



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2022 – 10:09 am BST

PDB ID : 7QG1  
Title : IRAK4 in complex with inhibitor  
Authors : Xue, Y.; Aagaard, A.; Robb, G.R.; Degorce, S.L.  
Deposited on : 2021-12-07  
Resolution : 2.07 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.28  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.28

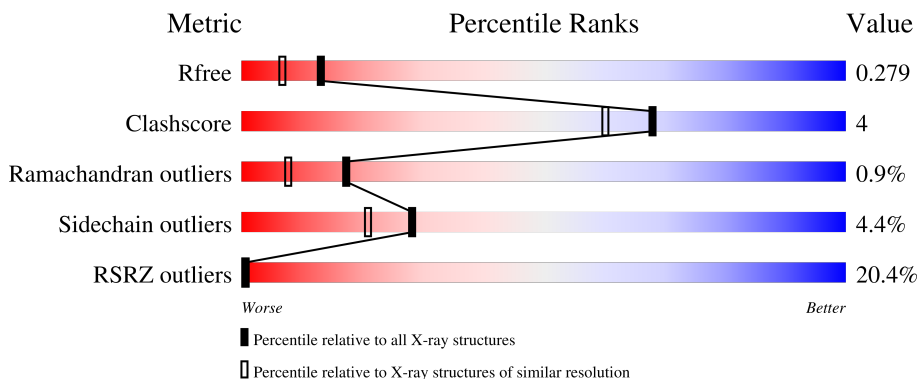
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	322	
1	B	322	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4657 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	266	2113	1332	356	409	2	14	0	0	0
1	B	282	2229	1398	376	439	2	14	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

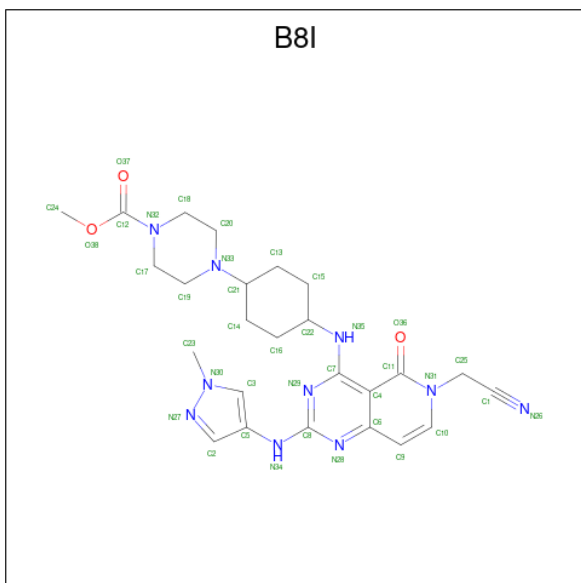
Chain	Residue	Modelled	Actual	Comment	Reference
A	139	MET	-	initiating methionine	UNP Q9NWZ3
A	140	HIS	-	expression tag	UNP Q9NWZ3
A	141	HIS	-	expression tag	UNP Q9NWZ3
A	142	HIS	-	expression tag	UNP Q9NWZ3
A	143	HIS	-	expression tag	UNP Q9NWZ3
A	144	HIS	-	expression tag	UNP Q9NWZ3
A	145	HIS	-	expression tag	UNP Q9NWZ3
A	146	HIS	-	expression tag	UNP Q9NWZ3
A	147	GLU	-	expression tag	UNP Q9NWZ3
A	148	ASN	-	expression tag	UNP Q9NWZ3
A	149	LEU	-	expression tag	UNP Q9NWZ3
A	150	TYR	-	expression tag	UNP Q9NWZ3
A	151	PHE	-	expression tag	UNP Q9NWZ3
A	152	GLN	-	expression tag	UNP Q9NWZ3
A	153	GLY	-	expression tag	UNP Q9NWZ3
B	139	MET	-	initiating methionine	UNP Q9NWZ3
B	140	HIS	-	expression tag	UNP Q9NWZ3
B	141	HIS	-	expression tag	UNP Q9NWZ3
B	142	HIS	-	expression tag	UNP Q9NWZ3
B	143	HIS	-	expression tag	UNP Q9NWZ3
B	144	HIS	-	expression tag	UNP Q9NWZ3
B	145	HIS	-	expression tag	UNP Q9NWZ3
B	146	HIS	-	expression tag	UNP Q9NWZ3
B	147	GLU	-	expression tag	UNP Q9NWZ3
B	148	ASN	-	expression tag	UNP Q9NWZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	149	LEU	-	expression tag	UNP Q9NWZ3
B	150	TYR	-	expression tag	UNP Q9NWZ3
B	151	PHE	-	expression tag	UNP Q9NWZ3
B	152	GLN	-	expression tag	UNP Q9NWZ3
B	153	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is methyl 4-[4-[[6-(cyanomethyl)-2-[(1-methylpyrazol-4-yl)amino]-5-oxidanyliden e-pyrido[4,3-d]pyrimidin-4-yl]amino]cyclohexyl]piperazine-1-carboxylate (three-letter code: B8I) (formula: C<sub>25</sub>H<sub>32</sub>N<sub>10</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
2	A	1	38	25	10	3	0	0
2	B	1	38	25	10	3	0	0

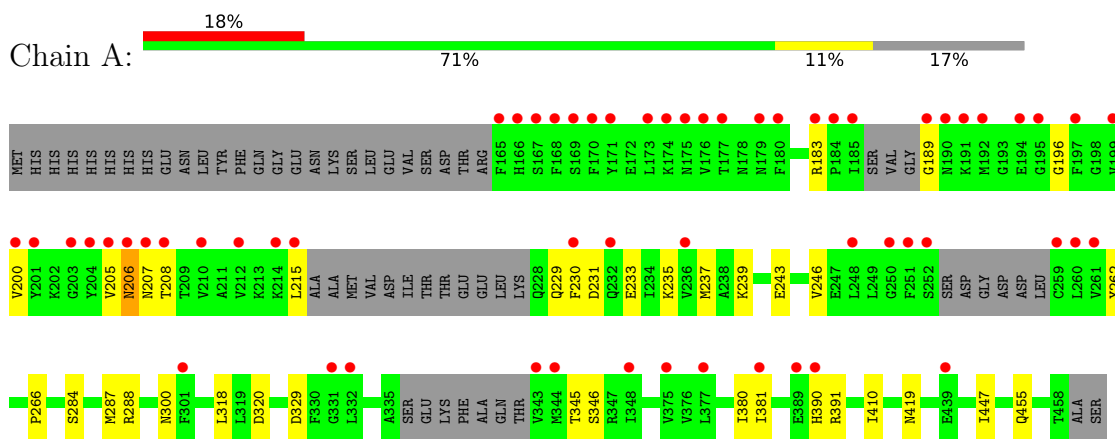
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	115	115	115	0	0
3	B	124	124	124	0	0

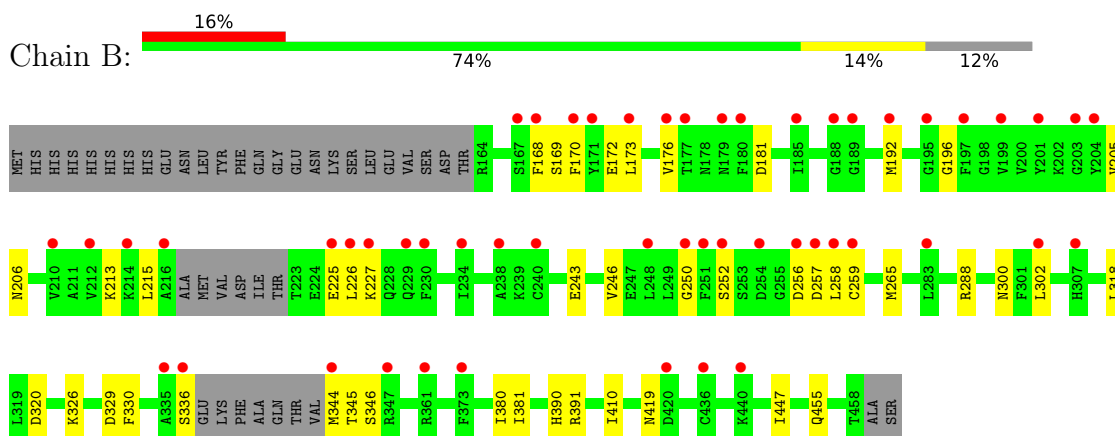
### 3 Residue-property plots [i](#)

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: 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, $\alpha$ , $\beta$ , $\gamma$	87.74Å 109.42Å 142.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.75 – 2.07 74.69 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.5 (86.75-2.07) 99.5 (74.69-2.07)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.07Å)	Xtrriage
Refinement program	BUSTER 2.11.6	Depositor
R, $R_{free}$	0.247 , 0.285 0.243 , 0.279	Depositor DCC
$R_{free}$ test set	2118 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtrriage
Anisotropy	0.534	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4657	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	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 20.42 % 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 8.7248e-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: B8I, TPO, 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	0.49	0/2126	0.65	0/2860
1	B	0.54	0/2244	0.68	0/3021
All	All	0.51	0/4370	0.67	0/5881

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	2113	0	2084	13	0
1	B	2229	0	2191	21	0
2	A	38	0	0	0	0
2	B	38	0	0	1	0
3	A	115	0	0	0	0
3	B	124	0	0	1	0
All	All	4657	0	4275	33	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 (33) 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:391:ARG:HA	1:B:390:HIS:HB3	1.60	0.82
1:A:390:HIS:HB3	1:B:391:ARG:HA	1.71	0.73
1:B:265:MET:HE1	1:B:326:LYS:HG3	1.72	0.72
1:B:265:MET:CE	1:B:326:LYS:HG3	2.25	0.66
1:B:205:VAL:HG23	3:B:650:HOH:O	1.96	0.66
1:A:237:MET:HE3	1:A:262:TYR:HE2	1.59	0.65
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.80	0.62
1:A:246:VAL:HG11	1:A:318:LEU:HD12	1.83	0.59
1:A:284:SER:H	1:A:287:MET:CE	2.19	0.54
1:B:302:LEU:HD11	1:B:330:PHE:HE1	1.75	0.52
1:B:227:LYS:HG2	1:B:258:LEU:HD11	1.93	0.51
1:B:252:SER:HB3	1:B:259:CYS:HB2	1.93	0.51
1:A:284:SER:H	1:A:287:MET:HE3	1.77	0.50
1:B:173:LEU:HA	1:B:176:VAL:HG22	1.94	0.49
1:A:266:PRO:HD2	1:A:320:ASP:HA	1.94	0.49
1:A:205:VAL:O	1:A:206:ASN:HB2	2.14	0.47
1:B:176:VAL:HG11	1:B:205:VAL:HG22	1.97	0.46
1:B:288:ARG:HB3	1:B:380:ILE:HG23	1.98	0.45
1:B:172:GLU:O	1:B:176:VAL:HG13	2.17	0.45
2:B:501:B8I:N29	2:B:501:B8I:C2	2.79	0.45
1:A:215:LEU:HD22	1:A:230:PHE:HB3	1.98	0.44
1:B:168:PHE:HE1	1:B:250:GLY:HA3	1.82	0.44
1:A:300:ASN:HA	1:A:447:ILE:HG21	2.00	0.44
1:B:215:LEU:HD23	1:B:226:LEU:HG	2.01	0.43
1:A:288:ARG:HB3	1:A:380:ILE:HG23	2.00	0.43
1:B:300:ASN:HA	1:B:447:ILE:HG21	2.01	0.42
1:A:381:ILE:HG21	1:A:410:ILE:HD11	2.00	0.42
1:B:265:MET:HE1	1:B:320:ASP:HB3	2.02	0.42
1:B:213:LYS:O	1:B:259:CYS:HA	2.19	0.42
1:B:381:ILE:HG21	1:B:410:ILE:HD11	2.01	0.42
1:A:183:ARG:O	1:A:189:GLY:HA3	2.19	0.42
1:B:170:PHE:HB2	1:B:257:ASP:HB3	2.02	0.42
1:B:169:SER:H	1:B:172:GLU:CD	2.23	0.41

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	254/322 (79%)	244 (96%)	7 (3%)	3 (1%)	13 4
1	B	274/322 (85%)	260 (95%)	12 (4%)	2 (1%)	22 11
All	All	528/644 (82%)	504 (96%)	19 (4%)	5 (1%)	17 8

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	196	GLY
1	A	208	THR
1	B	196	GLY
1	B	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	231/280 (82%)	220 (95%)	11 (5%)	25 18
1	B	244/280 (87%)	234 (96%)	10 (4%)	30 23
All	All	475/560 (85%)	454 (96%)	21 (4%)	28 21

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	VAL

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Mol	Chain	Res	Type
1	A	207	ASN
1	A	229	GLN
1	A	231	ASP
1	A	233	GLU
1	A	235	LYS
1	A	239	LYS
1	A	243	GLU
1	A	329	ASP
1	A	419	ASN
1	A	455	GLN
1	B	192	MET
1	B	206	ASN
1	B	225	GLU
1	B	243	GLU
1	B	256	ASP
1	B	329	ASP
1	B	336	SER
1	B	344	MET
1	B	419	ASN
1	B	455	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	419	ASN
1	B	206	ASN
1	B	419	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](#)

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	TPO	A	345	1	8,10,11	1.27	1 (12%)	10,14,16	1.25	1 (10%)
1	SEP	B	346	1	8,9,10	0.77	0	8,12,14	1.42	1 (12%)
1	TPO	B	345	1	8,10,11	1.26	1 (12%)	10,14,16	1.20	1 (10%)
1	SEP	A	346	1	8,9,10	0.90	0	8,12,14	1.22	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	TPO	A	345	1	-	5/9/11/13	-
1	SEP	B	346	1	-	0/5/8/10	-
1	TPO	B	345	1	-	5/9/11/13	-
1	SEP	A	346	1	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	345	TPO	CB-CA	2.32	1.59	1.53
1	A	345	TPO	CB-CA	2.15	1.58	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	TPO	O2P-P-OG1	2.43	116.89	105.99
1	B	346	SEP	OG-CB-CA	2.42	110.50	108.14
1	B	345	TPO	O2P-P-OG1	2.35	116.51	105.99
1	A	346	SEP	OG-CB-CA	2.12	110.20	108.14

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
1	B	345	TPO	O-C-CA-CB
1	A	345	TPO	CB-OG1-P-O1P
1	B	345	TPO	CB-OG1-P-O1P
1	A	345	TPO	CB-OG1-P-O2P
1	A	345	TPO	CB-OG1-P-O3P
1	B	345	TPO	CB-OG1-P-O2P
1	B	345	TPO	CB-OG1-P-O3P

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](#)

2 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	B8I	B	501	-	39,42,42	1.55	8 (20%)	46,59,59	1.52	7 (15%)
2	B8I	A	501	-	39,42,42	1.58	8 (20%)	46,59,59	1.45	6 (13%)

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	B8I	B	501	-	-	3/17/41/41	0/5/5/5
2	B8I	A	501	-	-	8/17/41/41	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	B8I	C7-C4	-5.05	1.38	1.44
2	A	501	B8I	C7-C4	-5.03	1.38	1.44
2	A	501	B8I	C4-C11	3.88	1.48	1.41
2	B	501	B8I	C2-C5	3.21	1.41	1.38
2	A	501	B8I	C2-C5	3.01	1.41	1.38
2	B	501	B8I	C4-C11	2.95	1.46	1.41
2	B	501	B8I	C25-N31	-2.74	1.43	1.48
2	A	501	B8I	C4-C6	-2.60	1.38	1.42
2	B	501	B8I	C12-N32	2.34	1.39	1.35
2	B	501	B8I	C4-C6	-2.31	1.38	1.42
2	A	501	B8I	C9-C6	2.31	1.45	1.41
2	B	501	B8I	C9-C6	2.25	1.45	1.41
2	A	501	B8I	C25-N31	-2.09	1.45	1.48
2	A	501	B8I	C6-N28	-2.08	1.34	1.37
2	A	501	B8I	C5-N34	-2.08	1.36	1.40
2	B	501	B8I	C6-N28	-2.07	1.34	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	B8I	C7-N35-C22	-4.27	116.04	124.16
2	A	501	B8I	C7-N35-C22	-3.80	116.94	124.16
2	B	501	B8I	C24-O38-C12	-3.70	111.06	115.34
2	A	501	B8I	C18-N32-C17	3.48	119.33	112.62
2	B	501	B8I	C15-C22-N35	-3.45	105.22	110.60
2	A	501	B8I	C3-N30-N27	3.29	114.43	111.56
2	B	501	B8I	C18-N32-C17	2.96	118.32	112.62
2	A	501	B8I	C24-O38-C12	-2.89	112.00	115.34
2	B	501	B8I	C3-N30-N27	2.63	113.85	111.56
2	B	501	B8I	C14-C16-C22	-2.53	108.69	111.48
2	A	501	B8I	C3-C5-C2	-2.44	104.88	106.02
2	B	501	B8I	C4-C7-N29	-2.10	118.69	122.18
2	A	501	B8I	C4-C7-N29	-2.04	118.80	122.18

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	B8I	O37-C12-N32-C17
2	A	501	B8I	O37-C12-N32-C18
2	A	501	B8I	O38-C12-N32-C17

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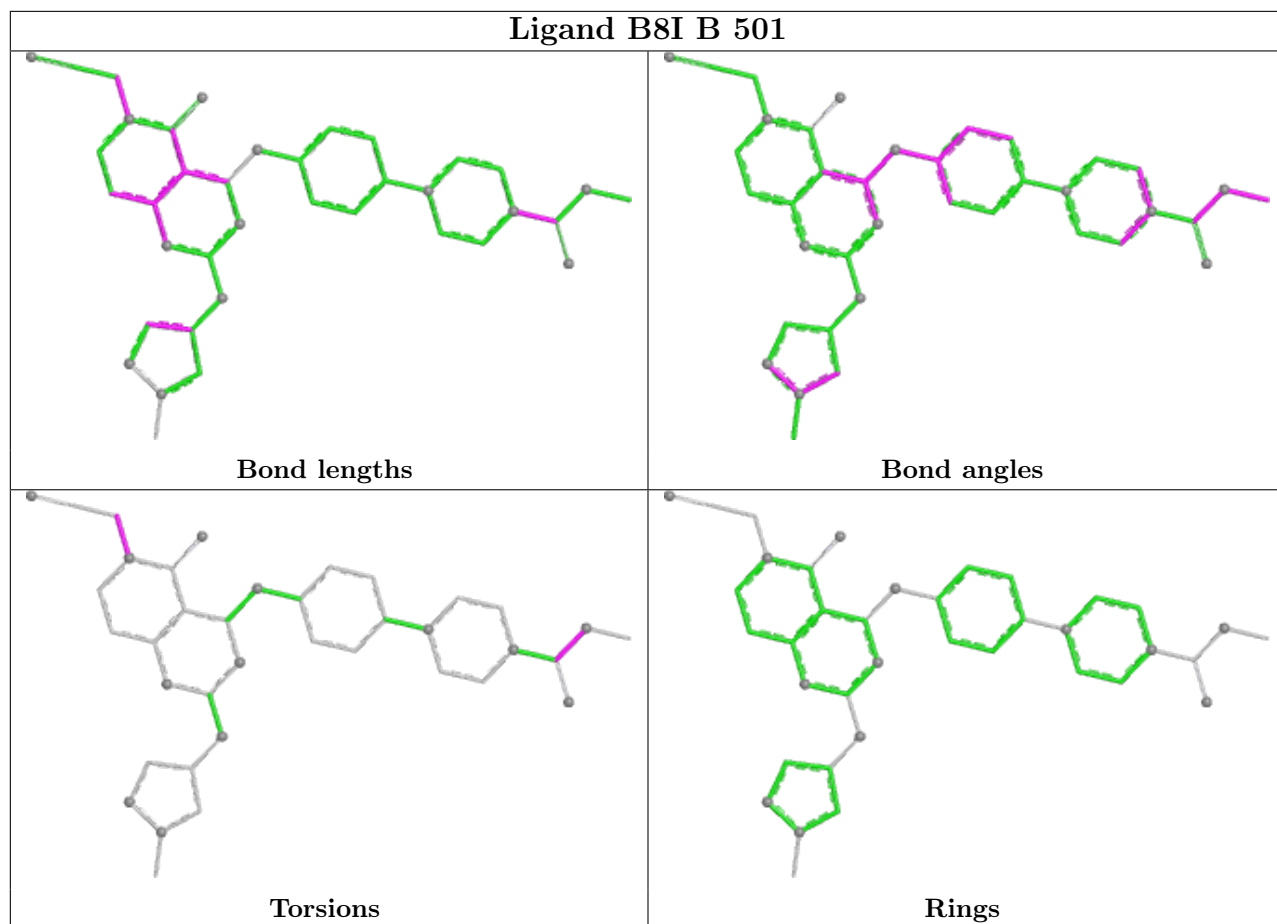
Mol	Chain	Res	Type	Atoms
2	A	501	B8I	O38-C12-N32-C18
2	A	501	B8I	N32-C12-O38-C24
2	A	501	B8I	O37-C12-O38-C24
2	A	501	B8I	C1-C25-N31-C10
2	B	501	B8I	N32-C12-O38-C24
2	B	501	B8I	O37-C12-O38-C24
2	B	501	B8I	C1-C25-N31-C10
2	A	501	B8I	C14-C21-N33-C20

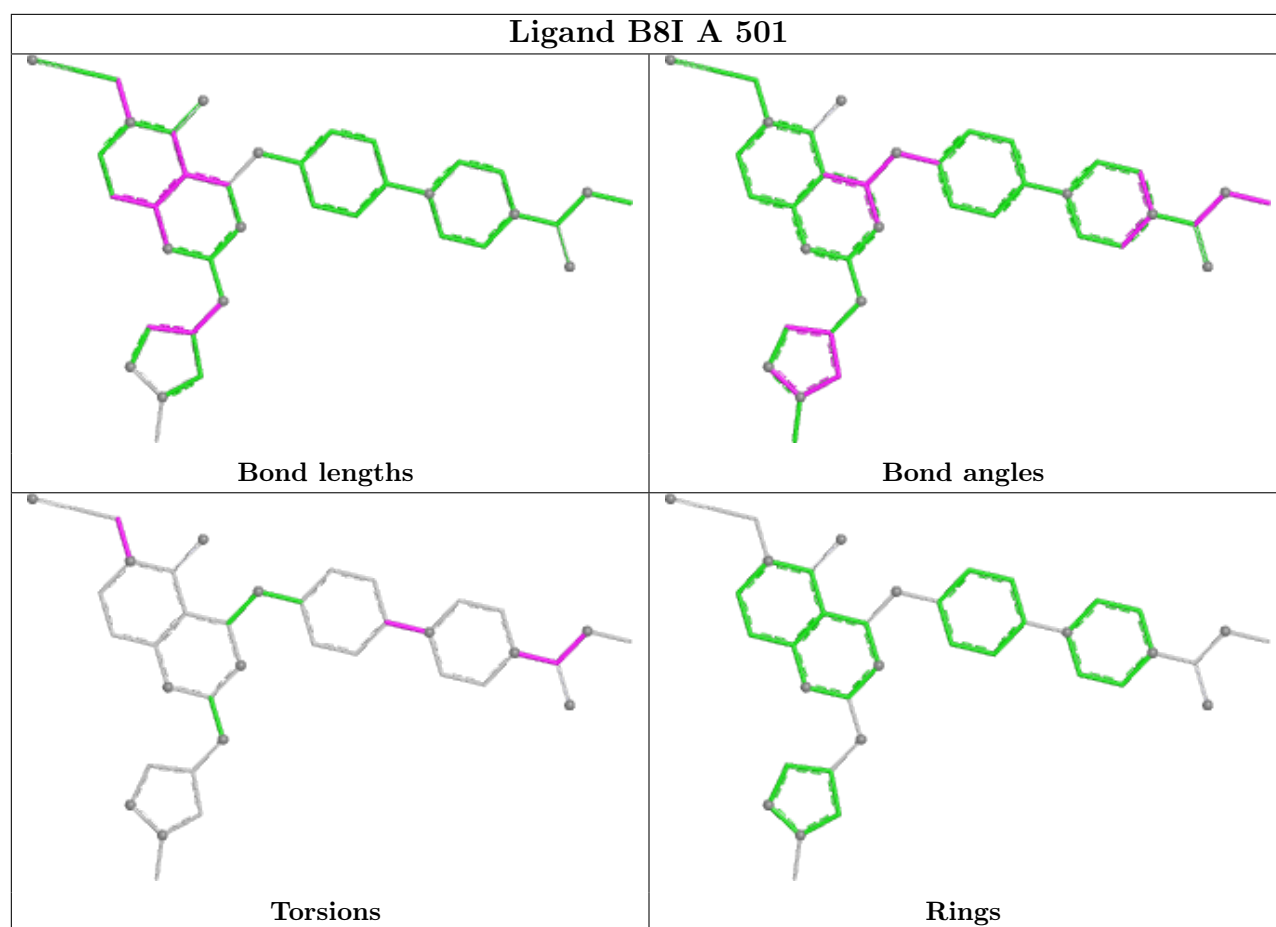
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	B8I	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	264/322 (81%)	1.49	59 (22%) 0 0	34, 59, 160, 170	0
1	B	280/322 (86%)	1.23	52 (18%) 1 1	33, 59, 97, 129	0
All	All	544/644 (84%)	1.36	111 (20%) 1 0	33, 59, 140, 170	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	TYR	12.7
1	A	236	VAL	9.3
1	B	257	ASP	9.0
1	B	168	PHE	8.2
1	A	230	PHE	7.9
1	A	170	PHE	7.3
1	A	179	ASN	7.2
1	B	259	CYS	6.6
1	A	176	VAL	6.6
1	A	190	ASN	6.4
1	A	251	PHE	6.0
1	A	165	PHE	6.0
1	A	248	LEU	5.7
1	A	203	GLY	5.7
1	A	167	SER	5.7
1	A	250	GLY	5.7
1	B	230	PHE	5.6
1	A	199	VAL	5.2
1	B	227	LYS	5.1
1	A	189	GLY	5.0
1	A	173	LEU	5.0
1	A	195	GLY	5.0
1	B	335	ALA	4.9
1	B	258	LEU	4.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	175	ASN	4.6
1	A	166	HIS	4.5
1	B	250	GLY	4.4
1	A	205	VAL	4.4
1	B	347	ARG	4.4
1	B	226	LEU	4.4
1	B	171	TYR	4.4
1	B	252	SER	4.3
1	A	185	ILE	4.2
1	A	214	LYS	4.2
1	A	180	PHE	4.2
1	A	207	ASN	4.1
1	B	170	PHE	4.1
1	B	189	GLY	4.1
1	A	168	PHE	4.1
1	B	176	VAL	4.1
1	A	169	SER	4.0
1	B	225	GLU	3.9
1	A	261	VAL	3.9
1	A	201	TYR	3.9
1	B	179	ASN	3.9
1	B	192	MET	3.8
1	A	332	LEU	3.8
1	A	252	SER	3.8
1	B	344	MET	3.8
1	B	188	GLY	3.7
1	A	197	PHE	3.6
1	A	177	THR	3.5
1	B	185	ILE	3.5
1	B	361	ARG	3.5
1	A	192	MET	3.4
1	B	254	ASP	3.4
1	B	234	ILE	3.3
1	A	174	LYS	3.2
1	B	436	CYS	3.2
1	A	439	GLU	3.1
1	B	373	PHE	3.1
1	A	215	LEU	3.1
1	B	180	PHE	3.0
1	A	232	GLN	3.0
1	A	348	ILE	2.9
1	B	336	SER	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	167	SER	2.9
1	B	229	GLN	2.8
1	A	259	CYS	2.8
1	A	343	VAL	2.8
1	B	216	ALA	2.7
1	A	184	PRO	2.7
1	A	204	TYR	2.7
1	B	195	GLY	2.6
1	B	177	THR	2.6
1	B	283	LEU	2.6
1	B	307	HIS	2.6
1	A	260	LEU	2.6
1	A	183	ARG	2.6
1	B	201	TYR	2.6
1	B	214	LYS	2.5
1	B	173	LEU	2.4
1	A	210	VAL	2.4
1	B	212	VAL	2.4
1	A	301	PHE	2.4
1	B	251	PHE	2.4
1	B	248	LEU	2.4
1	A	381	ILE	2.4
1	B	197	PHE	2.3
1	A	212	VAL	2.3
1	A	194	GLU	2.3
1	A	208	THR	2.3
1	A	191	LYS	2.3
1	A	331	GLY	2.2
1	B	203	GLY	2.2
1	B	238	ALA	2.2
1	B	210	VAL	2.2
1	B	256	ASP	2.2
1	A	206	ASN	2.2
1	A	377	LEU	2.2
1	B	440	LYS	2.2
1	B	199	VAL	2.1
1	A	200	VAL	2.1
1	B	420	ASP	2.1
1	B	302	LEU	2.0
1	A	375	VAL	2.0
1	A	344	MET	2.0
1	A	390	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	389	GLU	2.0
1	B	204	TYR	2.0
1	B	240	CYS	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	A	346	10/11	0.80	0.26	100,103,107,108	0
1	TPO	B	345	11/12	0.81	0.15	111,113,114,114	0
1	SEP	B	346	10/11	0.81	0.13	111,113,117,117	0
1	TPO	A	345	11/12	0.88	0.13	92,93,99,100	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

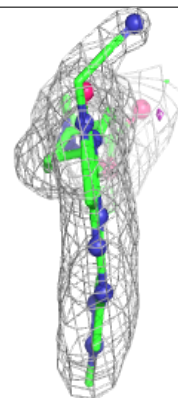
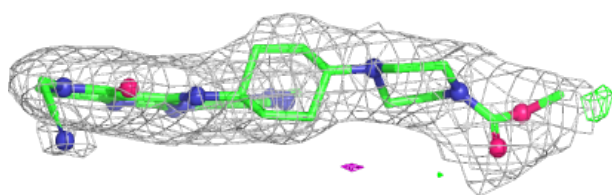
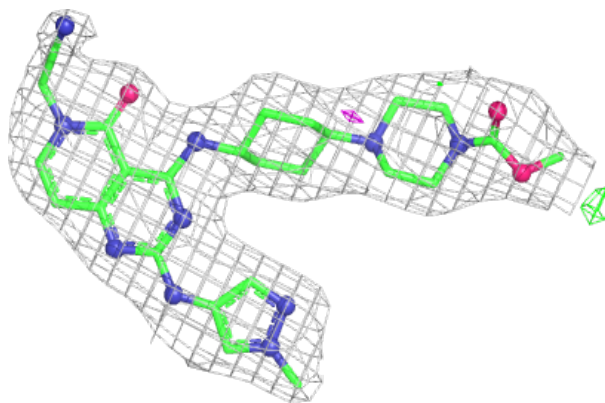
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	B8I	A	501	38/38	0.95	0.15	40,49,71,74	0
2	B8I	B	501	38/38	0.95	0.14	30,39,67,69	0

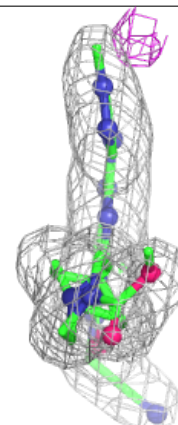
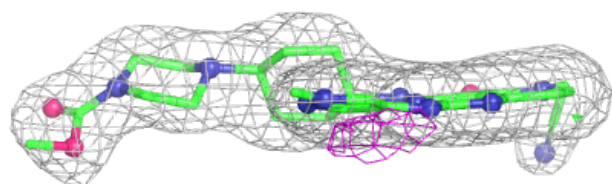
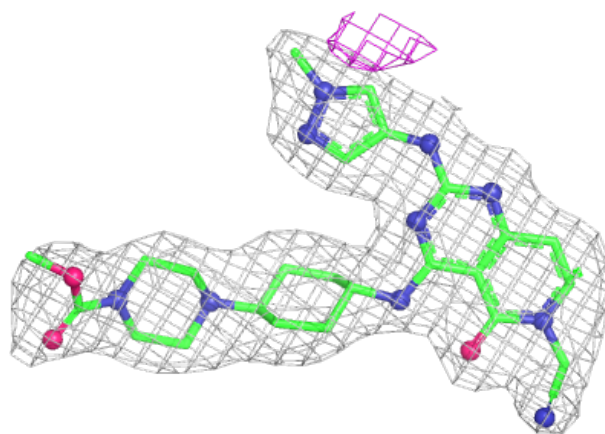
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around B8I 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 B8I 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.