



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:41 AM UTC

PDB ID : 5T61 / pdb_00005t61
Title : TUNGSTEN-CONTAINING FORMYLMETHANOFURAN DEHYDROGENASE FROM METHANOTHERMOBACTER WOLFEII, TRICLINIC FORM AT 2.55 Å
Authors : Wagner, T.; Ermler, U.; Shima, S.
Deposited on : 2016-09-01
Resolution : 2.55 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

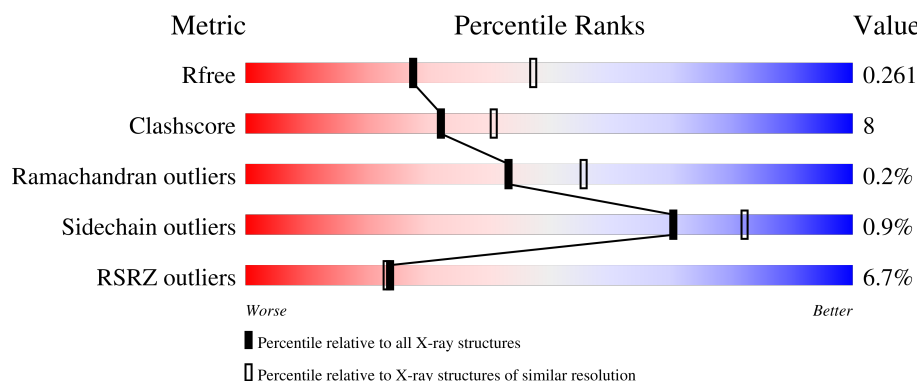
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	569	3% 86% 14%
1	G	569	8% 85% 14% .
1	M	569	13% 82% 17%
1	S	569	2% 86% 13% .

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Mol	Chain	Length	Quality of chain
1	Y	569	
1	e	569	
1	k	569	
1	q	569	
2	B	432	
2	H	432	
2	N	432	
2	T	432	
2	Z	432	
2	f	432	
2	l	432	
2	r	432	
3	C	270	
3	I	270	
3	O	270	
3	U	270	
3	a	270	
3	g	270	
3	m	270	
3	s	270	
4	D	130	
4	J	130	
4	P	130	
4	V	130	
4	b	130	

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Mol	Chain	Length	Quality of chain
4	h	130	
4	n	130	
4	t	130	
5	E	82	
5	K	82	
5	Q	82	
5	W	82	
5	c	82	
5	i	82	
5	o	82	
5	u	82	
6	F	349	
6	L	349	
6	R	349	
6	X	349	
6	d	349	
6	j	349	
6	p	349	
6	v	349	

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
14	H2S	l	505	-	-	X	-

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 114321 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	0	0
			4419	2812	735	849	23			
1	G	568	Total	C	N	O	S	0	0	0
			4411	2807	734	848	22			
1	M	568	Total	C	N	O	S	0	0	0
			4411	2807	734	848	22			
1	S	569	Total	C	N	O	S	0	0	0
			4419	2812	735	849	23			
1	Y	568	Total	C	N	O	S	0	0	0
			4411	2807	734	848	22			
1	e	569	Total	C	N	O	S	0	0	0
			4419	2812	735	849	23			
1	k	568	Total	C	N	O	S	0	0	0
			4411	2807	734	848	22			
1	q	569	Total	C	N	O	S	0	0	0
			4419	2812	735	849	23			

- Molecule 2 is a protein called Tungsten formylmethanofuran dehydrogenase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	429	Total	C	N	O	S	0	0	0
			3364	2115	590	629	30			
2	H	427	Total	C	N	O	S	0	0	0
			3352	2109	587	626	30			
2	N	430	Total	C	N	O	S	0	0	0
			3369	2118	591	630	30			
2	T	429	Total	C	N	O	S	0	0	0
			3364	2115	590	629	30			
2	Z	428	Total	C	N	O	S	0	0	0
			3357	2112	588	627	30			
2	f	427	Total	C	N	O	S	0	0	0
			3352	2109	587	626	30			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	l	428	Total	C	N	O	S	0	0	0
			3357	2112	588	627	30			
2	r	428	Total	C	N	O	S	0	0	0
			3357	2112	588	627	30			

- Molecule 3 is a protein called Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	267	Total	C	N	O	S	0	0	0
			1982	1246	334	389	13			
3	I	269	Total	C	N	O	S	0	0	0
			1994	1254	336	391	13			
3	O	268	Total	C	N	O	S	0	0	0
			1987	1249	335	390	13			
3	U	268	Total	C	N	O	S	0	0	0
			1987	1249	335	390	13			
3	a	268	Total	C	N	O	S	0	0	0
			1987	1249	335	390	13			
3	g	268	Total	C	N	O	S	0	0	0
			1987	1249	335	390	13			
3	m	268	Total	C	N	O	S	0	0	0
			1987	1249	335	390	13			
3	s	269	Total	C	N	O	S	0	0	0
			1994	1254	336	391	13			

- Molecule 4 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	J	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	P	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	V	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	b	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	h	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	n	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	t	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			

- Molecule 5 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	K	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	Q	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	W	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	c	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	i	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	o	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	u	81	Total	C	N	O	S	0	0	0
			581	359	97	116	9			

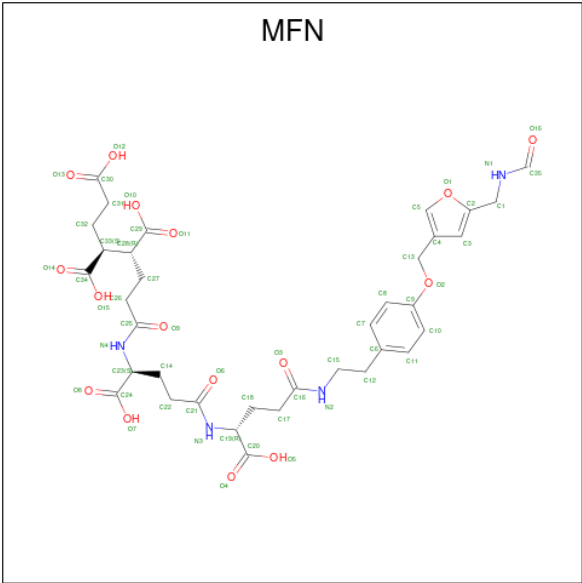
- Molecule 6 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	345	Total	C	N	O	S	0	0	0
			2629	1626	438	523	42			
6	L	348	Total	C	N	O	S	0	0	0
			2656	1641	441	532	42			
6	R	341	Total	C	N	O	S	0	0	0
			2602	1611	434	515	42			
6	X	344	Total	C	N	O	S	0	0	0
			2627	1625	437	523	42			
6	d	340	Total	C	N	O	S	0	0	0
			2595	1606	433	514	42			
6	j	344	Total	C	N	O	S	0	0	0
			2625	1624	437	522	42			
6	p	348	Total	C	N	O	S	0	0	0
			2656	1641	441	532	42			
6	v	346	Total	C	N	O	S	0	0	0
			2643	1634	439	528	42			

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Zn	0	0
			2	2		
7	G	2	Total	Zn	0	0
			2	2		
7	M	2	Total	Zn	0	0
			2	2		
7	S	2	Total	Zn	0	0
			2	2		
7	Y	2	Total	Zn	0	0
			2	2		
7	e	2	Total	Zn	0	0
			2	2		
7	k	2	Total	Zn	0	0
			2	2		
7	q	2	Total	Zn	0	0
			2	2		

- Molecule 8 is N-[4,5,7-TRICARBOXYHEPTANOYL]-L-GAMMA-GLUTAMYL-N-{2-[4-({5-[(FORMYLAMINO)METHYL]-3-FURYL}METHOXY)PHENYL]ETHYL}-D-GLUTAMINE (CCD ID: MFN) (formula: C₃₅H₄₄N₄O₁₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			53	34	4	15		
8	G	1	Total	C	N	O	0	0
			53	34	4	15		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	0	0
			53	34	4	15		
8	S	1	Total	C	N	O	0	0
			53	34	4	15		
8	Y	1	Total	C	N	O	0	0
			53	34	4	15		
8	e	1	Total	C	N	O	0	0
			53	34	4	15		
8	k	1	Total	C	N	O	0	0
			53	34	4	15		
8	q	1	Total	C	N	O	0	0
			53	34	4	15		

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Na	0	0
			1	1		
9	G	1	Total	Na	0	0
			1	1		
9	M	1	Total	Na	0	0
			1	1		
9	S	1	Total	Na	0	0
			1	1		
9	e	1	Total	Na	0	0
			1	1		
9	k	1	Total	Na	0	0
			1	1		
9	q	1	Total	Na	0	0
			1	1		

- Molecule 10 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	K	0	0
			1	1		
10	B	1	Total	K	0	0
			1	1		
10	E	1	Total	K	0	0
			1	1		
10	F	4	Total	K	0	0
			4	4		

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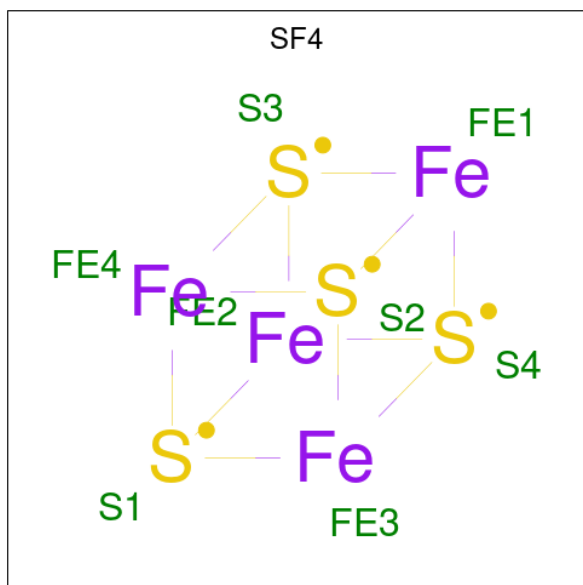
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	G	1	Total K 1 1	0	0
10	K	1	Total K 1 1	0	0
10	L	3	Total K 3 3	0	0
10	M	2	Total K 2 2	0	0
10	N	1	Total K 1 1	0	0
10	Q	1	Total K 1 1	0	0
10	R	3	Total K 3 3	0	0
10	S	2	Total K 2 2	0	0
10	T	1	Total K 1 1	0	0
10	X	3	Total K 3 3	0	0
10	Y	1	Total K 1 1	0	0
10	Z	1	Total K 1 1	0	0
10	c	1	Total K 1 1	0	0
10	d	2	Total K 2 2	0	0
10	e	4	Total K 4 4	0	0
10	i	1	Total K 1 1	0	0
10	j	6	Total K 6 6	0	0
10	k	1	Total K 1 1	0	0
10	o	1	Total K 1 1	0	0
10	p	3	Total K 3 3	0	0
10	q	2	Total K 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	r	1	Total	K	0	0
			1	1		
10	u	1	Total	K	0	0
			1	1		
10	v	7	Total	K	0	0
			7	7		

- Molecule 11 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			8	4	4		
11	E	1	Total	Fe	S	0	0
			8	4	4		
11	E	1	Total	Fe	S	0	0
			8	4	4		
11	F	1	Total	Fe	S	0	0
			8	4	4		
11	F	1	Total	Fe	S	0	0
			8	4	4		
11	F	1	Total	Fe	S	0	0
			8	4	4		
11	F	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	F	1	Total 8	Fe 4	S 4	0	0
11	F	1	Total 8	Fe 4	S 4	0	0
11	F	1	Total 8	Fe 4	S 4	0	0
11	F	1	Total 8	Fe 4	S 4	0	0
11	H	1	Total 8	Fe 4	S 4	0	0
11	K	1	Total 8	Fe 4	S 4	0	0
11	K	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	L	1	Total 8	Fe 4	S 4	0	0
11	N	1	Total 8	Fe 4	S 4	0	0
11	Q	1	Total 8	Fe 4	S 4	0	0
11	Q	1	Total 8	Fe 4	S 4	0	0
11	R	1	Total 8	Fe 4	S 4	0	0
11	R	1	Total 8	Fe 4	S 4	0	0
11	R	1	Total 8	Fe 4	S 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	R	1	Total 8	Fe 4	S 4	0	0
11	R	1	Total 8	Fe 4	S 4	0	0
11	R	1	Total 8	Fe 4	S 4	0	0
11	R	1	Total 8	Fe 4	S 4	0	0
11	R	1	Total 8	Fe 4	S 4	0	0
11	R	1	Total 8	Fe 4	S 4	0	0
11	T	1	Total 8	Fe 4	S 4	0	0
11	W	1	Total 8	Fe 4	S 4	0	0
11	W	1	Total 8	Fe 4	S 4	0	0
11	X	1	Total 8	Fe 4	S 4	0	0
11	X	1	Total 8	Fe 4	S 4	0	0
11	X	1	Total 8	Fe 4	S 4	0	0
11	X	1	Total 8	Fe 4	S 4	0	0
11	X	1	Total 8	Fe 4	S 4	0	0
11	X	1	Total 8	Fe 4	S 4	0	0
11	X	1	Total 8	Fe 4	S 4	0	0
11	X	1	Total 8	Fe 4	S 4	0	0
11	X	1	Total 8	Fe 4	S 4	0	0
11	Z	1	Total 8	Fe 4	S 4	0	0
11	c	1	Total 8	Fe 4	S 4	0	0
11	c	1	Total 8	Fe 4	S 4	0	0
11	d	1	Total 8	Fe 4	S 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	d	1	Total 8	Fe 4	S 4	0	0
11	d	1	Total 8	Fe 4	S 4	0	0
11	d	1	Total 8	Fe 4	S 4	0	0
11	d	1	Total 8	Fe 4	S 4	0	0
11	d	1	Total 8	Fe 4	S 4	0	0
11	d	1	Total 8	Fe 4	S 4	0	0
11	d	1	Total 8	Fe 4	S 4	0	0
11	d	1	Total 8	Fe 4	S 4	0	0
11	f	1	Total 8	Fe 4	S 4	0	0
11	i	1	Total 8	Fe 4	S 4	0	0
11	i	1	Total 8	Fe 4	S 4	0	0
11	j	1	Total 8	Fe 4	S 4	0	0
11	j	1	Total 8	Fe 4	S 4	0	0
11	j	1	Total 8	Fe 4	S 4	0	0
11	j	1	Total 8	Fe 4	S 4	0	0
11	j	1	Total 8	Fe 4	S 4	0	0
11	j	1	Total 8	Fe 4	S 4	0	0
11	j	1	Total 8	Fe 4	S 4	0	0
11	j	1	Total 8	Fe 4	S 4	0	0
11	l	1	Total 8	Fe 4	S 4	0	0
11	o	1	Total 8	Fe 4	S 4	0	0

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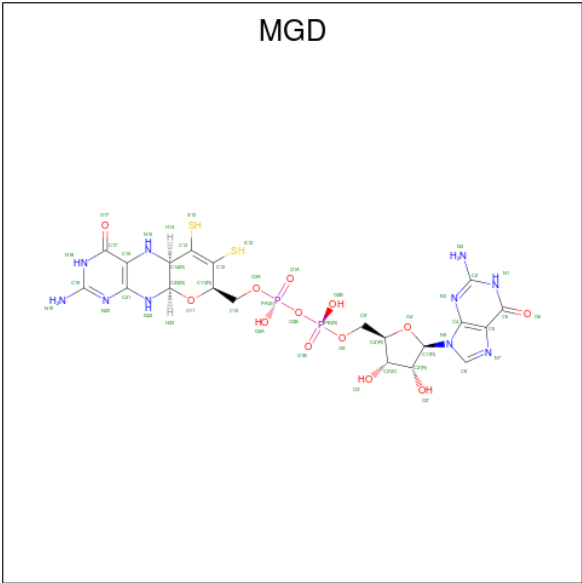
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	o	1	Total	Fe	S	0	0
			8	4	4		
11	p	1	Total	Fe	S	0	0
			8	4	4		
11	p	1	Total	Fe	S	0	0
			8	4	4		
11	p	1	Total	Fe	S	0	0
			8	4	4		
11	p	1	Total	Fe	S	0	0
			8	4	4		
11	p	1	Total	Fe	S	0	0
			8	4	4		
11	p	1	Total	Fe	S	0	0
			8	4	4		
11	p	1	Total	Fe	S	0	0
			8	4	4		
11	r	1	Total	Fe	S	0	0
			8	4	4		
11	u	1	Total	Fe	S	0	0
			8	4	4		
11	u	1	Total	Fe	S	0	0
			8	4	4		
11	v	1	Total	Fe	S	0	0
			8	4	4		
11	v	1	Total	Fe	S	0	0
			8	4	4		
11	v	1	Total	Fe	S	0	0
			8	4	4		
11	v	1	Total	Fe	S	0	0
			8	4	4		
11	v	1	Total	Fe	S	0	0
			8	4	4		
11	v	1	Total	Fe	S	0	0
			8	4	4		
11	v	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 12 is TUNGSTEN ION (CCD ID: W) (formula: W).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	1	Total	W	0	0
			1	1		
12	H	1	Total	W	0	0
			1	1		
12	N	1	Total	W	0	0
			1	1		
12	T	1	Total	W	0	0
			1	1		
12	Z	1	Total	W	0	0
			1	1		
12	f	1	Total	W	0	0
			1	1		
12	l	1	Total	W	0	0
			1	1		
12	r	1	Total	W	0	0
			1	1		

- Molecule 13 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-O XA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



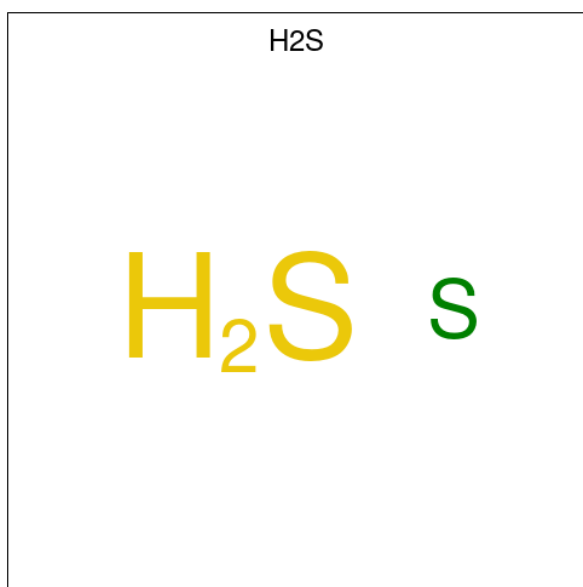
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	B	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	B	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	H	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	H	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	N	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	N	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	T	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	T	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	Z	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	Z	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	f	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	f	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	l	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	l	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	r	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
13	r	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 14 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H₂S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total S 1 1	0	0
14	H	1	Total S 1 1	0	0
14	N	1	Total S 1 1	0	0
14	T	1	Total S 1 1	0	0
14	Z	1	Total S 1 1	0	0
14	f	1	Total S 1 1	0	0
14	l	1	Total S 1 1	0	0
14	r	1	Total S 1 1	0	0

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total Mg 1 1	0	0
15	H	1	Total Mg 1 1	0	0
15	O	1	Total Mg 1 1	0	0
15	T	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	Z	1	Total 1	Mg 1	0	0
15	f	1	Total 1	Mg 1	0	0
15	l	1	Total 1	Mg 1	0	0
15	r	1	Total 1	Mg 1	0	0

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	N	1	Total 1	Cl 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	22	Total 22	O 22	0	0
17	B	12	Total 12	O 12	0	0
17	C	7	Total 7	O 7	0	0
17	D	2	Total 2	O 2	0	0
17	E	1	Total 1	O 1	0	0
17	F	25	Total 25	O 25	0	0
17	G	14	Total 14	O 14	0	0
17	H	20	Total 20	O 20	0	0
17	I	17	Total 17	O 17	0	0
17	J	4	Total 4	O 4	0	0
17	K	8	Total 8	O 8	0	0
17	L	26	Total 26	O 26	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	M	5	Total O 5 5	0	0
17	N	24	Total O 24 24	0	0
17	O	9	Total O 9 9	0	0
17	P	4	Total O 4 4	0	0
17	Q	2	Total O 2 2	0	0
17	R	6	Total O 6 6	0	0
17	S	59	Total O 59 59	0	0
17	T	29	Total O 29 29	0	0
17	U	10	Total O 10 10	0	0
17	V	9	Total O 9 9	0	0
17	W	3	Total O 3 3	0	0
17	X	19	Total O 19 19	0	0
17	Y	17	Total O 17 17	0	0
17	Z	19	Total O 19 19	0	0
17	a	12	Total O 12 12	0	0
17	b	4	Total O 4 4	0	0
17	c	3	Total O 3 3	0	0
17	d	3	Total O 3 3	0	0
17	e	40	Total O 40 40	0	0
17	f	21	Total O 21 21	0	0
17	g	3	Total O 3 3	0	0

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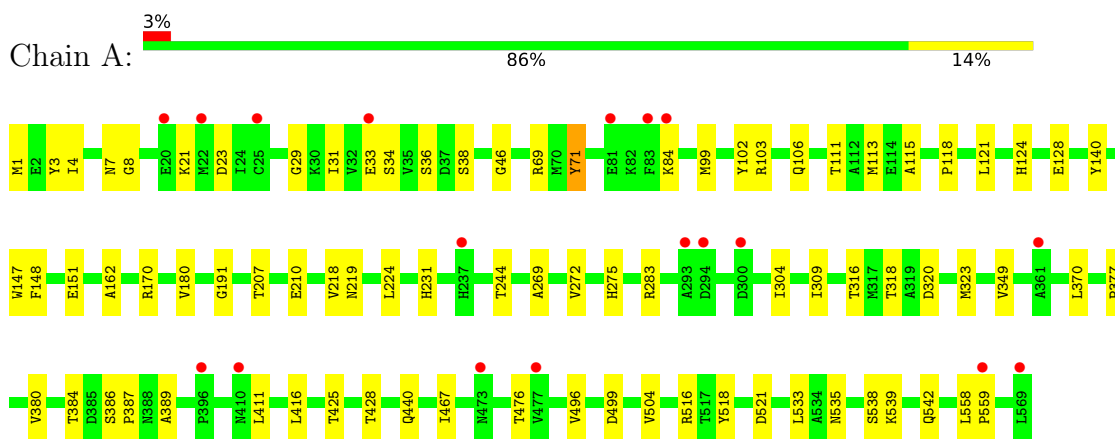
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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17	i	8	Total O 8 8	0	0
17	j	20	Total O 20 20	0	0
17	k	9	Total O 9 9	0	0
17	l	20	Total O 20 20	0	0
17	m	7	Total O 7 7	0	0
17	n	4	Total O 4 4	0	0
17	o	2	Total O 2 2	0	0
17	p	18	Total O 18 18	0	0
17	q	27	Total O 27 27	0	0
17	r	16	Total O 16 16	0	0
17	s	3	Total O 3 3	0	0
17	t	3	Total O 3 3	0	0
17	u	1	Total O 1 1	0	0
17	v	13	Total O 13 13	0	0

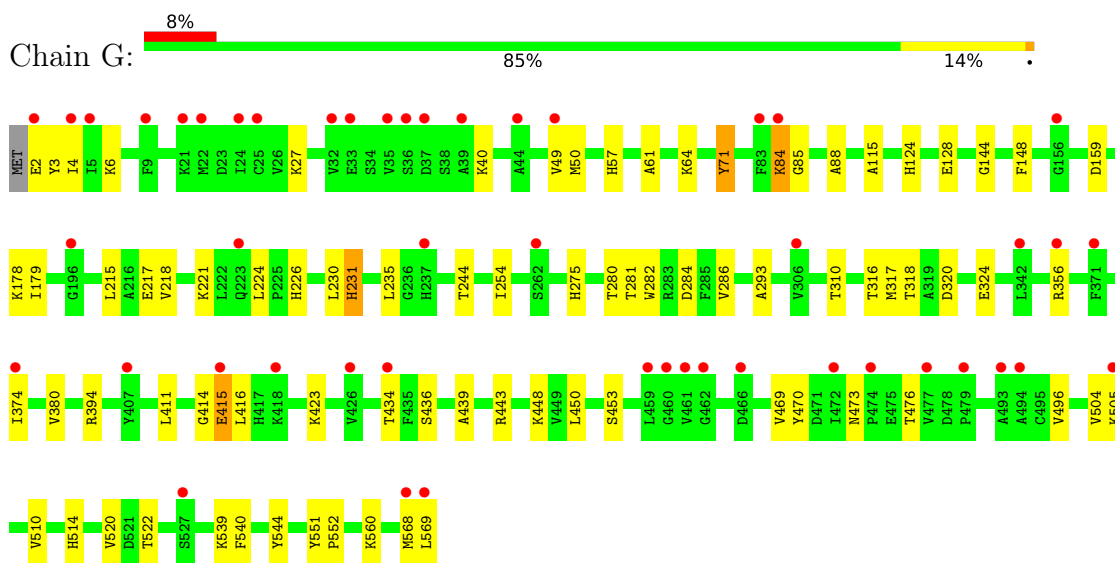
3 Residue-property plots [i](#)

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.

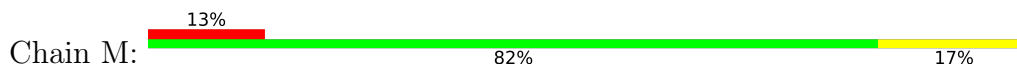
- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

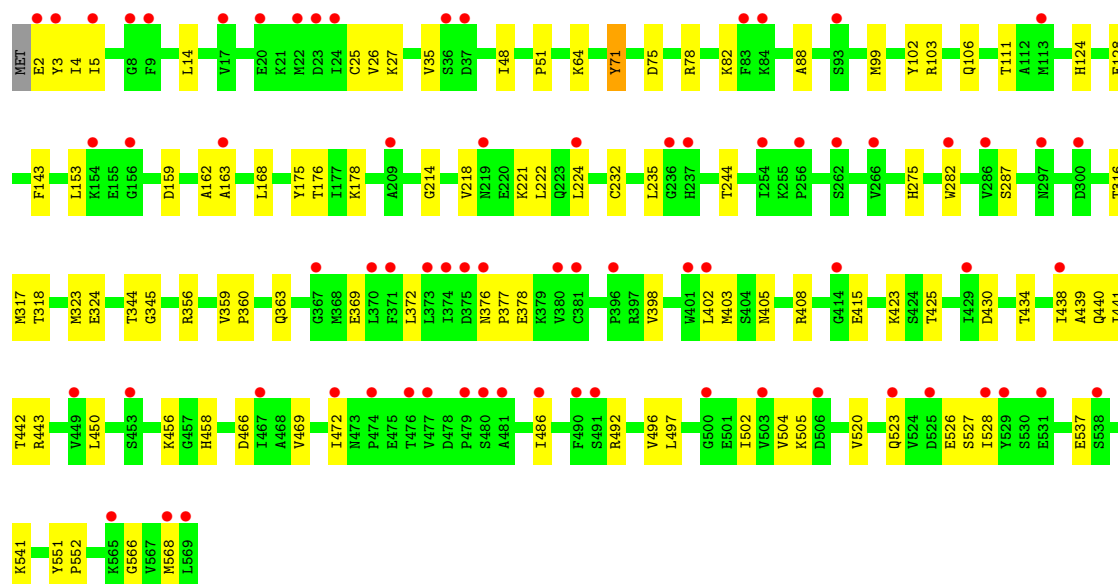


- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

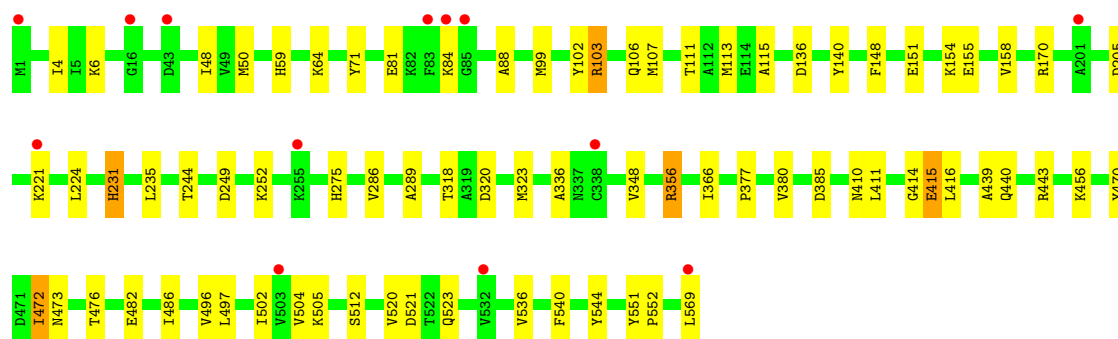
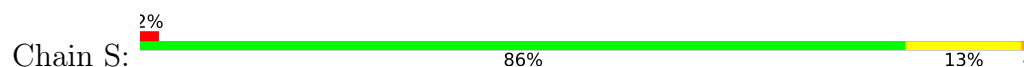


- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

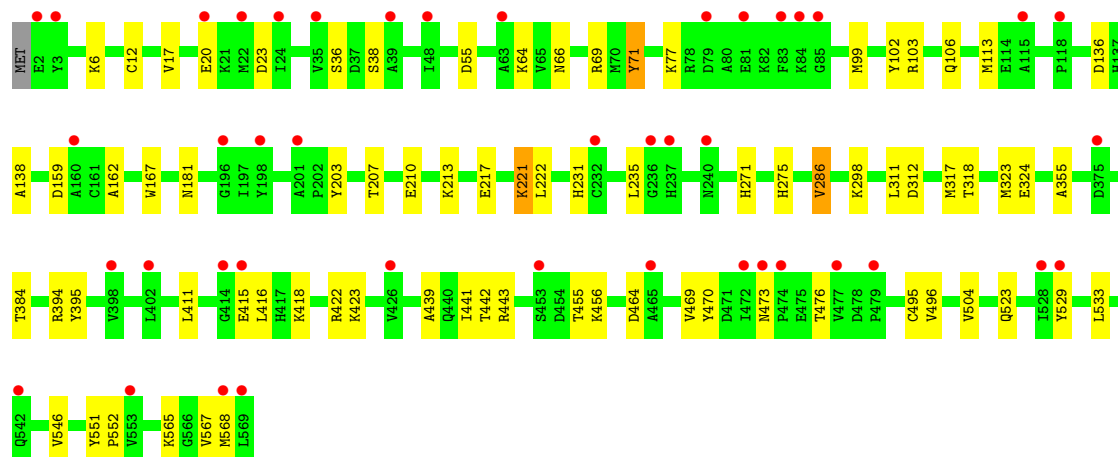
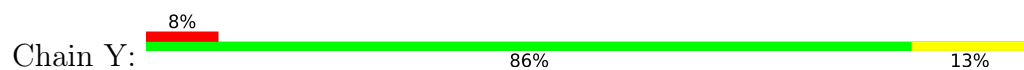




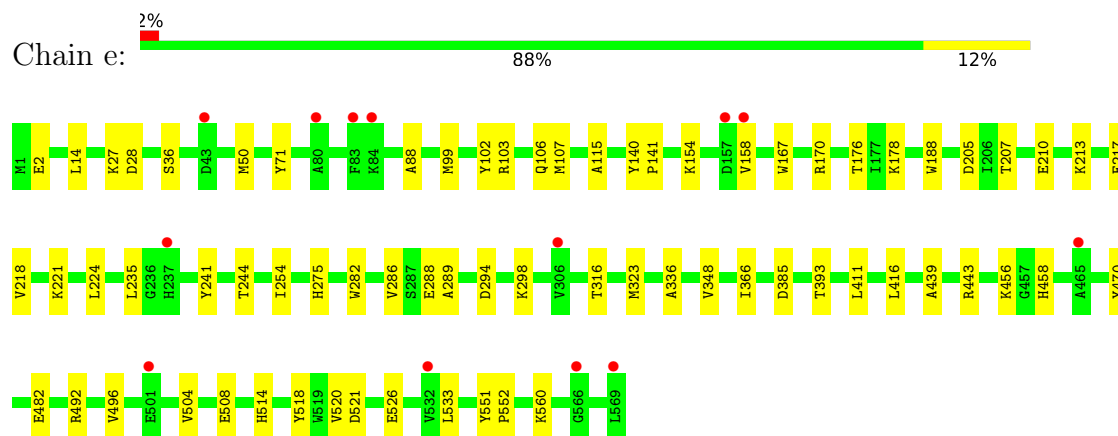
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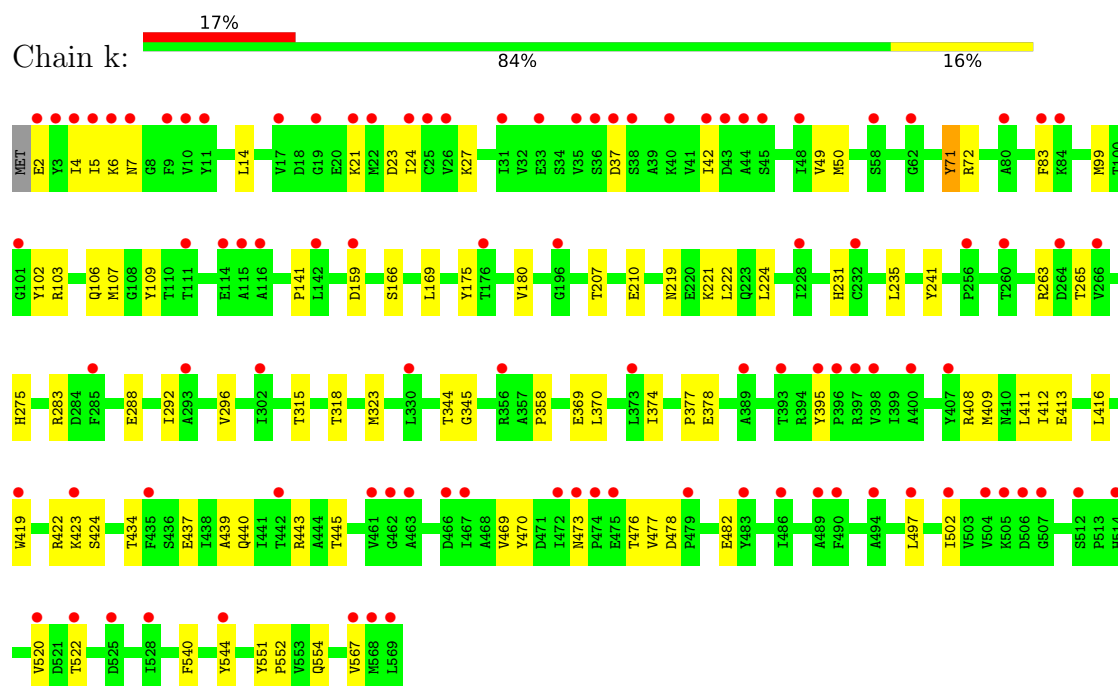
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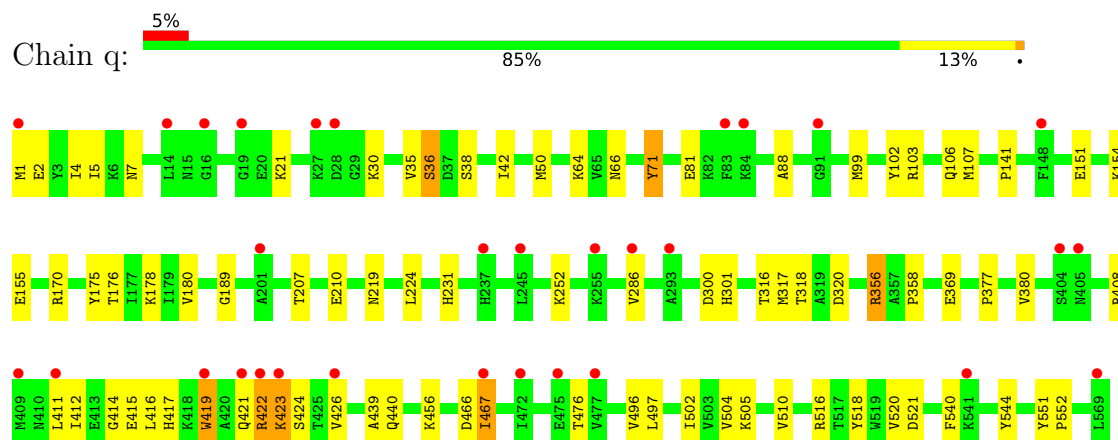
• Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA



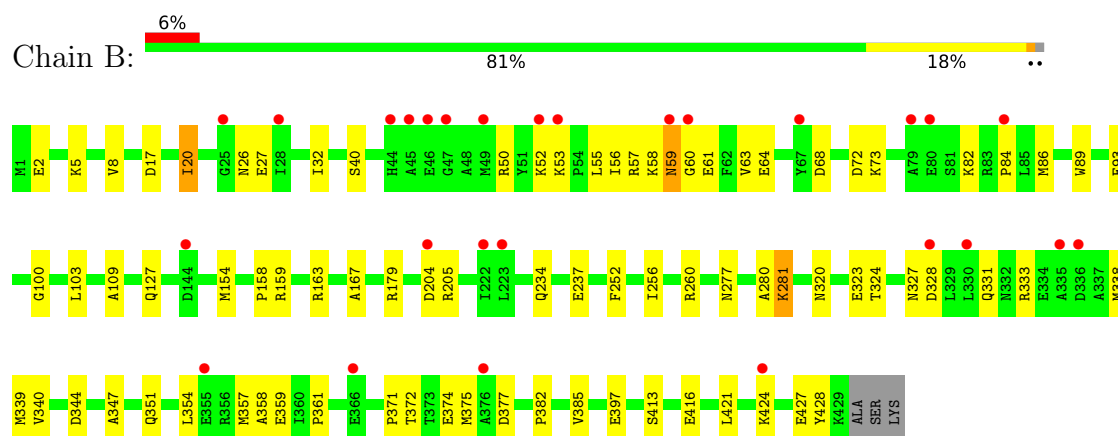
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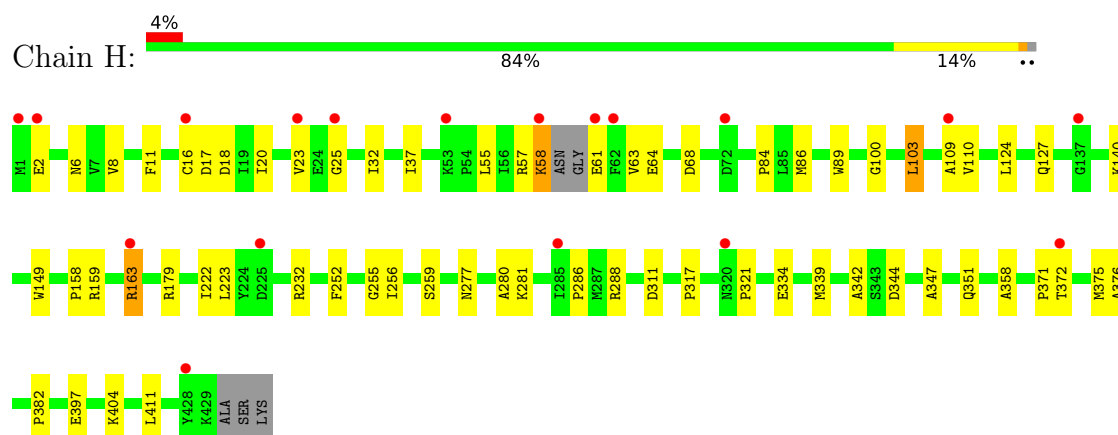
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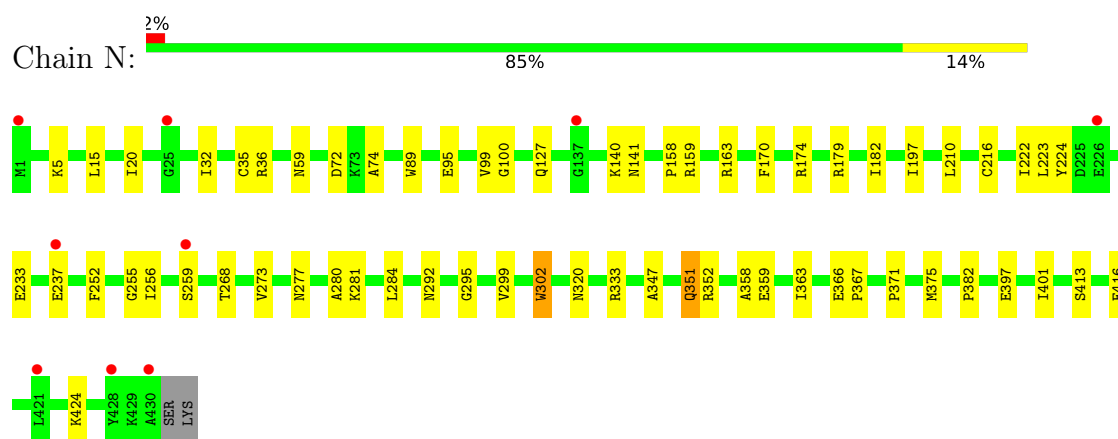
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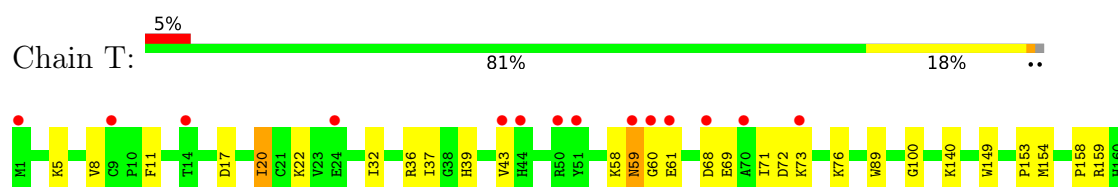
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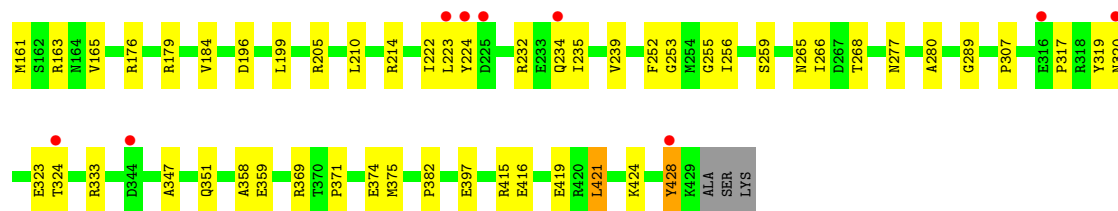


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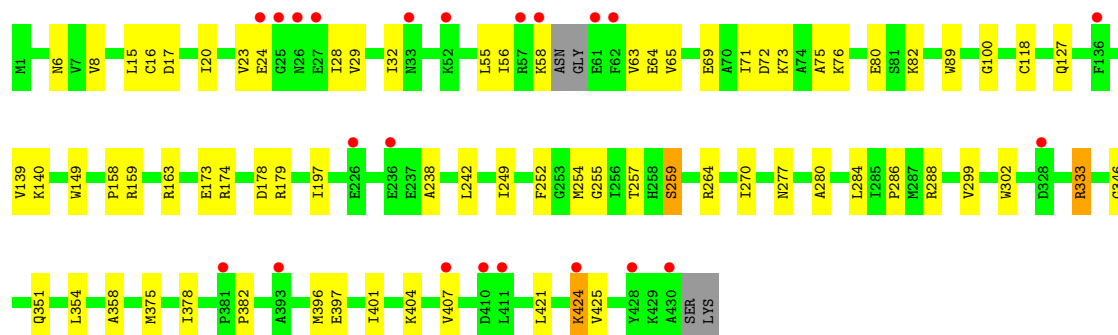
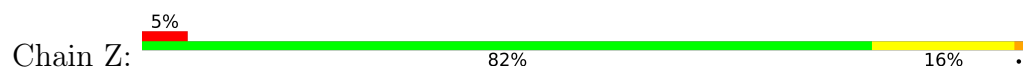


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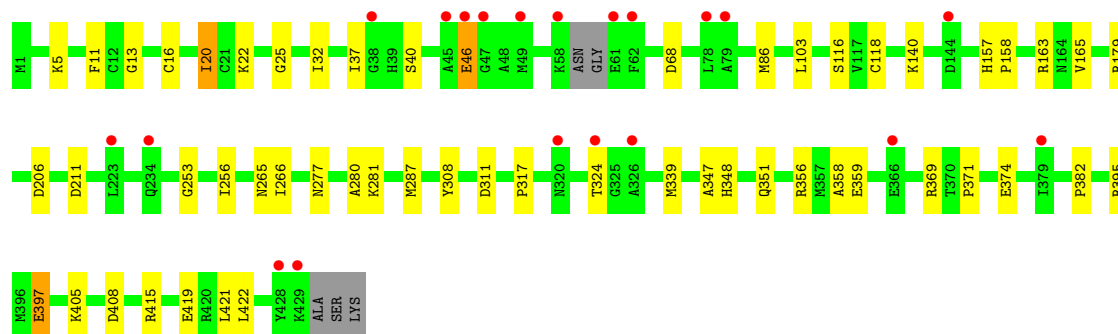
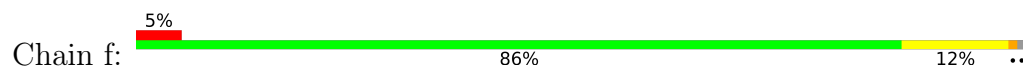




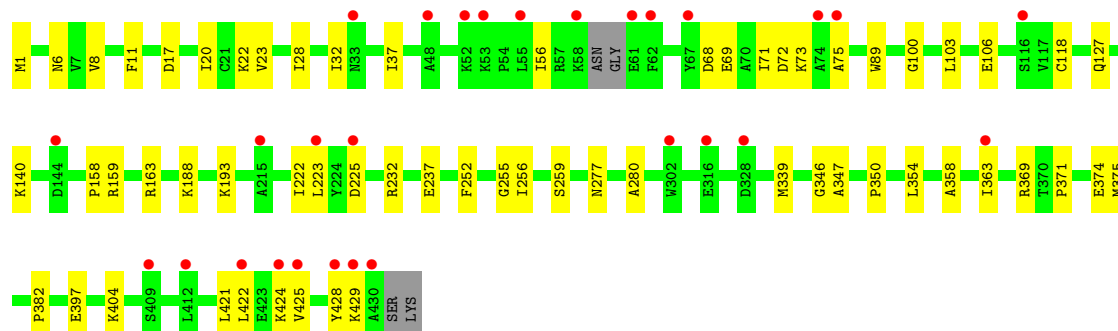
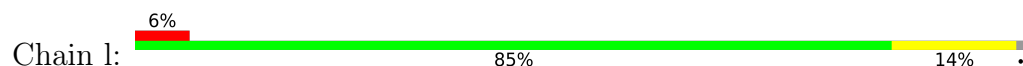
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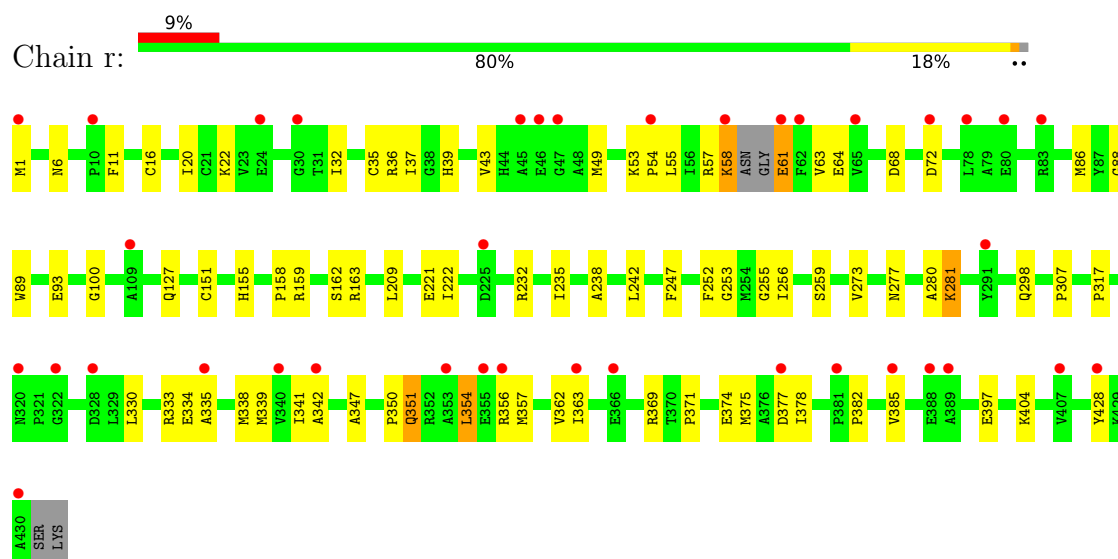
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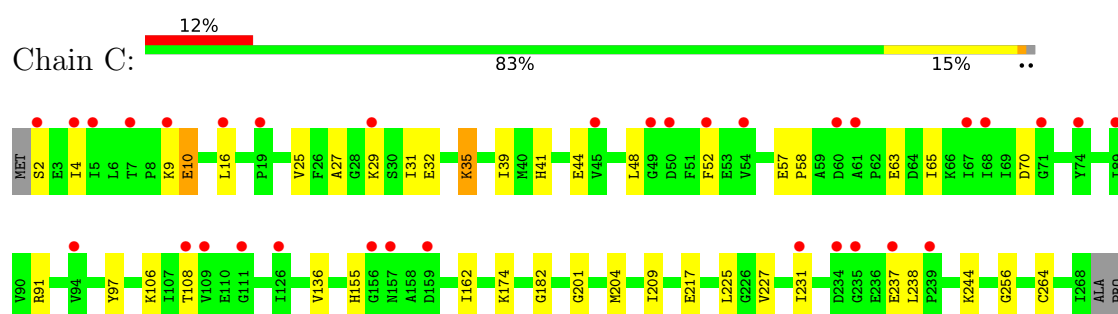
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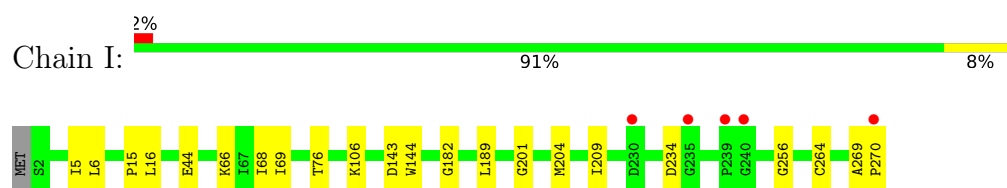
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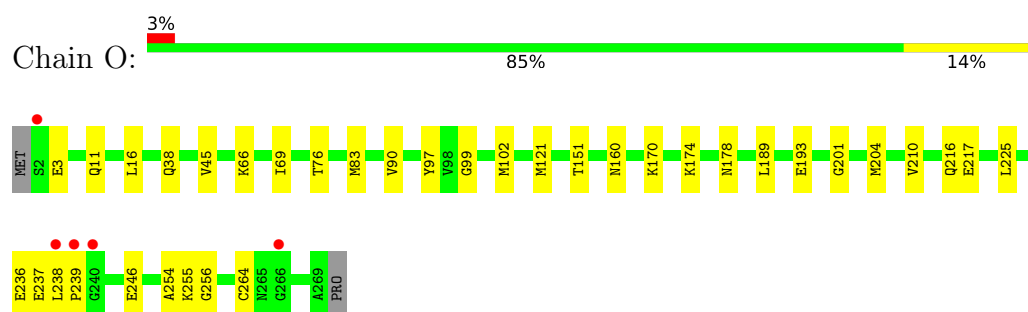
• Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C



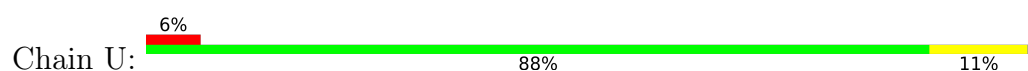
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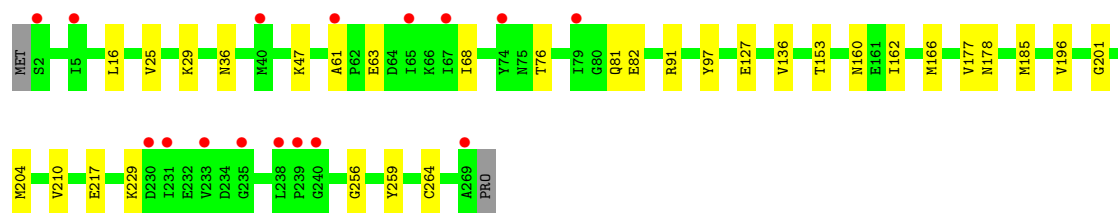


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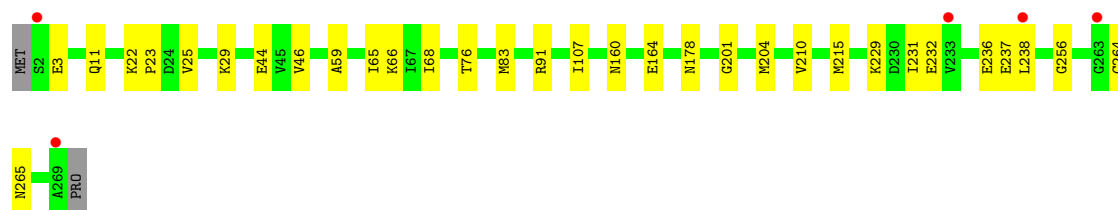
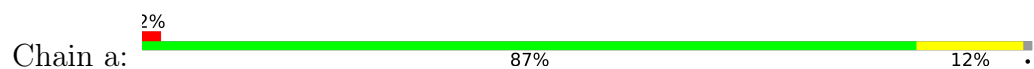


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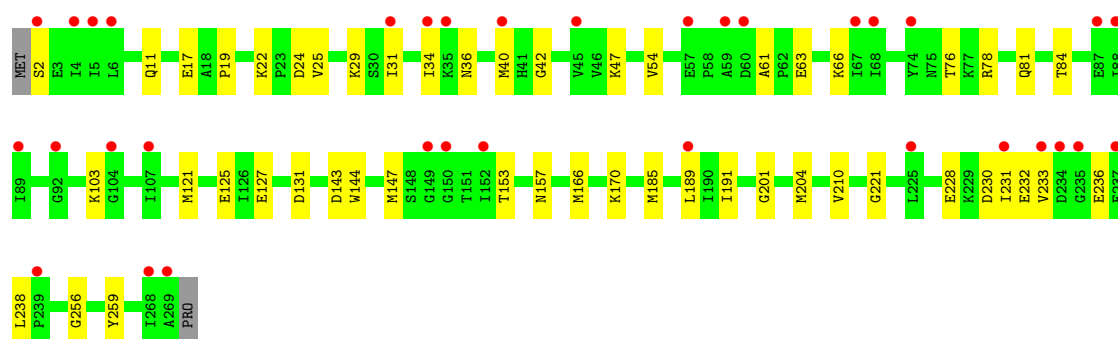
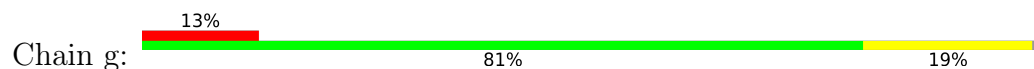




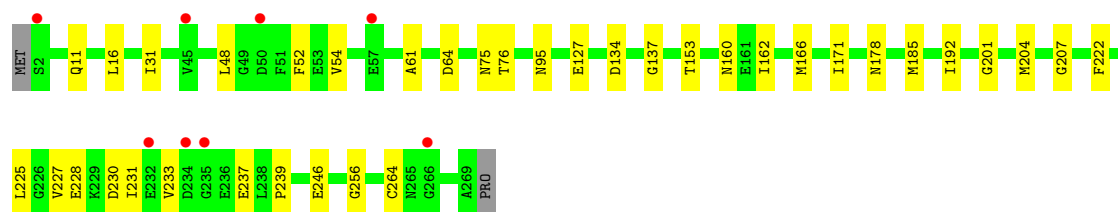
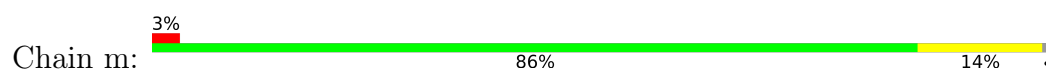
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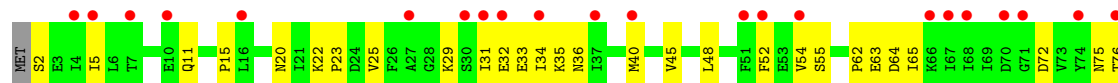
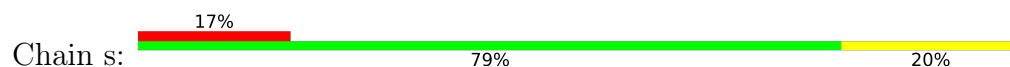
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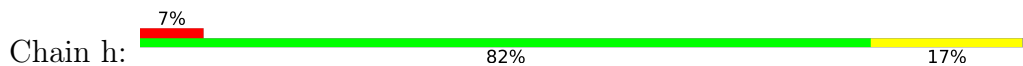


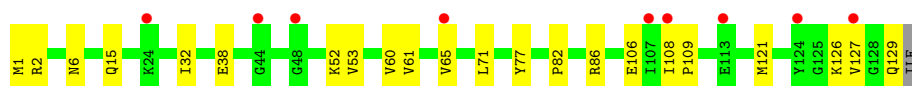
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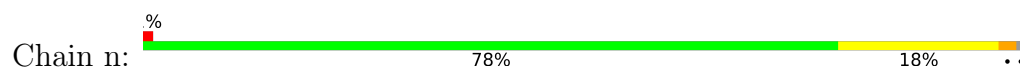
- Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C



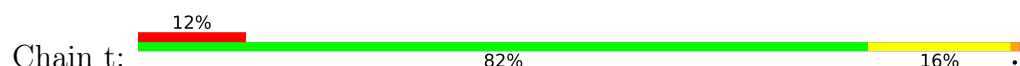




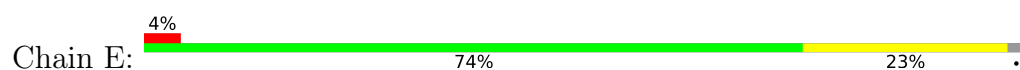
- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD



- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD



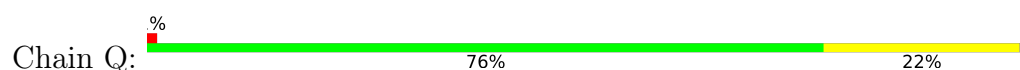
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



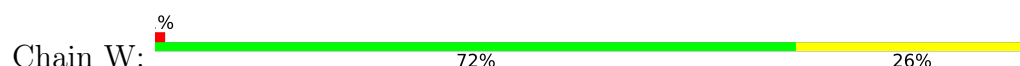
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



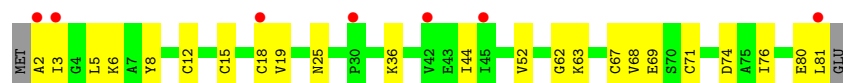
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



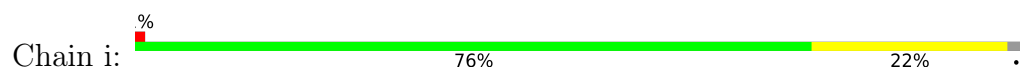
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



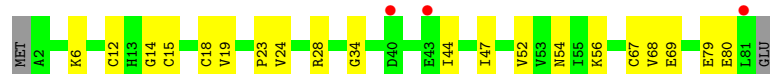
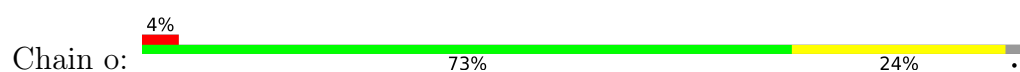
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



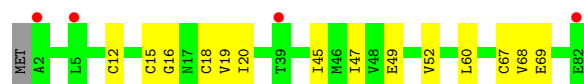
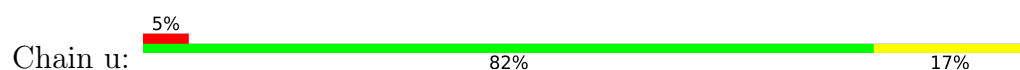
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



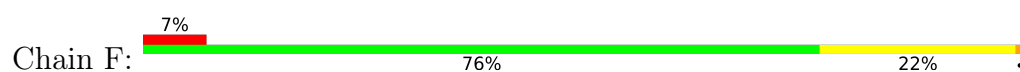
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



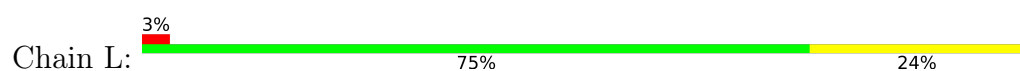
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG

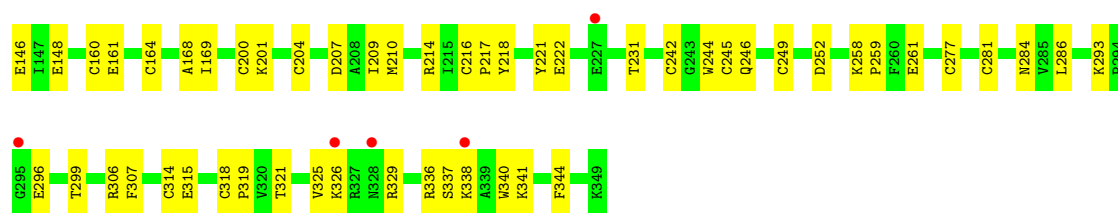


- Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF

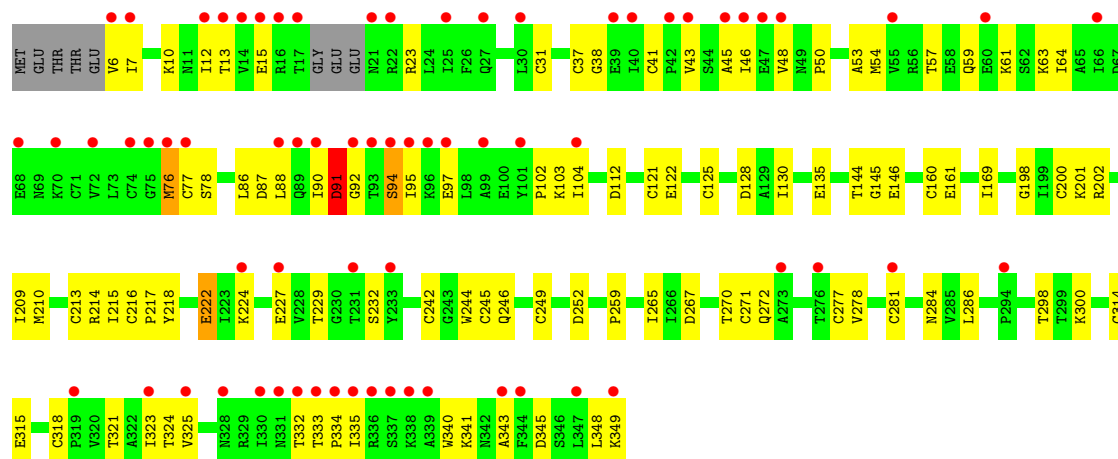


- Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF

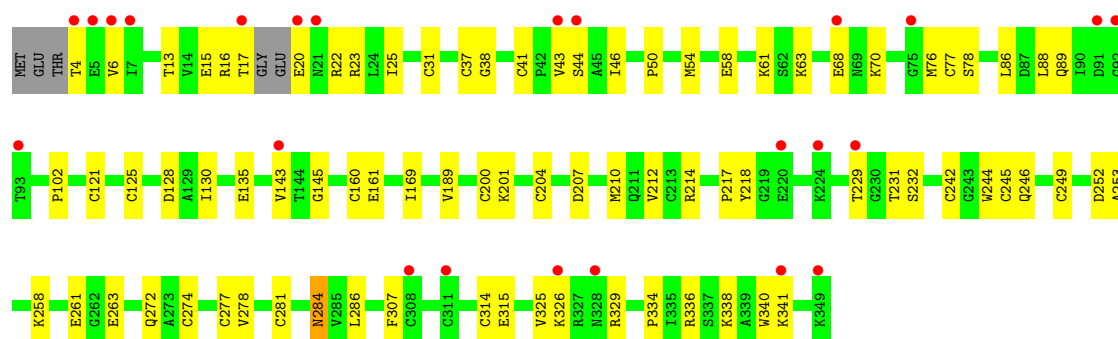
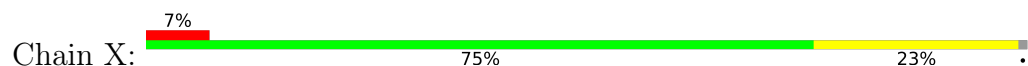




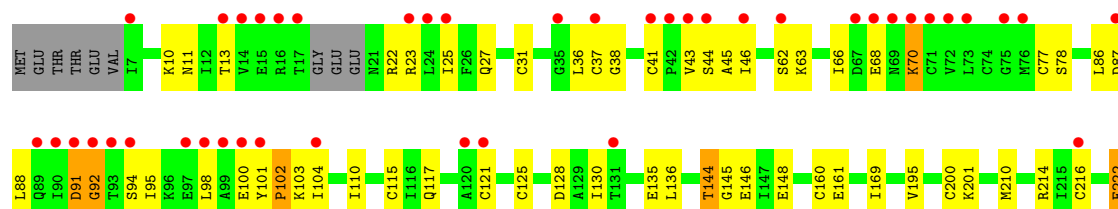
• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF

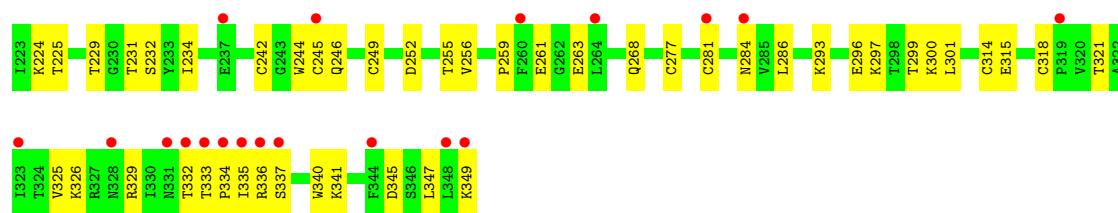


• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF

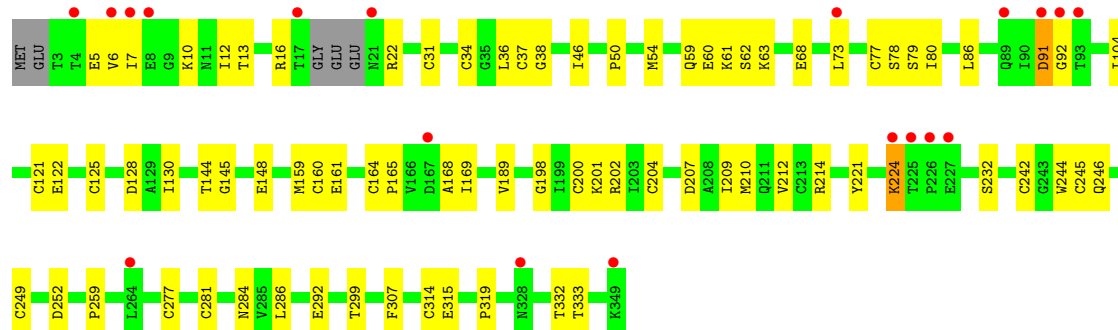
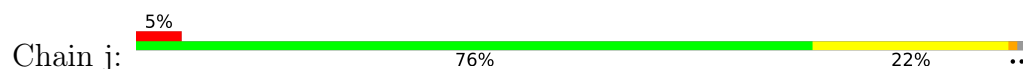


• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF

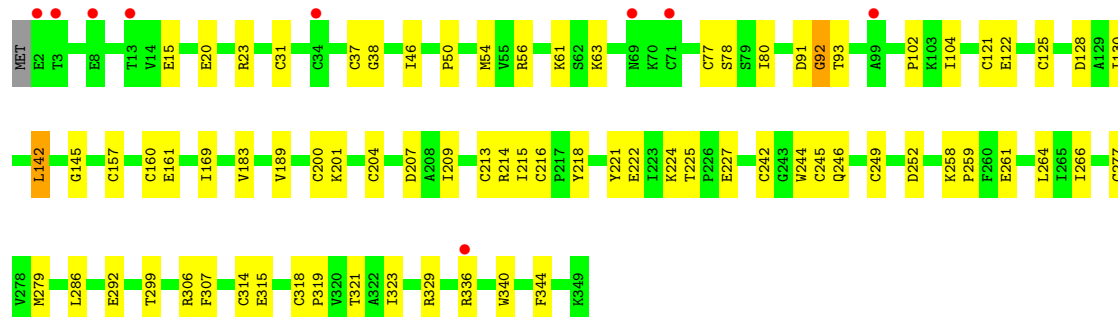
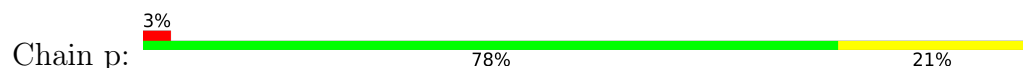




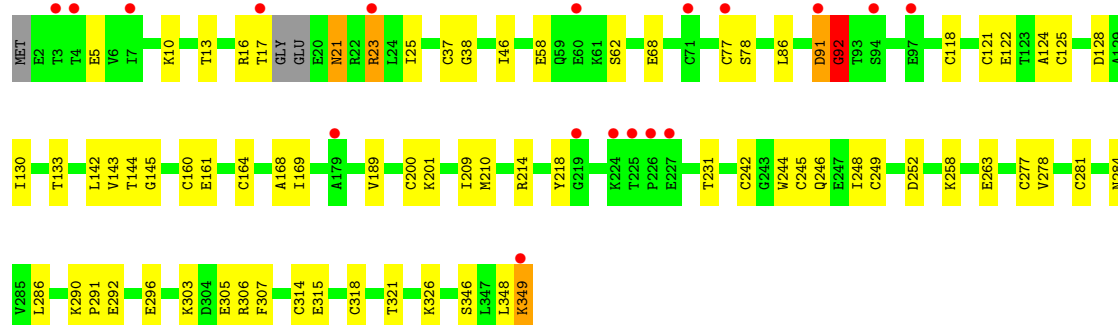
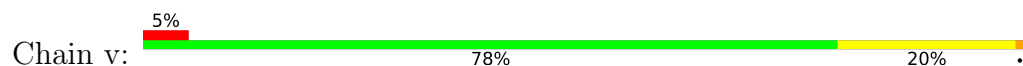
• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF



• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF



• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	174.18Å 173.68Å 183.16Å 89.98° 95.42° 92.14°	Depositor
Resolution (Å)	48.97 – 2.55 48.97 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.97-2.55) 96.7 (48.97-2.55)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.229 , 0.259 0.231 , 0.261	Depositor DCC
R_{free} test set	34086 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.118 for -h,k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	114321	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MFN, SF4, NA, ZN, K, MG, H2S, MGD, KCX, CL, W

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	0.35	4/4523 (0.1%)	0.49	0/6161
1	G	0.24	0/4515	0.50	0/6151
1	M	0.30	0/4515	0.57	0/6151
1	S	0.28	1/4523 (0.0%)	0.51	1/6161 (0.0%)
1	Y	0.27	1/4515 (0.0%)	0.56	2/6151 (0.0%)
1	e	0.23	0/4523	0.49	0/6161
1	k	0.27	0/4515	0.55	0/6151
1	q	0.41	4/4523 (0.1%)	0.62	10/6161 (0.2%)
2	B	0.24	0/3434	0.55	3/4647 (0.1%)
2	H	0.28	1/3421 (0.0%)	0.54	4/4628 (0.1%)
2	N	0.21	0/3439	0.53	0/4654
2	T	0.26	0/3434	0.54	1/4647 (0.0%)
2	Z	0.36	5/3426 (0.1%)	0.57	0/4635
2	f	0.24	1/3421 (0.0%)	0.50	0/4628
2	l	0.24	0/3426	0.53	1/4635 (0.0%)
2	r	0.39	5/3426 (0.1%)	0.61	6/4635 (0.1%)
3	C	0.29	0/2014	0.61	3/2710 (0.1%)
3	I	0.29	0/2027	0.50	0/2729
3	O	0.19	0/2019	0.48	0/2717
3	U	0.20	0/2019	0.51	0/2717
3	a	0.21	0/2019	0.53	0/2717
3	g	0.27	0/2019	0.59	2/2717 (0.1%)
3	m	0.21	0/2019	0.50	0/2717
3	s	0.29	0/2027	0.57	0/2729
4	D	0.21	0/1016	0.50	0/1379
4	J	0.19	0/1016	0.46	0/1379
4	P	0.18	0/1016	0.48	0/1379
4	V	0.18	0/1016	0.50	0/1379
4	b	0.19	0/1016	0.49	0/1379
4	h	0.21	0/1016	0.53	0/1379
4	n	0.26	0/1016	0.56	1/1379 (0.1%)
4	t	0.31	0/1016	0.62	1/1379 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	E	0.23	0/579	0.46	0/787
5	K	0.32	0/579	0.55	0/787
5	Q	0.23	0/579	0.51	0/787
5	W	0.19	0/579	0.49	0/787
5	c	0.18	0/579	0.50	0/787
5	i	0.21	0/579	0.53	0/787
5	o	0.22	0/579	0.45	0/787
5	u	0.21	0/588	0.53	0/799
6	F	0.25	0/2667	0.54	1/3616 (0.0%)
6	L	0.27	0/2695	0.56	1/3655 (0.0%)
6	R	0.32	0/2640	0.67	5/3579 (0.1%)
6	X	0.32	0/2665	0.64	4/3613 (0.1%)
6	d	0.36	0/2633	0.65	2/3569 (0.1%)
6	j	0.23	0/2663	0.56	1/3611 (0.0%)
6	p	0.27	0/2695	0.54	1/3655 (0.0%)
6	v	0.40	4/2681 (0.1%)	0.62	1/3635 (0.0%)
All	All	0.28	26/113850 (0.0%)	0.55	51/154383 (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	k	0	1
2	T	0	1
2	Z	0	1
6	F	0	1
6	L	0	1
6	R	0	1
6	d	0	1
6	p	0	1
6	v	0	1
All	All	0	9

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	558	LEU	CA-CB	10.60	1.68	1.53
1	q	423	LYS	CB-CG	-9.75	1.23	1.52
6	v	23	ARG	NE-CZ	-9.13	1.23	1.33
2	Z	333	ARG	NE-CZ	-8.82	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	r	58	LYS	CD-CE	-8.57	1.26	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	r	58	LYS	CD-CE-NZ	-14.10	66.79	111.90
6	v	92	GLY	N-CA-C	11.99	141.59	113.18
1	q	423	LYS	CB-CA-C	-9.25	95.67	110.85
6	X	58	GLU	CB-CA-C	8.71	124.58	110.29
4	t	1	MET	CA-CB-CG	8.01	130.11	114.10

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	91	ASP	Peptide
6	L	91	ASP	Peptide
6	R	91	ASP	Peptide
2	T	58	LYS	Peptide
2	Z	173	GLU	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	4419	0	4273	48	0
1	G	4411	0	4261	56	0
1	M	4411	0	4260	85	0
1	S	4419	0	4272	50	0
1	Y	4411	0	4260	79	0
1	e	4419	0	4272	39	1
1	k	4411	0	4260	70	0
1	q	4419	0	4272	75	0
2	B	3364	0	3307	62	0
2	H	3352	0	3297	41	0
2	N	3369	0	3312	41	0
2	T	3364	0	3307	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	3357	0	3302	56	0
2	f	3352	0	3297	37	0
2	l	3357	0	3302	50	0
2	r	3357	0	3300	67	0
3	C	1982	0	1950	35	0
3	I	1994	0	1962	15	0
3	O	1987	0	1955	31	0
3	U	1987	0	1955	20	0
3	a	1987	0	1955	21	0
3	g	1987	0	1955	54	0
3	m	1987	0	1955	25	0
3	s	1994	0	1962	43	0
4	D	997	0	1021	18	0
4	J	997	0	1022	17	0
4	P	997	0	1022	11	0
4	V	997	0	1022	8	0
4	b	997	0	1022	16	0
4	h	997	0	1022	14	0
4	n	997	0	1022	22	0
4	t	997	0	1022	24	0
5	E	572	0	567	15	0
5	K	572	0	567	14	0
5	Q	572	0	567	13	0
5	W	572	0	567	16	0
5	c	572	0	567	14	0
5	i	572	0	567	13	0
5	o	572	0	567	22	0
5	u	581	0	573	11	0
6	F	2629	0	2588	50	1
6	L	2656	0	2607	56	0
6	R	2602	0	2565	73	0
6	X	2627	0	2584	65	0
6	d	2595	0	2556	75	0
6	j	2625	0	2585	59	0
6	p	2656	0	2607	67	0
6	v	2643	0	2597	57	0
7	A	2	0	0	0	0
7	G	2	0	0	0	0
7	M	2	0	0	0	0
7	S	2	0	0	0	0
7	Y	2	0	0	0	0
7	e	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	k	2	0	0	0	0
7	q	2	0	0	0	0
8	A	53	0	37	0	0
8	G	53	0	37	2	0
8	M	53	0	37	3	0
8	S	53	0	37	3	0
8	Y	53	0	37	4	0
8	e	53	0	37	3	0
8	k	53	0	37	5	0
8	q	53	0	37	2	0
9	A	1	0	0	0	0
9	G	1	0	0	0	0
9	M	1	0	0	0	0
9	S	1	0	0	0	0
9	e	1	0	0	0	0
9	k	1	0	0	0	0
9	q	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	E	1	0	0	0	0
10	F	4	0	0	0	0
10	G	1	0	0	0	0
10	K	1	0	0	0	0
10	L	3	0	0	0	0
10	M	2	0	0	0	0
10	N	1	0	0	0	0
10	Q	1	0	0	0	0
10	R	3	0	0	0	0
10	S	2	0	0	0	0
10	T	1	0	0	0	0
10	X	3	0	0	0	0
10	Y	1	0	0	0	0
10	Z	1	0	0	0	0
10	c	1	0	0	0	0
10	d	2	0	0	0	0
10	e	4	0	0	0	0
10	i	1	0	0	0	0
10	j	6	0	0	0	0
10	k	1	0	0	0	0
10	o	1	0	0	0	0
10	p	3	0	0	0	0
10	q	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	r	1	0	0	0	0
10	u	1	0	0	0	0
10	v	7	0	0	0	0
11	B	8	0	0	0	0
11	E	16	0	0	1	0
11	F	72	0	0	0	0
11	H	8	0	0	0	0
11	K	16	0	0	0	0
11	L	64	0	0	0	0
11	N	8	0	0	0	0
11	Q	16	0	0	0	0
11	R	72	0	0	0	0
11	T	8	0	0	0	0
11	W	16	0	0	0	0
11	X	64	0	0	0	0
11	Z	8	0	0	0	0
11	c	16	0	0	0	0
11	d	72	0	0	0	0
11	f	8	0	0	0	0
11	i	16	0	0	1	0
11	j	64	0	0	0	0
11	l	8	0	0	0	0
11	o	16	0	0	0	0
11	p	72	0	0	0	0
11	r	8	0	0	0	0
11	u	16	0	0	0	0
11	v	64	0	0	0	0
12	B	1	0	0	0	0
12	H	1	0	0	0	0
12	N	1	0	0	0	0
12	T	1	0	0	0	0
12	Z	1	0	0	0	0
12	f	1	0	0	0	0
12	l	1	0	0	1	0
12	r	1	0	0	0	0
13	B	94	0	44	1	0
13	H	94	0	44	2	0
13	N	94	0	44	0	0
13	T	94	0	44	1	0
13	Z	94	0	44	1	0
13	f	94	0	44	0	0
13	l	94	0	44	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	r	94	0	44	1	0
14	B	1	0	0	0	0
14	H	1	0	0	0	0
14	N	1	0	0	0	0
14	T	1	0	0	0	0
14	Z	1	0	0	1	0
14	f	1	0	0	1	0
14	l	1	0	0	4	0
14	r	1	0	0	0	0
15	B	1	0	0	0	0
15	H	1	0	0	0	0
15	O	1	0	0	0	0
15	T	1	0	0	0	0
15	Z	1	0	0	0	0
15	f	1	0	0	0	0
15	l	1	0	0	0	0
15	r	1	0	0	0	0
16	N	1	0	0	1	0
17	A	22	0	0	1	0
17	B	12	0	0	0	0
17	C	7	0	0	0	0
17	D	2	0	0	1	0
17	E	1	0	0	0	0
17	F	25	0	0	0	0
17	G	14	0	0	0	0
17	H	20	0	0	0	0
17	I	17	0	0	1	0
17	J	4	0	0	0	0
17	K	8	0	0	1	0
17	L	26	0	0	0	0
17	M	5	0	0	0	0
17	N	24	0	0	0	0
17	O	9	0	0	0	0
17	P	4	0	0	0	0
17	Q	2	0	0	0	0
17	R	6	0	0	0	0
17	S	59	0	0	0	0
17	T	29	0	0	1	0
17	U	10	0	0	0	0
17	V	9	0	0	0	0
17	W	3	0	0	0	0
17	X	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Y	17	0	0	2	0
17	Z	19	0	0	0	0
17	a	12	0	0	0	0
17	b	4	0	0	0	0
17	c	3	0	0	0	0
17	d	3	0	0	1	0
17	e	40	0	0	0	0
17	f	21	0	0	1	0
17	g	3	0	0	0	0
17	h	3	0	0	0	0
17	i	8	0	0	0	0
17	j	20	0	0	1	0
17	k	9	0	0	0	0
17	l	20	0	0	0	0
17	m	7	0	0	0	0
17	n	4	0	0	0	0
17	o	2	0	0	0	0
17	p	18	0	0	1	0
17	q	27	0	0	1	0
17	r	16	0	0	0	0
17	s	3	0	0	0	0
17	t	3	0	0	0	0
17	u	1	0	0	0	0
17	v	13	0	0	0	0
All	All	114321	0	110257	1783	1

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 8.

The worst 5 of 1783 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)
3:g:170:LYS:NZ	3:g:189:LEU:CD2	1.87	1.37
1:Y:418:LYS:NZ	1:Y:422:ARG:NH1	1.72	1.34
1:Y:418:LYS:NZ	1:Y:422:ARG:HH11	0.89	1.33
1:Y:17:VAL:HG23	1:Y:20:GLU:OE1	1.15	1.27
2:l:106:GLU:O	2:l:429:LYS:NZ	1.68	1.26

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:336:ARG:NH1	1:e:526:GLU:OE1[1_544]	2.01	0.19

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	566/569 (100%)	540 (95%)	25 (4%)	1 (0%)	43	56
1	G	565/569 (99%)	538 (95%)	25 (4%)	2 (0%)	30	39
1	M	565/569 (99%)	542 (96%)	23 (4%)	0	100	100
1	S	566/569 (100%)	540 (95%)	25 (4%)	1 (0%)	43	56
1	Y	565/569 (99%)	539 (95%)	26 (5%)	0	100	100
1	e	566/569 (100%)	542 (96%)	24 (4%)	0	100	100
1	k	565/569 (99%)	540 (96%)	25 (4%)	0	100	100
1	q	566/569 (100%)	542 (96%)	24 (4%)	0	100	100
2	B	427/432 (99%)	407 (95%)	18 (4%)	2 (0%)	24	34
2	H	423/432 (98%)	405 (96%)	16 (4%)	2 (0%)	24	34
2	N	428/432 (99%)	413 (96%)	13 (3%)	2 (0%)	24	34
2	T	427/432 (99%)	409 (96%)	14 (3%)	4 (1%)	14	20
2	Z	424/432 (98%)	409 (96%)	14 (3%)	1 (0%)	43	56
2	f	423/432 (98%)	405 (96%)	16 (4%)	2 (0%)	24	34
2	l	424/432 (98%)	408 (96%)	15 (4%)	1 (0%)	43	56
2	r	424/432 (98%)	409 (96%)	13 (3%)	2 (0%)	24	34
3	C	265/270 (98%)	256 (97%)	9 (3%)	0	100	100
3	I	267/270 (99%)	258 (97%)	9 (3%)	0	100	100
3	O	266/270 (98%)	257 (97%)	9 (3%)	0	100	100
3	U	266/270 (98%)	257 (97%)	9 (3%)	0	100	100
3	a	266/270 (98%)	257 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	g	266/270 (98%)	257 (97%)	9 (3%)	0	100	100
3	m	266/270 (98%)	256 (96%)	10 (4%)	0	100	100
3	s	267/270 (99%)	258 (97%)	9 (3%)	0	100	100
4	D	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	J	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	P	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	V	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	b	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	h	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	n	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	t	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
5	E	78/82 (95%)	78 (100%)	0	0	100	100
5	K	78/82 (95%)	78 (100%)	0	0	100	100
5	Q	78/82 (95%)	78 (100%)	0	0	100	100
5	W	78/82 (95%)	78 (100%)	0	0	100	100
5	c	78/82 (95%)	78 (100%)	0	0	100	100
5	i	78/82 (95%)	78 (100%)	0	0	100	100
5	o	78/82 (95%)	78 (100%)	0	0	100	100
5	u	79/82 (96%)	79 (100%)	0	0	100	100
6	F	341/349 (98%)	337 (99%)	3 (1%)	1 (0%)	36	45
6	L	346/349 (99%)	340 (98%)	5 (1%)	1 (0%)	36	45
6	R	337/349 (97%)	330 (98%)	7 (2%)	0	100	100
6	X	340/349 (97%)	336 (99%)	4 (1%)	0	100	100
6	d	336/349 (96%)	331 (98%)	3 (1%)	2 (1%)	21	29
6	j	340/349 (97%)	336 (99%)	4 (1%)	0	100	100
6	p	346/349 (99%)	342 (99%)	3 (1%)	1 (0%)	36	45
6	v	342/349 (98%)	337 (98%)	4 (1%)	1 (0%)	36	45
All	All	14422/14656 (98%)	13934 (97%)	462 (3%)	26 (0%)	43	56

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	LYS

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Mol	Chain	Res	Type
6	F	92	GLY
1	G	415	GLU
6	L	92	GLY
1	S	415	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	470/470 (100%)	467 (99%)	3 (1%)	78	87
1	G	469/470 (100%)	466 (99%)	3 (1%)	78	87
1	M	469/470 (100%)	468 (100%)	1 (0%)	87	93
1	S	470/470 (100%)	463 (98%)	7 (2%)	57	74
1	Y	469/470 (100%)	467 (100%)	2 (0%)	84	90
1	e	470/470 (100%)	467 (99%)	3 (1%)	78	87
1	k	469/470 (100%)	468 (100%)	1 (0%)	87	93
1	q	470/470 (100%)	466 (99%)	4 (1%)	70	82
2	B	359/361 (99%)	355 (99%)	4 (1%)	65	79
2	H	358/361 (99%)	354 (99%)	4 (1%)	65	79
2	N	359/361 (99%)	355 (99%)	4 (1%)	65	79
2	T	359/361 (99%)	355 (99%)	4 (1%)	65	79
2	Z	358/361 (99%)	354 (99%)	4 (1%)	65	79
2	f	358/361 (99%)	353 (99%)	5 (1%)	59	75
2	l	358/361 (99%)	357 (100%)	1 (0%)	86	92
2	r	358/361 (99%)	354 (99%)	4 (1%)	65	79
3	C	202/204 (99%)	200 (99%)	2 (1%)	68	80
3	I	203/204 (100%)	201 (99%)	2 (1%)	68	80
3	O	202/204 (99%)	200 (99%)	2 (1%)	68	80
3	U	202/204 (99%)	201 (100%)	1 (0%)	81	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	a	202/204 (99%)	198 (98%)	4 (2%)	48	67
3	g	202/204 (99%)	201 (100%)	1 (0%)	81	88
3	m	202/204 (99%)	200 (99%)	2 (1%)	68	80
3	s	203/204 (100%)	199 (98%)	4 (2%)	48	67
4	D	110/111 (99%)	109 (99%)	1 (1%)	70	82
4	J	110/111 (99%)	109 (99%)	1 (1%)	70	82
4	P	110/111 (99%)	110 (100%)	0	100	100
4	V	110/111 (99%)	108 (98%)	2 (2%)	51	70
4	b	110/111 (99%)	110 (100%)	0	100	100
4	h	110/111 (99%)	109 (99%)	1 (1%)	70	82
4	n	110/111 (99%)	108 (98%)	2 (2%)	51	70
4	t	110/111 (99%)	110 (100%)	0	100	100
5	E	65/67 (97%)	65 (100%)	0	100	100
5	K	65/67 (97%)	64 (98%)	1 (2%)	57	74
5	Q	65/67 (97%)	65 (100%)	0	100	100
5	W	65/67 (97%)	63 (97%)	2 (3%)	35	53
5	c	65/67 (97%)	64 (98%)	1 (2%)	57	74
5	i	65/67 (97%)	64 (98%)	1 (2%)	57	74
5	o	65/67 (97%)	65 (100%)	0	100	100
5	u	66/67 (98%)	65 (98%)	1 (2%)	57	74
6	F	308/312 (99%)	302 (98%)	6 (2%)	50	69
6	L	311/312 (100%)	309 (99%)	2 (1%)	78	87
6	R	305/312 (98%)	302 (99%)	3 (1%)	68	80
6	X	308/312 (99%)	305 (99%)	3 (1%)	68	80
6	d	304/312 (97%)	301 (99%)	3 (1%)	68	80
6	j	308/312 (99%)	305 (99%)	3 (1%)	68	80
6	p	311/312 (100%)	308 (99%)	3 (1%)	68	80
6	v	310/312 (99%)	305 (98%)	5 (2%)	55	73
All	All	12107/12200 (99%)	11994 (99%)	113 (1%)	70	82

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	X	284	ASN
6	v	142	LEU
6	d	222	GLU
6	v	58	GLU
2	r	221	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
3	m	38	GLN
3	s	155	HIS
6	p	331	ASN
1	q	299	ASN
1	S	299	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	KCX	G	178	7,1	10,11,12	2.13	1 (10%)	6,12,14	1.70	1 (16%)
1	KCX	k	178	7,1	10,11,12	0.60	0	6,12,14	0.79	0
1	KCX	A	178	7,1	10,11,12	0.58	0	6,12,14	0.69	0
1	KCX	Y	178	7,1	10,11,12	0.60	0	6,12,14	0.72	0
1	KCX	q	178	7,1	10,11,12	2.16	1 (10%)	6,12,14	1.38	1 (16%)
1	KCX	e	178	7,1	10,11,12	2.15	1 (10%)	6,12,14	1.73	1 (16%)
1	KCX	M	178	7,1	10,11,12	2.17	1 (10%)	6,12,14	1.51	1 (16%)
1	KCX	S	178	7,1	10,11,12	0.66	0	6,12,14	0.68	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	KCX	G	178	7,1	-	0/9/10/12	-
1	KCX	k	178	7,1	-	0/9/10/12	-
1	KCX	A	178	7,1	-	1/9/10/12	-
1	KCX	Y	178	7,1	-	0/9/10/12	-
1	KCX	q	178	7,1	-	0/9/10/12	-
1	KCX	e	178	7,1	-	0/9/10/12	-
1	KCX	M	178	7,1	-	0/9/10/12	-
1	KCX	S	178	7,1	-	0/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	178	KCX	OQ1-CX	6.47	1.33	1.21
1	q	178	KCX	OQ1-CX	6.44	1.33	1.21
1	e	178	KCX	OQ1-CX	6.35	1.33	1.21
1	G	178	KCX	OQ1-CX	6.33	1.33	1.21

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	178	KCX	OQ1-CX-NZ	-4.15	118.61	124.92
1	G	178	KCX	OQ1-CX-NZ	-4.04	118.78	124.92
1	M	178	KCX	OQ1-CX-NZ	-3.59	119.47	124.92
1	q	178	KCX	OQ1-CX-NZ	-3.16	120.11	124.92

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	178	KCX	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 221 ligands modelled in this entry, 97 are monoatomic and 8 are modelled with single atom - leaving 116 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	$\# Z > 2$
11	SF4	F	406	6	0,12,12	-	-	-		
11	SF4	d	408	6	0,12,12	-	-	-		
13	MGD	H	503	12	47,52,52	1.40	7 (14%)	58,81,81	1.88	13 (22%)
11	SF4	j	504	6	0,12,12	-	-	-		
11	SF4	X	501	6	0,12,12	-	-	-		
11	SF4	o	102	5	0,12,12	-	-	-		
8	MFN	Y	603	7	54,54,56	1.86	8 (14%)	63,71,73	2.39	16 (25%)
11	SF4	R	405	6	0,12,12	-	-	-		
11	SF4	p	407	6	0,12,12	-	-	-		
11	SF4	d	401	6	0,12,12	-	-	-		
13	MGD	r	504	12	47,52,52	1.48	7 (14%)	58,81,81	2.06	13 (22%)
11	SF4	j	507	6	0,12,12	-	-	-		
11	SF4	F	401	6	0,12,12	-	-	-		
13	MGD	T	504	12	47,52,52	1.47	7 (14%)	58,81,81	2.14	13 (22%)
13	MGD	Z	504	12	47,52,52	1.48	7 (14%)	58,81,81	2.10	15 (25%)
11	SF4	X	508	6	0,12,12	-	-	-		
11	SF4	j	505	6	0,12,12	-	-	-		
11	SF4	F	402	6	0,12,12	-	-	-		
11	SF4	u	101	5	0,12,12	-	-	-		
11	SF4	j	503	6	0,12,12	-	-	-		
11	SF4	E	102	5	0,12,12	-	-	-		
11	SF4	p	401	6	0,12,12	-	-	-		
11	SF4	v	508	6	0,12,12	-	-	-		
11	SF4	L	504	6	0,12,12	-	-	-		
11	SF4	F	408	6	0,12,12	-	-	-		
11	SF4	d	409	6	0,12,12	-	-	-		
11	SF4	v	505	6	0,12,12	-	-	-		
13	MGD	f	503	12	47,52,52	1.43	7 (14%)	58,81,81	1.86	11 (18%)
11	SF4	K	102	5	0,12,12	-	-	-		
11	SF4	H	501	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SF4	p	402	6	0,12,12	-	-	-		
11	SF4	d	407	6	0,12,12	-	-	-		
11	SF4	X	507	6	0,12,12	-	-	-		
11	SF4	R	401	6	0,12,12	-	-	-		
8	MFN	M	603	7	54,54,56	1.88	8 (14%)	63,71,73	2.44	20 (31%)
11	SF4	L	502	6	0,12,12	-	-	-		
11	SF4	L	508	6	0,12,12	-	-	-		
13	MGD	l	503	12	47,52,52	1.41	7 (14%)	58,81,81	1.98	13 (22%)
11	SF4	X	504	6	0,12,12	-	-	-		
11	SF4	Z	501	2	0,12,12	-	-	-		
11	SF4	f	501	2	0,12,12	-	-	-		
13	MGD	r	503	12	47,52,52	1.41	6 (12%)	58,81,81	1.93	13 (22%)
11	SF4	i	101	5	0,12,12	-	-	-		
11	SF4	L	507	6	0,12,12	-	-	-		
11	SF4	v	503	6	0,12,12	-	-	-		
11	SF4	F	404	6	0,12,12	-	-	-		
11	SF4	d	404	6	0,12,12	-	-	-		
11	SF4	R	408	6	0,12,12	-	-	-		
11	SF4	F	409	6	0,12,12	-	-	-		
11	SF4	R	406	6	0,12,12	-	-	-		
11	SF4	v	504	6	0,12,12	-	-	-		
11	SF4	R	407	6	0,12,12	-	-	-		
11	SF4	v	506	6	0,12,12	-	-	-		
11	SF4	F	405	6	0,12,12	-	-	-		
11	SF4	R	402	6	0,12,12	-	-	-		
11	SF4	i	102	5	0,12,12	-	-	-		
13	MGD	N	503	12	47,52,52	1.37	4 (8%)	58,81,81	1.92	12 (20%)
8	MFN	k	603	7	54,54,56	1.87	9 (16%)	63,71,73	2.90	22 (34%)
11	SF4	R	404	6	0,12,12	-	-	-		
8	MFN	A	603	7	54,54,56	1.98	12 (22%)	63,71,73	2.17	15 (23%)
11	SF4	c	102	5	0,12,12	-	-	-		
8	MFN	G	603	7	54,54,56	1.86	8 (14%)	63,71,73	2.26	14 (22%)
11	SF4	N	501	2	0,12,12	-	-	-		
11	SF4	l	501	2	0,12,12	-	-	-		
11	SF4	j	502	6	0,12,12	-	-	-		
13	MGD	l	504	12	47,52,52	1.48	7 (14%)	58,81,81	2.07	14 (24%)
11	SF4	X	505	6	0,12,12	-	-	-		
11	SF4	Q	102	5	0,12,12	-	-	-		
11	SF4	p	408	6	0,12,12	-	-	-		
11	SF4	p	409	6	0,12,12	-	-	-		
11	SF4	Q	101	5	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SF4	E	101	5	0,12,12	-	-	-		
11	SF4	T	501	2	0,12,12	-	-	-		
11	SF4	p	406	6	0,12,12	-	-	-		
11	SF4	u	102	5	0,12,12	-	-	-		
11	SF4	R	409	6	0,12,12	-	-	-		
11	SF4	v	501	6	0,12,12	-	-	-		
11	SF4	K	101	5	0,12,12	-	-	-		
11	SF4	L	503	6	0,12,12	-	-	-		
11	SF4	c	101	5	0,12,12	-	-	-		
11	SF4	X	506	6	0,12,12	-	-	-		
11	SF4	d	405	6	0,12,12	-	-	-		
11	SF4	p	403	6	0,12,12	-	-	-		
11	SF4	W	201	5	0,12,12	-	-	-		
11	SF4	L	506	6	0,12,12	-	-	-		
11	SF4	d	402	6	0,12,12	-	-	-		
11	SF4	v	502	6	0,12,12	-	-	-		
11	SF4	B	501	2	0,12,12	-	-	-		
11	SF4	F	403	6	0,12,12	-	-	-		
13	MGD	Z	503	12	47,52,52	1.40	6 (12%)	58,81,81	1.97	13 (22%)
8	MFN	q	603	-	54,54,56	1.91	11 (20%)	63,71,73	2.18	14 (22%)
11	SF4	X	502	6	0,12,12	-	-	-		
11	SF4	d	406	6	0,12,12	-	-	-		
13	MGD	B	503	12	47,52,52	1.40	6 (12%)	58,81,81	1.96	13 (22%)
13	MGD	H	504	12	47,52,52	1.46	7 (14%)	58,81,81	2.10	11 (18%)
11	SF4	L	501	6	0,12,12	-	-	-		
11	SF4	o	101	5	0,12,12	-	-	-		
11	SF4	L	505	6	0,12,12	-	-	-		
11	SF4	v	507	6	0,12,12	-	-	-		
11	SF4	r	501	2	0,12,12	-	-	-		
13	MGD	f	504	12	47,52,52	1.46	8 (17%)	58,81,81	2.11	13 (22%)
11	SF4	j	506	6	0,12,12	-	-	-		
13	MGD	N	504	12	47,52,52	1.46	7 (14%)	58,81,81	2.06	14 (24%)
11	SF4	X	503	6	0,12,12	-	-	-		
11	SF4	F	407	6	0,12,12	-	-	-		
8	MFN	S	603	-	54,54,56	1.94	9 (16%)	63,71,73	2.23	16 (25%)
11	SF4	p	404	6	0,12,12	-	-	-		
11	SF4	d	403	6	0,12,12	-	-	-		
13	MGD	T	503	12	47,52,52	1.41	7 (14%)	58,81,81	1.90	13 (22%)
11	SF4	W	200	5	0,12,12	-	-	-		
13	MGD	B	504	12	47,52,52	1.47	8 (17%)	58,81,81	2.06	14 (24%)
11	SF4	p	405	6	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SF4	j	501	6	0,12,12	-	-	-		
11	SF4	R	403	6	0,12,12	-	-	-		
8	MFN	e	603	-	54,54,56	1.89	9 (16%)	63,71,73	2.42	13 (20%)
11	SF4	j	508	6	0,12,12	-	-	-		

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
11	SF4	F	406	6	-	-	0/6/5/5
13	MGD	H	503	12	-	8/22/66/66	0/6/6/6
11	SF4	d	408	6	-	-	0/6/5/5
11	SF4	j	504	6	-	-	0/6/5/5
11	SF4	X	501	6	-	-	0/6/5/5
11	SF4	o	102	5	-	-	0/6/5/5
8	MFN	Y	603	7	-	28/61/61/63	0/2/2/2
11	SF4	R	405	6	-	-	0/6/5/5
13	MGD	r	504	12	-	1/22/66/66	0/6/6/6
11	SF4	d	401	6	-	-	0/6/5/5
11	SF4	p	407	6	-	-	0/6/5/5
11	SF4	j	507	6	-	-	0/6/5/5
13	MGD	T	504	12	-	1/22/66/66	0/6/6/6
11	SF4	F	401	6	-	-	0/6/5/5
13	MGD	Z	504	12	-	1/22/66/66	0/6/6/6
11	SF4	X	508	6	-	-	0/6/5/5
11	SF4	j	505	6	-	-	0/6/5/5
11	SF4	F	402	6	-	-	0/6/5/5
11	SF4	u	101	5	-	-	0/6/5/5
11	SF4	j	503	6	-	-	0/6/5/5
11	SF4	E	102	5	-	-	0/6/5/5
11	SF4	p	401	6	-	-	0/6/5/5
11	SF4	v	508	6	-	-	0/6/5/5
11	SF4	L	504	6	-	-	0/6/5/5
11	SF4	d	409	6	-	-	0/6/5/5
11	SF4	v	505	6	-	-	0/6/5/5
13	MGD	f	503	12	-	8/22/66/66	0/6/6/6
11	SF4	K	102	5	-	-	0/6/5/5
11	SF4	H	501	2	-	-	0/6/5/5
11	SF4	p	402	6	-	-	0/6/5/5
11	SF4	d	407	6	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SF4	X	507	6	-	-	0/6/5/5
11	SF4	R	401	6	-	-	0/6/5/5
11	SF4	L	502	6	-	-	0/6/5/5
11	SF4	L	508	6	-	-	0/6/5/5
13	MGD	l	503	12	-	6/22/66/66	0/6/6/6
11	SF4	X	504	6	-	-	0/6/5/5
11	SF4	Z	501	2	-	-	0/6/5/5
11	SF4	f	501	2	-	-	0/6/5/5
13	MGD	r	503	12	-	9/22/66/66	0/6/6/6
11	SF4	i	101	5	-	-	0/6/5/5
11	SF4	L	507	6	-	-	0/6/5/5
11	SF4	v	503	6	-	-	0/6/5/5
11	SF4	F	404	6	-	-	0/6/5/5
11	SF4	d	404	6	-	-	0/6/5/5
11	SF4	R	408	6	-	-	0/6/5/5
11	SF4	F	409	6	-	-	0/6/5/5
11	SF4	R	406	6	-	-	0/6/5/5
11	SF4	v	504	6	-	-	0/6/5/5
11	SF4	R	407	6	-	-	0/6/5/5
11	SF4	v	506	6	-	-	0/6/5/5
11	SF4	F	405	6	-	-	0/6/5/5
11	SF4	R	402	6	-	-	0/6/5/5
11	SF4	i	102	5	-	-	0/6/5/5
13	MGD	N	503	12	-	7/22/66/66	0/6/6/6
8	MFN	k	603	7	-	19/61/61/63	0/2/2/2
11	SF4	R	404	6	-	-	0/6/5/5
8	MFN	A	603	7	-	12/61/61/63	0/2/2/2
11	SF4	c	102	5	-	-	0/6/5/5
8	MFN	G	603	7	-	17/61/61/63	0/2/2/2
11	SF4	N	501	2	-	-	0/6/5/5
11	SF4	l	501	2	-	-	0/6/5/5
11	SF4	j	502	6	-	-	0/6/5/5
13	MGD	l	504	12	-	1/22/66/66	0/6/6/6
11	SF4	X	505	6	-	-	0/6/5/5
11	SF4	Q	102	5	-	-	0/6/5/5
11	SF4	p	408	6	-	-	0/6/5/5
11	SF4	p	409	6	-	-	0/6/5/5
11	SF4	Q	101	5	-	-	0/6/5/5
11	SF4	E	101	5	-	-	0/6/5/5
11	SF4	T	501	2	-	-	0/6/5/5
11	SF4	p	406	6	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SF4	u	102	5	-	-	0/6/5/5
11	SF4	R	409	6	-	-	0/6/5/5
11	SF4	v	501	6	-	-	0/6/5/5
11	SF4	K	101	5	-	-	0/6/5/5
11	SF4	L	503	6	-	-	0/6/5/5
11	SF4	c	101	5	-	-	0/6/5/5
11	SF4	X	506	6	-	-	0/6/5/5
11	SF4	d	405	6	-	-	0/6/5/5
11	SF4	p	403	6	-	-	0/6/5/5
11	SF4	W	201	5	-	-	0/6/5/5
11	SF4	L	506	6	-	-	0/6/5/5
11	SF4	d	402	6	-	-	0/6/5/5
11	SF4	v	502	6	-	-	0/6/5/5
11	SF4	B	501	2	-	-	0/6/5/5
11	SF4	F	403	6	-	-	0/6/5/5
13	MGD	Z	503	12	-	9/22/66/66	0/6/6/6
8	MFN	q	603	-	-	19/61/61/63	0/2/2/2
11	SF4	X	502	6	-	-	0/6/5/5
11	SF4	d	406	6	-	-	0/6/5/5
13	MGD	B	503	12	-	8/22/66/66	0/6/6/6
13	MGD	H	504	12	-	1/22/66/66	0/6/6/6
11	SF4	L	501	6	-	-	0/6/5/5
11	SF4	o	101	5	-	-	0/6/5/5
11	SF4	L	505	6	-	-	0/6/5/5
11	SF4	v	507	6	-	-	0/6/5/5
11	SF4	r	501	2	-	-	0/6/5/5
13	MGD	f	504	12	-	1/22/66/66	0/6/6/6
11	SF4	j	501	6	-	-	0/6/5/5
13	MGD	N	504	12	-	0/22/66/66	0/6/6/6
11	SF4	j	506	6	-	-	0/6/5/5
11	SF4	X	503	6	-	-	0/6/5/5
11	SF4	F	407	6	-	-	0/6/5/5
8	MFN	S	603	-	-	20/61/61/63	0/2/2/2
8	MFN	e	603	-	-	21/61/61/63	0/2/2/2
11	SF4	p	404	6	-	-	0/6/5/5
11	SF4	d	403	6	-	-	0/6/5/5
13	MGD	T	503	12	-	3/22/66/66	0/6/6/6
13	MGD	B	504	12	-	1/22/66/66	0/6/6/6
11	SF4	W	200	5	-	-	0/6/5/5
11	SF4	p	405	6	-	-	0/6/5/5
8	MFN	M	603	7	-	19/61/61/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SF4	R	403	6	-	-	0/6/5/5
11	SF4	F	408	6	-	-	0/6/5/5
11	SF4	j	508	6	-	-	0/6/5/5

The worst 5 of 182 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	e	603	MFN	C21-N3	6.66	1.48	1.34
8	S	603	MFN	C21-N3	6.66	1.48	1.34
8	k	603	MFN	C21-N3	6.11	1.47	1.34
8	Y	603	MFN	C21-N3	6.05	1.46	1.34
8	A	603	MFN	C21-N3	5.97	1.46	1.34

The worst 5 of 338 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	e	603	MFN	C1-C2-C3	-12.75	122.05	134.23
8	k	603	MFN	C1-C2-C3	-11.64	123.11	134.23
8	Y	603	MFN	C1-C2-C3	-11.60	123.15	134.23
8	G	603	MFN	C1-C2-C3	-11.26	123.48	134.23
8	M	603	MFN	C1-C2-C3	-11.16	123.57	134.23

There are no chirality outliers.

5 of 220 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	603	MFN	N1-C1-C2-O1
8	A	603	MFN	N1-C1-C2-C3
8	A	603	MFN	C6-C12-C15-N2
8	A	603	MFN	C31-C32-C33-C28
8	A	603	MFN	C31-C32-C33-C34

There are no ring outliers.

16 monomers are involved in 33 short contacts:

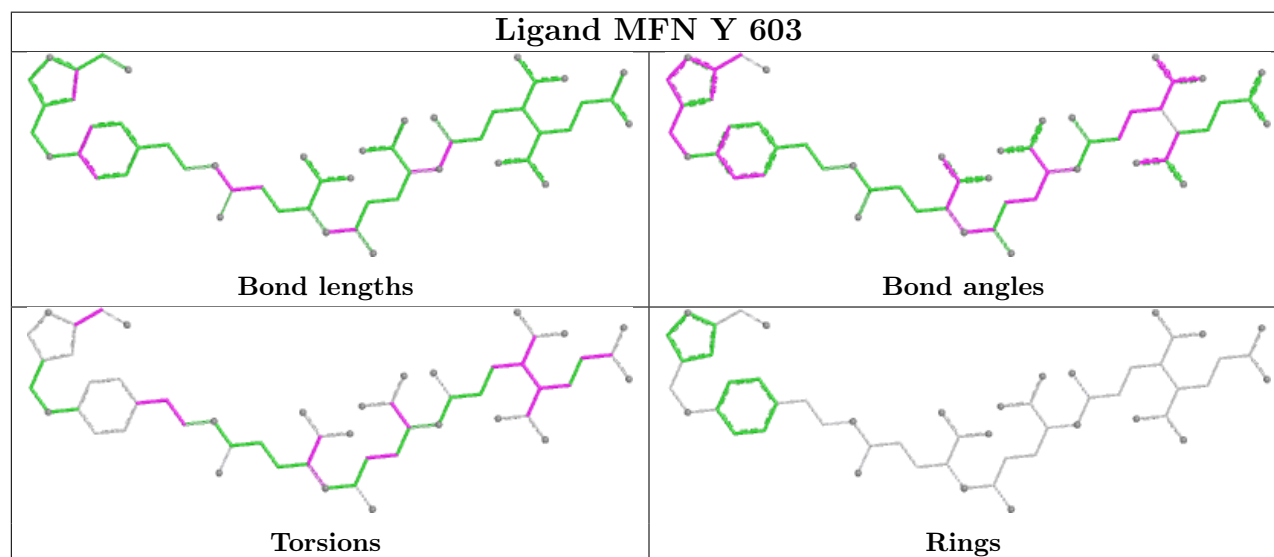
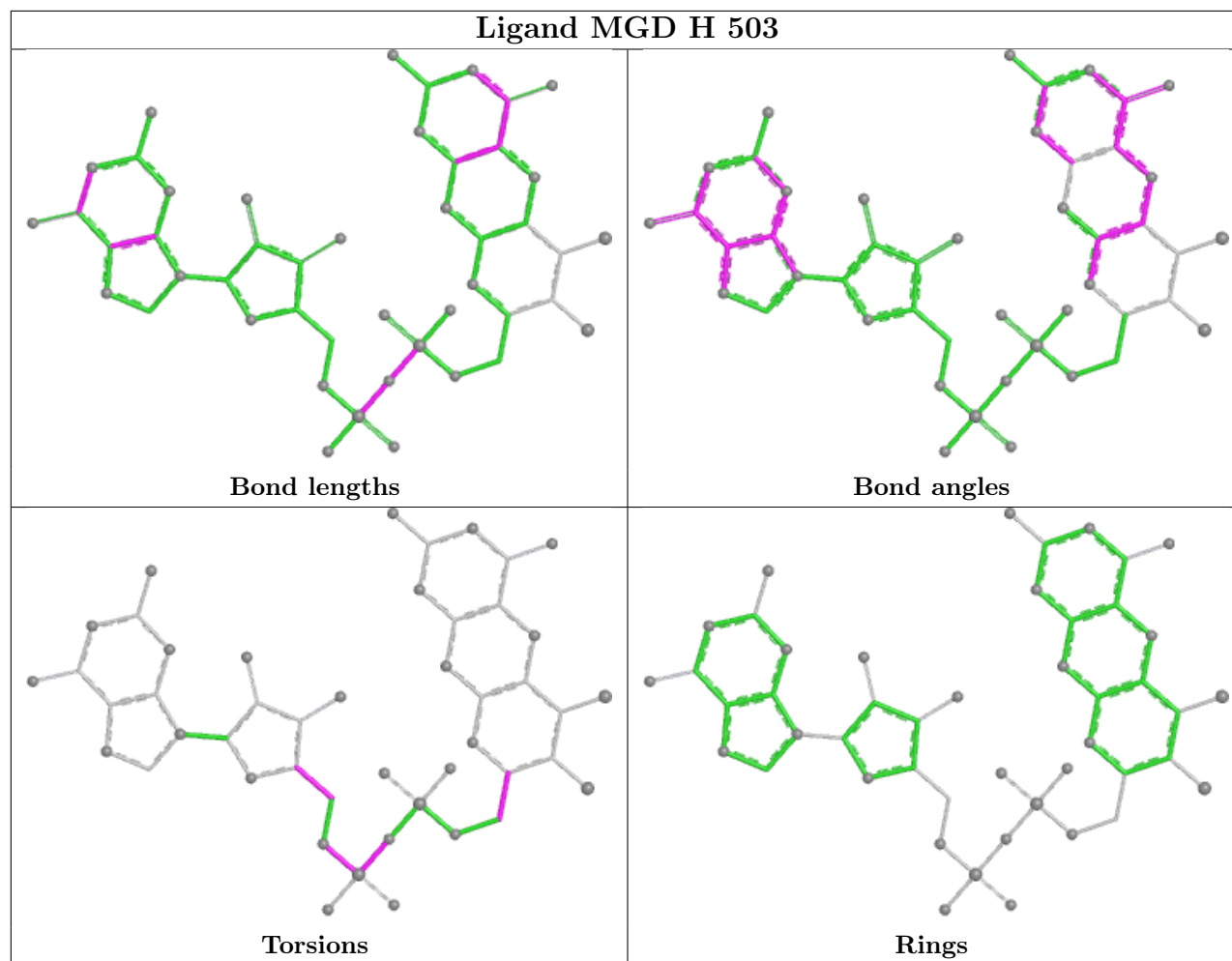
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	H	503	MGD	2	0
8	Y	603	MFN	4	0
13	T	504	MGD	1	0
13	Z	504	MGD	1	0
8	M	603	MFN	3	0

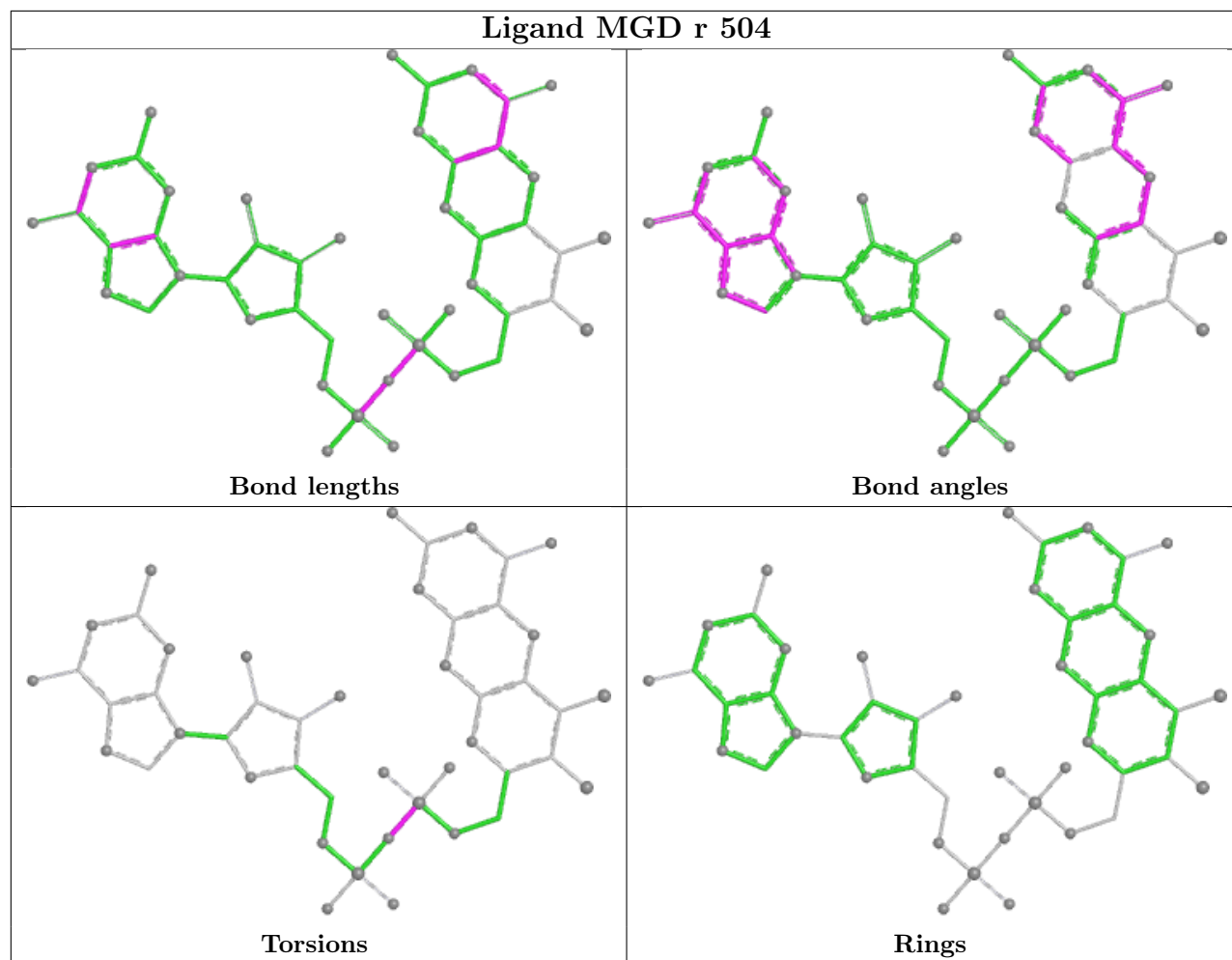
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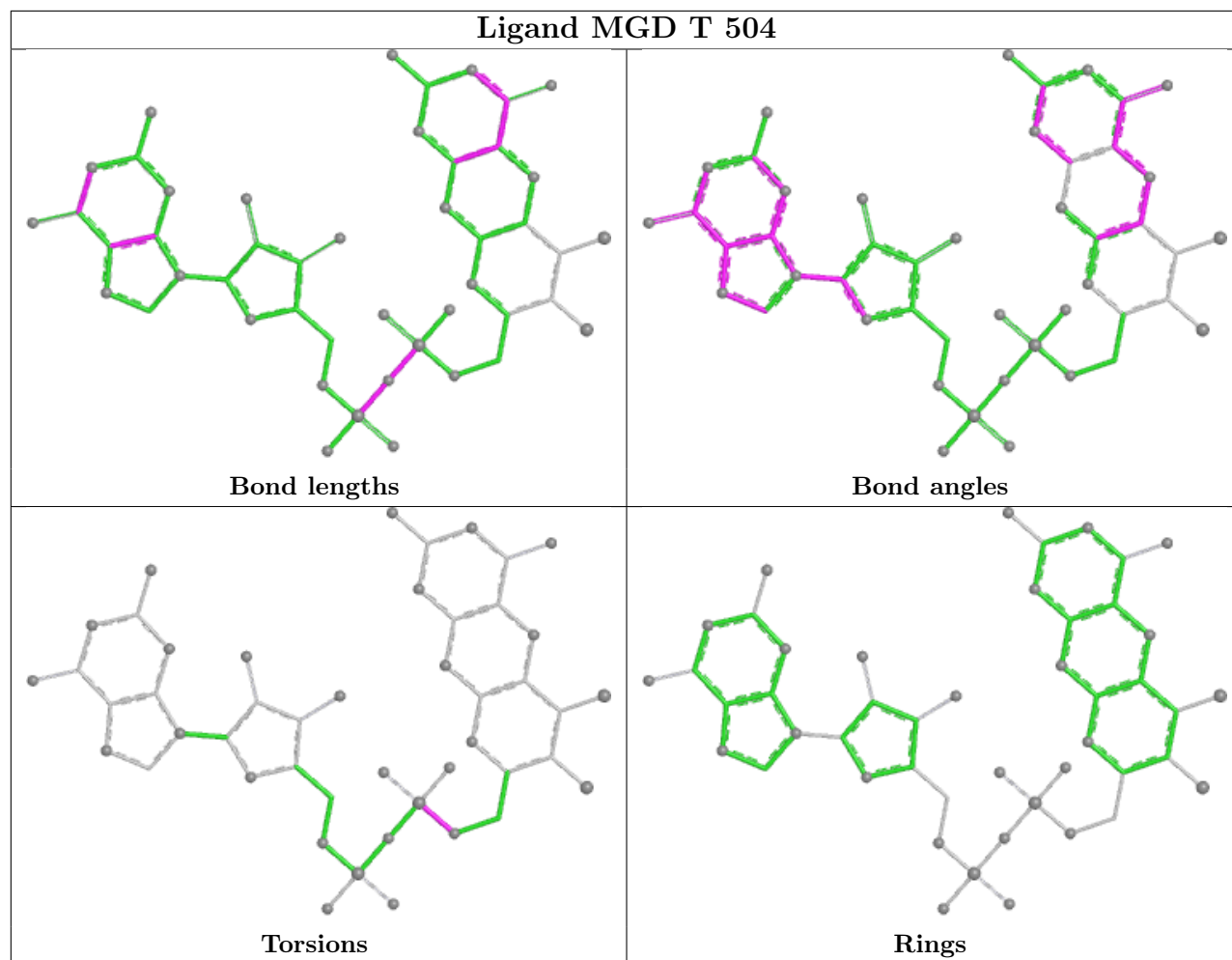
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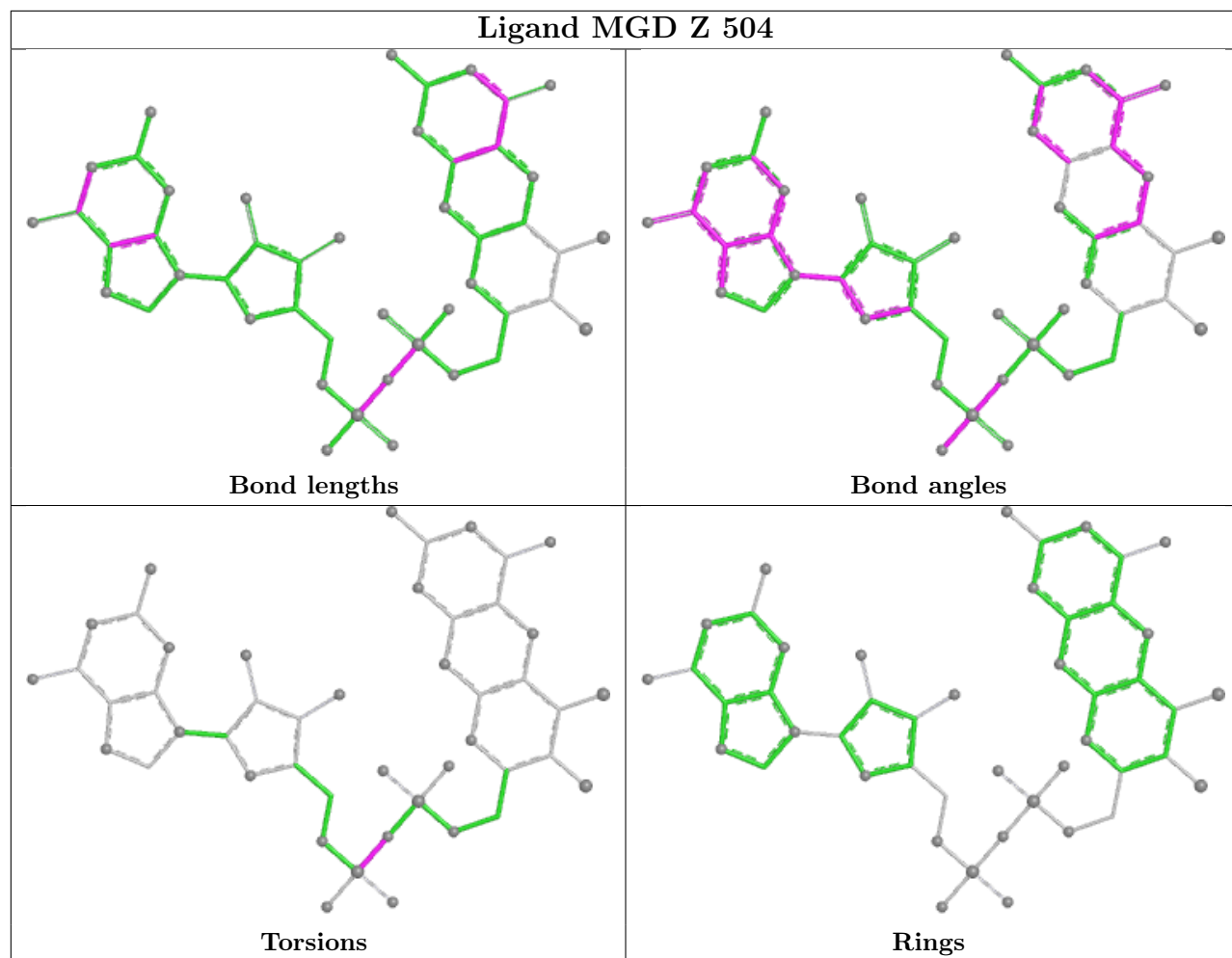
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	l	503	MGD	1	0
13	r	503	MGD	1	0
11	i	102	SF4	1	0
8	k	603	MFN	5	0
8	G	603	MFN	2	0
13	l	504	MGD	2	0
11	E	101	SF4	1	0
8	q	603	MFN	2	0
13	B	503	MGD	1	0
8	S	603	MFN	3	0
8	e	603	MFN	3	0

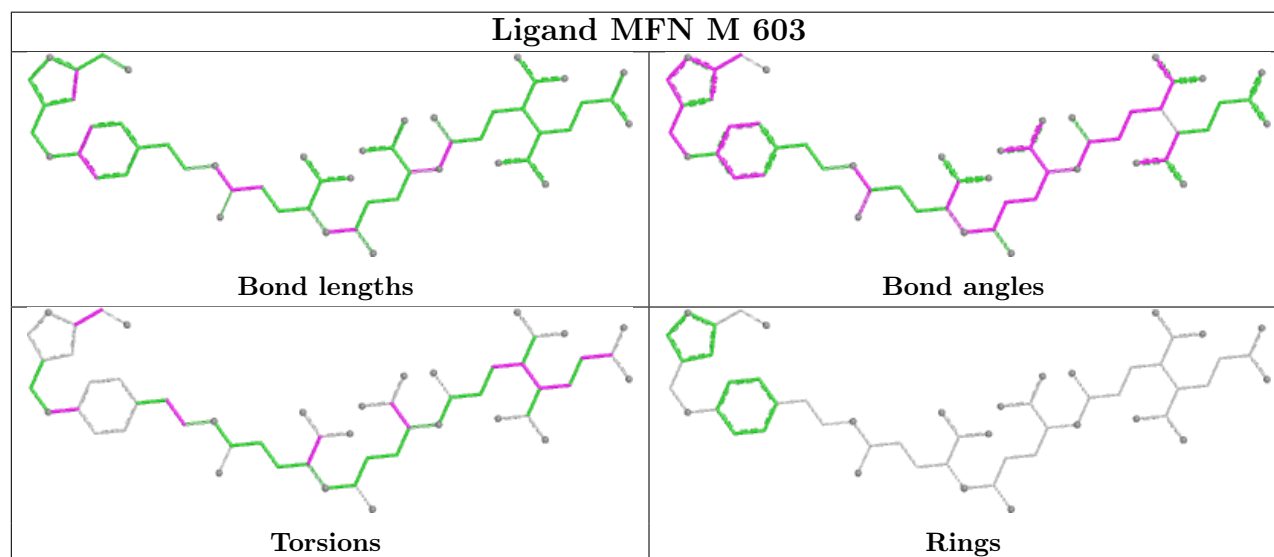
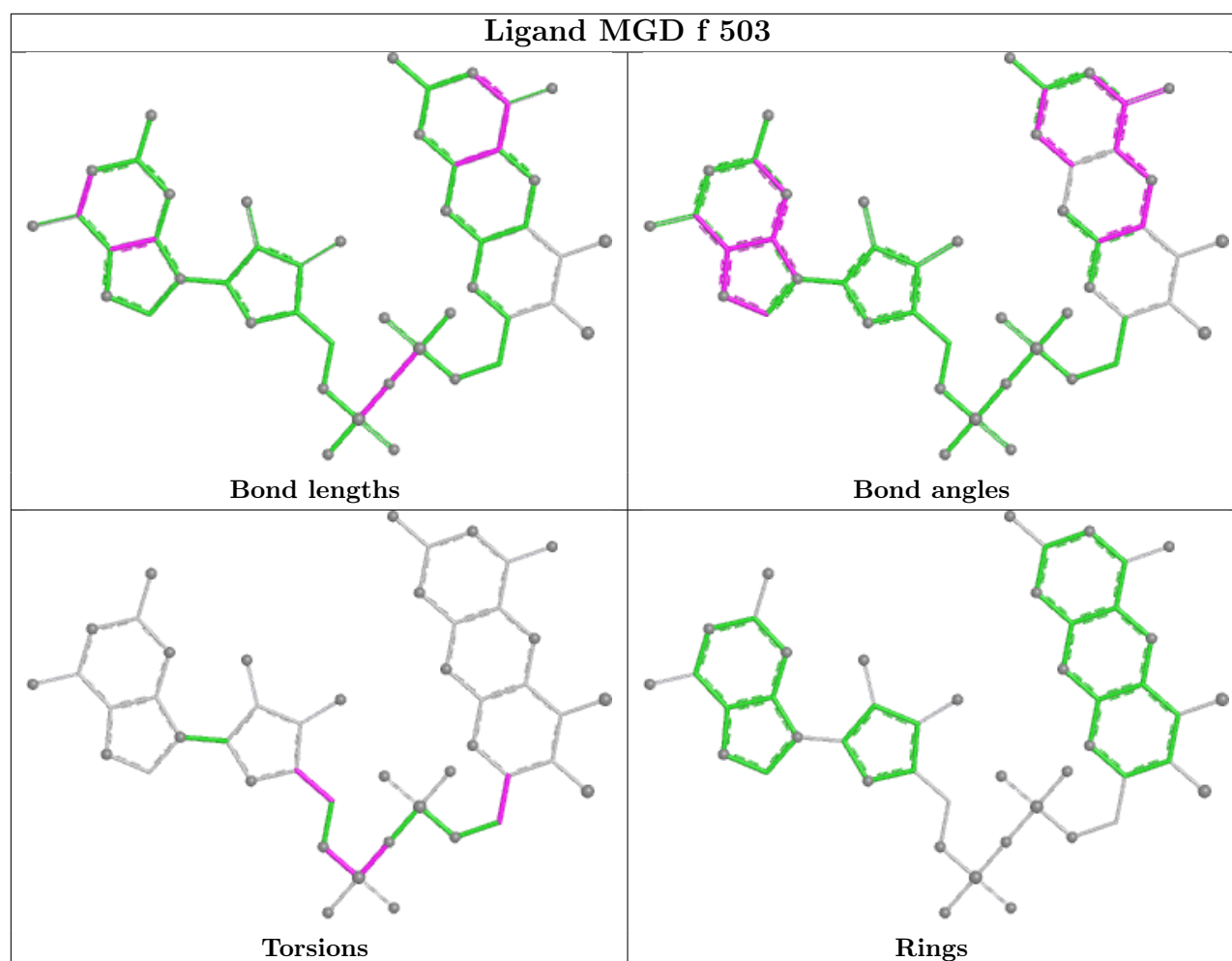
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

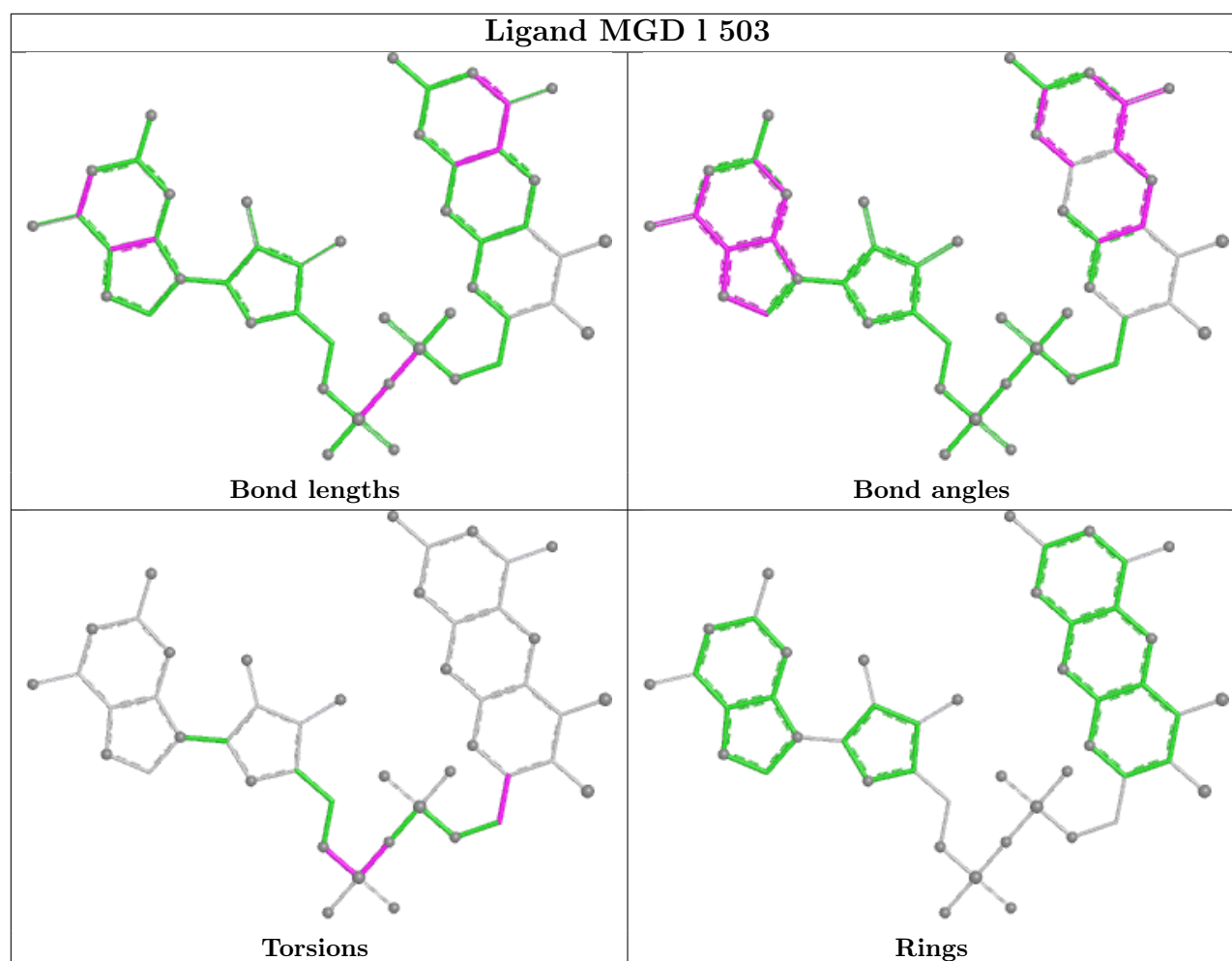


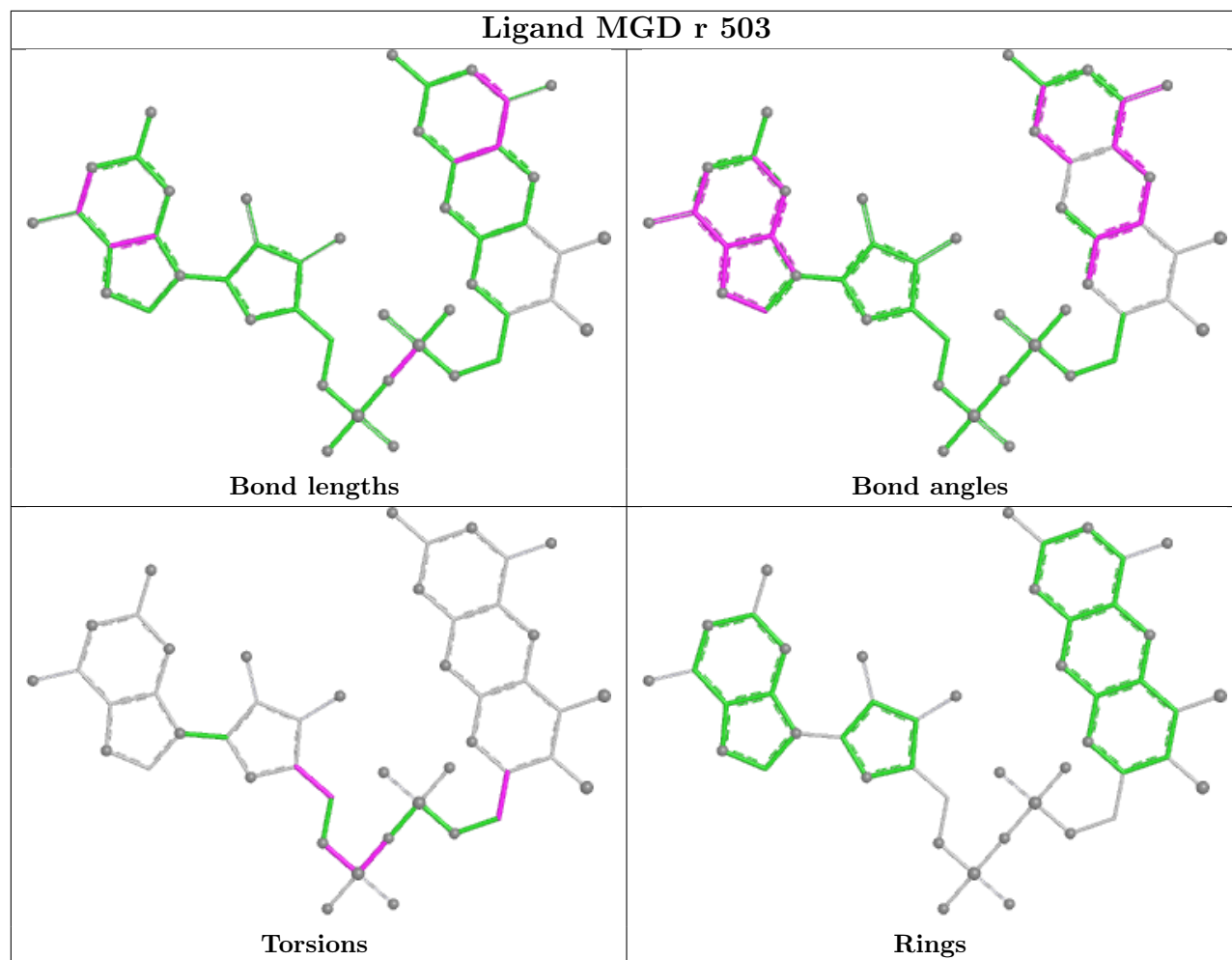


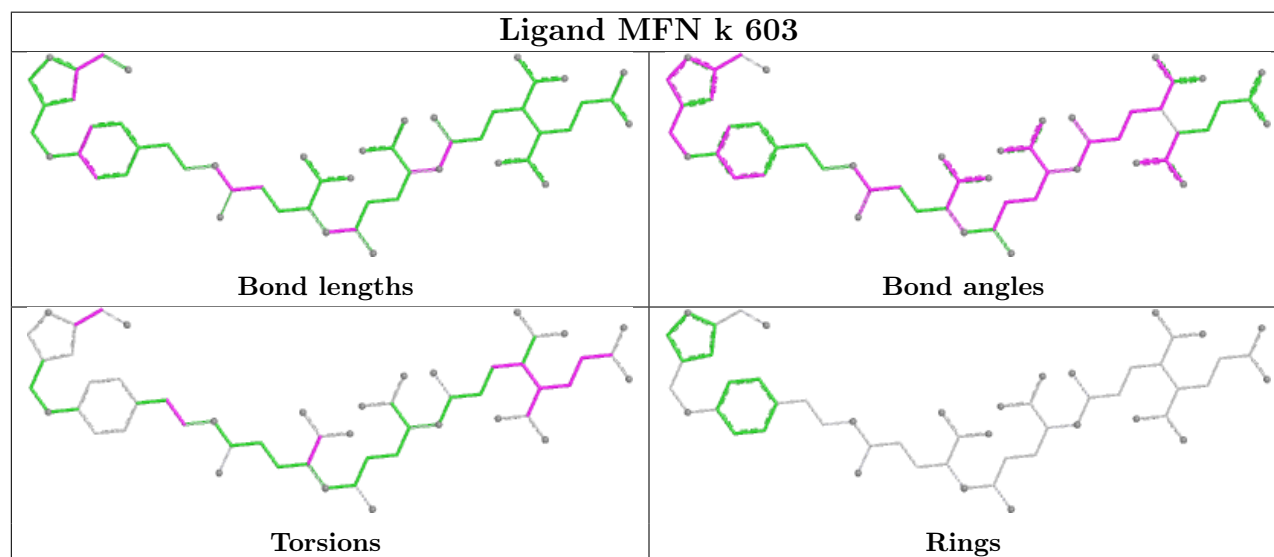
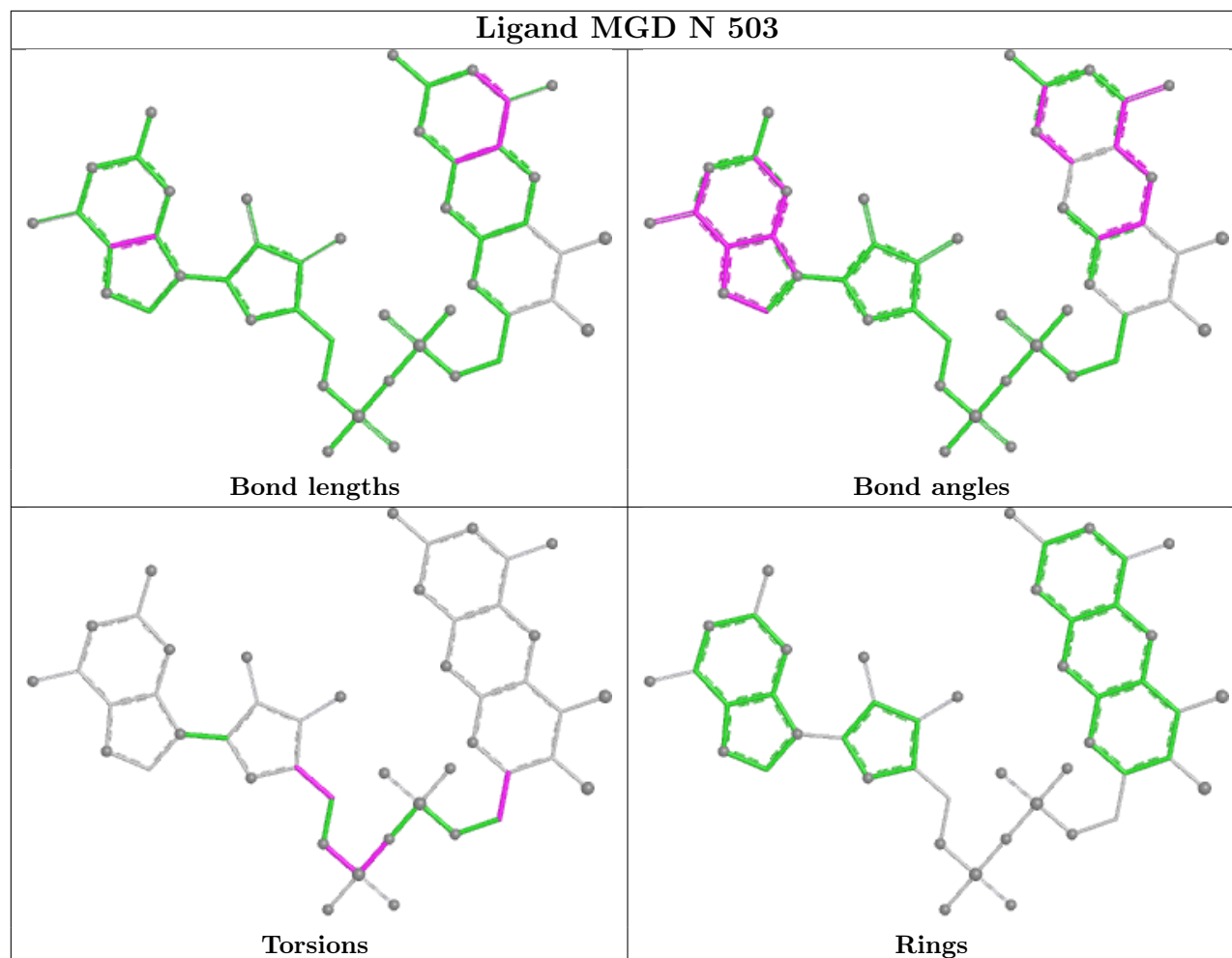


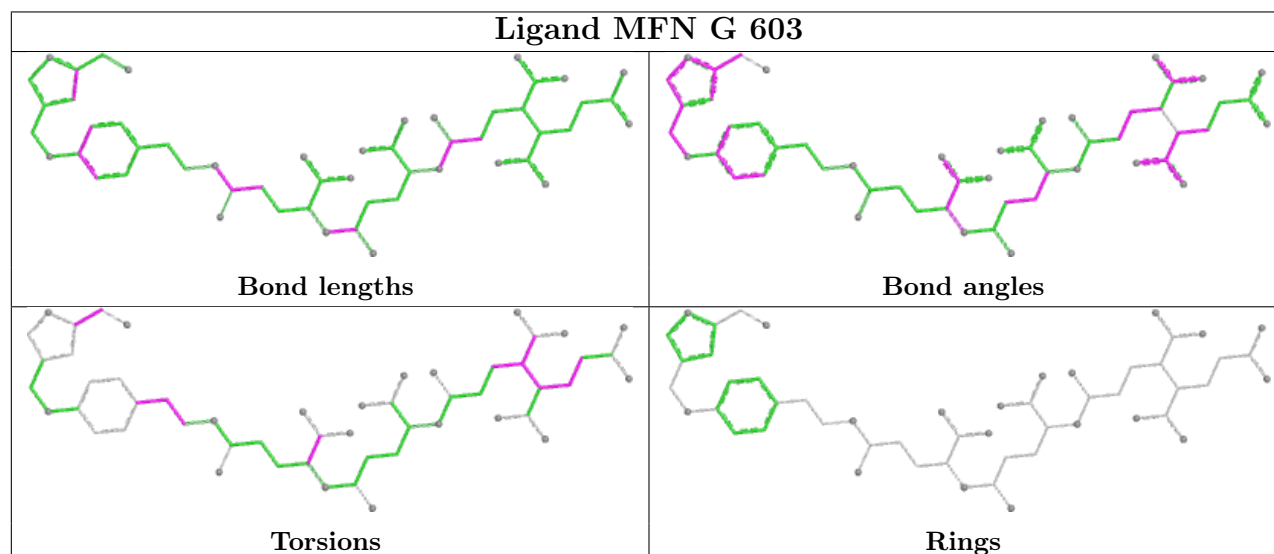
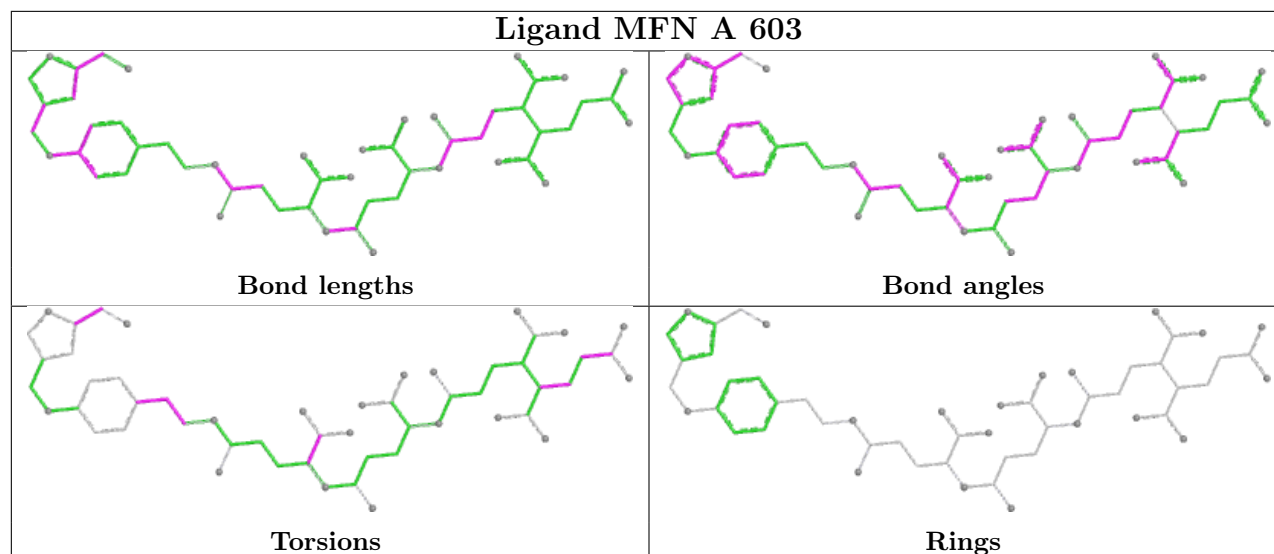


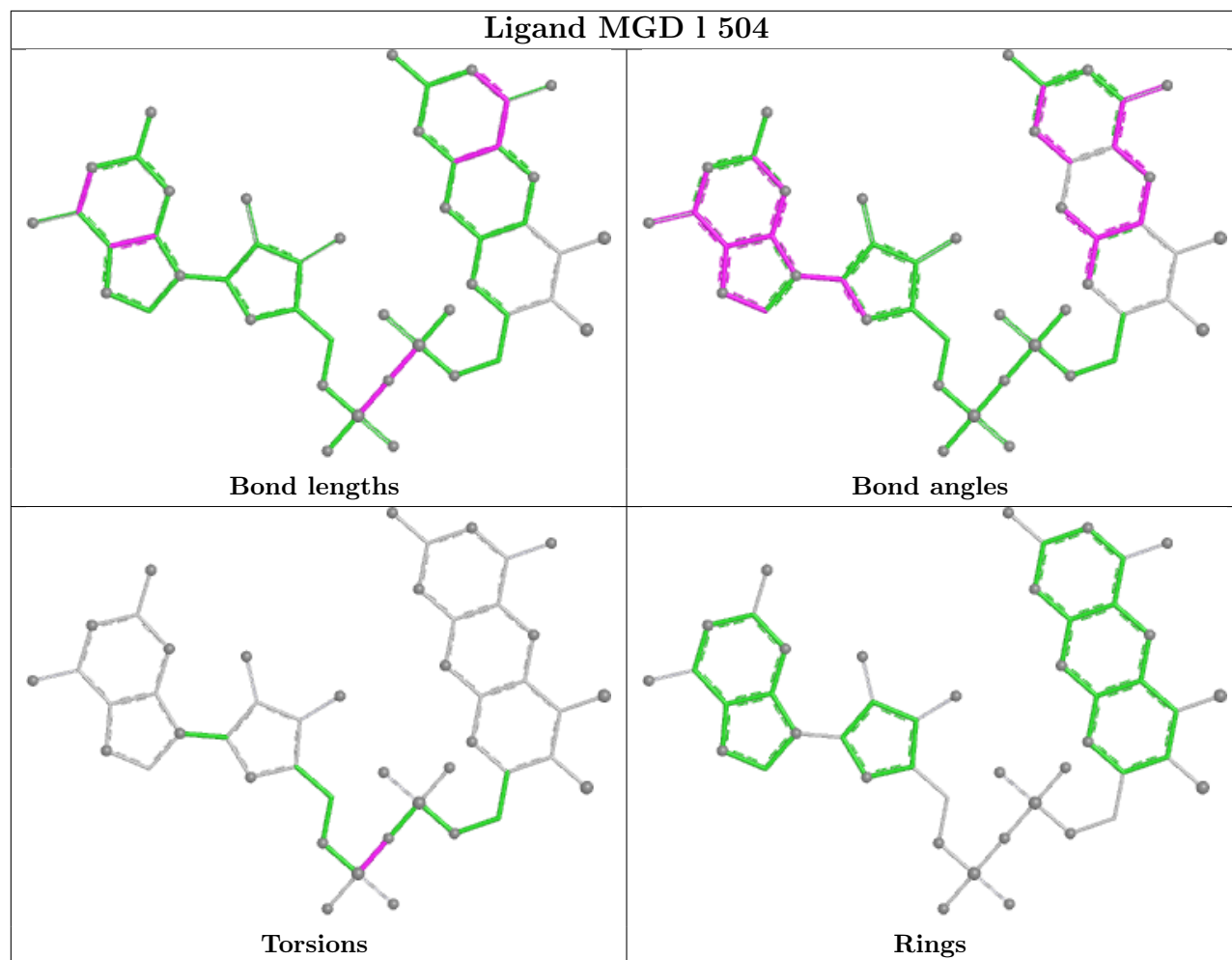


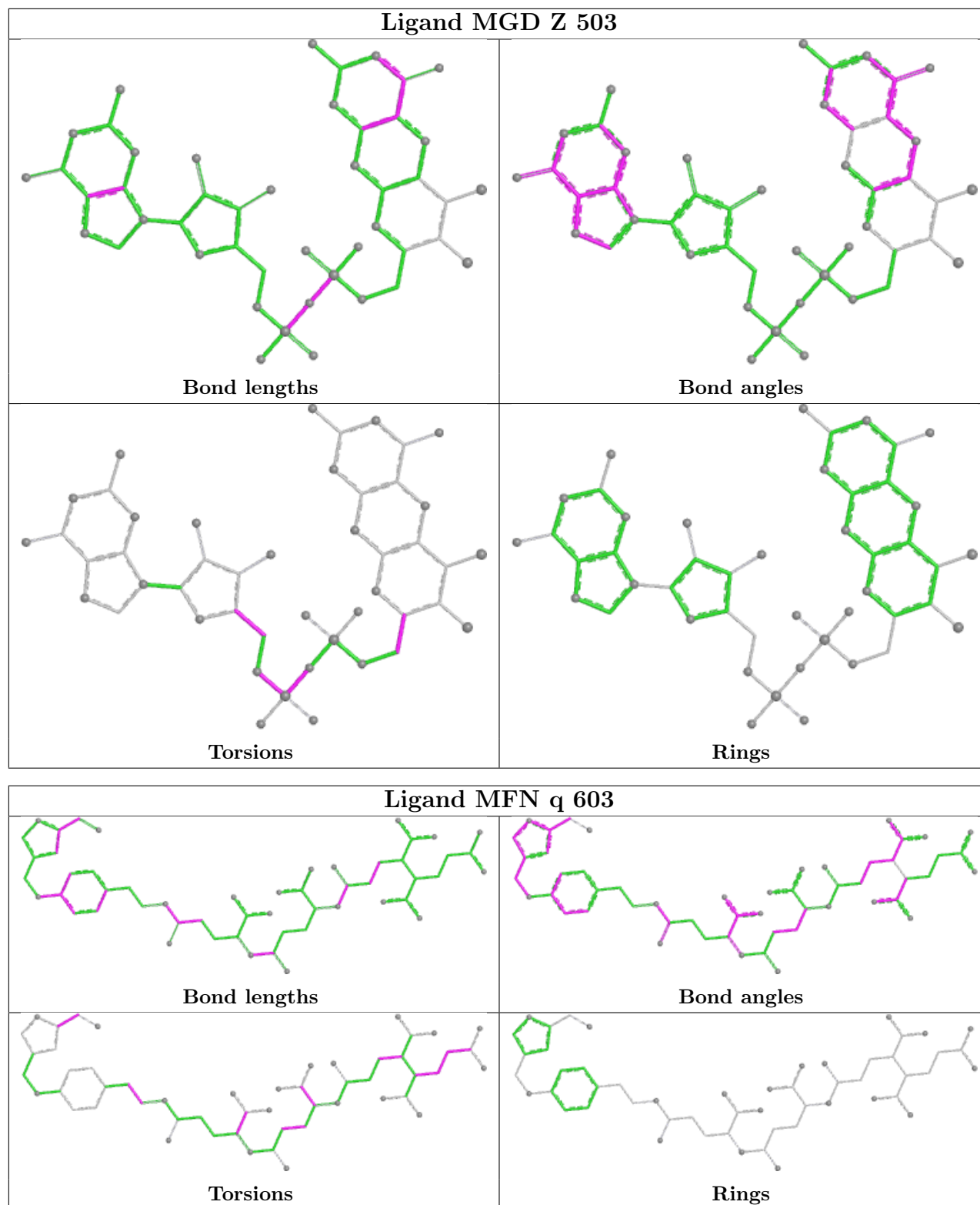


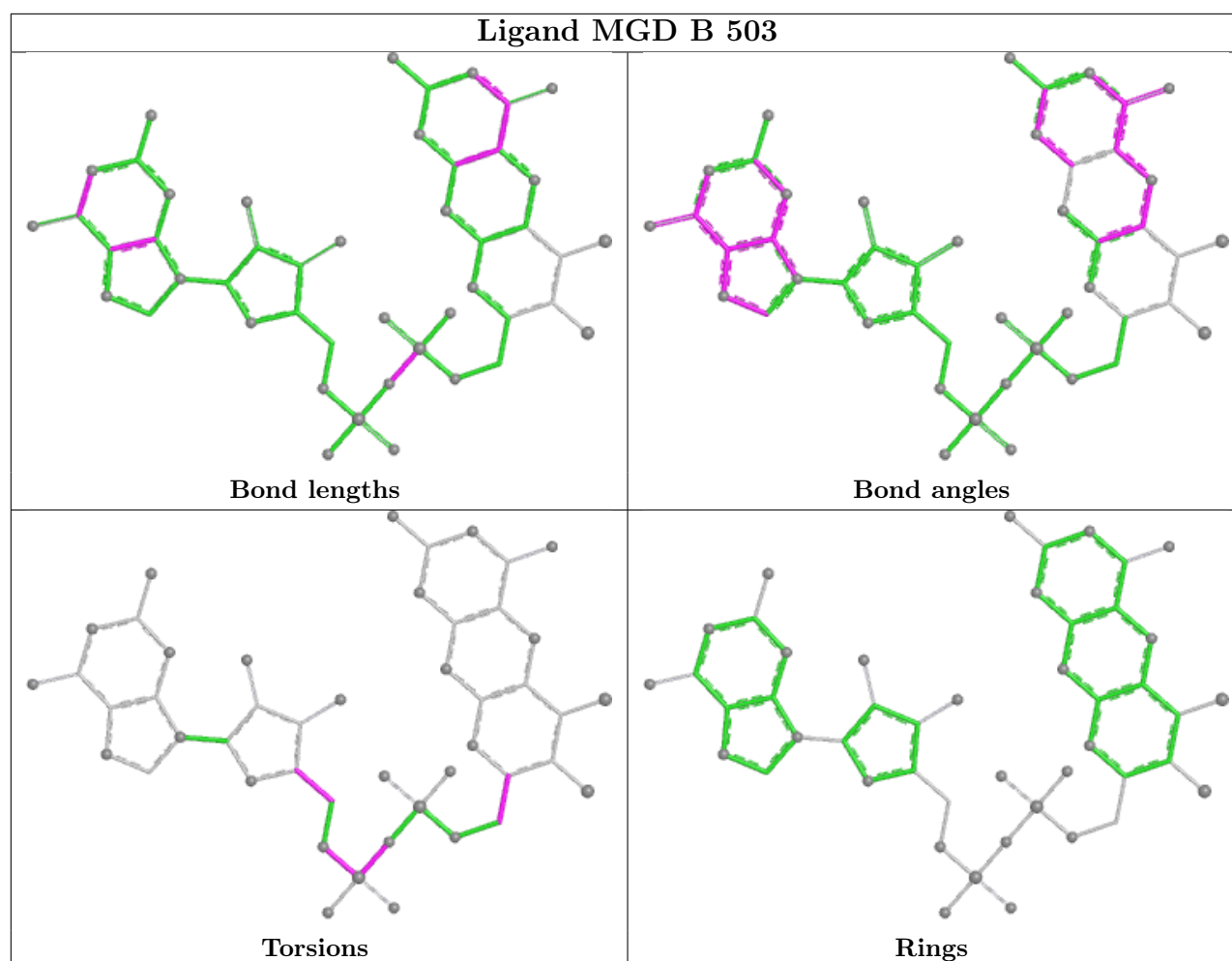


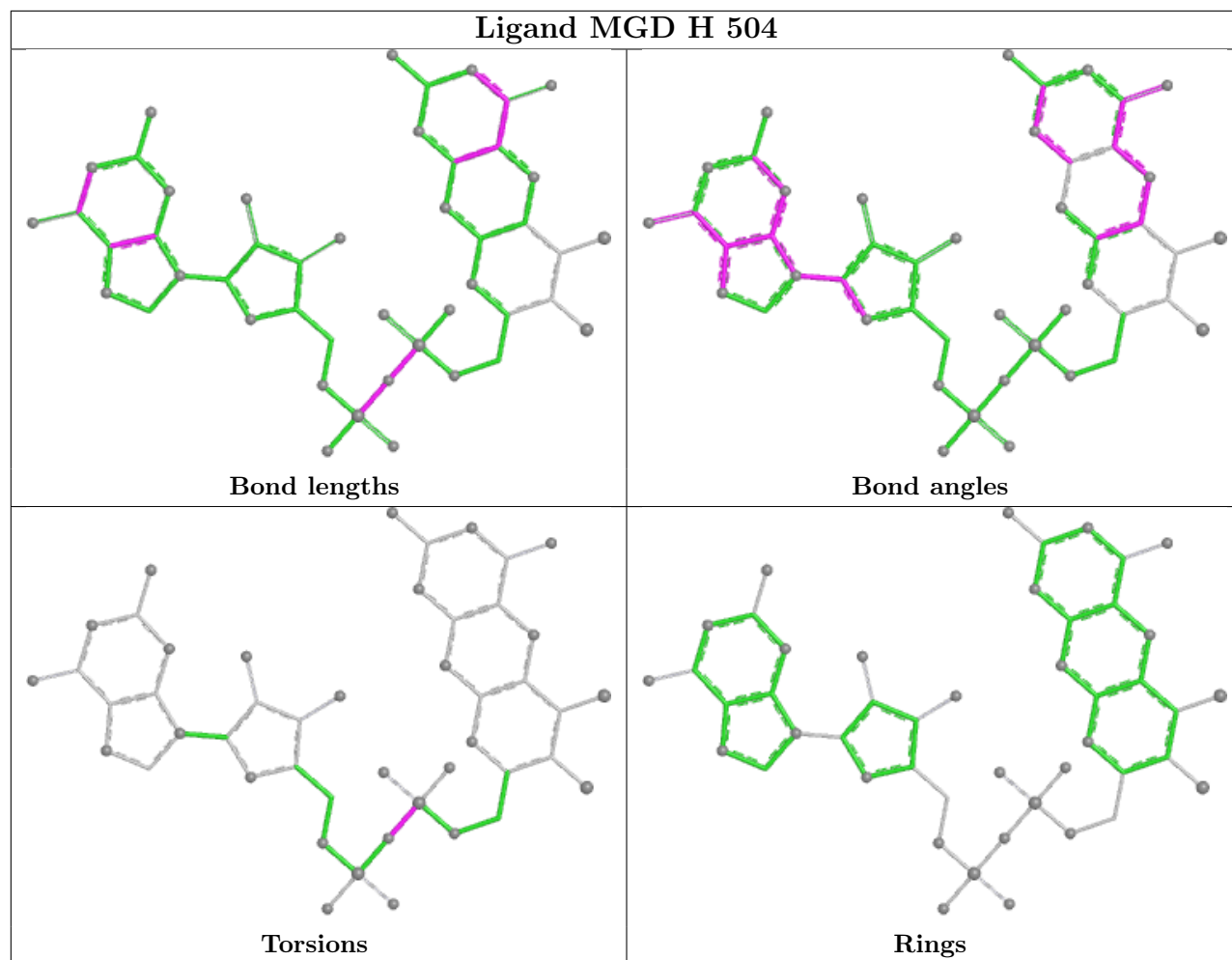


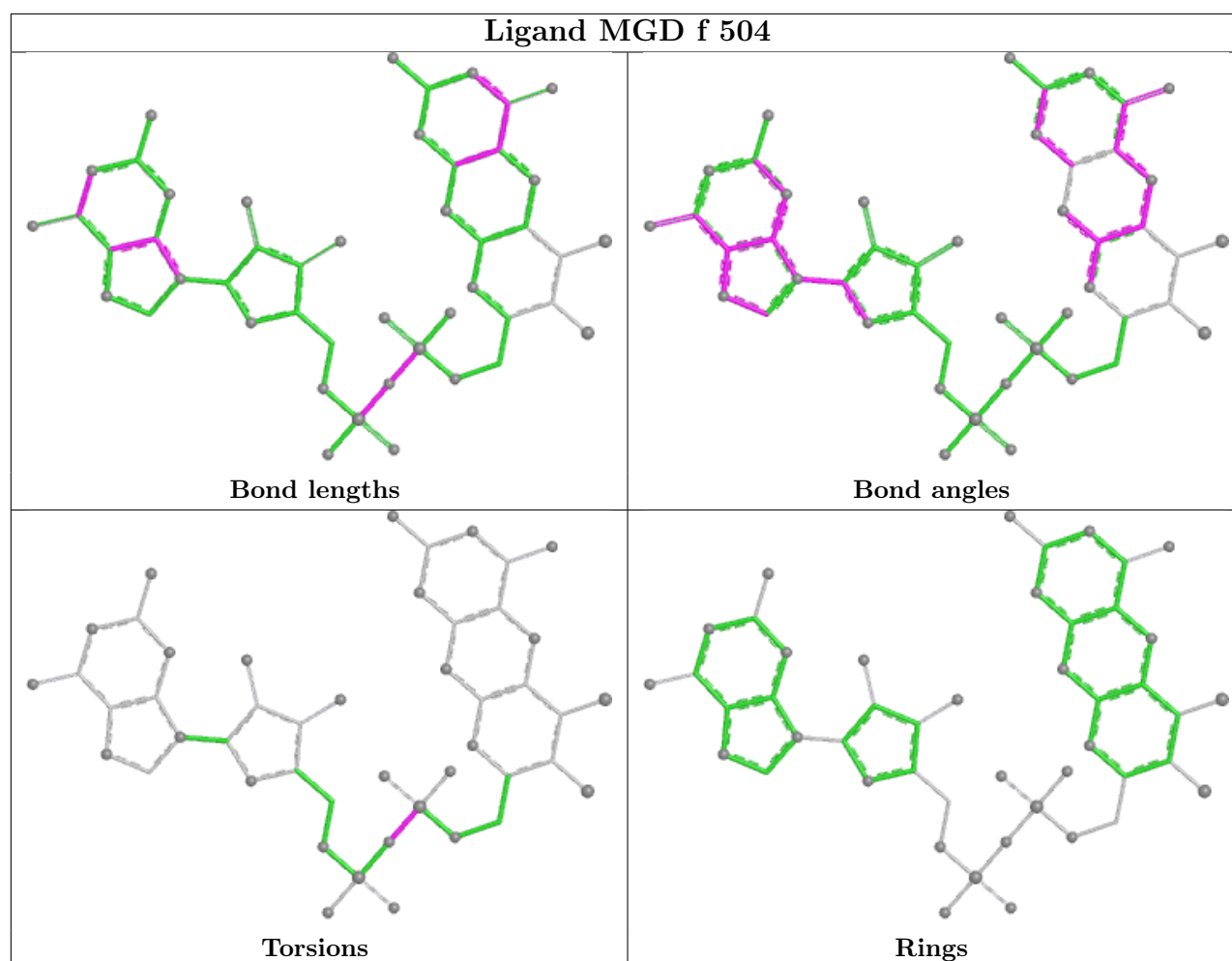


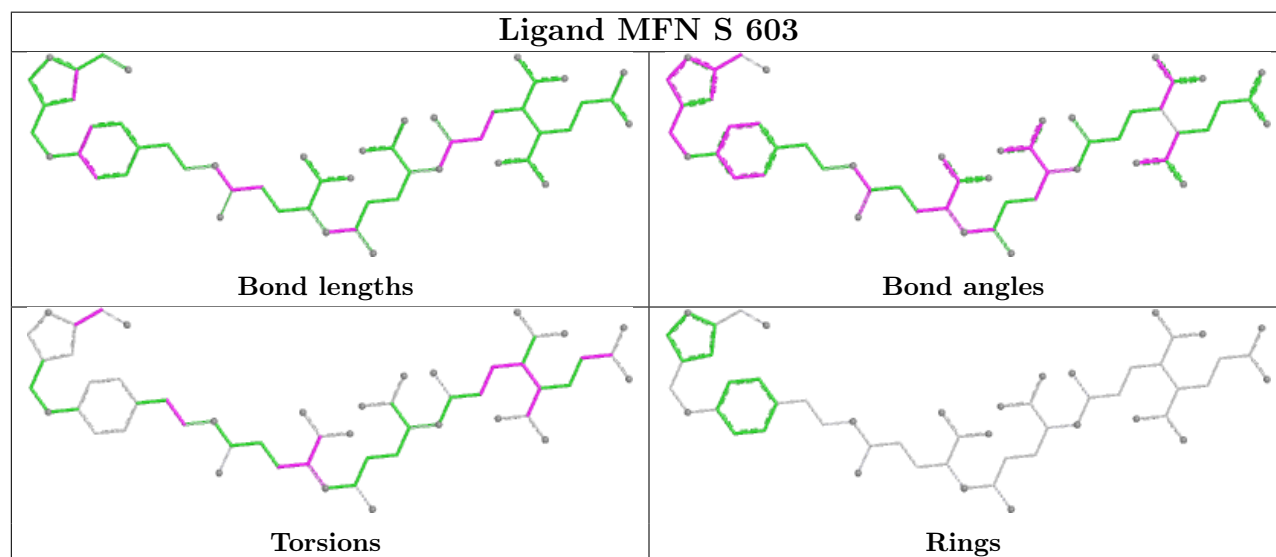
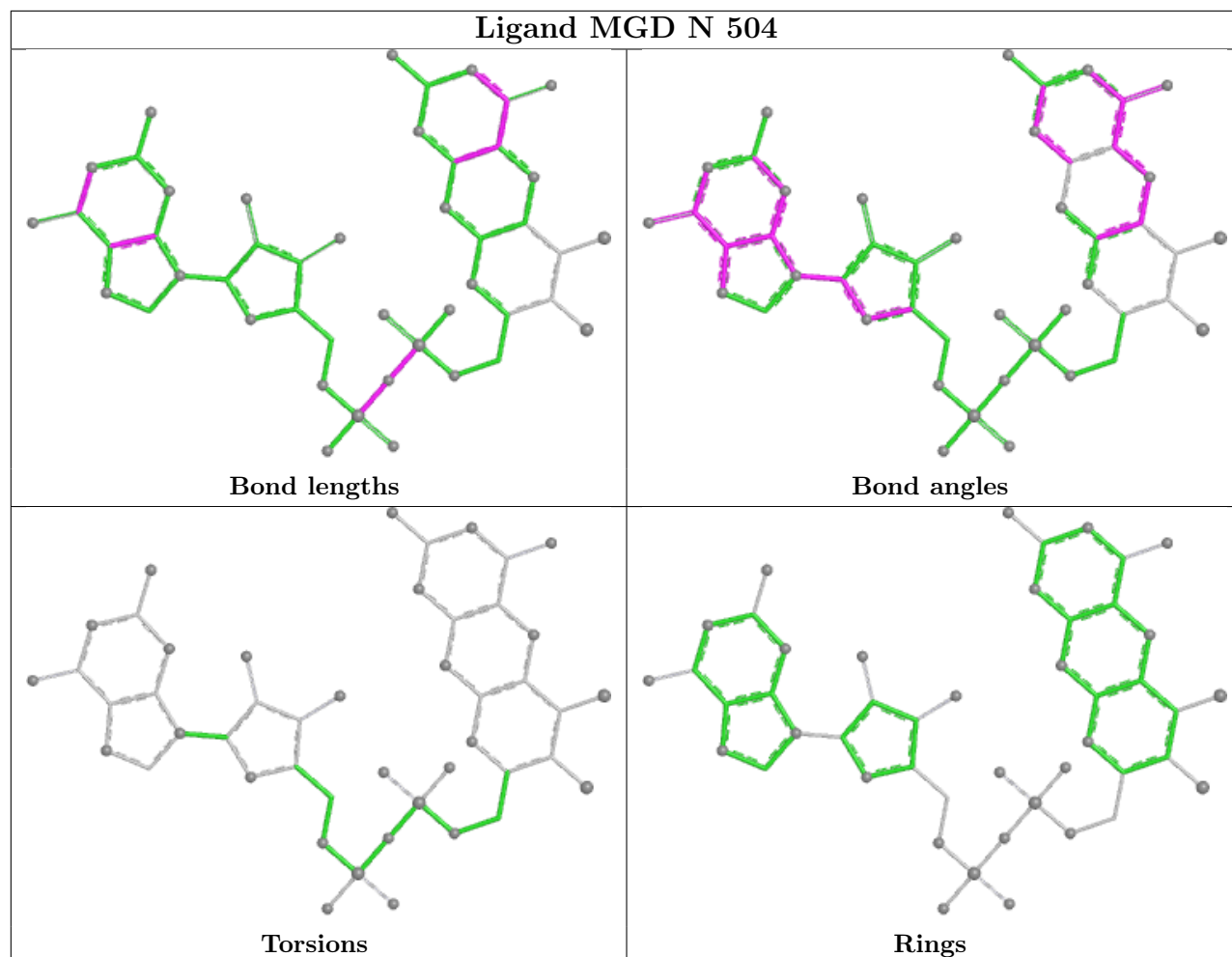


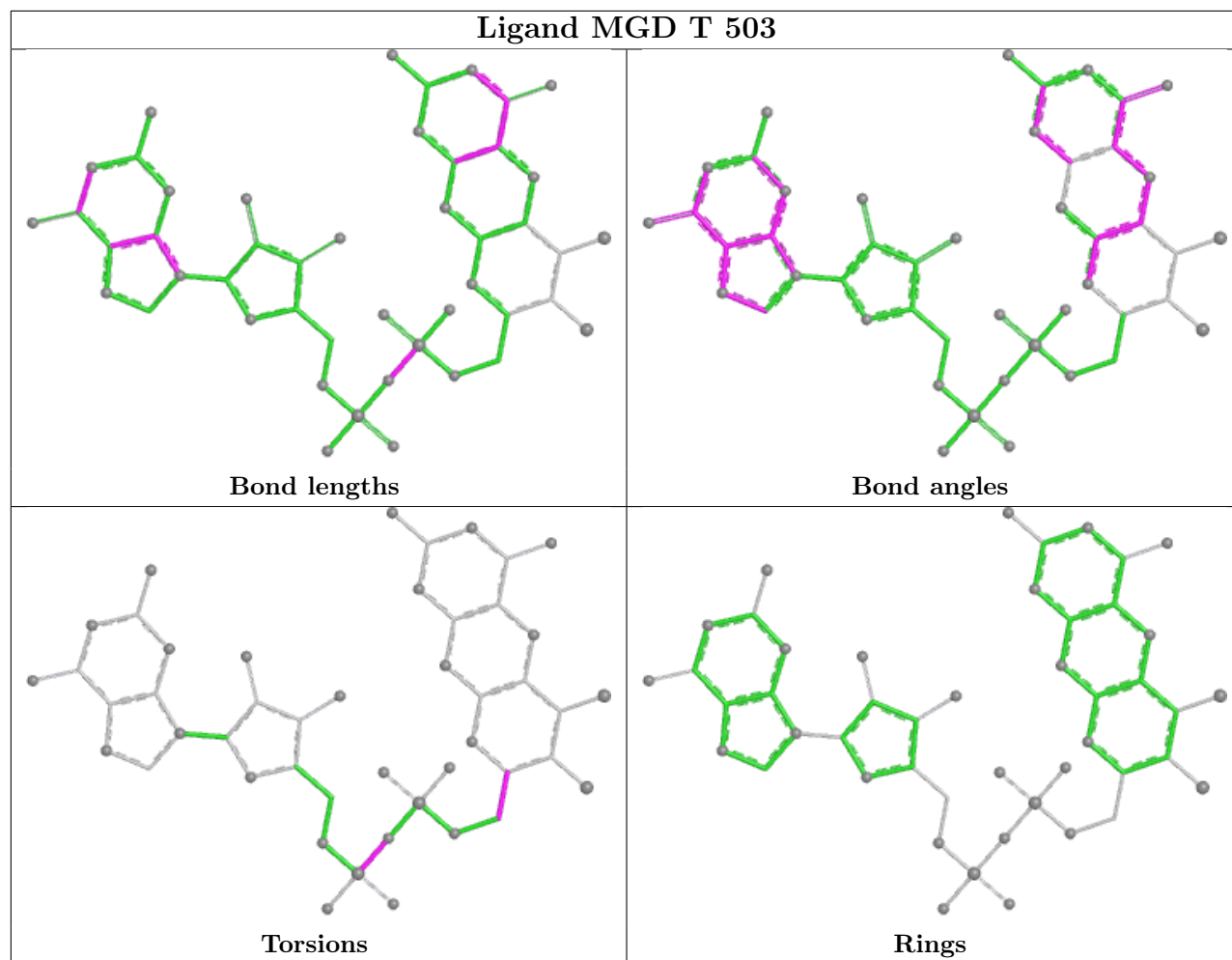


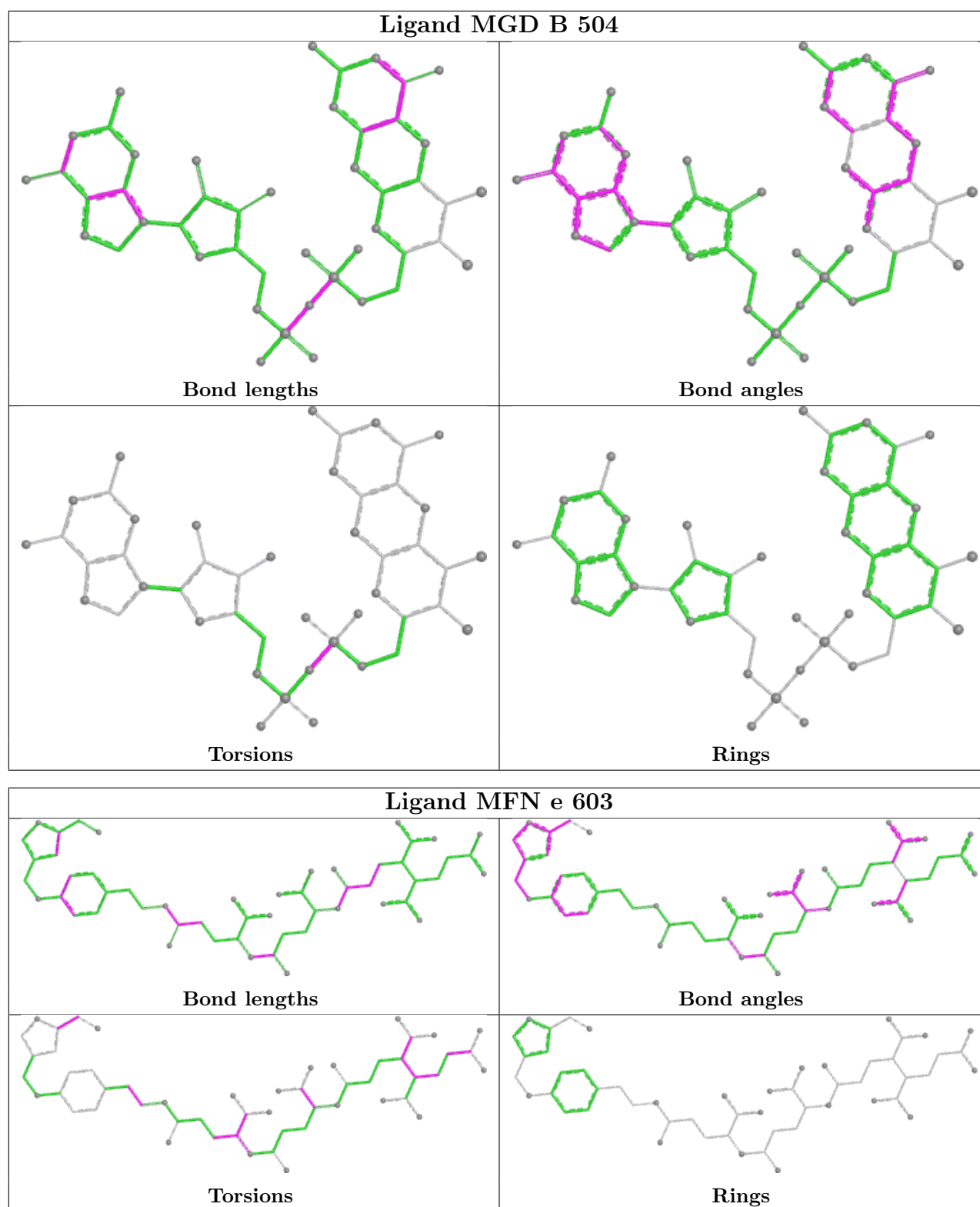












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	q	1
1	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	356:ARG	C	357:ALA	N	1.20
1	S	356:ARG	C	357:ALA	N	1.18

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, 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	568/569 (99%)	0.59	18 (3%)	50	51	29, 43, 63, 91	0
1	G	567/569 (99%)	0.85	48 (8%)	16	16	31, 48, 73, 117	0
1	M	567/569 (99%)	1.16	72 (12%)	8	7	34, 55, 81, 113	0
1	S	568/569 (99%)	0.33	13 (2%)	61	62	25, 36, 54, 94	0
1	Y	567/569 (99%)	0.92	43 (7%)	20	19	31, 51, 75, 109	0
1	e	568/569 (99%)	0.33	13 (2%)	61	62	27, 37, 53, 88	0
1	k	567/569 (99%)	1.27	97 (17%)	4	3	33, 56, 80, 102	0
1	q	568/569 (99%)	0.70	31 (5%)	30	30	31, 46, 66, 105	0
2	B	429/432 (99%)	0.69	27 (6%)	26	25	29, 42, 69, 124	0
2	H	427/432 (98%)	0.49	18 (4%)	40	41	26, 38, 61, 87	0
2	N	430/432 (99%)	0.44	9 (2%)	63	64	30, 39, 57, 71	0
2	T	429/432 (99%)	0.62	23 (5%)	31	31	26, 39, 65, 104	0
2	Z	428/432 (99%)	0.63	22 (5%)	33	33	28, 40, 64, 122	0
2	f	427/432 (98%)	0.57	20 (4%)	36	36	25, 39, 61, 109	0
2	l	428/432 (99%)	0.73	28 (6%)	25	24	29, 43, 68, 98	0
2	r	428/432 (99%)	0.84	38 (8%)	15	14	29, 44, 69, 106	0
3	C	267/270 (98%)	1.10	33 (12%)	8	7	35, 53, 78, 108	0
3	I	269/270 (99%)	0.35	5 (1%)	66	66	26, 38, 56, 90	0
3	O	268/270 (99%)	0.46	7 (2%)	57	58	30, 41, 61, 86	0
3	U	268/270 (99%)	0.73	16 (5%)	27	27	28, 46, 70, 110	0
3	a	268/270 (99%)	0.42	5 (1%)	66	66	30, 39, 55, 83	0
3	g	268/270 (99%)	0.97	34 (12%)	8	7	31, 50, 78, 101	0
3	m	268/270 (99%)	0.54	8 (2%)	52	54	28, 41, 62, 93	0
3	s	269/270 (99%)	1.23	47 (17%)	4	3	36, 56, 80, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
4	D	129/130 (99%)	1.07	12 (9%) 14 13	36, 52, 70, 91	0
4	J	129/130 (99%)	0.34	1 (0%) 82 84	31, 41, 56, 66	0
4	P	129/130 (99%)	0.20	1 (0%) 82 84	29, 38, 54, 65	0
4	V	129/130 (99%)	0.63	3 (2%) 61 62	33, 43, 58, 68	0
4	b	129/130 (99%)	0.47	2 (1%) 70 71	33, 41, 56, 83	0
4	h	129/130 (99%)	0.85	9 (6%) 22 21	34, 48, 65, 84	0
4	n	129/130 (99%)	0.46	1 (0%) 82 84	34, 42, 61, 78	0
4	t	129/130 (99%)	0.99	15 (11%) 9 8	37, 51, 70, 83	0
5	E	80/82 (97%)	0.83	3 (3%) 44 45	33, 42, 57, 67	0
5	K	80/82 (97%)	0.60	1 (1%) 75 75	32, 40, 55, 72	0
5	Q	80/82 (97%)	0.75	1 (1%) 75 75	34, 44, 60, 69	0
5	W	80/82 (97%)	0.64	1 (1%) 75 75	31, 39, 52, 68	0
5	c	80/82 (97%)	0.91	7 (8%) 15 15	37, 46, 63, 72	0
5	i	80/82 (97%)	0.57	1 (1%) 75 75	28, 37, 50, 70	0
5	o	80/82 (97%)	0.86	3 (3%) 44 45	34, 43, 57, 71	0
5	u	81/82 (98%)	0.77	4 (4%) 35 34	32, 40, 61, 84	0
6	F	345/349 (98%)	0.74	26 (7%) 20 19	29, 40, 67, 116	0
6	L	348/349 (99%)	0.51	9 (2%) 57 58	28, 38, 60, 83	0
6	R	341/349 (97%)	1.19	69 (20%) 3 2	29, 48, 87, 147	0
6	X	344/349 (98%)	0.72	24 (6%) 22 21	29, 41, 71, 107	0
6	d	340/349 (97%)	1.15	62 (18%) 3 3	28, 49, 96, 130	0
6	j	344/349 (98%)	0.66	19 (5%) 30 30	26, 39, 69, 99	0
6	p	348/349 (99%)	0.53	9 (2%) 57 58	29, 37, 58, 85	0
6	v	346/349 (99%)	0.54	18 (5%) 33 32	27, 38, 63, 87	0
All	All	14540/14656 (99%)	0.71	976 (6%) 24 23	25, 43, 71, 147	0

The worst 5 of 976 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	83	PHE	8.3
2	l	430	ALA	6.7
1	q	467	ILE	5.9
1	A	83	PHE	5.9
6	R	17	THR	5.9

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, 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	KCX	k	178	12/13	0.92	0.15	39,45,52,53	0
1	KCX	M	178	12/13	0.94	0.12	41,47,48,50	0
1	KCX	e	178	12/13	0.94	0.09	21,27,33,35	0
1	KCX	G	178	12/13	0.94	0.11	33,38,40,44	0
1	KCX	A	178	12/13	0.95	0.08	28,35,40,43	0
1	KCX	Y	178	12/13	0.95	0.12	36,43,50,51	0
1	KCX	q	178	12/13	0.95	0.08	31,35,42,44	0
1	KCX	S	178	12/13	0.97	0.07	25,29,38,39	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, 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
8	MFN	M	603	53/55	0.79	0.21	46,85,111,116	0
8	MFN	k	603	53/55	0.80	0.20	51,77,108,110	0
10	K	v	515	1/1	0.82	0.15	78,78,78,78	0
8	MFN	q	603	53/55	0.84	0.17	40,85,115,121	0
8	MFN	A	603	53/55	0.84	0.17	40,72,97,107	0
8	MFN	Y	603	53/55	0.85	0.17	44,75,101,103	0
9	NA	q	604	1/1	0.85	0.18	47,47,47,47	0
8	MFN	G	603	53/55	0.85	0.17	43,68,86,90	0
9	NA	G	604	1/1	0.86	0.23	54,54,54,54	0
8	MFN	e	603	53/55	0.87	0.15	35,59,92,101	0
10	K	L	511	1/1	0.88	0.12	80,80,80,80	0
8	MFN	S	603	53/55	0.88	0.13	30,56,87,89	0
10	K	Z	506	1/1	0.89	0.13	63,63,63,63	0
16	CL	N	506	1/1	0.89	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	NA	A	604	1/1	0.90	0.14	41,41,41,41	0
10	K	v	511	1/1	0.90	0.10	53,53,53,53	0
10	K	e	608	1/1	0.91	0.09	68,68,68,68	0
9	NA	M	604	1/1	0.91	0.18	56,56,56,56	0
10	K	d	411	1/1	0.93	0.11	60,60,60,60	0
10	K	X	511	1/1	0.94	0.10	59,59,59,59	0
10	K	T	506	1/1	0.94	0.09	59,59,59,59	0
13	MGD	Z	503	47/47	0.94	0.10	29,37,45,56	0
14	H2S	l	505	1/1	0.94	0.24	66,66,66,66	0
14	H2S	r	505	1/1	0.94	0.13	52,52,52,52	0
10	K	v	510	1/1	0.94	0.07	57,57,57,57	0
11	SF4	R	403	8/8	0.95	0.06	67,74,83,94	0
11	SF4	c	102	8/8	0.95	0.08	42,53,64,69	0
11	SF4	d	403	8/8	0.95	0.06	60,74,85,92	0
11	SF4	l	501	8/8	0.95	0.07	30,37,53,53	0
13	MGD	T	504	47/47	0.95	0.10	25,37,43,55	0
10	K	R	411	1/1	0.95	0.07	59,59,59,59	0
13	MGD	Z	504	47/47	0.95	0.09	23,37,43,65	0
13	MGD	f	503	47/47	0.95	0.09	26,37,43,46	0
13	MGD	r	503	47/47	0.95	0.09	37,46,53,55	0
13	MGD	r	504	47/47	0.95	0.09	27,36,45,47	0
9	NA	e	604	1/1	0.95	0.09	30,30,30,30	0
10	K	v	514	1/1	0.95	0.09	42,42,42,42	0
10	K	M	606	1/1	0.95	0.10	55,55,55,55	0
10	K	v	509	1/1	0.96	0.08	58,58,58,58	0
11	SF4	d	404	8/8	0.96	0.06	44,57,65,69	0
11	SF4	d	405	8/8	0.96	0.05	38,43,61,62	0
11	SF4	d	406	8/8	0.96	0.06	34,42,54,61	0
11	SF4	f	501	8/8	0.96	0.08	38,41,64,66	0
11	SF4	i	101	8/8	0.96	0.05	26,34,41,47	0
11	SF4	j	505	8/8	0.96	0.05	33,47,54,55	0
10	K	X	510	1/1	0.96	0.06	52,52,52,52	0
11	SF4	p	402	8/8	0.96	0.06	28,37,44,57	0
13	MGD	B	503	47/47	0.96	0.09	34,40,48,51	0
13	MGD	H	503	47/47	0.96	0.08	29,35,41,47	0
13	MGD	T	503	47/47	0.96	0.09	28,38,46,47	0
10	K	N	507	1/1	0.96	0.06	55,55,55,55	0
10	K	F	412	1/1	0.96	0.06	53,53,53,53	0
10	K	R	412	1/1	0.96	0.06	61,61,61,61	0
11	SF4	F	407	8/8	0.96	0.05	29,31,44,53	0
13	MGD	l	504	47/47	0.96	0.09	25,36,47,50	0
10	K	L	509	1/1	0.96	0.06	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	SF4	R	404	8/8	0.96	0.06	48,54,65,78	0
11	SF4	R	407	8/8	0.96	0.06	23,35,43,46	0
11	SF4	X	504	8/8	0.96	0.06	25,30,48,57	0
15	MG	B	507	1/1	0.96	0.13	36,36,36,36	0
15	MG	r	507	1/1	0.96	0.14	34,34,34,34	0
10	K	p	411	1/1	0.96	0.07	57,57,57,57	0
11	SF4	R	402	8/8	0.97	0.06	28,41,51,59	0
10	K	j	512	1/1	0.97	0.08	58,58,58,58	0
10	K	j	514	1/1	0.97	0.16	48,48,48,48	0
11	SF4	R	405	8/8	0.97	0.05	32,44,55,65	0
10	K	p	410	1/1	0.97	0.10	63,63,63,63	0
11	SF4	R	409	8/8	0.97	0.04	31,35,47,50	0
11	SF4	T	501	8/8	0.97	0.06	28,39,53,60	0
11	SF4	W	200	8/8	0.97	0.05	32,40,47,54	0
11	SF4	W	201	8/8	0.97	0.04	21,33,41,47	0
10	K	F	410	1/1	0.97	0.07	53,53,53,53	0
11	SF4	X	505	8/8	0.97	0.05	33,46,57,60	0
11	SF4	X	506	8/8	0.97	0.04	22,31,42,42	0
11	SF4	X	507	8/8	0.97	0.05	30,31,40,48	0
11	SF4	Z	501	8/8	0.97	0.05	26,36,44,53	0
11	SF4	c	101	8/8	0.97	0.06	39,45,51,66	0
10	K	p	412	1/1	0.97	0.07	53,53,53,53	0
11	SF4	d	401	8/8	0.97	0.04	34,50,53,59	0
11	SF4	d	402	8/8	0.97	0.06	37,48,56,66	0
10	K	q	605	1/1	0.97	0.06	47,47,47,47	0
10	K	r	506	1/1	0.97	0.08	57,57,57,57	0
10	K	L	510	1/1	0.97	0.05	52,52,52,52	0
10	K	F	411	1/1	0.97	0.06	38,38,38,38	0
11	SF4	d	407	8/8	0.97	0.04	34,42,53,55	0
9	NA	k	604	1/1	0.97	0.08	52,52,52,52	0
10	K	v	512	1/1	0.97	0.09	56,56,56,56	0
11	SF4	i	102	8/8	0.97	0.05	20,31,41,52	0
11	SF4	j	501	8/8	0.97	0.05	27,38,44,57	0
11	SF4	j	502	8/8	0.97	0.05	18,31,50,53	0
11	SF4	j	503	8/8	0.97	0.04	33,38,44,49	0
11	SF4	j	504	8/8	0.97	0.05	25,37,42,51	0
10	K	v	513	1/1	0.97	0.07	59,59,59,59	0
11	SF4	j	507	8/8	0.97	0.04	16,26,43,45	0
10	K	F	413	1/1	0.97	0.05	40,40,40,40	0
11	SF4	o	102	8/8	0.97	0.05	31,38,49,51	0
10	K	R	410	1/1	0.97	0.04	40,40,40,40	0
11	SF4	p	403	8/8	0.97	0.07	20,35,47,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	SF4	p	404	8/8	0.97	0.05	20,30,41,42	0
11	SF4	p	406	8/8	0.97	0.05	24,37,43,44	0
11	SF4	p	409	8/8	0.97	0.04	28,41,43,45	0
11	SF4	u	101	8/8	0.97	0.05	25,39,46,61	0
11	SF4	v	503	8/8	0.97	0.04	27,31,39,44	0
11	SF4	v	505	8/8	0.97	0.05	33,39,51,51	0
11	SF4	v	507	8/8	0.97	0.04	21,33,45,47	0
11	SF4	v	508	8/8	0.97	0.05	27,41,48,52	0
11	SF4	B	501	8/8	0.97	0.05	29,38,55,56	0
13	MGD	B	504	47/47	0.97	0.08	27,36,42,44	0
11	SF4	E	102	8/8	0.97	0.06	33,37,52,61	0
13	MGD	H	504	47/47	0.97	0.08	21,32,38,41	0
13	MGD	N	503	47/47	0.97	0.08	26,34,43,48	0
13	MGD	N	504	47/47	0.97	0.08	24,32,40,44	0
11	SF4	F	401	8/8	0.97	0.05	26,38,46,46	0
11	SF4	F	403	8/8	0.97	0.05	41,48,60,66	0
11	SF4	F	405	8/8	0.97	0.05	29,37,49,56	0
10	K	K	103	1/1	0.97	0.05	48,48,48,48	0
11	SF4	F	408	8/8	0.97	0.05	26,33,40,49	0
13	MGD	f	504	47/47	0.97	0.08	23,33,38,43	0
13	MGD	l	503	47/47	0.97	0.08	30,37,44,51	0
11	SF4	F	409	8/8	0.97	0.04	18,29,38,39	0
11	SF4	H	501	8/8	0.97	0.05	28,33,40,45	0
11	SF4	K	102	8/8	0.97	0.04	27,41,47,60	0
11	SF4	L	504	8/8	0.97	0.05	25,31,39,41	0
11	SF4	L	508	8/8	0.97	0.06	27,34,46,52	0
11	SF4	N	501	8/8	0.97	0.07	30,38,48,55	0
15	MG	Z	507	1/1	0.97	0.12	30,30,30,30	0
15	MG	l	506	1/1	0.97	0.05	32,32,32,32	0
11	SF4	Q	102	8/8	0.97	0.06	32,45,54,63	0
11	SF4	R	401	8/8	0.97	0.05	31,47,53,59	0
10	K	j	510	1/1	0.98	0.07	49,49,49,49	0
11	SF4	j	506	8/8	0.98	0.04	25,30,42,43	0
10	K	j	511	1/1	0.98	0.04	35,35,35,35	0
11	SF4	j	508	8/8	0.98	0.04	22,36,40,59	0
10	K	Q	103	1/1	0.98	0.07	53,53,53,53	0
11	SF4	o	101	8/8	0.98	0.04	27,35,45,55	0
11	SF4	R	406	8/8	0.98	0.04	33,36,50,59	0
11	SF4	p	401	8/8	0.98	0.04	24,34,47,52	0
11	SF4	E	101	8/8	0.98	0.06	36,43,51,58	0
11	SF4	R	408	8/8	0.98	0.03	21,28,40,41	0
10	K	j	513	1/1	0.98	0.04	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	SF4	p	405	8/8	0.98	0.04	17,21,36,39	0
10	K	X	509	1/1	0.98	0.05	42,42,42,42	0
11	SF4	p	407	8/8	0.98	0.04	25,32,44,51	0
11	SF4	F	402	8/8	0.98	0.04	18,36,46,49	0
11	SF4	r	501	8/8	0.98	0.05	31,43,47,51	0
10	K	o	103	1/1	0.98	0.04	42,42,42,42	0
11	SF4	u	102	8/8	0.98	0.06	26,34,43,46	0
11	SF4	v	501	8/8	0.98	0.04	20,33,44,46	0
11	SF4	v	502	8/8	0.98	0.04	15,26,36,42	0
11	SF4	X	501	8/8	0.98	0.05	34,41,58,62	0
11	SF4	v	504	8/8	0.98	0.05	18,36,41,42	0
11	SF4	X	502	8/8	0.98	0.04	22,36,39,53	0
11	SF4	v	506	8/8	0.98	0.04	19,27,43,47	0
11	SF4	X	503	8/8	0.98	0.04	28,33,40,61	0
11	SF4	F	404	8/8	0.98	0.04	22,35,44,57	0
7	ZN	q	602	1/1	0.98	0.03	39,39,39,39	0
11	SF4	F	406	8/8	0.98	0.04	20,35,46,49	0
10	K	B	506	1/1	0.98	0.10	54,54,54,54	0
11	SF4	X	508	8/8	0.98	0.04	26,29,41,46	0
9	NA	S	604	1/1	0.98	0.05	32,32,32,32	0
10	K	c	103	1/1	0.98	0.04	57,57,57,57	0
10	K	q	606	1/1	0.98	0.07	47,47,47,47	0
11	SF4	K	101	8/8	0.98	0.04	25,34,43,52	0
10	K	d	410	1/1	0.98	0.04	47,47,47,47	0
11	SF4	L	501	8/8	0.98	0.04	21,34,47,49	0
11	SF4	L	502	8/8	0.98	0.05	27,40,50,52	0
11	SF4	L	503	8/8	0.98	0.04	24,34,46,47	0
10	K	u	103	1/1	0.98	0.11	53,53,53,53	0
11	SF4	L	506	8/8	0.98	0.03	15,26,33,44	0
11	SF4	d	408	8/8	0.98	0.05	20,34,50,59	0
11	SF4	d	409	8/8	0.98	0.04	24,29,38,60	0
14	H2S	Z	505	1/1	0.98	0.11	63,63,63,63	0
11	SF4	L	507	8/8	0.98	0.04	21,27,40,43	0
10	K	S	605	1/1	0.98	0.04	32,32,32,32	0
10	K	e	605	1/1	0.98	0.06	34,34,34,34	0
15	MG	T	507	1/1	0.98	0.10	27,27,27,27	0
11	SF4	Q	101	8/8	0.98	0.04	23,36,48,49	0
10	K	e	606	1/1	0.98	0.04	37,37,37,37	0
10	K	S	606	1/1	0.98	0.08	46,46,46,46	0
10	K	i	103	1/1	0.98	0.03	36,36,36,36	0
11	SF4	L	505	8/8	0.99	0.03	22,32,41,49	0
7	ZN	M	601	1/1	0.99	0.02	51,51,51,51	0

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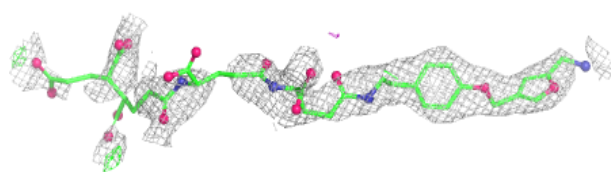
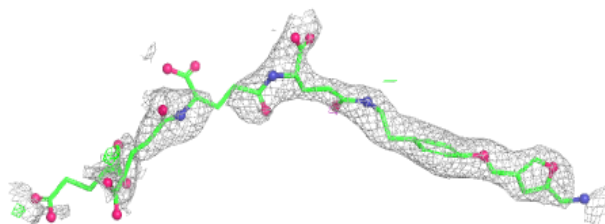
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	K	k	605	1/1	0.99	0.03	36,36,36,36	0
11	SF4	p	408	8/8	0.99	0.03	21,34,40,44	0
7	ZN	M	602	1/1	0.99	0.06	46,46,46,46	0
10	K	Y	604	1/1	0.99	0.10	38,38,38,38	0
7	ZN	S	601	1/1	0.99	0.04	40,40,40,40	0
10	K	M	605	1/1	0.99	0.03	37,37,37,37	0
7	ZN	S	602	1/1	0.99	0.02	32,32,32,32	0
10	K	A	605	1/1	0.99	0.04	49,49,49,49	0
7	ZN	Y	602	1/1	0.99	0.04	47,47,47,47	0
10	K	E	103	1/1	0.99	0.04	43,43,43,43	0
14	H2S	B	505	1/1	0.99	0.08	44,44,44,44	0
14	H2S	H	505	1/1	0.99	0.11	41,41,41,41	0
14	H2S	N	505	1/1	0.99	0.10	50,50,50,50	0
14	H2S	T	505	1/1	0.99	0.10	50,50,50,50	0
10	K	e	607	1/1	0.99	0.04	51,51,51,51	0
14	H2S	f	505	1/1	0.99	0.06	38,38,38,38	0
7	ZN	e	602	1/1	0.99	0.03	34,34,34,34	0
7	ZN	k	601	1/1	0.99	0.03	46,46,46,46	0
10	K	j	509	1/1	0.99	0.08	37,37,37,37	0
15	MG	H	506	1/1	0.99	0.06	24,24,24,24	0
15	MG	O	301	1/1	0.99	0.10	31,31,31,31	0
12	W	Z	502	1/1	0.99	0.11	63,63,63,63	0
7	ZN	q	601	1/1	0.99	0.03	39,39,39,39	0
15	MG	f	506	1/1	0.99	0.10	28,28,28,28	0
7	ZN	A	601	1/1	0.99	0.03	40,40,40,40	0
10	K	G	605	1/1	0.99	0.05	62,62,62,62	0
7	ZN	G	602	1/1	0.99	0.02	40,40,40,40	0
12	W	f	502	1/1	1.00	0.10	52,52,52,52	0
12	W	l	502	1/1	1.00	0.08	48,48,48,48	0
12	W	r	502	1/1	1.00	0.05	48,48,48,48	0
7	ZN	A	602	1/1	1.00	0.02	41,41,41,41	0
7	ZN	Y	601	1/1	1.00	0.04	45,45,45,45	0
7	ZN	k	602	1/1	1.00	0.02	44,44,44,44	0
7	ZN	G	601	1/1	1.00	0.02	41,41,41,41	0
12	W	B	502	1/1	1.00	0.04	43,43,43,43	0
12	W	H	502	1/1	1.00	0.04	37,37,37,37	0
12	W	N	502	1/1	1.00	0.02	34,34,34,34	0
12	W	T	502	1/1	1.00	0.08	49,49,49,49	0
7	ZN	e	601	1/1	1.00	0.02	38,38,38,38	0

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.

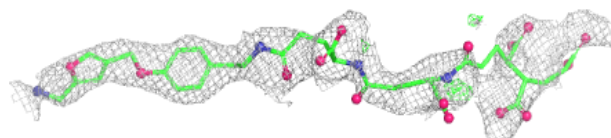
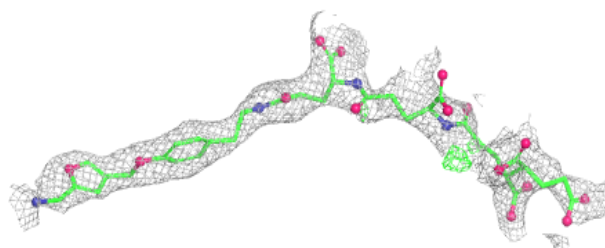
Electron density around MFN M 603:

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



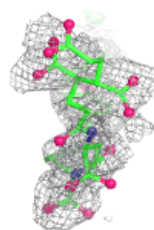
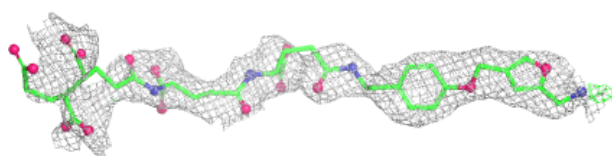
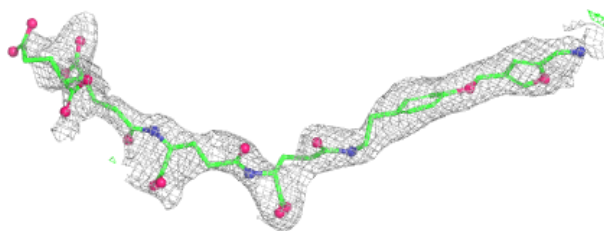
Electron density around MFN k 603:

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

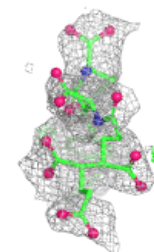
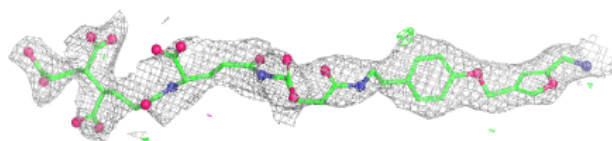
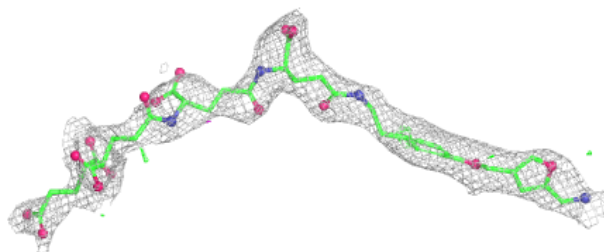


Electron density around MFN q 603:

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

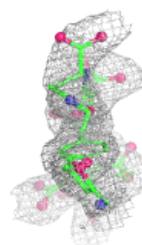
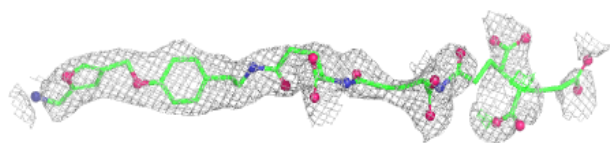
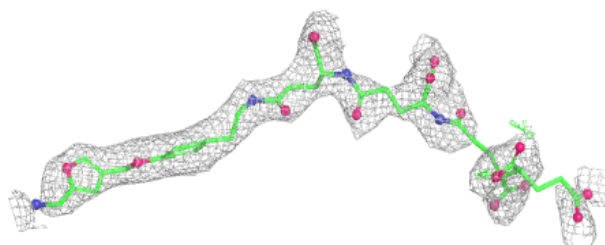
**Electron density around MFN A 603:**

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

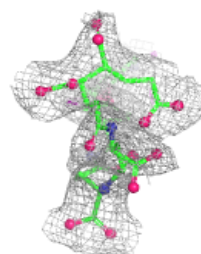
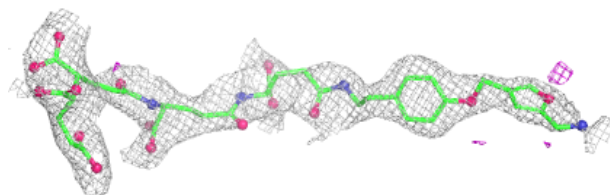
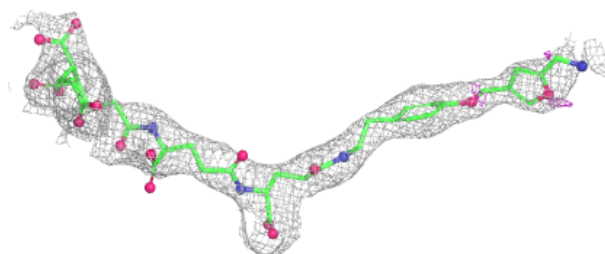


Electron density around MFN Y 603:

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

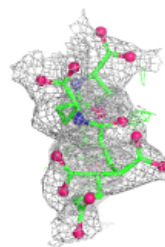
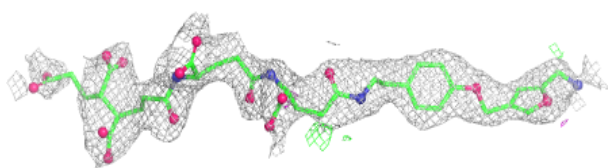
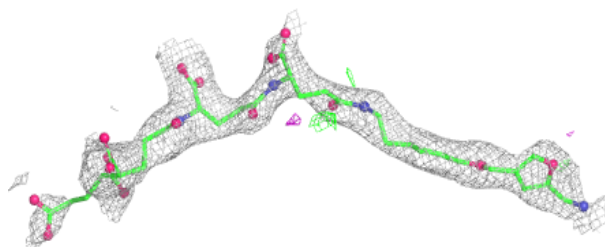
**Electron density around MFN G 603:**

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

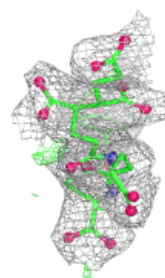
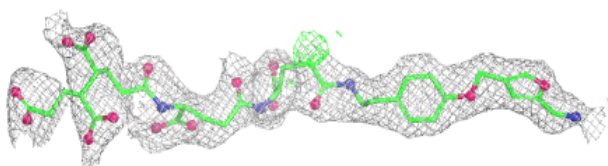
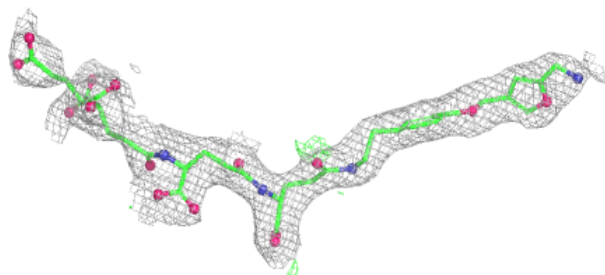


Electron density around MFN e 603:

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

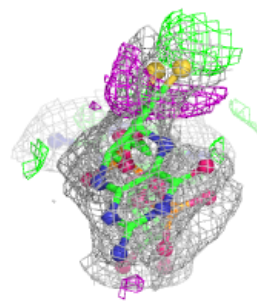
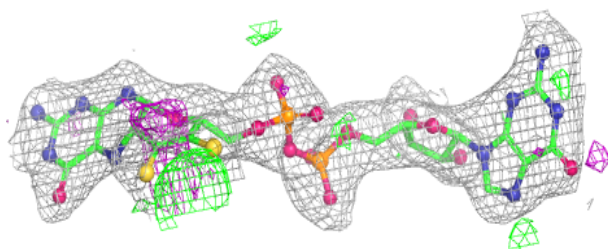
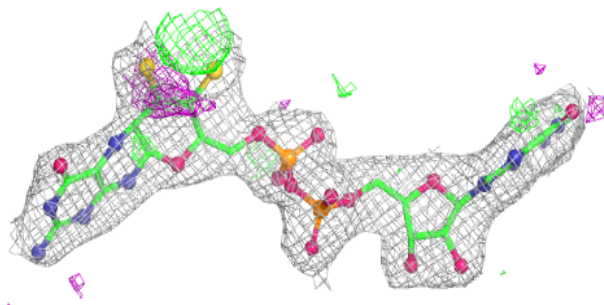
**Electron density around MFN S 603:**

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

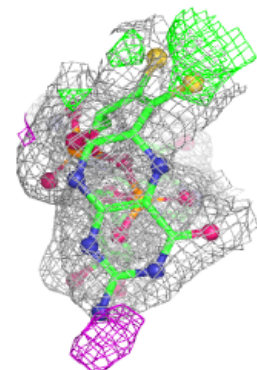
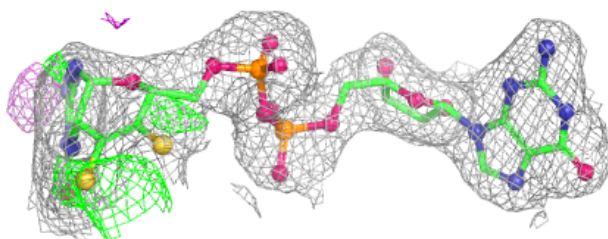
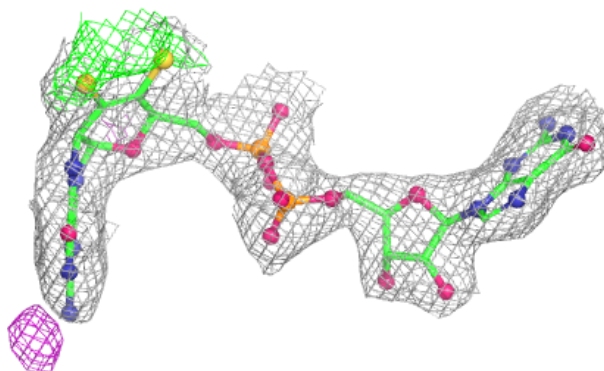


Electron density around MGD Z 503:

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

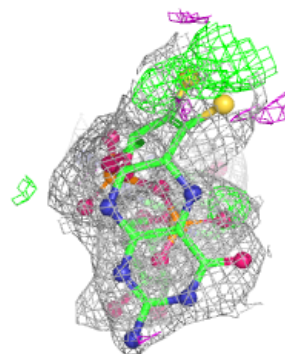
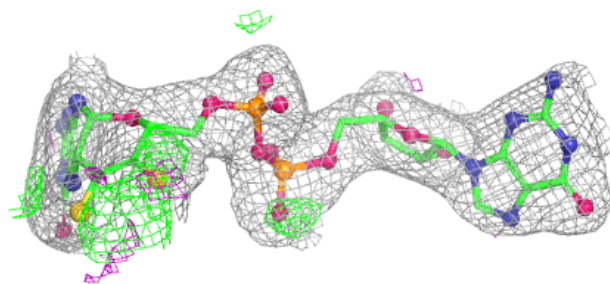
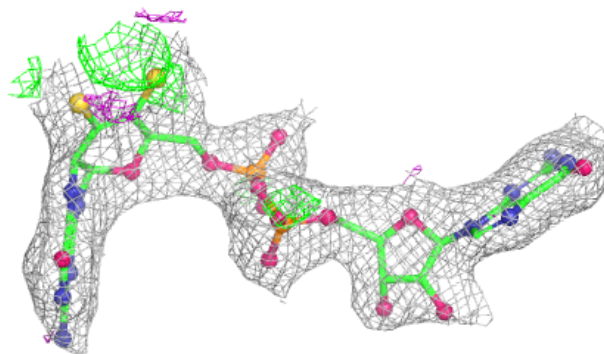
**Electron density around MGD T 504:**

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

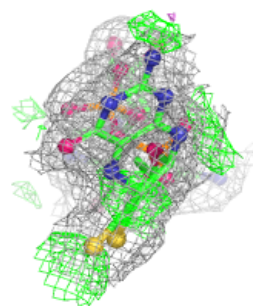
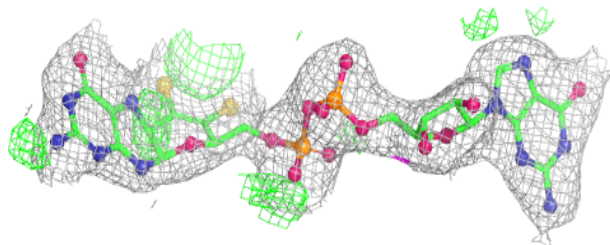
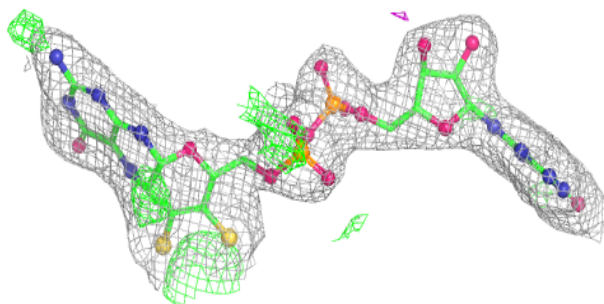


Electron density around MGD Z 504:

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

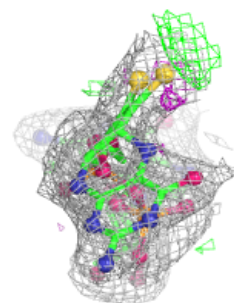
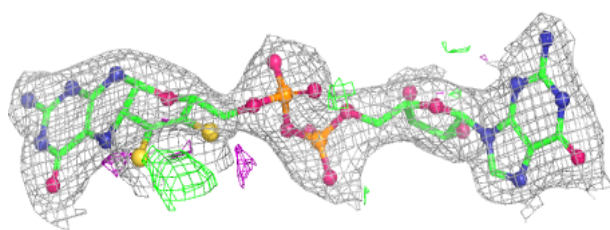
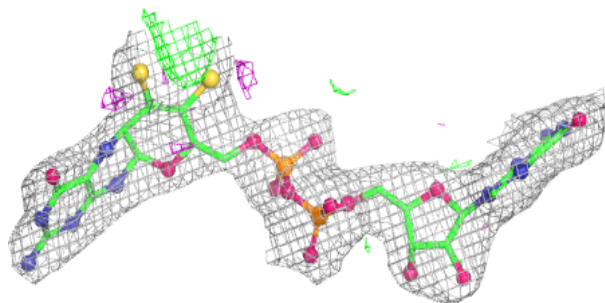
**Electron density around MGD f 503:**

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

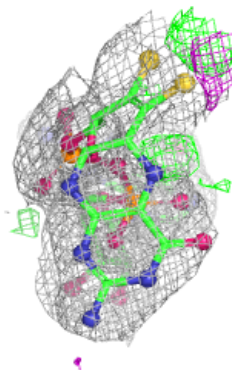
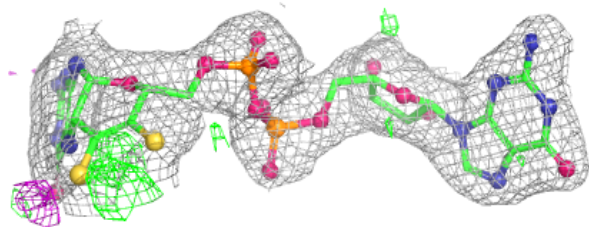
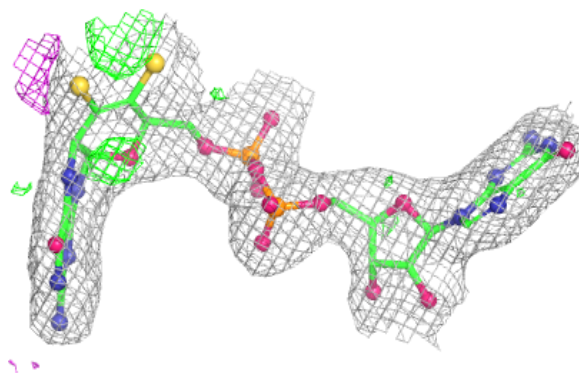


Electron density around MGD r 503:

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

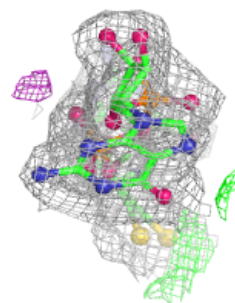
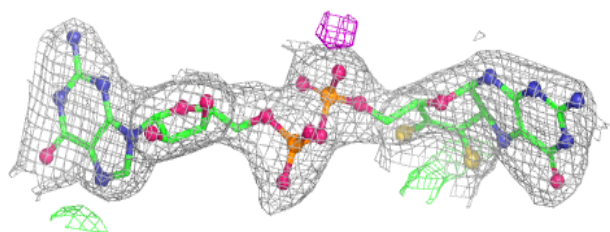
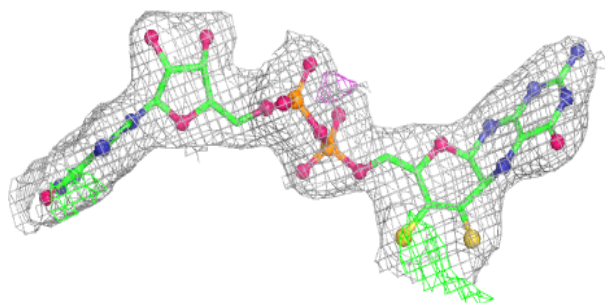
**Electron density around MGD r 504:**

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

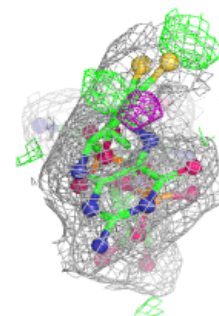
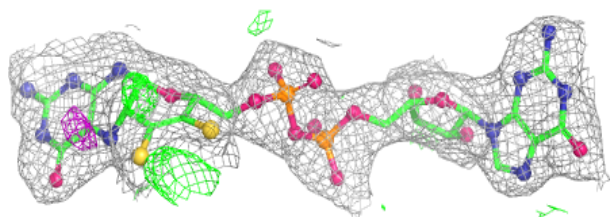
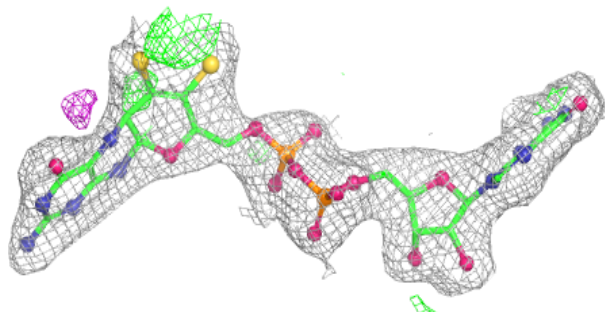


Electron density around MGD B 503:

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

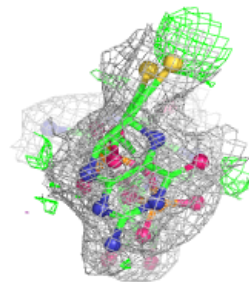
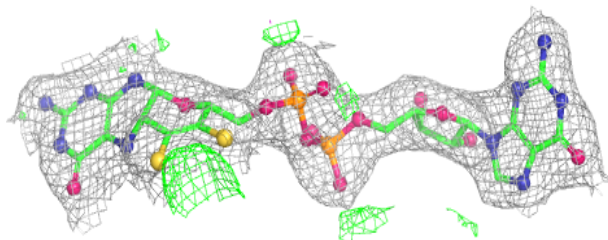
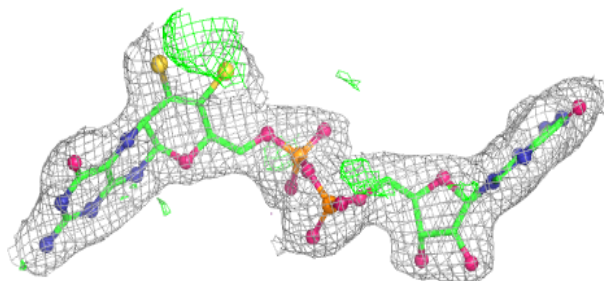
**Electron density around MGD H 503:**

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

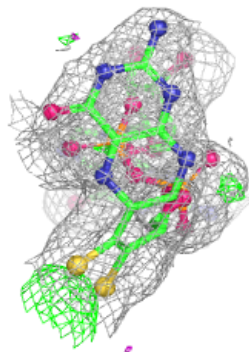
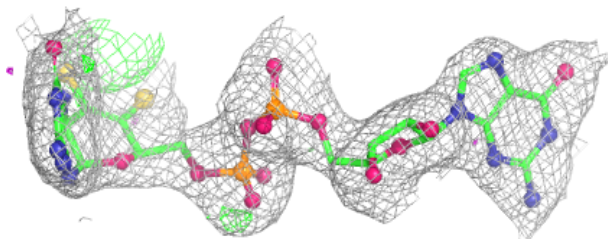
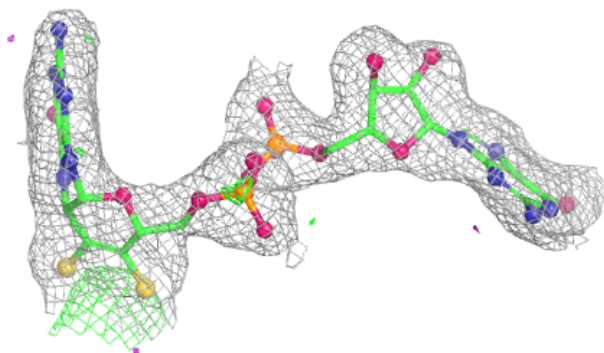


Electron density around MGD T 503:

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

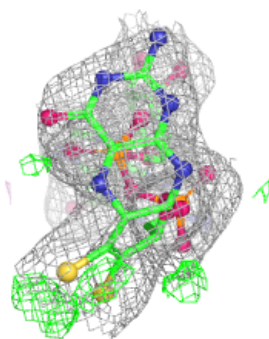
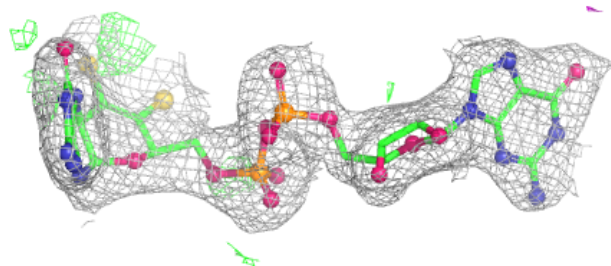
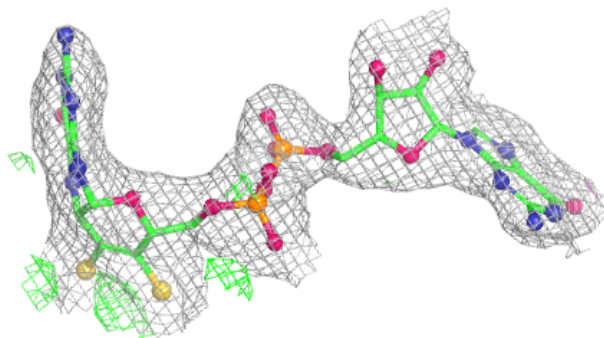
**Electron density around MGD I 504:**

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

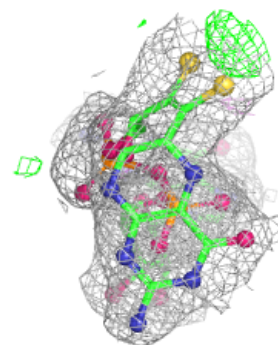
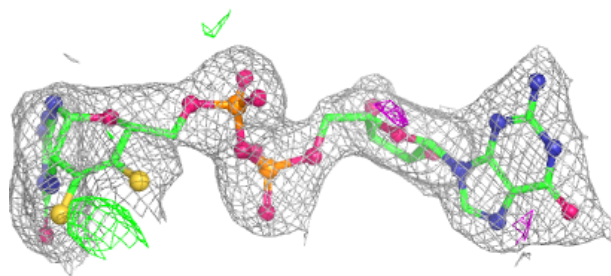
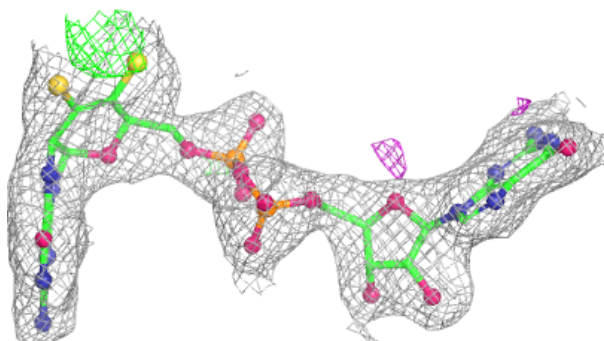


Electron density around MGD B 504:

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

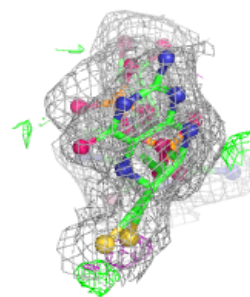
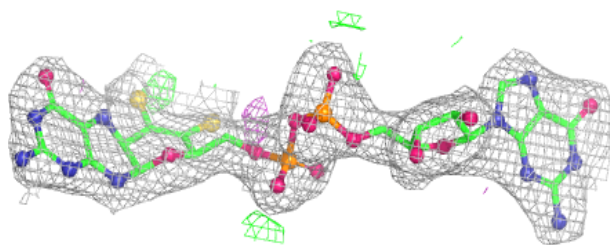
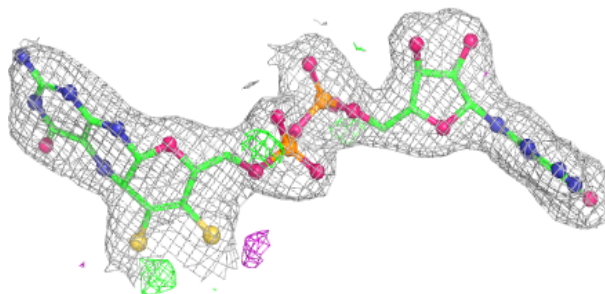
**Electron density around MGD H 504:**

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

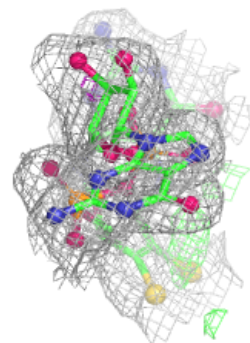
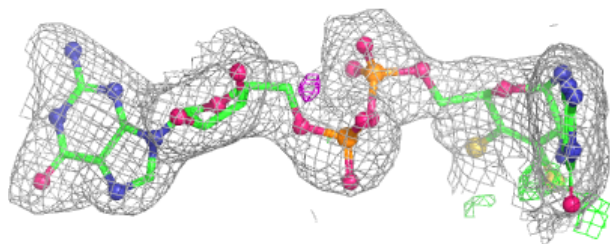
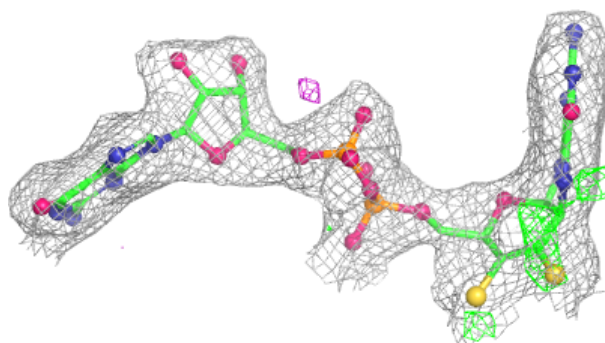


Electron density around MGD N 503:

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

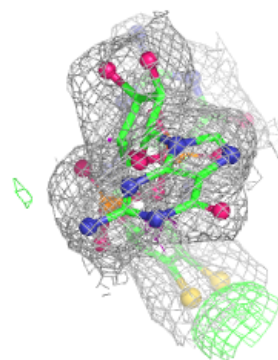
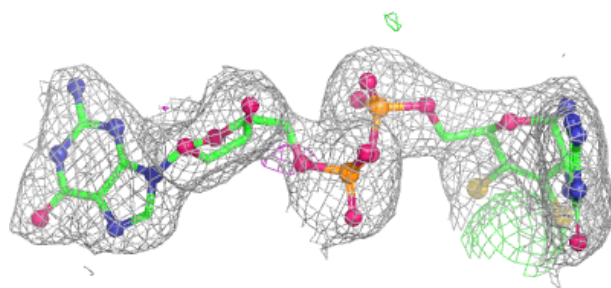
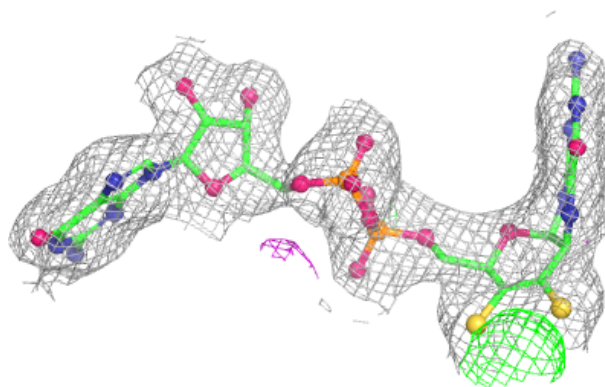
**Electron density around MGD N 504:**

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

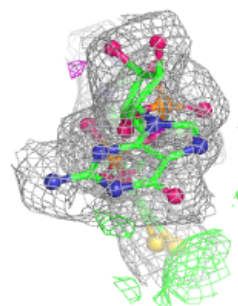
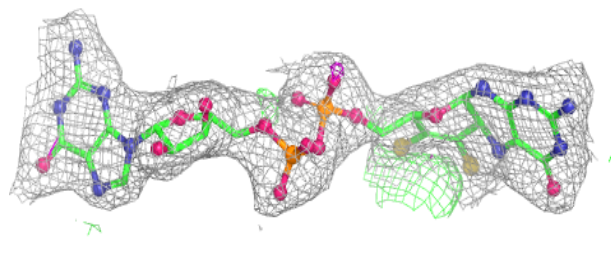
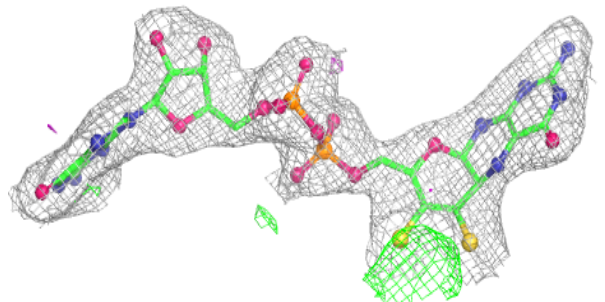


Electron density around MGD f 504:

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

**Electron density around MGD l 503:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.