



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:52 pm BST

PDB ID : 5K7I  
Title : IRAK4 in complex with AZ3864  
Authors : Ferguson, A.D.  
Deposited on : 2016-05-26  
Resolution : 2.31 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 : 2.11  
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) : 2.11

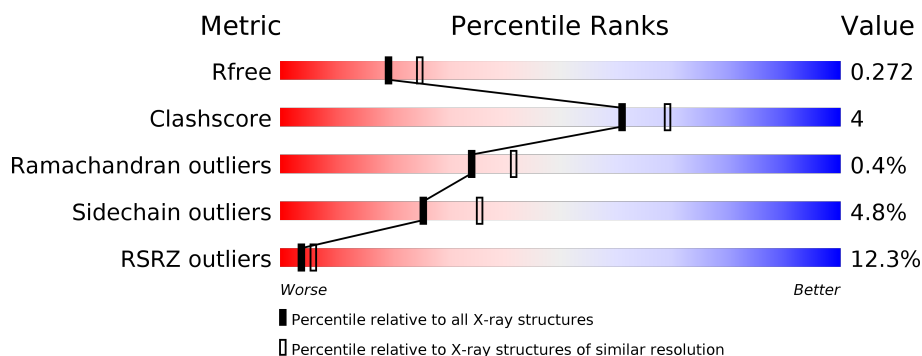
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	

## 2 Entry composition [i](#)

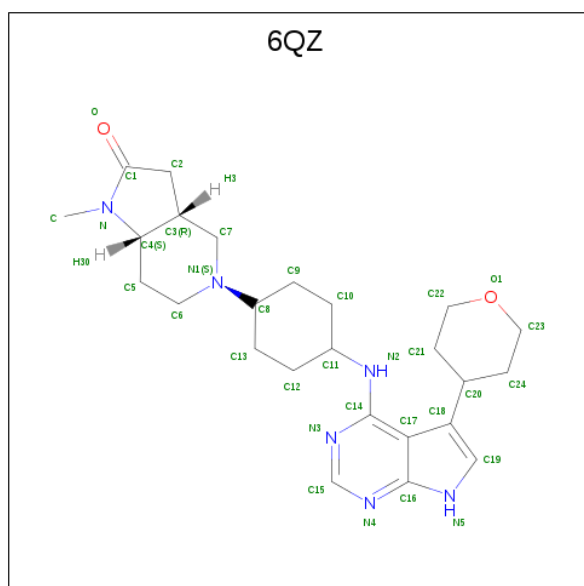
There are 4 unique types of molecules in this entry. The entry contains 4497 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	274	Total	C	N	O	P	S	0	0	0
			2174	1370	368	420	2	14			
1	B	273	Total	C	N	O	P	S	0	0	0
			2175	1370	367	422	2	14			

- Molecule 2 is (3 {a} {R},7 {a} {S})-1-methyl-5-[4-[[5-(oxan-4-yl)-7 {H}-pyrrolo[2,3-d]pyrimidin-4-yl]amino]cyclohexyl]-3,3 {a},4,6,7,7 {a}-hexahydropyrrolo[3,2-c]pyridin-2-one (three-letter code: 6QZ) (formula: C<sub>25</sub>H<sub>36</sub>N<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	25	6	2		
2	B	1	Total	C	N	O	0	0
			33	25	6	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

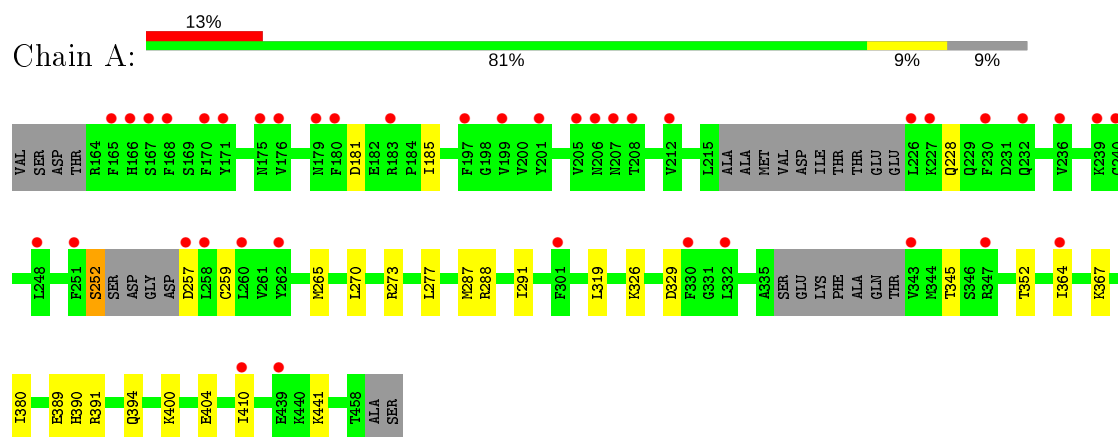
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	45	Total	O	0	0
			45	45		

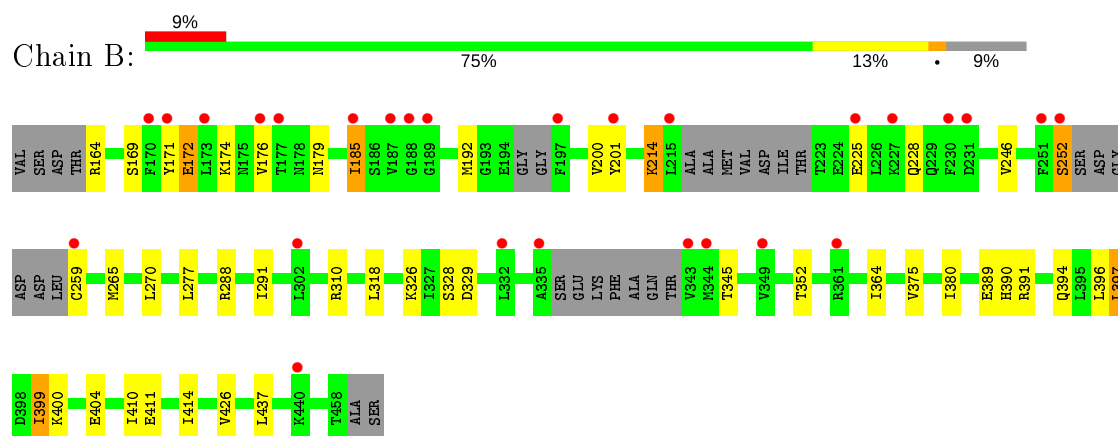
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.54Å 110.53Å 142.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.21 – 2.31 71.21 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.1 (71.21-2.31) 99.1 (71.21-2.31)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.32Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.7	Depositor
R, $R_{free}$	0.219 , 0.257 0.233 , 0.272	Depositor DCC
$R_{free}$ test set	1495 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 65.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4497	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.45 % 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 5.6884e-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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6QZ, TPO, SO4, SEP

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	0.48	0/2188	0.65	0/2944
1	B	0.49	0/2188	0.67	0/2943
All	All	0.49	0/4376	0.66	0/5887

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

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	2174	0	2154	14	0
1	B	2175	0	2151	27	0
2	A	33	0	0	0	0
2	B	33	0	0	0	0
3	B	5	0	0	0	0
4	A	32	0	0	1	0
4	B	45	0	0	0	0
All	All	4497	0	4305	39	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 4.

All (39) 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:265:MET:CE	1:B:326:LYS:HG3	2.21	0.71
1:B:265:MET:HE2	1:B:326:LYS:HG3	1.76	0.66
1:A:265:MET:CE	1:A:326:LYS:HG3	2.26	0.65
1:A:265:MET:HE1	1:A:326:LYS:HG3	1.79	0.63
1:B:201:TYR:HE2	1:B:214:LYS:HD2	1.64	0.62
1:A:391:ARG:HA	1:B:390:HIS:HB3	1.83	0.60
1:A:390:HIS:HB3	1:B:391:ARG:HA	1.83	0.59
1:B:171:TYR:O	1:B:172:GLU:HB2	2.04	0.56
1:B:396:LEU:HD12	1:B:399:ILE:HD13	1.86	0.56
1:A:287:MET:HG2	4:A:632:HOH:O	2.08	0.54
1:B:396:LEU:O	1:B:399:ILE:HB	2.06	0.53
1:B:201:TYR:CE2	1:B:214:LYS:HD2	2.43	0.53
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.91	0.53
1:B:375:VAL:HG22	1:B:397:LEU:HD13	1.91	0.52
1:A:367:LYS:HD3	1:A:441:LYS:HD2	1.93	0.50
1:A:345:TPO:HB	1:A:364:ILE:HD11	1.93	0.50
1:A:252:SER:HB3	1:A:259:CYS:HB2	1.93	0.50
1:B:389:GLU:HA	1:B:394:GLN:NE2	2.28	0.49
1:B:185:ILE:HD11	1:B:192:MET:HG2	1.95	0.49
1:B:400:LYS:HE2	1:B:404:GLU:OE2	2.13	0.49
1:A:400:LYS:HE2	1:A:404:GLU:OE2	2.13	0.48
1:B:397:LEU:HD11	1:B:437:LEU:HD22	1.96	0.48
1:B:270:LEU:HD13	1:B:291:ILE:HG21	1.96	0.48
1:B:252:SER:HB2	1:B:259:CYS:HB2	1.96	0.47
1:A:270:LEU:HD13	1:A:291:ILE:HG21	1.96	0.47
1:B:288:ARG:HB3	1:B:380:ILE:HG23	1.96	0.47
1:B:345:TPO:HB	1:B:364:ILE:HD11	1.96	0.47
1:A:389:GLU:HA	1:A:394:GLN:NE2	2.30	0.46
1:B:265:MET:HE1	1:B:326:LYS:HG3	1.97	0.45
1:B:214:LYS:H	1:B:214:LYS:HG3	1.66	0.45
1:A:265:MET:HE2	1:A:326:LYS:HG3	1.96	0.44
1:A:288:ARG:HB3	1:A:380:ILE:HG23	1.98	0.44
1:B:246:VAL:HG11	1:B:328:SER:HB3	2.03	0.41
1:A:273:ARG:HG3	1:A:319:LEU:HD12	2.03	0.41
1:B:174:LYS:HE2	1:B:179:ASN:OD1	2.21	0.41
1:B:310:ARG:HD3	1:B:364:ILE:HG23	2.02	0.41
1:B:172:GLU:O	1:B:176:VAL:HG13	2.20	0.41
1:B:397:LEU:CD1	1:B:437:LEU:HD22	2.51	0.40
1:B:414:ILE:HG12	1:B:426:VAL:HG11	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	264/301 (88%)	256 (97%)	7 (3%)	1 (0%)	34	41
1	B	261/301 (87%)	253 (97%)	7 (3%)	1 (0%)	34	41
All	All	525/602 (87%)	509 (97%)	14 (3%)	2 (0%)	34	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	GLU
1	A	181	ASP

### 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	238/260 (92%)	230 (97%)	8 (3%)	37	51
1	B	239/260 (92%)	224 (94%)	15 (6%)	18	24
All	All	477/520 (92%)	454 (95%)	23 (5%)	25	35

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	ILE

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Mol	Chain	Res	Type
1	A	228	GLN
1	A	252	SER
1	A	257	ASP
1	A	277	LEU
1	A	329	ASP
1	A	352	THR
1	A	410	ILE
1	B	164	ARG
1	B	169	SER
1	B	185	ILE
1	B	200	VAL
1	B	214	LYS
1	B	225	GLU
1	B	228	GLN
1	B	252	SER
1	B	277	LEU
1	B	329	ASP
1	B	352	THR
1	B	397	LEU
1	B	399	ILE
1	B	410	ILE
1	B	411	GLU

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	293	GLN
1	A	394	GLN
1	B	293	GLN
1	B	394	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	B	346	1	8,9,10	0.95	0	8,12,14	1.46	1 (12%)
1	TPO	A	345	1	8,10,11	1.18	1 (12%)	10,14,16	1.09	1 (10%)
1	SEP	A	346	1	8,9,10	0.93	0	8,12,14	1.39	1 (12%)
1	TPO	B	345	1	8,10,11	1.14	0	10,14,16	1.09	1 (10%)

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	B	346	1	-	0/5/8/10	-
1	TPO	A	345	1	-	2/9/11/13	-
1	SEP	A	346	1	-	0/5/8/10	-
1	TPO	B	345	1	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	TPO	CB-CA	2.32	1.59	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	SEP	OG-P-O1P	2.71	114.08	106.47
1	A	346	SEP	OG-P-O1P	2.69	114.01	106.47
1	B	345	TPO	O3P-P-OG1	2.38	116.64	105.99
1	A	345	TPO	O3P-P-OG1	2.35	116.54	105.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1

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Mol	Chain	Res	Type	Atoms
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	345	TPO	1	0
1	B	345	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	6QZ	A	501	-	37,38,38	1.10	1 (2%)	43,55,55	1.18	2 (4%)
3	SO4	B	501	-	4,4,4	0.22	0	6,6,6	0.15	0
2	6QZ	B	502	-	37,38,38	0.97	2 (5%)	43,55,55	1.22	2 (4%)

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	6QZ	A	501	-	-	6/10/55/55	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6QZ	B	502	-	-	5/10/55/55	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	6QZ	C18-C17	5.22	1.46	1.40
2	B	502	6QZ	C4-N	3.40	1.51	1.46
2	B	502	6QZ	C18-C17	3.34	1.44	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	6QZ	C6-C5-C4	5.91	119.19	109.91
2	A	501	6QZ	C6-C5-C4	5.44	118.46	109.91
2	B	502	6QZ	C13-C8-N1	2.71	119.56	112.52
2	A	501	6QZ	C9-C8-N1	2.55	119.14	112.52

There are no chirality outliers.

All (11) torsion outliers are listed below:

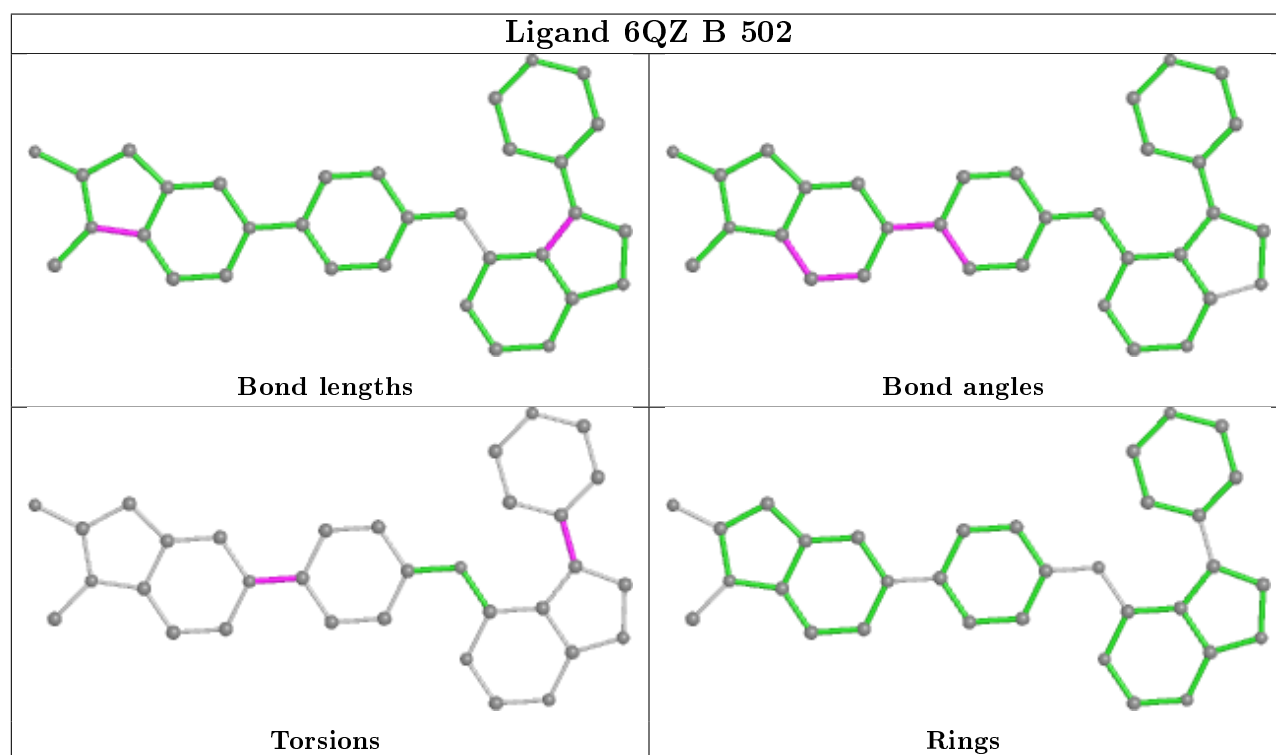
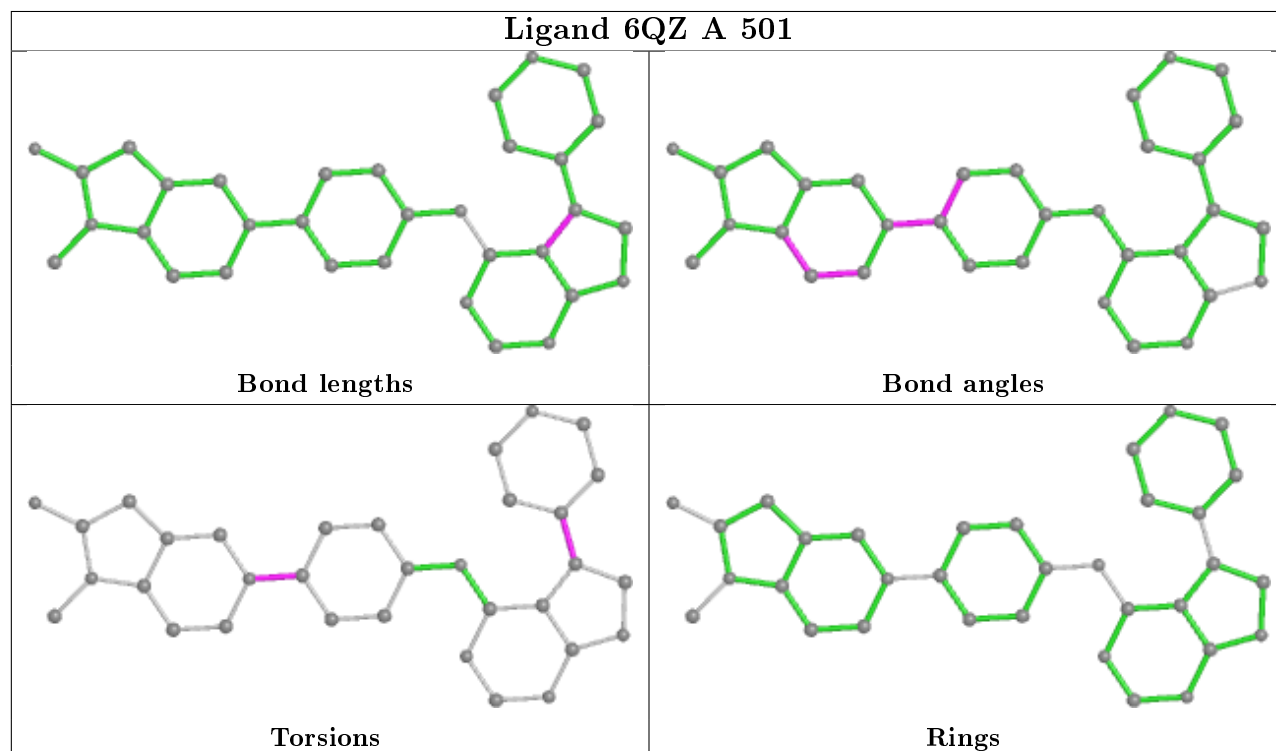
Mol	Chain	Res	Type	Atoms
2	A	501	6QZ	C13-C8-N1-C6
2	B	502	6QZ	C9-C8-N1-C7
2	B	502	6QZ	C9-C8-N1-C6
2	B	502	6QZ	C13-C8-N1-C7
2	B	502	6QZ	C13-C8-N1-C6
2	A	501	6QZ	C9-C8-N1-C6
2	A	501	6QZ	C13-C8-N1-C7
2	A	501	6QZ	C9-C8-N1-C7
2	A	501	6QZ	C19-C18-C20-C21
2	A	501	6QZ	C19-C18-C20-C24
2	B	502	6QZ	C19-C18-C20-C24

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	272/301 (90%)	0.98	40 (14%) 2 3	44, 77, 148, 170	0
1	B	271/301 (90%)	0.84	27 (9%) 7 10	47, 79, 123, 156	0
All	All	543/602 (90%)	0.91	67 (12%) 4 6	44, 78, 142, 170	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	ASN	8.8
1	A	171	TYR	8.1
1	A	197	PHE	6.2
1	A	239	LYS	6.0
1	A	236	VAL	5.9
1	A	230	PHE	5.6
1	B	176	VAL	5.5
1	B	171	TYR	5.4
1	B	343	VAL	5.1
1	A	251	PHE	4.7
1	A	165	PHE	4.7
1	A	332	LEU	4.7
1	B	188	GLY	4.4
1	A	168	PHE	4.3
1	B	230	PHE	4.3
1	B	197	PHE	4.0
1	A	240	CYS	3.8
1	A	301	PHE	3.7
1	A	232	GLN	3.7
1	A	330	PHE	3.6
1	B	259	CYS	3.6
1	B	173	LEU	3.5
1	B	215	LEU	3.4
1	B	177	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	205	VAL	3.2
1	A	176	VAL	3.1
1	A	260	LEU	3.1
1	A	226	LEU	3.1
1	A	206	ASN	3.0
1	A	167	SER	2.9
1	A	199	VAL	2.9
1	B	344	MET	2.9
1	A	347	ARG	2.9
1	B	185	ILE	2.8
1	B	231	ASP	2.8
1	A	262	TYR	2.7
1	A	212	VAL	2.7
1	A	343	VAL	2.7
1	B	187	VAL	2.7
1	A	207	ASN	2.7
1	B	227	LYS	2.7
1	B	335	ALA	2.6
1	A	257	ASP	2.6
1	A	166	HIS	2.6
1	A	180	PHE	2.6
1	A	439	GLU	2.6
1	B	440	LYS	2.6
1	B	302	LEU	2.5
1	A	175	ASN	2.5
1	B	361	ARG	2.5
1	A	248	LEU	2.5
1	B	201	TYR	2.5
1	B	251	PHE	2.5
1	A	208	THR	2.4
1	A	258	LEU	2.3
1	A	364	ILE	2.3
1	B	349	VAL	2.3
1	B	189	GLY	2.3
1	A	183	ARG	2.3
1	B	252	SER	2.3
1	A	201	TYR	2.2
1	A	170	PHE	2.2
1	B	170	PHE	2.1
1	B	225	GLU	2.1
1	B	332	LEU	2.0
1	A	227	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	410	ILE	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	B	346	10/11	0.71	0.24	147,158,168,170	0
1	TPO	B	345	11/12	0.77	0.20	134,143,148,151	0
1	SEP	A	346	10/11	0.80	0.26	130,137,150,151	0
1	TPO	A	345	11/12	0.86	0.17	117,124,130,133	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

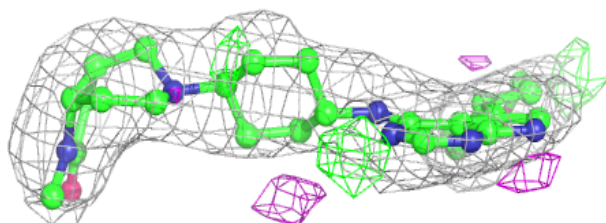
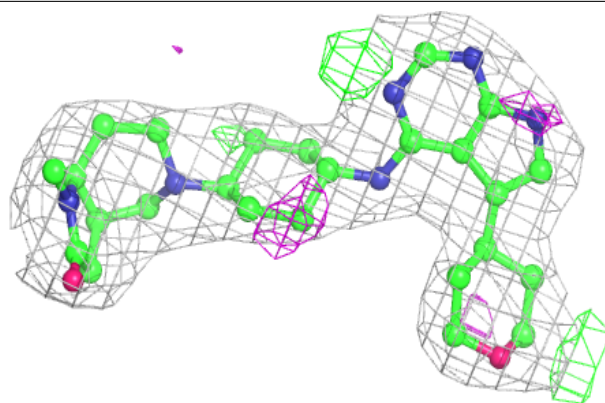
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	SO4	B	501	5/5	0.83	0.21	121,121,123,125	0
2	6QZ	A	501	33/33	0.90	0.16	54,63,81,84	0
2	6QZ	B	502	33/33	0.95	0.17	40,52,58,59	0

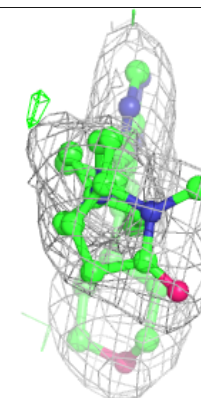
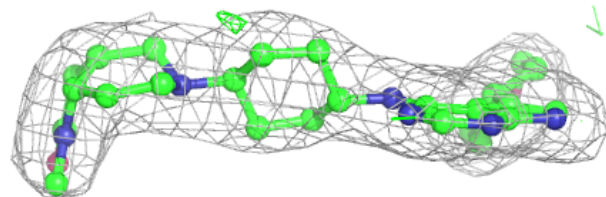
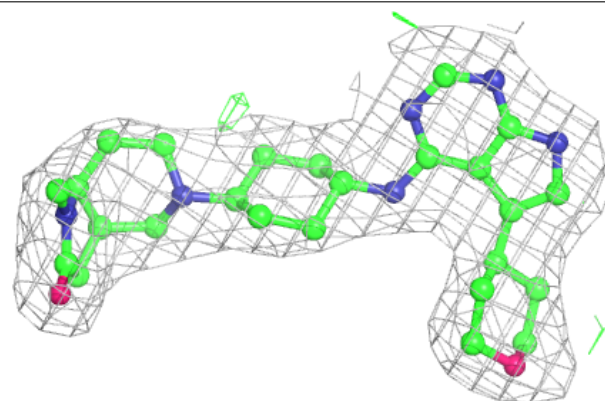
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around 6QZ 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 6QZ 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)



## 6.5 Other polymers

There are no such residues in this entry.