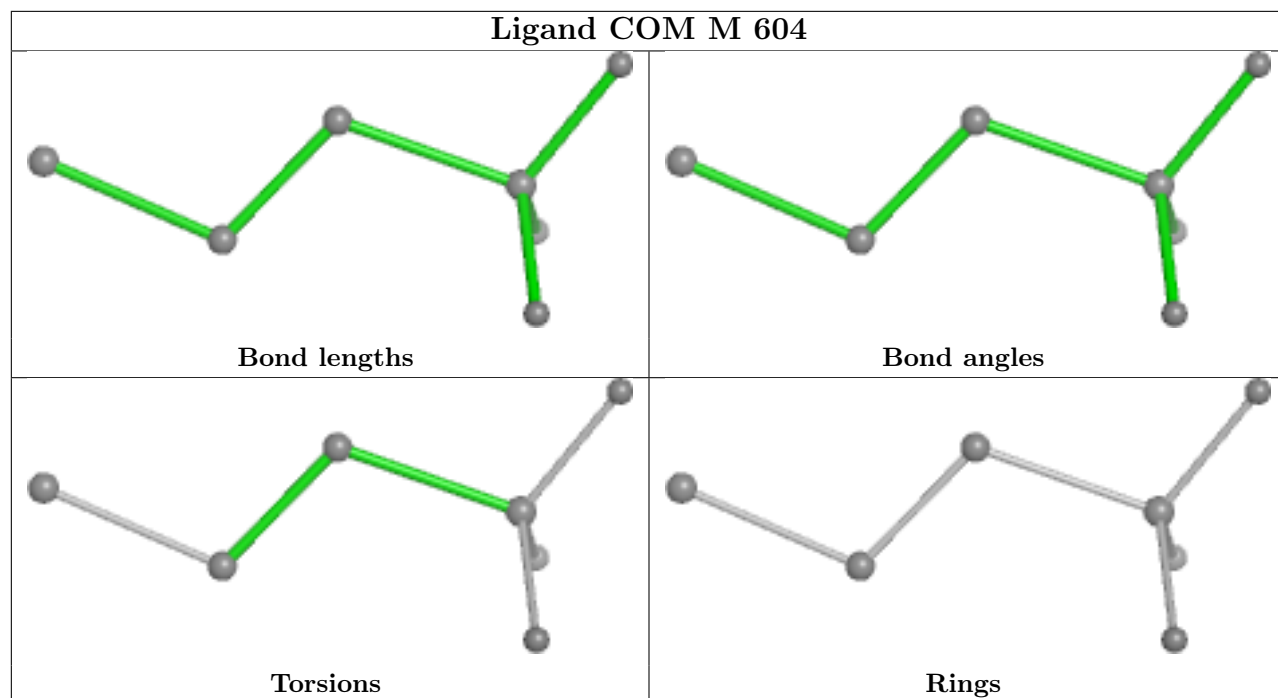
Torsions



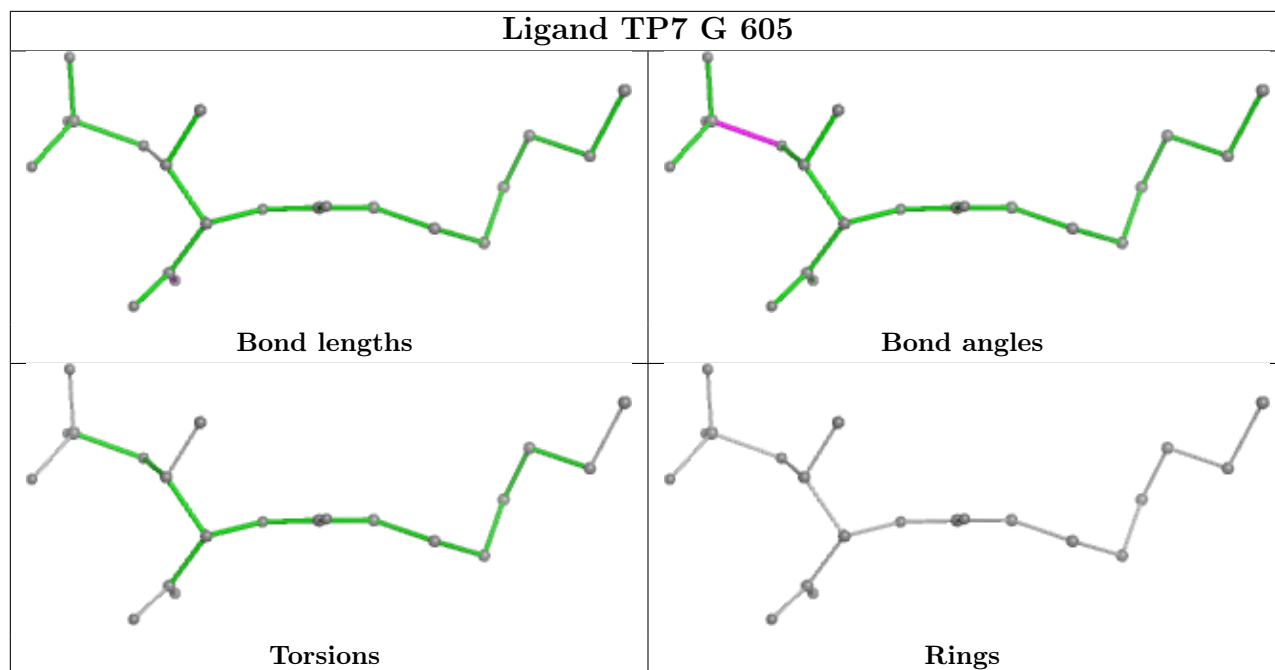
Rings



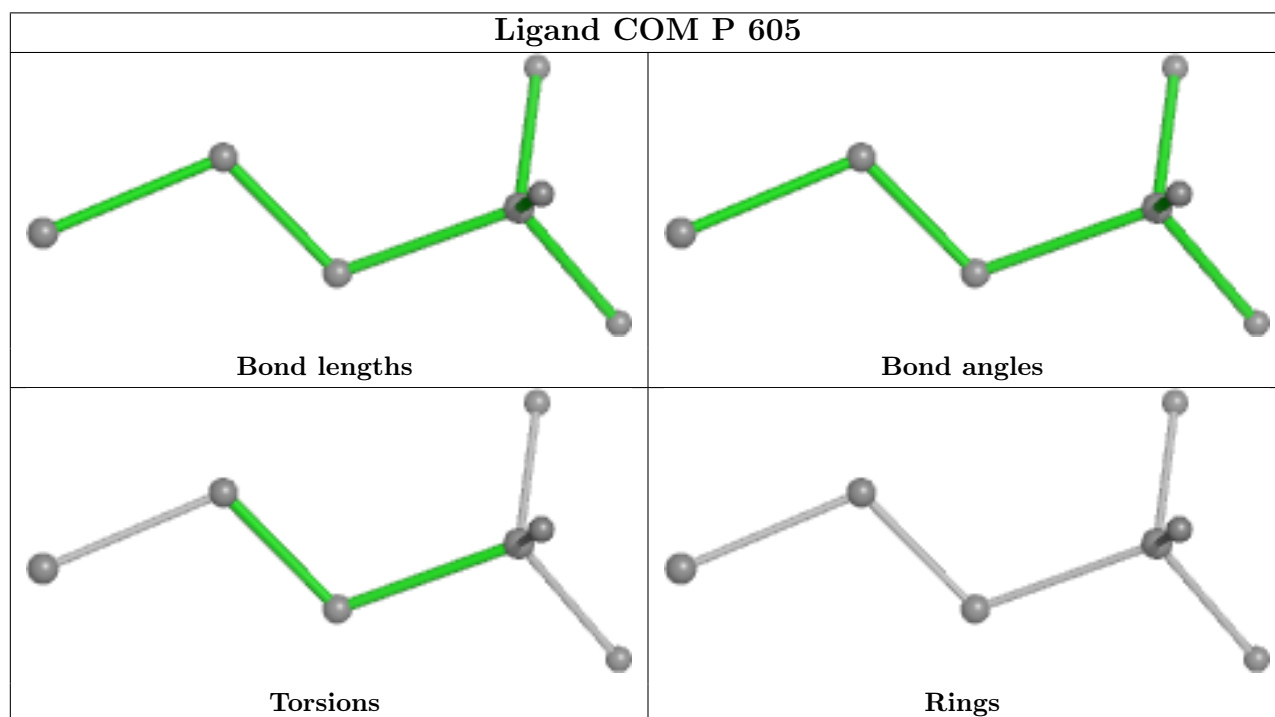




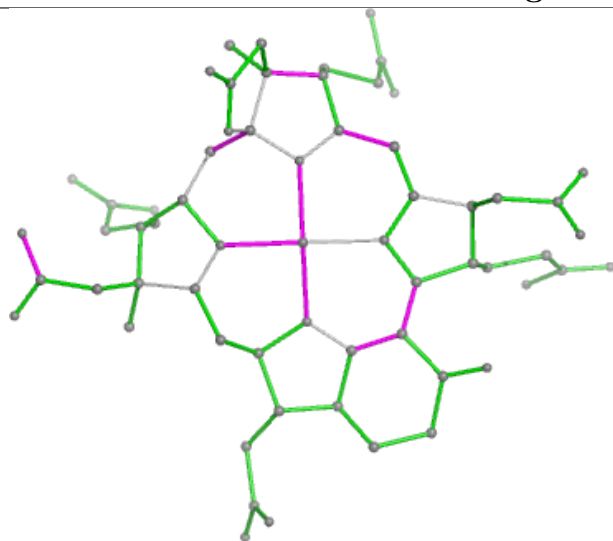
## Ligand TP7 G 605



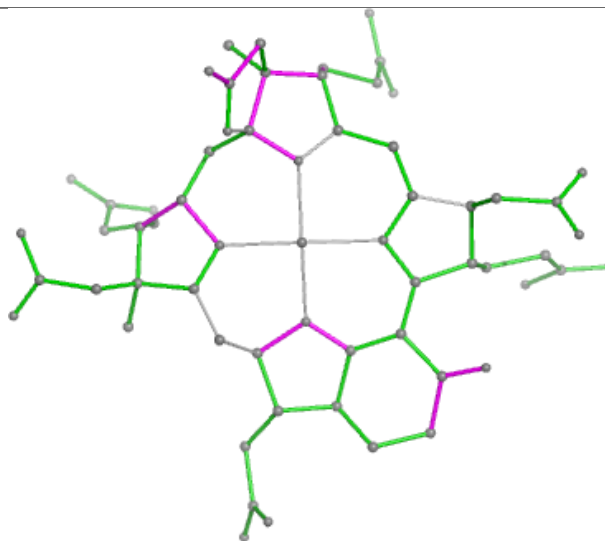
## Ligand COM P 605



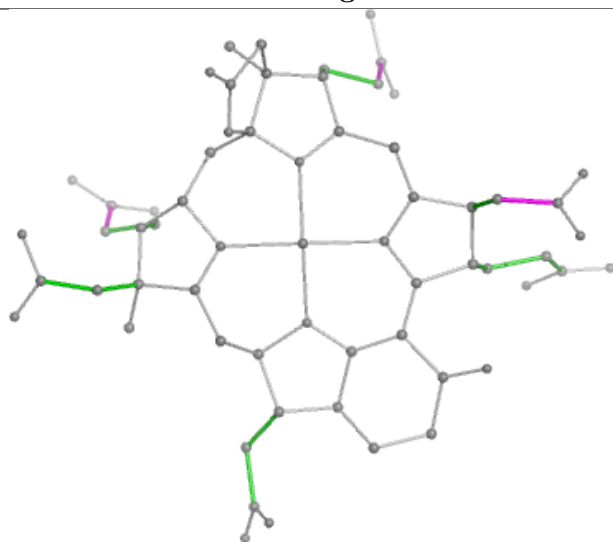
## Ligand F43 S 603



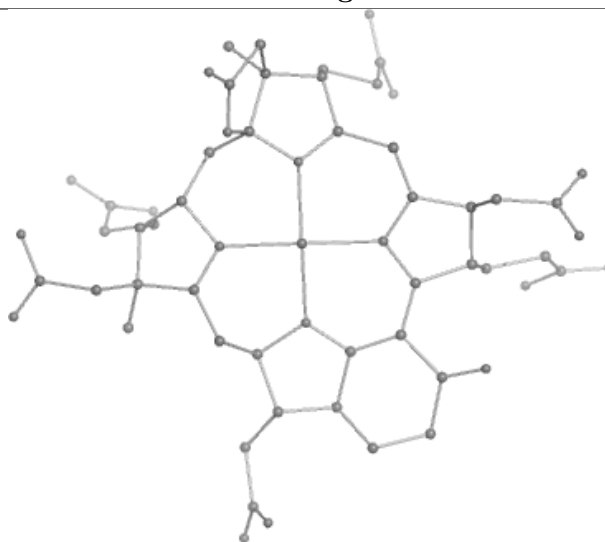
Bond lengths



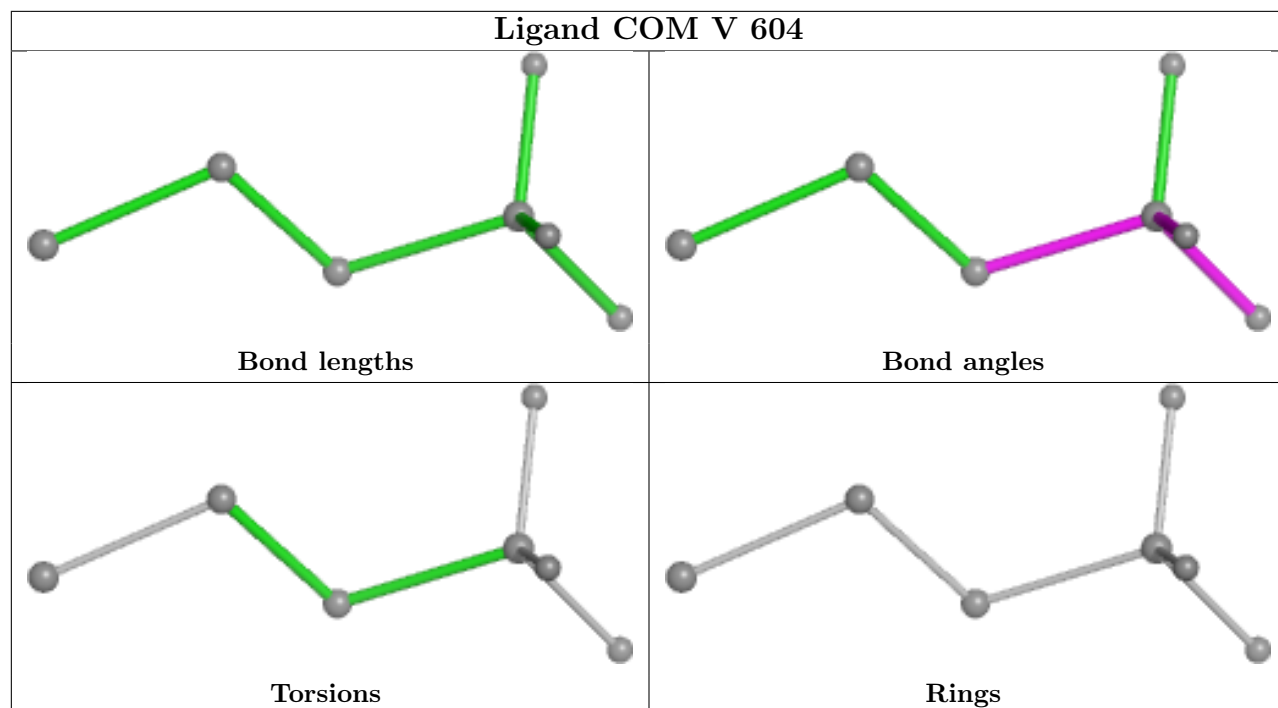
Bond angles



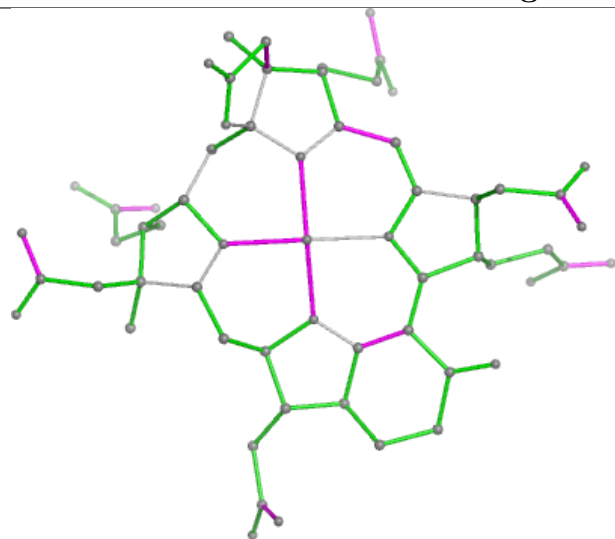
Torsions



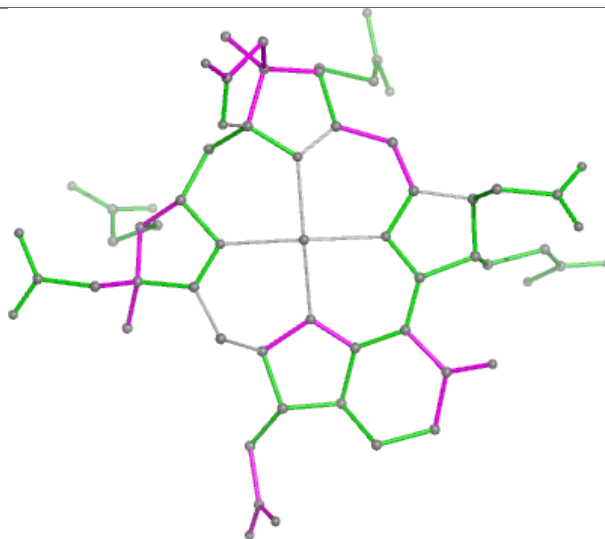
Rings



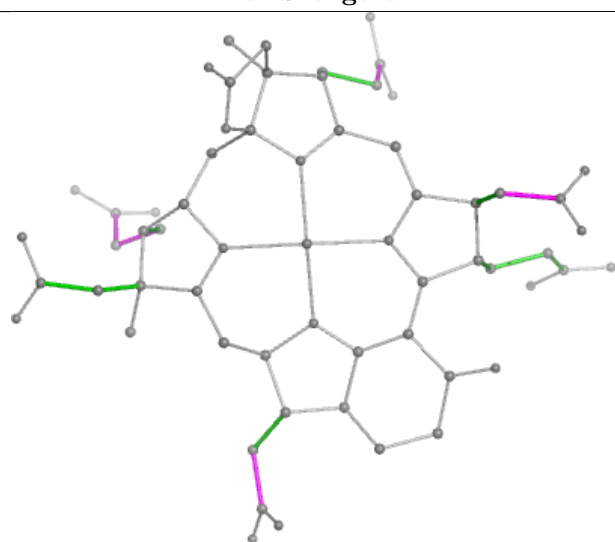
## Ligand F43 M 603



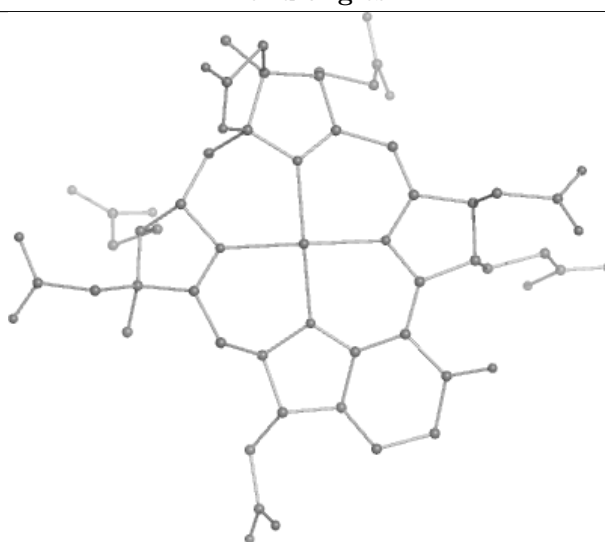
Bond lengths



Bond angles

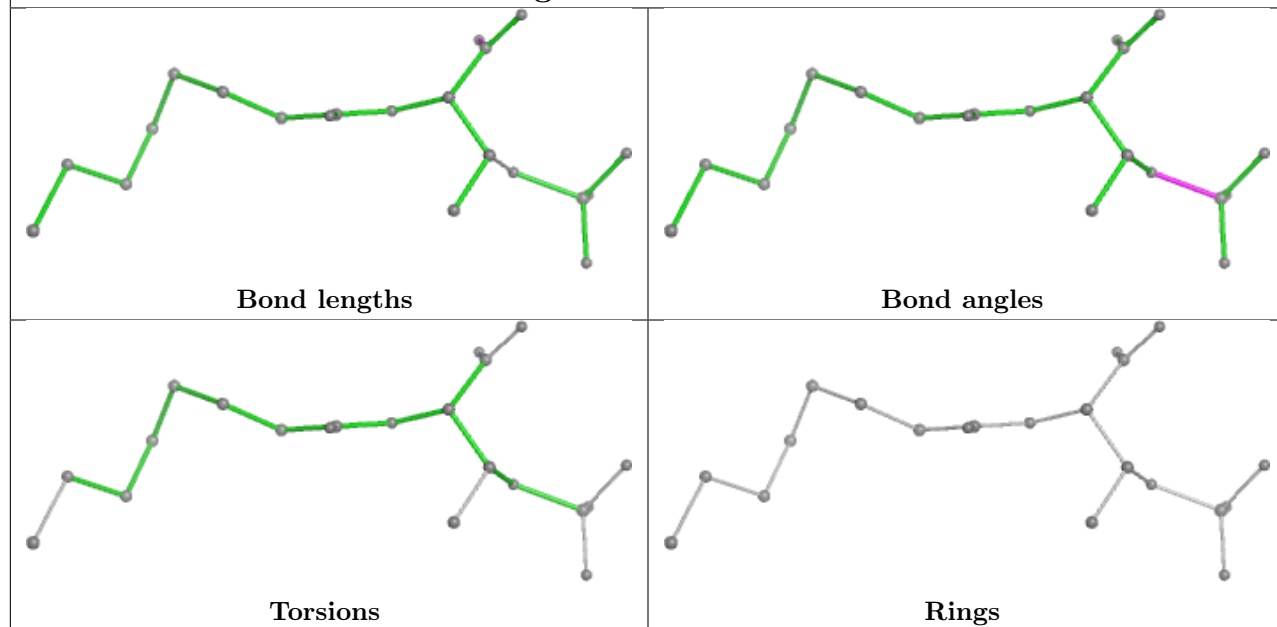


Torsions

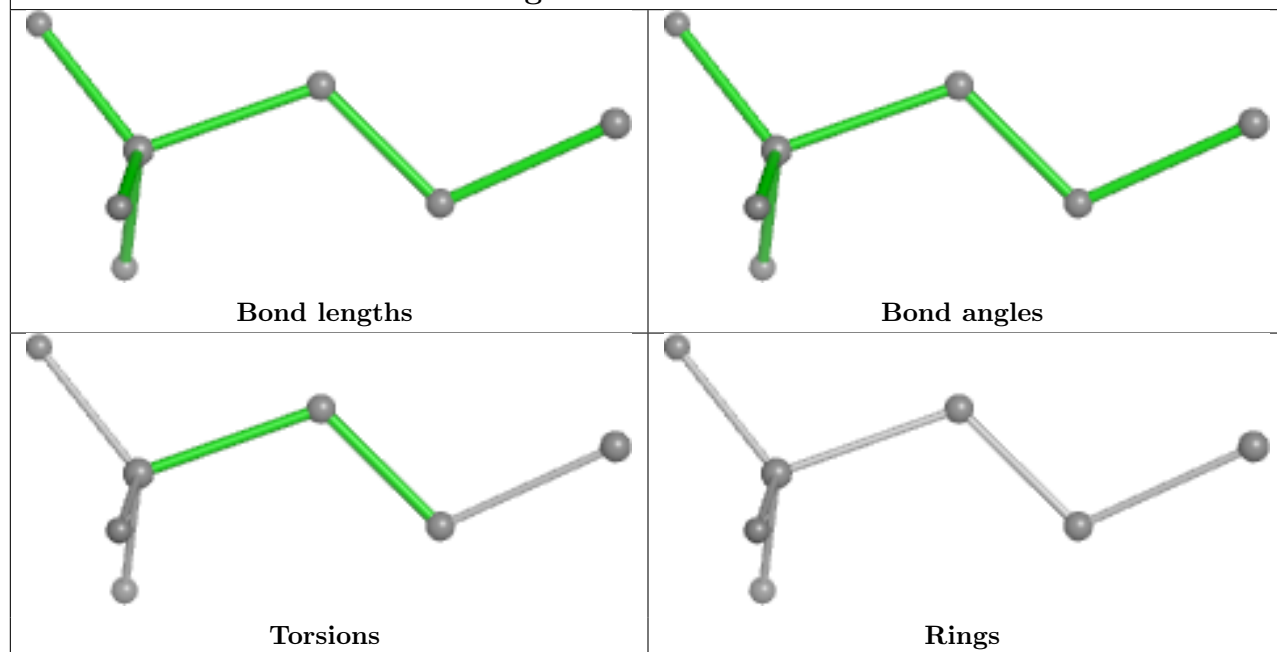


Rings

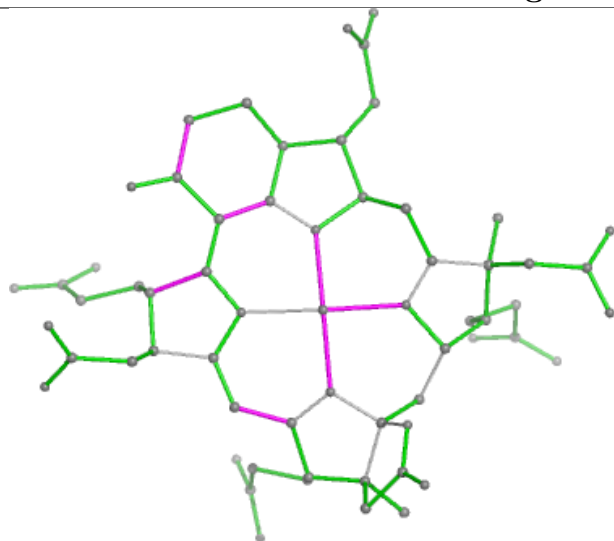
## Ligand TP7 V 603



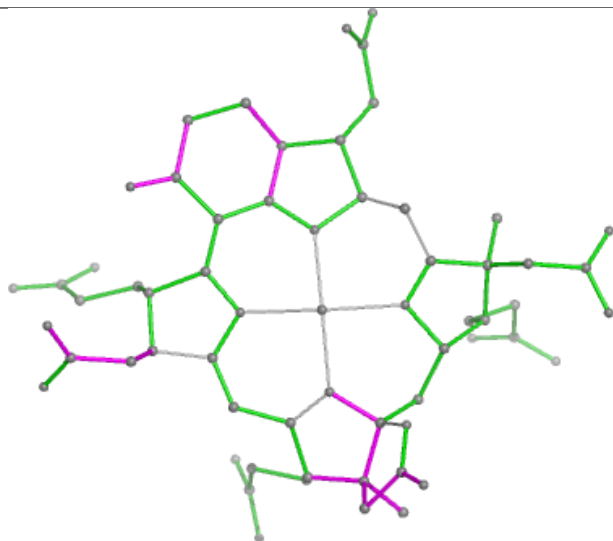
## Ligand COM A 605



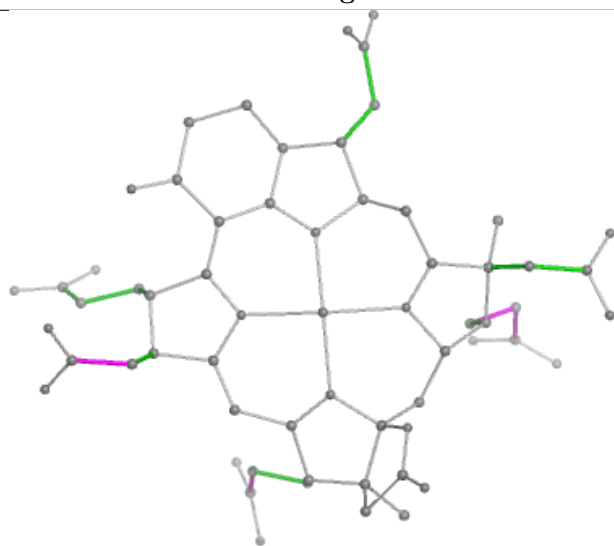
## Ligand F43 S 608



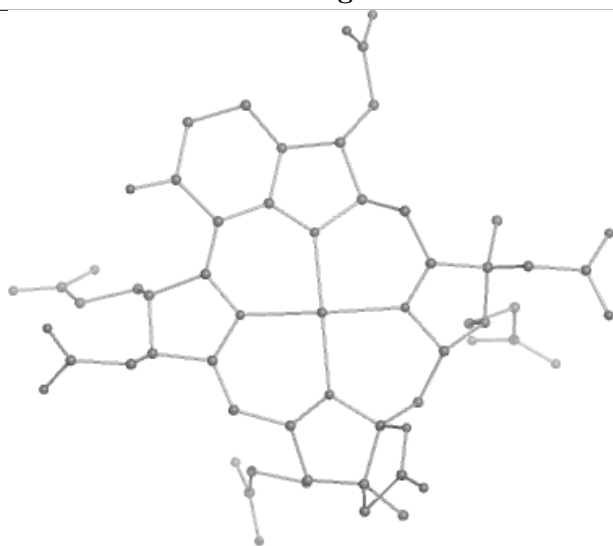
Bond lengths



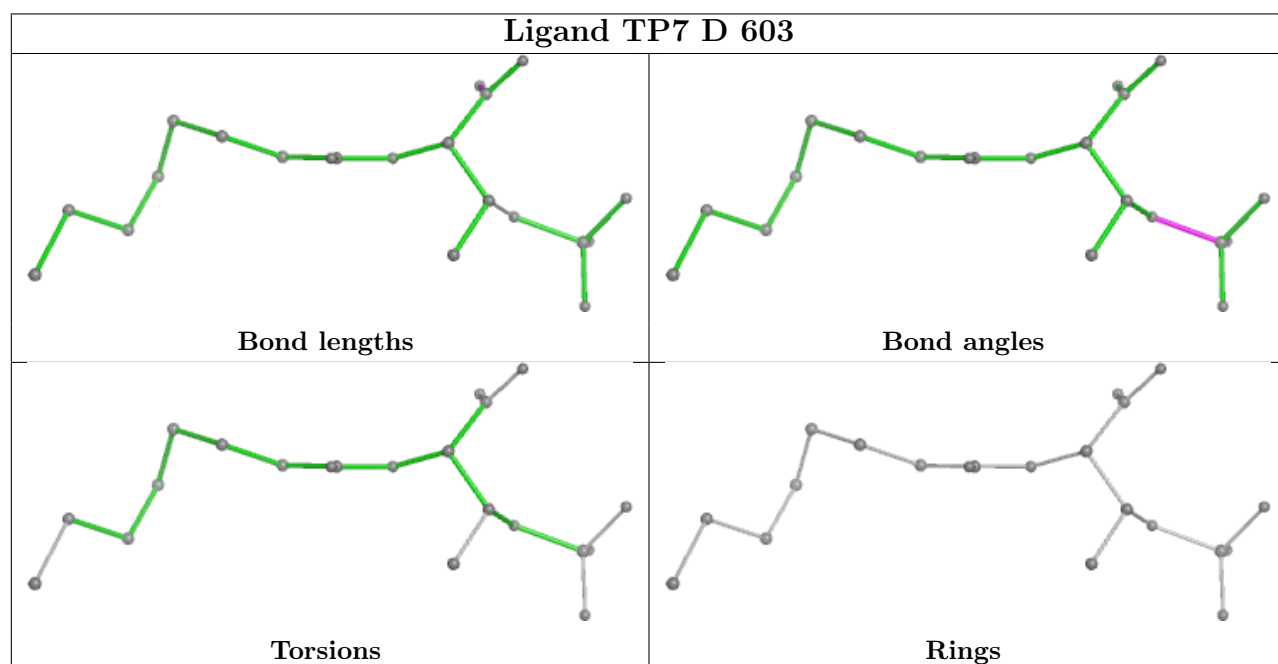
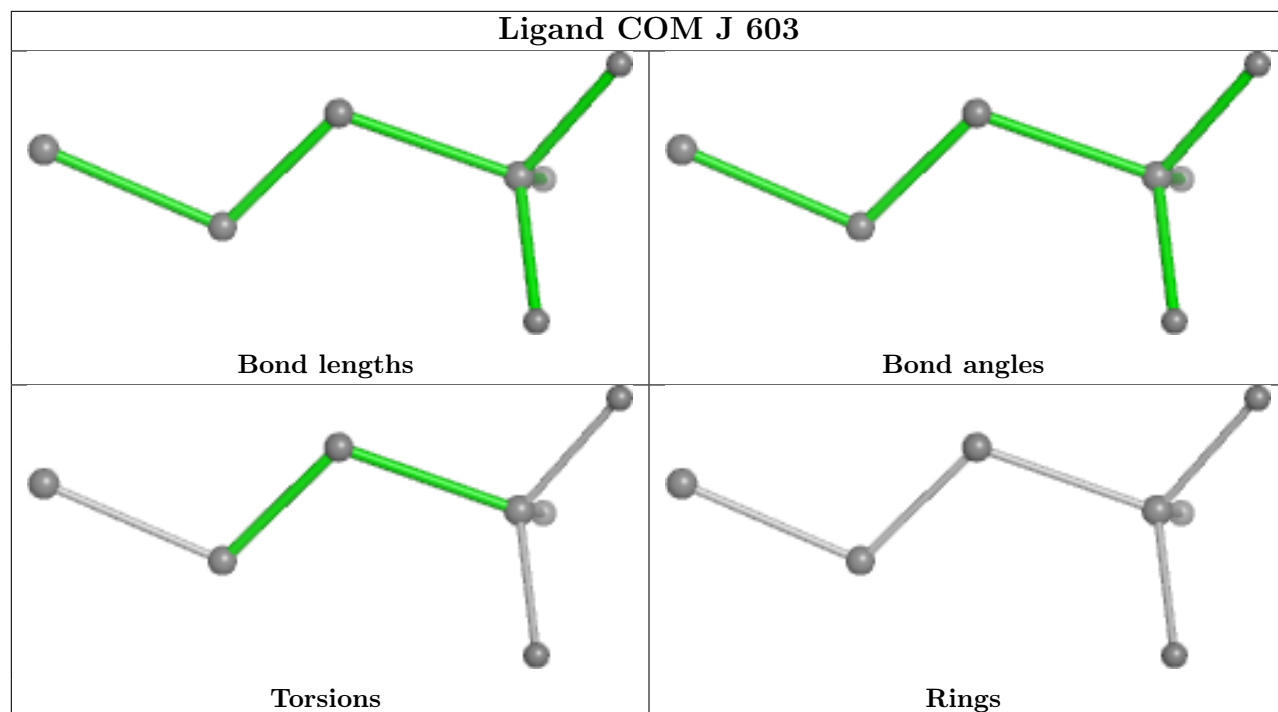
Bond angles



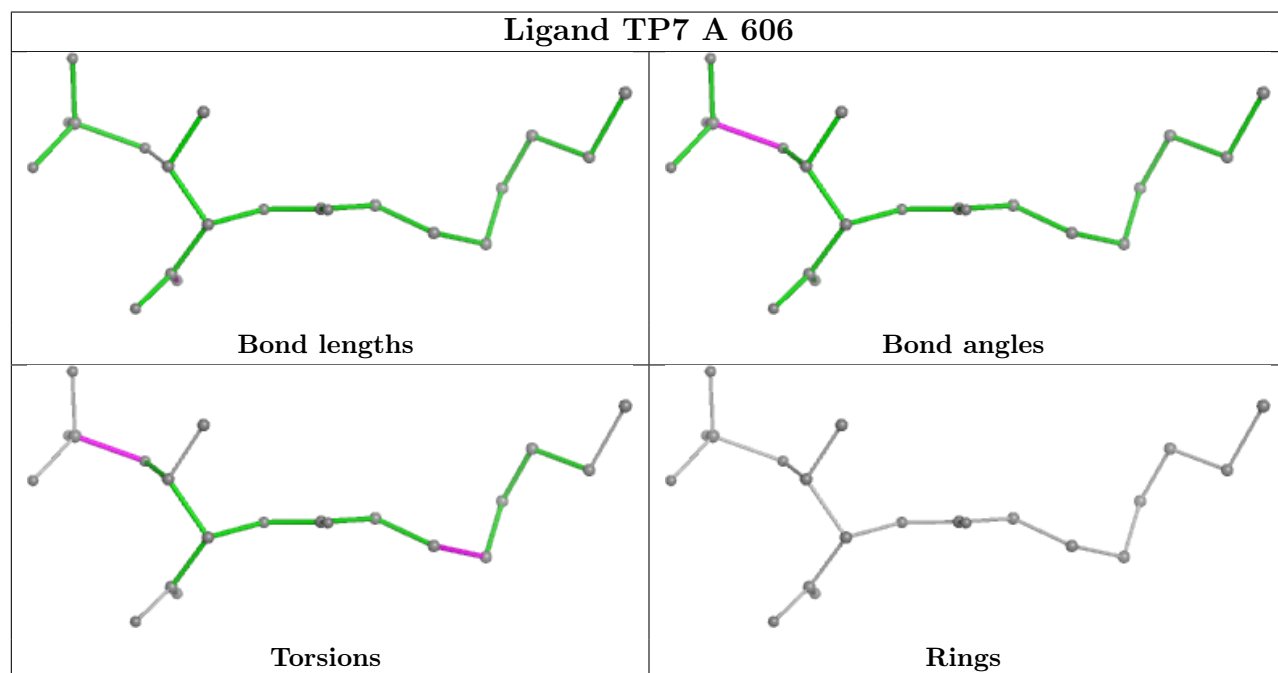
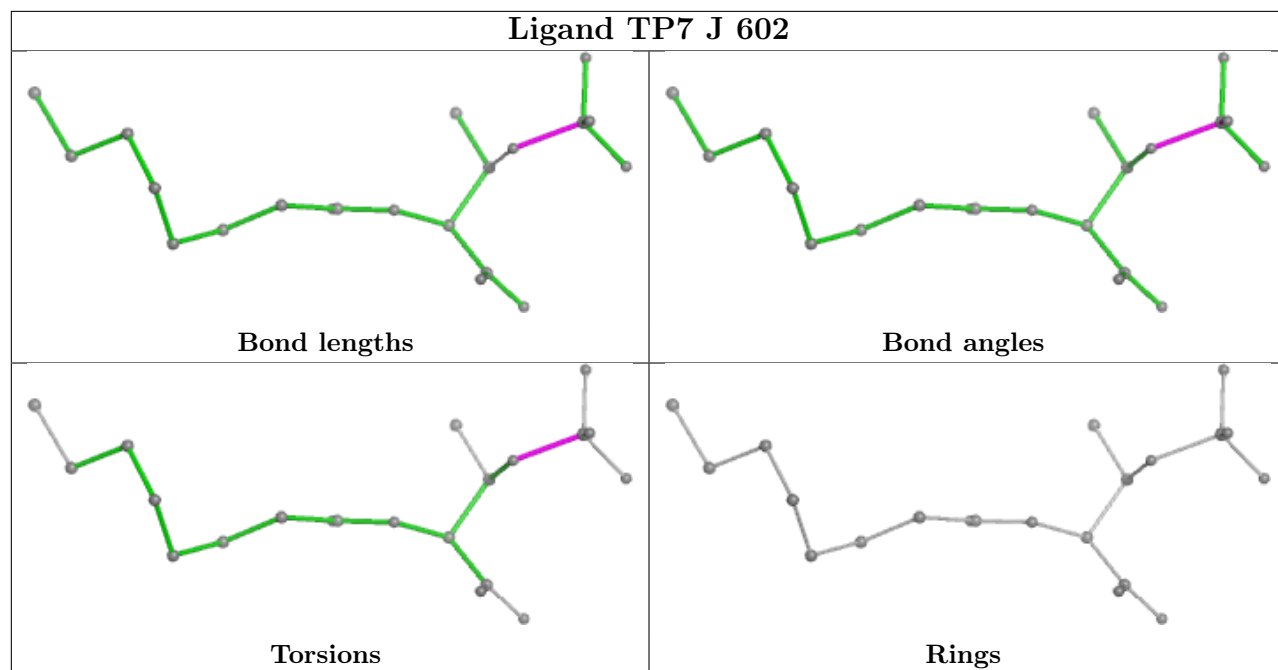
Torsions



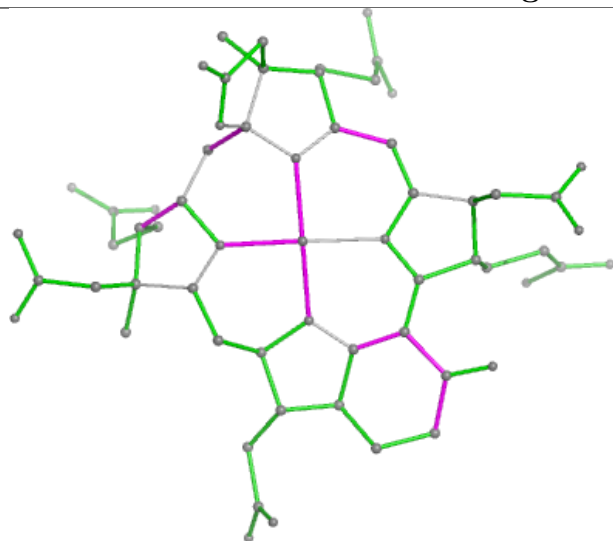
Rings



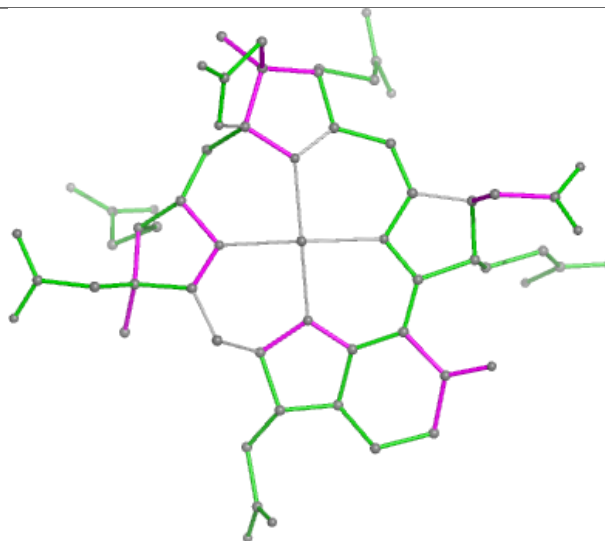




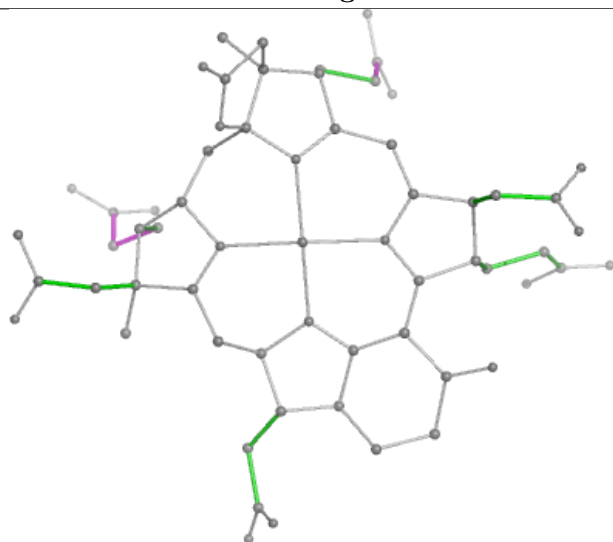
## Ligand F43 A 604



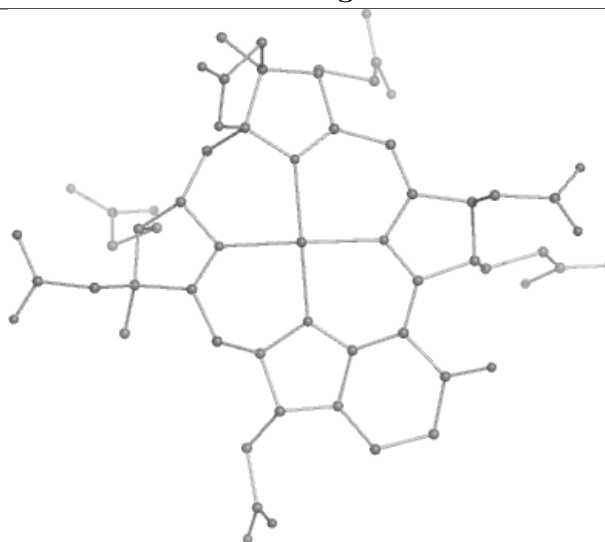
Bond lengths



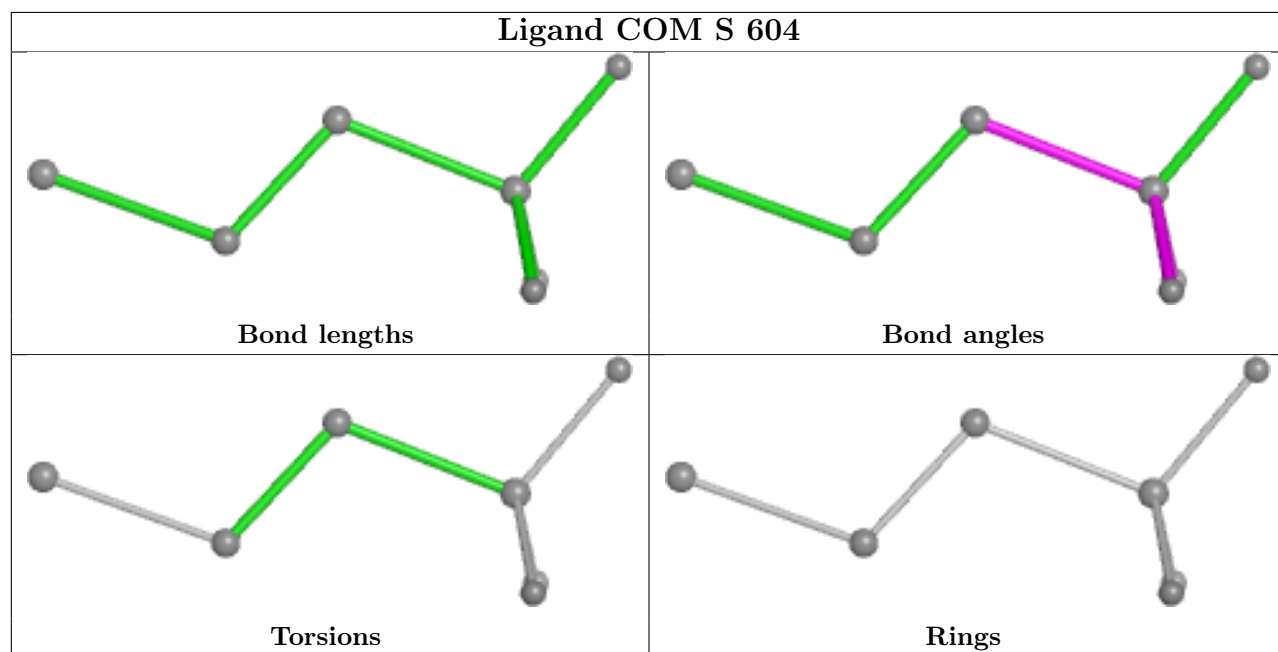
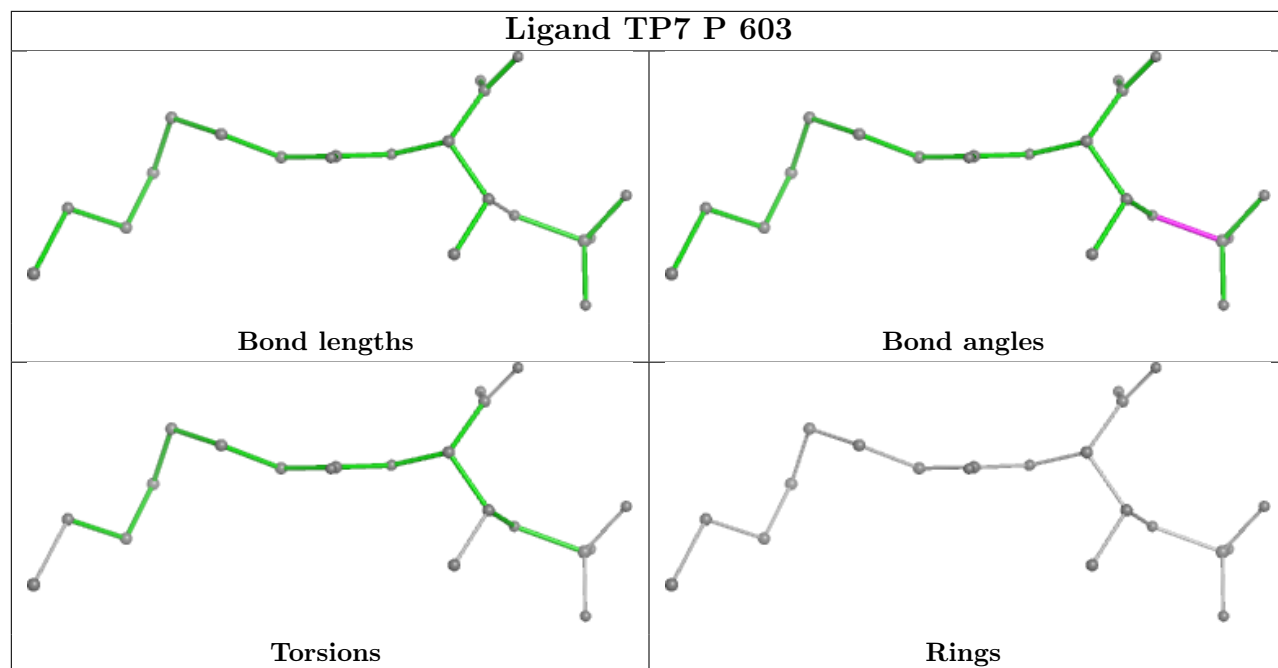
Bond angles



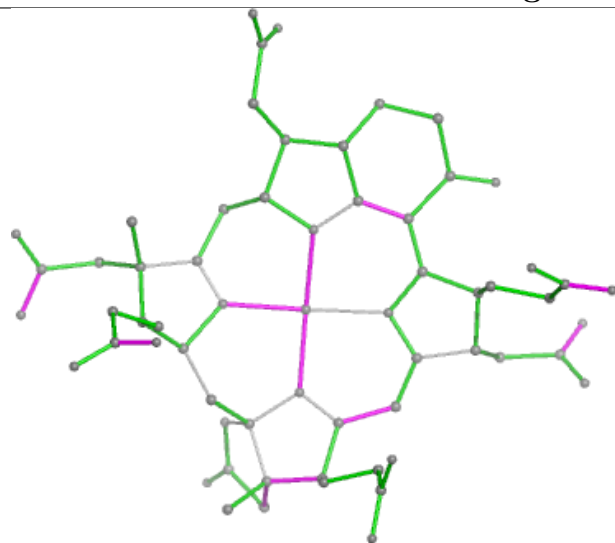
Torsions



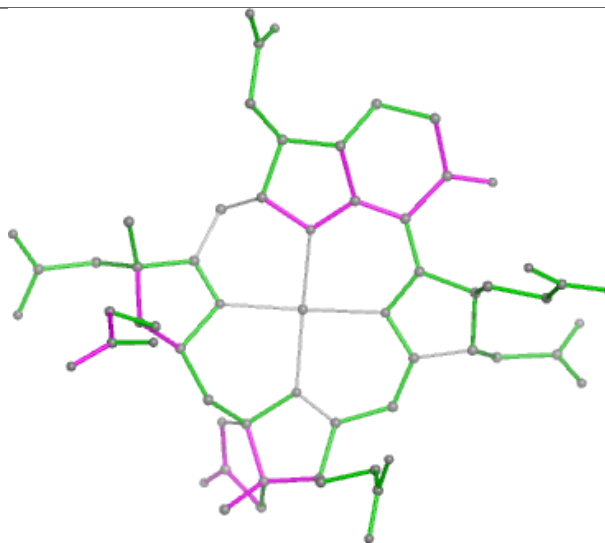
Rings



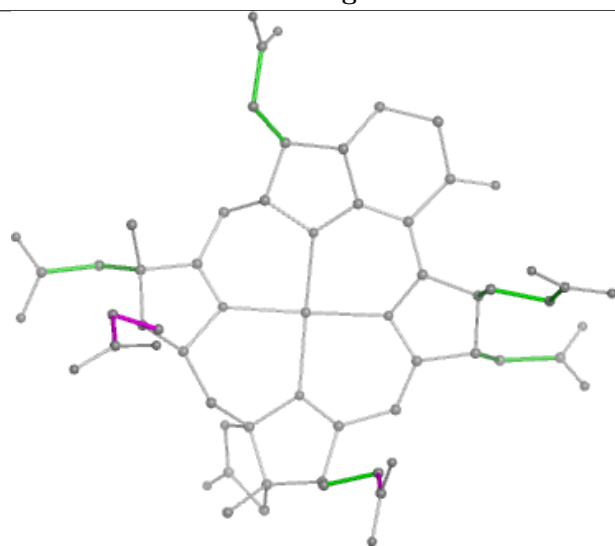
## Ligand F43 G 603



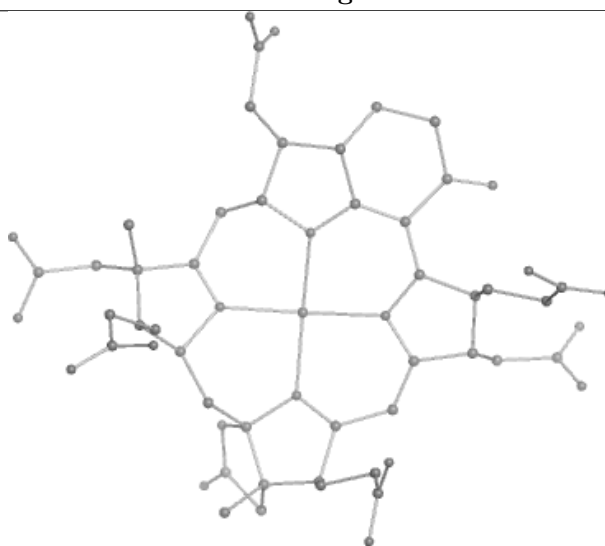
Bond lengths



Bond angles

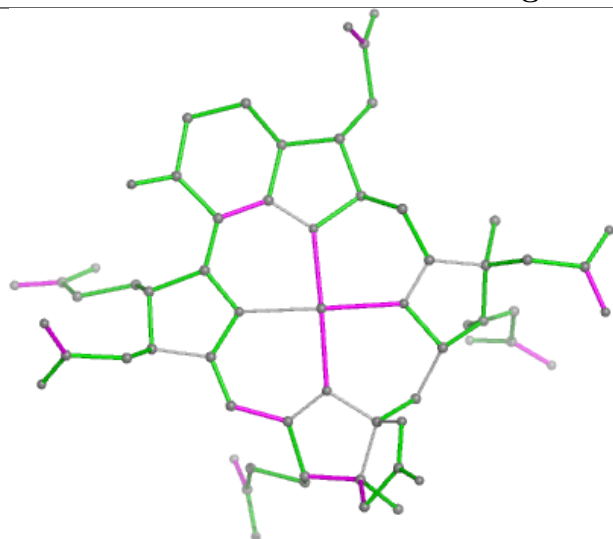


Torsions

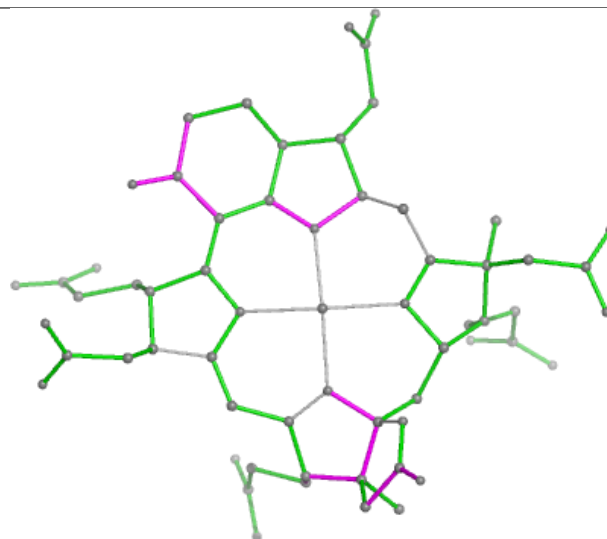


Rings

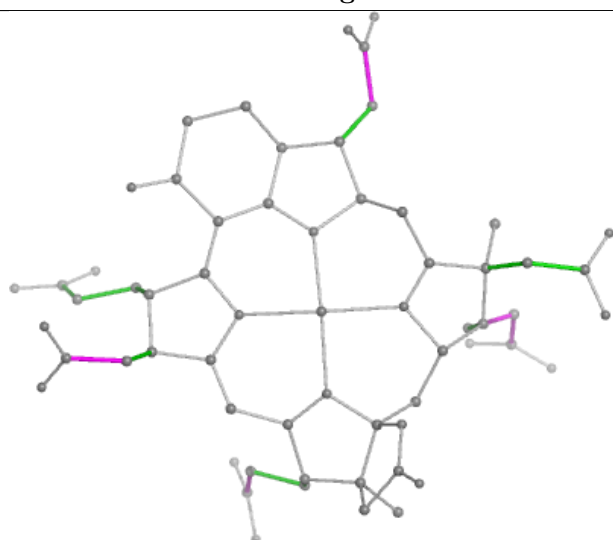
## Ligand F43 A 613



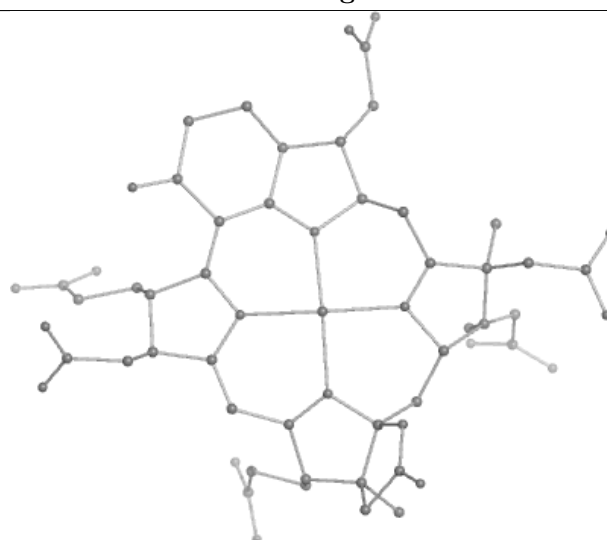
Bond lengths



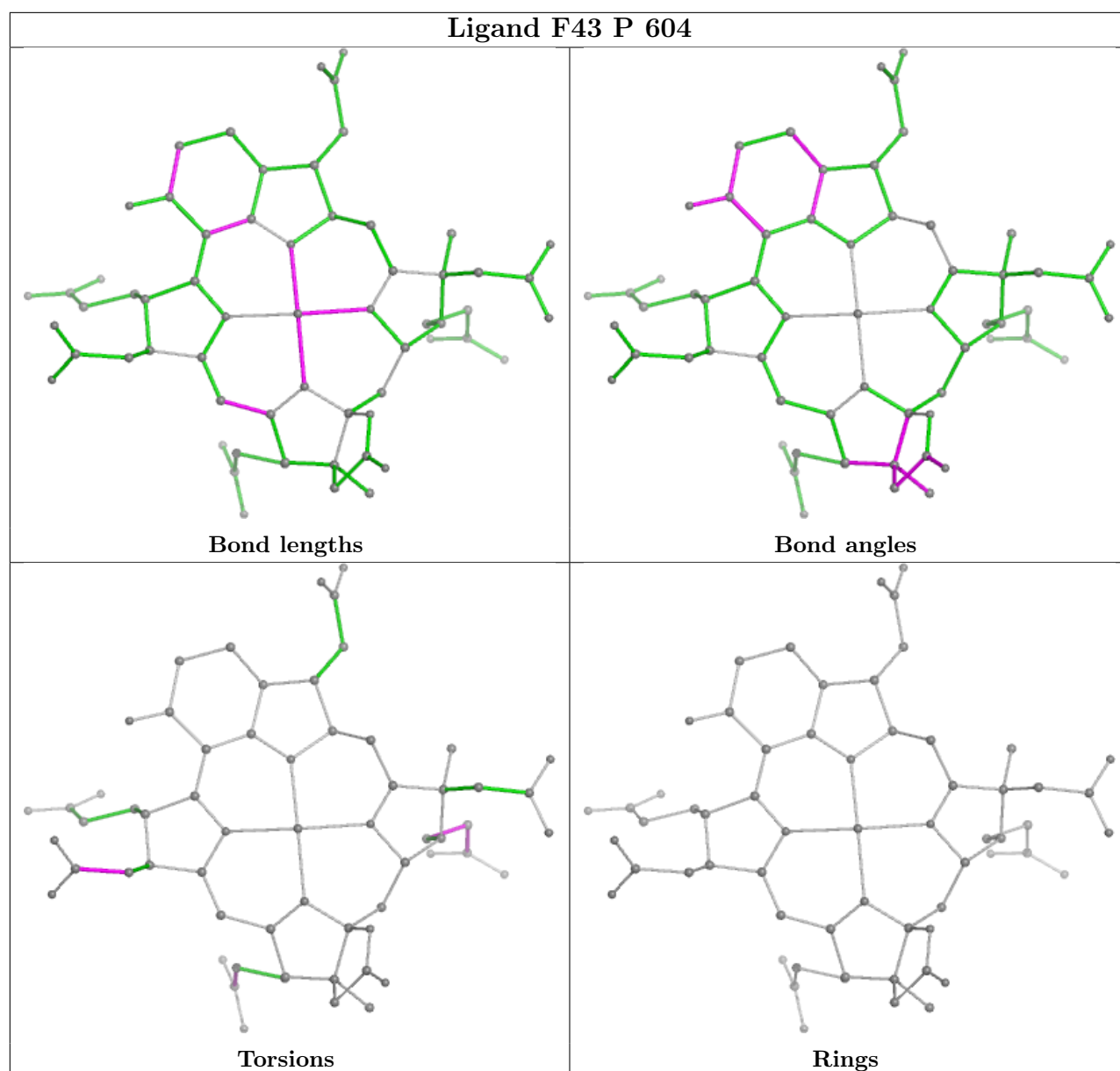
Bond angles



Torsions



Rings



## 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	553/561 (98%)	-1.07	3 (0%) 87 92	4, 9, 20, 47	5 (0%)
1	D	553/561 (98%)	-1.07	3 (0%) 87 92	4, 8, 19, 46	8 (1%)
1	G	553/561 (98%)	-1.05	3 (0%) 87 92	5, 9, 20, 49	5 (0%)
1	J	551/561 (98%)	-1.01	1 (0%) 92 95	6, 11, 21, 35	5 (0%)
1	M	553/561 (98%)	-0.94	3 (0%) 87 92	7, 12, 23, 51	4 (0%)
1	P	553/561 (98%)	-0.93	3 (0%) 87 92	7, 12, 23, 51	6 (1%)
1	S	553/561 (98%)	-0.70	5 (0%) 81 89	9, 17, 27, 47	3 (0%)
1	V	551/561 (98%)	-0.79	1 (0%) 92 95	7, 16, 27, 40	4 (0%)
2	B	433/434 (99%)	-0.99	1 (0%) 92 95	5, 11, 20, 35	9 (2%)
2	E	433/434 (99%)	-0.96	1 (0%) 92 95	5, 10, 20, 41	12 (2%)
2	H	433/434 (99%)	-0.85	1 (0%) 92 95	7, 13, 25, 42	5 (1%)
2	K	433/434 (99%)	-0.80	1 (0%) 92 95	6, 15, 25, 38	8 (1%)
2	N	433/434 (99%)	-0.59	2 (0%) 87 92	9, 19, 30, 41	5 (1%)
2	Q	433/434 (99%)	-0.69	1 (0%) 92 95	8, 17, 28, 41	8 (1%)
2	T	433/434 (99%)	-0.07	5 (1%) 76 85	12, 28, 38, 48	5 (1%)
2	W	433/434 (99%)	-0.20	2 (0%) 87 92	12, 26, 36, 46	4 (0%)
3	C	264/265 (99%)	-0.94	1 (0%) 89 94	7, 12, 24, 37	4 (1%)
3	F	264/265 (99%)	-0.97	0 100 100	5, 11, 22, 32	7 (2%)
3	I	264/265 (99%)	-0.96	1 (0%) 89 94	6, 12, 21, 34	2 (0%)
3	L	264/265 (99%)	-0.74	1 (0%) 89 94	9, 17, 27, 39	3 (1%)
3	O	264/265 (99%)	-0.72	1 (0%) 89 94	9, 17, 28, 43	2 (0%)
3	R	264/265 (99%)	-0.81	1 (0%) 89 94	8, 15, 26, 37	3 (1%)
3	U	264/265 (99%)	-0.28	1 (0%) 89 94	13, 25, 36, 48	2 (0%)
3	X	264/265 (99%)	-0.51	1 (0%) 89 94	11, 20, 31, 45	4 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	9996/10080 (99%)	-0.80	43 (0%) 89 94	4, 14, 30, 51	123 (1%)

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	561	VAL	5.9
1	M	560	GLY	5.8
1	D	561	VAL	5.5
1	G	561	VAL	5.5
1	S	561	VAL	5.2

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	MHS	G	266	11/12	0.98	0.04	7,9,11,11	0
1	MHS	V	266	11/12	0.98	0.04	14,16,19,19	0
1	AGM	A	280	12/13	0.98	0.04	4,5,7,7	0
1	AGM	G	280	12/13	0.98	0.04	5,6,8,8	0
1	AGM	S	280	12/13	0.98	0.04	14,15,16,16	0
1	AGM	V	280	12/13	0.98	0.05	12,13,14,15	0
1	MGN	P	410	10/11	0.98	0.03	4,7,8,9	0
1	TRX	D	437	15/16	0.98	0.03	4,5,6,6	0
1	TRX	V	437	15/16	0.98	0.04	12,12,13,14	0
1	DYA	A	460	8/9	0.98	0.03	4,6,8,8	0
1	DYA	D	460	8/9	0.98	0.03	4,6,8,8	0
1	DYA	M	460	8/9	0.98	0.03	9,10,10,14	0
1	DYA	P	460	8/9	0.98	0.04	8,9,11,12	0
1	DYA	S	460	8/9	0.98	0.04	15,19,19,21	0
1	DYA	V	460	8/9	0.98	0.04	13,14,17,17	0
1	MHS	P	266	11/12	0.99	0.04	9,10,12,12	0
1	MGN	D	410	10/11	0.99	0.03	4,4,5,8	0
1	MGN	G	410	10/11	0.99	0.03	3,5,6,7	0
1	MGN	J	410	10/11	0.99	0.02	7,8,8,9	0
1	MGN	M	410	10/11	0.99	0.03	6,7,8,9	0
1	MHS	S	266	11/12	0.99	0.04	14,15,17,17	0
1	MGN	S	410	10/11	0.99	0.04	12,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MGN	V	410	10/11	0.99	0.03	7,9,11,11	0
1	TRX	A	437	15/16	0.99	0.03	4,5,6,6	0
1	MHS	D	266	11/12	0.99	0.03	4,6,8,9	0
1	TRX	G	437	15/16	0.99	0.03	5,6,6,7	0
1	TRX	J	437	15/16	0.99	0.02	7,8,10,10	0
1	TRX	M	437	15/16	0.99	0.04	8,8,9,9	0
1	TRX	P	437	15/16	0.99	0.03	8,8,9,9	0
1	TRX	S	437	15/16	0.99	0.04	14,15,16,16	0
1	MHS	A	266	11/12	0.99	0.03	5,6,8,8	0
1	AGM	D	280	12/13	0.99	0.04	4,5,5,6	0
1	MHS	J	266	11/12	0.99	0.03	6,8,10,12	0
1	DYA	G	460	8/9	0.99	0.03	5,7,10,10	0
1	DYA	J	460	8/9	0.99	0.03	9,10,11,12	0
1	AGM	J	280	12/13	0.99	0.04	6,7,9,9	0
1	AGM	M	280	12/13	0.99	0.04	7,9,10,10	0
1	AGM	P	280	12/13	0.99	0.04	6,8,9,9	0
1	MHS	M	266	11/12	0.99	0.03	8,9,10,11	0
1	SMC	M	462	7/8	0.99	0.03	10,11,12,13	0
1	SMC	P	462	7/8	0.99	0.04	9,10,10,11	0
1	SMC	S	462	7/8	0.99	0.04	17,17,19,20	0
1	SMC	V	462	7/8	0.99	0.05	15,16,17,17	0
1	GL3	G	455	4/5	1.00	0.03	5,5,5,6	0
1	GL3	J	455	4/5	1.00	0.01	7,7,8,8	0
1	GL3	M	455	4/5	1.00	0.02	7,7,8,8	0
1	GL3	P	455	4/5	1.00	0.02	7,7,7,8	0
1	GL3	S	455	4/5	1.00	0.02	14,15,15,16	0
1	SMC	A	462	7/8	1.00	0.04	5,6,7,8	0
1	SMC	D	462	7/8	1.00	0.03	5,6,7,7	0
1	SMC	G	462	7/8	1.00	0.03	6,7,7,8	0
1	SMC	J	462	7/8	1.00	0.03	10,10,11,11	0
1	GL3	V	455	4/5	1.00	0.04	10,11,11,13	0
1	MGN	A	410	10/11	1.00	0.02	3,5,6,7	0
1	GL3	A	455	4/5	1.00	0.02	5,5,5,6	0
1	GL3	D	455	4/5	1.00	0.02	4,4,5,5	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
12	EDO	F	303	4/4	0.69	0.18	50,60,60,60	0
10	GOL	R	302	6/6	0.72	0.19	49,59,61,62	0
11	MPD	N	502	8/8	0.74	0.16	43,52,53,53	0
12	EDO	G	608	4/4	0.74	0.21	49,59,60,60	0
12	EDO	P	608	4/4	0.75	0.19	42,50,51,51	0
12	EDO	A	611	4/4	0.76	0.21	49,59,59,60	0
12	EDO	A	612	4/4	0.77	0.17	47,56,57,58	0
10	GOL	Q	502	6/6	0.77	0.16	43,52,53,54	0
12	EDO	S	607	4/4	0.81	0.15	40,48,49,50	0
11	MPD	K	504[A]	8/8	0.84	0.15	23,28,30,32	22
10	GOL	G	607	6/6	0.84	0.13	41,49,51,53	0
11	MPD	H	503	8/8	0.84	0.12	35,44,46,46	0
11	MPD	J	606	8/8	0.84	0.14	38,46,48,49	0
11	MPD	V	606	8/8	0.86	0.12	33,43,45,46	0
12	EDO	D	608	4/4	0.86	0.14	39,47,48,49	0
10	GOL	M	607	6/6	0.87	0.12	42,51,52,53	0
10	GOL	A	608	6/6	0.88	0.12	40,48,51,52	0
10	GOL	A	610	6/6	0.88	0.12	38,46,50,51	0
11	MPD	J	605	8/8	0.89	0.12	22,34,36,39	0
10	GOL	D	607	6/6	0.89	0.12	41,49,49,49	0
11	MPD	B	502	8/8	0.90	0.10	28,34,38,38	0
12	EDO	N	503	4/4	0.91	0.10	29,34,41,41	0
11	MPD	P	607	8/8	0.92	0.10	24,32,34,34	0
11	MPD	D	606	8/8	0.92	0.10	20,30,31,32	0
11	MPD	K	503	8/8	0.92	0.09	26,31,36,36	0
11	MPD	A	609	8/8	0.92	0.09	19,26,31,31	0
10	GOL	M	606	6/6	0.92	0.10	21,25,28,28	0
12	EDO	V	607	4/4	0.92	0.09	39,47,49,50	0
6	CL	U	301	1/1	0.93	0.20	60,60,60,60	0
10	GOL	L	302	6/6	0.93	0.10	24,32,38,39	0
10	GOL	V	605	6/6	0.94	0.08	23,26,31,31	0
6	CL	T	501	1/1	0.94	0.17	55,55,55,55	0
10	GOL	O	302	6/6	0.94	0.09	28,33,39,40	0
10	GOL	F	302	6/6	0.95	0.08	18,26,32,35	0
10	GOL	D	605	6/6	0.95	0.07	19,23,27,27	0
10	GOL	S	606	6/6	0.95	0.08	25,27,32,32	0
6	CL	X	301	1/1	0.95	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
10	GOL	A	607	6/6	0.96	0.07	17,21,26,26	0
10	GOL	J	604	6/6	0.96	0.06	21,24,28,28	0
10	GOL	G	606	6/6	0.96	0.07	19,23,27,27	0
10	GOL	P	606	6/6	0.96	0.06	23,26,31,31	0
5	NA	V	601	1/1	0.97	0.06	19,19,19,19	1
5	NA	A	602	1/1	0.97	0.05	9,9,9,9	1
5	NA	D	601	1/1	0.97	0.09	19,19,19,19	1
7	F43	S	603	62/62	0.98	0.06	10,13,16,18	0
6	CL	W	501	1/1	0.98	0.08	41,41,41,41	0
5	NA	H	501	1/1	0.98	0.10	34,34,34,34	0
6	CL	I	301	1/1	0.99	0.09	20,20,20,20	0
6	CL	N	501	1/1	0.99	0.04	30,30,30,30	0
6	CL	R	301	1/1	0.99	0.04	27,27,27,27	0
7	F43	A	604	62/62	0.99	0.03	3,5,8,10	0
7	F43	A	613	62/62	0.99	0.03	2,5,8,10	0
7	F43	G	603	62/62	0.99	0.04	3,5,9,10	0
7	F43	G	609	62/62	0.99	0.03	5,7,11,12	0
7	F43	M	603	62/62	0.99	0.03	5,7,10,12	0
5	NA	P	601	1/1	0.99	0.03	15,15,15,15	1
7	F43	S	608	62/62	0.99	0.03	8,10,12,16	0
8	COM	S	604	7/7	0.99	0.03	13,14,14,14	0
9	TP7	A	606	21/21	0.99	0.03	4,6,8,9	0
9	TP7	D	603	21/21	0.99	0.03	4,6,7,9	0
9	TP7	G	605	21/21	0.99	0.03	6,7,8,9	0
9	TP7	J	602	21/21	0.99	0.03	7,9,9,10	0
9	TP7	M	605	21/21	0.99	0.03	7,9,11,11	0
9	TP7	P	603	21/21	0.99	0.03	6,8,11,11	0
9	TP7	S	605	21/21	0.99	0.04	12,16,17,19	0
9	TP7	V	603	21/21	0.99	0.04	11,14,16,16	0
6	CL	F	301	1/1	1.00	0.04	16,16,16,16	0
6	CL	G	602	1/1	1.00	0.04	15,15,15,15	0
6	CL	H	502	1/1	1.00	0.03	19,19,19,19	0
7	F43	P	604	62/62	1.00	0.03	5,6,10,12	0
4	K	G	601	1/1	1.00	0.00	7,7,7,7	0
6	CL	J	601	1/1	1.00	0.03	19,19,19,19	0
8	COM	A	605	7/7	1.00	0.01	5,5,6,6	0
8	COM	D	604	7/7	1.00	0.02	4,5,5,6	0
8	COM	G	604	7/7	1.00	0.02	5,6,6,7	0
8	COM	J	603	7/7	1.00	0.02	7,8,8,9	0
8	COM	M	604	7/7	1.00	0.02	7,8,9,9	0
8	COM	P	605	7/7	1.00	0.02	6,7,8,9	0
6	CL	K	501	1/1	1.00	0.03	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	COM	V	604	7/7	1.00	0.03	11,12,13,13	0
6	CL	K	502	1/1	1.00	0.08	22,22,22,22	0
6	CL	L	301	1/1	1.00	0.08	24,24,24,24	0
6	CL	M	602	1/1	1.00	0.04	17,17,17,17	0
4	K	M	601	1/1	1.00	0.01	9,9,9,9	0
6	CL	O	301	1/1	1.00	0.04	30,30,30,30	0
6	CL	P	602	1/1	1.00	0.04	20,20,20,20	0
6	CL	Q	501	1/1	1.00	0.03	26,26,26,26	0
4	K	S	601	1/1	1.00	0.01	11,11,11,11	0
6	CL	S	602	1/1	1.00	0.02	24,24,24,24	0
4	K	A	601	1/1	1.00	0.01	6,6,6,6	0
6	CL	A	603	1/1	1.00	0.01	15,15,15,15	0
6	CL	V	602	1/1	1.00	0.03	17,17,17,17	0
6	CL	B	501	1/1	1.00	0.03	18,18,18,18	0
6	CL	C	301	1/1	1.00	0.07	18,18,18,18	0
6	CL	D	602	1/1	1.00	0.02	17,17,17,17	0
6	CL	E	501	1/1	1.00	0.03	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.