



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 02:32 PM BST

PDB ID : 5KX8  
Title : Irak4-inhibitor co-structure  
Authors : Fischmann, T.O.  
Deposited on : 2016-07-20  
Resolution : 2.67 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 : 2.13.1  
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) : 2.13.1

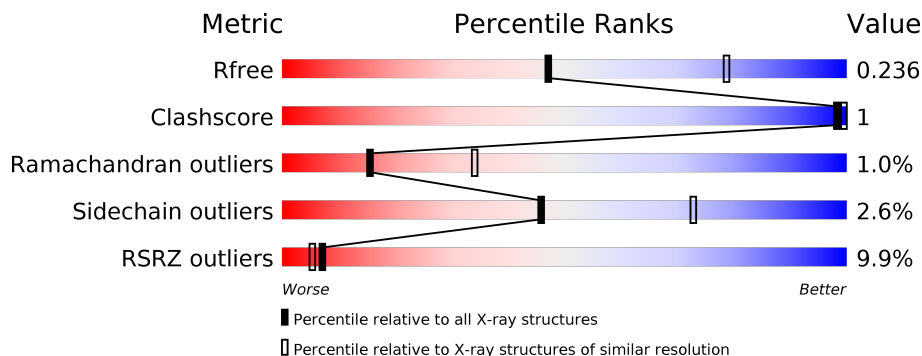
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	301	
1	B	301	
1	C	301	
1	D	301	

## 2 Entry composition [i](#)

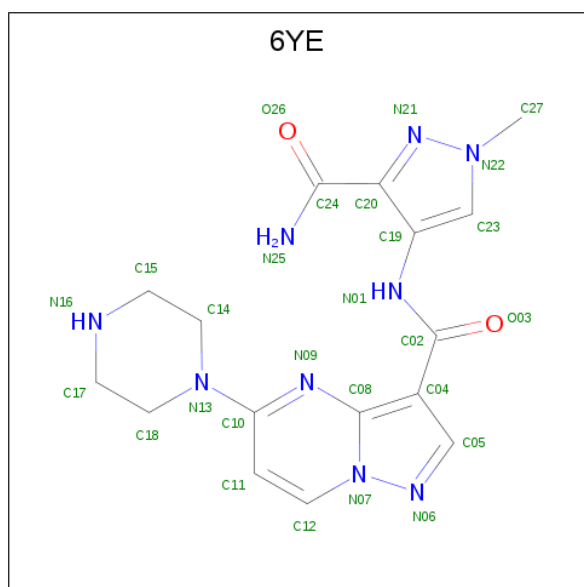
There are 3 unique types of molecules in this entry. The entry contains 9115 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	288	Total	C	N	O	P	S	0	0	3
			2262	1415	382	448	3	14			
1	B	281	Total	C	N	O	P	S	0	0	2
			2204	1381	371	435	3	14			
1	C	290	Total	C	N	O	P	S	0	0	3
			2260	1415	379	449	3	14			
1	D	286	Total	C	N	O	P	S	0	0	1
			2254	1412	380	445	3	14			

- Molecule 2 is {N}-(3-aminocarbonyl-1-methyl-pyrazol-4-yl)-5-piperazin-1-yl-pyrazolo[1,5-a]pyrimidine-3-carboxamide (three-letter code: 6YE) (formula: C<sub>16</sub>H<sub>19</sub>N<sub>9</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			27	16	9	2		
2	B	1	Total	C	N	O	0	0
			27	16	9	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			27	16	9	2		
2	D	1	Total	C	N	O	0	0
			27	16	9	2		

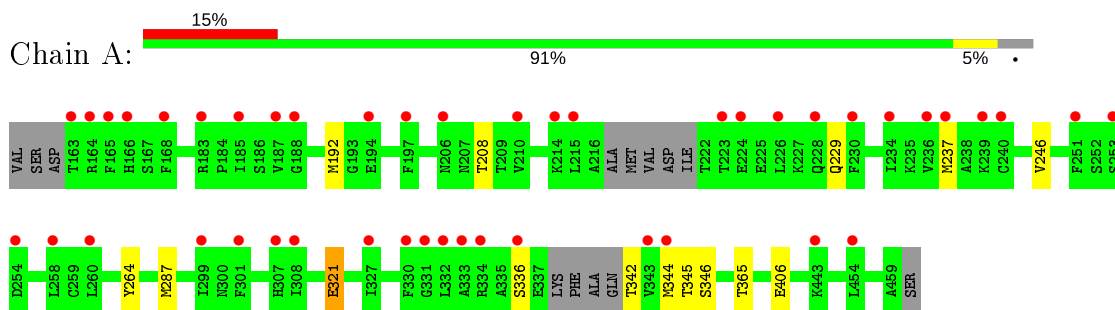
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	B	5	Total	O	0	0
			5	5		
3	C	9	Total	O	0	0
			9	9		
3	D	8	Total	O	0	0
			8	8		

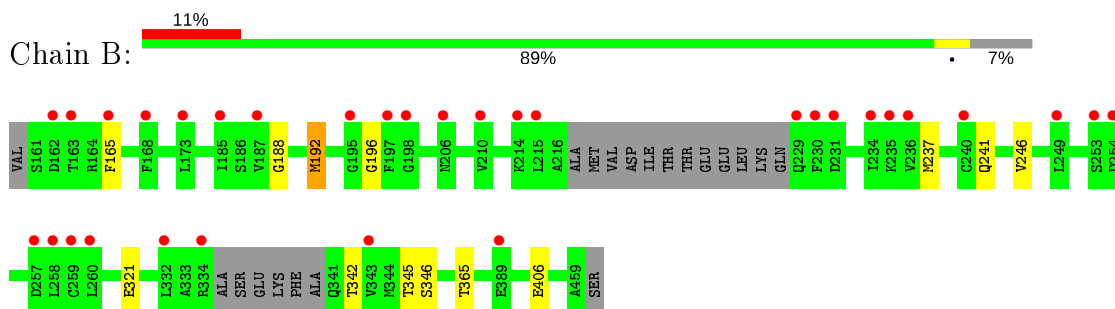
### 3 Residue-property plots [i](#)

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.

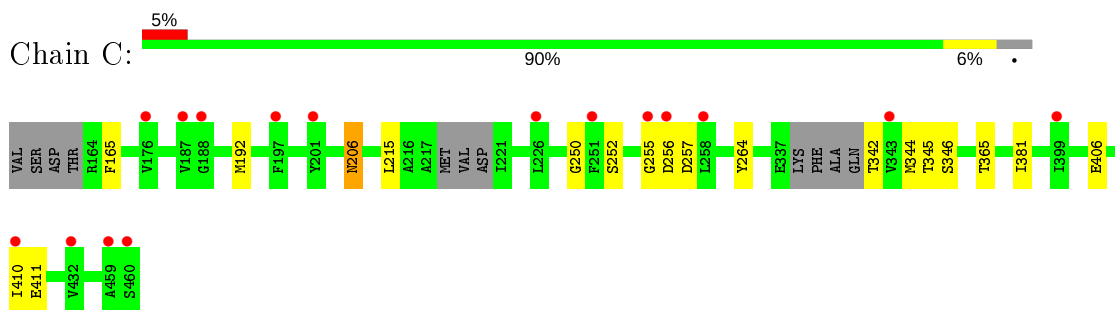
- Molecule 1: Interleukin-1 receptor-associated kinase 4



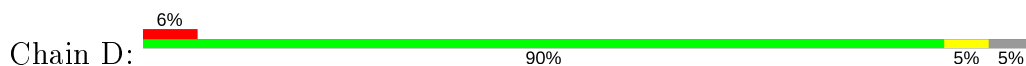
- Molecule 1: Interleukin-1 receptor-associated kinase 4

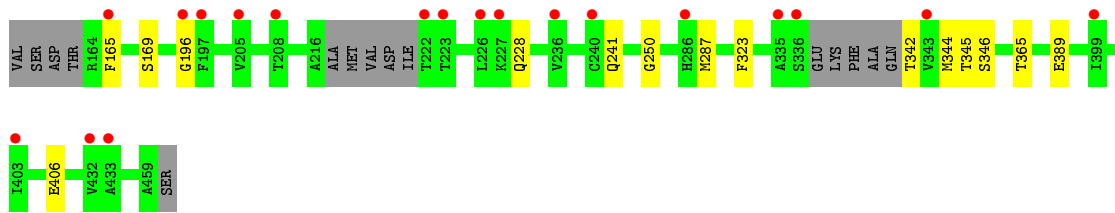


- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4





## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.70Å 139.88Å 87.44Å 90.00° 125.25° 90.00°	Depositor
Resolution (Å)	45.00 – 2.67 45.00 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.00-2.67) 87.8 (45.00-2.67)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 2.69Å)	Xtrriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.204 , 0.233 0.210 , 0.236	Depositor DCC
$R_{free}$ test set	2015 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.4	Xtrriage
Anisotropy	0.501	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 57.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.186 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9115	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2729e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: TPO, SEP, 6YE

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	0.51	0/2266	0.61	0/3053
1	B	0.51	0/2207	0.63	0/2972
1	C	0.51	0/2264	0.63	0/3051
1	D	0.53	0/2258	0.62	0/3042
All	All	0.51	0/8995	0.62	0/12118

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	2262	0	2221	2	0
1	B	2204	0	2154	2	0
1	C	2260	0	2212	3	0
1	D	2254	0	2216	3	0
2	A	27	0	0	0	0
2	B	27	0	0	1	0
2	C	27	0	0	0	0
2	D	27	0	0	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	9	0	0	0	0
3	D	8	0	0	0	0
All	All	9115	0	8803	10	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (10) 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:D:287:MET:HE2	1:D:323:PHE:HB2	1.86	0.56
1:B:192:MET:HG2	2:B:501:6YE:C20	2.36	0.56
1:A:237:MET:HE1	1:A:246:VAL:HG23	1.92	0.50
1:D:287:MET:CE	1:D:323:PHE:HB2	2.40	0.50
1:B:237:MET:CE	1:B:246:VAL:HG23	2.46	0.45
1:C:165:PHE:HB3	1:C:250:GLY:HA2	2.00	0.43
1:C:381:ILE:HG21	1:C:410:ILE:HD11	2.01	0.43
1:A:192:MET:HE2	1:A:264:TYR:HE1	1.83	0.41
1:C:192:MET:HE2	1:C:264:TYR:HE1	1.85	0.41
1:D:165:PHE:HB3	1:D:250:GLY:HA2	2.04	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	280/301 (93%)	266 (95%)	12 (4%)	2 (1%)	22	44
1	B	272/301 (90%)	253 (93%)	15 (6%)	4 (2%)	10	23
1	C	282/301 (94%)	265 (94%)	14 (5%)	3 (1%)	14	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	278/301 (92%)	265 (95%)	11 (4%)	2 (1%)	22	44
All	All	1112/1204 (92%)	1049 (94%)	52 (5%)	11 (1%)	15	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLU
1	B	406	GLU
1	C	406	GLU
1	D	406	GLU
1	B	321	GLU
1	C	206	ASN
1	C	255	GLY
1	D	196	GLY
1	A	321	GLU
1	B	196	GLY
1	B	188	GLY

### 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	247/259 (95%)	240 (97%)	7 (3%)	43	70
1	B	240/259 (93%)	236 (98%)	4 (2%)	60	82
1	C	245/259 (95%)	237 (97%)	8 (3%)	38	64
1	D	246/259 (95%)	240 (98%)	6 (2%)	49	75
All	All	978/1036 (94%)	953 (97%)	25 (3%)	46	73

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	THR
1	A	229	GLN
1	A	287	MET

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Mol	Chain	Res	Type
1	A	321	GLU
1	A	336	SER
1	A	344	MET
1	A	365	THR
1	B	165	PHE
1	B	192	MET
1	B	241	GLN
1	B	365	THR
1	C	206	ASN
1	C	215	LEU
1	C	252	SER
1	C	256	ASP
1	C	257	ASP
1	C	344	MET
1	C	365	THR
1	C	411	GLU
1	D	169	SER
1	D	228	GLN
1	D	241	GLN
1	D	344	MET
1	D	365	THR
1	D	389	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	229	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

12 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	SEP	A	346	1	8,9,10	0.90	0	8,12,14	1.40	2 (25%)
1	TPO	B	342	1	8,10,11	0.90	0	10,14,16	1.39	1 (10%)
1	SEP	B	346	1	8,9,10	0.72	0	8,12,14	1.20	1 (12%)
1	TPO	D	342	1	8,10,11	1.04	1 (12%)	10,14,16	1.38	1 (10%)
1	TPO	B	345	1	8,10,11	1.02	0	10,14,16	1.19	1 (10%)
1	TPO	D	345	1	8,10,11	1.22	1 (12%)	10,14,16	1.24	1 (10%)
1	SEP	C	346	1	8,9,10	1.05	0	8,12,14	1.06	1 (12%)
1	TPO	A	342	1	8,10,11	0.95	0	10,14,16	1.34	1 (10%)
1	TPO	A	345	1	8,10,11	0.93	0	10,14,16	1.13	1 (10%)
1	TPO	C	342	1	8,10,11	0.90	0	10,14,16	1.37	1 (10%)
1	TPO	C	345	1	8,10,11	1.17	1 (12%)	10,14,16	1.19	1 (10%)
1	SEP	D	346	1	8,9,10	1.08	1 (12%)	8,12,14	1.10	1 (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
1	SEP	A	346	1	-	0/5/8/10	-
1	TPO	B	342	1	-	1/9/11/13	-
1	SEP	B	346	1	-	0/5/8/10	-
1	TPO	D	342	1	-	1/9/11/13	-
1	TPO	B	345	1	-	3/9/11/13	-
1	TPO	D	345	1	-	3/9/11/13	-
1	SEP	C	346	1	-	0/5/8/10	-
1	TPO	A	342	1	-	0/9/11/13	-
1	TPO	A	345	1	-	3/9/11/13	-
1	TPO	C	342	1	-	0/9/11/13	-
1	TPO	C	345	1	-	4/9/11/13	-
1	SEP	D	346	1	-	0/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	345	TPO	P-OG1	-2.37	1.54	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	342	TPO	P-OG1	-2.22	1.55	1.59
1	C	345	TPO	P-OG1	-2.19	1.55	1.59
1	D	346	SEP	P-O1P	2.15	1.57	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	TPO	P-OG1-CB	-3.07	113.93	123.21
1	C	342	TPO	P-OG1-CB	-2.99	114.17	123.21
1	A	342	TPO	P-OG1-CB	-2.99	114.18	123.21
1	D	342	TPO	P-OG1-CB	-2.97	114.23	123.21
1	A	346	SEP	P-OG-CB	-2.88	110.37	118.30
1	B	346	SEP	P-OG-CB	-2.74	110.74	118.30
1	D	346	SEP	P-OG-CB	-2.57	111.22	118.30
1	C	346	SEP	P-OG-CB	-2.35	111.83	118.30
1	C	345	TPO	P-OG1-CB	-2.24	116.44	123.21
1	A	346	SEP	OG-CB-CA	2.22	110.30	108.14
1	D	345	TPO	P-OG1-CB	-2.15	116.71	123.21
1	A	345	TPO	P-OG1-CB	-2.10	116.87	123.21
1	B	345	TPO	P-OG1-CB	-2.05	117.02	123.21

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	345	TPO	N-CA-CB-OG1
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	A	345	TPO	CB-OG1-P-O1P
1	C	345	TPO	N-CA-CB-OG1
1	B	345	TPO	CB-OG1-P-O1P
1	B	342	TPO	CB-OG1-P-O3P
1	D	342	TPO	CB-OG1-P-O3P
1	D	345	TPO	CB-OG1-P-O1P
1	C	345	TPO	CB-OG1-P-O1P
1	C	345	TPO	CB-OG1-P-O2P
1	B	345	TPO	O-C-CA-CB
1	C	345	TPO	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](#)

4 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$
2	6YE	C	501	-	21,30,30	1.53	2 (9%)	24,43,43	1.03	1 (4%)
2	6YE	D	501	-	21,30,30	1.27	3 (14%)	24,43,43	1.35	3 (12%)
2	6YE	A	501	-	21,30,30	1.81	2 (9%)	24,43,43	1.01	0
2	6YE	B	501	-	21,30,30	1.39	2 (9%)	24,43,43	1.54	5 (20%)

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
2	6YE	C	501	-	-	0/8/24/24	0/4/4/4
2	6YE	D	501	-	-	0/8/24/24	0/4/4/4
2	6YE	A	501	-	-	2/8/24/24	0/4/4/4
2	6YE	B	501	-	-	0/8/24/24	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	6YE	C23-C19	5.97	1.44	1.38
2	C	501	6YE	C10-N09	5.49	1.40	1.32
2	A	501	6YE	C10-N09	4.42	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	6YE	C23-C19	3.93	1.42	1.38
2	D	501	6YE	C10-N09	3.51	1.37	1.32
2	B	501	6YE	C10-N09	3.40	1.37	1.32
2	C	501	6YE	C23-C19	2.87	1.41	1.38
2	D	501	6YE	C23-C19	2.44	1.40	1.38
2	D	501	6YE	C04-C02	-2.18	1.46	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	6YE	N09-C10-N13	-3.81	114.06	117.43
2	B	501	6YE	C17-C18-N13	3.53	118.12	110.48
2	D	501	6YE	C04-C02-N01	3.18	119.54	114.79
2	D	501	6YE	O03-C02-C04	-3.09	117.45	121.72
2	D	501	6YE	N09-C10-N13	-2.44	115.27	117.43
2	B	501	6YE	C04-C02-N01	2.38	118.35	114.79
2	B	501	6YE	C18-N13-C10	-2.13	115.45	120.39
2	B	501	6YE	O03-C02-C04	-2.02	118.93	121.72
2	C	501	6YE	C24-C20-N21	2.01	125.60	120.57

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	6YE	C11-C10-N13-C18
2	A	501	6YE	N09-C10-N13-C18

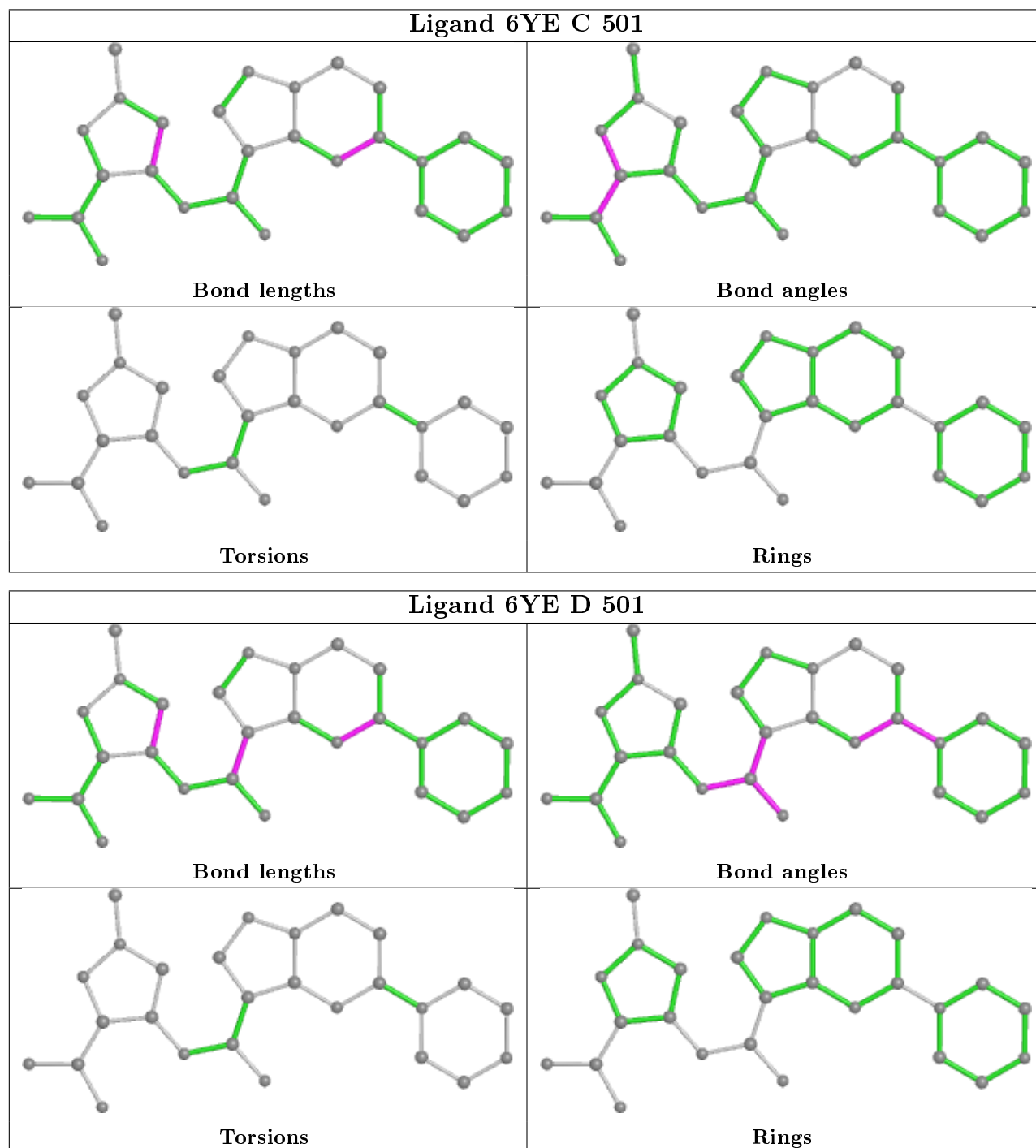
There are no ring outliers.

1 monomer is involved in 1 short contact:

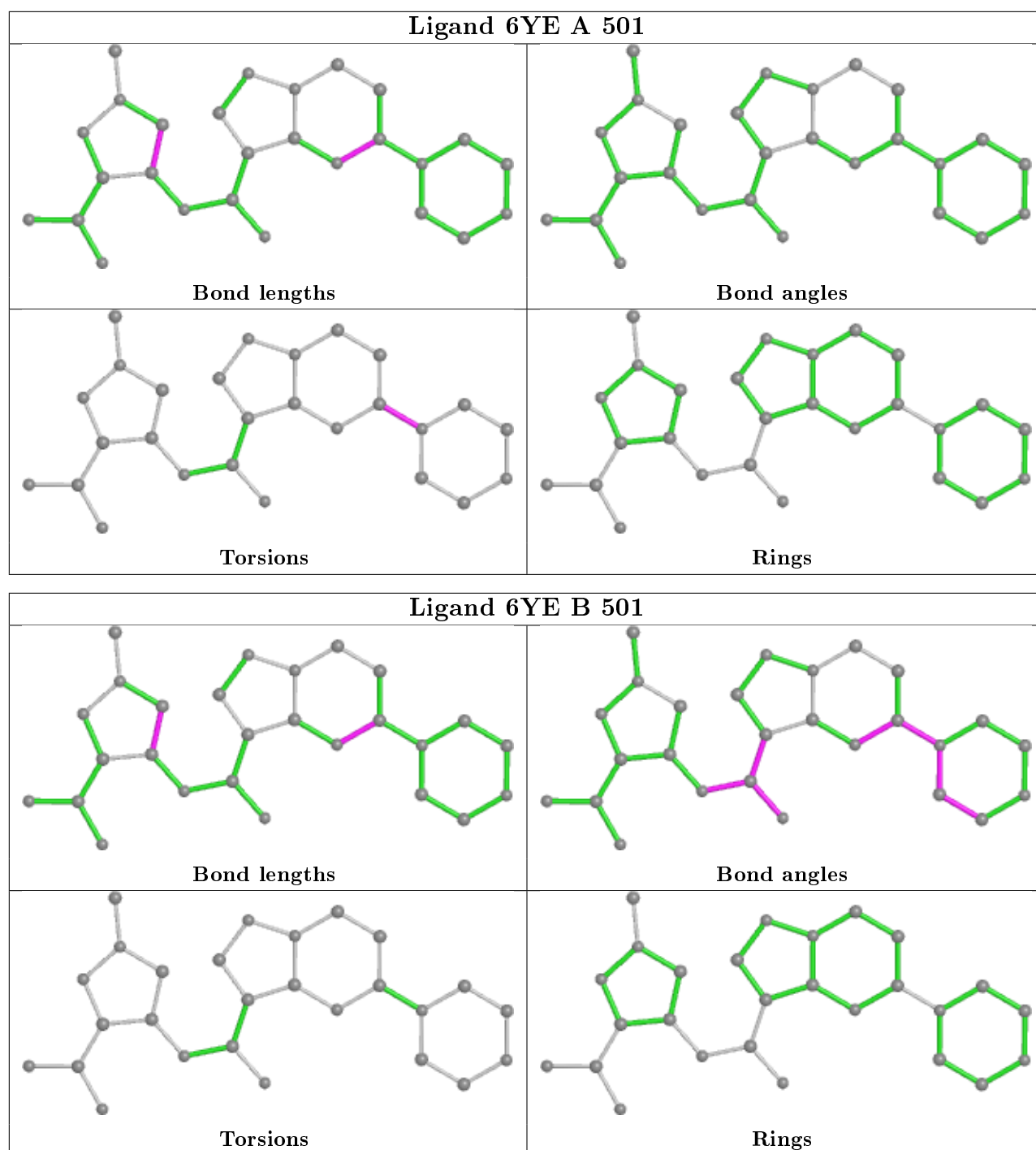
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	6YE	1	0

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.







## 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	285/301 (94%)	1.07	45 (15%) <b>2</b> <b>1</b>	45, 86, 132, 144	0
1	B	278/301 (92%)	1.03	32 (11%) <b>4</b> <b>3</b>	45, 80, 137, 165	0
1	C	287/301 (95%)	0.60	16 (5%) <b>24</b> <b>22</b>	42, 73, 112, 123	0
1	D	283/301 (94%)	0.58	19 (6%) <b>17</b> <b>15</b>	43, 68, 107, 141	0
All	All	1133/1204 (94%)	0.82	112 (9%) <b>7</b> <b>5</b>	42, 75, 128, 165	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	PHE	13.6
1	A	240	CYS	11.6
1	B	240	CYS	10.8
1	B	230	PHE	8.8
1	A	226	LEU	7.3
1	B	236	VAL	6.2
1	C	460	SER	5.6
1	B	163	THR	5.4
1	B	215	LEU	5.4
1	B	334	ARG	5.4
1	A	185	ILE	5.3
1	A	253	SER	4.9
1	C	255	GLY	4.9
1	A	223	THR	4.7
1	C	197	PHE	4.5
1	A	332	LEU	4.5
1	A	343	VAL	4.5
1	B	332	LEU	4.4
1	D	197	PHE	4.4
1	A	164	ARG	4.3
1	B	168	PHE	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	236	VAL	4.0
1	A	188	GLY	4.0
1	B	165	PHE	3.9
1	A	230	PHE	3.8
1	B	198	GLY	3.8
1	B	343	VAL	3.7
1	C	187	VAL	3.7
1	C	343	VAL	3.7
1	A	215	LEU	3.5
1	A	254	ASP	3.5
1	A	166	HIS	3.5
1	D	165	PHE	3.5
1	B	253	SER	3.4
1	A	260	LEU	3.4
1	B	234	ILE	3.4
1	C	256	ASP	3.4
1	D	226	LEU	3.4
1	A	334	ARG	3.3
1	B	214	LYS	3.3
1	A	336	SER	3.2
1	A	299	ILE	3.2
1	B	260	LEU	3.2
1	A	251	PHE	3.2
1	A	258	LEU	3.2
1	A	197	PHE	3.2
1	B	249	LEU	3.2
1	B	195	GLY	3.1
1	B	173	LEU	3.1
1	A	234	ILE	3.0
1	B	258	LEU	3.0
1	B	257	ASP	2.9
1	A	165	PHE	2.9
1	A	239	LYS	2.9
1	D	240	CYS	2.9
1	C	251	PHE	2.8
1	D	223	THR	2.8
1	A	187	VAL	2.8
1	B	187	VAL	2.8
1	C	410	ILE	2.8
1	A	168	PHE	2.7
1	A	163	THR	2.7
1	C	188	GLY	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	206	ASN	2.7
1	C	459	ALA	2.6
1	A	210	VAL	2.6
1	A	333	ALA	2.6
1	A	301	PHE	2.6
1	D	399	ILE	2.6
1	A	237	MET	2.6
1	B	206	ASN	2.5
1	A	308	ILE	2.5
1	C	226	LEU	2.5
1	B	185	ILE	2.5
1	C	176	VAL	2.4
1	A	454	LEU	2.4
1	D	343	VAL	2.4
1	A	214	LYS	2.4
1	B	162	ASP	2.4
1	D	196	GLY	2.4
1	B	259	CYS	2.4
1	D	286	HIS	2.3
1	B	235	LYS	2.3
1	A	331	GLY	2.3
1	C	399	ILE	2.3
1	A	443	LYS	2.3
1	A	327	ILE	2.2
1	D	336	SER	2.2
1	B	254	ASP	2.2
1	A	224	GLU	2.2
1	D	433	ALA	2.1
1	B	229	GLN	2.1
1	A	194	GLU	2.1
1	B	389	GLU	2.1
1	A	330	PHE	2.1
1	B	210	VAL	2.1
1	D	403	ILE	2.1
1	C	258	LEU	2.1
1	D	227	LYS	2.1
1	D	335	ALA	2.1
1	A	228	GLN	2.1
1	A	183	ARG	2.0
1	D	208	THR	2.0
1	C	432	VAL	2.0
1	D	236	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	201	TYR	2.0
1	D	222	THR	2.0
1	A	344	MET	2.0
1	A	307	HIS	2.0
1	D	432	VAL	2.0
1	B	231	ASP	2.0
1	D	205	VAL	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	SEP	D	346	10/11	0.72	0.17	108,113,119,120	0
1	SEP	B	346	10/11	0.73	0.18	124,127,133,133	0
1	SEP	A	346	10/11	0.74	0.16	120,124,129,129	0
1	TPO	A	342	11/12	0.75	0.25	124,125,130,131	0
1	TPO	D	342	11/12	0.76	0.18	113,118,127,128	0
1	SEP	C	346	10/11	0.77	0.14	101,109,120,120	0
1	TPO	C	342	11/12	0.83	0.17	109,112,120,121	0
1	TPO	B	342	11/12	0.89	0.19	123,125,129,129	0
1	TPO	B	345	11/12	0.89	0.17	120,124,126,127	0
1	TPO	A	345	11/12	0.90	0.16	118,121,123,123	0
1	TPO	C	345	11/12	0.91	0.19	96,98,102,103	0
1	TPO	D	345	11/12	0.93	0.13	104,106,108,109	0

## 6.3 Carbohydrates [i](#)

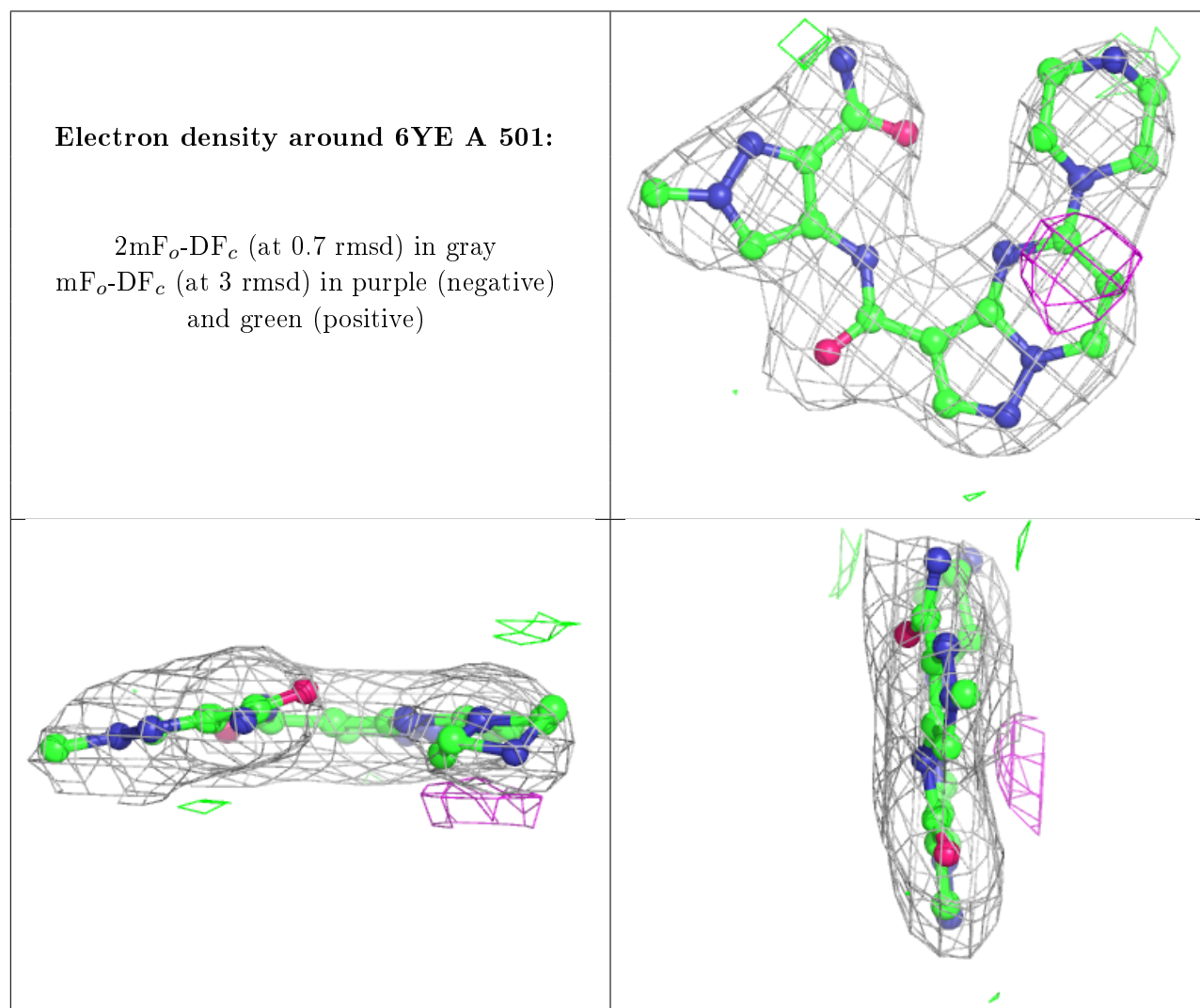
There are no monosaccharides in this entry.

## 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.

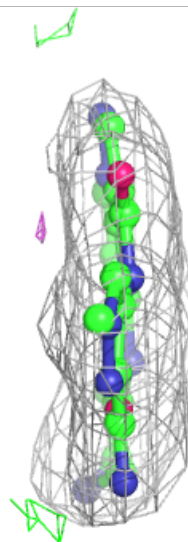
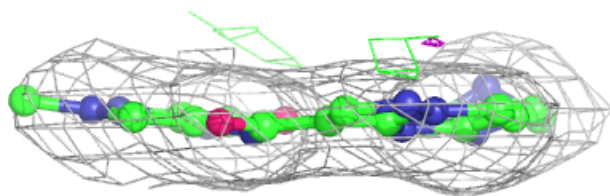
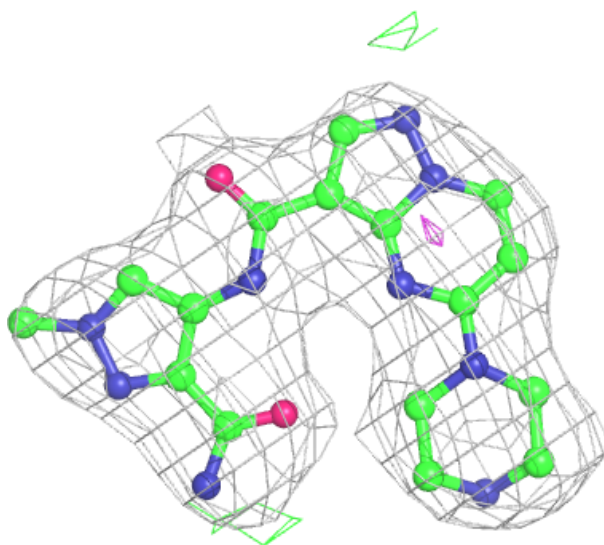
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	6YE	A	501	27/27	0.95	0.19	56,66,80,82	0
2	6YE	B	501	27/27	0.95	0.20	57,62,75,77	0
2	6YE	C	501	27/27	0.97	0.20	44,53,57,59	0
2	6YE	D	501	27/27	0.97	0.19	34,47,55,57	0

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.



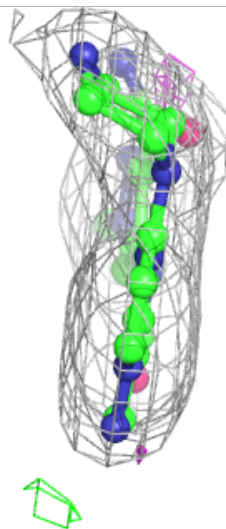
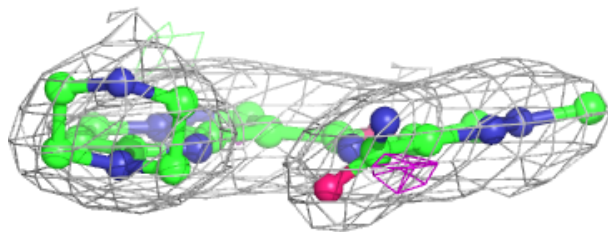
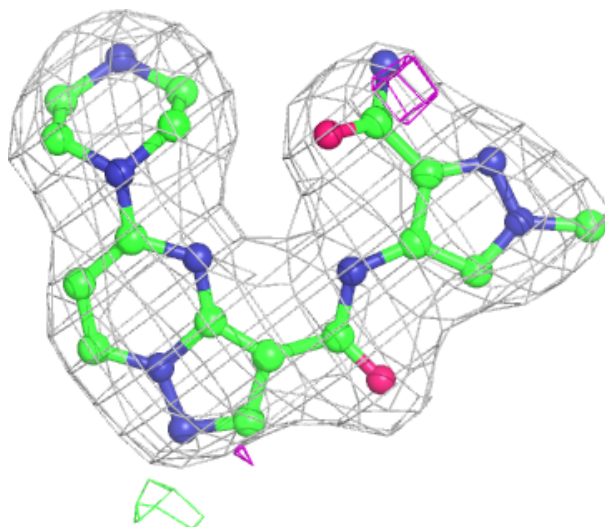
**Electron density around 6YE B 501:**

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

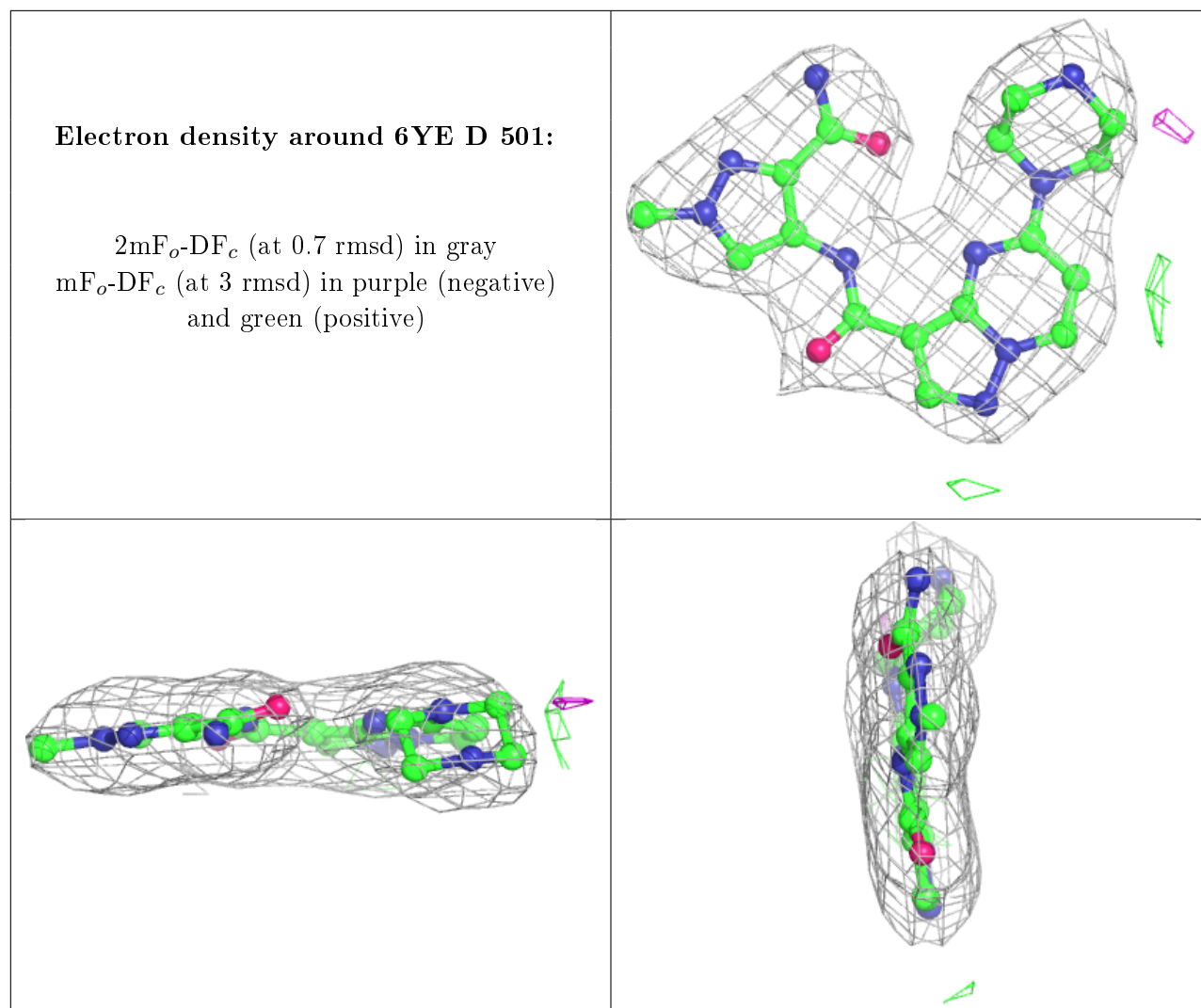


**Electron density around 6YE C 501:**

$2mF_o-DF_c$  (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.