



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2020 – 09:21 am GMT

PDB ID : 6RB5  
Title : Trypanothione reductase in complex with 4-(((3-(8-(2-((1R,2S,5R)-6,6-dimethylbicyclo[3.1.1]heptan-2-yl)ethyl)-4-oxo-1-phenyl-1,3,8-triazaspiro[4.5]decan-3-yl)propyl)(methyl)amino)methyl)-4-hydroxypiperidine-1-carboximidamide  
Authors : Ilari, A.; Fiorillo, A.; Battista, T.; Mocci, S.  
Deposited on : 2019-04-09  
Resolution : 1.98 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 : 2.14.6  
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) : 2.14.6

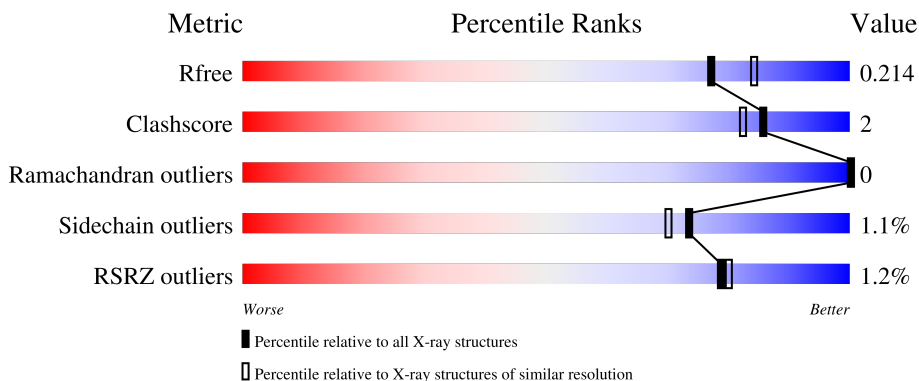
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 on 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	512	 2% 92% . .
1	B	512	 % 93% . .

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 8412 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 Trypanothione reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	490	3784	2406	641	717	20	0	9	0
1	B	489	3773	2400	640	713	20	0	9	0

There are 40 discrepancies between the modelled and reference sequences:

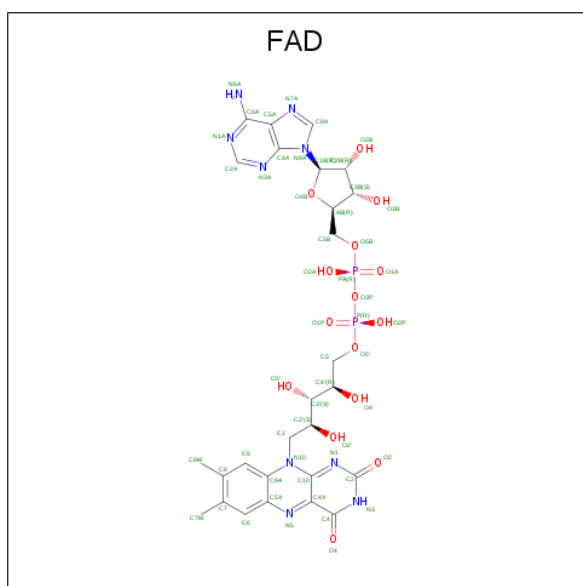
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q389T8
A	-18	GLY	-	expression tag	UNP Q389T8
A	-17	SER	-	expression tag	UNP Q389T8
A	-16	SER	-	expression tag	UNP Q389T8
A	-15	HIS	-	expression tag	UNP Q389T8
A	-14	HIS	-	expression tag	UNP Q389T8
A	-13	HIS	-	expression tag	UNP Q389T8
A	-12	HIS	-	expression tag	UNP Q389T8
A	-11	HIS	-	expression tag	UNP Q389T8
A	-10	HIS	-	expression tag	UNP Q389T8
A	-9	SER	-	expression tag	UNP Q389T8
A	-8	SER	-	expression tag	UNP Q389T8
A	-7	GLY	-	expression tag	UNP Q389T8
A	-6	LEU	-	expression tag	UNP Q389T8
A	-5	VAL	-	expression tag	UNP Q389T8
A	-4	PRO	-	expression tag	UNP Q389T8
A	-3	ARG	-	expression tag	UNP Q389T8
A	-2	GLY	-	expression tag	UNP Q389T8
A	-1	SER	-	expression tag	UNP Q389T8
A	0	HIS	-	expression tag	UNP Q389T8
B	-19	MET	-	initiating methionine	UNP Q389T8
B	-18	GLY	-	expression tag	UNP Q389T8
B	-17	SER	-	expression tag	UNP Q389T8
B	-16	SER	-	expression tag	UNP Q389T8
B	-15	HIS	-	expression tag	UNP Q389T8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q389T8
B	-13	HIS	-	expression tag	UNP Q389T8
B	-12	HIS	-	expression tag	UNP Q389T8
B	-11	HIS	-	expression tag	UNP Q389T8
B	-10	HIS	-	expression tag	UNP Q389T8
B	-9	SER	-	expression tag	UNP Q389T8
B	-8	SER	-	expression tag	UNP Q389T8
B	-7	GLY	-	expression tag	UNP Q389T8
B	-6	LEU	-	expression tag	UNP Q389T8
B	-5	VAL	-	expression tag	UNP Q389T8
B	-4	PRO	-	expression tag	UNP Q389T8
B	-3	ARG	-	expression tag	UNP Q389T8
B	-2	GLY	-	expression tag	UNP Q389T8
B	-1	SER	-	expression tag	UNP Q389T8
B	0	HIS	-	expression tag	UNP Q389T8

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



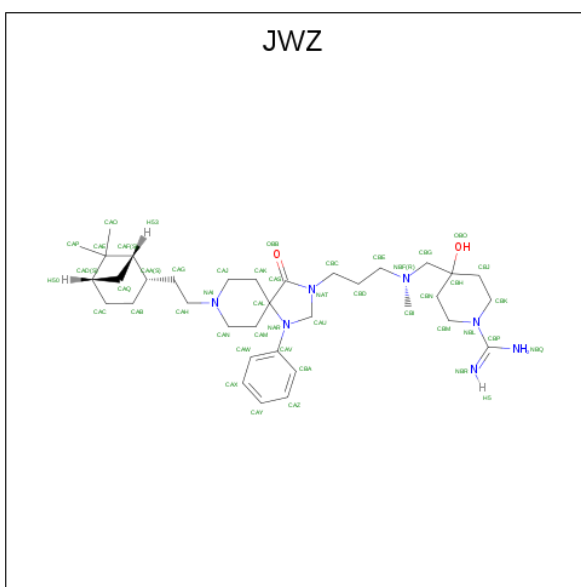
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	53	27	9	15	2	0	0
2	B	1	53	27	9	15	2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



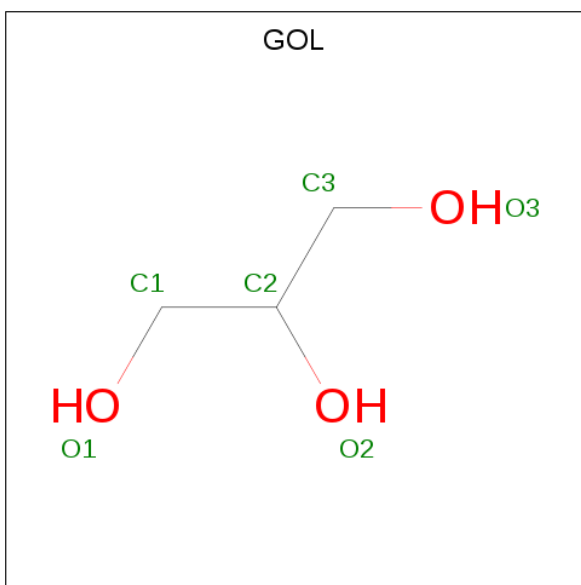
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
3	A	1	5	4	1	0	0
3	A	1	5	4	1	0	0
3	A	1	5	4	1	0	0
3	A	1	5	4	1	0	0
3	A	1	5	4	1	0	0
3	B	1	5	4	1	0	0
3	B	1	5	4	1	0	0
3	B	1	5	4	1	0	0
3	B	1	5	4	1	0	0

- Molecule 4 is 4-(((3-(8-(2-((1R,2S,5R)-6,6-dimethylbicyclo[3.1.1]heptan-2-yl)ethyl)-4-oxo-1-phenyl-1,3,8-triazaspiro[4.5]decan-3-yl)propyl)(methyl)amino)methyl)-4-hydroxypiperidine-1-carboximidamide (three-letter code: JWZ) (formula: C<sub>35</sub>H<sub>57</sub>N<sub>7</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	44	35	7	2	0	0
4	A	1	44	35	7	2	0	0
4	B	1	44	35	7	2	0	0
4	B	1	44	35	7	2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

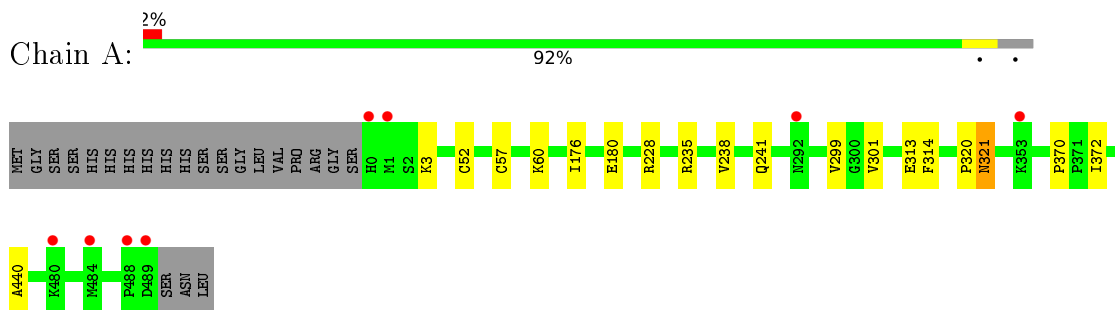
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	232	Total O 232 232	0	0
6	B	255	Total O 255 255	0	0

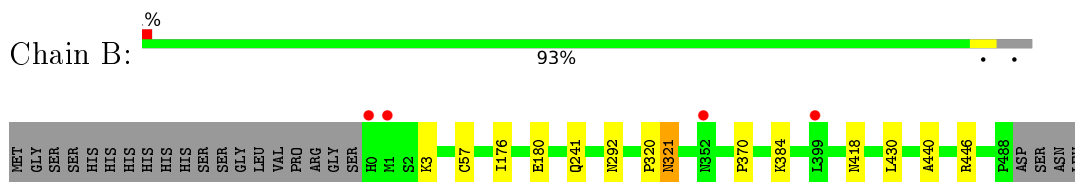
### 3 Residue-property plots [i](#)

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: Trypanothione reductase



- Molecule 1: Trypanothione reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.07Å 132.62Å 161.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.38 – 1.98 102.38 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.7 (102.38-1.98) 99.7 (102.38-1.98)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 1.98Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.183 , 0.207 0.189 , 0.214	Depositor DCC
$R_{free}$ test set	4839 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtrriage
Anisotropy	0.541	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8412	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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: GOL, JWZ, SO4, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.35	0/3879	0.57	0/5261
1	B	0.36	0/3874	0.58	0/5254
All	All	0.36	0/7753	0.57	0/10515

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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	3784	0	3792	14	0
1	B	3773	0	3788	11	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
3	A	30	0	0	0	0
3	B	20	0	0	0	0
4	A	88	0	0	6	0
4	B	88	0	0	5	0
5	A	12	0	16	2	0
5	B	24	0	32	0	0
6	A	232	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	255	0	0	0	0
All	All	8412	0	7690	35	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 (35) 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:A:321[A]:ASN:HD22	1:A:321[A]:ASN:H	1.11	0.96
1:B:321[A]:ASN:HD22	1:B:321[A]:ASN:H	1.25	0.83
1:A:321[A]:ASN:ND2	1:A:321[A]:ASN:H	1.92	0.60
1:B:446[B]:ARG:HG3	1:B:446[B]:ARG:HH11	1.69	0.57
1:A:321[A]:ASN:HD22	1:A:321[A]:ASN:N	1.88	0.56
1:B:321[A]:ASN:HD22	1:B:321[A]:ASN:N	1.98	0.56
1:B:320[B]:PRO:O	1:B:321[B]:ASN:HB2	2.05	0.56
4:A:509:JWZ:CAP	4:A:509:JWZ:CAB	2.84	0.55
4:B:506:JWZ:CAB	4:B:506:JWZ:CAP	2.85	0.55
4:B:507:JWZ:CAB	4:B:507:JWZ:CAP	2.84	0.55
4:A:508:JWZ:CBC	4:A:508:JWZ:CBJ	2.85	0.54
4:A:508:JWZ:CAB	4:A:508:JWZ:CAP	2.85	0.54
4:A:509:JWZ:CBI	4:A:509:JWZ:CBN	2.85	0.54
1:A:238[A]:VAL:HG21	1:A:372:ILE:HD11	1.91	0.51
1:B:446[B]:ARG:HG3	1:B:446[B]:ARG:NH1	2.23	0.51
1:A:241:GLN:OE1	1:A:370:PRO:HG3	2.11	0.51
1:B:370:PRO:HG2	1:B:430:LEU:HD11	1.91	0.51
1:B:241:GLN:OE1	1:B:370:PRO:HG3	2.12	0.50
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.95	0.49
4:B:507:JWZ:CAK	4:B:507:JWZ:CAW	2.92	0.47
1:A:320[B]:PRO:O	1:A:321[B]:ASN:HB2	2.15	0.46
1:A:235:ARG:HH22	5:A:511:GOL:H2	1.81	0.46
1:B:321[A]:ASN:H	1:B:321[A]:ASN:ND2	2.05	0.45
4:A:509:JWZ:CBG	4:A:509:JWZ:CAU	2.95	0.44
1:A:228[B]:ARG:NE	5:A:511:GOL:O2	2.50	0.44
4:A:508:JWZ:CAK	4:A:508:JWZ:CBA	2.95	0.43
4:B:507:JWZ:CBG	4:B:507:JWZ:CBC	2.96	0.43
1:A:299:VAL:HG23	1:A:301:VAL:HG23	2.01	0.43
4:B:506:JWZ:CAG	4:B:506:JWZ:CAP	2.98	0.42
1:A:176:ILE:HB	1:A:180:GLU:HB2	2.01	0.42
1:B:292[B]:ASN:HD22	1:B:292[B]:ASN:HA	1.67	0.41
1:A:52:CYS:HB3	6:A:614:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313[B]:GLU:HG2	1:A:314:PHE:CD1	2.56	0.41
1:B:176:ILE:HB	1:B:180:GLU:HB2	2.02	0.41
1:A:321[B]:ASN:HD22	1:A:321[B]:ASN:N	2.18	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	497/512 (97%)	487 (98%)	10 (2%)	0	100	100
1	B	496/512 (97%)	486 (98%)	10 (2%)	0	100	100
All	All	993/1024 (97%)	973 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	412/422 (98%)	407 (99%)	5 (1%)	71	67
1	B	411/422 (97%)	405 (98%)	6 (2%)	65	59
All	All	823/844 (98%)	812 (99%)	11 (1%)	73	64

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	57	CYS
1	A	60	LYS
1	A	321[A]	ASN
1	A	321[B]	ASN
1	B	3	LYS
1	B	57	CYS
1	B	321[A]	ASN
1	B	321[B]	ASN
1	B	384	LYS
1	B	418	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	152	GLN
1	A	292	ASN
1	B	418	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](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

22 ligands 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
4	JWZ	A	509	-	47,49,49	1.15	7 (14%)	62,74,74	1.63	11 (17%)
4	JWZ	B	507	-	47,49,49	1.21	7 (14%)	62,74,74	1.87	14 (22%)
3	SO4	A	504	-	4,4,4	0.35	0	6,6,6	0.10	0
3	SO4	A	503	-	4,4,4	0.33	0	6,6,6	0.08	0
5	GOL	B	509	-	5,5,5	0.33	0	5,5,5	0.13	0
3	SO4	A	505	-	4,4,4	0.33	0	6,6,6	0.07	0
3	SO4	A	506	-	4,4,4	0.30	0	6,6,6	0.13	0
5	GOL	A	511	-	5,5,5	0.40	0	5,5,5	0.74	0
4	JWZ	A	508	-	47,49,49	1.52	8 (17%)	62,74,74	1.95	13 (20%)
2	FAD	B	501	-	51,58,58	1.96	8 (15%)	60,89,89	2.07	10 (16%)
3	SO4	B	504	-	4,4,4	0.36	0	6,6,6	0.14	0
5	GOL	B	511	-	5,5,5	0.30	0	5,5,5	0.37	0
3	SO4	B	503	-	4,4,4	0.36	0	6,6,6	0.09	0
3	SO4	B	502	-	4,4,4	0.32	0	6,6,6	0.13	0
2	FAD	A	501	-	51,58,58	1.99	9 (17%)	60,89,89	2.04	9 (15%)
3	SO4	B	505	-	4,4,4	0.32	0	6,6,6	0.09	0
5	GOL	B	510	-	5,5,5	0.29	0	5,5,5	0.27	0
5	GOL	B	508	-	5,5,5	0.47	0	5,5,5	0.45	0
3	SO4	A	502	-	4,4,4	0.34	0	6,6,6	0.08	0
5	GOL	A	510	-	5,5,5	0.25	0	5,5,5	0.13	0
4	JWZ	B	506	-	47,49,49	1.28	7 (14%)	62,74,74	1.87	7 (11%)
3	SO4	A	507	-	4,4,4	0.36	0	6,6,6	0.11	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
4	JWZ	A	509	-	-	7/24/93/93	0/7/6/6
5	GOL	A	511	-	-	2/4/4/4	-
4	JWZ	B	507	-	-	4/24/93/93	0/7/6/6
5	GOL	B	509	-	-	0/4/4/4	-
4	JWZ	A	508	-	-	10/24/93/93	0/7/6/6
2	FAD	A	501	-	-	4/30/50/50	0/6/6/6
2	FAD	B	501	-	-	4/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	510	-	-	0/4/4/4	-
5	GOL	B	510	-	-	2/4/4/4	-
5	GOL	B	508	-	-	3/4/4/4	-
5	GOL	B	511	-	-	1/4/4/4	-
4	JWZ	B	506	-	-	11/24/93/93	0/7/6/6

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C4X-C10	10.14	1.49	1.38
2	B	501	FAD	C4X-C10	9.94	1.48	1.38
4	A	508	JWZ	CAU-NAT	-4.83	1.41	1.45
2	A	501	FAD	C4-C4X	4.60	1.49	1.41
2	B	501	FAD	C4-C4X	4.40	1.48	1.41
2	B	501	FAD	C9A-C5X	4.07	1.50	1.42
2	A	501	FAD	C9A-C5X	3.94	1.50	1.42
4	A	508	JWZ	CAV-NAR	-3.87	1.31	1.41
4	B	506	JWZ	CAV-NAR	-3.77	1.32	1.41
4	B	507	JWZ	CAV-NAR	-3.41	1.33	1.41
2	A	501	FAD	C8-C7	3.40	1.49	1.40
2	B	501	FAD	C9A-N10	3.35	1.43	1.38
4	A	508	JWZ	CAL-NAR	-3.31	1.45	1.48
2	B	501	FAD	C8-C7	3.28	1.49	1.40
4	A	508	JWZ	CBJ-CBH	-3.24	1.49	1.52
4	A	509	JWZ	CAV-NAR	-3.19	1.33	1.41
2	A	501	FAD	C9A-N10	3.18	1.42	1.38
4	A	508	JWZ	CBN-CBH	-2.97	1.50	1.52
4	B	507	JWZ	CAM-CAL	-2.94	1.50	1.54
4	B	506	JWZ	CAU-NAT	-2.84	1.43	1.45
4	B	507	JWZ	CBN-CBH	2.81	1.55	1.52
4	B	506	JWZ	CAK-CAL	-2.78	1.51	1.54
4	B	507	JWZ	CAS-NAT	-2.74	1.32	1.34
4	A	508	JWZ	CAL-CAS	-2.63	1.38	1.53
4	B	506	JWZ	CAL-CAS	-2.57	1.39	1.53
2	A	501	FAD	C10-N1	2.54	1.36	1.33
4	A	509	JWZ	CAS-NAT	-2.53	1.32	1.34
4	A	508	JWZ	CAS-NAT	-2.43	1.32	1.34
4	A	509	JWZ	CAM-CAL	-2.43	1.51	1.54
4	B	507	JWZ	CAL-CAS	-2.42	1.40	1.53
4	B	506	JWZ	CAL-NAR	-2.40	1.45	1.48
4	B	507	JWZ	CAE-CAD	-2.40	1.47	1.55
4	A	509	JWZ	CAL-CAS	-2.40	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	509	JWZ	CAQ-CAF	-2.38	1.50	1.55
2	B	501	FAD	C10-N1	2.25	1.36	1.33
2	A	501	FAD	C5A-C4A	2.20	1.46	1.40
4	B	506	JWZ	CAE-CAF	-2.20	1.51	1.56
4	A	509	JWZ	CAK-CAL	-2.16	1.51	1.54
4	B	506	JWZ	CAS-NAT	-2.15	1.32	1.34
4	A	508	JWZ	CAE-CAF	-2.13	1.51	1.56
2	B	501	FAD	C5A-C4A	2.11	1.46	1.40
2	B	501	FAD	C2A-N3A	2.11	1.35	1.32
4	A	509	JWZ	CAE-CAF	-2.10	1.51	1.56
2	A	501	FAD	C2A-N3A	2.08	1.35	1.32
4	B	507	JWZ	CAQ-CAF	-2.05	1.50	1.55
2	A	501	FAD	C4X-N5	2.02	1.36	1.33

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	506	JWZ	CBC-NAT-CAS	8.46	132.84	123.58
2	A	501	FAD	C4-N3-C2	8.44	122.27	115.14
2	B	501	FAD	C4-N3-C2	8.21	122.08	115.14
4	A	508	JWZ	CBC-NAT-CAS	7.10	131.35	123.58
2	B	501	FAD	C1'-N10-C9A	6.64	123.52	118.29
4	B	506	JWZ	CAM-CAL-NAR	-6.57	108.00	112.85
4	B	507	JWZ	CAK-CAL-NAR	-6.45	108.09	112.85
4	A	508	JWZ	CAM-CAL-NAR	-6.42	108.11	112.85
2	A	501	FAD	C1'-N10-C9A	6.12	123.11	118.29
2	B	501	FAD	C4-C4X-C10	-5.95	116.01	119.95
4	A	509	JWZ	CAM-CAL-NAR	-5.91	108.48	112.85
2	A	501	FAD	C4-C4X-C10	-5.60	116.25	119.95
4	A	509	JWZ	OBB-CAS-NAT	-5.03	121.53	125.87
4	A	508	JWZ	CBM-NBL-CBK	4.83	121.93	112.62
2	A	501	FAD	C4X-N5-C5X	4.69	121.46	116.77
2	B	501	FAD	C4X-N5-C5X	4.69	121.46	116.77
4	B	506	JWZ	CAU-NAT-CAS	-4.60	108.77	113.44
4	B	507	JWZ	CAU-NAT-CAS	-4.37	109.01	113.44
4	A	508	JWZ	OBB-CAS-NAT	-4.35	122.12	125.87
4	B	507	JWZ	OBB-CAS-NAT	-4.16	122.28	125.87
4	B	507	JWZ	CAK-CAJ-NAI	4.04	115.22	111.23
4	B	506	JWZ	OBB-CAS-NAT	-3.98	122.44	125.87
4	A	508	JWZ	CAU-NAT-CAS	-3.85	109.54	113.44
2	A	501	FAD	C4-C4X-N5	3.81	122.95	118.60
2	B	501	FAD	N3A-C2A-N1A	-3.77	122.79	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	N3A-C2A-N1A	-3.74	122.83	128.68
2	B	501	FAD	C4-C4X-N5	3.74	122.87	118.60
4	A	509	JWZ	CAU-NAT-CAS	-3.66	109.73	113.44
4	B	507	JWZ	CBC-NAT-CAS	3.59	127.51	123.58
4	A	509	JWZ	CAM-CAN-NAI	3.47	114.66	111.23
2	A	501	FAD	C4X-C4-N3	-3.46	118.70	123.43
4	B	507	JWZ	CAM-CAL-NAR	-3.33	110.39	112.85
2	B	501	FAD	C4X-C4-N3	-3.27	118.97	123.43
2	B	501	FAD	C4A-C5A-N7A	-3.12	106.15	109.40
4	B	507	JWZ	CAQ-CAF-CAE	-3.10	82.84	87.44
4	B	507	JWZ	CBM-NBL-CBK	3.08	118.56	112.62
4	A	508	JWZ	CAK-CAL-NAR	-3.08	110.58	112.85
2	A	501	FAD	C4A-C5A-N7A	-3.02	106.25	109.40
4	B	507	JWZ	CAU-NAR-CAV	2.90	122.65	118.32
4	B	507	JWZ	CBN-CBH-CBJ	2.88	113.22	109.85
4	B	507	JWZ	CAM-CAN-NAI	2.85	114.05	111.23
4	B	506	JWZ	CBM-NBL-CBK	2.84	118.08	112.62
4	B	506	JWZ	CAO-CAE-CAP	2.83	115.17	108.67
4	A	508	JWZ	CAQ-CAD-CAE	-2.75	83.75	87.86
4	A	509	JWZ	CBM-NBL-CBK	2.69	117.80	112.62
4	B	506	JWZ	CAM-CAN-NAI	2.68	113.88	111.23
4	A	509	JWZ	CAK-CAJ-NAI	2.67	113.86	111.23
4	A	509	JWZ	CBC-NAT-CAS	2.60	126.42	123.58
4	A	508	JWZ	CAN-CAM-CAL	2.49	115.21	113.06
2	B	501	FAD	C1B-N9A-C4A	-2.49	122.27	126.64
4	A	508	JWZ	CAQ-CAF-CAE	-2.46	83.79	87.44
4	A	508	JWZ	CAO-CAE-CAP	2.41	114.22	108.67
4	A	508	JWZ	CAF-CAE-CAD	2.34	87.66	85.24
4	A	509	JWZ	CAK-CAL-NAR	-2.26	111.18	112.85
4	B	507	JWZ	CAF-CAE-CAD	2.24	87.55	85.24
4	A	508	JWZ	CBN-CBM-NBL	2.19	115.26	110.92
4	B	507	JWZ	CAQ-CAF-CAA	-2.14	103.96	107.66
4	A	508	JWZ	CBN-CBH-CBJ	-2.12	107.38	109.85
4	A	509	JWZ	CAJ-NAI-CAN	2.11	113.57	108.83
2	A	501	FAD	C1B-N9A-C4A	-2.10	122.96	126.64
4	B	507	JWZ	CAK-CAL-CAM	2.04	113.09	110.96
4	A	509	JWZ	CBN-CBH-CBJ	2.02	112.21	109.85
4	A	509	JWZ	CAH-NAI-CAN	-2.01	106.09	111.23
2	B	501	FAD	C9A-N10-C10	-2.00	119.29	121.91

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	509	JWZ	NBF-CBG-CBH-CBJ
4	A	509	JWZ	CBH-CBG-NBF-CBI
4	A	509	JWZ	CBD-CBE-NBF-CBG
4	B	507	JWZ	NBF-CBG-CBH-CBJ
4	B	507	JWZ	NBF-CBG-CBH-CBN
4	A	508	JWZ	CBD-CBC-NAT-CAS
4	A	508	JWZ	CBD-CBC-NAT-CAU
5	B	508	GOL	C1-C2-C3-O3
5	B	508	GOL	O2-C2-C3-O3
4	B	506	JWZ	NBF-CBG-CBH-CBJ
4	B	506	JWZ	NBF-CBG-CBH-CBN
4	B	506	JWZ	CBD-CBC-NAT-CAS
4	B	506	JWZ	CBD-CBC-NAT-CAU
4	B	506	JWZ	CBC-CBD-CBE-NBF
4	A	508	JWZ	CBD-CBE-NBF-CBI
4	B	506	JWZ	NAT-CBC-CBD-CBE
4	A	508	JWZ	CAG-CAH-NAI-CAN
4	A	508	JWZ	CAG-CAH-NAI-CAJ
4	B	506	JWZ	CAG-CAH-NAI-CAJ
4	B	506	JWZ	CAG-CAH-NAI-CAN
5	B	510	GOL	O1-C1-C2-C3
4	B	506	JWZ	CAA-CAG-CAH-NAI
4	A	509	JWZ	NBF-CBG-CBH-CBN
4	A	509	JWZ	NAT-CBC-CBD-CBE
4	A	508	JWZ	NAT-CBC-CBD-CBE
4	A	508	JWZ	CBD-CBE-NBF-CBG
4	A	508	JWZ	CAF-CAA-CAG-CAH
5	A	511	GOL	O2-C2-C3-O3
5	B	508	GOL	O1-C1-C2-O2
2	B	501	FAD	PA-O3P-P-O5'
2	A	501	FAD	PA-O3P-P-O5'
2	A	501	FAD	O4B-C4B-C5B-O5B
4	A	508	JWZ	CBC-CBD-CBE-NBF
4	B	507	JWZ	NAT-CBC-CBD-CBE
4	A	509	JWZ	NBQ-CBP-NBL-CBK
4	B	506	JWZ	NBQ-CBP-NBL-CBK
4	B	507	JWZ	CAA-CAG-CAH-NAI
2	B	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	P-O3P-PA-O2A
5	B	510	GOL	O1-C1-C2-O2
4	A	508	JWZ	CAB-CAA-CAG-CAH
2	A	501	FAD	PA-O3P-P-O1P
5	B	511	GOL	C1-C2-C3-O3

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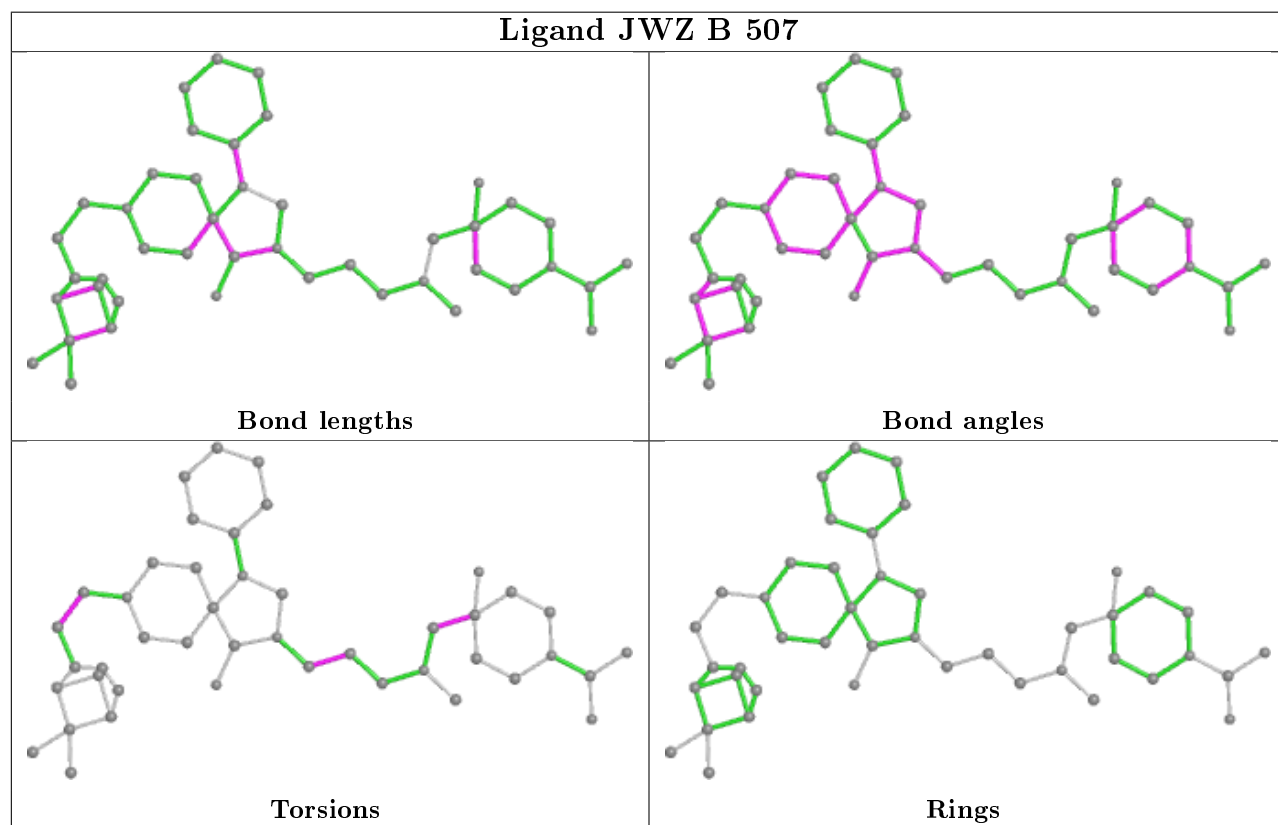
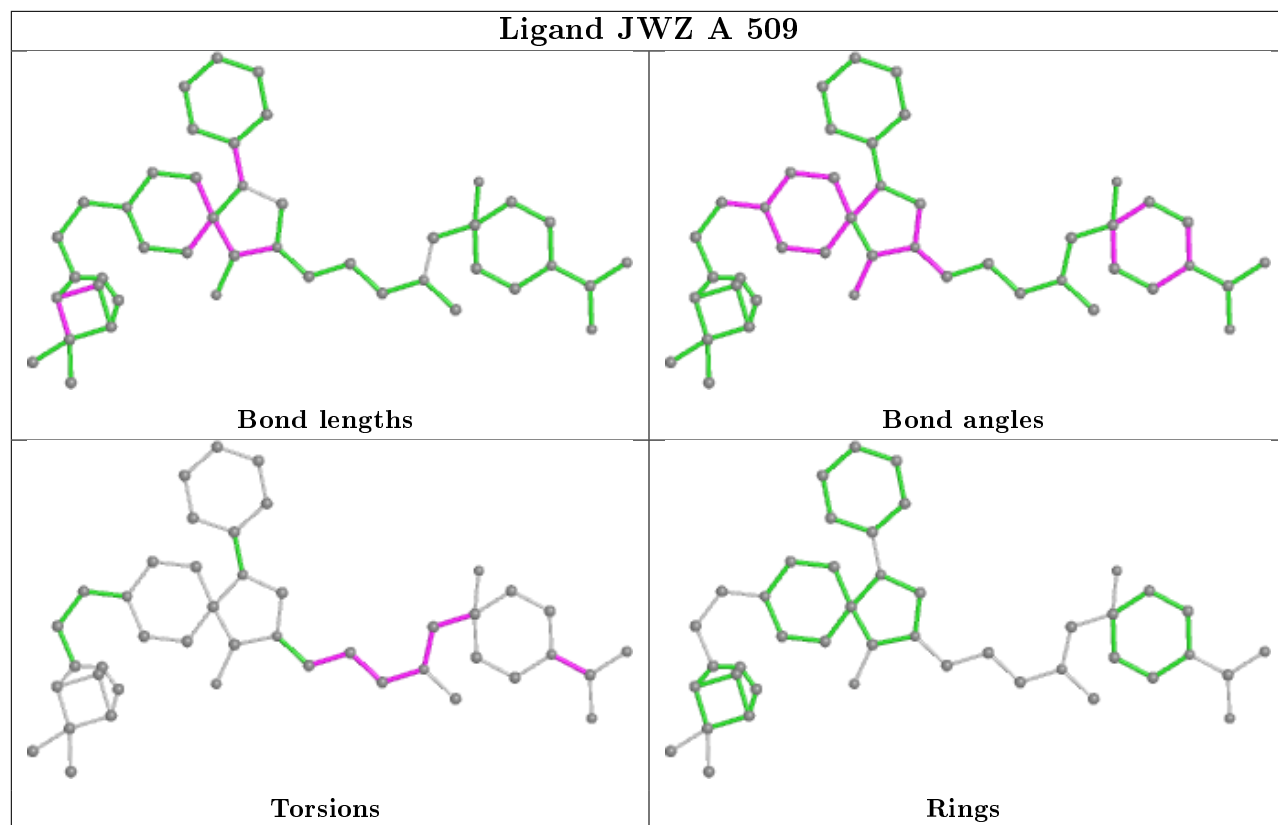
Mol	Chain	Res	Type	Atoms
4	A	509	JWZ	CBC-CBD-CBE-NBF
2	A	501	FAD	C3B-C4B-C5B-O5B
2	B	501	FAD	P-O3P-PA-O1A
5	A	511	GOL	C1-C2-C3-O3
4	B	506	JWZ	NBF-CBG-CBH-OBO

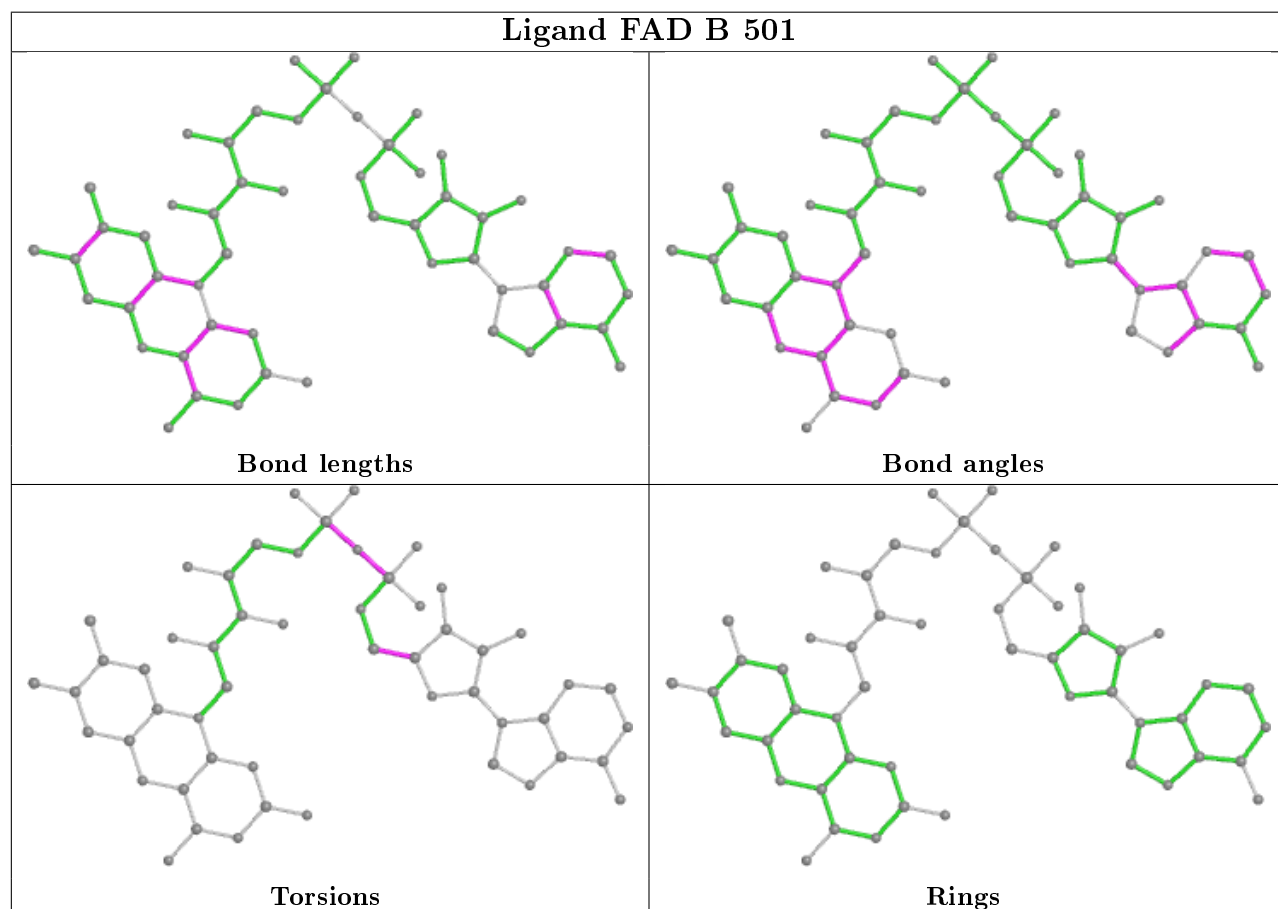
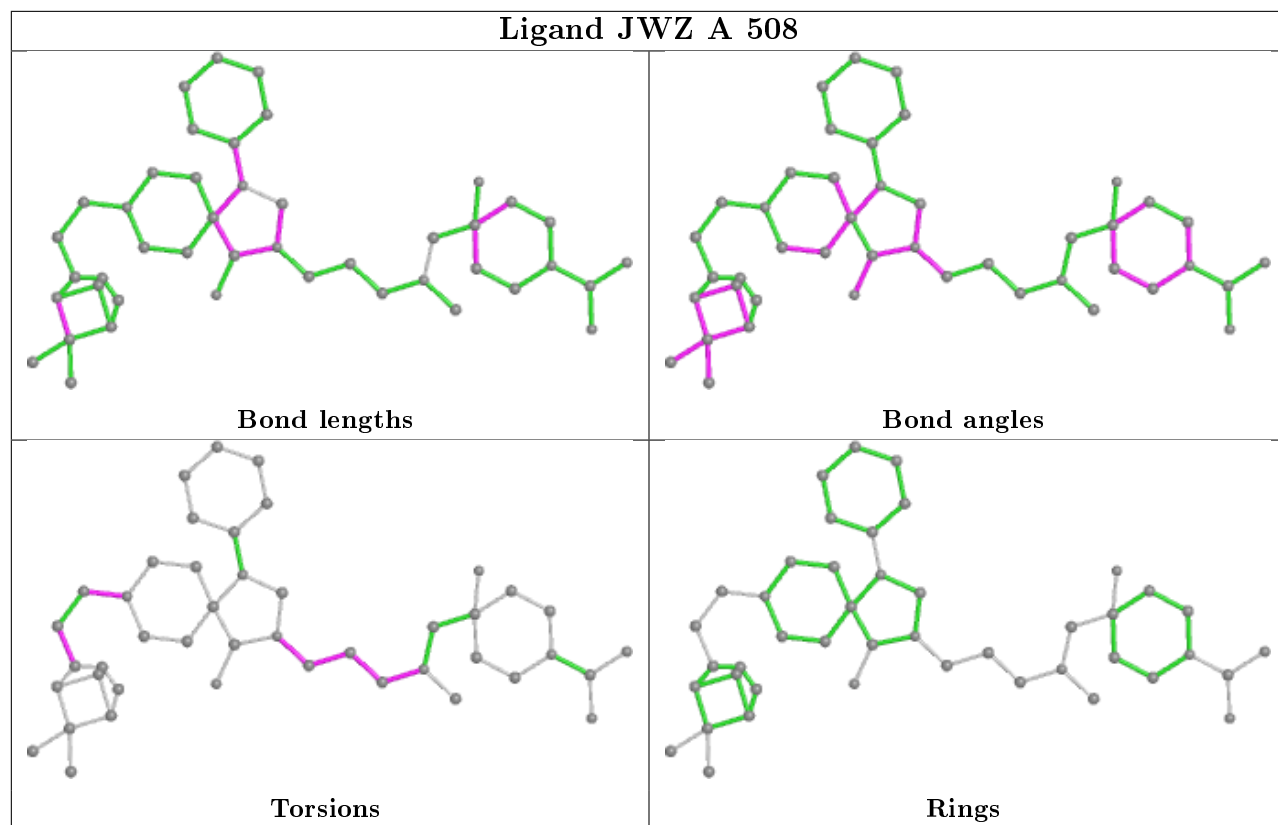
There are no ring outliers.

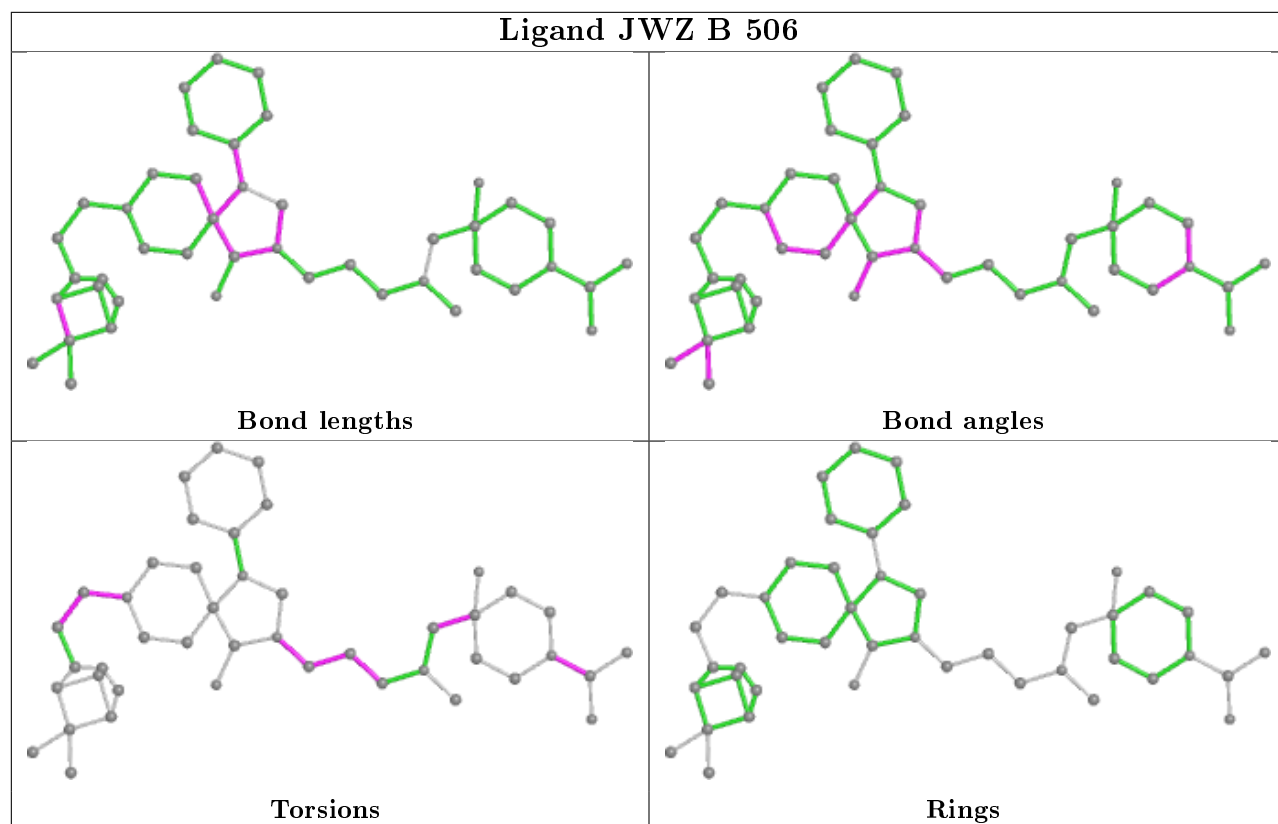
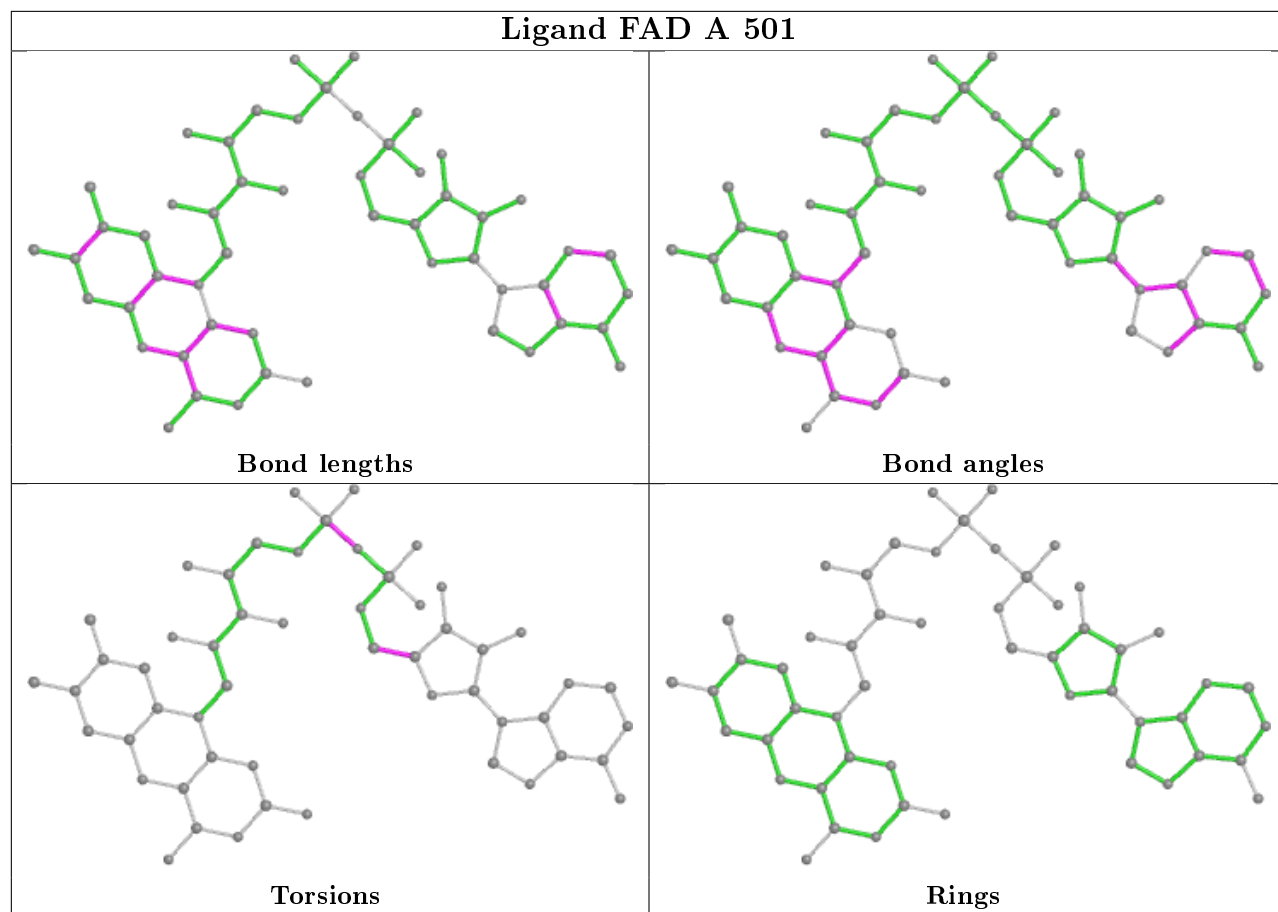
5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	509	JWZ	3	0
4	B	507	JWZ	3	0
5	A	511	GOL	2	0
4	A	508	JWZ	3	0
4	B	506	JWZ	2	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	490/512 (95%)	0.23	8 (1%) 72 73	25, 34, 56, 90	0
1	B	489/512 (95%)	0.21	4 (0%) 86 87	25, 32, 51, 85	1 (0%)
All	All	979/1024 (95%)	0.22	12 (1%) 79 80	25, 33, 53, 90	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	HIS	4.7
1	B	399	LEU	4.1
1	B	352	ASN	3.2
1	B	0	HIS	2.5
1	A	292	ASN	2.4
1	A	488	PRO	2.3
1	A	489	ASP	2.3
1	A	484	MET	2.2
1	A	480	LYS	2.2
1	B	1	MET	2.1
1	A	353	LYS	2.1
1	A	1	MET	2.1

### 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](#)

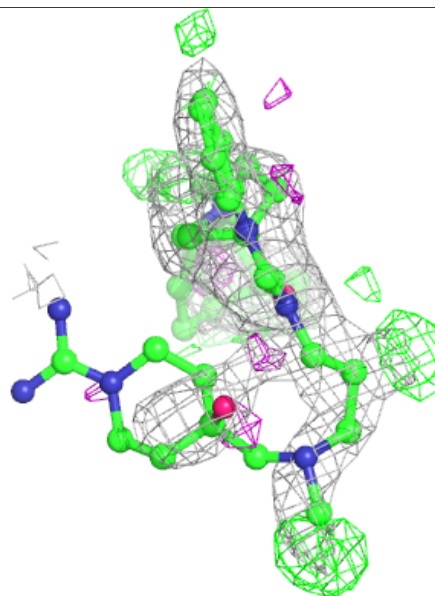
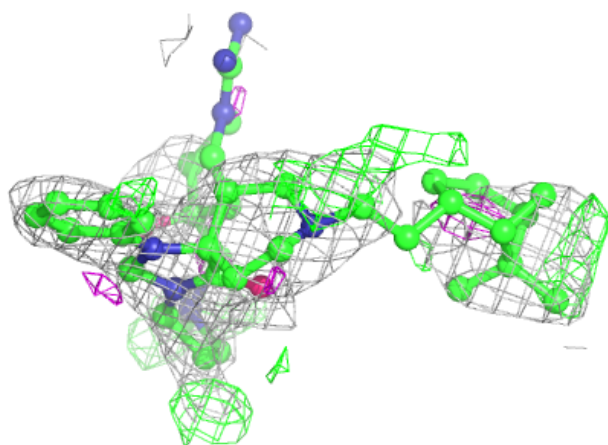
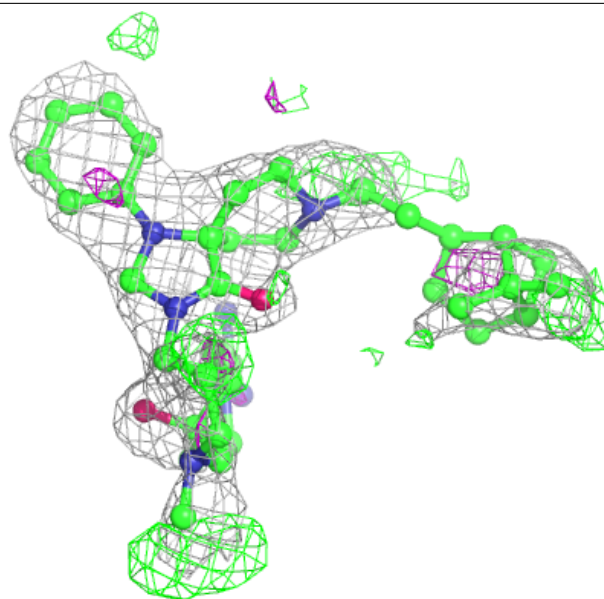
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

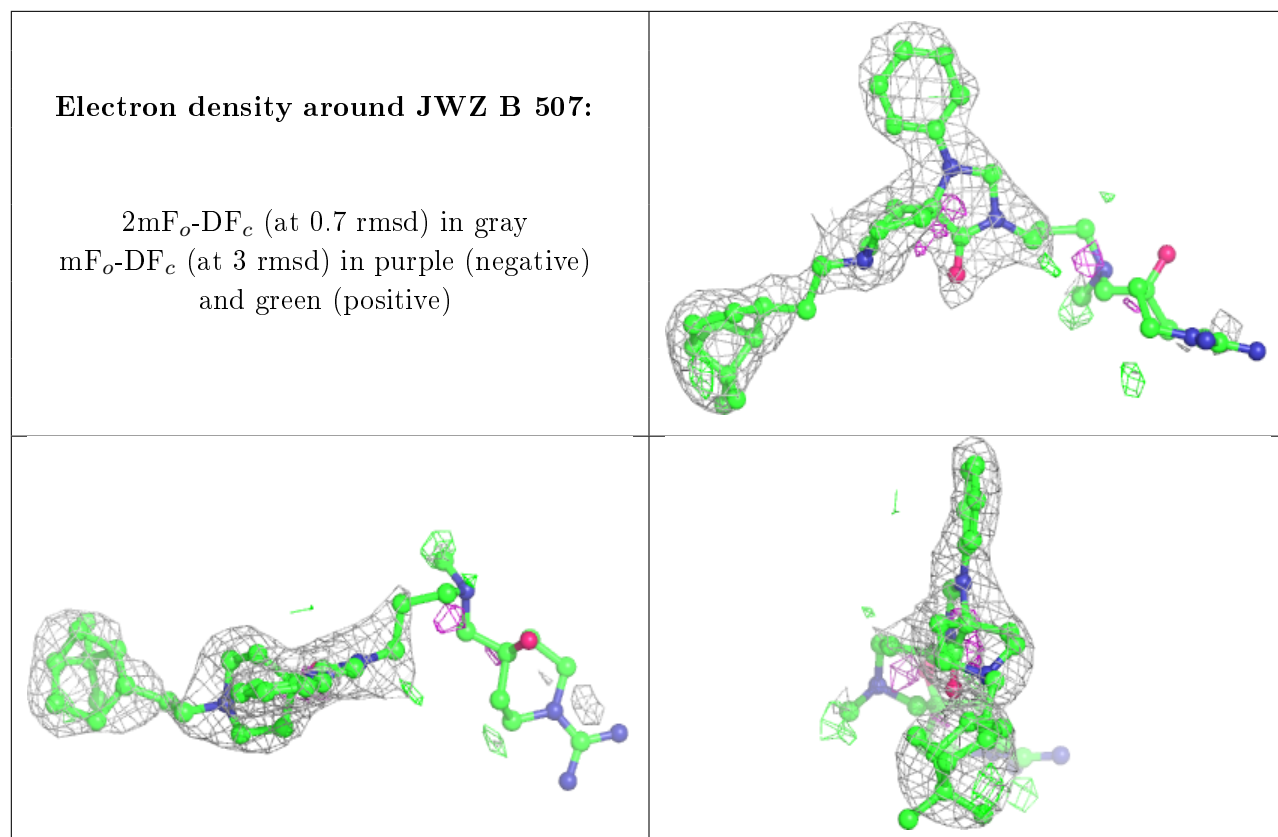
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	B	509	6/6	0.66	0.20	64,66,67,68	0
5	GOL	A	511	6/6	0.69	0.20	59,59,60,62	0
5	GOL	B	510	6/6	0.69	0.18	62,64,65,66	0
4	JWZ	B	506	44/44	0.71	0.29	70,80,106,108	0
4	JWZ	B	507	44/44	0.73	0.30	81,85,127,128	0
3	SO4	A	504	5/5	0.74	0.28	89,91,94,95	0
5	GOL	B	511	6/6	0.77	0.17	62,65,65,68	0
4	JWZ	A	508	44/44	0.80	0.23	58,71,83,84	0
3	SO4	A	502	5/5	0.82	0.17	83,84,86,86	0
4	JWZ	A	509	44/44	0.82	0.34	69,76,115,117	0
3	SO4	A	505	5/5	0.84	0.25	101,102,103,103	0
3	SO4	B	504	5/5	0.84	0.21	73,74,77,78	0
3	SO4	B	503	5/5	0.85	0.21	69,69,73,75	0
5	GOL	A	510	6/6	0.88	0.23	62,63,63,65	0
3	SO4	A	503	5/5	0.88	0.21	83,85,86,87	0
3	SO4	B	505	5/5	0.90	0.22	92,93,94,96	0
5	GOL	B	508	6/6	0.91	0.20	39,42,48,53	0
3	SO4	A	506	5/5	0.92	0.17	81,84,86,88	0
3	SO4	A	507	5/5	0.93	0.15	68,72,73,76	0
3	SO4	B	502	5/5	0.96	0.15	61,62,65,65	0
2	FAD	A	501	53/53	0.98	0.12	25,26,28,29	0
2	FAD	B	501	53/53	0.98	0.11	24,26,28,28	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 JWZ B 506:**

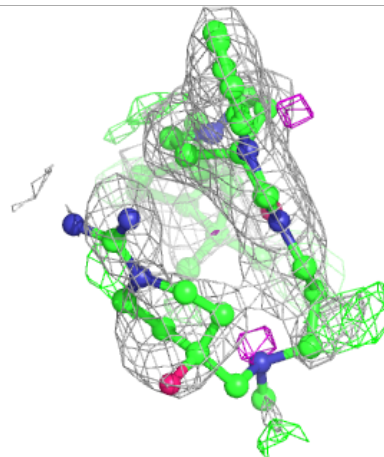
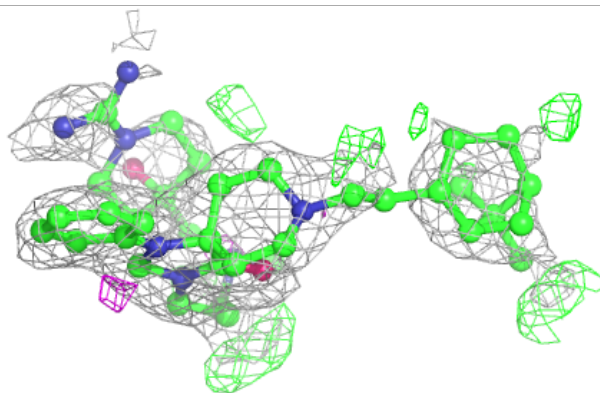
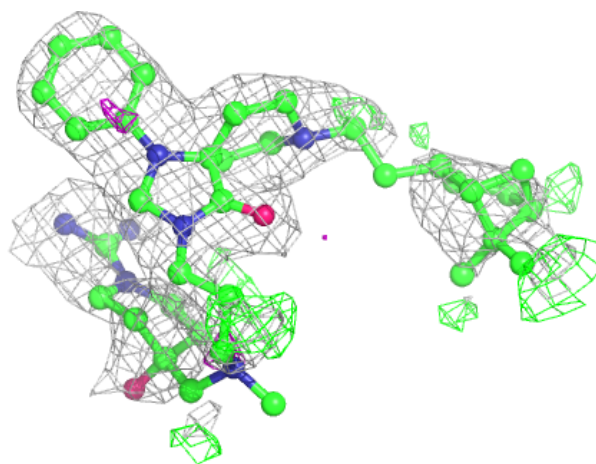
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

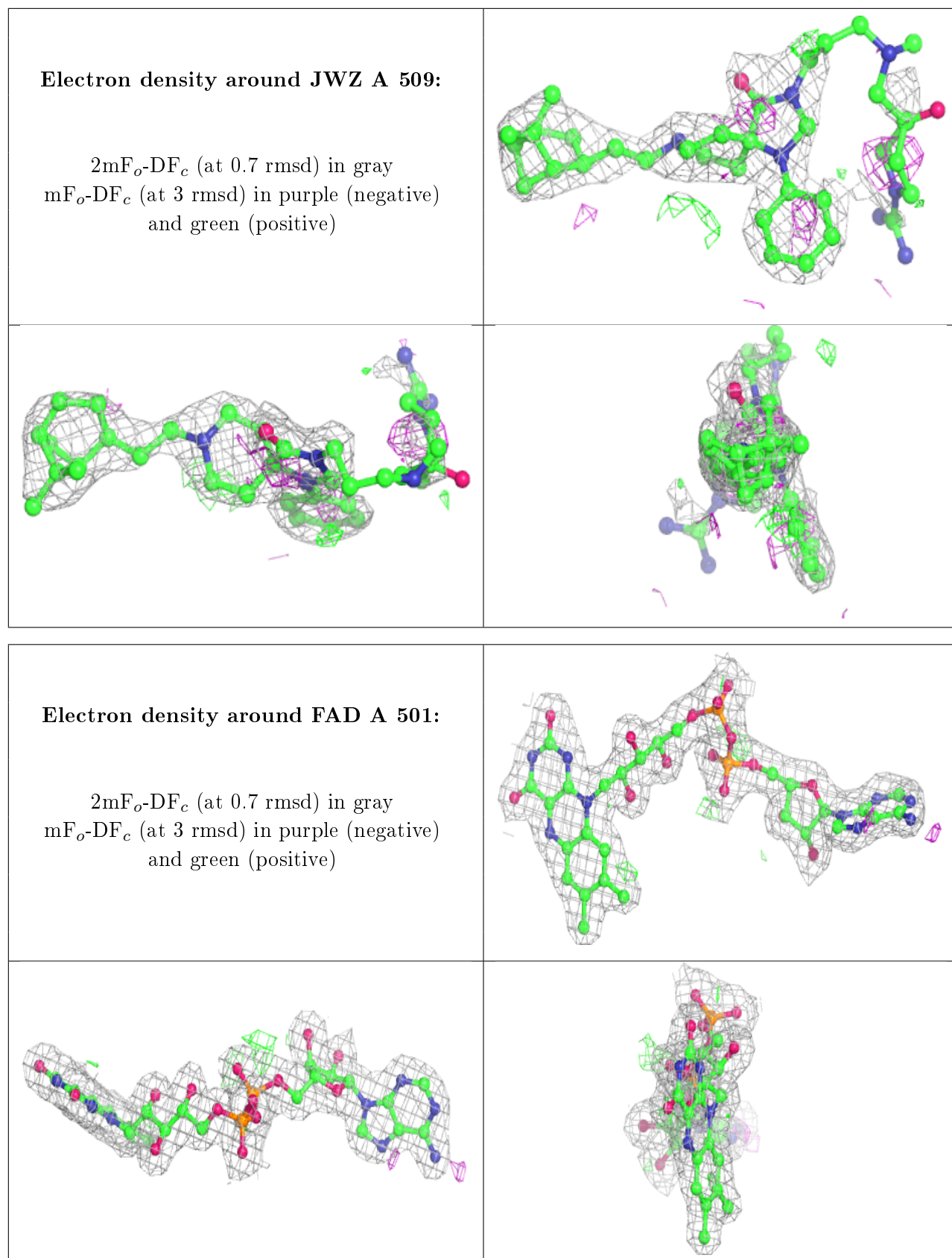


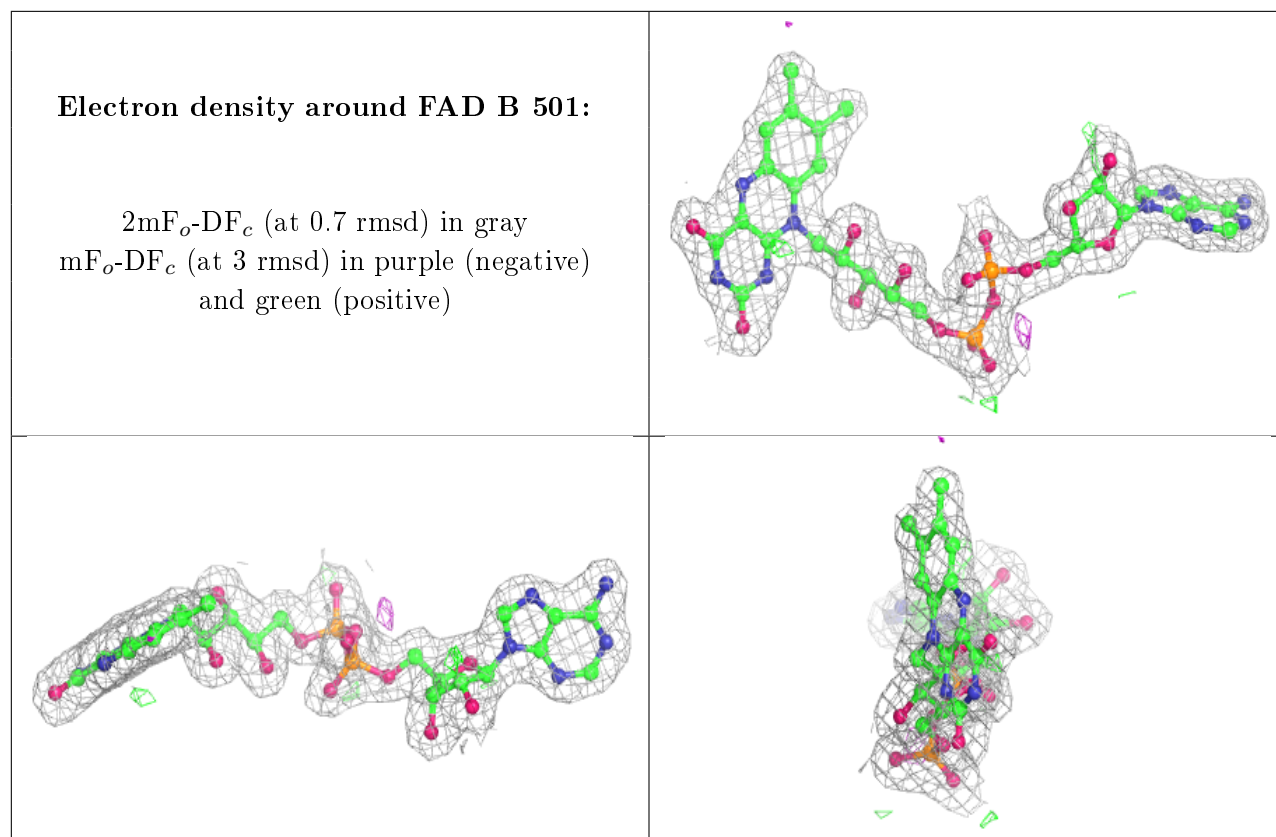


**Electron density around JWZ A 508:**

$2mF_o-DF_c$  (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.