



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 02:48 pm GMT

PDB ID : 5T61  
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

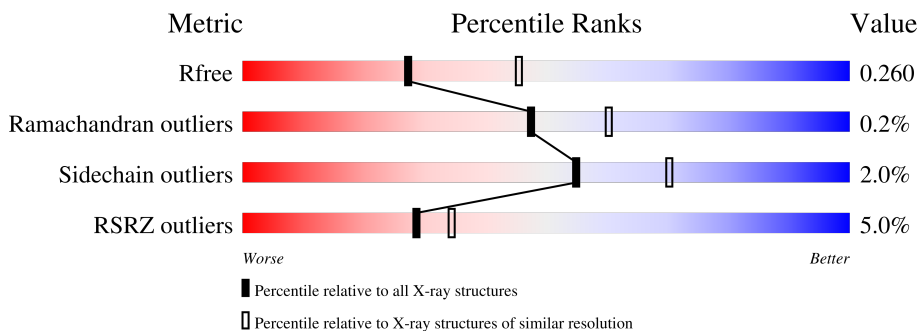
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	1284 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	569	 2% 99%
1	G	569	 5% 98%
1	M	569	 12% 98%
1	S	569	 2% 98%
1	Y	569	 10% 99%
1	e	569	 2% 98%

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Mol	Chain	Length	Quality of chain
1	k	569	10% 98%
1	q	569	4% 98%
2	B	432	3% 96%
2	H	432	4% 96%
2	N	432	6% 97%
2	T	432	4% 96%
2	Z	432	7% 96%
2	f	432	4% 96%
2	l	432	8% 97%
2	r	432	5% 95%
3	C	270	9% 98%
3	I	270	2% 98%
3	O	270	% 98%
3	U	270	6% 98%
3	a	270	% 97%
3	g	270	8% 98%
3	m	270	% 97%
3	s	270	8% 99%
4	D	130	5% 98%
4	J	130	2% 98%
4	P	130	3% 99%
4	V	130	4% 97%
4	b	130	2% 99%
4	h	130	3% 98%
4	n	130	4% 97%

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Mol	Chain	Length	Quality of chain
4	t	130	6% 97% ..
5	E	82	% 93% 5% .
5	K	82	% 93% 5% .
5	Q	82	% 93% 5% .
5	W	82	4% 90% 7% .
5	c	82	4% 93% 5% .
5	i	82	% 91% 6% .
5	o	82	% 93% 5% .
5	u	82	% 91% 7% .
6	F	349	5% 95% ... .
6	L	349	% 97% .
6	R	349	11% 94% ..
6	X	349	4% 96% ..
6	d	349	12% 94% ... .
6	j	349	4% 96% ..
6	p	349	3% 96% .
6	v	349	2% 95% ... .

## 2 Entry composition

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
			Total	C	N	O	S			
1	A	569	4419	2812	735	849	23	0	0	0
1	G	568	4411	2807	734	848	22	0	0	0
1	M	568	4411	2807	734	848	22	0	0	0
1	S	569	4419	2812	735	849	23	0	0	0
1	Y	568	4411	2807	734	848	22	0	0	0
1	e	569	4419	2812	735	849	23	0	0	0
1	k	568	4411	2807	734	848	22	0	0	0
1	q	569	4419	2812	735	849	23	0	0	0

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

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

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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
			Total	C	N	O	S			
4	t	129	997	637	162	189	9	0	0	0

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

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

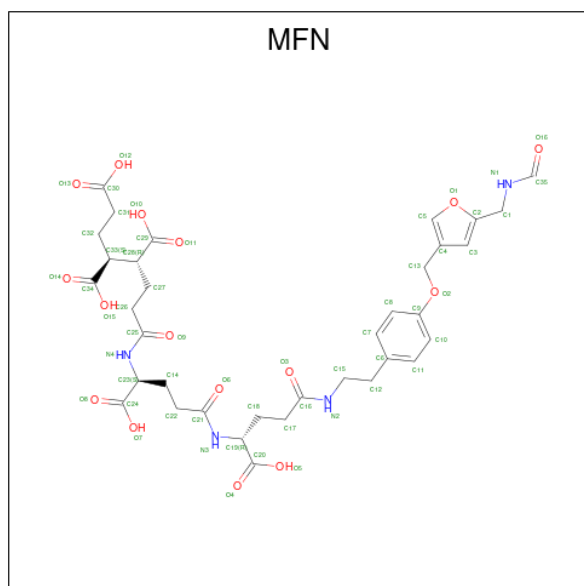
- Molecule 6 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdF.

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

- Molecule 7 is ZINC ION (three-letter code: 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 (three-letter code: MFN) (formula: C<sub>35</sub>H<sub>44</sub>N<sub>4</sub>O<sub>16</sub>).



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 (three-letter code: 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 (three-letter code: 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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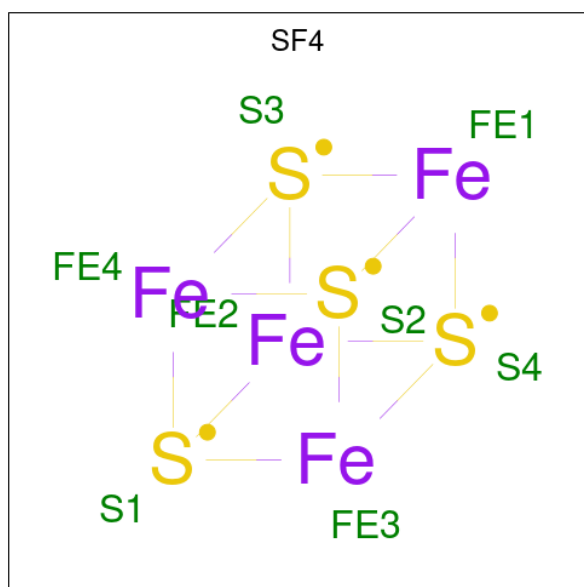
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	G	1	Total K 1 1	0	0
10	K	1	Total K 1 1	0	0
10	L	3	Total K 3 3	0	0
10	M	2	Total K 2 2	0	0
10	N	1	Total K 1 1	0	0
10	Q	1	Total K 1 1	0	0
10	R	3	Total K 3 3	0	0
10	S	2	Total K 2 2	0	0
10	T	1	Total K 1 1	0	0
10	X	3	Total K 3 3	0	0
10	Y	1	Total K 1 1	0	0
10	Z	1	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 1 1	0	0
10	u	1	Total K 1 1	0	0
10	v	7	Total K 7 7	0	0

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

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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	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	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
			Total	Fe	S		
11	d	1	8	4	4	0	0
11	d	1	8	4	4	0	0
11	d	1	8	4	4	0	0
11	d	1	8	4	4	0	0
11	d	1	8	4	4	0	0
11	d	1	8	4	4	0	0
11	d	1	8	4	4	0	0
11	d	1	8	4	4	0	0
11	d	1	8	4	4	0	0
11	f	1	8	4	4	0	0
11	i	1	8	4	4	0	0
11	i	1	8	4	4	0	0
11	j	1	8	4	4	0	0
11	j	1	8	4	4	0	0
11	j	1	8	4	4	0	0
11	j	1	8	4	4	0	0
11	j	1	8	4	4	0	0
11	j	1	8	4	4	0	0
11	j	1	8	4	4	0	0
11	j	1	8	4	4	0	0
11	j	1	8	4	4	0	0
11	l	1	8	4	4	0	0
11	o	1	8	4	4	0	0

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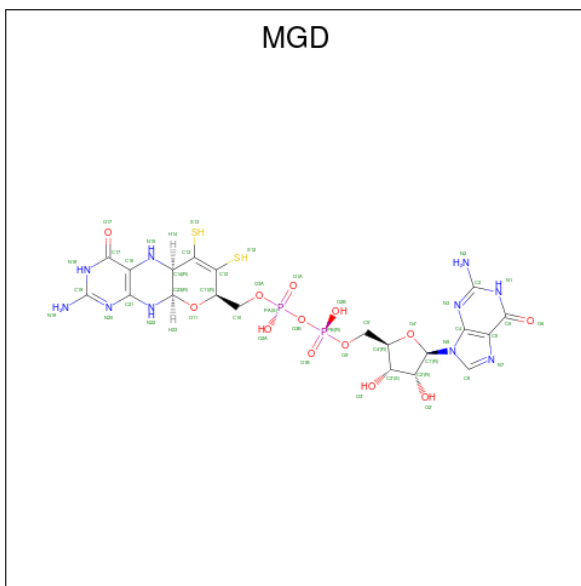
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	o	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total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

- Molecule 12 is TUNGSTEN ION (three-letter code: W) (formula: W).

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

- Molecule 13 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).



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

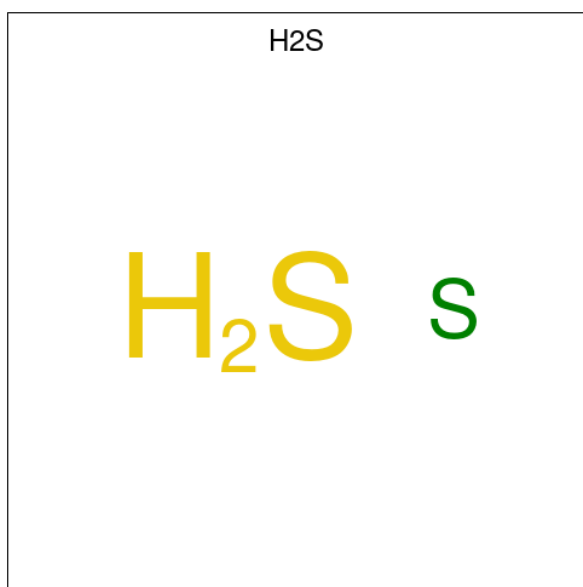
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
13	H	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	H	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	N	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	N	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	T	1	Total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

- Molecule 14 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H<sub>2</sub>S).



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 (three-letter code: 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

*Continued on next page...*

*Continued from previous page...*

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 (three-letter code: 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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

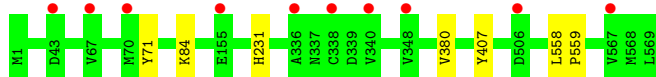
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	h	3	Total O 3 3	0	0
17	i	8	Total O 8 8	0	0
17	j	20	Total O 20 20	0	0
17	k	9	Total O 9 9	0	0
17	l	20	Total O 20 20	0	0
17	m	7	Total O 7 7	0	0
17	n	4	Total O 4 4	0	0
17	o	2	Total O 2 2	0	0
17	p	18	Total O 18 18	0	0
17	q	27	Total O 27 27	0	0
17	r	16	Total O 16 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.

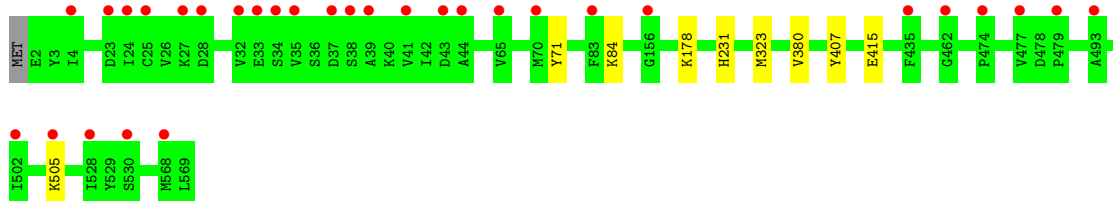
- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

Chain A: 



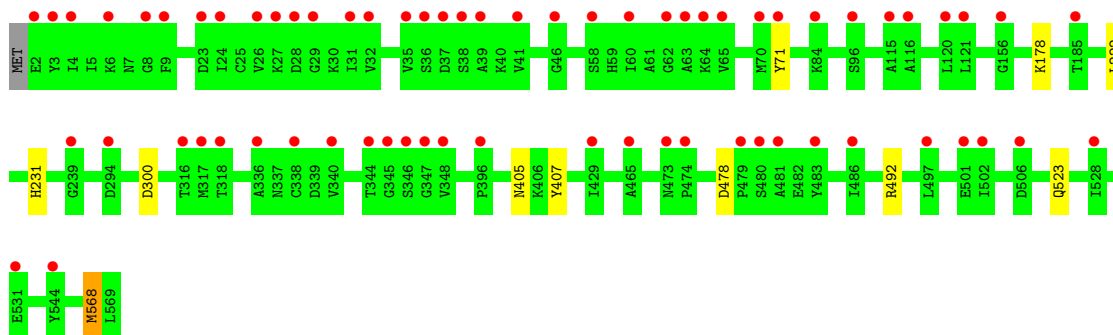
- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

Chain G: 



- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

Chain M: 



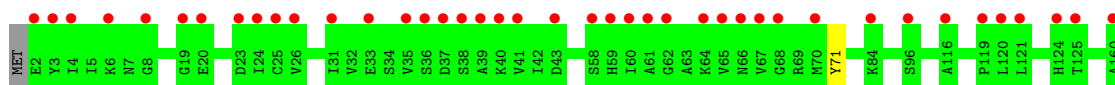
- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

Chain S: 





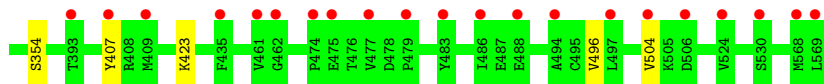
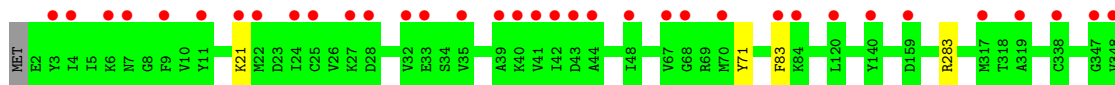
- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA



- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA



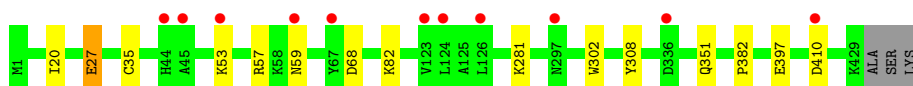
- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA



- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

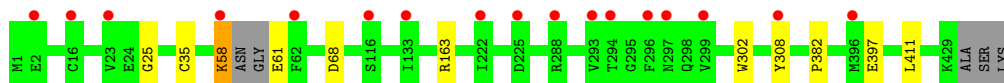


- Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B



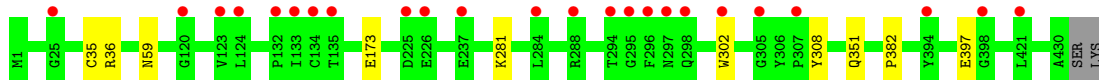
- Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

Chain H: 



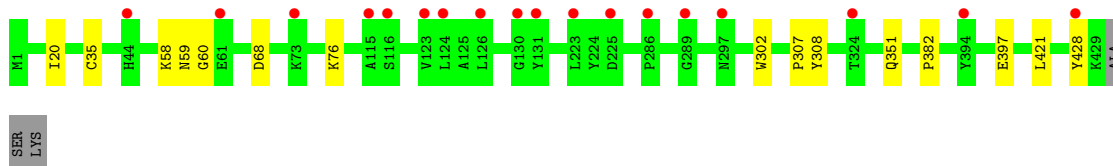
• Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

Chain N: 



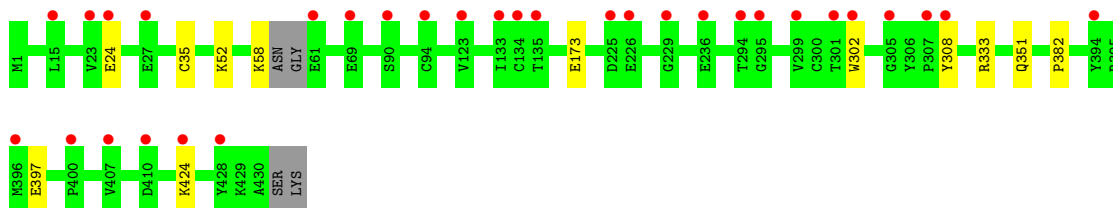
• Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

Chain T: 



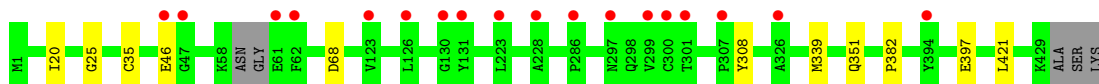
• Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

Chain Z: 



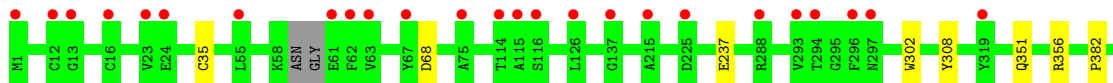
• Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

Chain f: 

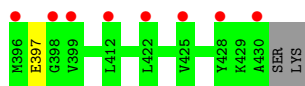


• Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

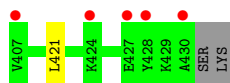
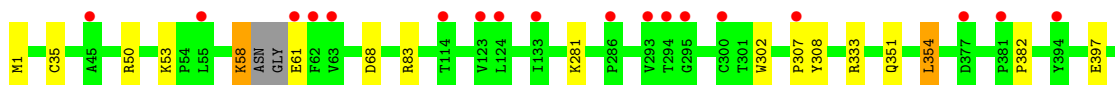
Chain l: 



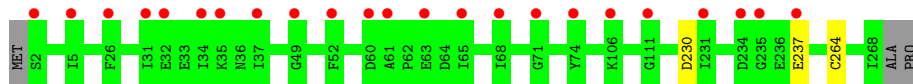




- Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B



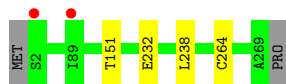
- Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C



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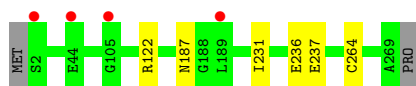


- Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C



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

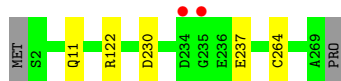




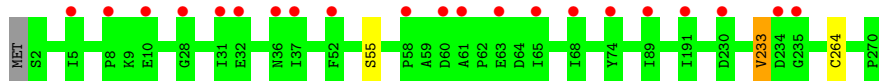
- Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C



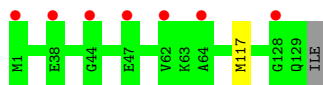
- Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C



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



- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD



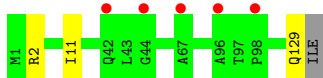
- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD



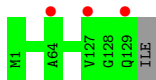
- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD



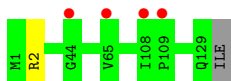
- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD



- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD



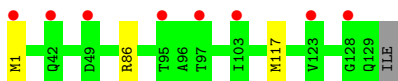
- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD



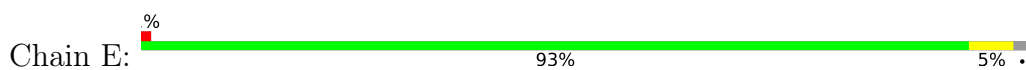
- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD



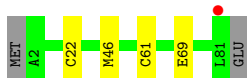
- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD



- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



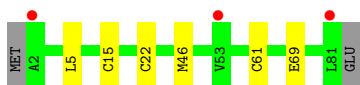
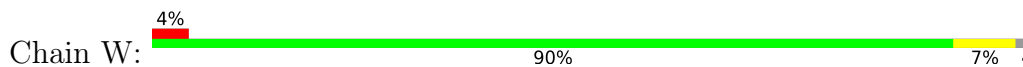
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



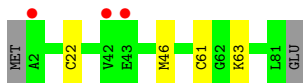
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



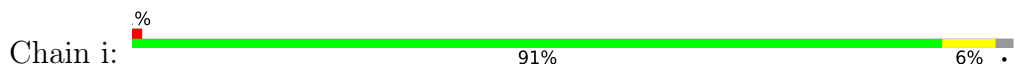
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



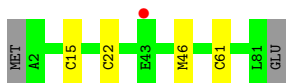
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



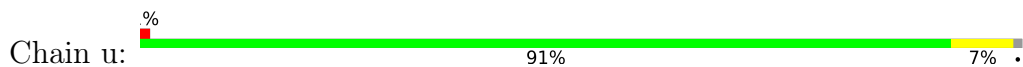
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG



- Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF

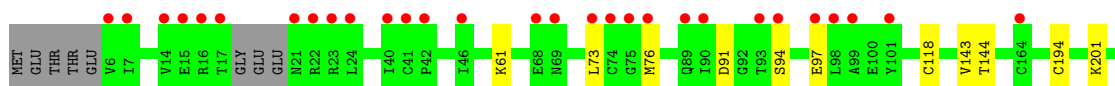
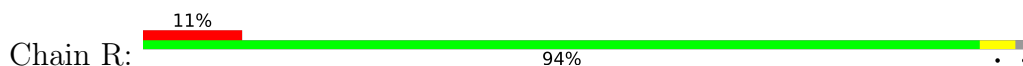




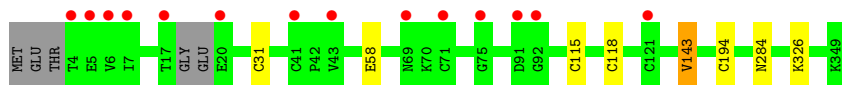
- Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF



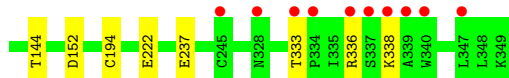
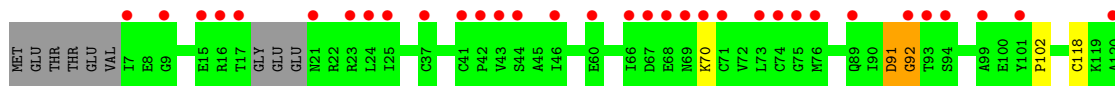
- Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF



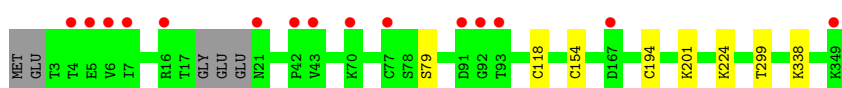
- Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF



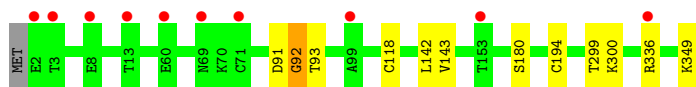
- Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.54Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.229 , 0.259 0.230 , 0.260	Depositor DCC
$R_{free}$ test set	34085 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtrriage
Anisotropy	0.213	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.118 for -h,k,-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	114321	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage'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.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.36	3/4523 (0.1%)	0.54	0/6161
1	G	0.32	0/4515	0.54	0/6151
1	M	0.34	0/4515	0.59	4/6151 (0.1%)
1	S	0.35	2/4523 (0.0%)	0.56	3/6161 (0.0%)
1	Y	0.34	0/4515	0.61	5/6151 (0.1%)
1	e	0.33	0/4523	0.54	1/6161 (0.0%)
1	k	0.34	0/4515	0.60	4/6151 (0.1%)
1	q	0.51	9/4523 (0.2%)	0.66	12/6161 (0.2%)
2	B	0.35	1/3434 (0.0%)	0.58	1/4647 (0.0%)
2	H	0.42	2/3421 (0.1%)	0.62	4/4628 (0.1%)
2	N	0.29	0/3439	0.56	1/4654 (0.0%)
2	T	0.35	2/3434 (0.1%)	0.58	4/4647 (0.1%)
2	Z	0.42	5/3426 (0.1%)	0.59	2/4635 (0.0%)
2	f	0.37	2/3421 (0.1%)	0.54	0/4628
2	l	0.33	1/3426 (0.0%)	0.56	2/4635 (0.0%)
2	r	0.50	4/3426 (0.1%)	0.70	10/4635 (0.2%)
3	C	0.36	0/2014	0.64	1/2710 (0.0%)
3	I	0.43	4/2027 (0.2%)	0.57	0/2729
3	O	0.29	0/2019	0.56	1/2717 (0.0%)
3	U	0.30	0/2019	0.58	1/2717 (0.0%)
3	a	0.30	0/2019	0.59	1/2717 (0.0%)
3	g	0.34	0/2019	0.63	2/2717 (0.1%)
3	m	0.31	0/2019	0.59	2/2717 (0.1%)
3	s	0.39	0/2027	0.63	1/2729 (0.0%)
4	D	0.30	0/1016	0.60	0/1379
4	J	0.29	0/1016	0.54	0/1379
4	P	0.27	0/1016	0.56	0/1379
4	V	0.28	0/1016	0.57	0/1379
4	b	0.29	0/1016	0.54	0/1379
4	h	0.30	0/1016	0.59	0/1379
4	n	0.31	0/1016	0.62	1/1379 (0.1%)
4	t	0.37	0/1016	0.71	2/1379 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
5	E	0.37	0/579	0.53	0/787
5	K	0.43	0/579	0.61	0/787
5	Q	0.32	0/579	0.54	0/787
5	W	0.31	0/579	0.56	0/787
5	c	0.30	0/579	0.57	0/787
5	i	0.33	0/579	0.60	1/787 (0.1%)
5	o	0.34	0/579	0.54	0/787
5	u	0.32	0/588	0.58	0/799
6	F	0.35	1/2667 (0.0%)	0.58	1/3616 (0.0%)
6	L	0.37	1/2695 (0.0%)	0.61	2/3655 (0.1%)
6	R	0.42	3/2640 (0.1%)	0.68	5/3579 (0.1%)
6	X	0.40	2/2665 (0.1%)	0.65	2/3613 (0.1%)
6	d	0.43	2/2633 (0.1%)	0.66	3/3569 (0.1%)
6	j	0.33	0/2663	0.58	0/3611
6	p	0.37	2/2695 (0.1%)	0.59	1/3655 (0.0%)
6	v	0.47	4/2681 (0.1%)	0.65	2/3635 (0.1%)
All	All	0.37	50/113850 (0.0%)	0.59	82/154383 (0.1%)

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

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	r	61	GLU	CD-OE1	13.10	1.40	1.25
2	H	61	GLU	CD-OE2	12.01	1.38	1.25
2	r	61	GLU	CD-OE2	11.46	1.38	1.25
1	q	423	LYS	CB-CG	-10.87	1.23	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	r	58	LYS	CD-CE	-9.80	1.26	1.51
1	q	419	TRP	CE3-CZ3	-9.51	1.22	1.38
2	f	46	GLU	CD-OE1	-9.35	1.15	1.25
2	H	61	GLU	CD-OE1	-8.88	1.15	1.25
2	f	46	GLU	CD-OE2	-8.33	1.16	1.25
1	q	419	TRP	CG-CD1	8.07	1.48	1.36
6	v	23	ARG	NE-CZ	-7.72	1.23	1.33
1	q	423	LYS	CD-CE	-7.60	1.32	1.51
2	Z	424	LYS	CE-NZ	-7.51	1.30	1.49
2	Z	333	ARG	NE-CZ	-7.46	1.23	1.33
1	q	419	TRP	CD1-NE1	7.20	1.50	1.38
2	Z	333	ARG	CZ-NH1	-7.03	1.24	1.33
1	S	356	ARG	C-N	-6.91	1.18	1.34
6	R	97	GLU	CD-OE1	-6.73	1.18	1.25
2	T	428	TYR	CD1-CE1	-6.41	1.29	1.39
3	I	44	GLU	CD-OE1	-6.31	1.18	1.25
1	q	415	GLU	CB-CG	-6.27	1.40	1.52
1	A	558	LEU	CA-CB	6.26	1.68	1.53
3	I	237	GLU	CD-OE1	-6.26	1.18	1.25
6	v	349	LYS	CD-CE	-6.20	1.35	1.51
2	Z	24	GLU	CG-CD	6.05	1.61	1.51
6	v	23	ARG	CZ-NH2	-6.00	1.25	1.33
1	q	415	GLU	CG-CD	-5.99	1.43	1.51
6	X	326	LYS	CE-NZ	5.95	1.64	1.49
1	q	356	ARG	C-N	-5.94	1.20	1.34
1	A	559	PRO	C-O	5.80	1.34	1.23
2	T	428	TYR	CB-CG	-5.78	1.43	1.51
6	d	237	GLU	CD-OE1	-5.64	1.19	1.25
1	S	286	VAL	CB-CG2	5.56	1.64	1.52
6	v	143	VAL	CB-CG2	5.54	1.64	1.52
6	d	237	GLU	CD-OE2	-5.53	1.19	1.25
6	X	143	VAL	CB-CG2	5.44	1.64	1.52
6	p	180	SER	C-N	5.44	1.44	1.34
3	I	44	GLU	CD-OE2	-5.41	1.19	1.25
3	I	237	GLU	CD-OE2	-5.41	1.19	1.25
6	F	143	VAL	CB-CG2	5.39	1.64	1.52
1	A	559	PRO	N-CA	-5.38	1.38	1.47
2	Z	333	ARG	CZ-NH2	-5.35	1.26	1.33
2	r	58	LYS	CE-NZ	-5.21	1.36	1.49
6	R	143	VAL	CB-CG2	5.14	1.63	1.52
2	B	27	GLU	CD-OE1	-5.14	1.20	1.25
6	p	143	VAL	CB-CG2	5.09	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	143	VAL	CB-CG2	5.09	1.63	1.52
6	R	97	GLU	CD-OE2	-5.07	1.20	1.25
2	l	237	GLU	CD-OE2	5.05	1.31	1.25
1	q	286	VAL	CB-CG2	5.04	1.63	1.52

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	r	58	LYS	CD-CE-NZ	-19.53	66.79	111.70
2	H	61	GLU	OE1-CD-OE2	12.47	138.26	123.30
2	r	354	LEU	CB-CG-CD1	-12.13	90.38	111.00
1	q	356	ARG	NE-CZ-NH1	-11.58	114.51	120.30
6	v	92	GLY	N-CA-C	11.39	141.59	113.10
1	Y	221	LYS	CD-CE-NZ	-9.99	88.71	111.70
4	t	1	MET	CA-CB-CG	9.89	130.11	113.30
2	H	163	ARG	NE-CZ-NH1	-9.40	115.60	120.30
2	r	1	MET	CG-SD-CE	-8.77	86.16	100.20
1	S	569	LEU	CB-CG-CD2	-8.74	96.14	111.00
1	q	467	ILE	CG1-CB-CG2	-8.66	92.35	111.40
1	Y	300	ASP	CB-CG-OD2	8.63	126.06	118.30
2	T	428	TYR	CB-CG-CD1	-8.58	115.85	121.00
6	R	76	MET	CG-SD-CE	-8.21	87.06	100.20
2	H	163	ARG	NE-CZ-NH2	8.02	124.31	120.30
6	p	92	GLY	N-CA-C	7.57	132.03	113.10
6	R	73	LEU	CB-CG-CD2	7.56	123.86	111.00
1	Y	569	LEU	CA-CB-CG	7.39	132.29	115.30
1	q	423	LYS	CB-CA-C	-7.36	95.67	110.40
2	H	58	LYS	CD-CE-NZ	-7.22	95.10	111.70
2	r	333	ARG	CG-CD-NE	-7.20	96.67	111.80
6	R	61	LYS	CD-CE-NZ	-7.19	95.16	111.70
1	q	356	ARG	NE-CZ-NH2	7.14	123.87	120.30
6	L	92	GLY	N-CA-C	7.13	130.92	113.10
6	X	58	GLU	CB-CA-C	7.09	124.58	110.40
6	d	92	GLY	N-CA-C	7.08	130.80	113.10
3	C	230	ASP	CB-CG-OD1	6.79	124.41	118.30
1	q	300	ASP	CB-CG-OD2	6.68	124.31	118.30
1	k	283	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	M	478	ASP	CB-CG-OD1	6.51	124.16	118.30
1	M	300	ASP	CB-CG-OD1	6.50	124.15	118.30
1	q	423	LYS	CD-CE-NZ	-6.50	96.76	111.70
6	F	92	GLY	N-CA-C	6.48	129.31	113.10
1	q	419	TRP	CH2-CZ2-CE2	-6.42	110.98	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	g	125	GLU	CB-CA-C	6.27	122.94	110.40
1	e	426	VAL	CG1-CB-CG2	6.16	120.76	110.90
4	n	103	ILE	CA-CB-CG1	-6.13	99.35	111.00
1	M	478	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	S	221	LYS	CD-CE-NZ	6.12	125.78	111.70
2	T	428	TYR	CB-CG-CD2	6.04	124.62	121.00
2	r	58	LYS	CB-CG-CD	-5.97	96.08	111.60
6	X	58	GLU	N-CA-CB	-5.95	99.90	110.60
2	l	237	GLU	CG-CD-OE1	-5.87	106.56	118.30
4	t	86	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	k	496	VAL	CG1-CB-CG2	-5.85	101.54	110.90
1	Y	300	ASP	CB-CG-OD1	-5.83	113.05	118.30
3	m	122	ARG	NE-CZ-NH1	5.82	123.21	120.30
3	s	233	VAL	CG1-CB-CG2	5.72	120.06	110.90
6	R	97	GLU	CA-CB-CG	5.71	125.96	113.40
1	q	422	ARG	CB-CG-CD	-5.66	96.89	111.60
2	T	76	LYS	CD-CE-NZ	-5.65	98.71	111.70
1	q	422	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	k	21	LYS	CD-CE-NZ	-5.58	98.86	111.70
2	B	27	GLU	CG-CD-OE1	5.56	129.42	118.30
2	T	428	TYR	CA-CB-CG	-5.56	102.84	113.40
2	r	61	GLU	CA-CB-CG	5.56	125.62	113.40
6	L	293	LYS	CD-CE-NZ	5.54	124.45	111.70
2	r	50	ARG	NE-CZ-NH2	5.50	123.05	120.30
2	Z	24	GLU	CG-CD-OE2	5.49	129.28	118.30
2	r	61	GLU	CG-CD-OE1	-5.46	107.38	118.30
1	S	505	LYS	CD-CE-NZ	-5.43	99.21	111.70
6	d	70	LYS	CB-CG-CD	-5.43	97.47	111.60
3	g	238	LEU	CB-CG-CD2	-5.38	101.86	111.00
2	r	421	LEU	CB-CG-CD2	-5.37	101.88	111.00
3	a	122	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	l	356	ARG	NE-CZ-NH1	5.31	122.96	120.30
2	Z	24	GLU	CG-CD-OE1	-5.28	107.74	118.30
1	k	504	VAL	CG1-CB-CG2	5.27	119.34	110.90
3	O	238	LEU	CB-CG-CD2	-5.25	102.07	111.00
1	M	568	MET	CA-CB-CG	5.24	122.20	113.30
3	U	141	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	q	419	TRP	CG-CD1-NE1	-5.18	104.92	110.10
3	m	230	ASP	CB-CG-OD2	5.15	122.94	118.30
6	R	61	LYS	CG-CD-CE	5.15	127.34	111.90
5	i	81	LEU	CB-CG-CD2	5.12	119.71	111.00
1	q	419	TRP	CZ3-CH2-CZ2	5.11	127.73	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	221	LYS	CB-CA-C	-5.09	100.22	110.40
1	q	422	ARG	CB-CA-C	5.08	120.56	110.40
6	d	333	THR	CA-CB-CG2	-5.08	105.29	112.40
6	v	23	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	N	173	GLU	CB-CA-C	-5.03	100.34	110.40
2	r	333	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (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
6	d	91	ASP	Peptide
1	k	83	PHE	Peptide
6	p	91	ASP	Peptide
6	v	91	ASP	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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%)	47 60
1	G	565/569 (99%)	538 (95%)	25 (4%)	2 (0%)	34 46
1	M	565/569 (99%)	542 (96%)	23 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	566/569 (100%)	540 (95%)	25 (4%)	1 (0%)	47	60
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%)	29	40
2	H	423/432 (98%)	405 (96%)	16 (4%)	2 (0%)	29	40
2	N	428/432 (99%)	413 (96%)	13 (3%)	2 (0%)	29	40
2	T	427/432 (99%)	409 (96%)	14 (3%)	4 (1%)	17	24
2	Z	424/432 (98%)	409 (96%)	14 (3%)	1 (0%)	47	60
2	f	423/432 (98%)	405 (96%)	16 (4%)	2 (0%)	29	40
2	l	424/432 (98%)	408 (96%)	15 (4%)	1 (0%)	47	60
2	r	424/432 (98%)	409 (96%)	13 (3%)	2 (0%)	29	40
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	41	51
6	L	346/349 (99%)	340 (98%)	5 (1%)	1 (0%)	41	51
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%)	25	34
6	j	340/349 (97%)	336 (99%)	4 (1%)	0	100	100
6	p	346/349 (99%)	342 (99%)	3 (1%)	1 (0%)	41	51
6	v	342/349 (98%)	337 (98%)	4 (1%)	1 (0%)	41	51
All	All	14422/14656 (98%)	13934 (97%)	462 (3%)	26 (0%)	47	60

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	LYS
6	F	92	GLY
1	G	415	GLU
6	L	92	GLY
1	S	415	GLU
2	T	60	GLY
6	d	92	GLY
6	p	92	GLY
6	v	92	GLY
2	B	59	ASN
2	T	59	ASN
2	N	59	ASN
2	T	382	PRO
2	Z	382	PRO
2	r	382	PRO
2	B	382	PRO
2	H	382	PRO
2	N	382	PRO

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Mol	Chain	Res	Type
2	f	382	PRO
2	l	382	PRO
1	G	84	LYS
6	d	102	PRO
2	H	25	GLY
2	f	25	GLY
2	r	307	PRO
2	T	307	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	470/470 (100%)	466 (99%)	4 (1%)	78	86
1	G	469/470 (100%)	463 (99%)	6 (1%)	69	80
1	M	469/470 (100%)	461 (98%)	8 (2%)	60	75
1	S	470/470 (100%)	461 (98%)	9 (2%)	57	72
1	Y	469/470 (100%)	465 (99%)	4 (1%)	78	86
1	e	470/470 (100%)	461 (98%)	9 (2%)	57	72
1	k	469/470 (100%)	465 (99%)	4 (1%)	78	86
1	q	470/470 (100%)	465 (99%)	5 (1%)	73	83
2	B	359/361 (99%)	346 (96%)	13 (4%)	35	47
2	H	358/361 (99%)	351 (98%)	7 (2%)	55	70
2	N	359/361 (99%)	352 (98%)	7 (2%)	57	72
2	T	359/361 (99%)	351 (98%)	8 (2%)	52	66
2	Z	358/361 (99%)	351 (98%)	7 (2%)	55	70
2	f	358/361 (99%)	350 (98%)	8 (2%)	52	66
2	l	358/361 (99%)	352 (98%)	6 (2%)	60	75
2	r	358/361 (99%)	347 (97%)	11 (3%)	40	54
3	C	202/204 (99%)	200 (99%)	2 (1%)	76	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	203/204 (100%)	200 (98%)	3 (2%)	65	77
3	O	202/204 (99%)	199 (98%)	3 (2%)	65	77
3	U	202/204 (99%)	199 (98%)	3 (2%)	65	77
3	a	202/204 (99%)	197 (98%)	5 (2%)	47	62
3	g	202/204 (99%)	200 (99%)	2 (1%)	76	84
3	m	202/204 (99%)	199 (98%)	3 (2%)	65	77
3	s	203/204 (100%)	200 (98%)	3 (2%)	65	77
4	D	110/111 (99%)	109 (99%)	1 (1%)	78	86
4	J	110/111 (99%)	109 (99%)	1 (1%)	78	86
4	P	110/111 (99%)	110 (100%)	0	100	100
4	V	110/111 (99%)	107 (97%)	3 (3%)	44	59
4	b	110/111 (99%)	110 (100%)	0	100	100
4	h	110/111 (99%)	109 (99%)	1 (1%)	78	86
4	n	110/111 (99%)	108 (98%)	2 (2%)	59	74
4	t	110/111 (99%)	109 (99%)	1 (1%)	78	86
5	E	65/67 (97%)	61 (94%)	4 (6%)	18	24
5	K	65/67 (97%)	61 (94%)	4 (6%)	18	24
5	Q	65/67 (97%)	61 (94%)	4 (6%)	18	24
5	W	65/67 (97%)	59 (91%)	6 (9%)	9	11
5	c	65/67 (97%)	61 (94%)	4 (6%)	18	24
5	i	65/67 (97%)	61 (94%)	4 (6%)	18	24
5	o	65/67 (97%)	61 (94%)	4 (6%)	18	24
5	u	66/67 (98%)	60 (91%)	6 (9%)	9	11
6	F	308/312 (99%)	299 (97%)	9 (3%)	42	57
6	L	311/312 (100%)	307 (99%)	4 (1%)	69	80
6	R	305/312 (98%)	298 (98%)	7 (2%)	50	65
6	X	308/312 (99%)	302 (98%)	6 (2%)	57	72
6	d	304/312 (97%)	296 (97%)	8 (3%)	46	61
6	j	308/312 (99%)	300 (97%)	8 (3%)	46	61
6	p	311/312 (100%)	303 (97%)	8 (3%)	46	61
6	v	310/312 (99%)	299 (96%)	11 (4%)	36	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	12107/12200 (99%)	11861 (98%)	246 (2%)	55 70

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	TYR
1	A	231	HIS
1	A	380	VAL
1	A	407	TYR
2	B	20	ILE
2	B	27	GLU
2	B	35	CYS
2	B	53	LYS
2	B	57	ARG
2	B	68	ASP
2	B	82	LYS
2	B	281	LYS
2	B	302	TRP
2	B	308	TYR
2	B	351	GLN
2	B	397	GLU
2	B	410	ASP
3	C	237	GLU
3	C	264	CYS
4	D	117	MET
5	E	15	CYS
5	E	22	CYS
5	E	46	MET
5	E	61	CYS
6	F	31	CYS
6	F	118	CYS
6	F	143	VAL
6	F	194	CYS
6	F	210	MET
6	F	222	GLU
6	F	240	VAL
6	F	306	ARG
6	F	328	ASN
1	G	71	TYR
1	G	231	HIS
1	G	323	MET
1	G	380	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	407	TYR
1	G	505	LYS
2	H	35	CYS
2	H	58	LYS
2	H	68	ASP
2	H	302	TRP
2	H	308	TYR
2	H	397	GLU
2	H	411	LEU
3	I	44	GLU
3	I	187	ASN
3	I	264	CYS
4	J	129	GLN
5	K	22	CYS
5	K	46	MET
5	K	61	CYS
5	K	69	GLU
6	L	2	GLU
6	L	118	CYS
6	L	194	CYS
6	L	201	LYS
1	M	71	TYR
1	M	222	LEU
1	M	231	HIS
1	M	405	ASN
1	M	407	TYR
1	M	492	ARG
1	M	523	GLN
1	M	568	MET
2	N	35	CYS
2	N	36	ARG
2	N	281	LYS
2	N	302	TRP
2	N	308	TYR
2	N	351	GLN
2	N	397	GLU
3	O	151	THR
3	O	232	GLU
3	O	264	CYS
5	Q	15	CYS
5	Q	22	CYS
5	Q	46	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	Q	61	CYS
6	R	94	SER
6	R	118	CYS
6	R	144	THR
6	R	194	CYS
6	R	201	LYS
6	R	210	MET
6	R	222	GLU
1	S	71	TYR
1	S	231	HIS
1	S	286	VAL
1	S	356	ARG
1	S	380	VAL
1	S	406	LYS
1	S	407	TYR
1	S	482	GLU
1	S	512	SER
2	T	20	ILE
2	T	35	CYS
2	T	68	ASP
2	T	302	TRP
2	T	308	TYR
2	T	351	GLN
2	T	397	GLU
2	T	421	LEU
3	U	187	ASN
3	U	223	LYS
3	U	264	CYS
4	V	2	ARG
4	V	11	ILE
4	V	129	GLN
5	W	5	LEU
5	W	15	CYS
5	W	22	CYS
5	W	46	MET
5	W	61	CYS
5	W	69	GLU
6	X	31	CYS
6	X	115	CYS
6	X	118	CYS
6	X	143	VAL
6	X	194	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	X	284	ASN
1	Y	71	TYR
1	Y	286	VAL
1	Y	407	TYR
1	Y	418	LYS
2	Z	35	CYS
2	Z	52	LYS
2	Z	58	LYS
2	Z	302	TRP
2	Z	308	TYR
2	Z	351	GLN
2	Z	397	GLU
3	a	187	ASN
3	a	231	ILE
3	a	236	GLU
3	a	237	GLU
3	a	264	CYS
5	c	22	CYS
5	c	46	MET
5	c	61	CYS
5	c	63	LYS
6	d	91	ASP
6	d	118	CYS
6	d	144	THR
6	d	152	ASP
6	d	194	CYS
6	d	222	GLU
6	d	336	ARG
6	d	338	LYS
1	e	71	TYR
1	e	83	PHE
1	e	231	HIS
1	e	273	GLN
1	e	283	ARG
1	e	286	VAL
1	e	407	TYR
1	e	456	LYS
1	e	482	GLU
2	f	20	ILE
2	f	35	CYS
2	f	68	ASP
2	f	308	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	f	339	MET
2	f	351	GLN
2	f	397	GLU
2	f	421	LEU
3	g	60	ASP
3	g	236	GLU
4	h	2	ARG
5	i	15	CYS
5	i	22	CYS
5	i	46	MET
5	i	61	CYS
6	j	79	SER
6	j	118	CYS
6	j	154	CYS
6	j	194	CYS
6	j	201	LYS
6	j	224	LYS
6	j	299	THR
6	j	338	LYS
1	k	71	TYR
1	k	354	SER
1	k	407	TYR
1	k	423	LYS
2	l	35	CYS
2	l	68	ASP
2	l	302	TRP
2	l	308	TYR
2	l	351	GLN
2	l	397	GLU
3	m	11	GLN
3	m	237	GLU
3	m	264	CYS
4	n	2	ARG
4	n	117	MET
5	o	15	CYS
5	o	22	CYS
5	o	46	MET
5	o	61	CYS
6	p	93	THR
6	p	118	CYS
6	p	142	LEU
6	p	194	CYS

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Mol	Chain	Res	Type
6	p	299	THR
6	p	300	LYS
6	p	336	ARG
6	p	349	LYS
1	q	22	MET
1	q	36	SER
1	q	71	TYR
1	q	380	VAL
1	q	407	TYR
2	r	35	CYS
2	r	53	LYS
2	r	58	LYS
2	r	68	ASP
2	r	83	ARG
2	r	281	LYS
2	r	302	TRP
2	r	308	TYR
2	r	351	GLN
2	r	354	LEU
2	r	397	GLU
3	s	55	SER
3	s	233	VAL
3	s	264	CYS
4	t	117	MET
5	u	5	LEU
5	u	15	CYS
5	u	22	CYS
5	u	46	MET
5	u	61	CYS
5	u	69	GLU
6	v	21	ASN
6	v	23	ARG
6	v	31	CYS
6	v	58	GLU
6	v	118	CYS
6	v	142	LEU
6	v	143	VAL
6	v	154	CYS
6	v	194	CYS
6	v	210	MET
6	v	336	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27)

such sidechains are listed below:

Mol	Chain	Res	Type
6	F	342	ASN
1	G	106	GLN
1	G	523	GLN
2	H	234	GLN
2	H	297	ASN
1	M	253	ASN
1	M	363	GLN
1	M	376	ASN
1	M	405	ASN
2	N	141	ASN
3	O	216	GLN
1	S	523	GLN
1	Y	15	ASN
1	Y	410	ASN
1	Y	523	GLN
3	a	265	ASN
6	d	246	GLN
6	d	268	GLN
2	f	44	HIS
1	k	7	ASN
1	k	106	GLN
1	k	126	HIS
1	q	253	ASN
2	r	332	ASN
3	s	81	GLN
6	v	21	ASN
6	v	284	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	k	178	7,1	9,11,12	0.60	0	5,12,14	0.88	0
1	KCX	A	178	7,1	9,11,12	0.58	0	5,12,14	0.71	0
1	KCX	S	178	7,1	9,11,12	0.67	0	5,12,14	0.71	0
1	KCX	G	178	7,1	9,11,12	2.17	1 (11%)	5,12,14	1.82	1 (20%)
1	KCX	M	178	7,1	9,11,12	2.22	1 (11%)	5,12,14	1.62	1 (20%)
1	KCX	e	178	7,1	9,11,12	2.19	1 (11%)	5,12,14	1.86	1 (20%)
1	KCX	q	178	7,1	9,11,12	2.21	1 (11%)	5,12,14	1.47	1 (20%)
1	KCX	Y	178	7,1	9,11,12	0.60	0	5,12,14	0.74	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	k	178	7,1	-	0/9/10/12	-
1	KCX	A	178	7,1	-	1/9/10/12	-
1	KCX	S	178	7,1	-	0/9/10/12	-
1	KCX	G	178	7,1	-	0/9/10/12	-
1	KCX	M	178	7,1	-	0/9/10/12	-
1	KCX	e	178	7,1	-	0/9/10/12	-
1	KCX	q	178	7,1	-	0/9/10/12	-
1	KCX	Y	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	6.42	1.33	1.21
1	q	178	KCX	OQ1-CX	6.39	1.33	1.21
1	e	178	KCX	OQ1-CX	6.29	1.33	1.21
1	G	178	KCX	OQ1-CX	6.27	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	-4.09	118.61	124.96
1	G	178	KCX	OQ1-CX-NZ	-3.99	118.78	124.96
1	M	178	KCX	OQ1-CX-NZ	-3.54	119.47	124.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	q	178	KCX	OQ1-CX-NZ	-3.13	120.11	124.96

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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	v	501	6	0,12,12	-	-	-	-	-
8	MFN	A	603	7	50,54,56	1.91	10 (20%)	59,71,73	1.77	12 (20%)
11	SF4	R	401	6	0,12,12	-	-	-	-	-
11	SF4	R	404	6	0,12,12	-	-	-	-	-
11	SF4	K	101	5	0,12,12	-	-	-	-	-
11	SF4	c	102	5	0,12,12	-	-	-	-	-
11	SF4	L	505	6	0,12,12	-	-	-	-	-
11	SF4	p	404	6	0,12,12	-	-	-	-	-
11	SF4	R	409	6	0,12,12	-	-	-	-	-
11	SF4	L	503	6	0,12,12	-	-	-	-	-
11	SF4	v	507	6	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	SF4	j	506	6	0,12,12	-	-	-		
11	SF4	p	402	6	0,12,12	-	-	-		
11	SF4	p	401	6	0,12,12	-	-	-		
11	SF4	p	409	6	0,12,12	-	-	-		
13	MGD	B	504	12	41,52,52	1.33	3 (7%)	40,81,81	1.43	6 (15%)
11	SF4	p	403	6	0,12,12	-	-	-		
11	SF4	j	501	6	0,12,12	-	-	-		
11	SF4	i	101	5	0,12,12	-	-	-		
11	SF4	r	501	2	0,12,12	-	-	-		
11	SF4	Z	501	2	0,12,12	-	-	-		
11	SF4	X	507	6	0,12,12	-	-	-		
13	MGD	f	503	12	41,52,52	1.31	3 (7%)	40,81,81	1.39	6 (15%)
11	SF4	F	401	6	0,12,12	-	-	-		
13	MGD	H	504	12	41,52,52	1.29	3 (7%)	40,81,81	1.42	5 (12%)
11	SF4	p	408	6	0,12,12	-	-	-		
11	SF4	L	502	6	0,12,12	-	-	-		
11	SF4	d	402	6	0,12,12	-	-	-		
11	SF4	u	102	5	0,12,12	-	-	-		
8	MFN	q	603	-	50,54,56	1.84	9 (18%)	59,71,73	1.74	11 (18%)
11	SF4	j	508	6	0,12,12	-	-	-		
11	SF4	v	506	6	0,12,12	-	-	-		
13	MGD	N	503	12	41,52,52	1.30	3 (7%)	40,81,81	1.48	7 (17%)
13	MGD	r	503	12	41,52,52	1.33	3 (7%)	40,81,81	1.45	7 (17%)
11	SF4	F	402	6	0,12,12	-	-	-		
13	MGD	r	504	12	41,52,52	1.37	4 (9%)	40,81,81	1.40	5 (12%)
11	SF4	W	200	5	0,12,12	-	-	-		
11	SF4	T	501	2	0,12,12	-	-	-		
11	SF4	d	403	6	0,12,12	-	-	-		
11	SF4	f	501	2	0,12,12	-	-	-		
11	SF4	v	505	6	0,12,12	-	-	-		
8	MFN	S	603	-	50,54,56	1.88	8 (16%)	59,71,73	1.78	14 (23%)
11	SF4	o	102	5	0,12,12	-	-	-		
11	SF4	c	101	5	0,12,12	-	-	-		
11	SF4	d	408	6	0,12,12	-	-	-		
11	SF4	L	506	6	0,12,12	-	-	-		
11	SF4	v	504	6	0,12,12	-	-	-		
11	SF4	i	102	5	0,12,12	-	-	-		
11	SF4	v	502	6	0,12,12	-	-	-		
11	SF4	o	101	5	0,12,12	-	-	-		
11	SF4	X	501	6	0,12,12	-	-	-		
11	SF4	N	501	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	SF4	j	504	6	0,12,12	-	-	-		
11	SF4	v	508	6	0,12,12	-	-	-		
11	SF4	R	403	6	0,12,12	-	-	-		
11	SF4	X	504	6	0,12,12	-	-	-		
8	MFN	k	603	7	50,54,56	1.80	7 (14%)	59,71,73	2.46	20 (33%)
13	MGD	T	503	12	41,52,52	1.34	3 (7%)	40,81,81	1.48	7 (17%)
13	MGD	B	503	12	41,52,52	1.30	3 (7%)	40,81,81	1.51	7 (17%)
11	SF4	l	501	2	0,12,12	-	-	-		
11	SF4	F	407	6	0,12,12	-	-	-		
13	MGD	T	504	12	41,52,52	1.31	4 (9%)	40,81,81	1.39	5 (12%)
11	SF4	H	501	2	0,12,12	-	-	-		
11	SF4	d	401	6	0,12,12	-	-	-		
11	SF4	v	503	6	0,12,12	-	-	-		
11	SF4	X	508	6	0,12,12	-	-	-		
11	SF4	F	404	6	0,12,12	-	-	-		
11	SF4	K	102	5	0,12,12	-	-	-		
11	SF4	L	508	6	0,12,12	-	-	-		
11	SF4	L	507	6	0,12,12	-	-	-		
8	MFN	e	603	-	50,54,56	1.83	7 (14%)	59,71,73	1.81	13 (22%)
11	SF4	R	402	6	0,12,12	-	-	-		
11	SF4	X	506	6	0,12,12	-	-	-		
11	SF4	d	407	6	0,12,12	-	-	-		
11	SF4	B	501	2	0,12,12	-	-	-		
13	MGD	H	503	12	41,52,52	1.29	3 (7%)	40,81,81	1.52	8 (20%)
11	SF4	u	101	5	0,12,12	-	-	-		
11	SF4	j	503	6	0,12,12	-	-	-		
11	SF4	R	408	6	0,12,12	-	-	-		
11	SF4	E	102	5	0,12,12	-	-	-		
11	SF4	F	405	6	0,12,12	-	-	-		
11	SF4	j	505	6	0,12,12	-	-	-		
11	SF4	Q	102	5	0,12,12	-	-	-		
13	MGD	l	503	12	41,52,52	1.29	4 (9%)	40,81,81	1.52	7 (17%)
11	SF4	X	505	6	0,12,12	-	-	-		
11	SF4	L	501	6	0,12,12	-	-	-		
11	SF4	X	502	6	0,12,12	-	-	-		
13	MGD	Z	504	12	41,52,52	1.34	4 (9%)	40,81,81	1.37	5 (12%)
11	SF4	F	406	6	0,12,12	-	-	-		
11	SF4	R	406	6	0,12,12	-	-	-		
11	SF4	Q	101	5	0,12,12	-	-	-		
11	SF4	j	507	6	0,12,12	-	-	-		
11	SF4	j	502	6	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	SF4	X	503	6	0,12,12	-	-	-		
11	SF4	F	408	6	0,12,12	-	-	-		
8	MFN	G	603	7	50,54,56	1.79	8 (16%)	59,71,73	1.76	11 (18%)
11	SF4	F	409	6	0,12,12	-	-	-		
11	SF4	d	406	6	0,12,12	-	-	-		
11	SF4	L	504	6	0,12,12	-	-	-		
13	MGD	f	504	12	41,52,52	1.33	3 (7%)	40,81,81	1.43	5 (12%)
11	SF4	W	201	5	0,12,12	-	-	-		
11	SF4	d	405	6	0,12,12	-	-	-		
11	SF4	F	403	6	0,12,12	-	-	-		
11	SF4	R	407	6	0,12,12	-	-	-		
13	MGD	Z	503	12	41,52,52	1.30	3 (7%)	40,81,81	1.49	6 (15%)
11	SF4	p	407	6	0,12,12	-	-	-		
13	MGD	N	504	12	41,52,52	1.34	4 (9%)	40,81,81	1.36	5 (12%)
11	SF4	p	405	6	0,12,12	-	-	-		
11	SF4	E	101	5	0,12,12	-	-	-		
11	SF4	R	405	6	0,12,12	-	-	-		
8	MFN	M	603	7	50,54,56	1.81	8 (16%)	59,71,73	2.02	18 (30%)
13	MGD	l	504	12	41,52,52	1.30	3 (7%)	40,81,81	1.39	4 (10%)
8	MFN	Y	603	7	50,54,56	1.79	7 (14%)	59,71,73	1.75	14 (23%)
11	SF4	d	404	6	0,12,12	-	-	-		
11	SF4	p	406	6	0,12,12	-	-	-		
11	SF4	d	409	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	v	501	6	-	-	0/6/5/5
8	MFN	A	603	7	-	10/57/61/63	0/2/2/2
11	SF4	R	401	6	-	-	0/6/5/5
11	SF4	R	404	6	-	-	0/6/5/5
11	SF4	K	101	5	-	-	0/6/5/5
11	SF4	c	102	5	-	-	0/6/5/5
11	SF4	L	505	6	-	-	0/6/5/5
11	SF4	p	404	6	-	-	0/6/5/5
11	SF4	R	409	6	-	-	0/6/5/5
11	SF4	L	503	6	-	-	0/6/5/5
11	SF4	v	507	6	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SF4	j	506	6	-	-	0/6/5/5
11	SF4	p	402	6	-	-	0/6/5/5
11	SF4	p	401	6	-	-	0/6/5/5
11	SF4	p	409	6	-	-	0/6/5/5
13	MGD	B	504	12	-	2/18/66/66	0/6/6/6
11	SF4	p	403	6	-	-	0/6/5/5
11	SF4	j	501	6	-	-	0/6/5/5
11	SF4	i	101	5	-	-	0/6/5/5
11	SF4	r	501	2	-	-	0/6/5/5
11	SF4	Z	501	2	-	-	0/6/5/5
11	SF4	X	507	6	-	-	0/6/5/5
13	MGD	f	503	12	-	8/18/66/66	0/6/6/6
13	MGD	H	504	12	-	1/18/66/66	0/6/6/6
11	SF4	F	401	6	-	-	0/6/5/5
11	SF4	p	408	6	-	-	0/6/5/5
11	SF4	L	502	6	-	-	0/6/5/5
11	SF4	d	402	6	-	-	0/6/5/5
11	SF4	u	102	5	-	-	0/6/5/5
8	MFN	q	603	-	-	17/57/61/63	0/2/2/2
11	SF4	j	508	6	-	-	0/6/5/5
11	SF4	v	506	6	-	-	0/6/5/5
13	MGD	N	503	12	-	7/18/66/66	0/6/6/6
13	MGD	r	503	12	-	7/18/66/66	0/6/6/6
11	SF4	F	402	6	-	-	0/6/5/5
13	MGD	r	504	12	-	0/18/66/66	0/6/6/6
11	SF4	W	200	5	-	-	0/6/5/5
11	SF4	T	501	2	-	-	0/6/5/5
11	SF4	d	403	6	-	-	0/6/5/5
11	SF4	f	501	2	-	-	0/6/5/5
11	SF4	v	505	6	-	-	0/6/5/5
8	MFN	S	603	-	-	17/57/61/63	0/2/2/2
11	SF4	o	102	5	-	-	0/6/5/5
11	SF4	c	101	5	-	-	0/6/5/5
11	SF4	d	408	6	-	-	0/6/5/5
11	SF4	L	506	6	-	-	0/6/5/5
11	SF4	v	504	6	-	-	0/6/5/5
11	SF4	i	102	5	-	-	0/6/5/5
11	SF4	v	502	6	-	-	0/6/5/5
11	SF4	o	101	5	-	-	0/6/5/5
11	SF4	X	501	6	-	-	0/6/5/5
11	SF4	N	501	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SF4	j	504	6	-	-	0/6/5/5
11	SF4	v	508	6	-	-	0/6/5/5
11	SF4	R	403	6	-	-	0/6/5/5
11	SF4	X	504	6	-	-	0/6/5/5
8	MFN	k	603	7	-	17/57/61/63	0/2/2/2
13	MGD	T	503	12	-	4/18/66/66	0/6/6/6
13	MGD	B	503	12	-	8/18/66/66	0/6/6/6
11	SF4	l	501	2	-	-	0/6/5/5
11	SF4	F	407	6	-	-	0/6/5/5
13	MGD	T	504	12	-	1/18/66/66	0/6/6/6
11	SF4	H	501	2	-	-	0/6/5/5
11	SF4	d	401	6	-	-	0/6/5/5
11	SF4	v	503	6	-	-	0/6/5/5
11	SF4	X	508	6	-	-	0/6/5/5
11	SF4	F	404	6	-	-	0/6/5/5
11	SF4	K	102	5	-	-	0/6/5/5
11	SF4	L	508	6	-	-	0/6/5/5
11	SF4	L	507	6	-	-	0/6/5/5
8	MFN	e	603	-	-	21/57/61/63	0/2/2/2
11	SF4	R	402	6	-	-	0/6/5/5
11	SF4	X	506	6	-	-	0/6/5/5
11	SF4	d	407	6	-	-	0/6/5/5
13	MGD	H	503	12	-	8/18/66/66	0/6/6/6
11	SF4	B	501	2	-	-	0/6/5/5
11	SF4	u	101	5	-	-	0/6/5/5
11	SF4	j	503	6	-	-	0/6/5/5
11	SF4	R	408	6	-	-	0/6/5/5
11	SF4	E	102	5	-	-	0/6/5/5
11	SF4	F	405	6	-	-	0/6/5/5
11	SF4	j	505	6	-	-	0/6/5/5
11	SF4	Q	102	5	-	-	0/6/5/5
13	MGD	l	503	12	-	7/18/66/66	0/6/6/6
11	SF4	X	505	6	-	-	0/6/5/5
11	SF4	L	501	6	-	-	0/6/5/5
11	SF4	X	502	6	-	-	0/6/5/5
13	MGD	Z	504	12	-	1/18/66/66	0/6/6/6
11	SF4	F	406	6	-	-	0/6/5/5
11	SF4	R	406	6	-	-	0/6/5/5
11	SF4	Q	101	5	-	-	0/6/5/5
11	SF4	j	507	6	-	-	0/6/5/5
11	SF4	j	502	6	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SF4	X	503	6	-	-	0/6/5/5
11	SF4	F	408	6	-	-	0/6/5/5
8	MFN	G	603	7	-	15/57/61/63	0/2/2/2
11	SF4	F	409	6	-	-	0/6/5/5
11	SF4	d	406	6	-	-	0/6/5/5
11	SF4	L	504	6	-	-	0/6/5/5
13	MGD	f	504	12	-	1/18/66/66	0/6/6/6
11	SF4	W	201	5	-	-	0/6/5/5
11	SF4	d	405	6	-	-	0/6/5/5
11	SF4	F	403	6	-	-	0/6/5/5
11	SF4	R	407	6	-	-	0/6/5/5
13	MGD	Z	503	12	-	8/18/66/66	0/6/6/6
11	SF4	p	407	6	-	-	0/6/5/5
13	MGD	N	504	12	-	1/18/66/66	0/6/6/6
11	SF4	p	405	6	-	-	0/6/5/5
11	SF4	E	101	5	-	-	0/6/5/5
11	SF4	R	405	6	-	-	0/6/5/5
8	MFN	M	603	7	-	18/57/61/63	0/2/2/2
13	MGD	l	504	12	-	1/18/66/66	0/6/6/6
8	MFN	Y	603	7	-	24/57/61/63	0/2/2/2
11	SF4	d	404	6	-	-	0/6/5/5
11	SF4	p	406	6	-	-	0/6/5/5
11	SF4	d	409	6	-	-	0/6/5/5

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	e	603	MFN	C21-N3	6.62	1.48	1.34
8	S	603	MFN	C21-N3	6.61	1.48	1.34
8	k	603	MFN	C21-N3	6.07	1.47	1.34
8	Y	603	MFN	C21-N3	6.01	1.46	1.34
8	A	603	MFN	C21-N3	5.93	1.46	1.34
13	r	504	MGD	C16-C21	5.90	1.48	1.38
13	Z	504	MGD	C16-C21	5.81	1.48	1.38
8	q	603	MFN	C21-N3	5.81	1.46	1.34
13	N	504	MGD	C16-C21	5.77	1.48	1.38
13	B	504	MGD	C16-C21	5.73	1.48	1.38
13	T	503	MGD	C16-C21	5.72	1.48	1.38
8	A	603	MFN	C16-N2	5.71	1.46	1.33
13	l	504	MGD	C16-C21	5.66	1.48	1.38
13	f	504	MGD	C16-C21	5.65	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	r	503	MGD	C16-C21	5.62	1.48	1.38
13	T	504	MGD	C16-C21	5.60	1.48	1.38
8	G	603	MFN	C21-N3	5.59	1.46	1.34
13	B	503	MGD	C16-C21	5.56	1.48	1.38
8	M	603	MFN	C16-N2	5.53	1.46	1.33
13	H	503	MGD	C16-C21	5.53	1.48	1.38
8	M	603	MFN	C21-N3	5.52	1.45	1.34
13	f	503	MGD	C16-C21	5.52	1.48	1.38
13	N	503	MGD	C16-C21	5.51	1.48	1.38
8	Y	603	MFN	C16-N2	5.48	1.45	1.33
13	H	504	MGD	C16-C21	5.46	1.48	1.38
8	k	603	MFN	C16-N2	5.46	1.45	1.33
13	Z	503	MGD	C16-C21	5.41	1.47	1.38
13	l	503	MGD	C16-C21	5.39	1.47	1.38
8	G	603	MFN	C16-N2	5.34	1.45	1.33
8	q	603	MFN	C16-N2	5.34	1.45	1.33
8	S	603	MFN	C16-N2	5.32	1.45	1.33
8	e	603	MFN	C16-N2	5.26	1.45	1.33
8	A	603	MFN	C25-N4	4.87	1.44	1.34
8	S	603	MFN	C25-N4	4.69	1.44	1.34
8	e	603	MFN	C25-N4	4.67	1.44	1.34
8	q	603	MFN	C25-N4	4.60	1.43	1.34
8	G	603	MFN	C25-N4	4.42	1.43	1.34
8	M	603	MFN	C25-N4	4.30	1.43	1.34
8	Y	603	MFN	C25-N4	4.15	1.42	1.34
8	k	603	MFN	C25-N4	4.08	1.42	1.34
8	k	603	MFN	C23-N4	-3.21	1.39	1.45
8	q	603	MFN	C8-C9	3.11	1.44	1.38
8	S	603	MFN	C8-C9	3.07	1.44	1.38
8	A	603	MFN	C8-C9	3.03	1.44	1.38
8	e	603	MFN	C8-C9	3.00	1.44	1.38
8	G	603	MFN	C8-C9	2.95	1.44	1.38
8	M	603	MFN	C8-C9	2.95	1.44	1.38
8	Y	603	MFN	C8-C9	2.92	1.44	1.38
8	A	603	MFN	C10-C9	2.91	1.44	1.38
8	k	603	MFN	C8-C9	2.88	1.44	1.38
8	M	603	MFN	C17-C16	2.83	1.56	1.51
8	S	603	MFN	C17-C16	2.83	1.56	1.51
8	M	603	MFN	C10-C9	2.78	1.44	1.38
8	k	603	MFN	C17-C16	2.70	1.56	1.51
13	N	504	MGD	C16-C17	2.69	1.49	1.42
13	r	504	MGD	C16-C17	2.67	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	q	603	MFN	C10-C9	2.65	1.43	1.38
8	A	603	MFN	C17-C16	2.64	1.56	1.51
13	B	503	MGD	C17-N18	-2.63	1.33	1.38
8	q	603	MFN	C17-C16	2.63	1.56	1.51
13	T	503	MGD	C17-N18	-2.62	1.34	1.38
8	Y	603	MFN	C10-C9	2.61	1.43	1.38
8	Y	603	MFN	C17-C16	2.60	1.56	1.51
13	Z	504	MGD	C17-N18	-2.59	1.34	1.38
8	S	603	MFN	C10-C9	2.59	1.43	1.38
8	G	603	MFN	C10-C9	2.59	1.43	1.38
8	G	603	MFN	C17-C16	2.58	1.56	1.51
13	B	504	MGD	C16-C17	2.56	1.48	1.42
13	Z	504	MGD	C16-C17	2.55	1.48	1.42
13	r	503	MGD	C16-C17	2.55	1.48	1.42
8	k	603	MFN	C10-C9	2.55	1.43	1.38
13	Z	503	MGD	C17-N18	-2.54	1.34	1.38
13	f	503	MGD	C16-C17	2.51	1.48	1.42
8	A	603	MFN	C26-C25	2.51	1.56	1.51
13	B	504	MGD	C17-N18	-2.50	1.34	1.38
13	N	503	MGD	C17-N18	-2.50	1.34	1.38
8	A	603	MFN	C13-C4	2.49	1.56	1.50
8	M	603	MFN	C23-N4	-2.49	1.40	1.45
13	r	503	MGD	C17-N18	-2.48	1.34	1.38
13	H	503	MGD	C17-N18	-2.48	1.34	1.38
8	e	603	MFN	C10-C9	2.47	1.43	1.38
13	T	504	MGD	C17-N18	-2.46	1.34	1.38
13	N	504	MGD	C17-N18	-2.45	1.34	1.38
13	f	504	MGD	C16-C17	2.45	1.48	1.42
13	T	504	MGD	C16-C17	2.44	1.48	1.42
13	l	503	MGD	C16-C17	2.44	1.48	1.42
13	f	504	MGD	C17-N18	-2.42	1.34	1.38
13	H	504	MGD	C17-N18	-2.41	1.34	1.38
8	Y	603	MFN	C23-N4	-2.39	1.40	1.45
13	Z	503	MGD	C16-C17	2.38	1.48	1.42
13	l	504	MGD	C17-N18	-2.37	1.34	1.38
13	N	503	MGD	C16-C17	2.37	1.48	1.42
13	H	503	MGD	C16-C17	2.37	1.48	1.42
13	T	503	MGD	C16-C17	2.35	1.48	1.42
13	B	503	MGD	C16-C17	2.34	1.48	1.42
13	f	503	MGD	C17-N18	-2.34	1.34	1.38
8	A	603	MFN	O2-C9	2.33	1.43	1.37
13	l	503	MGD	C17-N18	-2.33	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	r	504	MGD	C17-N18	-2.31	1.34	1.38
8	S	603	MFN	C26-C25	2.27	1.55	1.51
8	e	603	MFN	C17-C16	2.26	1.55	1.51
13	l	504	MGD	C16-C17	2.25	1.48	1.42
8	G	603	MFN	C26-C25	2.24	1.55	1.51
8	q	603	MFN	C13-C4	2.22	1.55	1.50
13	H	504	MGD	C16-C17	2.20	1.48	1.42
8	e	603	MFN	C26-C25	2.19	1.55	1.51
13	r	504	MGD	C6-N1	-2.14	1.34	1.37
8	M	603	MFN	C13-C4	2.09	1.55	1.50
8	G	603	MFN	C13-C4	2.09	1.55	1.50
8	A	603	MFN	C27-C26	2.09	1.59	1.52
13	T	504	MGD	C6-N1	-2.09	1.34	1.37
8	S	603	MFN	C13-C4	2.08	1.55	1.50
8	q	603	MFN	C26-C25	2.07	1.55	1.51
13	l	503	MGD	C6-N1	-2.02	1.34	1.37
13	Z	504	MGD	C6-N1	-2.02	1.34	1.37
13	N	504	MGD	C6-N1	-2.01	1.34	1.37
8	q	603	MFN	O2-C9	2.01	1.42	1.37

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	k	603	MFN	C24-C23-N4	-7.85	91.97	110.55
8	k	603	MFN	C22-C14-C23	-6.65	100.73	113.16
8	A	603	MFN	C8-C9-C10	-6.17	110.67	120.18
8	M	603	MFN	C8-C9-C10	-5.83	111.20	120.18
8	q	603	MFN	C8-C9-C10	-5.73	111.34	120.18
8	G	603	MFN	C8-C9-C10	-5.64	111.49	120.18
8	e	603	MFN	C1-C2-C3	-5.50	122.05	129.54
8	Y	603	MFN	C8-C9-C10	-5.44	111.80	120.18
8	k	603	MFN	C8-C9-C10	-5.43	111.81	120.18
8	S	603	MFN	C8-C9-C10	-5.40	111.86	120.18
8	e	603	MFN	C8-C9-C10	-5.11	112.30	120.18
8	k	603	MFN	C26-C27-C28	-5.03	99.02	113.86
8	k	603	MFN	C1-C2-C3	-4.73	123.11	129.54
8	Y	603	MFN	C1-C2-C3	-4.69	123.15	129.54
8	k	603	MFN	C26-C25-N4	-4.63	107.81	115.83
13	f	504	MGD	C19-N20-C21	4.61	121.75	113.43
13	Z	504	MGD	C19-N20-C21	4.60	121.73	113.43
13	Z	503	MGD	C19-N20-C21	4.60	121.72	113.43
13	H	504	MGD	C19-N20-C21	4.59	121.71	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	l	503	MGD	C19-N20-C21	4.56	121.66	113.43
8	Y	603	MFN	C22-C14-C23	-4.53	104.69	113.16
13	f	503	MGD	C19-N20-C21	4.53	121.60	113.43
13	H	503	MGD	C19-N20-C21	4.52	121.59	113.43
8	M	603	MFN	C22-C14-C23	-4.52	104.71	113.16
13	B	503	MGD	C19-N20-C21	4.49	121.53	113.43
8	k	603	MFN	C27-C26-C25	4.48	123.05	113.04
8	G	603	MFN	C1-C2-C3	-4.45	123.48	129.54
13	r	504	MGD	C19-N20-C21	4.45	121.47	113.43
8	G	603	MFN	C22-C14-C23	-4.45	104.83	113.16
8	q	603	MFN	C22-C14-C23	-4.45	104.84	113.16
13	N	504	MGD	C19-N20-C21	4.44	121.45	113.43
13	r	503	MGD	C19-N20-C21	4.44	121.44	113.43
13	T	503	MGD	C19-N20-C21	4.43	121.42	113.43
13	B	504	MGD	C19-N20-C21	4.41	121.40	113.43
8	M	603	MFN	C1-C2-C3	-4.39	123.57	129.54
13	T	504	MGD	C19-N20-C21	4.38	121.34	113.43
13	N	503	MGD	C19-N20-C21	4.38	121.33	113.43
13	l	504	MGD	C19-N20-C21	4.34	121.27	113.43
8	S	603	MFN	C1-C2-C3	-4.05	124.03	129.54
8	q	603	MFN	C1-C2-C3	-4.05	124.03	129.54
8	e	603	MFN	C24-C23-N4	-3.91	101.30	110.55
8	S	603	MFN	C19-N3-C21	3.87	131.61	121.65
8	S	603	MFN	C24-C23-N4	-3.81	101.52	110.55
8	M	603	MFN	C20-C19-N3	-3.80	101.55	110.55
8	A	603	MFN	C1-C2-C3	-3.80	124.38	129.54
8	M	603	MFN	C26-C27-C28	-3.71	102.92	113.86
8	q	603	MFN	C20-C19-N3	-3.46	102.35	110.55
8	e	603	MFN	O2-C13-C4	-3.38	99.03	109.16
13	H	503	MGD	PA-O3B-PB	-3.19	121.89	132.83
8	M	603	MFN	C24-C23-N4	-3.18	103.00	110.55
8	A	603	MFN	C11-C10-C9	3.16	123.59	119.73
8	k	603	MFN	O2-C13-C4	-3.09	99.89	109.16
13	B	503	MGD	C5-C6-N1	3.05	119.34	113.95
13	T	503	MGD	PA-O3B-PB	-2.98	122.59	132.83
8	S	603	MFN	O2-C13-C4	-2.98	100.21	109.16
8	A	603	MFN	C20-C19-N3	-2.97	103.52	110.55
8	Y	603	MFN	O2-C13-C4	-2.96	100.29	109.16
8	M	603	MFN	C11-C10-C9	2.95	123.34	119.73
8	A	603	MFN	C26-C25-N4	2.94	120.92	115.83
8	e	603	MFN	C19-N3-C21	2.89	129.07	121.65
13	Z	503	MGD	C5-C6-N1	2.88	119.03	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	k	603	MFN	C14-C22-C21	2.85	119.41	113.04
13	l	503	MGD	C5-C6-N1	2.85	118.98	113.95
8	q	603	MFN	C11-C10-C9	2.84	123.20	119.73
8	G	603	MFN	C20-C19-N3	-2.83	103.86	110.55
13	H	504	MGD	O17-C17-C16	-2.81	120.79	127.24
13	N	503	MGD	C5-C6-N1	2.80	118.90	113.95
8	A	603	MFN	O7-C24-O8	-2.79	117.76	124.09
8	G	603	MFN	O2-C13-C4	-2.78	100.82	109.16
13	B	504	MGD	O11-C23-N22	-2.77	105.72	108.57
13	B	503	MGD	PA-O3B-PB	-2.74	123.41	132.83
8	S	603	MFN	O3-C16-N2	-2.74	117.84	123.01
13	r	504	MGD	C5-C6-N1	2.73	118.77	113.95
13	N	503	MGD	PA-O3B-PB	-2.72	123.48	132.83
8	k	603	MFN	C20-C19-N3	-2.72	104.11	110.55
8	e	603	MFN	O7-C24-O8	-2.71	117.93	124.09
13	f	503	MGD	PA-O3B-PB	-2.69	123.61	132.83
13	l	503	MGD	O17-C17-C16	-2.67	121.12	127.24
13	Z	503	MGD	C8-N7-C5	2.67	108.08	102.99
8	e	603	MFN	O15-C34-C33	2.67	121.38	114.03
8	M	603	MFN	O7-C24-O8	-2.67	118.03	124.09
13	H	503	MGD	C5-C6-N1	2.67	118.66	113.95
13	r	503	MGD	C5-C6-N1	2.67	118.66	113.95
13	f	504	MGD	O17-C17-C16	-2.66	121.13	127.24
13	l	503	MGD	C8-N7-C5	2.65	108.03	102.99
13	r	503	MGD	C8-N7-C5	2.64	108.02	102.99
13	N	503	MGD	C8-N7-C5	2.63	108.00	102.99
13	T	504	MGD	C8-N7-C5	2.63	108.00	102.99
13	r	504	MGD	C8-N7-C5	2.63	107.99	102.99
13	Z	503	MGD	O17-C17-C16	-2.62	121.23	127.24
13	l	504	MGD	O17-C17-C16	-2.62	121.23	127.24
13	Z	504	MGD	C5-C6-N1	2.62	118.57	113.95
13	T	504	MGD	C5-C6-N1	2.61	118.56	113.95
13	B	503	MGD	C8-N7-C5	2.60	107.95	102.99
8	G	603	MFN	C11-C10-C9	2.60	122.92	119.73
13	l	504	MGD	C8-N7-C5	2.60	107.94	102.99
8	Y	603	MFN	C19-N3-C21	2.60	128.33	121.65
8	S	603	MFN	C11-C10-C9	2.60	122.91	119.73
13	T	503	MGD	C8-N7-C5	2.59	107.92	102.99
8	M	603	MFN	O2-C13-C4	-2.58	101.42	109.16
13	N	504	MGD	C17-C16-N15	2.58	123.68	116.76
13	l	503	MGD	C17-C16-N15	2.58	123.68	116.76
13	N	504	MGD	C5-C6-N1	2.57	118.49	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	f	503	MGD	C8-N7-C5	2.57	107.88	102.99
13	f	504	MGD	C8-N7-C5	2.57	107.88	102.99
13	B	504	MGD	C8-N7-C5	2.56	107.86	102.99
13	l	504	MGD	C5-C6-N1	2.54	118.44	113.95
13	H	503	MGD	C8-N7-C5	2.53	107.81	102.99
13	H	503	MGD	O17-C17-C16	-2.52	121.46	127.24
13	B	503	MGD	O6-C6-C5	-2.52	119.44	124.37
13	T	503	MGD	O17-C17-C16	-2.52	121.46	127.24
13	T	504	MGD	O17-C17-C16	-2.52	121.46	127.24
13	B	504	MGD	C5-C6-N1	2.52	118.40	113.95
8	G	603	MFN	O15-C34-C33	2.52	120.96	114.03
13	N	503	MGD	O17-C17-C16	-2.52	121.47	127.24
13	T	503	MGD	C5-C6-N1	2.51	118.39	113.95
8	e	603	MFN	O7-C24-C23	2.51	121.74	113.40
8	M	603	MFN	C27-C26-C25	2.50	118.63	113.04
8	q	603	MFN	O5-C20-C19	2.50	121.72	113.40
13	f	503	MGD	O17-C17-C16	-2.50	121.51	127.24
13	Z	504	MGD	C8-N7-C5	2.49	107.74	102.99
8	k	603	MFN	O15-C34-C33	2.49	120.89	114.03
8	k	603	MFN	C11-C10-C9	2.49	122.78	119.73
8	M	603	MFN	O10-C29-C28	2.49	120.87	114.03
8	Y	603	MFN	C11-C10-C9	2.49	122.77	119.73
13	B	503	MGD	O17-C17-C16	-2.46	121.59	127.24
13	N	504	MGD	C8-N7-C5	2.46	107.67	102.99
13	r	504	MGD	C17-C16-N15	2.45	123.35	116.76
8	k	603	MFN	O3-C16-N2	-2.44	118.41	123.01
13	r	503	MGD	C17-C16-N15	2.44	123.30	116.76
8	k	603	MFN	O10-C29-C28	2.43	120.72	114.03
13	f	504	MGD	O11-C23-N22	-2.43	106.07	108.57
8	k	603	MFN	C17-C16-N2	2.42	120.50	116.42
13	H	503	MGD	C17-C16-N15	2.41	123.23	116.76
13	f	504	MGD	C5-C6-N1	2.41	118.21	113.95
13	H	504	MGD	C5-C6-N1	2.41	118.20	113.95
8	q	603	MFN	O10-C29-C28	2.40	120.64	114.03
8	M	603	MFN	O3-C16-N2	-2.40	118.49	123.01
8	A	603	MFN	O5-C20-C19	2.37	121.28	113.40
13	f	503	MGD	C17-C16-N15	2.37	123.12	116.76
13	H	504	MGD	C8-N7-C5	2.37	107.50	102.99
13	B	504	MGD	O17-C17-C16	-2.34	121.88	127.24
8	M	603	MFN	C22-C21-N3	-2.34	111.78	115.83
13	l	503	MGD	PA-O3B-PB	-2.32	124.85	132.83
13	f	503	MGD	C5-C6-N1	2.32	118.05	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Z	503	MGD	C17-C16-N15	2.32	122.99	116.76
8	S	603	MFN	O7-C24-O8	-2.31	118.85	124.09
8	q	603	MFN	O3-C16-N2	-2.30	118.67	123.01
8	A	603	MFN	C22-C14-C23	-2.29	108.88	113.16
8	M	603	MFN	O15-C34-C33	2.29	120.33	114.03
8	M	603	MFN	C26-C25-N4	-2.28	111.87	115.83
13	r	503	MGD	PA-O3B-PB	-2.28	125.00	132.83
8	G	603	MFN	C26-C27-C28	-2.27	107.16	113.86
13	r	504	MGD	O17-C17-C16	-2.27	122.04	127.24
8	Y	603	MFN	O15-C34-C33	2.26	120.26	114.03
8	Y	603	MFN	C20-C19-N3	-2.26	105.20	110.55
13	r	503	MGD	O17-C17-C16	-2.25	122.08	127.24
8	A	603	MFN	C27-C26-C25	-2.25	108.02	113.04
8	M	603	MFN	C19-N3-C21	2.25	127.42	121.65
13	B	503	MGD	C17-C16-N15	2.24	122.77	116.76
8	k	603	MFN	O15-C34-O14	-2.23	119.03	124.09
8	e	603	MFN	C3-C4-C5	2.22	108.78	105.12
13	N	504	MGD	O17-C17-C16	-2.22	122.15	127.24
8	k	603	MFN	O9-C25-C26	2.22	126.07	122.02
8	e	603	MFN	C11-C10-C9	2.22	122.44	119.73
8	G	603	MFN	O5-C20-C19	2.20	120.72	113.40
8	Y	603	MFN	O5-C20-C19	2.20	120.71	113.40
8	k	603	MFN	O7-C24-O8	-2.20	119.10	124.09
8	e	603	MFN	O10-C29-O11	-2.20	119.10	124.09
8	A	603	MFN	O10-C29-C28	2.20	120.07	114.03
13	N	503	MGD	C17-C16-N15	2.19	122.63	116.76
13	Z	504	MGD	O17-C17-C16	-2.19	122.23	127.24
8	M	603	MFN	C7-C8-C9	2.18	122.40	119.73
8	Y	603	MFN	O10-C29-O11	-2.18	119.13	124.09
8	S	603	MFN	O5-C20-C19	2.18	120.65	113.40
13	Z	504	MGD	C17-C16-N15	2.17	122.60	116.76
8	k	603	MFN	C3-C4-C5	2.17	108.69	105.12
8	A	603	MFN	C17-C16-N2	2.16	120.06	116.42
13	B	504	MGD	C17-C16-N15	2.15	122.52	116.76
8	q	603	MFN	O15-C34-C33	2.14	119.93	114.03
13	r	503	MGD	O11-C23-C14	-2.14	107.54	108.96
13	T	503	MGD	C17-C16-N15	2.14	122.49	116.76
8	S	603	MFN	O10-C29-C28	2.13	119.90	114.03
8	Y	603	MFN	C3-C4-C5	2.12	108.62	105.12
8	e	603	MFN	O10-C29-C28	2.12	119.88	114.03
8	G	603	MFN	O10-C29-O11	-2.10	119.31	124.09
8	Y	603	MFN	C26-C27-C28	-2.10	107.65	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Y	603	MFN	C24-C23-N4	-2.10	105.57	110.55
8	A	603	MFN	O15-C34-C33	2.10	119.81	114.03
13	H	503	MGD	O6-C6-C5	-2.10	120.27	124.37
13	Z	503	MGD	O6-C6-C5	-2.09	120.29	124.37
13	H	503	MGD	O11-C23-C14	-2.09	107.57	108.96
8	q	603	MFN	O5-C20-O4	-2.07	119.39	124.09
8	q	603	MFN	C26-C27-C28	-2.06	107.77	113.86
13	N	503	MGD	O6-C6-C5	-2.06	120.34	124.37
8	S	603	MFN	C18-C19-N3	2.06	115.03	110.88
8	M	603	MFN	C14-C23-N4	-2.05	106.73	110.88
13	T	503	MGD	O11-C23-C14	-2.05	107.60	108.96
8	S	603	MFN	C14-C23-C24	2.03	115.26	110.35
8	e	603	MFN	O5-C20-C19	2.03	120.14	113.40
13	l	503	MGD	O6-C6-C5	-2.02	120.44	124.37
8	S	603	MFN	C3-C4-C5	2.02	108.44	105.12
8	Y	603	MFN	O3-C16-N2	-2.01	119.21	123.01
8	S	603	MFN	C7-C8-C9	2.01	122.19	119.73
13	H	504	MGD	O6-C6-C5	-2.01	120.44	124.37
8	G	603	MFN	O15-C34-O14	-2.01	119.53	124.09
13	T	504	MGD	C17-C16-N15	2.00	122.14	116.76
8	k	603	MFN	O5-C20-O4	-2.00	119.54	124.09

There are no chirality outliers.

All (204) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	603	MFN	C6-C12-C15-N2
8	A	603	MFN	C31-C32-C33-C28
8	A	603	MFN	C31-C32-C33-C34
8	G	603	MFN	C26-C27-C28-C29
8	G	603	MFN	C6-C12-C15-N2
8	G	603	MFN	C31-C32-C33-C28
8	G	603	MFN	C31-C32-C33-C34
8	M	603	MFN	C26-C27-C28-C29
8	M	603	MFN	C26-C27-C28-C33
8	M	603	MFN	C27-C28-C33-C34
8	M	603	MFN	C29-C28-C33-C32
8	M	603	MFN	C29-C28-C33-C34
8	M	603	MFN	C6-C12-C15-N2
8	M	603	MFN	C31-C32-C33-C28
8	M	603	MFN	C31-C32-C33-C34
8	S	603	MFN	C18-C19-N3-C21

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Mol	Chain	Res	Type	Atoms
8	S	603	MFN	C26-C27-C28-C29
8	S	603	MFN	C29-C28-C33-C34
8	S	603	MFN	C17-C18-C19-N3
8	S	603	MFN	C6-C12-C15-N2
8	Y	603	MFN	C26-C27-C28-C29
8	Y	603	MFN	C26-C27-C28-C33
8	Y	603	MFN	C6-C12-C15-N2
8	Y	603	MFN	C31-C32-C33-C28
8	Y	603	MFN	C31-C32-C33-C34
8	e	603	MFN	C27-C28-C33-C32
8	e	603	MFN	C29-C28-C33-C32
8	e	603	MFN	C29-C28-C33-C34
8	e	603	MFN	C6-C12-C15-N2
8	e	603	MFN	C31-C32-C33-C34
8	k	603	MFN	C26-C27-C28-C29
8	k	603	MFN	C26-C27-C28-C33
8	k	603	MFN	C27-C28-C33-C34
8	k	603	MFN	C29-C28-C33-C32
8	k	603	MFN	C29-C28-C33-C34
8	k	603	MFN	C6-C12-C15-N2
8	k	603	MFN	C31-C32-C33-C28
8	k	603	MFN	C31-C32-C33-C34
8	k	603	MFN	C28-C33-C34-O15
8	q	603	MFN	C26-C27-C28-C29
8	q	603	MFN	C26-C27-C28-C33
8	q	603	MFN	C6-C12-C15-N2
8	q	603	MFN	C31-C32-C33-C28
8	q	603	MFN	C31-C32-C33-C34
13	B	503	MGD	C5'-O5'-PB-O2B
13	B	503	MGD	O3A-C10-C11-C12
13	H	503	MGD	C5'-O5'-PB-O1B
13	H	503	MGD	C5'-O5'-PB-O2B
13	H	503	MGD	O3A-C10-C11-C12
13	N	503	MGD	C5'-O5'-PB-O2B
13	N	503	MGD	O3A-C10-C11-C12
13	T	503	MGD	PA-O3B-PB-O5'
13	T	503	MGD	O3A-C10-C11-C12
13	Z	503	MGD	PA-O3B-PB-O5'
13	Z	503	MGD	C5'-O5'-PB-O1B
13	Z	503	MGD	C5'-O5'-PB-O2B
13	Z	503	MGD	O3A-C10-C11-C12
13	f	503	MGD	C5'-O5'-PB-O1B

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Mol	Chain	Res	Type	Atoms
13	f	503	MGD	C5'-O5'-PB-O2B
13	f	503	MGD	O3A-C10-C11-C12
13	l	503	MGD	C5'-O5'-PB-O2B
13	l	503	MGD	O3A-C10-C11-C12
13	r	503	MGD	C5'-O5'-PB-O1B
13	r	503	MGD	C5'-O5'-PB-O2B
13	r	503	MGD	O3A-C10-C11-C12
8	e	603	MFN	C18-C19-N3-C21
8	e	603	MFN	C17-C18-C19-N3
13	B	503	MGD	O4'-C4'-C5'-O5'
13	H	503	MGD	O4'-C4'-C5'-O5'
8	Y	603	MFN	C18-C19-N3-C21
8	q	603	MFN	C30-C31-C32-C33
8	S	603	MFN	C17-C18-C19-C20
13	H	503	MGD	C3'-C4'-C5'-O5'
8	S	603	MFN	C18-C19-C20-O5
8	k	603	MFN	C30-C31-C32-C33
8	G	603	MFN	C30-C31-C32-C33
8	S	603	MFN	C18-C19-C20-O4
8	Y	603	MFN	C23-C14-C22-C21
8	M	603	MFN	C8-C9-O2-C13
8	G	603	MFN	N3-C19-C20-O4
8	G	603	MFN	N3-C19-C20-O5
8	e	603	MFN	N3-C19-C20-O4
8	q	603	MFN	C23-C14-C22-C21
8	e	603	MFN	N4-C23-C24-O8
8	e	603	MFN	N3-C19-C20-O5
8	A	603	MFN	C18-C19-C20-O4
8	q	603	MFN	C18-C19-C20-O4
8	S	603	MFN	C25-C26-C27-C28
13	B	503	MGD	C3'-C4'-C5'-O5'
8	M	603	MFN	C27-C28-C33-C32
8	k	603	MFN	C27-C28-C33-C32
8	A	603	MFN	C18-C19-C20-O5
8	Y	603	MFN	C18-C19-C20-O4
8	Y	603	MFN	C18-C19-C20-O5
8	q	603	MFN	C18-C19-C20-O5
13	f	503	MGD	O4'-C4'-C5'-O5'
8	G	603	MFN	C27-C28-C33-C34
8	e	603	MFN	C27-C28-C33-C34
8	A	603	MFN	N3-C19-C20-O4
8	Y	603	MFN	N4-C23-C24-O7

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Mol	Chain	Res	Type	Atoms
8	e	603	MFN	N4-C23-C24-O7
8	q	603	MFN	N4-C23-C24-O7
8	q	603	MFN	N3-C19-C20-O4
8	q	603	MFN	N3-C19-C20-O5
8	e	603	MFN	C17-C18-C19-C20
8	Y	603	MFN	C29-C28-C33-C34
13	B	503	MGD	O3A-C10-C11-O11
13	H	503	MGD	O3A-C10-C11-O11
13	N	503	MGD	O3A-C10-C11-O11
13	T	503	MGD	O3A-C10-C11-O11
13	Z	503	MGD	O3A-C10-C11-O11
13	f	503	MGD	O3A-C10-C11-O11
13	l	503	MGD	O3A-C10-C11-O11
8	A	603	MFN	N3-C19-C20-O5
8	M	603	MFN	N3-C19-C20-O4
8	Y	603	MFN	N4-C23-C24-O8
8	Y	603	MFN	N3-C19-C20-O4
8	Y	603	MFN	N3-C19-C20-O5
8	q	603	MFN	N4-C23-C24-O8
13	B	503	MGD	PA-O3B-PB-O5'
13	H	503	MGD	PA-O3B-PB-O5'
13	N	503	MGD	PA-O3B-PB-O5'
13	Z	504	MGD	PA-O3B-PB-O5'
13	f	503	MGD	PA-O3B-PB-O5'
13	l	503	MGD	PA-O3B-PB-O5'
13	l	504	MGD	PA-O3B-PB-O5'
13	r	503	MGD	PA-O3B-PB-O5'
8	A	603	MFN	C15-C12-C6-C7
8	k	603	MFN	C32-C33-C34-O14
8	M	603	MFN	N3-C19-C20-O5
8	k	603	MFN	N3-C19-C20-O4
8	k	603	MFN	N3-C19-C20-O5
8	G	603	MFN	C33-C28-C29-O10
8	G	603	MFN	C33-C28-C29-O11
8	Y	603	MFN	C33-C28-C29-O10
8	Y	603	MFN	C33-C28-C29-O11
13	B	503	MGD	C5'-O5'-PB-O3B
13	N	503	MGD	C5'-O5'-PB-O3B
13	N	504	MGD	C10-O3A-PA-O3B
13	T	504	MGD	C10-O3A-PA-O3B
13	Z	503	MGD	C5'-O5'-PB-O3B
13	f	503	MGD	C5'-O5'-PB-O3B

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Mol	Chain	Res	Type	Atoms
13	f	504	MGD	C10-O3A-PA-O3B
13	l	503	MGD	C5'-O5'-PB-O3B
13	B	504	MGD	PB-O3B-PA-O1A
13	B	503	MGD	C5'-O5'-PB-O1B
13	N	503	MGD	C5'-O5'-PB-O1B
13	l	503	MGD	C5'-O5'-PB-O1B
8	S	603	MFN	N3-C19-C20-O5
8	q	603	MFN	C14-C23-C24-O8
13	r	503	MGD	O4'-C4'-C5'-O5'
8	S	603	MFN	C27-C28-C33-C32
8	Y	603	MFN	C27-C28-C33-C32
8	M	603	MFN	N4-C23-C24-O8
8	q	603	MFN	C14-C23-C24-O7
8	S	603	MFN	N3-C19-C20-O4
13	N	503	MGD	O4'-C4'-C5'-O5'
8	S	603	MFN	C27-C28-C33-C34
8	S	603	MFN	C29-C28-C33-C32
8	Y	603	MFN	C27-C28-C33-C34
8	Y	603	MFN	C29-C28-C33-C32
8	Y	603	MFN	O13-C30-C31-C32
8	M	603	MFN	O12-C30-C31-C32
8	M	603	MFN	C14-C23-C24-O8
8	Y	603	MFN	O12-C30-C31-C32
8	M	603	MFN	O13-C30-C31-C32
8	G	603	MFN	C29-C28-C33-C34
13	r	503	MGD	O3A-C10-C11-O11
8	A	603	MFN	O12-C30-C31-C32
8	A	603	MFN	O13-C30-C31-C32
8	e	603	MFN	O12-C30-C31-C32
8	e	603	MFN	O13-C30-C31-C32
8	q	603	MFN	O13-C30-C31-C32
13	Z	503	MGD	O4'-C4'-C5'-O5'
8	S	603	MFN	O12-C30-C31-C32
8	M	603	MFN	C14-C23-C24-O7
13	f	503	MGD	C3'-C4'-C5'-O5'
8	S	603	MFN	O13-C30-C31-C32
8	G	603	MFN	C26-C27-C28-C33
8	S	603	MFN	C32-C33-C34-O15
8	Y	603	MFN	C27-C28-C29-O10
8	Y	603	MFN	C27-C28-C29-O11
8	Y	603	MFN	C32-C33-C34-O15
8	e	603	MFN	C27-C28-C29-O10

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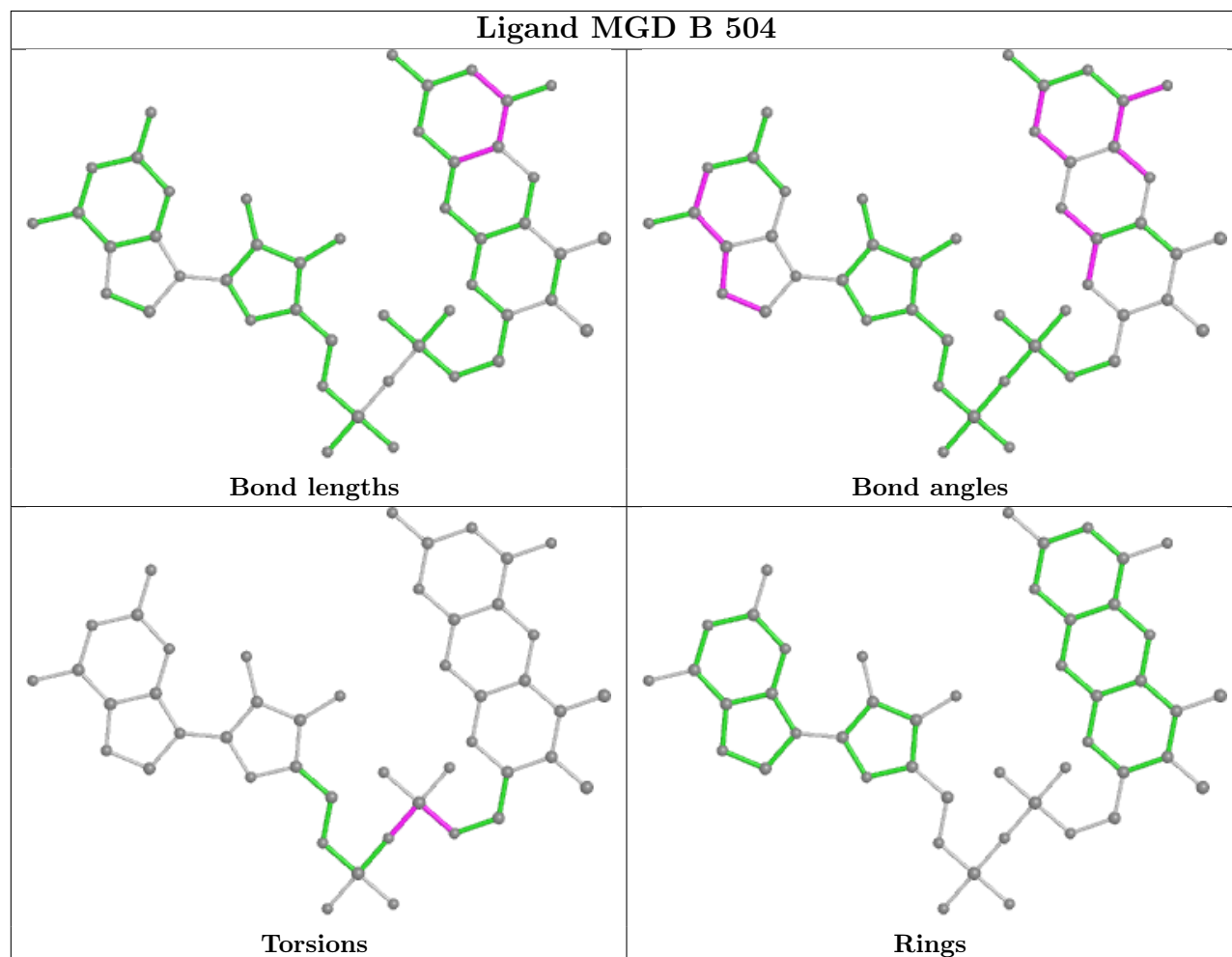
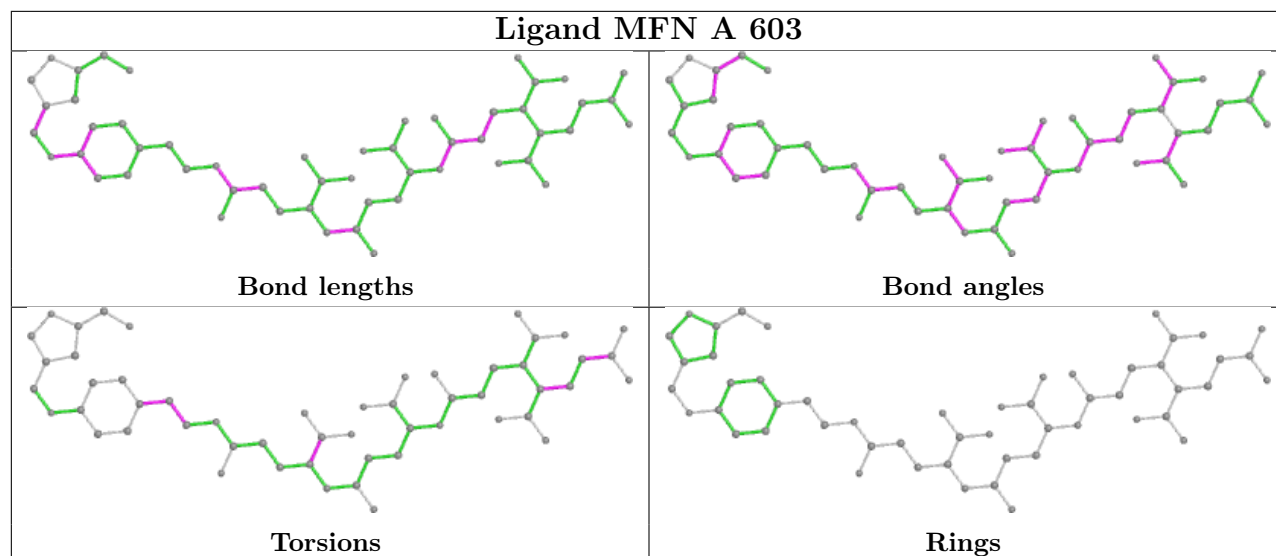
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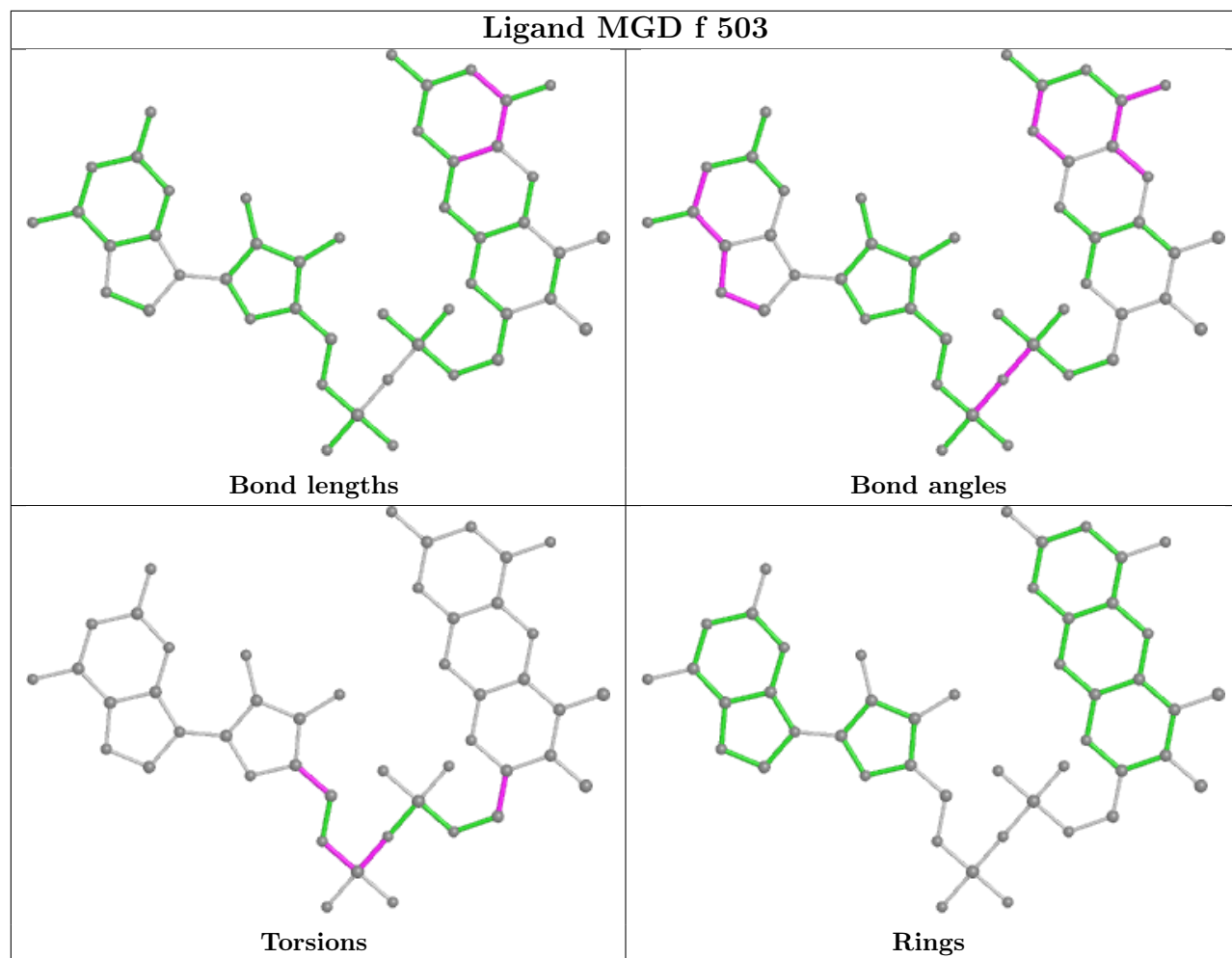
Mol	Chain	Res	Type	Atoms
8	e	603	MFN	C27-C28-C29-O11
8	k	603	MFN	C32-C33-C34-O15
8	M	603	MFN	N4-C23-C24-O7
8	G	603	MFN	C18-C19-C20-O4
8	e	603	MFN	C14-C23-C24-O8
13	B	504	MGD	C10-O3A-PA-O3B
13	H	503	MGD	C5'-O5'-PB-O3B
13	H	504	MGD	C10-O3A-PA-O3B
13	r	503	MGD	C5'-O5'-PB-O3B
13	T	503	MGD	O4'-C4'-C5'-O5'
13	Z	503	MGD	PA-O3B-PB-O1B
8	G	603	MFN	C15-C12-C6-C7
8	q	603	MFN	O12-C30-C31-C32
8	G	603	MFN	C18-C19-C20-O5
8	k	603	MFN	O12-C30-C31-C32
13	l	503	MGD	O4'-C4'-C5'-O5'
8	e	603	MFN	C30-C31-C32-C33
8	e	603	MFN	C14-C23-C24-O7
8	k	603	MFN	O13-C30-C31-C32
8	e	603	MFN	C16-C17-C18-C19

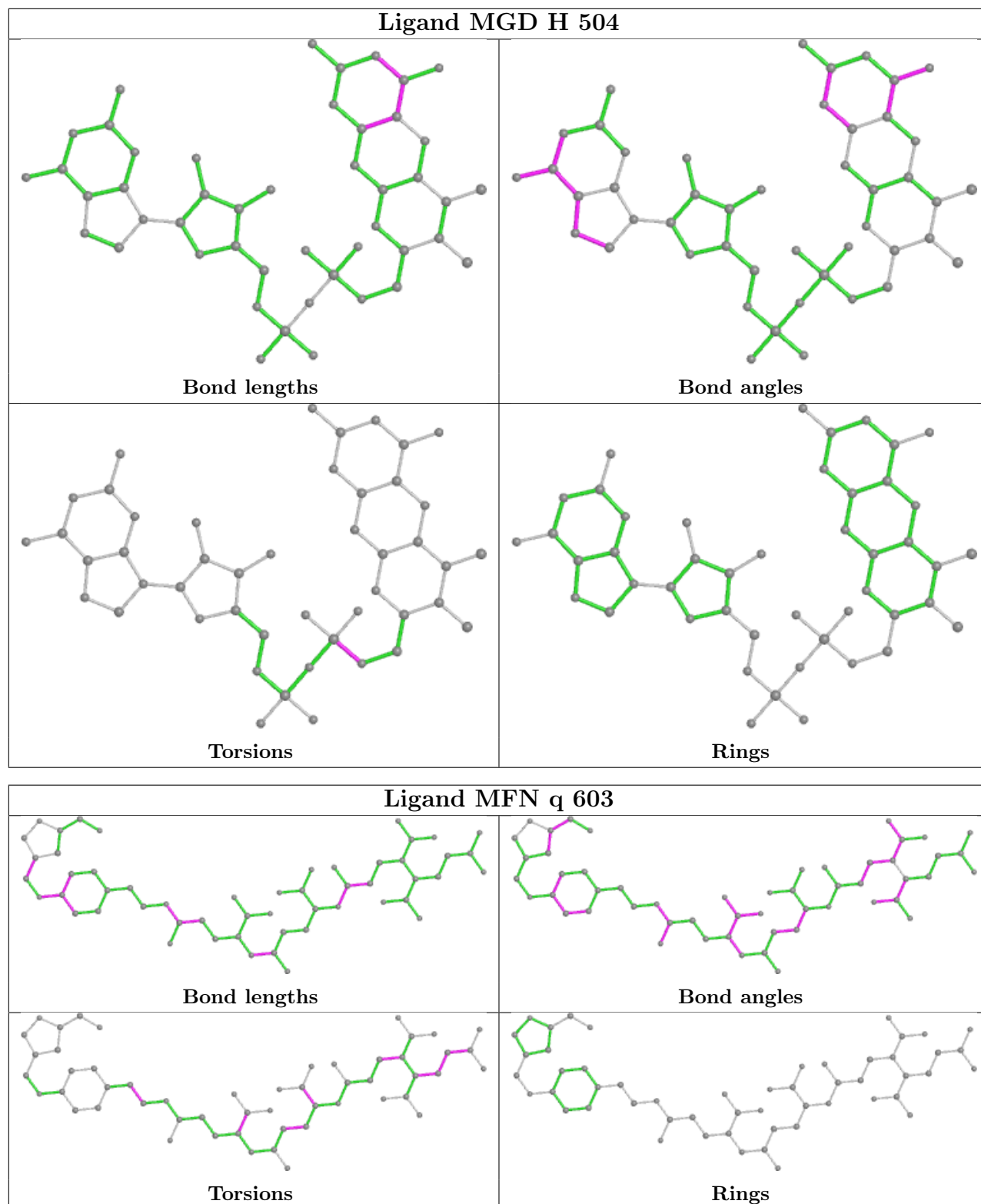
There are no ring outliers.

No monomer is involved in short contacts.

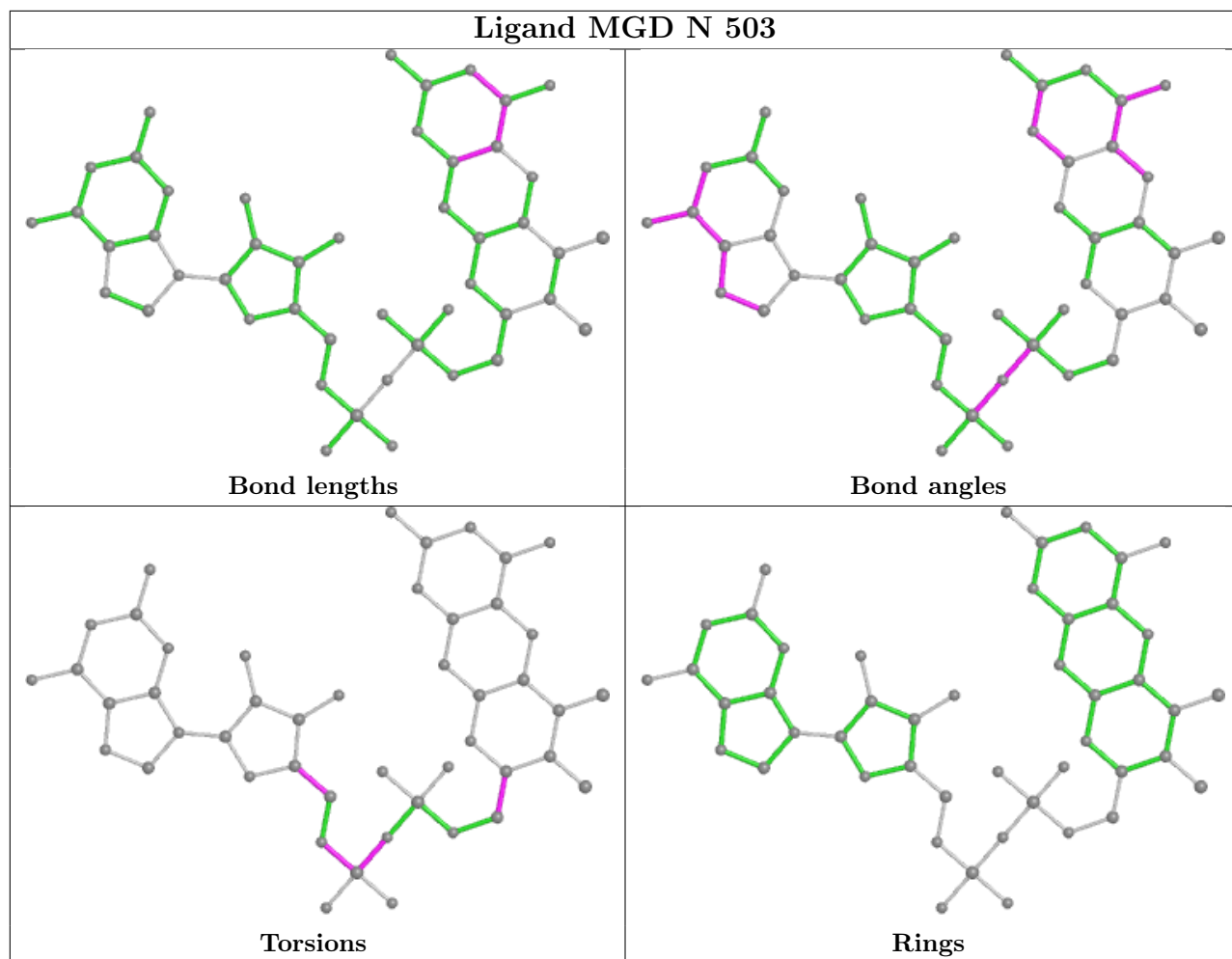
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

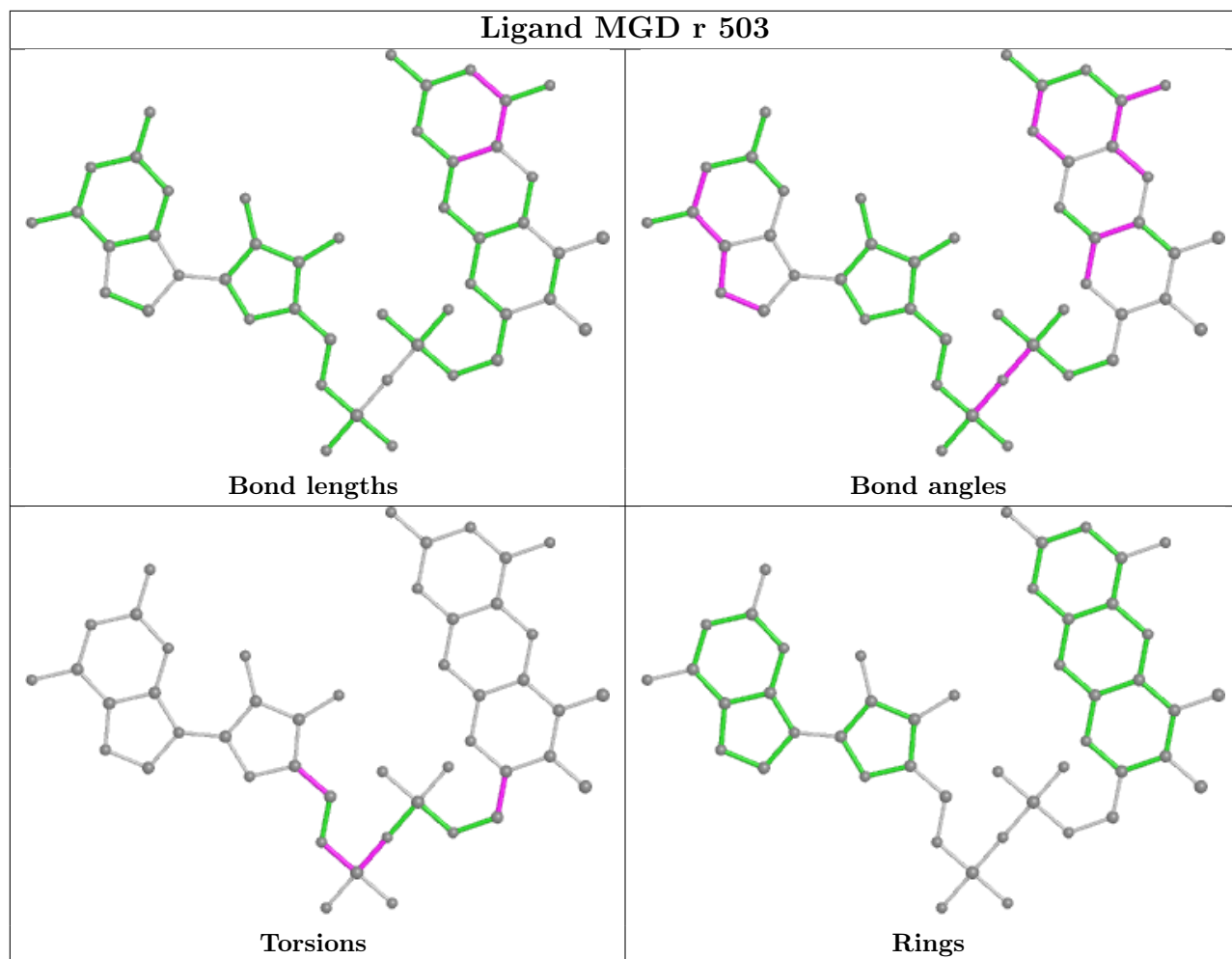


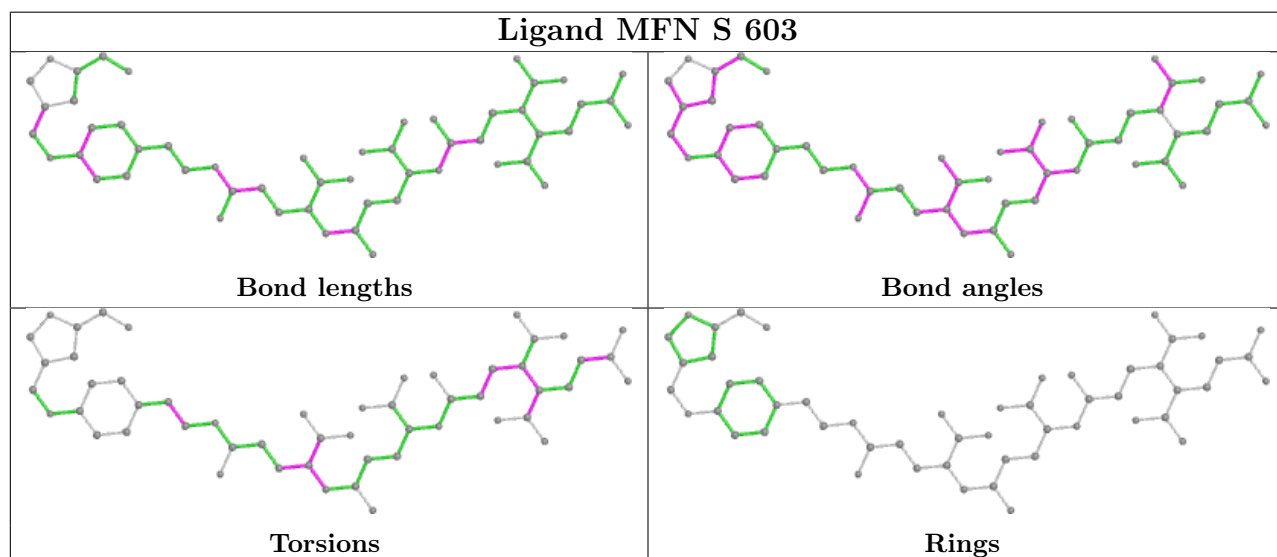
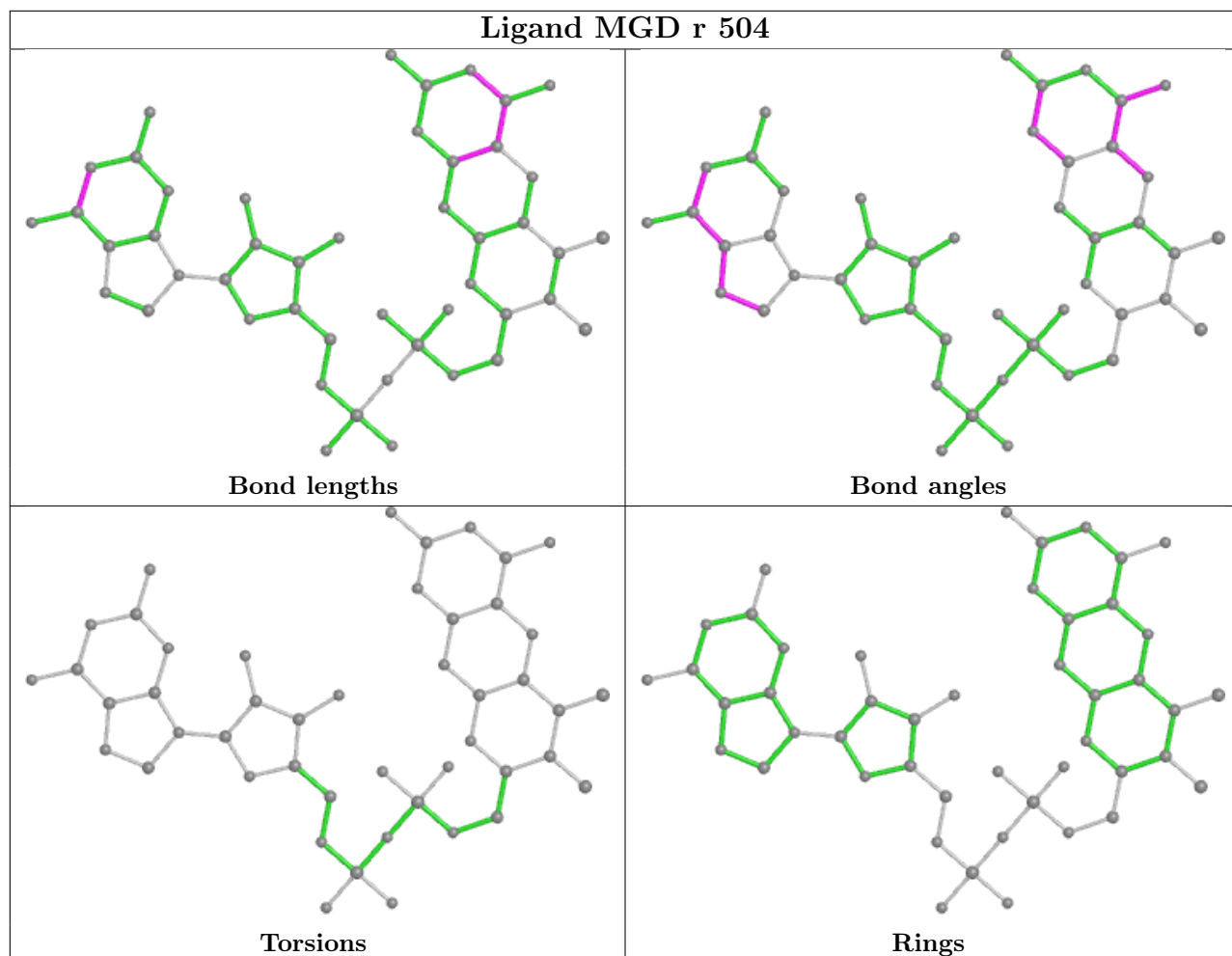


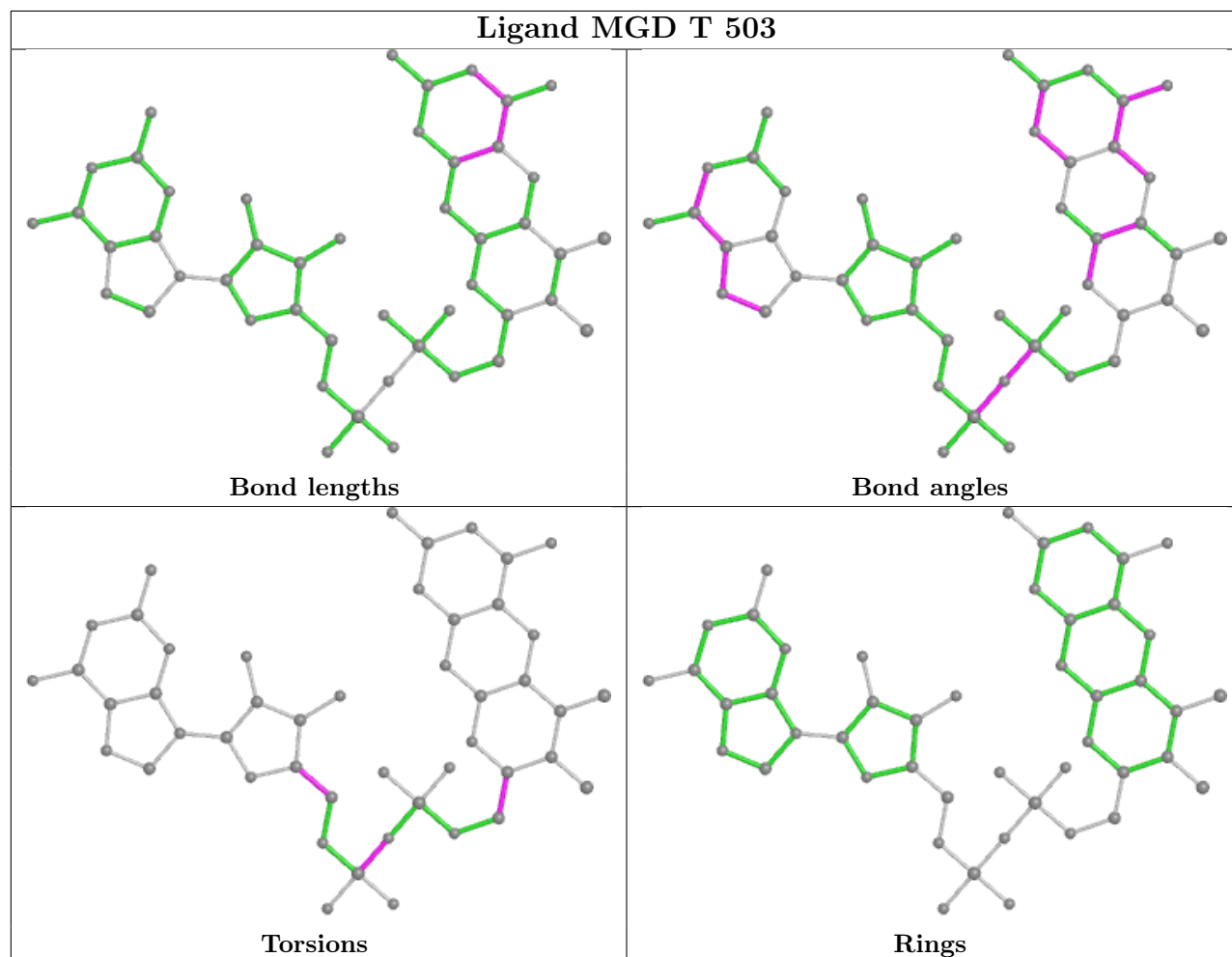
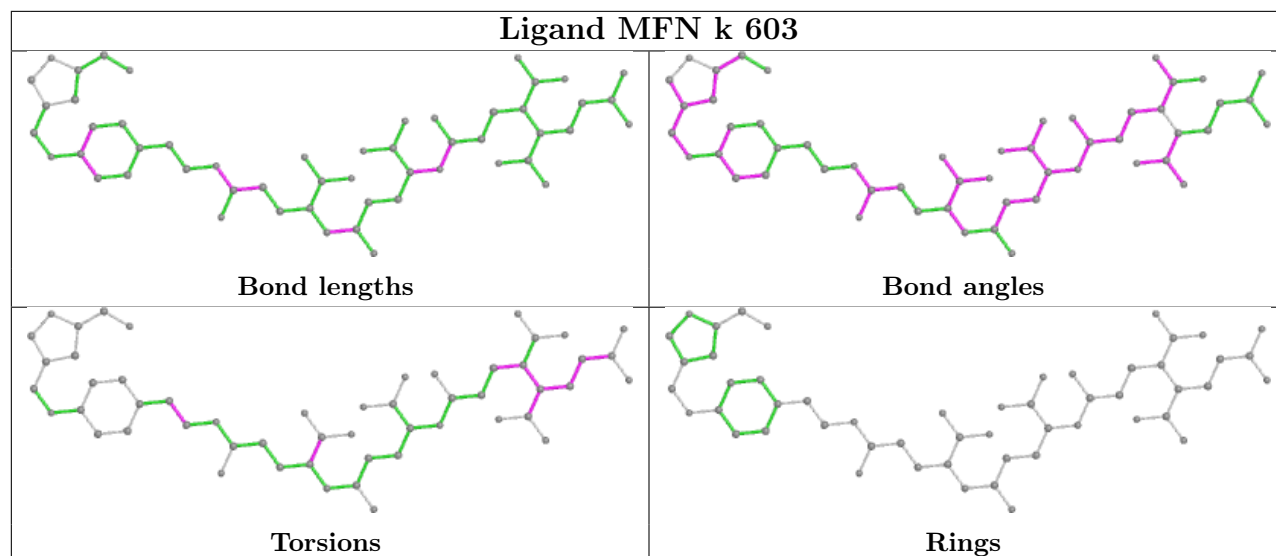


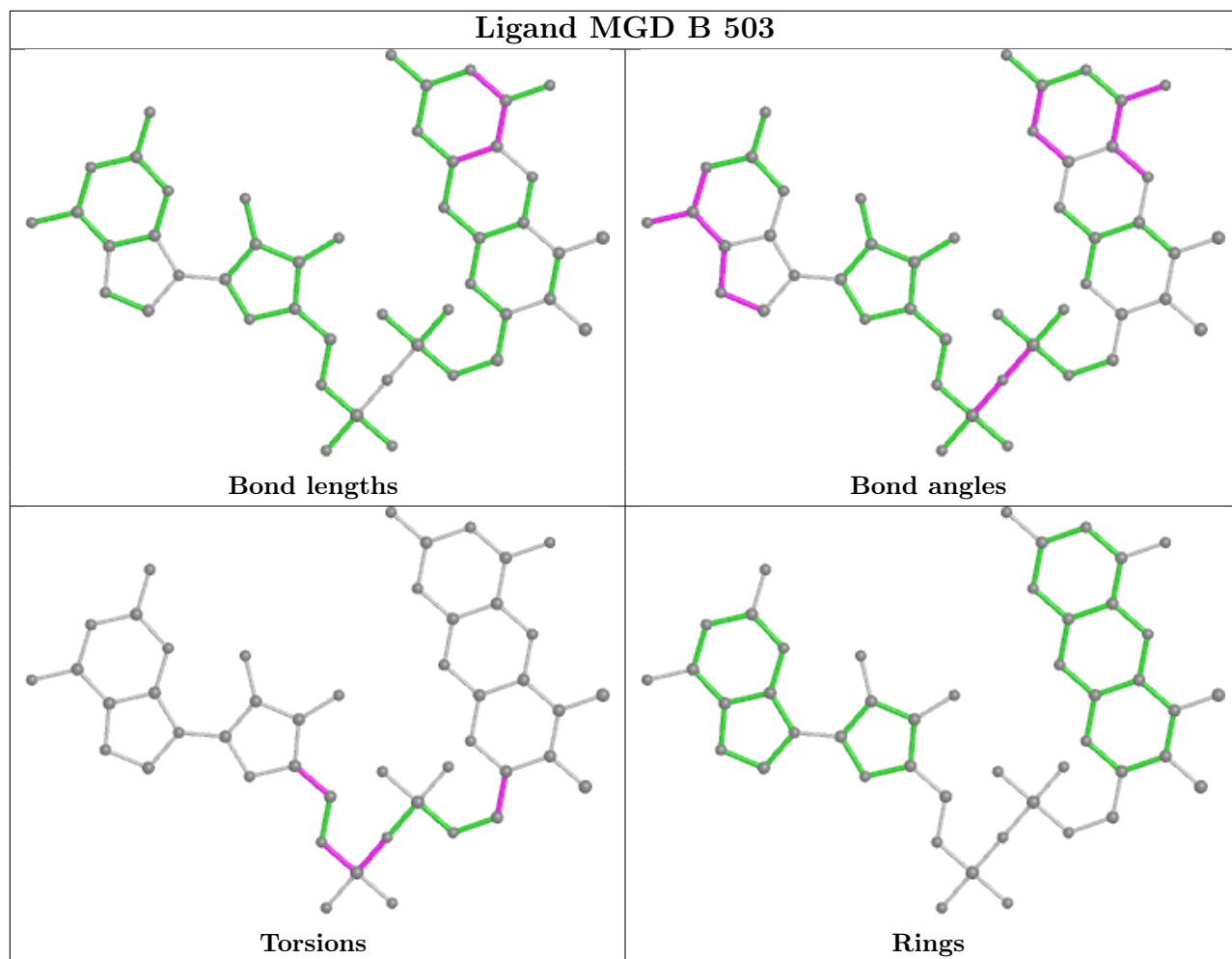


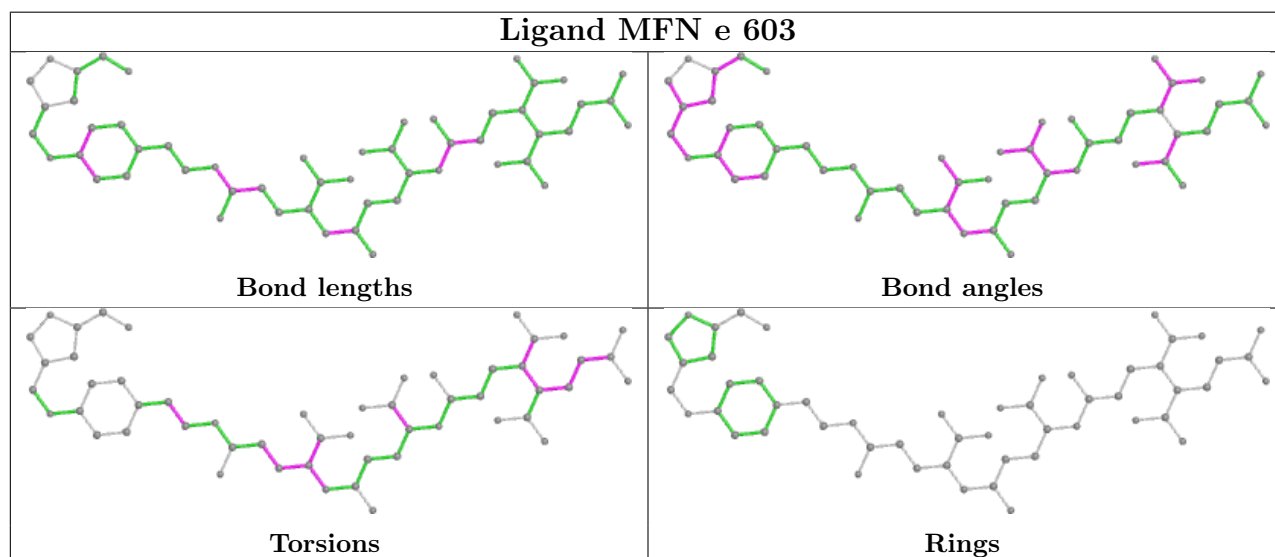
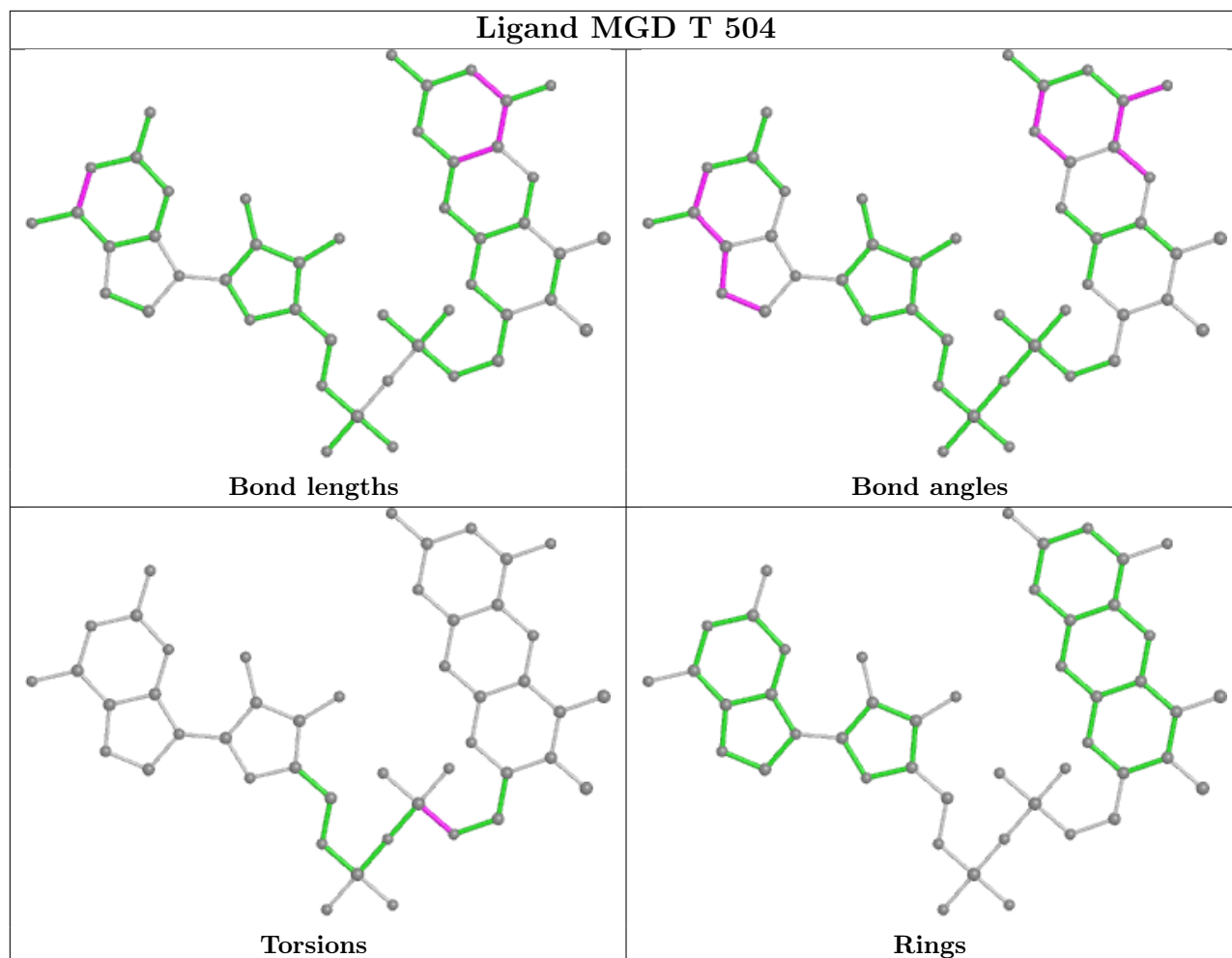


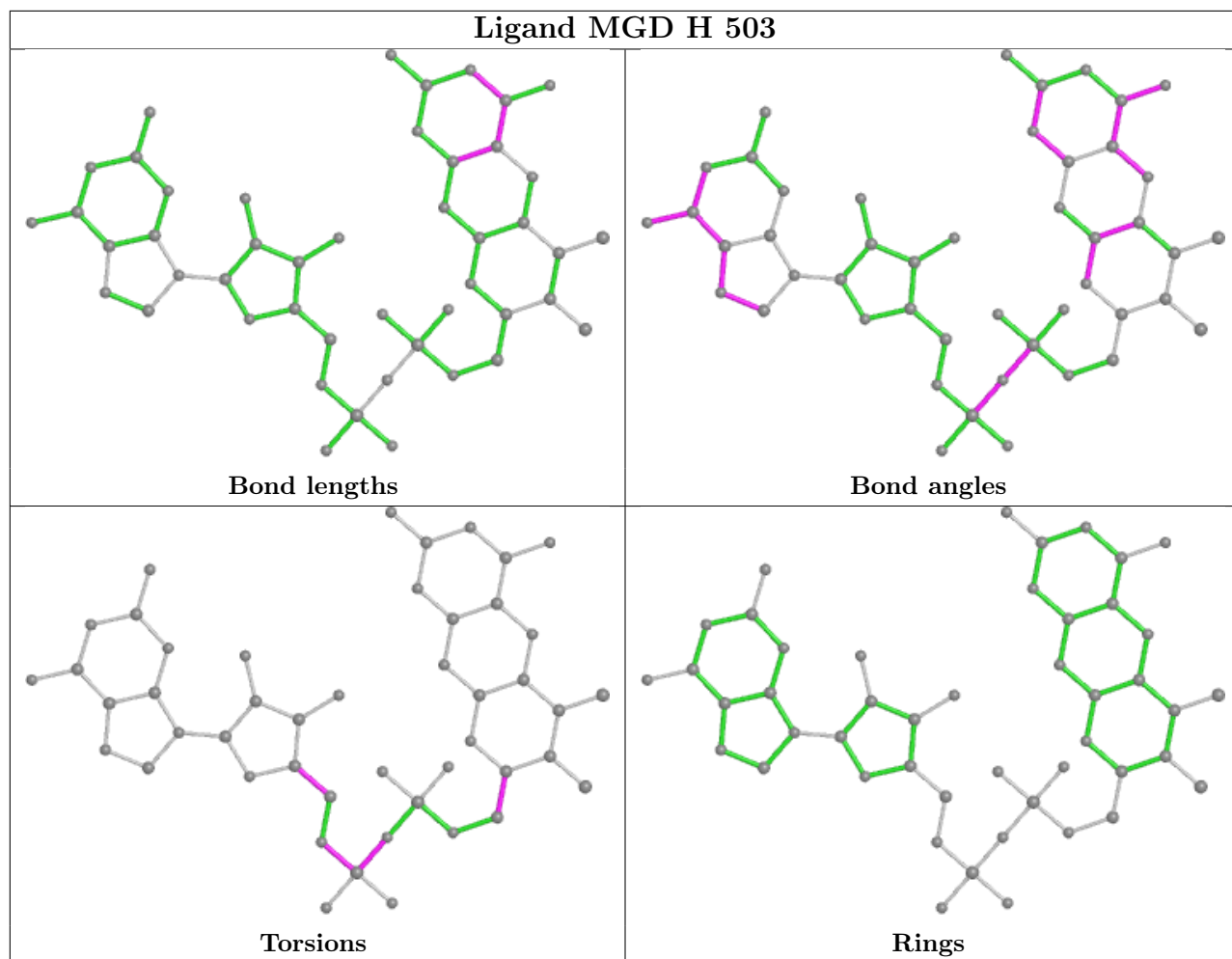


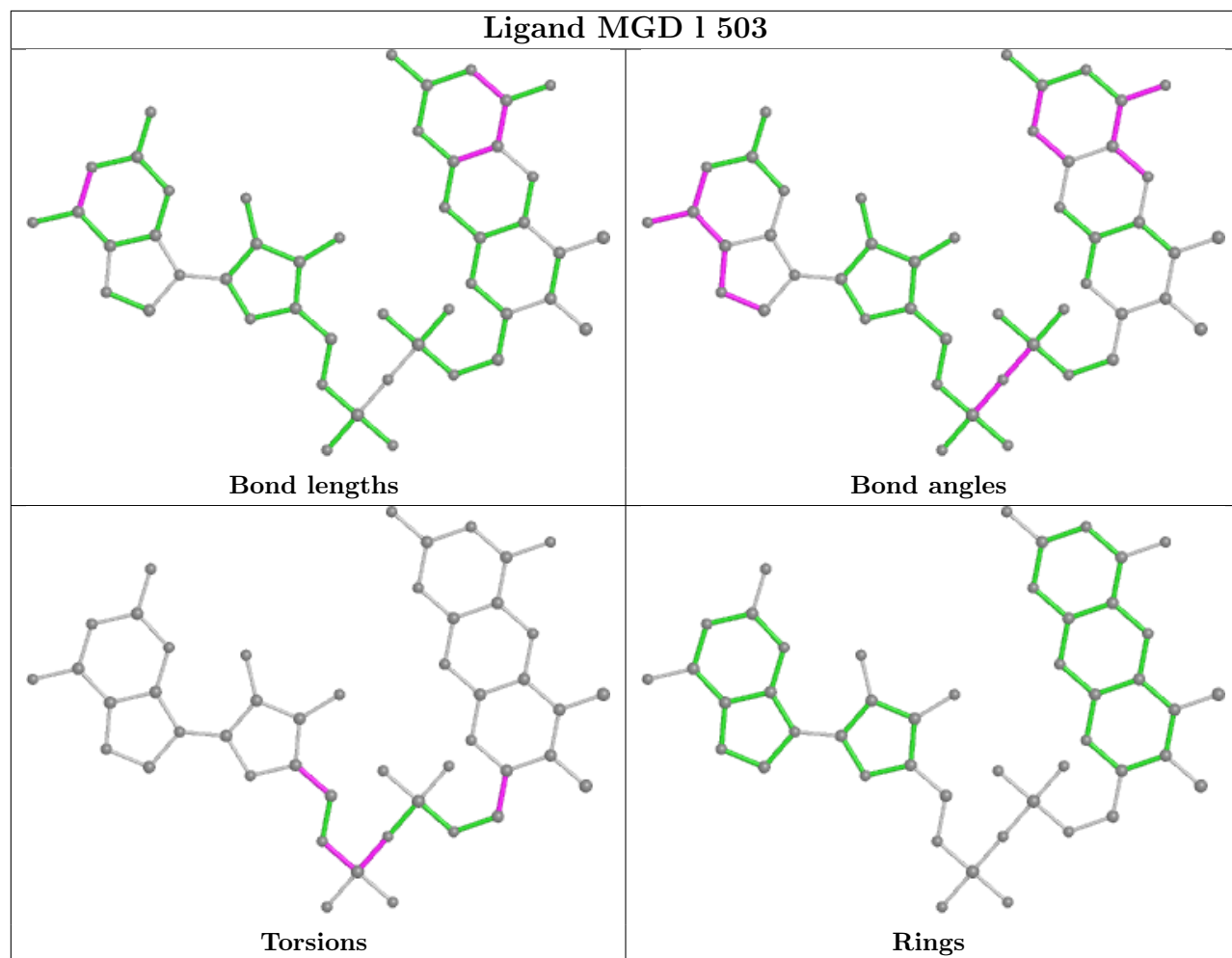




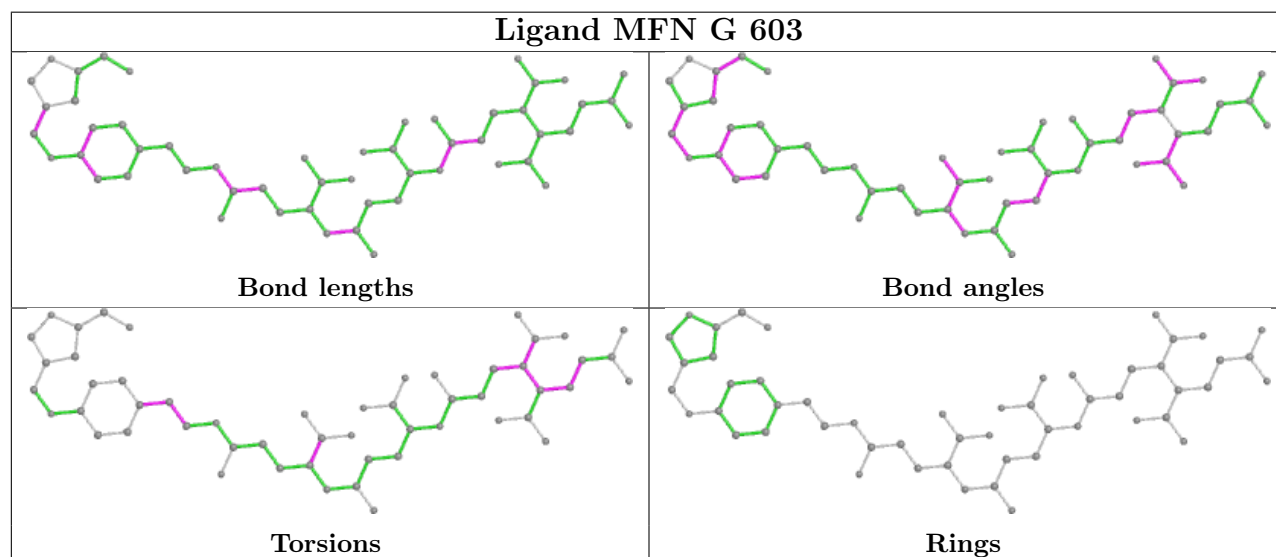
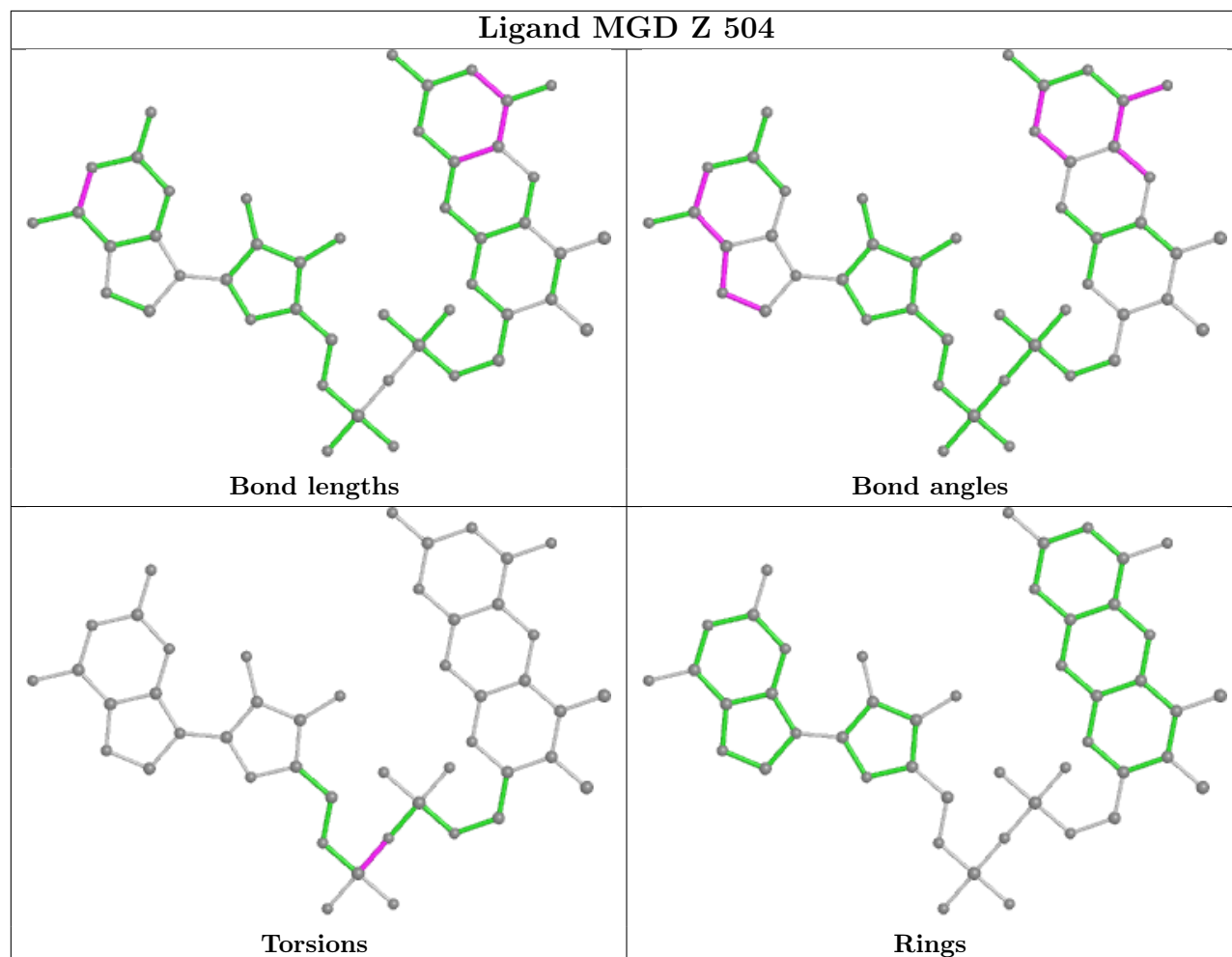


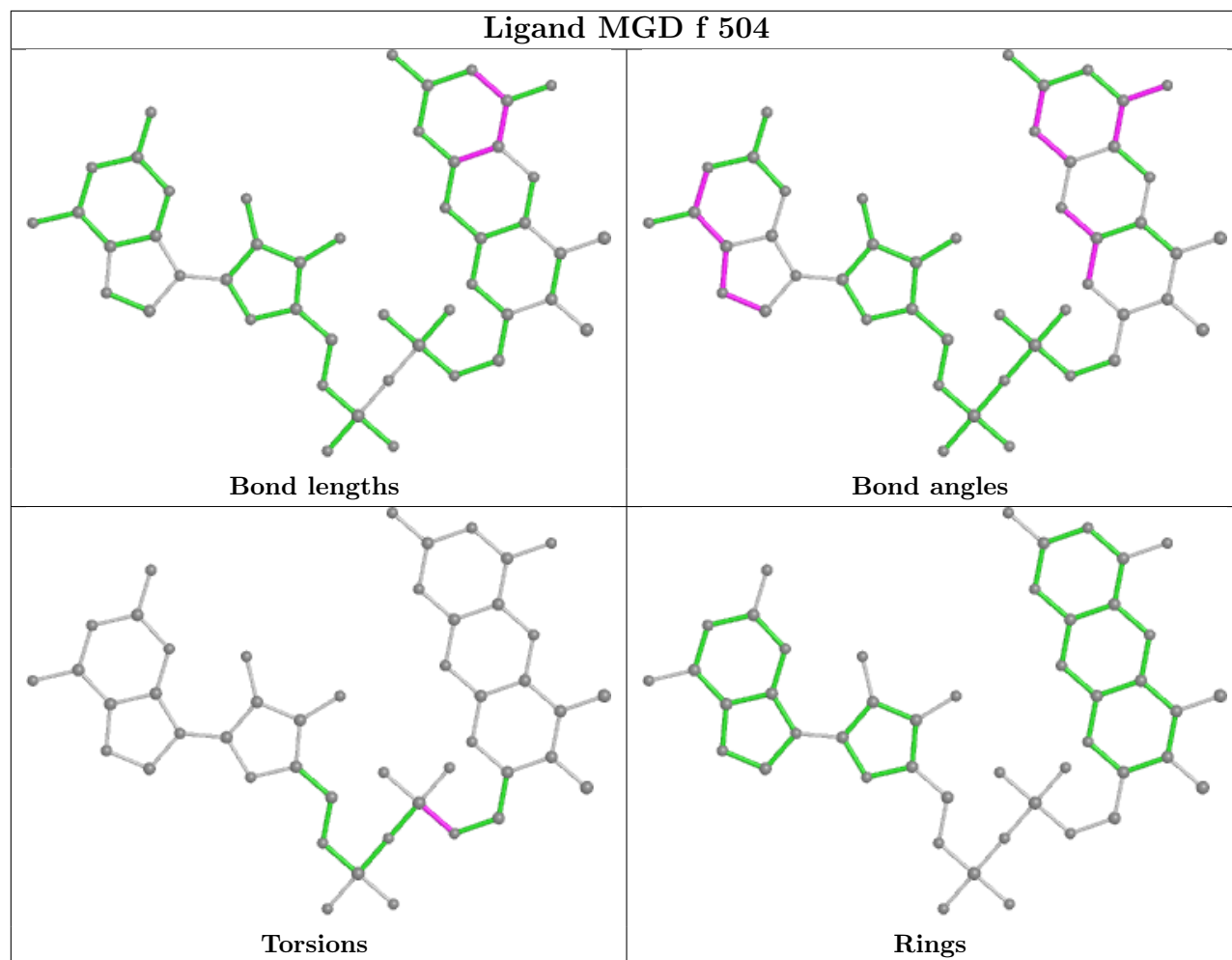


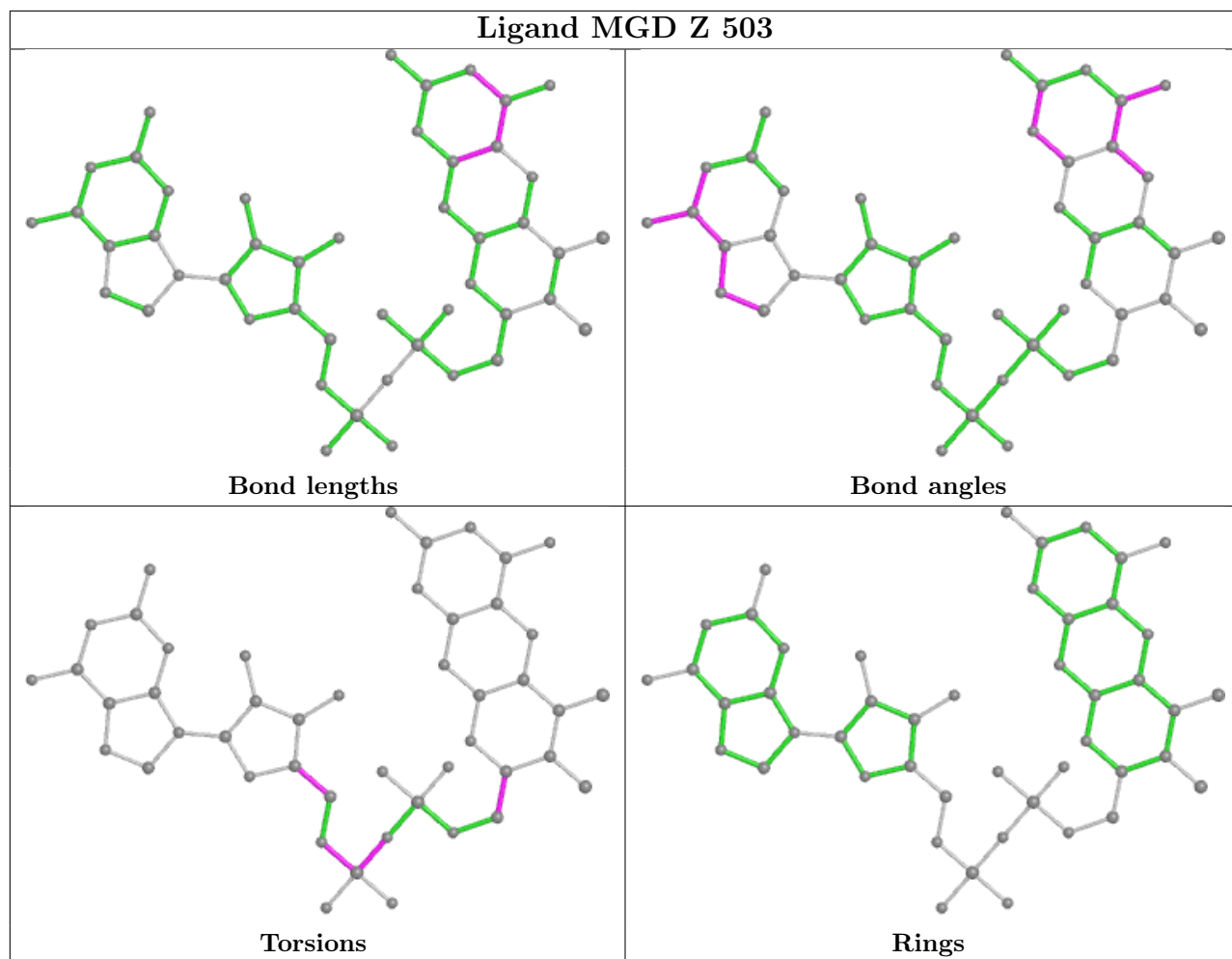


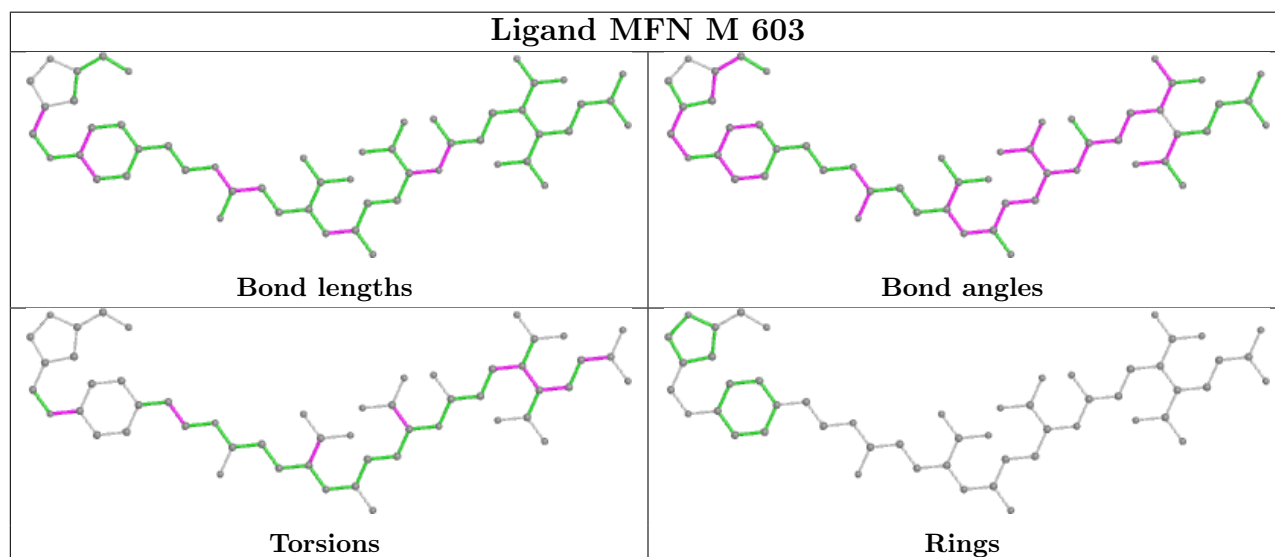
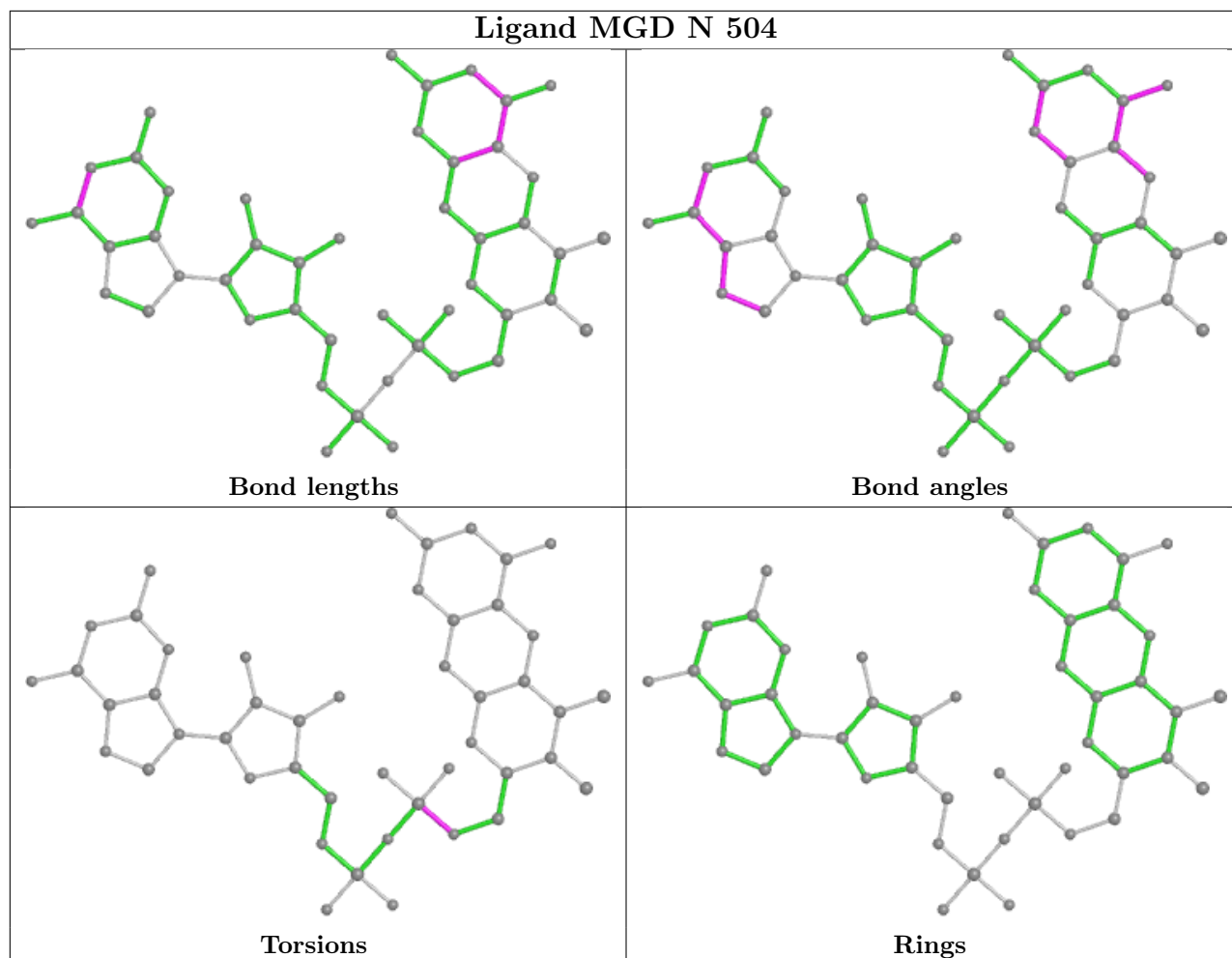


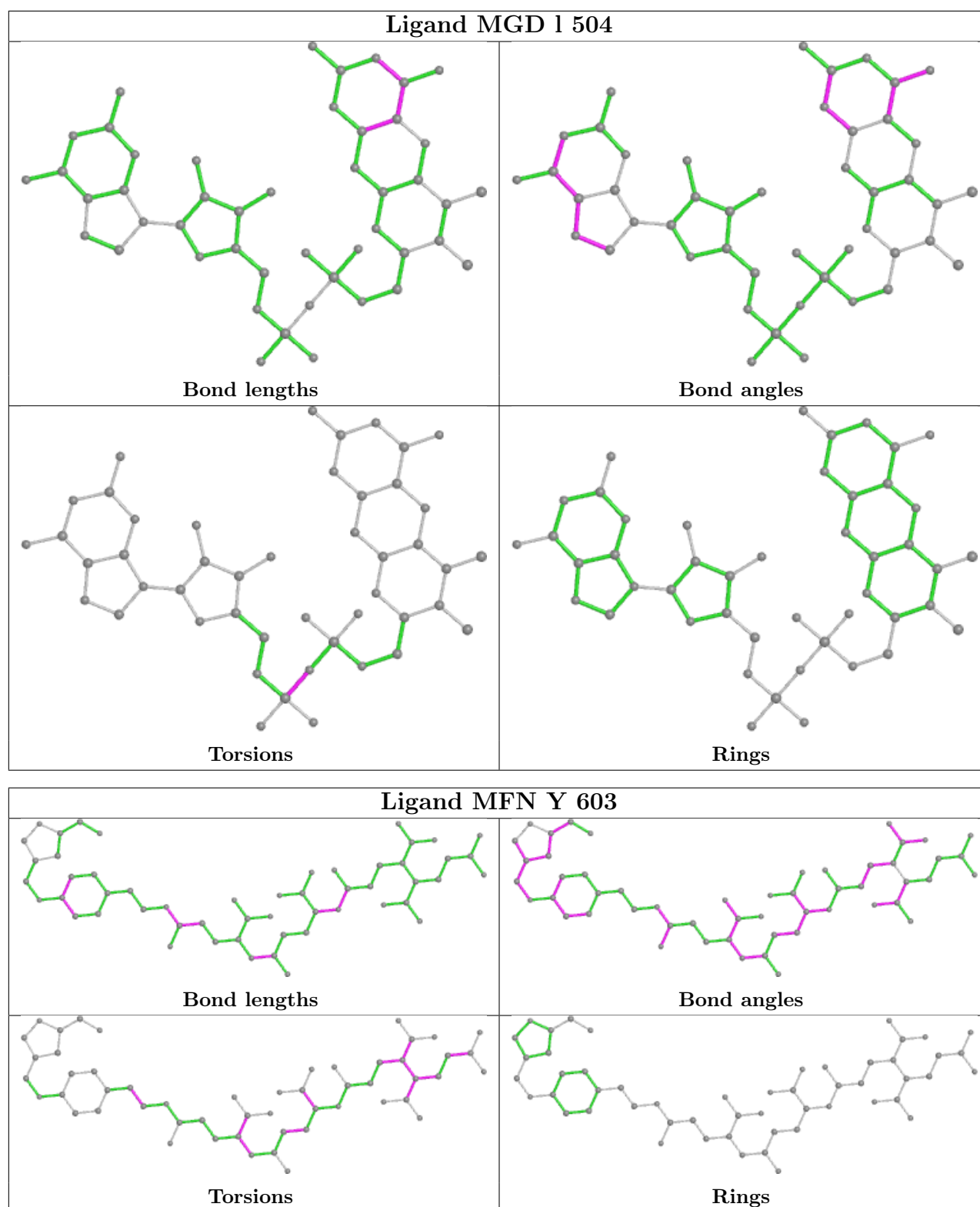












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	568/569 (99%)	0.26	10 (1%) 68 74	29, 43, 63, 91	0
1	G	567/569 (99%)	0.44	31 (5%) 25 30	31, 48, 73, 117	0
1	M	567/569 (99%)	0.73	67 (11%) 4 6	34, 55, 81, 113	0
1	S	568/569 (99%)	0.11	10 (1%) 68 74	25, 36, 54, 94	0
1	Y	567/569 (99%)	0.62	57 (10%) 7 8	31, 51, 75, 109	0
1	e	568/569 (99%)	0.14	14 (2%) 57 63	27, 37, 53, 88	0
1	k	567/569 (99%)	0.71	56 (9%) 7 9	33, 56, 80, 102	0
1	q	568/569 (99%)	0.40	20 (3%) 44 51	31, 46, 66, 105	0
2	B	429/432 (99%)	0.47	11 (2%) 56 62	29, 42, 69, 124	0
2	H	427/432 (98%)	0.40	17 (3%) 38 45	26, 38, 61, 87	0
2	N	430/432 (99%)	0.39	24 (5%) 24 29	30, 39, 57, 71	0
2	T	429/432 (99%)	0.45	18 (4%) 36 42	26, 39, 65, 104	0
2	Z	428/432 (99%)	0.53	31 (7%) 15 18	28, 40, 64, 122	0
2	f	427/432 (98%)	0.39	18 (4%) 36 42	25, 39, 61, 109	0
2	l	428/432 (99%)	0.60	33 (7%) 13 17	29, 43, 68, 98	0
2	r	428/432 (99%)	0.57	23 (5%) 25 30	29, 44, 69, 106	0
3	C	267/270 (98%)	0.60	23 (8%) 10 12	35, 53, 78, 108	0
3	I	269/270 (99%)	0.04	5 (1%) 66 73	26, 38, 56, 90	0
3	O	268/270 (99%)	0.02	2 (0%) 87 90	30, 41, 61, 86	0
3	U	268/270 (99%)	0.34	15 (5%) 24 29	28, 46, 70, 110	0
3	a	268/270 (99%)	0.06	4 (1%) 73 79	30, 39, 55, 83	0
3	g	268/270 (99%)	0.46	21 (7%) 13 16	31, 50, 78, 101	0
3	m	268/270 (99%)	0.04	2 (0%) 87 90	28, 41, 62, 93	0
3	s	269/270 (99%)	0.65	21 (7%) 13 16	36, 56, 80, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
4	D	129/130 (99%)	0.49	7 (5%) 25 30	36, 52, 70, 91	0
4	J	129/130 (99%)	0.19	2 (1%) 72 78	31, 41, 56, 66	0
4	P	129/130 (99%)	0.07	4 (3%) 49 56	29, 38, 54, 65	0
4	V	129/130 (99%)	0.26	5 (3%) 39 45	33, 43, 58, 68	0
4	b	129/130 (99%)	0.17	3 (2%) 60 67	33, 41, 56, 83	0
4	h	129/130 (99%)	0.41	4 (3%) 49 56	34, 48, 65, 84	0
4	n	129/130 (99%)	0.22	5 (3%) 39 45	34, 42, 61, 78	0
4	t	129/130 (99%)	0.51	8 (6%) 20 24	37, 51, 70, 83	0
5	E	80/82 (97%)	0.20	1 (1%) 77 82	33, 42, 57, 67	0
5	K	80/82 (97%)	0.17	1 (1%) 77 82	32, 40, 55, 72	0
5	Q	80/82 (97%)	0.24	1 (1%) 77 82	34, 44, 60, 69	0
5	W	80/82 (97%)	0.16	3 (3%) 40 47	31, 39, 52, 68	0
5	c	80/82 (97%)	0.35	3 (3%) 40 47	37, 46, 63, 72	0
5	i	80/82 (97%)	0.08	1 (1%) 77 82	28, 37, 50, 70	0
5	o	80/82 (97%)	0.23	1 (1%) 77 82	34, 43, 57, 71	0
5	u	81/82 (98%)	0.15	1 (1%) 79 84	32, 40, 61, 84	0
6	F	345/349 (98%)	0.32	16 (4%) 32 39	29, 40, 67, 116	0
6	L	348/349 (99%)	0.09	3 (0%) 84 88	28, 38, 60, 83	0
6	R	341/349 (97%)	0.66	37 (10%) 5 7	29, 48, 87, 147	0
6	X	344/349 (98%)	0.32	14 (4%) 37 44	29, 41, 71, 107	0
6	d	340/349 (97%)	0.70	43 (12%) 3 4	28, 49, 96, 130	0
6	j	344/349 (98%)	0.30	15 (4%) 34 41	26, 39, 69, 99	0
6	p	348/349 (99%)	0.15	10 (2%) 51 59	29, 37, 58, 85	0
6	v	346/349 (99%)	0.16	7 (2%) 65 72	27, 38, 63, 87	0
All	All	14540/14656 (99%)	0.38	728 (5%) 28 34	25, 43, 71, 147	0

All (728) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	X	6	VAL	7.5
6	R	14	VAL	7.3
1	k	4	ILE	7.3
6	d	336	ARG	6.7
6	j	6	VAL	6.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	U	235	GLY	6.5
1	k	462	GLY	6.3
1	k	6	LYS	6.1
6	R	17	THR	6.1
6	d	17	THR	6.0
6	j	7	ILE	6.0
6	d	75	GLY	5.9
6	d	99	ALA	5.9
6	j	4	THR	5.8
6	d	76	MET	5.8
6	R	6	VAL	5.7
2	B	45	ALA	5.7
6	X	4	THR	5.7
3	g	234	ASP	5.5
6	R	15	GLU	5.4
1	M	8	GLY	5.3
1	Y	3	TYR	5.2
1	G	32	VAL	5.1
1	Y	84	LYS	5.1
6	R	334	PRO	5.1
1	Y	35	VAL	5.0
1	M	156	GLY	5.0
6	R	21	ASN	4.9
6	X	92	GLY	4.9
3	s	32	GLU	4.9
3	U	231	ILE	4.9
3	s	52	PHE	4.8
1	k	486	ILE	4.8
3	s	37	ILE	4.8
6	d	334	PRO	4.7
6	X	7	ILE	4.7
6	R	337	SER	4.6
1	q	419	TRP	4.6
2	l	55	LEU	4.6
1	k	35	VAL	4.6
6	R	97	GLU	4.6
6	p	2	GLU	4.6
6	d	245	CYS	4.5
6	R	7	ILE	4.5
1	G	25	CYS	4.4
6	R	99	ALA	4.4
2	r	430	ALA	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	d	42	PRO	4.3
1	Y	4	ILE	4.3
1	q	467	ILE	4.3
1	Y	41	VAL	4.3
3	C	61	ALA	4.3
6	d	69	ASN	4.2
1	M	345	GLY	4.2
1	S	569	LEU	4.2
6	j	92	GLY	4.2
1	Y	24	ILE	4.1
1	G	505	LYS	4.1
2	T	428	TYR	4.1
3	g	37	ILE	4.1
6	F	25	ILE	4.1
5	c	2	ALA	4.1
3	s	65	ILE	4.1
1	M	4	ILE	4.0
4	h	65	VAL	4.0
1	Y	36	SER	4.0
6	R	340	TRP	4.0
1	k	569	LEU	4.0
4	P	45	ILE	4.0
3	s	28	GLY	4.0
6	R	336	ARG	4.0
6	R	333	THR	4.0
5	Q	2	ALA	4.0
2	Z	61	GLU	3.9
3	s	5	ILE	3.9
1	M	39	ALA	3.9
2	Z	410	ASP	3.9
3	g	233	VAL	3.9
1	M	346	SER	3.9
2	r	293	VAL	3.9
3	C	60	ASP	3.8
1	k	479	PRO	3.8
1	G	477	VAL	3.8
6	X	43	VAL	3.8
6	d	41	CYS	3.8
1	Y	65	VAL	3.8
2	T	123	VAL	3.8
1	M	38	SER	3.8
6	R	42	PRO	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	l	294	THR	3.8
1	k	9	PHE	3.7
6	R	74	CYS	3.7
3	s	68	ILE	3.7
1	M	24	ILE	3.7
6	d	71	CYS	3.6
6	d	46	ILE	3.6
1	S	67	VAL	3.6
1	k	22	MET	3.6
3	C	68	ILE	3.6
1	Y	474	PRO	3.6
1	G	83	PHE	3.6
1	k	40	LYS	3.6
1	k	42	ILE	3.6
6	X	5	GLU	3.6
1	M	465	ALA	3.6
3	s	234	ASP	3.6
3	C	52	PHE	3.5
2	r	61	GLU	3.5
6	R	41	CYS	3.5
1	M	528	ILE	3.5
1	M	3	TYR	3.5
1	M	502	ILE	3.5
3	U	238	LEU	3.5
2	r	294	THR	3.5
6	v	179	ALA	3.5
3	O	2	SER	3.5
3	C	2	SER	3.5
2	N	123	VAL	3.5
1	M	23	ASP	3.4
3	C	234	ASP	3.4
6	d	74	CYS	3.4
4	D	1	MET	3.4
3	g	237	GLU	3.4
4	b	127	VAL	3.4
2	r	424	LYS	3.4
6	d	89	GLN	3.4
6	R	24	LEU	3.4
1	M	41	VAL	3.4
2	H	225	ASP	3.4
3	C	37	ILE	3.4
3	s	61	ALA	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	156	GLY	3.4
3	g	34	ILE	3.4
1	k	25	CYS	3.4
6	d	16	ARG	3.3
2	B	59	ASN	3.3
4	h	109	PRO	3.3
1	G	28	ASP	3.3
1	M	71	TYR	3.3
2	Z	428	TYR	3.3
6	d	92	GLY	3.3
1	G	35	VAL	3.3
2	l	293	VAL	3.3
2	Z	27	GLU	3.3
2	r	45	ALA	3.3
6	d	339	ALA	3.3
1	G	37	ASP	3.3
2	H	23	VAL	3.3
1	M	9	PHE	3.3
6	F	16	ARG	3.3
6	d	337	SER	3.3
1	k	44	ALA	3.2
6	F	68	GLU	3.2
1	M	70	MET	3.2
1	A	506	ASP	3.2
2	B	123	VAL	3.2
2	l	63	VAL	3.2
1	M	64	LYS	3.2
1	M	116	ALA	3.2
2	l	430	ALA	3.2
6	d	120	ALA	3.2
1	S	83	PHE	3.2
2	B	44	HIS	3.2
6	d	333	THR	3.2
3	a	2	SER	3.2
2	B	336	ASP	3.2
3	C	71	GLY	3.2
6	j	167	ASP	3.2
1	q	255	LYS	3.2
1	M	120	LEU	3.2
6	R	93	THR	3.1
6	d	70	LYS	3.1
1	Y	67	VAL	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	k	159	ASP	3.1
6	R	73	LEU	3.1
3	I	5	ILE	3.1
1	M	347	GLY	3.1
1	Y	116	ALA	3.1
2	l	297	ASN	3.1
3	U	239	PRO	3.1
4	J	129	GLN	3.1
1	Y	2	GLU	3.1
1	e	316	THR	3.1
2	l	75	ALA	3.1
1	A	567	VAL	3.1
2	H	293	VAL	3.1
6	d	7	ILE	3.1
1	Y	37	ASP	3.1
1	M	336	ALA	3.1
6	R	339	ALA	3.1
1	e	65	VAL	3.1
1	q	28	ASP	3.0
2	H	16	CYS	3.0
6	p	71	CYS	3.0
6	d	9	GLY	3.0
1	k	475	GLU	3.0
6	R	22	ARG	3.0
3	C	35	LYS	3.0
3	U	54	VAL	3.0
1	Y	60	ILE	3.0
6	R	90	ILE	3.0
6	R	75	GLY	3.0
6	F	71	CYS	3.0
1	M	63	ALA	3.0
6	F	9	GLY	3.0
2	l	114	THR	3.0
3	U	233	VAL	3.0
6	R	76	MET	3.0
3	C	231	ILE	3.0
1	G	493	ALA	3.0
1	M	121	LEU	3.0
1	Y	58	SER	2.9
6	R	16	ARG	2.9
6	R	89	GLN	2.9
3	s	36	ASN	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	r	407	VAL	2.9
2	Z	229	GLY	2.9
6	j	5	GLU	2.9
1	G	27	LYS	2.9
2	f	299	VAL	2.9
1	Y	415	GLU	2.9
2	H	296	PHE	2.9
1	k	7	ASN	2.9
1	Y	465	ALA	2.9
6	F	77	CYS	2.9
1	Y	346	SER	2.9
6	p	69	ASN	2.9
1	Y	121	LEU	2.9
5	W	81	LEU	2.9
6	j	93	THR	2.9
1	k	568	MET	2.9
6	d	340	TRP	2.9
2	H	294	THR	2.9
2	Z	424	LYS	2.9
2	l	23	VAL	2.9
6	v	7	ILE	2.9
1	M	27	LYS	2.9
1	G	34	SER	2.8
2	T	116	SER	2.8
2	Z	226	GLU	2.8
4	t	128	GLY	2.8
1	Y	96	SER	2.8
3	g	2	SER	2.8
3	s	58	PRO	2.8
1	Y	338	CYS	2.8
6	R	164	CYS	2.8
1	M	317	MET	2.8
1	M	26	VAL	2.8
1	q	41	VAL	2.8
1	k	435	PHE	2.8
2	r	62	PHE	2.8
1	k	39	ALA	2.8
2	r	114	THR	2.8
6	j	77	CYS	2.8
2	Z	302	TRP	2.8
2	Z	123	VAL	2.8
2	Z	407	VAL	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	f	61	GLU	2.8
2	H	62	PHE	2.8
6	d	328	ASN	2.8
2	l	24	GLU	2.8
3	s	60	ASP	2.8
1	q	19	GLY	2.8
2	N	297	ASN	2.8
3	U	240	GLY	2.8
1	S	70	MET	2.8
1	Y	340	VAL	2.8
1	G	4	ILE	2.8
6	p	60	GLU	2.8
2	Z	305	GLY	2.8
1	q	43	ASP	2.8
4	t	1	MET	2.8
1	q	477	VAL	2.7
5	o	43	GLU	2.7
1	e	338	CYS	2.7
1	Y	39	ALA	2.7
1	k	84	LYS	2.7
1	e	70	MET	2.7
2	N	394	TYR	2.7
2	Z	294	THR	2.7
2	Z	394	TYR	2.7
5	W	2	ALA	2.7
2	T	223	LEU	2.7
2	f	223	LEU	2.7
1	M	2	GLU	2.7
2	l	225	ASP	2.7
6	d	338	LYS	2.7
6	d	23	ARG	2.7
1	Y	528	ILE	2.7
2	H	222	ILE	2.7
4	J	108	ILE	2.7
1	k	506	ASP	2.7
1	A	338	CYS	2.7
3	s	10	GLU	2.7
1	Y	160	ALA	2.7
1	Y	31	ILE	2.7
3	m	234	ASP	2.7
2	N	124	LEU	2.7
1	G	70	MET	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	H	2	GLU	2.7
2	H	297	ASN	2.7
1	Y	477	VAL	2.7
4	t	123	VAL	2.7
6	j	91	ASP	2.7
3	g	239	PRO	2.7
3	U	46	VAL	2.7
6	d	94	SER	2.7
6	d	25	ILE	2.7
2	N	295	GLY	2.7
2	l	67	TYR	2.7
1	Y	375	ASP	2.7
1	Y	25	CYS	2.6
6	j	43	VAL	2.6
1	q	259	ALA	2.6
2	Z	301	THR	2.6
2	T	286	PRO	2.6
2	B	53	LYS	2.6
1	k	41	VAL	2.6
1	G	44	ALA	2.6
3	I	269	ALA	2.6
2	f	297	ASN	2.6
4	h	44	GLY	2.6
1	Y	23	ASP	2.6
3	C	237	GLU	2.6
6	X	91	ASP	2.6
2	T	131	TYR	2.6
3	g	74	TYR	2.6
1	Y	61	ALA	2.6
2	T	44	HIS	2.6
3	g	46	VAL	2.6
3	s	235	GLY	2.6
6	X	17	THR	2.6
1	M	60	ILE	2.6
1	k	43	ASP	2.6
2	N	133	ILE	2.6
3	I	270	PRO	2.6
3	s	31	ILE	2.6
6	X	71	CYS	2.6
1	Y	33	GLU	2.6
1	k	477	VAL	2.6
2	r	63	VAL	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	49	GLY	2.6
3	U	269	ALA	2.6
2	N	307	PRO	2.6
2	Z	236	GLU	2.6
1	Y	124	HIS	2.6
2	N	305	GLY	2.6
2	f	46	GLU	2.6
1	M	6	LYS	2.6
6	F	349	LYS	2.6
1	k	347	GLY	2.6
2	l	16	CYS	2.6
1	A	336	ALA	2.6
1	e	319	ALA	2.6
1	e	465	ALA	2.6
1	Y	26	VAL	2.6
2	Z	135	THR	2.6
3	g	59	ALA	2.6
1	k	497	LEU	2.6
6	d	73	LEU	2.6
1	M	36	SER	2.6
1	e	43	ASP	2.6
2	l	288	ARG	2.6
6	X	75	GLY	2.6
6	v	97	GLU	2.6
1	M	35	VAL	2.5
2	r	300	CYS	2.5
1	M	396	PRO	2.5
5	K	81	LEU	2.5
1	G	24	ILE	2.5
1	k	70	MET	2.5
3	g	235	GLY	2.5
6	F	97	GLU	2.5
1	G	39	ALA	2.5
1	M	185	THR	2.5
4	V	96	ALA	2.5
1	M	65	VAL	2.5
2	Z	400	PRO	2.5
1	M	338	CYS	2.5
6	d	37	CYS	2.5
6	v	71	CYS	2.5
1	M	531	GLU	2.5
1	k	68	GLY	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	l	61	GLU	2.5
1	k	3	TYR	2.5
1	k	407	TYR	2.5
4	V	67	ALA	2.5
1	k	67	VAL	2.5
2	N	288	ARG	2.5
6	R	23	ARG	2.5
1	Y	345	GLY	2.5
2	T	225	ASP	2.5
3	C	34	ILE	2.5
6	d	66	ILE	2.5
1	M	480	SER	2.5
1	q	36	SER	2.5
1	e	67	VAL	2.5
5	W	53	VAL	2.5
6	R	98	LEU	2.5
1	M	29	GLY	2.5
1	S	16	GLY	2.5
2	T	297	ASN	2.5
2	f	47	GLY	2.5
6	X	69	ASN	2.5
6	R	46	ILE	2.5
4	n	2	ARG	2.5
1	Y	40	LYS	2.5
1	M	28	ASP	2.5
1	M	316	THR	2.5
4	D	64	ALA	2.5
6	p	99	ALA	2.5
1	A	340	VAL	2.5
1	k	120	LEU	2.5
3	C	235	GLY	2.5
3	C	63	GLU	2.5
1	Y	336	ALA	2.5
2	l	215	ALA	2.5
1	M	239	GLY	2.5
1	e	237	HIS	2.5
2	H	299	VAL	2.5
2	f	394	TYR	2.5
2	l	399	VAL	2.5
4	n	127	VAL	2.5
6	d	24	LEU	2.5
1	M	429	ILE	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	65	ILE	2.5
1	k	409	MET	2.5
1	Y	8	GLY	2.5
2	N	237	GLU	2.5
2	N	294	THR	2.5
6	X	20	GLU	2.5
2	B	67	TYR	2.4
2	l	62	PHE	2.4
3	U	5	ILE	2.4
2	N	132	PRO	2.4
2	Z	307	PRO	2.4
2	r	286	PRO	2.4
6	L	69	ASN	2.4
1	k	319	ALA	2.4
1	Y	59	HIS	2.4
2	N	284	LEU	2.4
6	d	101	TYR	2.4
1	S	43	ASP	2.4
1	Y	43	ASP	2.4
2	N	302	TRP	2.4
5	c	43	GLU	2.4
1	M	474	PRO	2.4
2	N	398	GLY	2.4
2	f	130	GLY	2.4
2	r	295	GLY	2.4
2	r	381	PRO	2.4
4	t	42	GLN	2.4
2	f	123	VAL	2.4
6	R	94	SER	2.4
1	k	83	PHE	2.4
3	C	5	ILE	2.4
3	U	79	ILE	2.4
3	s	89	ILE	2.4
3	a	105	GLY	2.4
2	r	307	PRO	2.4
6	F	93	THR	2.4
6	d	68	GLU	2.4
1	A	348	VAL	2.4
2	Z	299	VAL	2.4
6	j	70	LYS	2.4
1	M	483	TYR	2.4
1	Y	66	ASN	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	Y	70	MET	2.4
1	k	474	PRO	2.4
6	L	160	CYS	2.4
3	g	32	GLU	2.4
1	G	43	ASP	2.4
2	Z	23	VAL	2.4
1	A	155	GLU	2.4
1	G	33	GLU	2.4
3	U	74	TYR	2.4
1	k	338	CYS	2.4
2	f	228	ALA	2.4
3	g	7	THR	2.4
2	l	116	SER	2.4
2	r	124	LEU	2.4
1	q	405	ASN	2.4
1	Y	119	PRO	2.4
3	g	31	ILE	2.4
2	f	62	PHE	2.4
6	R	101	TYR	2.4
2	T	324	THR	2.4
2	B	124	LEU	2.4
2	T	126	LEU	2.4
5	E	12	CYS	2.4
3	U	56	GLY	2.3
3	s	63	GLU	2.3
1	Y	62	GLY	2.3
1	Y	237	HIS	2.3
1	k	32	VAL	2.3
1	q	567	VAL	2.3
3	a	44	GLU	2.3
6	R	335	ILE	2.3
1	M	84	LYS	2.3
1	q	44	ALA	2.3
1	G	38	SER	2.3
1	G	462	GLY	2.3
2	B	126	LEU	2.3
6	p	8	GLU	2.3
1	M	348	VAL	2.3
1	e	567	VAL	2.3
4	b	129	GLN	2.3
1	Y	64	LYS	2.3
2	l	396	MET	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	R	344	PHE	2.3
1	M	58	SER	2.3
2	r	394	TYR	2.3
3	s	74	TYR	2.3
2	T	124	LEU	2.3
6	j	42	PRO	2.3
1	G	435	PHE	2.3
1	M	96	SER	2.3
1	M	115	ALA	2.3
2	B	297	ASN	2.3
2	Z	94	CYS	2.3
2	T	61	GLU	2.3
3	C	106	LYS	2.3
1	e	340	VAL	2.3
2	l	1	MET	2.3
1	k	48	ILE	2.3
1	q	63	ALA	2.3
1	q	418	LYS	2.3
2	Z	90	SER	2.3
4	D	44	GLY	2.3
6	p	3	THR	2.3
2	N	134	CYS	2.3
6	d	347	LEU	2.3
1	k	27	LYS	2.3
1	Y	19	GLY	2.3
1	e	347	GLY	2.3
3	C	111	GLY	2.3
1	M	486	ILE	2.3
3	g	152	ILE	2.3
1	k	494	ALA	2.3
3	C	26	PHE	2.3
1	M	318	THR	2.3
1	Y	476	THR	2.3
2	l	398	GLY	2.2
6	F	72	VAL	2.2
3	C	31	ILE	2.2
3	C	32	GLU	2.2
1	e	120	LEU	2.2
2	Z	15	LEU	2.2
2	l	422	LEU	2.2
4	n	43	LEU	2.2
2	l	428	TYR	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	M	479	PRO	2.2
6	R	69	ASN	2.2
2	N	25	GLY	2.2
2	l	13	GLY	2.2
1	M	340	VAL	2.2
4	P	96	ALA	2.2
1	Y	344	THR	2.2
4	t	97	THR	2.2
2	N	298	GLN	2.2
2	Z	308	TYR	2.2
4	P	38	GLU	2.2
6	d	67	ASP	2.2
1	k	504	VAL	2.2
2	Z	396	MET	2.2
1	M	31	ILE	2.2
1	k	24	ILE	2.2
6	F	3	THR	2.2
2	l	126	LEU	2.2
2	l	412	LEU	2.2
1	k	33	GLU	2.2
3	g	58	PRO	2.2
6	j	21	ASN	2.2
2	H	308	TYR	2.2
1	A	70	MET	2.2
6	F	128	ASP	2.2
1	k	11	TYR	2.2
1	k	530	SER	2.2
1	G	41	VAL	2.2
1	M	32	VAL	2.2
3	I	233	VAL	2.2
4	b	64	ALA	2.2
6	d	60	GLU	2.2
1	G	502	ILE	2.2
1	G	528	ILE	2.2
1	M	344	THR	2.2
6	d	93	THR	2.2
2	N	421	LEU	2.2
2	l	137	GLY	2.2
4	V	44	GLY	2.2
1	e	422	ARG	2.2
2	T	394	TYR	2.2
1	S	94	VAL	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	i	2	ALA	2.2
2	Z	133	ILE	2.2
2	r	377	ASP	2.2
3	g	70	ASP	2.2
2	N	296	PHE	2.2
6	v	219	GLY	2.2
4	V	98	PRO	2.2
1	Y	20	GLU	2.2
2	Z	24	GLU	2.2
2	Z	295	GLY	2.1
3	g	71	GLY	2.1
6	p	13	THR	2.1
6	p	336	ARG	2.1
1	M	501	GLU	2.1
2	f	286	PRO	2.1
4	D	47	GLU	2.1
3	a	189	LEU	2.1
6	X	121	CYS	2.1
1	q	37	ASP	2.1
1	S	336	ALA	2.1
1	k	461	VAL	2.1
2	l	425	VAL	2.1
1	Y	482	GLU	2.1
6	d	15	GLU	2.1
2	r	133	ILE	2.1
3	g	231	ILE	2.1
1	M	497	LEU	2.1
2	f	126	LEU	2.1
5	u	81	LEU	2.1
1	Y	38	SER	2.1
1	M	506	ASP	2.1
1	M	473	ASN	2.1
2	N	226	GLU	2.1
3	I	232	GLU	2.1
6	d	21	ASN	2.1
1	A	67	VAL	2.1
1	k	140	TYR	2.1
3	C	74	TYR	2.1
6	j	349	LYS	2.1
1	S	4	ILE	2.1
2	f	307	PRO	2.1
3	O	89	ILE	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	k	28	ASP	2.1
1	k	488	GLU	2.1
3	g	33	GLU	2.1
2	H	396	MET	2.1
2	N	120	GLY	2.1
1	G	65	VAL	2.1
1	k	348	VAL	2.1
2	T	115	ALA	2.1
2	Z	134	CYS	2.1
6	v	77	CYS	2.1
2	H	133	ILE	2.1
1	A	43	ASP	2.1
1	Y	120	LEU	2.1
2	H	288	ARG	2.1
6	L	113	GLU	2.1
1	G	530	SER	2.1
2	H	116	SER	2.1
2	N	225	ASP	2.1
2	r	123	VAL	2.1
1	M	544	TYR	2.1
2	l	319	TYR	2.1
2	r	427	GLU	2.1
6	F	17	THR	2.1
6	R	68	GLU	2.1
6	p	153	THR	2.1
2	Z	225	ASP	2.1
3	s	191	ILE	2.1
3	s	230	ASP	2.1
2	r	55	LEU	2.1
1	M	46	GLY	2.1
1	q	283	ARG	2.1
1	G	474	PRO	2.1
1	Y	360	PRO	2.1
2	H	58	LYS	2.1
2	f	326	ALA	2.1
2	l	115	ALA	2.1
1	k	393	THR	2.1
4	D	62	VAL	2.1
1	G	23	ASP	2.1
1	M	294	ASP	2.1
2	B	410	ASP	2.1
2	f	131	TYR	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	t	103	ILE	2.1
6	d	44	SER	2.1
1	Y	68	GLY	2.1
1	q	345	GLY	2.1
2	f	300	CYS	2.1
2	l	12	CYS	2.1
4	D	128	GLY	2.1
4	n	42	GLN	2.1
6	X	41	CYS	2.1
1	q	422	ARG	2.1
4	n	1	MET	2.0
1	M	37	ASP	2.0
6	F	91	ASP	2.0
2	r	428	TYR	2.0
4	P	42	GLN	2.0
6	F	64	ILE	2.0
2	T	130	GLY	2.0
2	T	289	GLY	2.0
3	m	235	GLY	2.0
3	U	234	ASP	2.0
1	M	481	ALA	2.0
1	S	259	ALA	2.0
1	Y	125	THR	2.0
1	k	524	VAL	2.0
2	N	135	THR	2.0
2	Z	69	GLU	2.0
2	f	301	THR	2.0
5	c	42	VAL	2.0
6	d	43	VAL	2.0
4	V	42	GLN	2.0
1	Y	6	LYS	2.0
1	k	483	TYR	2.0
6	R	40	ILE	2.0
6	j	16	ARG	2.0
1	G	479	PRO	2.0
1	G	568	MET	2.0
1	k	317	MET	2.0
4	D	38	GLU	2.0
1	k	21	LYS	2.0
2	T	73	LYS	2.0
3	U	241	ALA	2.0
4	t	95	THR	2.0

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Mol	Chain	Res	Type	RSRZ
6	F	194	CYS	2.0
1	M	62	GLY	2.0
4	h	108	ILE	2.0
2	l	296	PHE	2.0
4	t	49	ASP	2.0
3	g	229	LYS	2.0
6	v	349	LYS	2.0
1	q	70	MET	2.0
3	s	8	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	KCX	G	178	12/13	0.94	0.16	33,38,40,44	0
1	KCX	e	178	12/13	0.94	0.16	21,27,33,35	0
1	KCX	M	178	12/13	0.95	0.19	41,47,48,50	0
1	KCX	k	178	12/13	0.95	0.20	39,45,52,53	0
1	KCX	A	178	12/13	0.96	0.17	28,35,40,43	0
1	KCX	q	178	12/13	0.96	0.15	31,35,42,44	0
1	KCX	Y	178	12/13	0.97	0.16	36,43,50,51	0
1	KCX	S	178	12/13	0.98	0.16	25,29,38,39	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	MFN	M	603	53/55	0.57	0.38	46,85,111,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	MFN	q	603	53/55	0.63	0.33	40,85,115,121	0
8	MFN	A	603	53/55	0.70	0.28	40,72,97,107	0
8	MFN	k	603	53/55	0.72	0.29	51,77,108,110	0
8	MFN	Y	603	53/55	0.74	0.30	44,75,101,103	0
10	K	v	515	1/1	0.80	0.10	78,78,78,78	0
8	MFN	e	603	53/55	0.82	0.25	35,59,92,101	0
8	MFN	S	603	53/55	0.83	0.22	30,56,87,89	0
8	MFN	G	603	53/55	0.83	0.25	43,68,86,90	0
16	CL	N	506	1/1	0.83	0.12	62,62,62,62	0
9	NA	G	604	1/1	0.87	0.49	54,54,54,54	0
10	K	L	511	1/1	0.87	0.16	80,80,80,80	0
10	K	R	412	1/1	0.89	0.07	61,61,61,61	0
10	K	e	608	1/1	0.90	0.10	68,68,68,68	0
9	NA	A	604	1/1	0.90	0.35	41,41,41,41	0
10	K	Z	506	1/1	0.90	0.11	63,63,63,63	0
9	NA	M	604	1/1	0.91	0.62	56,56,56,56	0
9	NA	q	604	1/1	0.91	0.36	47,47,47,47	0
10	K	X	511	1/1	0.92	0.10	59,59,59,59	0
10	K	v	512	1/1	0.92	0.12	56,56,56,56	0
11	SF4	X	504	8/8	0.93	0.08	25,30,48,57	0
10	K	v	514	1/1	0.93	0.10	42,42,42,42	0
10	K	R	411	1/1	0.94	0.07	59,59,59,59	0
10	K	v	509	1/1	0.94	0.07	58,58,58,58	0
10	K	F	411	1/1	0.94	0.07	38,38,38,38	0
11	SF4	d	404	8/8	0.94	0.07	44,57,65,69	0
11	SF4	l	501	8/8	0.94	0.15	30,37,53,53	0
15	MG	r	507	1/1	0.94	0.41	34,34,34,34	0
10	K	v	513	1/1	0.94	0.09	59,59,59,59	0
10	K	c	103	1/1	0.95	0.05	57,57,57,57	0
10	K	T	506	1/1	0.95	0.13	59,59,59,59	0
10	K	p	411	1/1	0.95	0.09	57,57,57,57	0
10	K	p	412	1/1	0.95	0.08	53,53,53,53	0
11	SF4	d	405	8/8	0.95	0.09	38,43,61,62	0
11	SF4	i	101	8/8	0.95	0.10	26,34,41,47	0
11	SF4	i	102	8/8	0.95	0.09	20,31,41,52	0
10	K	X	510	1/1	0.95	0.08	52,52,52,52	0
13	MGD	T	504	47/47	0.95	0.19	25,37,43,55	0
13	MGD	Z	503	47/47	0.95	0.17	29,37,45,56	0
13	MGD	Z	504	47/47	0.95	0.17	23,37,43,65	0
10	K	K	103	1/1	0.95	0.08	48,48,48,48	0
9	NA	e	604	1/1	0.95	0.30	30,30,30,30	0
11	SF4	F	405	8/8	0.96	0.08	29,37,49,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	SF4	F	407	8/8	0.96	0.08	29,31,44,53	0
11	SF4	F	408	8/8	0.96	0.09	26,33,40,49	0
11	SF4	H	501	8/8	0.96	0.14	28,33,40,45	0
11	SF4	N	501	8/8	0.96	0.16	30,38,48,55	0
11	SF4	R	401	8/8	0.96	0.08	31,47,53,59	0
11	SF4	R	403	8/8	0.96	0.06	67,74,83,94	0
11	SF4	R	404	8/8	0.96	0.08	48,54,65,78	0
11	SF4	R	407	8/8	0.96	0.09	23,35,43,46	0
10	K	M	606	1/1	0.96	0.17	55,55,55,55	0
11	SF4	X	505	8/8	0.96	0.06	33,46,57,60	0
11	SF4	X	507	8/8	0.96	0.09	30,31,40,48	0
11	SF4	Z	501	8/8	0.96	0.12	26,36,44,53	0
11	SF4	c	101	8/8	0.96	0.09	39,45,51,66	0
11	SF4	c	102	8/8	0.96	0.11	42,53,64,69	0
11	SF4	d	401	8/8	0.96	0.09	34,50,53,59	0
11	SF4	d	403	8/8	0.96	0.05	60,74,85,92	0
10	K	L	509	1/1	0.96	0.08	43,43,43,43	0
10	K	d	411	1/1	0.96	0.09	60,60,60,60	0
11	SF4	d	408	8/8	0.96	0.09	20,34,50,59	0
11	SF4	f	501	8/8	0.96	0.18	38,41,64,66	0
10	K	v	510	1/1	0.96	0.11	57,57,57,57	0
10	K	v	511	1/1	0.96	0.09	53,53,53,53	0
11	SF4	j	501	8/8	0.96	0.08	27,38,44,57	0
11	SF4	j	502	8/8	0.96	0.08	18,31,50,53	0
11	SF4	j	505	8/8	0.96	0.06	33,47,54,55	0
10	K	F	412	1/1	0.96	0.05	53,53,53,53	0
11	SF4	p	406	8/8	0.96	0.08	24,37,43,44	0
11	SF4	p	409	8/8	0.96	0.07	28,41,43,45	0
11	SF4	v	507	8/8	0.96	0.07	21,33,45,47	0
10	K	j	513	1/1	0.96	0.05	53,53,53,53	0
10	K	o	103	1/1	0.96	0.09	42,42,42,42	0
10	K	p	410	1/1	0.96	0.12	63,63,63,63	0
13	MGD	r	503	47/47	0.96	0.17	37,46,53,55	0
13	MGD	r	504	47/47	0.96	0.17	27,36,45,47	0
11	SF4	B	501	8/8	0.96	0.13	29,38,55,56	0
11	SF4	F	401	8/8	0.96	0.10	26,38,46,46	0
11	SF4	X	501	8/8	0.97	0.09	34,41,58,62	0
11	SF4	X	502	8/8	0.97	0.08	22,36,39,53	0
10	K	j	510	1/1	0.97	0.05	49,49,49,49	0
11	SF4	F	402	8/8	0.97	0.10	18,36,46,49	0
11	SF4	X	506	8/8	0.97	0.09	22,31,42,42	0
11	SF4	F	403	8/8	0.97	0.08	41,48,60,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	SF4	X	508	8/8	0.97	0.08	26,29,41,46	0
10	K	F	413	1/1	0.97	0.13	40,40,40,40	0
11	SF4	F	406	8/8	0.97	0.06	20,35,46,49	0
10	K	j	514	1/1	0.97	0.12	48,48,48,48	0
10	K	N	507	1/1	0.97	0.09	55,55,55,55	0
11	SF4	d	402	8/8	0.97	0.11	37,48,56,66	0
11	SF4	F	409	8/8	0.97	0.08	18,29,38,39	0
10	K	Q	103	1/1	0.97	0.10	53,53,53,53	0
11	SF4	K	102	8/8	0.97	0.08	27,41,47,60	0
11	SF4	d	406	8/8	0.97	0.10	34,42,54,61	0
11	SF4	L	501	8/8	0.97	0.05	21,34,47,49	0
11	SF4	d	409	8/8	0.97	0.06	24,29,38,60	0
11	SF4	L	502	8/8	0.97	0.10	27,40,50,52	0
11	SF4	L	503	8/8	0.97	0.08	24,34,46,47	0
11	SF4	L	508	8/8	0.97	0.09	27,34,46,52	0
10	K	e	607	1/1	0.97	0.06	51,51,51,51	0
11	SF4	Q	101	8/8	0.97	0.07	23,36,48,49	0
11	SF4	j	503	8/8	0.97	0.08	33,38,44,49	0
11	SF4	j	504	8/8	0.97	0.10	25,37,42,51	0
11	SF4	Q	102	8/8	0.97	0.10	32,45,54,63	0
11	SF4	j	506	8/8	0.97	0.07	25,30,42,43	0
11	SF4	j	507	8/8	0.97	0.09	16,26,43,45	0
10	K	B	506	1/1	0.97	0.12	54,54,54,54	0
11	SF4	o	101	8/8	0.97	0.10	27,35,45,55	0
11	SF4	o	102	8/8	0.97	0.09	31,38,49,51	0
11	SF4	p	401	8/8	0.97	0.08	24,34,47,52	0
11	SF4	p	402	8/8	0.97	0.11	28,37,44,57	0
11	SF4	p	403	8/8	0.97	0.10	20,35,47,51	0
11	SF4	p	404	8/8	0.97	0.09	20,30,41,42	0
11	SF4	R	402	8/8	0.97	0.11	28,41,51,59	0
11	SF4	p	407	8/8	0.97	0.07	25,32,44,51	0
10	K	r	506	1/1	0.97	0.14	57,57,57,57	0
11	SF4	r	501	8/8	0.97	0.14	31,43,47,51	0
11	SF4	u	101	8/8	0.97	0.10	25,39,46,61	0
11	SF4	v	502	8/8	0.97	0.07	15,26,36,42	0
11	SF4	v	503	8/8	0.97	0.09	27,31,39,44	0
11	SF4	v	505	8/8	0.97	0.09	33,39,51,51	0
11	SF4	E	101	8/8	0.97	0.10	36,43,51,58	0
11	SF4	v	508	8/8	0.97	0.07	27,41,48,52	0
13	MGD	B	503	47/47	0.97	0.17	34,40,48,51	0
13	MGD	B	504	47/47	0.97	0.16	27,36,42,44	0
13	MGD	H	504	47/47	0.97	0.17	21,32,38,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
13	MGD	N	504	47/47	0.97	0.15	24,32,40,44	0
13	MGD	T	503	47/47	0.97	0.19	28,38,46,47	0
11	SF4	R	405	8/8	0.97	0.07	32,44,55,65	0
11	SF4	R	406	8/8	0.97	0.07	33,36,50,59	0
11	SF4	E	102	8/8	0.97	0.11	33,37,52,61	0
13	MGD	f	503	47/47	0.97	0.17	26,37,43,46	0
13	MGD	f	504	47/47	0.97	0.14	23,33,38,43	0
13	MGD	l	503	47/47	0.97	0.15	30,37,44,51	0
13	MGD	l	504	47/47	0.97	0.17	25,36,47,50	0
11	SF4	R	409	8/8	0.97	0.09	31,35,47,50	0
11	SF4	T	501	8/8	0.97	0.15	28,39,53,60	0
15	MG	B	507	1/1	0.97	0.32	36,36,36,36	0
11	SF4	W	200	8/8	0.97	0.09	32,40,47,54	0
11	SF4	W	201	8/8	0.97	0.07	21,33,41,47	0
10	K	u	103	1/1	0.98	0.15	53,53,53,53	0
11	SF4	p	408	8/8	0.98	0.09	21,34,40,44	0
10	K	e	605	1/1	0.98	0.12	34,34,34,34	0
10	K	e	606	1/1	0.98	0.17	37,37,37,37	0
11	SF4	d	407	8/8	0.98	0.08	34,42,53,55	0
11	SF4	u	102	8/8	0.98	0.11	26,34,43,46	0
11	SF4	v	501	8/8	0.98	0.07	20,33,44,46	0
10	K	S	605	1/1	0.98	0.17	32,32,32,32	0
11	SF4	R	408	8/8	0.98	0.06	21,28,40,41	0
11	SF4	v	504	8/8	0.98	0.11	18,36,41,42	0
10	K	S	606	1/1	0.98	0.09	46,46,46,46	0
11	SF4	v	506	8/8	0.98	0.08	19,27,43,47	0
11	SF4	K	101	8/8	0.98	0.10	25,34,43,52	0
10	K	j	509	1/1	0.98	0.09	37,37,37,37	0
10	K	M	605	1/1	0.98	0.21	37,37,37,37	0
10	K	X	509	1/1	0.98	0.10	42,42,42,42	0
13	MGD	H	503	47/47	0.98	0.16	29,35,41,47	0
10	K	E	103	1/1	0.98	0.06	43,43,43,43	0
13	MGD	N	503	47/47	0.98	0.15	26,34,43,48	0
11	SF4	X	503	8/8	0.98	0.10	28,33,40,61	0
11	SF4	L	504	8/8	0.98	0.11	25,31,39,41	0
11	SF4	L	505	8/8	0.98	0.07	22,32,41,49	0
11	SF4	L	506	8/8	0.98	0.07	15,26,33,44	0
11	SF4	j	508	8/8	0.98	0.08	22,36,40,59	0
11	SF4	L	507	8/8	0.98	0.09	21,27,40,43	0
10	K	F	410	1/1	0.98	0.09	53,53,53,53	0
9	NA	S	604	1/1	0.98	0.15	32,32,32,32	0
10	K	L	510	1/1	0.98	0.04	52,52,52,52	0

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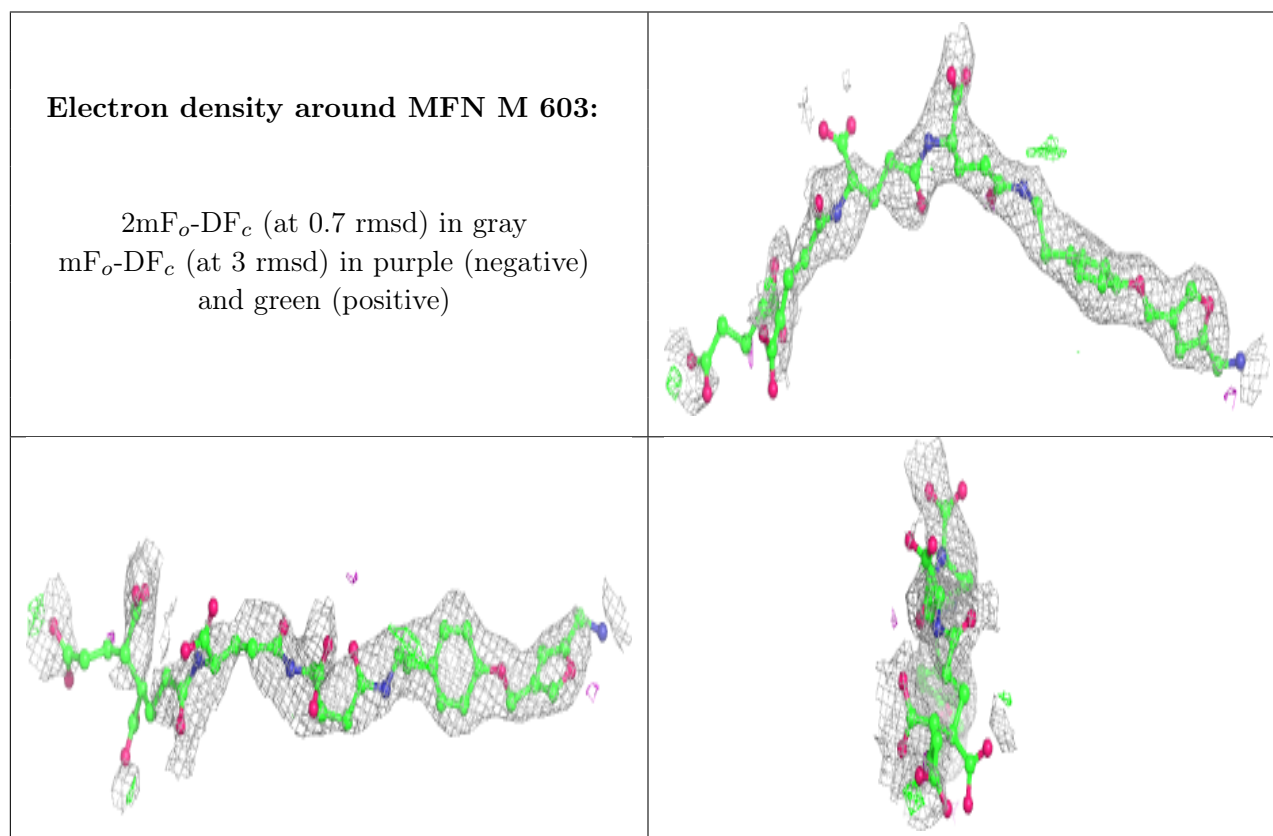
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	K	d	410	1/1	0.98	0.06	47,47,47,47	0
10	K	q	606	1/1	0.98	0.27	47,47,47,47	0
11	SF4	F	404	8/8	0.98	0.07	22,35,44,57	0
15	MG	H	506	1/1	0.98	0.20	24,24,24,24	0
15	MG	T	507	1/1	0.98	0.29	27,27,27,27	0
15	MG	Z	507	1/1	0.98	0.23	30,30,30,30	0
15	MG	f	506	1/1	0.98	0.31	28,28,28,28	0
15	MG	l	506	1/1	0.98	0.18	32,32,32,32	0
11	SF4	p	405	8/8	0.98	0.08	17,21,36,39	0
7	ZN	M	601	1/1	0.98	0.13	51,51,51,51	0
12	W	Z	502	1/1	0.99	0.21	63,63,63,63	0
7	ZN	e	601	1/1	0.99	0.12	38,38,38,38	0
7	ZN	e	602	1/1	0.99	0.12	34,34,34,34	0
7	ZN	k	601	1/1	0.99	0.13	46,46,46,46	0
7	ZN	k	602	1/1	0.99	0.13	44,44,44,44	0
7	ZN	q	601	1/1	0.99	0.09	39,39,39,39	0
10	K	i	103	1/1	0.99	0.08	36,36,36,36	0
9	NA	k	604	1/1	0.99	0.31	52,52,52,52	0
10	K	R	410	1/1	0.99	0.04	40,40,40,40	0
10	K	j	511	1/1	0.99	0.05	35,35,35,35	0
10	K	j	512	1/1	0.99	0.05	58,58,58,58	0
7	ZN	q	602	1/1	0.99	0.12	39,39,39,39	0
10	K	A	605	1/1	0.99	0.17	49,49,49,49	0
10	K	k	605	1/1	0.99	0.21	36,36,36,36	0
7	ZN	A	602	1/1	0.99	0.12	41,41,41,41	0
7	ZN	G	602	1/1	0.99	0.12	40,40,40,40	0
7	ZN	A	601	1/1	0.99	0.13	40,40,40,40	0
14	H2S	N	505	1/1	0.99	0.25	50,50,50,50	0
14	H2S	T	505	1/1	0.99	0.25	50,50,50,50	0
14	H2S	Z	505	1/1	0.99	0.20	63,63,63,63	0
14	H2S	l	505	1/1	0.99	0.29	66,66,66,66	0
14	H2S	r	505	1/1	0.99	0.18	52,52,52,52	0
7	ZN	M	602	1/1	0.99	0.07	46,46,46,46	0
10	K	q	605	1/1	0.99	0.16	47,47,47,47	0
15	MG	O	301	1/1	0.99	0.24	31,31,31,31	0
7	ZN	S	601	1/1	0.99	0.15	40,40,40,40	0
7	ZN	S	602	1/1	0.99	0.13	32,32,32,32	0
10	K	Y	604	1/1	0.99	0.31	38,38,38,38	0
10	K	G	605	1/1	0.99	0.17	62,62,62,62	0
7	ZN	Y	601	1/1	0.99	0.08	45,45,45,45	0
7	ZN	Y	602	1/1	0.99	0.09	47,47,47,47	0
12	W	T	502	1/1	1.00	0.18	49,49,49,49	0

*Continued on next page...*

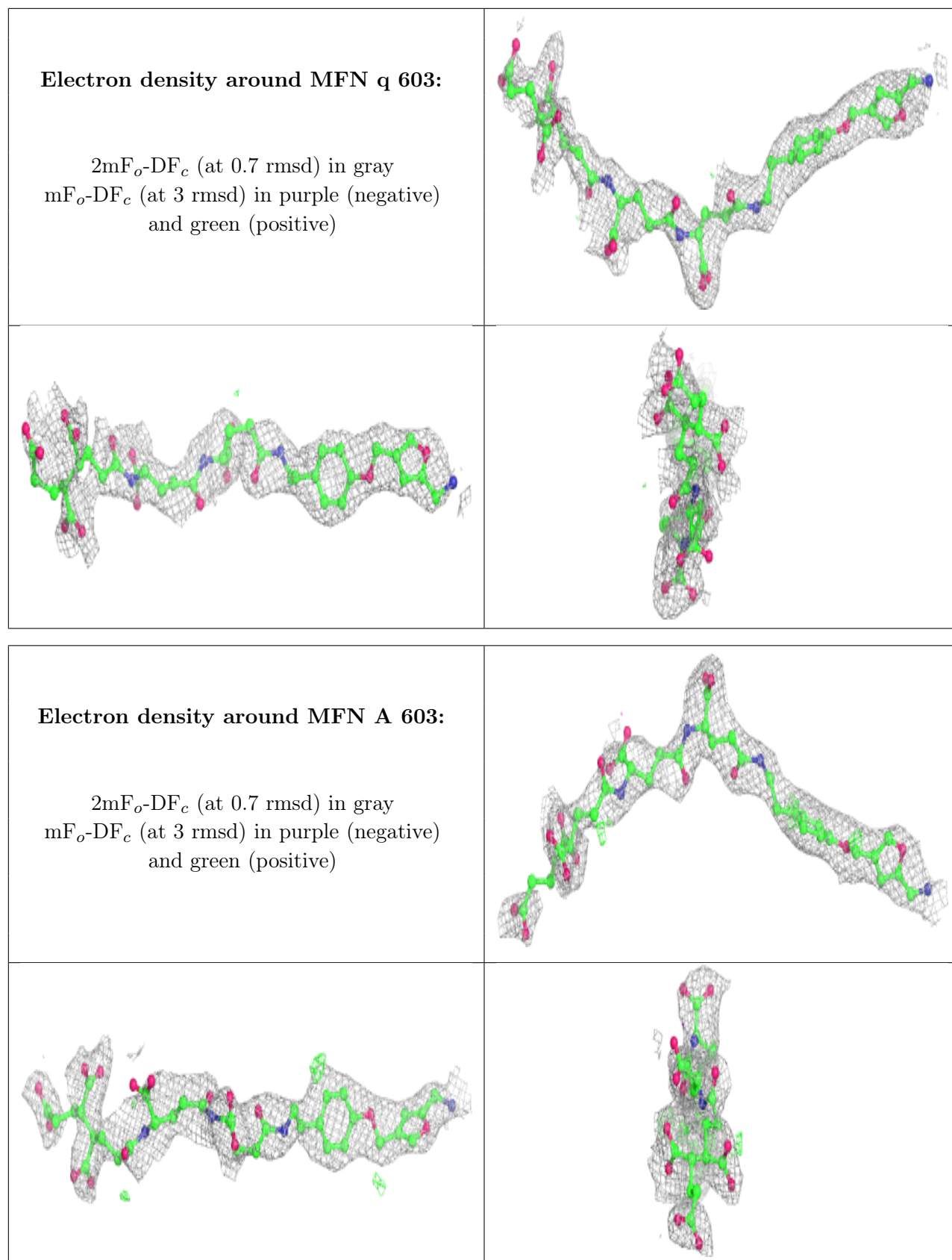
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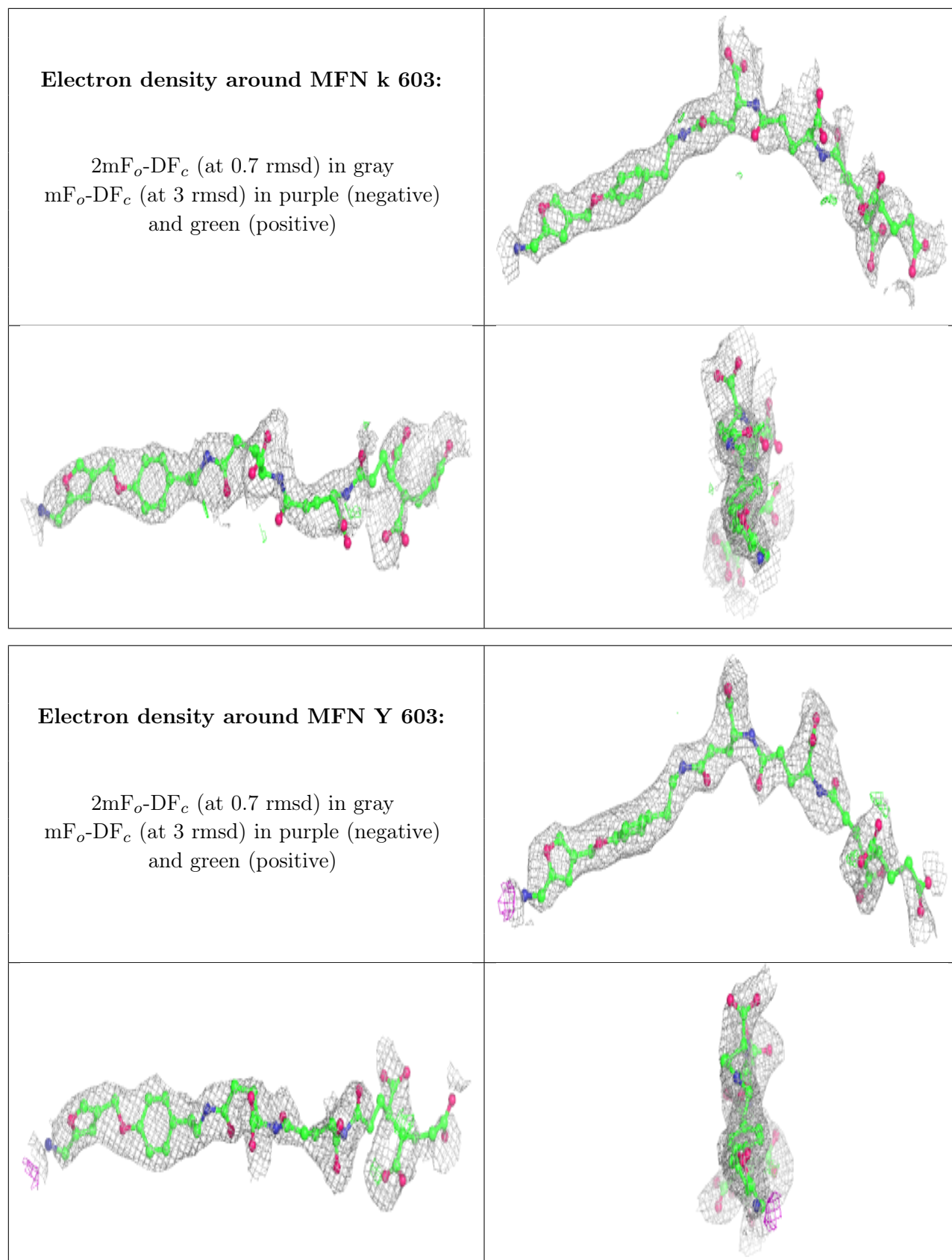
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	ZN	G	601	1/1	1.00	0.11	41,41,41,41	0
12	W	f	502	1/1	1.00	0.20	52,52,52,52	0
12	W	l	502	1/1	1.00	0.17	48,48,48,48	0
12	W	r	502	1/1	1.00	0.14	48,48,48,48	0
14	H2S	B	505	1/1	1.00	0.11	44,44,44,44	0
14	H2S	H	505	1/1	1.00	0.17	41,41,41,41	0
12	W	B	502	1/1	1.00	0.13	43,43,43,43	0
12	W	H	502	1/1	1.00	0.14	37,37,37,37	0
12	W	N	502	1/1	1.00	0.12	34,34,34,34	0
14	H2S	f	505	1/1	1.00	0.16	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.



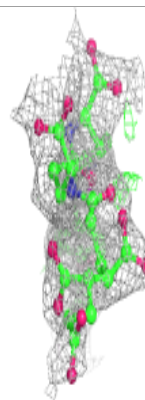
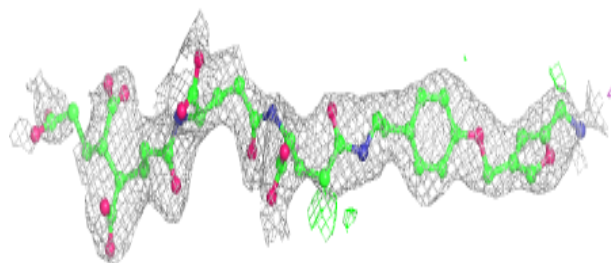
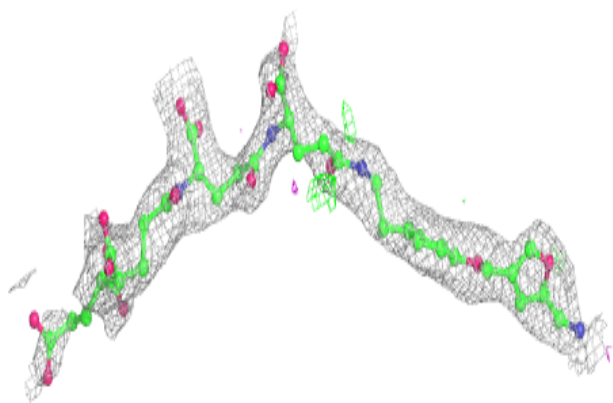




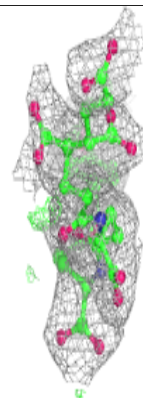
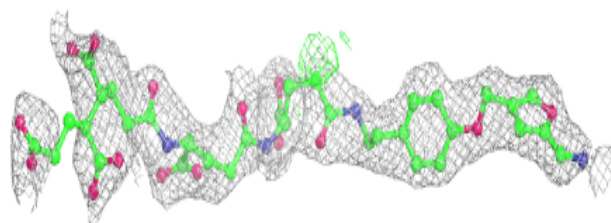
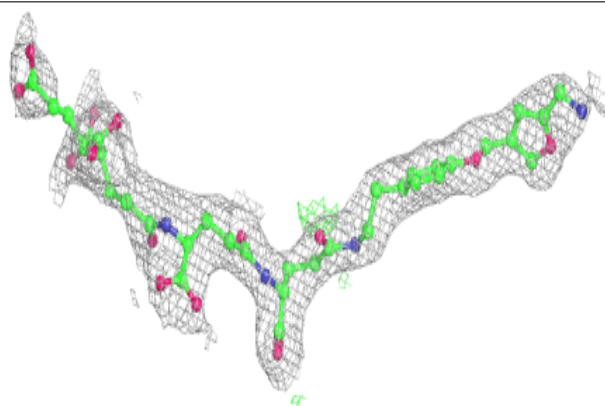


**Electron density around MFN e 603:**

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

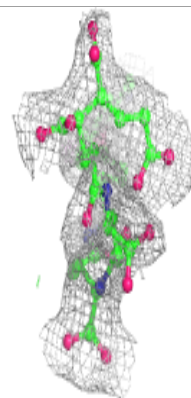
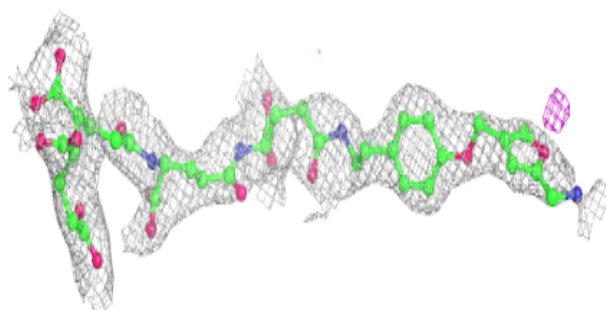
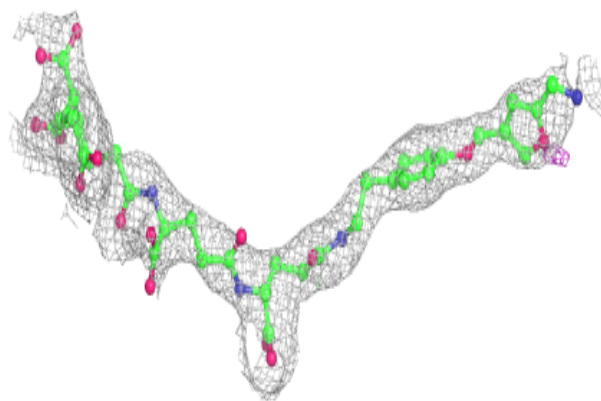
**Electron density around MFN S 603:**

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

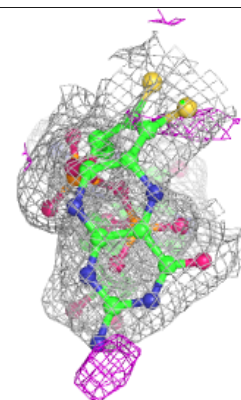
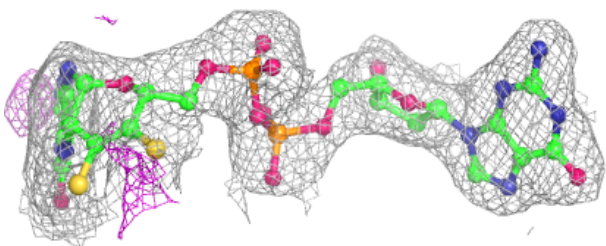
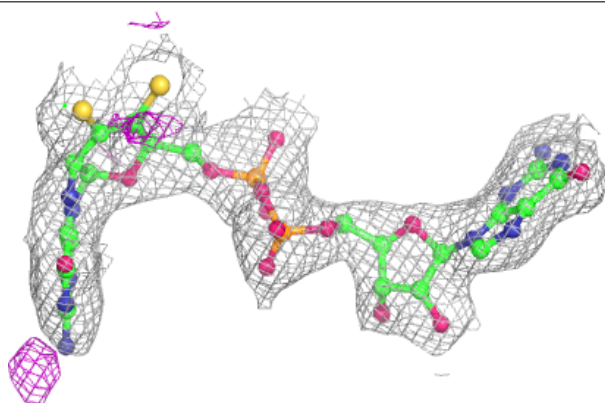


**Electron density around MFN G 603:**

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

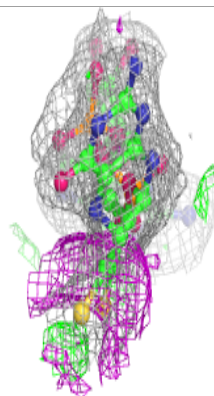
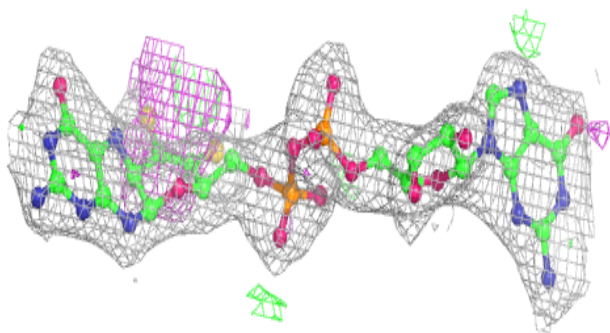
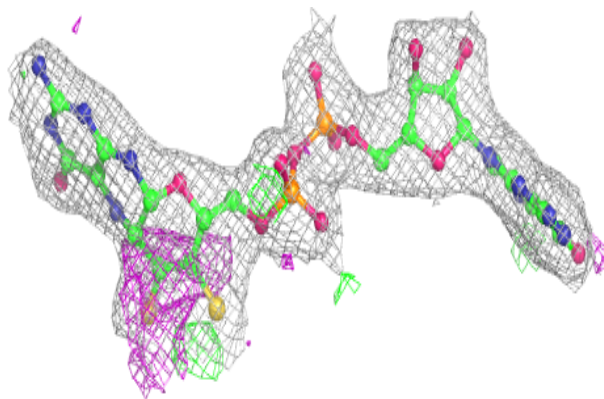
**Electron density around MGD T 504:**

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

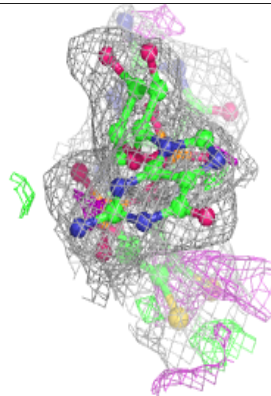
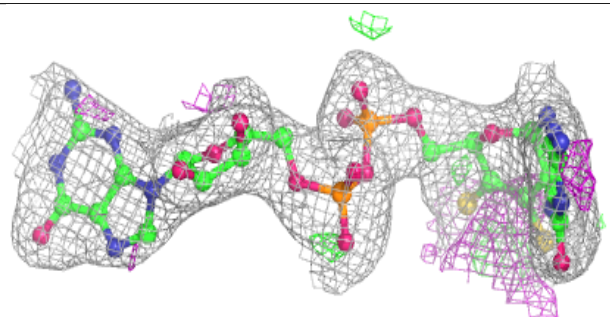
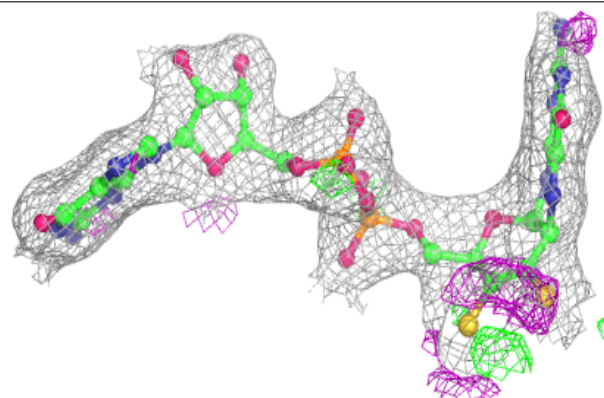


**Electron density around MGD Z 503:**

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

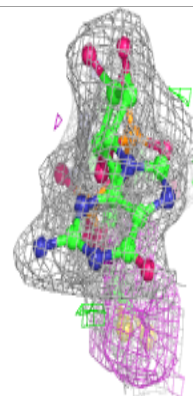
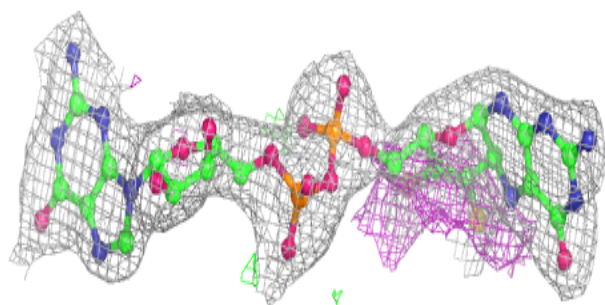
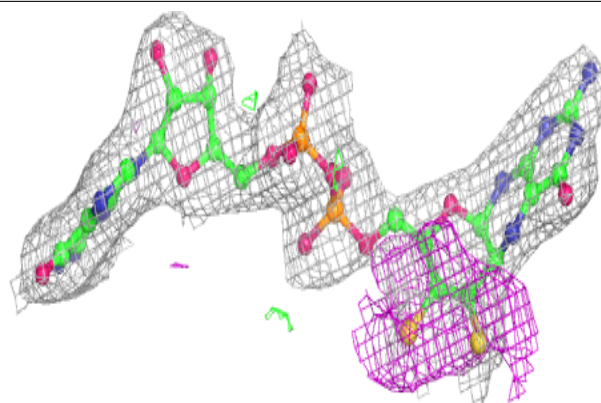
**Electron density around MGD Z 504:**

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

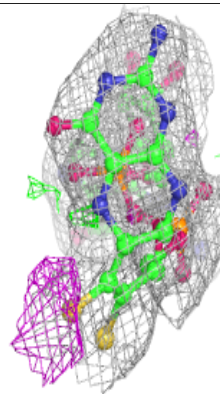
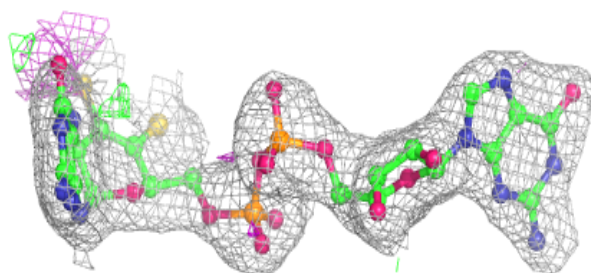
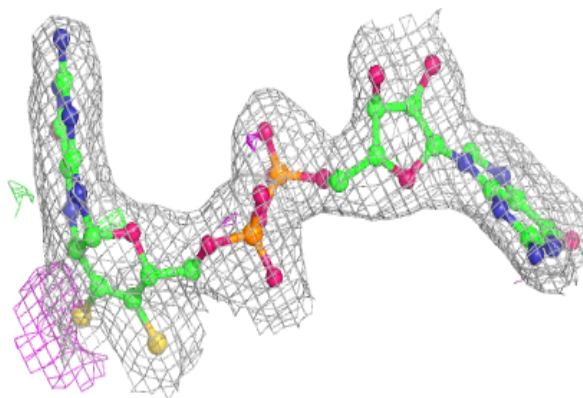


**Electron density around MGD r 503:**

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

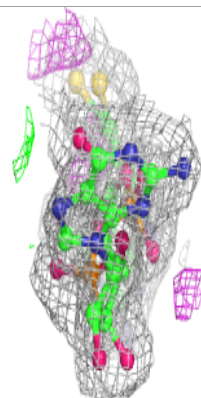
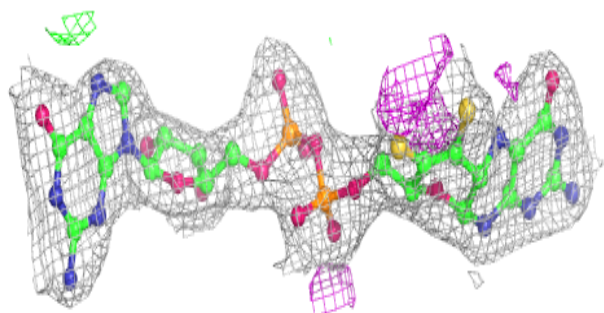
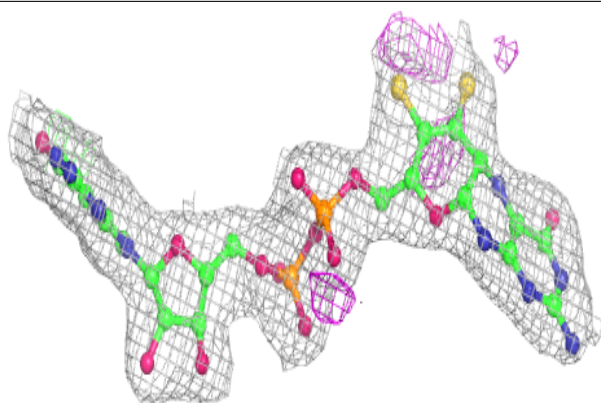
**Electron density around MGD r 504:**

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

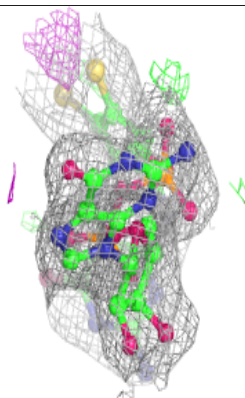
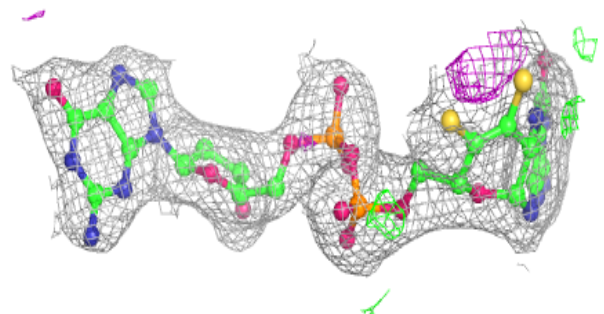
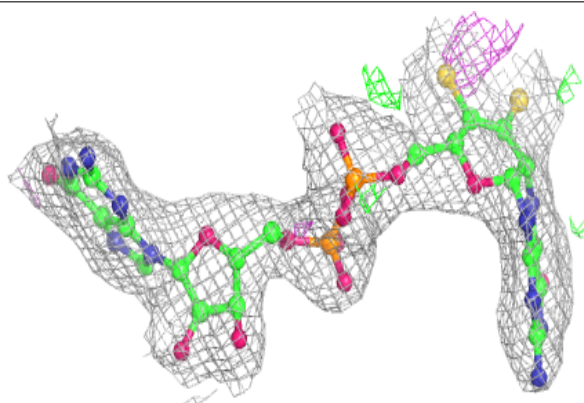


**Electron density around MGD B 503:**

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

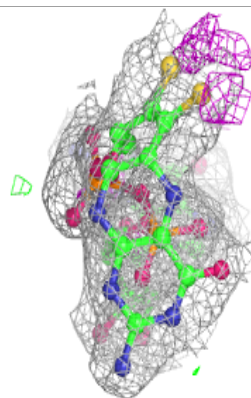
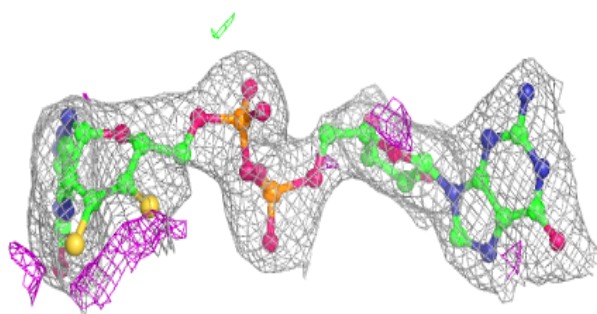
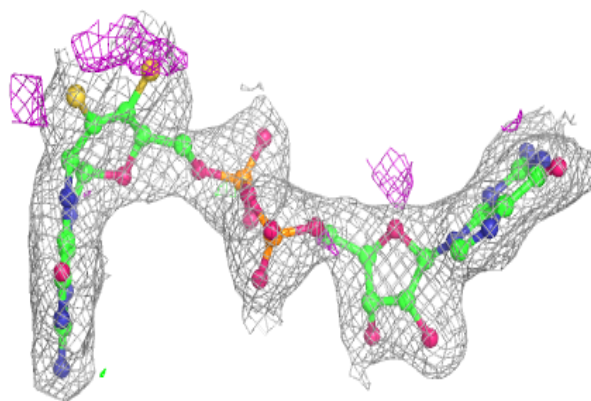
**Electron density around MGD B 504:**

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and green (positive)

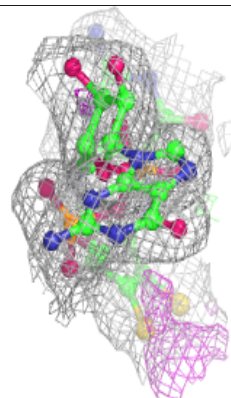
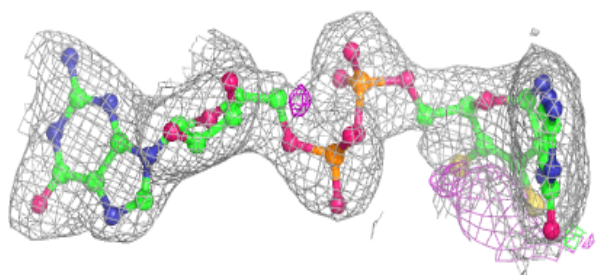
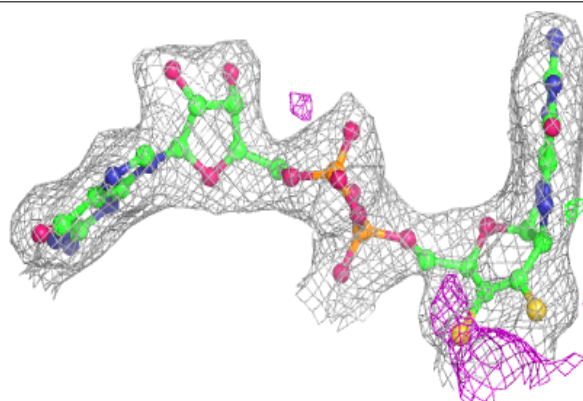


**Electron density around MGD H 504:**

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

**Electron density around MGD N 504:**

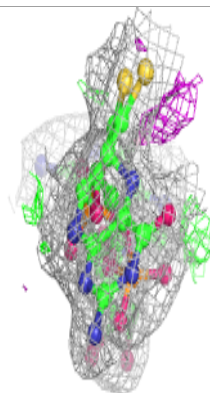
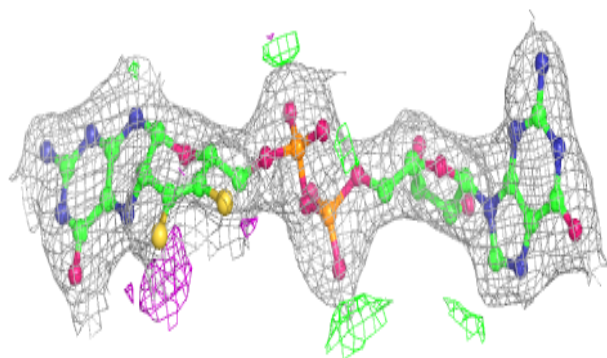
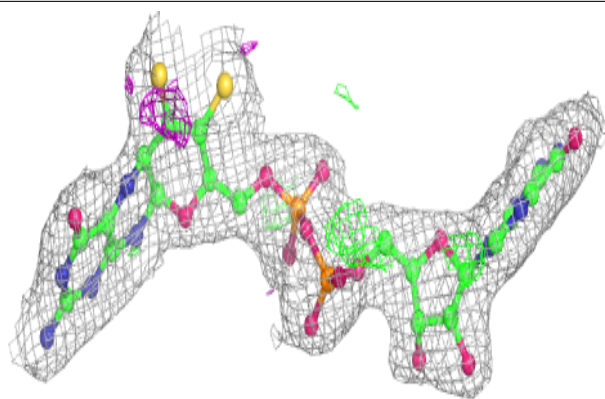
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



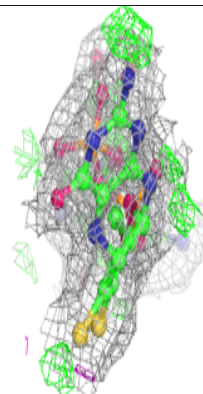
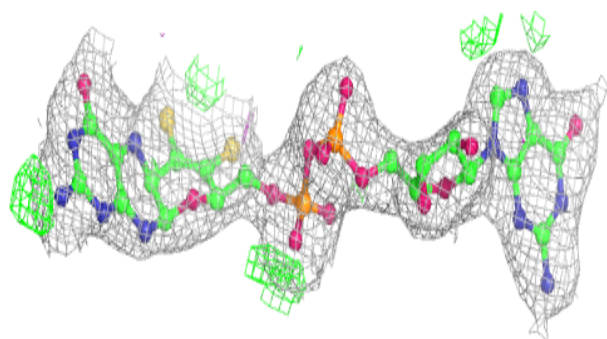
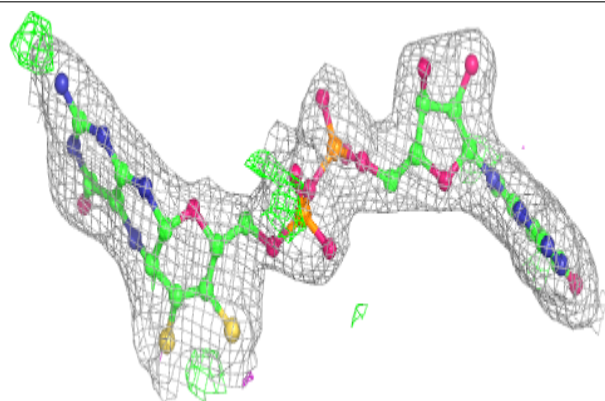


**Electron density around MGD T 503:**

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

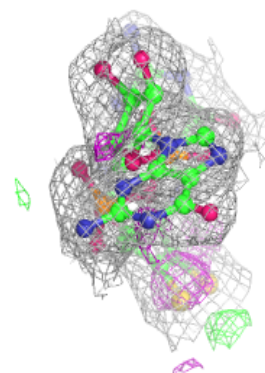
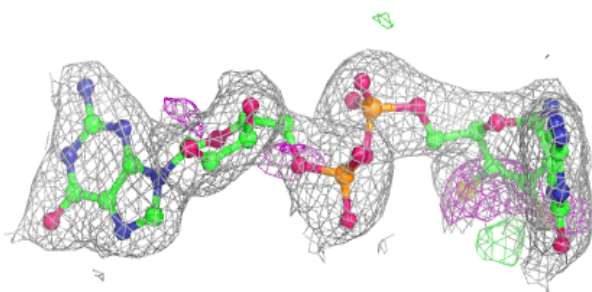
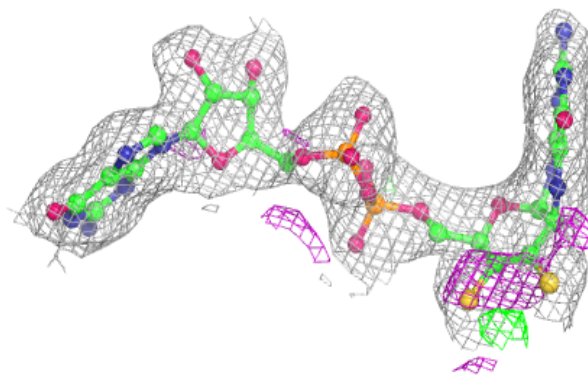
**Electron density around MGD f 503:**

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and green (positive)

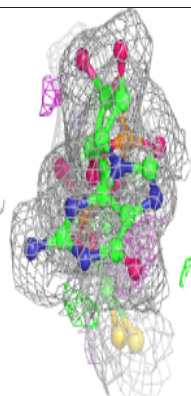
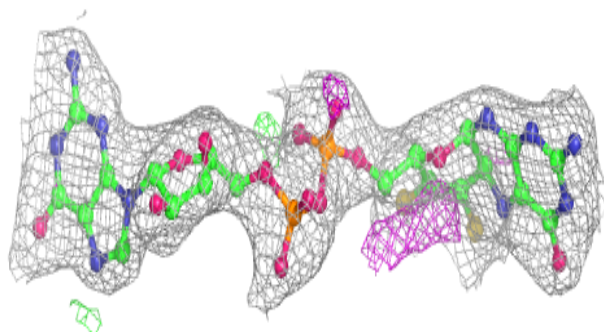
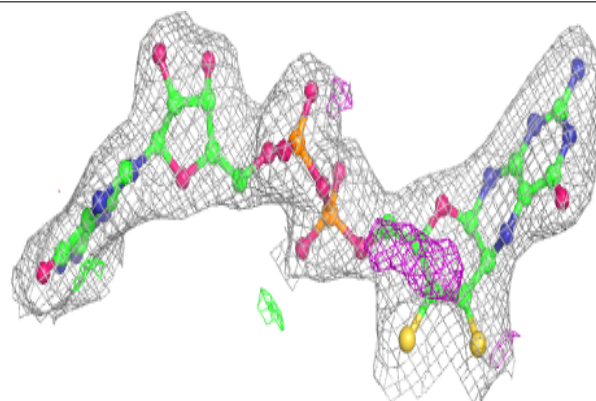


**Electron density around MGD f 504:**

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

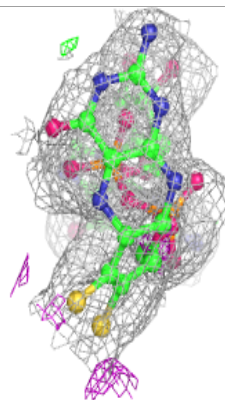
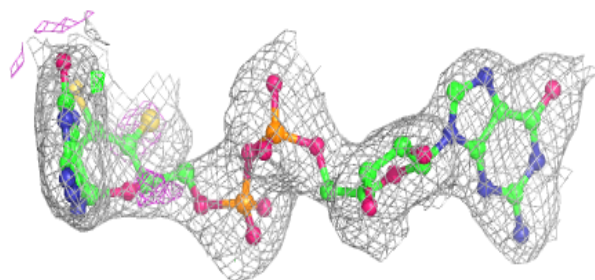
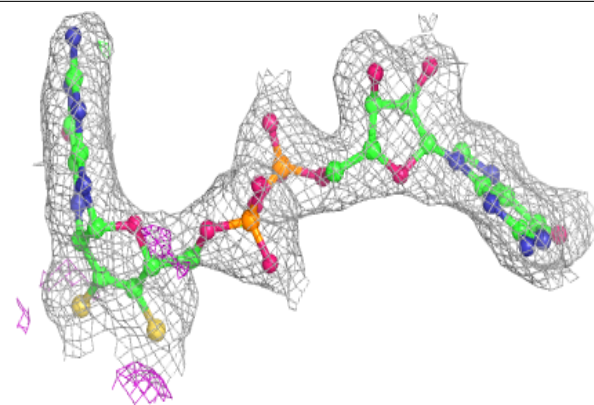
**Electron density around MGD l 503:**

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

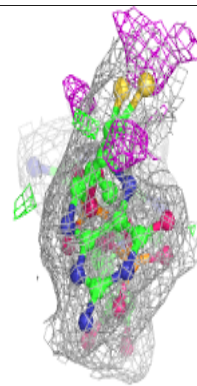
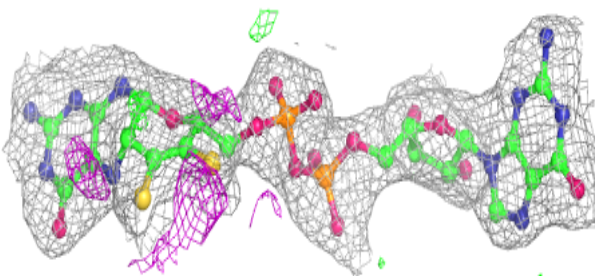
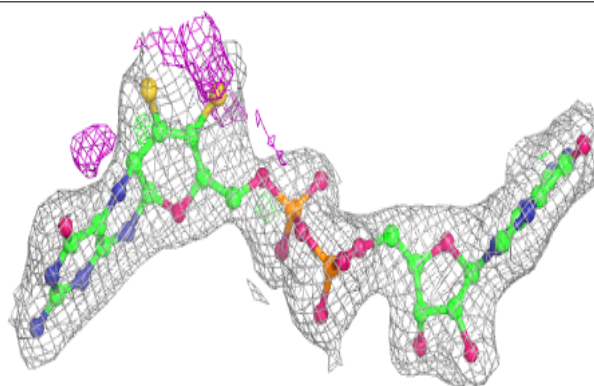


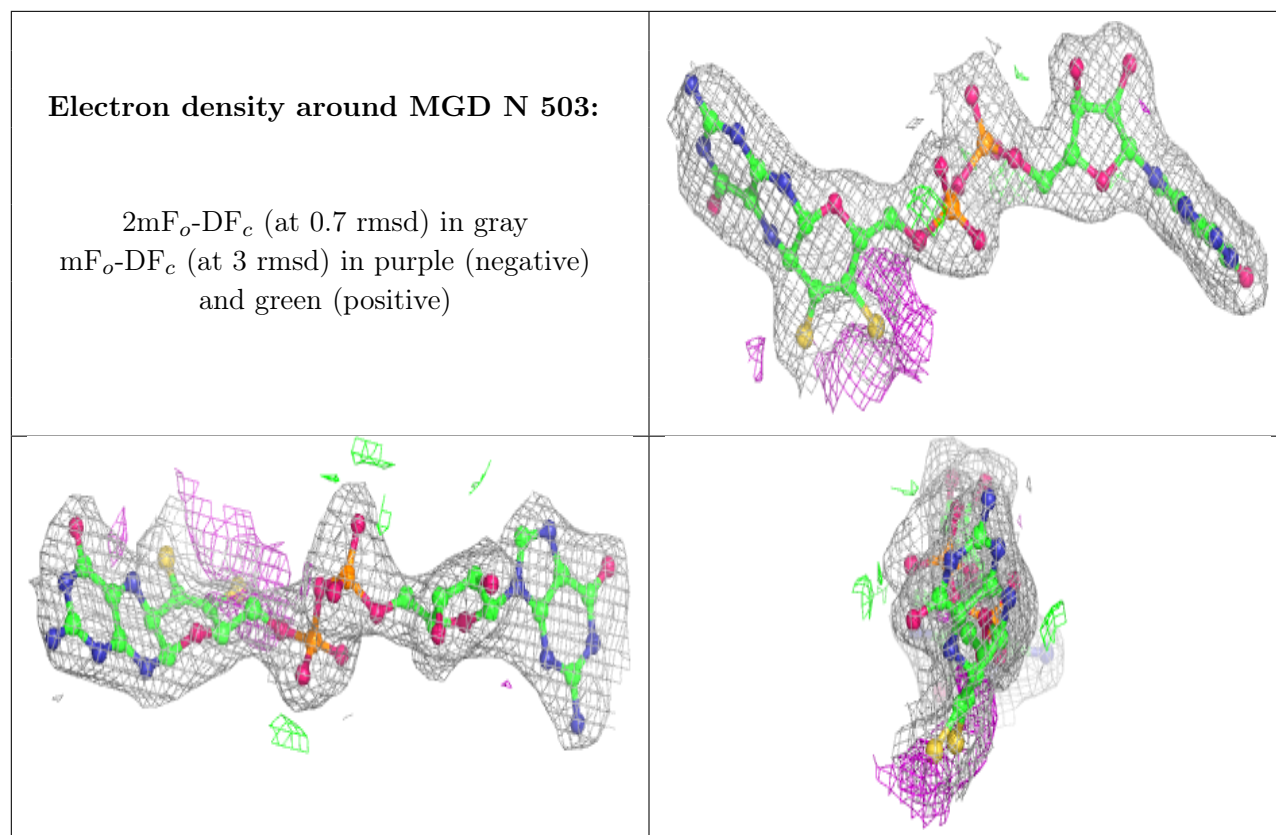
**Electron density around MGD I 504:**

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

**Electron density around MGD 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.