



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2021 – 12:36 PM EDT

PDB ID : 7MJW  
Title : Methylated MiaB in the complex with 5'-deoxyadenosine, methionine and RNA  
Authors : Esakova, O.A.; Grove, T.L.; Yennawar, N.H.; Arcinas, A.J.; Wang, B.; Krebs, C.; Almo, S.C.; Booker, S.J.  
Deposited on : 2021-04-20  
Resolution : 1.40 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.1  
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) : 2.23.1

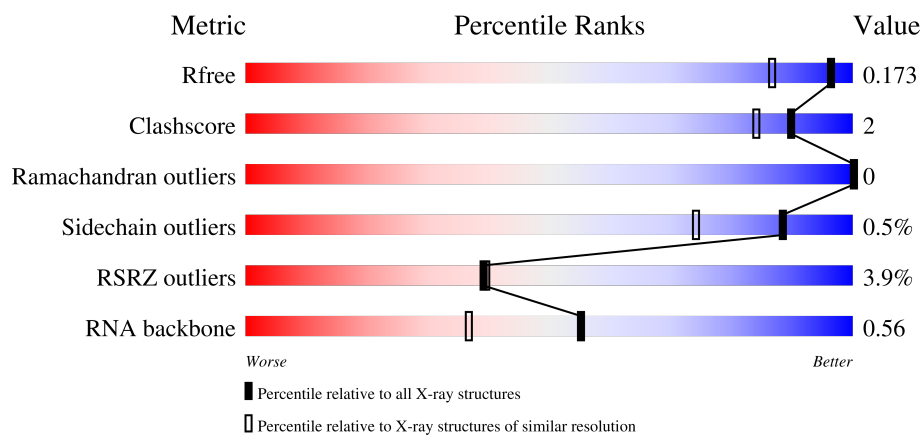
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)
RNA backbone	3102	1000 (2.34-0.62)

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	457	<div> <div>4%</div> <div>92%</div> <div>6%</div> <div>•</div> </div>
1	B	457	<div> <div>3%</div> <div>90%</div> <div>6%</div> <div>•</div> </div>
2	G	13	<div> <div>38%</div> <div>62%</div> </div>
2	M	13	<div> <div>46%</div> <div>54%</div> </div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9006 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.

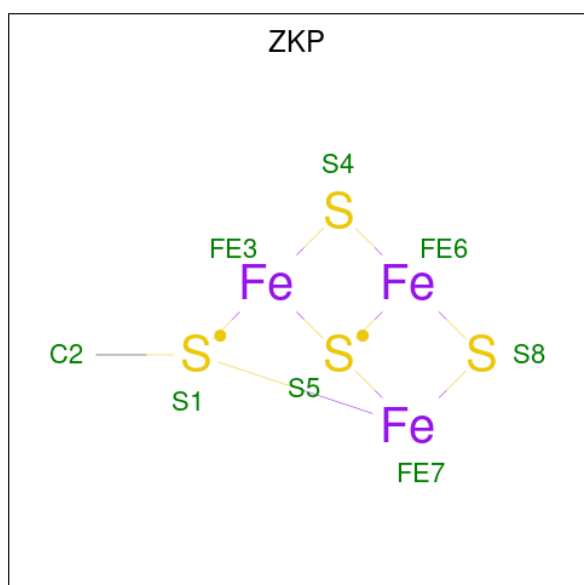
- Molecule 1 is a protein called tRNA-2-methylthio-N(6)-dimethylallyladosine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	13	0
			3547	2217	628	675	27			
1	B	441	Total	C	N	O	S	0	25	0
			3601	2261	626	685	29			

- Molecule 2 is a RNA chain called RNA (5'-R(\*GP\*GP\*AP\*CP\*UP\*GP\*AP\*AP\*(MIA)P\*AP\*UP\*CP\*C)-3').

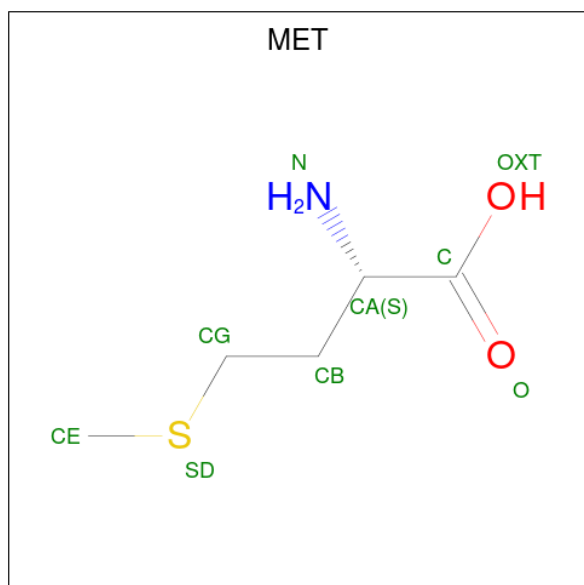
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	13	Total	C	N	O	P	0	0	0
			281	130	53	86	12			
2	G	13	Total	C	N	O	P	0	0	0
			281	130	53	86	12			

- Molecule 3 is FE3-S4 methylated cluster (three-letter code: ZKP) (formula:  $\text{CH}_3\text{Fe}_3\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



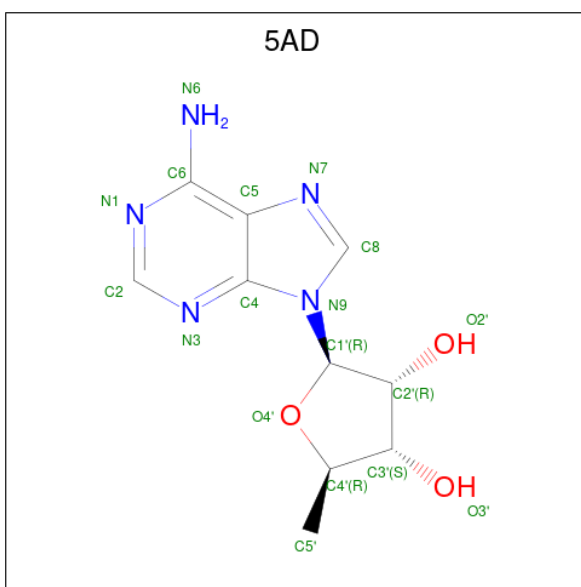
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Fe	S	0	0
			8	1	3	4		
3	B	1	Total	C	Fe	S	0	0
			8	1	3	4		

- Molecule 4 is METHIONINE (three-letter code: MET) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



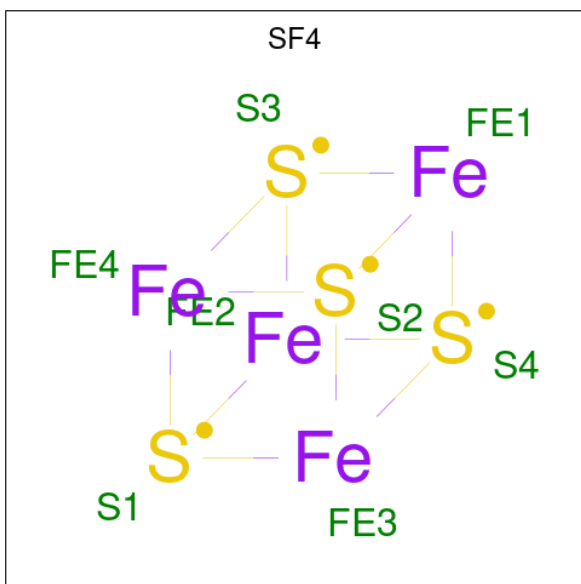
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
4	B	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

- Molecule 5 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>5</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			18	10	5	3		
5	B	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		
7	G	1	Total	Mg	0	0
			1	1		

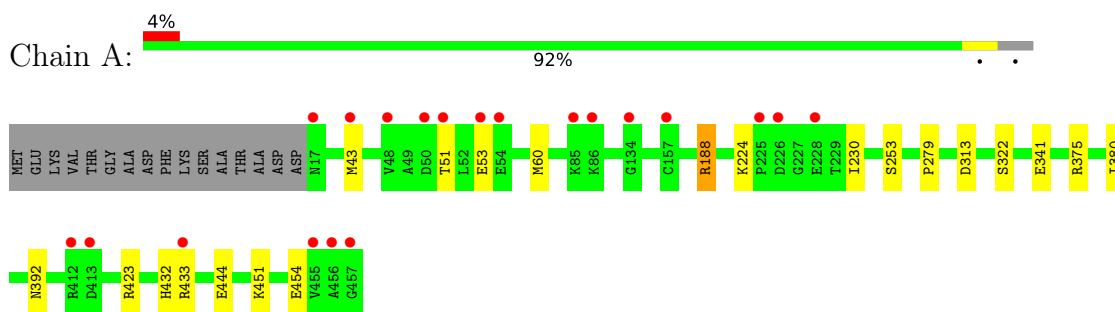
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	519	Total	O	0	0
			519	519		
8	M	80	Total	O	0	0
			80	80		
8	B	534	Total	O	0	0
			534	534		
8	G	74	Total	O	0	0
			74	74		

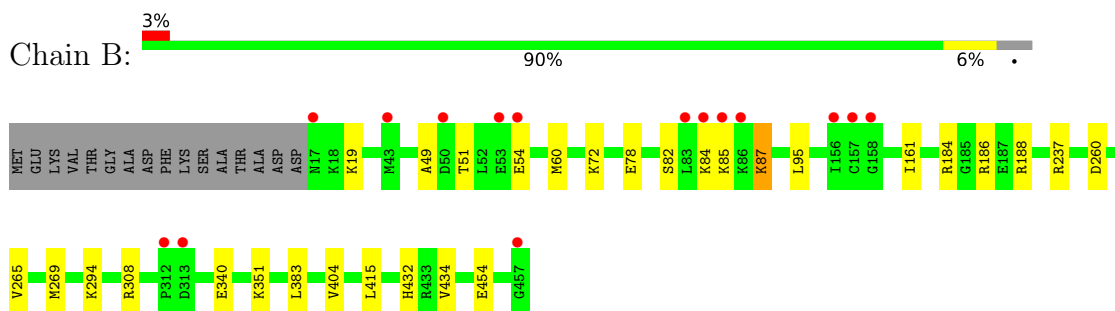
### 3 Residue-property plots [i](#)

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.

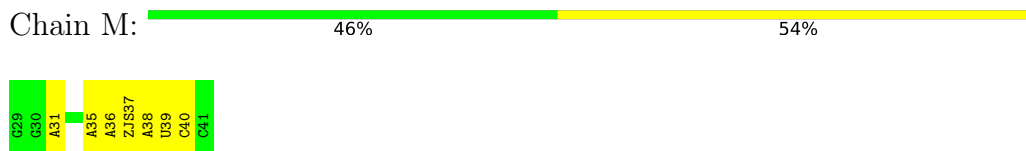
- Molecule 1: tRNA-2-methylthio-N(6)-dimethylallyladenosine synthase



- Molecule 1: tRNA-2-methylthio-N(6)-dimethylallyladenosine synthase



- Molecule 2: RNA (5'-R(\*GP\*GP\*AP\*CP\*UP\*GP\*AP\*AP\*(MIA)P\*AP\*UP\*CP\*C)-3')



- Molecule 2: RNA (5'-R(\*GP\*GP\*AP\*CP\*UP\*GP\*AP\*AP\*(MIA)P\*AP\*UP\*CP\*C)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.90Å 97.41Å 80.74Å 90.00° 108.08° 90.00°	Depositor
Resolution (Å)	39.08 – 1.40 39.08 – 1.35	Depositor EDS
% Data completeness (in resolution range)	78.5 (39.08-1.40) 86.9 (39.08-1.35)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.35Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.149 , 0.174 0.149 , 0.173	Depositor DCC
$R_{free}$ test set	2000 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.9	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9006	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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: 5AD, ZKP, ZJS, SF4, MG

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	0.77	1/3642 (0.0%)	0.88	2/4907 (0.0%)
1	B	0.80	2/3732 (0.1%)	0.93	3/5027 (0.1%)
2	G	1.57	4/283 (1.4%)	1.83	10/437 (2.3%)
2	M	1.42	3/283 (1.1%)	1.83	9/437 (2.1%)
All	All	0.86	10/7940 (0.1%)	1.01	24/10808 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	35	A	N9-C4	7.40	1.42	1.37
2	G	34	G	C8-N7	6.70	1.34	1.30
1	B	184	ARG	CG-CD	6.14	1.67	1.51
1	B	351	LYS	CB-CG	-6.06	1.36	1.52
1	A	313	ASP	CB-CG	5.96	1.64	1.51
2	M	35	A	C5-C4	-5.90	1.34	1.38
2	M	35	A	C8-N7	-5.83	1.27	1.31
2	M	36	A	N3-C4	-5.83	1.31	1.34
2	G	40	C	P-OP2	-5.80	1.39	1.49
2	G	31	A	N3-C4	5.08	1.38	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	35	A	C5-C6-N1	-8.78	113.31	117.70
2	G	35	A	C8-N9-C4	-8.70	102.32	105.80
2	M	39	U	C5-C6-N1	-7.82	118.79	122.70
2	M	35	A	C2-N3-C4	-7.34	106.93	110.60
2	M	35	A	N7-C8-N9	7.03	117.32	113.80
1	A	313	ASP	CB-CG-OD2	6.85	124.46	118.30
1	B	260	ASP	CB-CG-OD1	6.54	124.19	118.30
2	M	35	A	C4-C5-C6	6.53	120.27	117.00
1	B	95	LEU	CB-CG-CD1	6.42	121.92	111.00
2	M	35	A	C8-N9-C4	-6.23	103.31	105.80
2	G	35	A	N9-C4-C5	6.20	108.28	105.80
1	B	60	MET	CG-SD-CE	-6.18	90.31	100.20
2	G	35	A	C5-C6-N1	-5.98	114.71	117.70
2	G	29	G	C5-C6-N1	-5.94	108.53	111.50
2	G	35	A	C2-N3-C4	-5.92	107.64	110.60
1	A	60	MET	CG-SD-CE	-5.88	90.79	100.20
2	G	34	G	N3-C4-N9	-5.86	122.48	126.00
2	M	35	A	C6-C5-N7	-5.80	128.24	132.30
2	M	40	C	N3-C4-C5	-5.68	119.63	121.90
2	G	35	A	N7-C8-N9	5.66	116.63	113.80
2	G	35	A	N3-C4-N9	-5.47	123.02	127.40
2	G	34	G	N9-C4-C5	5.47	107.59	105.40
2	G	39	U	C5-C6-N1	-5.09	120.16	122.70
2	M	31	A	N7-C8-N9	-5.00	111.30	113.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	ARG	Sidechain
1	B	186	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3547	0	3572	13	0
1	B	3601	0	3662	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	281	0	132	1	0
2	M	281	0	132	1	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
4	A	9	0	8	0	0
4	B	9	0	8	0	0
5	A	18	0	13	1	0
5	B	18	0	13	1	0
6	A	8	0	0	0	0
6	B	8	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	G	1	0	0	0	0
8	A	519	0	0	4	0
8	B	534	0	0	2	0
8	G	74	0	0	1	0
8	M	80	0	0	0	0
All	All	9006	0	7540	28	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294[A]:LYS:HE3	8:B:729:HOH:O	1.76	0.85
1:B:161:ILE:HG13	1:B:434:VAL:HG12	1.68	0.76
1:A:444:GLU:HG2	1:A:451[A]:LYS:HB2	1.73	0.71
1:A:444:GLU:HG2	1:A:451[B]:LYS:HB2	1.83	0.59
1:A:51:THR:HB	1:A:53:GLU:OE1	2.02	0.59
1:B:19:LYS:HB3	1:B:49:ALA:HB2	1.88	0.56
1:A:432:HIS:HE2	1:A:454:GLU:CD	2.09	0.55
1:A:375:ARG:HD3	1:B:78[A]:GLU:HG3	1.87	0.55
1:B:340[B]:GLU:HG3	1:B:383:LEU:HD21	1.92	0.52
1:B:82:SER:O	1:B:85[D]:LYS:HG3	2.12	0.50
1:A:433[B]:ARG:HD3	8:A:670:HOH:O	2.12	0.49
1:B:87:LYS:HE3	1:B:87:LYS:HB3	1.58	0.48
5:B:503:5AD:H5'1	2:G:37:ZJS:C2	2.46	0.46
1:B:237[B]:ARG:NH2	8:B:611:HOH:O	2.47	0.45
1:A:322[B]:SER:OG	1:A:380:ILE:HD12	2.17	0.45
1:B:51:THR:OG1	1:B:54:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43[A]:MET:HB3	8:A:778:HOH:O	2.16	0.44
1:A:341[A]:GLU:HG3	8:A:870:HOH:O	2.16	0.44
1:B:72:LYS:HD3	8:G:205:HOH:O	2.18	0.44
1:A:392:ASN:OD1	1:A:423[A]:ARG:HD3	2.18	0.44
5:A:503:5AD:H5'1	2:M:37:ZJS:C2	2.47	0.44
1:A:224:LYS:HE2	1:A:230:ILE:HD11	2.00	0.43
1:A:454:GLU:HG2	8:A:615:HOH:O	2.19	0.42
1:B:84:LYS:HB3	1:B:84:LYS:HE3	1.79	0.42
1:B:265:VAL:O	1:B:269[B]:MET:HG3	2.20	0.42
1:B:404:VAL:HG11	1:B:415:LEU:HD13	2.02	0.42
1:A:253:SER:O	1:A:279:PRO:HD2	2.20	0.41
1:B:432:HIS:NE2	1:B:454:GLU:OE2	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	452/457 (99%)	442 (98%)	10 (2%)	0	100	100
1	B	464/457 (102%)	455 (98%)	9 (2%)	0	100	100
All	All	916/914 (100%)	897 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	399/398 (100%)	398 (100%)	1 (0%)	92	81
1	B	411/398 (103%)	408 (99%)	3 (1%)	84	66
All	All	810/796 (102%)	806 (100%)	4 (0%)	88	74

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	ARG
1	B	87	LYS
1	B	188	ARG
1	B	308	ARG

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

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	11/13 (84%)	1 (9%)	0
2	M	11/13 (84%)	1 (9%)	0
All	All	22/26 (84%)	2 (9%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	M	38	A
2	G	38	A

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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
3	ZKP	B	501	1	3,10,10	7.36	3 (100%)	-		
6	SF4	B	504	1,4	0,12,12	0.00	-	-		
5	5AD	A	503	-	17,20,20	3.27	7 (41%)	15,30,30	2.41	5 (33%)
5	5AD	B	503	-	17,20,20	2.73	6 (35%)	15,30,30	2.48	6 (40%)
6	SF4	A	504	1,4	0,12,12	0.00	-	-		
4	MET	A	502	6	4,8,8	0.70	0	2,9,9	0.53	0
3	ZKP	A	501	1	3,10,10	7.58	3 (100%)	-		
4	MET	B	502	6	4,8,8	1.02	0	2,9,9	0.61	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
3	ZKP	B	501	1	-	-	0/3/3/3
6	SF4	B	504	1,4	-	-	0/6/5/5
5	5AD	A	503	-	-	0/0/20/20	0/3/3/3
5	5AD	B	503	-	-	0/0/20/20	0/3/3/3
6	SF4	A	504	1,4	-	-	0/6/5/5
4	MET	A	502	6	-	1/4/8/8	-
3	ZKP	A	501	1	-	-	0/3/3/3
4	MET	B	502	6	-	1/4/8/8	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	ZKP	S1-FE3	-9.98	2.23	2.37
3	A	501	ZKP	S1-FE3	-9.91	2.23	2.37
5	A	503	5AD	O4'-C1'	8.40	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	503	5AD	C3'-C4'	6.64	1.62	1.52
3	A	501	ZKP	S1-FE7	-6.62	2.27	2.37
3	B	501	ZKP	C2-S1	-6.14	1.68	1.82
5	B	503	5AD	O4'-C1'	6.04	1.49	1.41
5	B	503	5AD	C3'-C4'	5.54	1.60	1.52
3	A	501	ZKP	C2-S1	-5.52	1.70	1.82
3	B	501	ZKP	S1-FE7	-5.04	2.30	2.37
5	A	503	5AD	C3'-C2'	-4.75	1.40	1.53
5	B	503	5AD	C3'-C2'	-4.56	1.40	1.53
5	A	503	5AD	C2'-C1'	3.35	1.58	1.53
5	A	503	5AD	C2-N3	3.11	1.37	1.32
5	B	503	5AD	C2'-C1'	2.78	1.58	1.53
5	A	503	5AD	C5-C4	-2.50	1.34	1.40
5	B	503	5AD	C2-N3	2.50	1.36	1.32
5	A	503	5AD	O4'-C4'	-2.44	1.37	1.44
5	B	503	5AD	C5-C4	-2.01	1.35	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	503	5AD	C5'-C4'-C3'	-6.40	108.98	115.70
5	A	503	5AD	C5'-C4'-C3'	-5.64	109.77	115.70
5	A	503	5AD	C5-C6-N6	4.15	126.65	120.35
5	B	503	5AD	O4'-C1'-C2'	-4.11	100.93	106.93
5	A	503	5AD	C3'-C2'-C1'	3.40	106.10	100.98
5	B	503	5AD	C5-C6-N6	3.21	125.23	120.35
5	A	503	5AD	O4'-C1'-C2'	-3.09	102.41	106.93
5	B	503	5AD	C3'-C2'-C1'	2.76	105.14	100.98
5	B	503	5AD	C1'-N9-C4	-2.61	122.06	126.64
5	A	503	5AD	C1'-N9-C4	-2.10	122.95	126.64
5	B	503	5AD	N3-C2-N1	-2.08	125.43	128.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

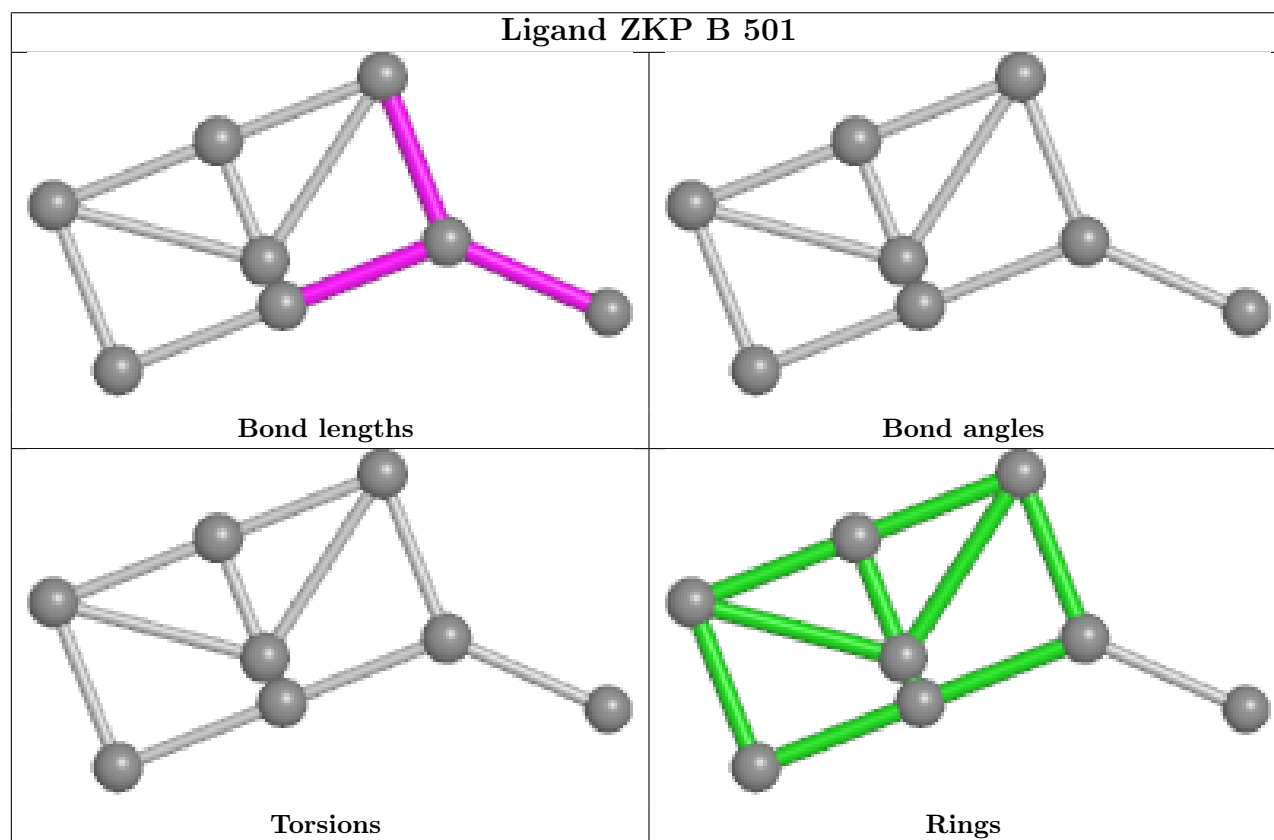
Mol	Chain	Res	Type	Atoms
4	A	502	MET	C-CA-CB-CG
4	B	502	MET	C-CA-CB-CG

There are no ring outliers.

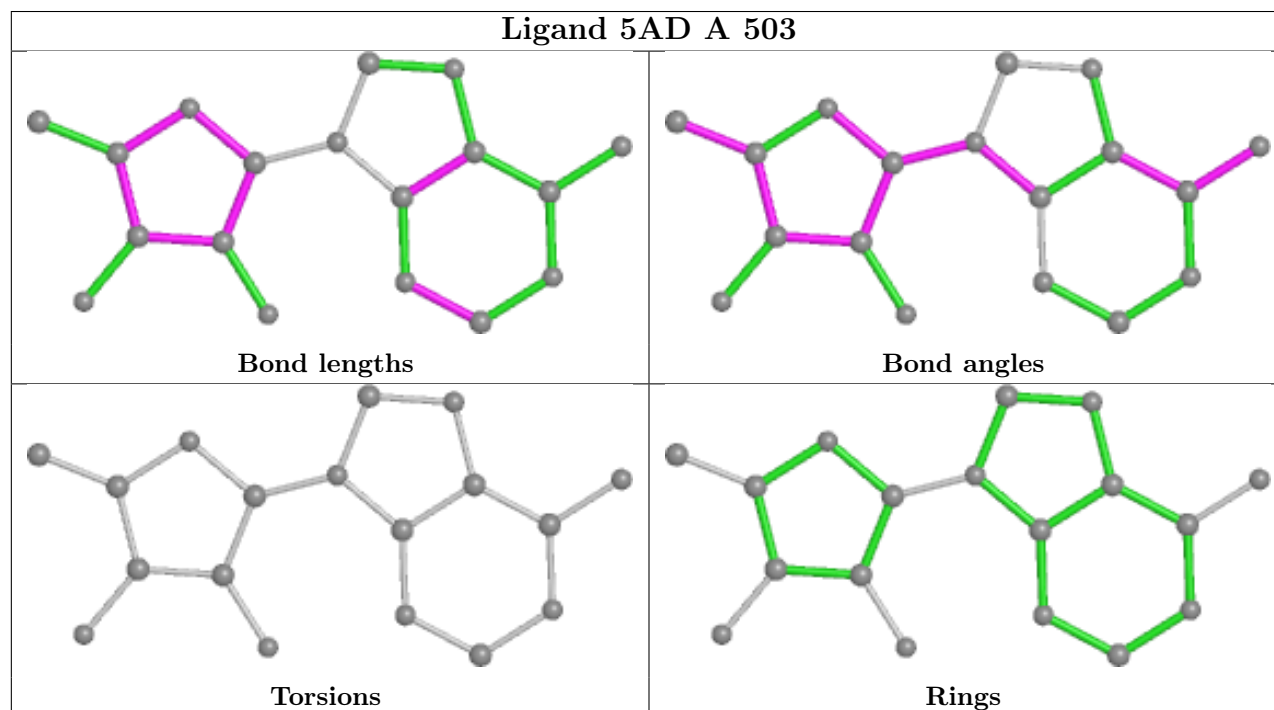
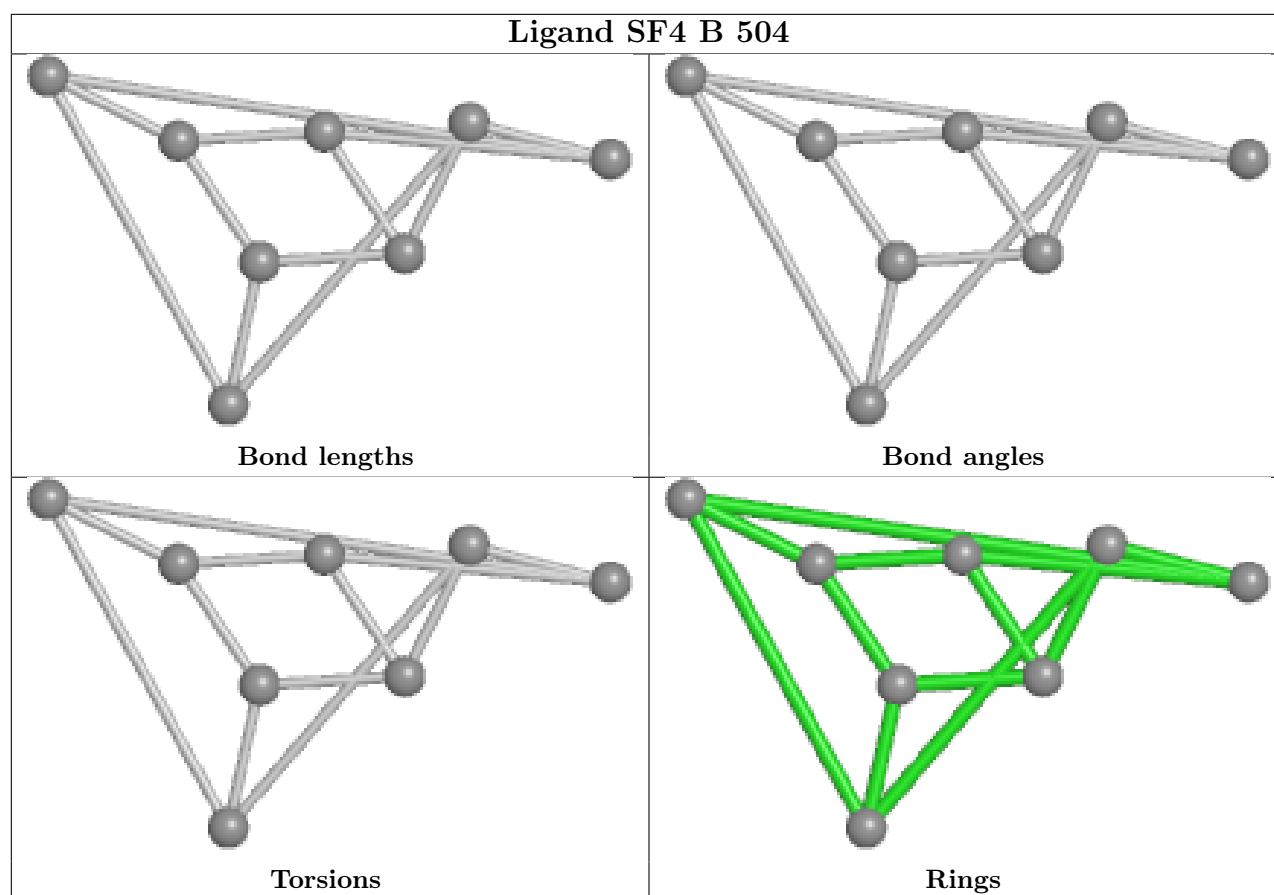
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	5AD	1	0
5	B	503	5AD	1	0

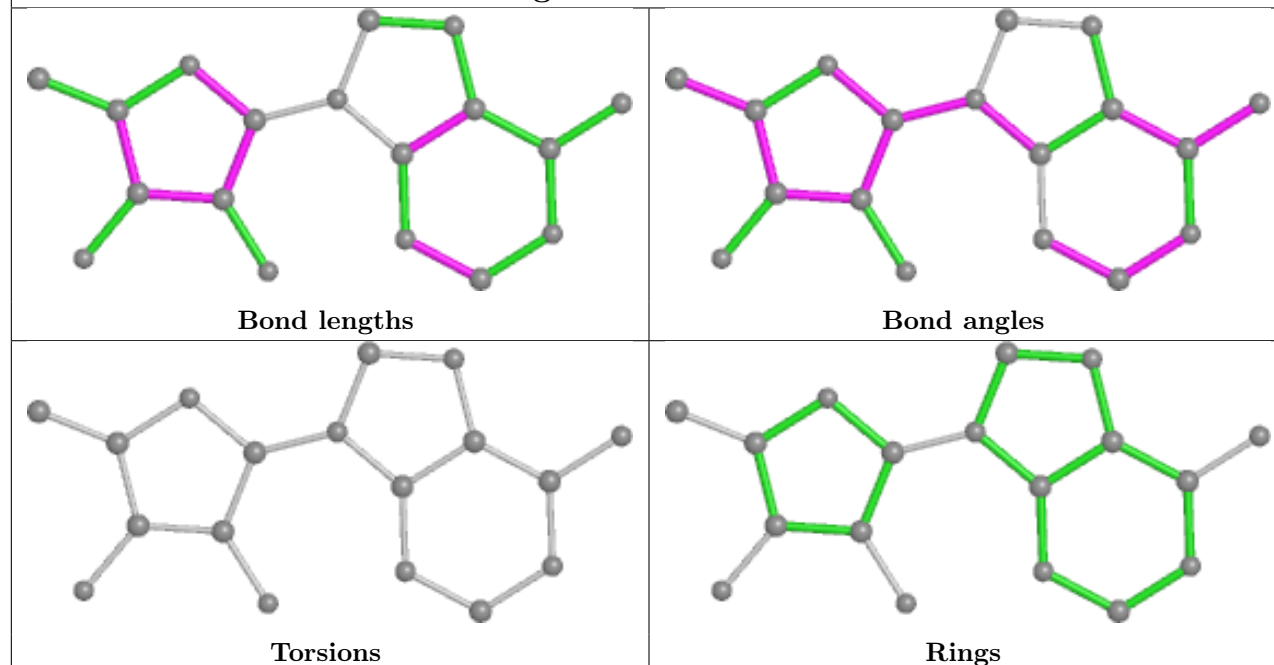
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



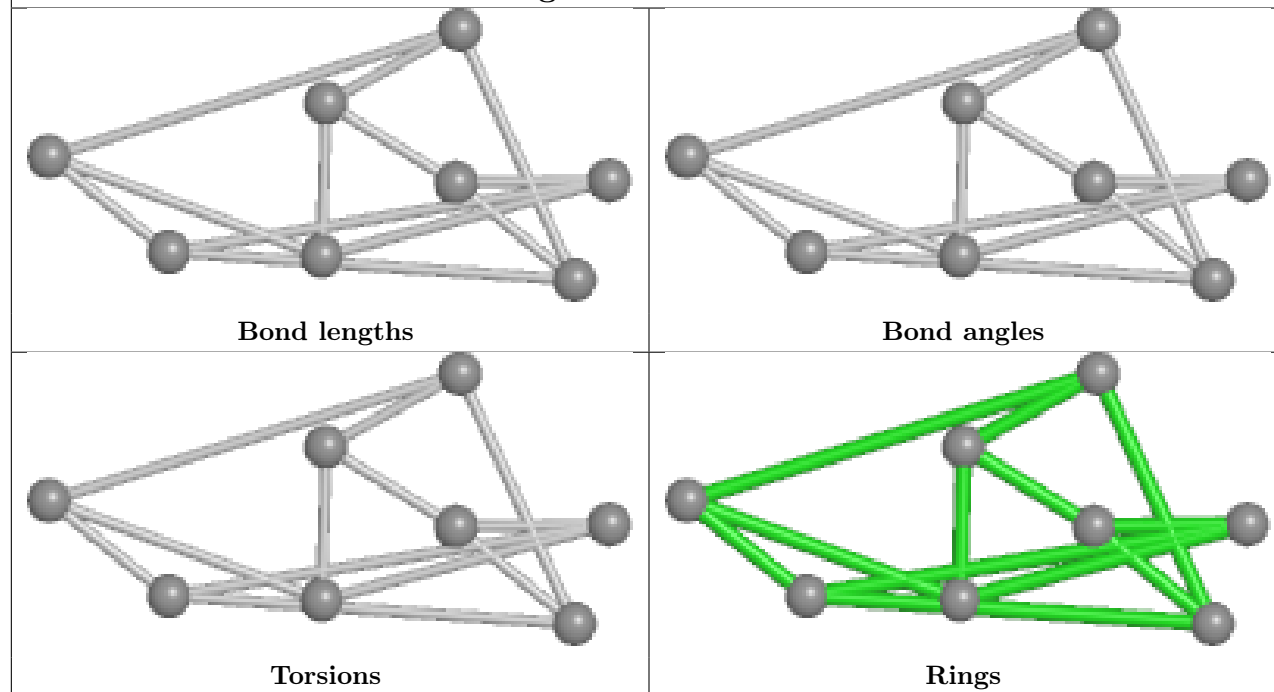


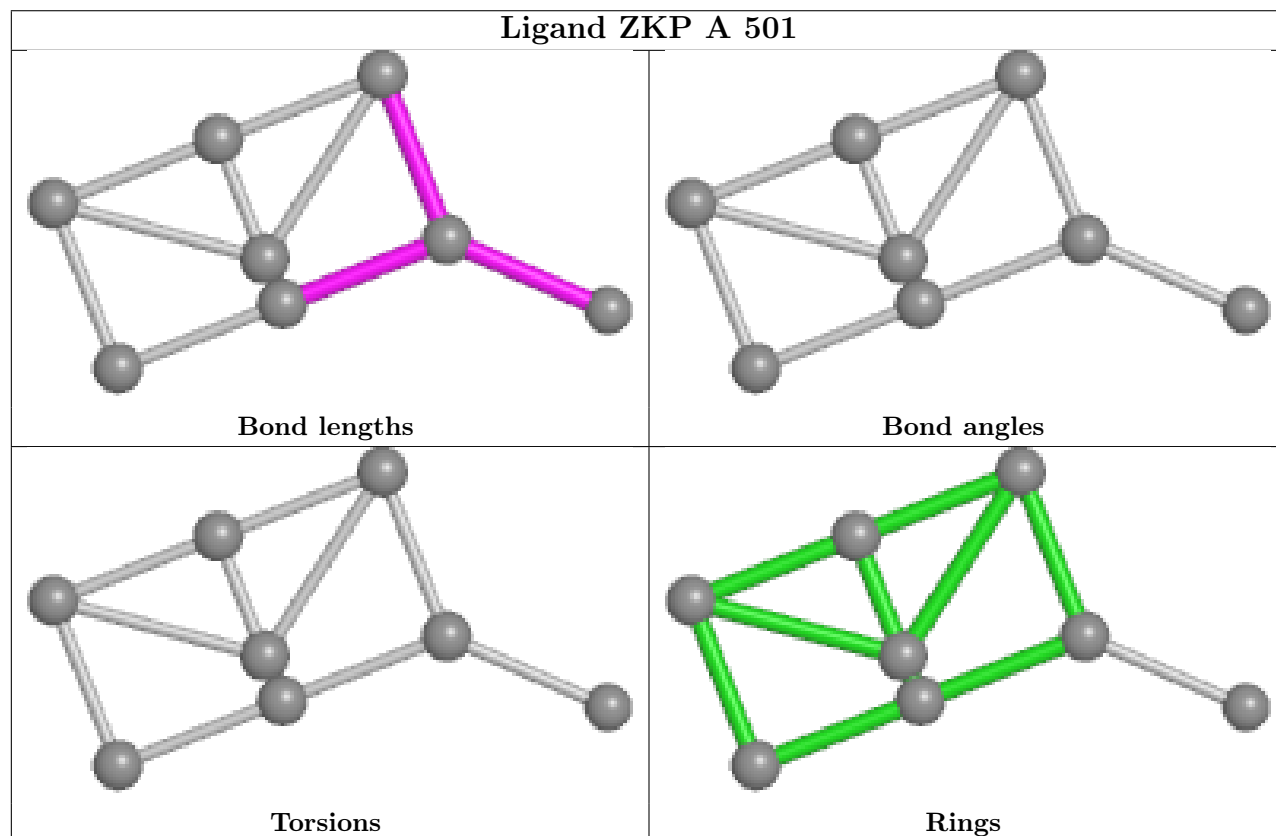
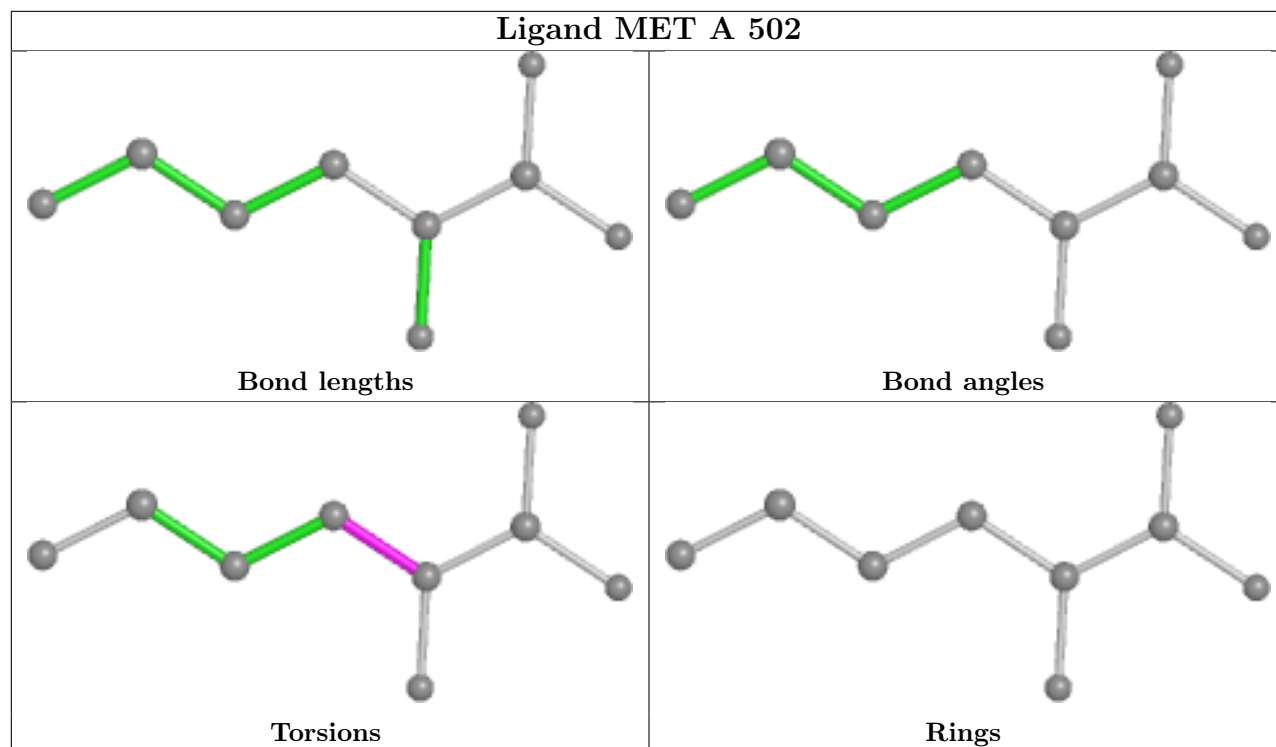


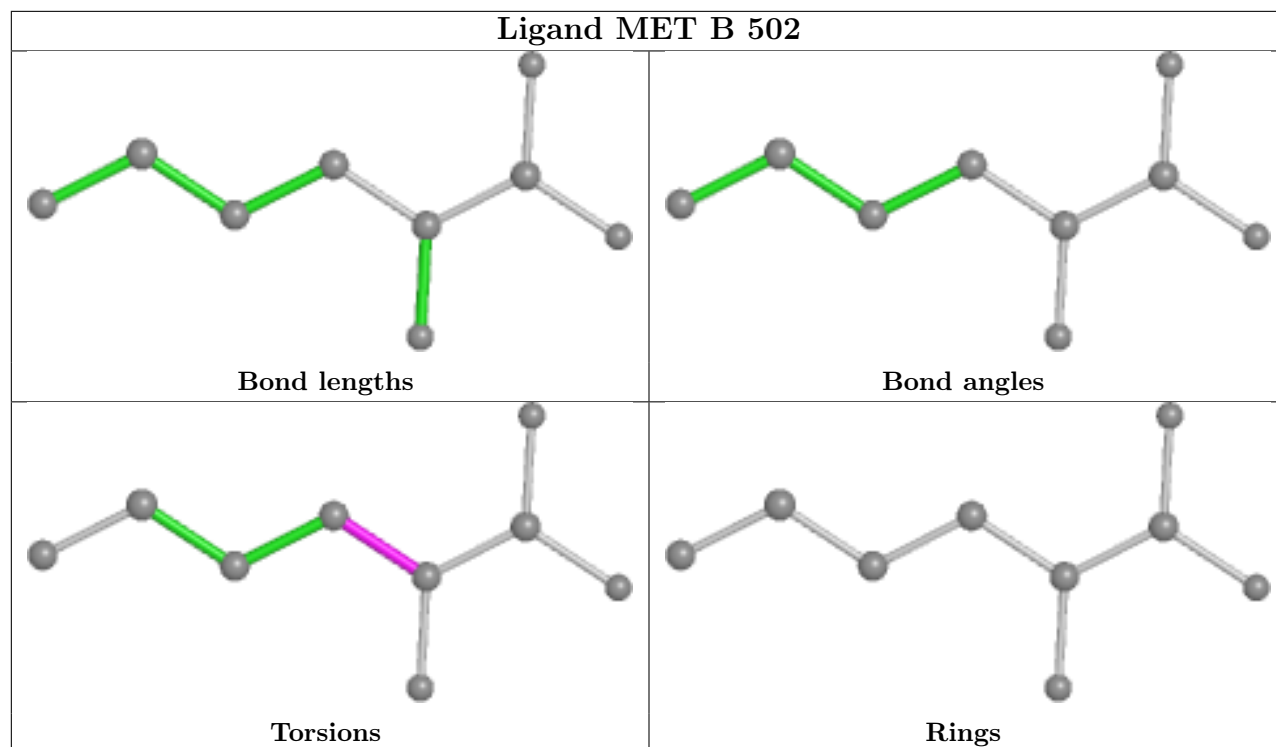
## Ligand 5AD B 503



## Ligand SF4 A 504







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	441/457 (96%)	-0.15	20 (4%) 33 33	10, 18, 31, 39	0
1	B	441/457 (96%)	-0.18	15 (3%) 45 44	9, 16, 28, 36	0
2	G	12/13 (92%)	-0.65	0 100 100	12, 17, 23, 24	0
2	M	12/13 (92%)	-0.58	0 100 100	12, 19, 23, 24	0
All	All	906/940 (96%)	-0.18	35 (3%) 39 39	9, 17, 30, 39	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	456	ALA	8.3
1	B	457	GLY	7.8
1	B	157	CYS	7.5
1	A	17	ASN	6.8
1	A	457	GLY	6.0
1	B	86[A]	LYS	4.9
1	A	50	ASP	4.5
1	B	85[B]	LYS	4.4
1	A	225	PRO	4.3
1	B	156	ILE	4.3
1	B	312	PRO	3.6
1	B	158	GLY	3.6
1	B	83	LEU	3.6
1	A	43[A]	MET	3.1
1	A	53	GLU	3.1
1	A	54	GLU	3.1
1	B	84	LYS	2.9
1	A	134	GLY	2.9
1	A	412	ARG	2.8
1	A	51	THR	2.8
1	B	50	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	226	ASP	2.6
1	B	17	ASN	2.5
1	A	86[A]	LYS	2.4
1	B	53	GLU	2.4
1	A	85	LYS	2.2
1	B	43[A]	MET	2.2
1	B	54	GLU	2.2
1	A	433[A]	ARG	2.1
1	A	48	VAL	2.1
1	B	313	ASP	2.1
1	A	413	ASP	2.1
1	A	228	GLU	2.0
1	A	455	VAL	2.0
1	A	157	CYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 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.

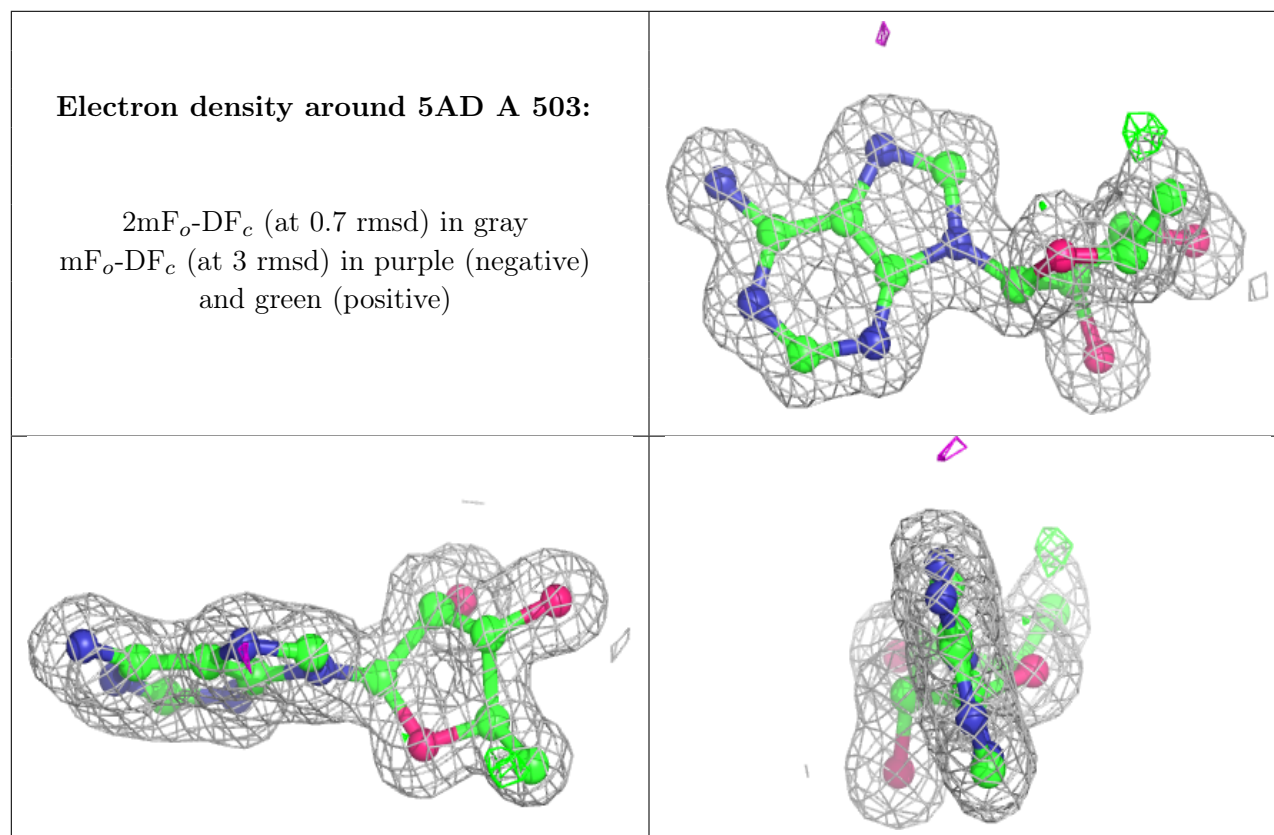
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	5AD	A	503	18/18	0.98	0.09	10,11,15,19	0
5	5AD	B	503	18/18	0.98	0.09	7,9,11,16	0
4	MET	A	502	9/9	0.99	0.09	10,10,11,12	0
4	MET	B	502	9/9	0.99	0.10	8,9,10,12	0
7	MG	A	505	1/1	0.99	0.05	15,15,15,15	0
7	MG	B	505	1/1	0.99	0.06	15,15,15,15	0
7	MG	G	101	1/1	0.99	0.04	17,17,17,17	0
6	SF4	B	504	8/8	1.00	0.07	7,8,9,9	0
3	ZKP	A	501	8/8	1.00	0.06	11,12,13,21	1

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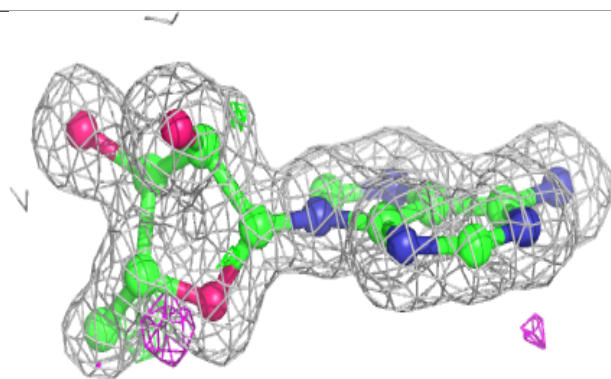
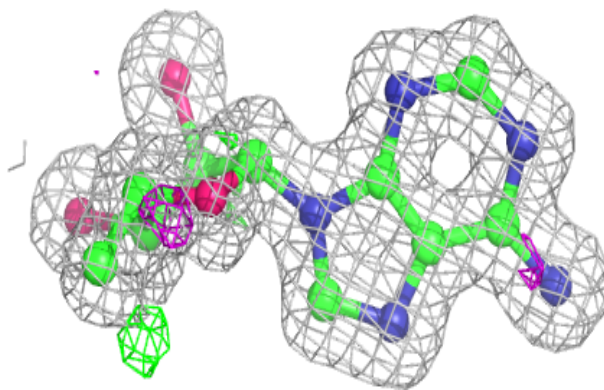
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZKP	B	501	8/8	1.00	0.08	10,11,12,24	1
6	SF4	A	504	8/8	1.00	0.06	10,11,11,12	0

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.

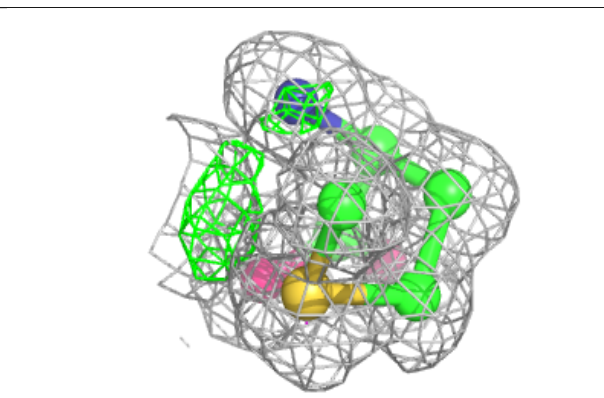
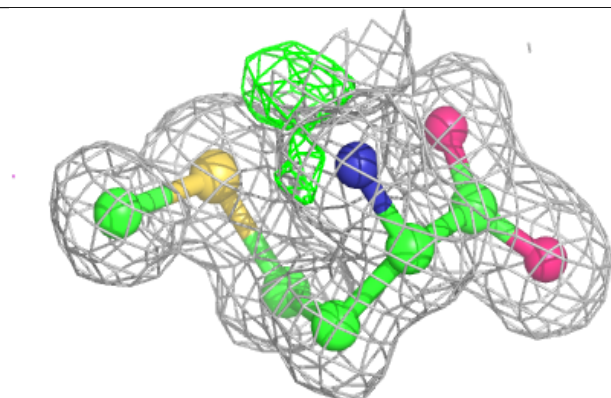
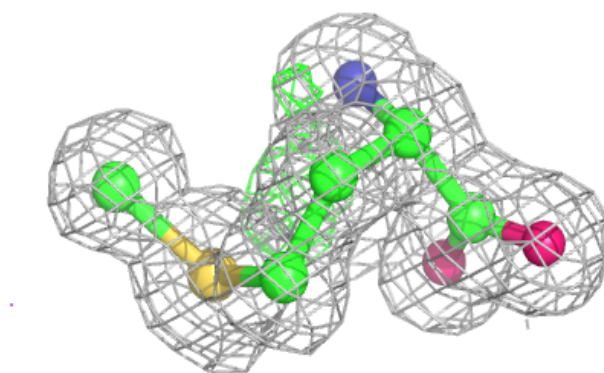


**Electron density around 5AD B 503:**

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

**Electron density around MET A 502:**

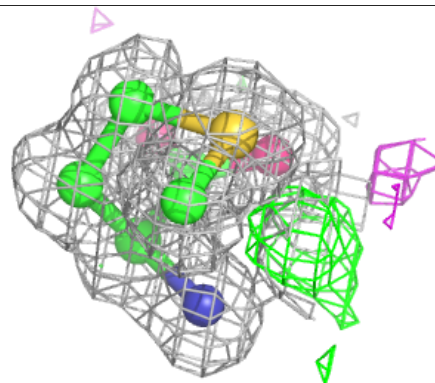
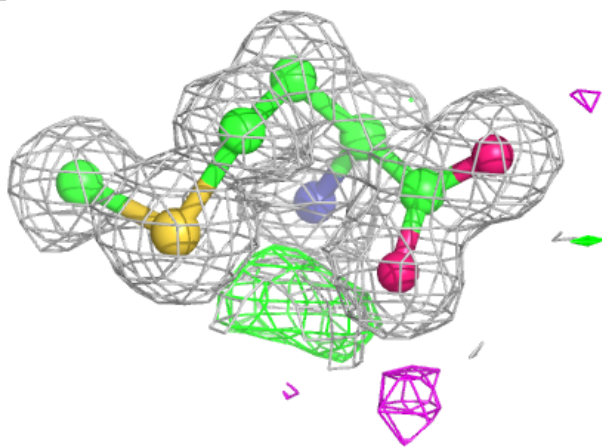
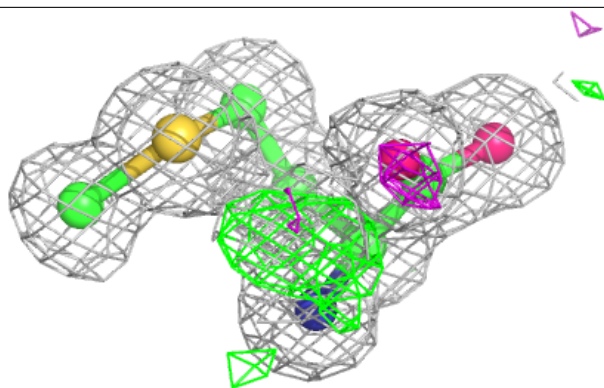
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





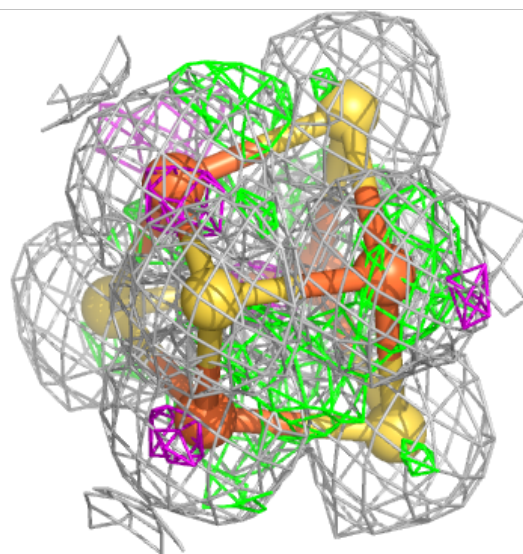
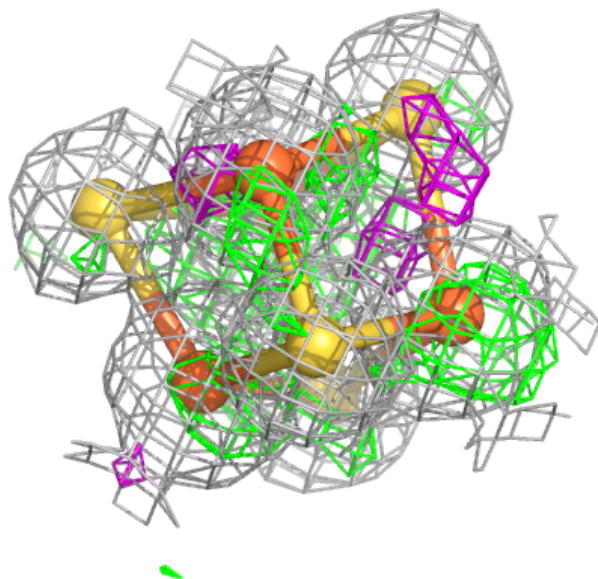
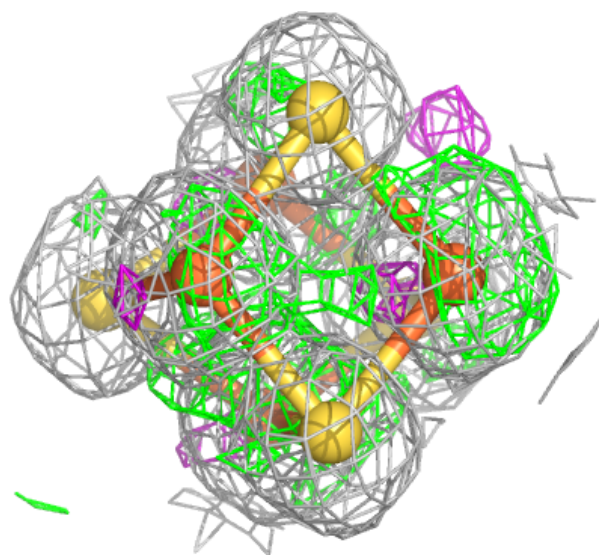
**Electron density around MET B 502:**

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



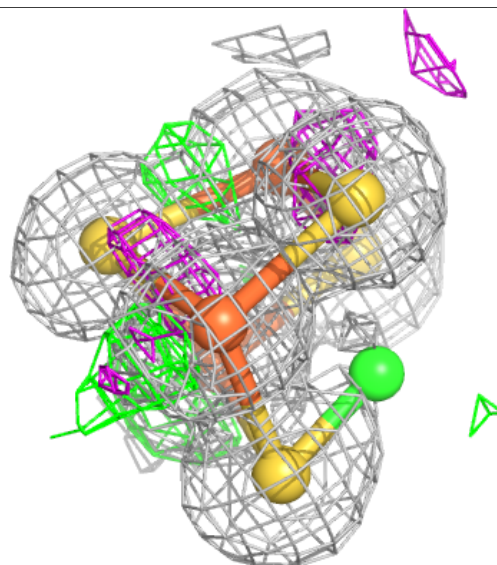
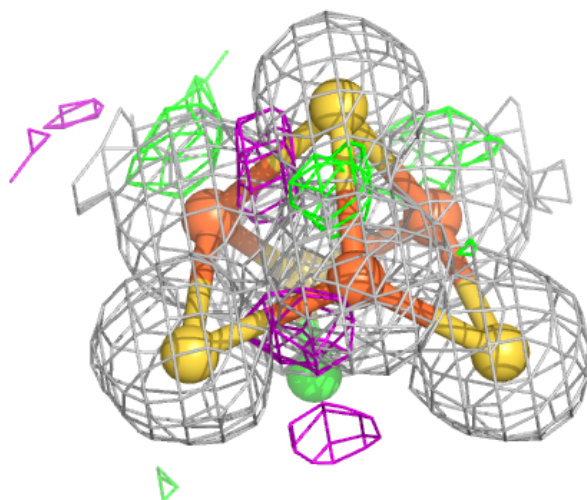
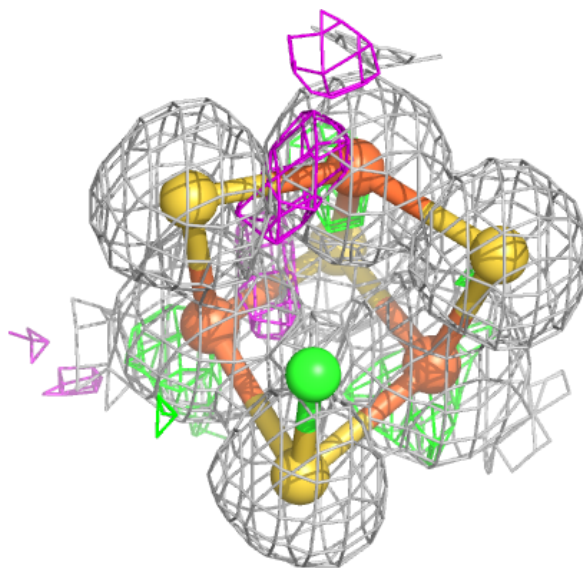
**Electron density around SF4 B 504:**

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



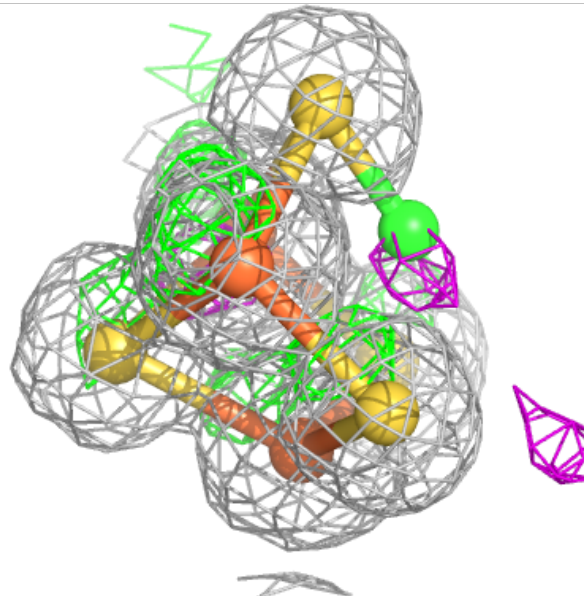
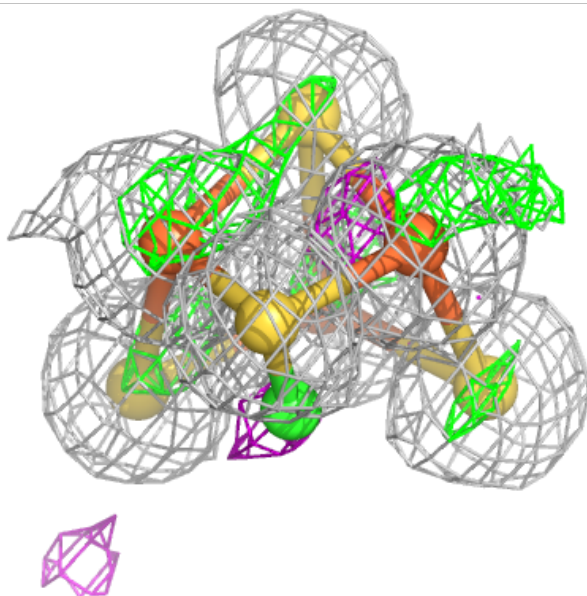
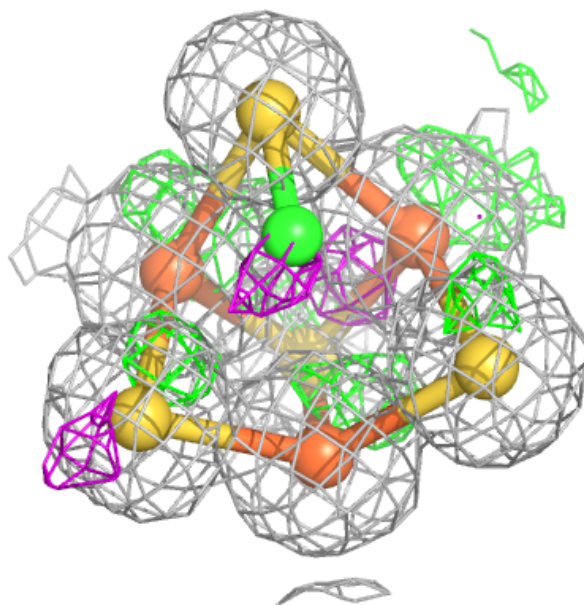
**Electron density around ZKP A 501:**

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



**Electron density around ZKP B 501:**

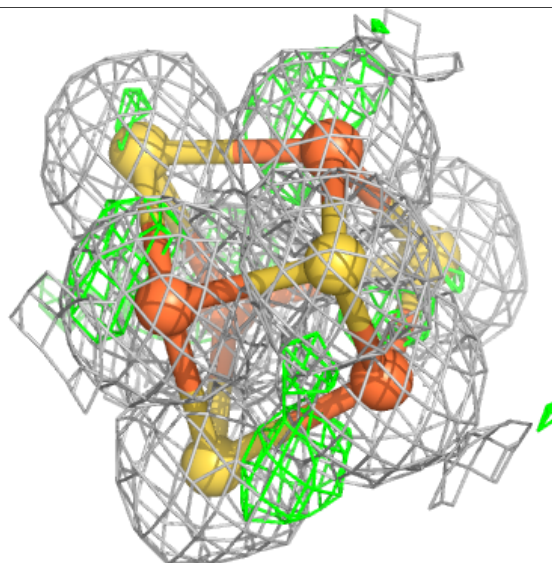
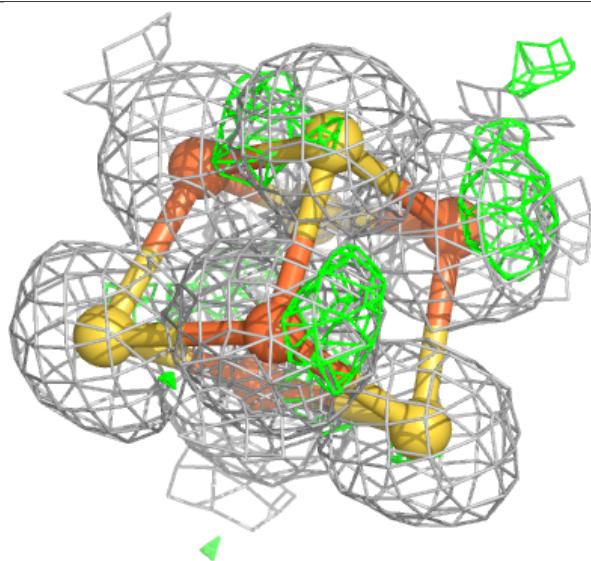
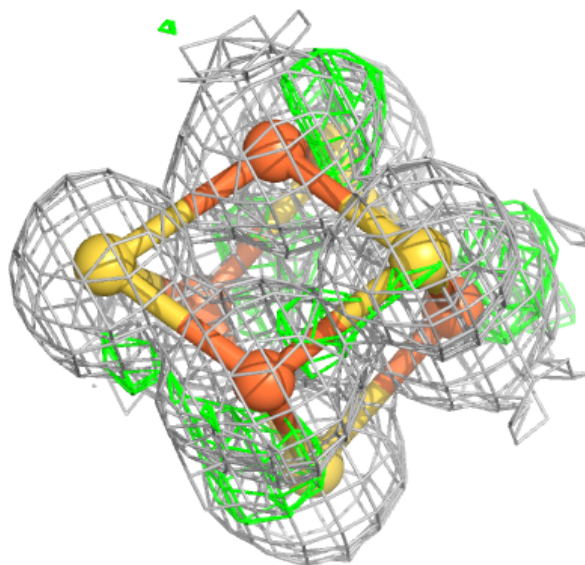
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around SF4 A 504:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.