



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:11 pm BST

PDB ID : 4BIE  
Title : Crystal Structures of Ask1-inhibitor Complexes  
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Deposited on : 2013-04-10  
Resolution : 2.36 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

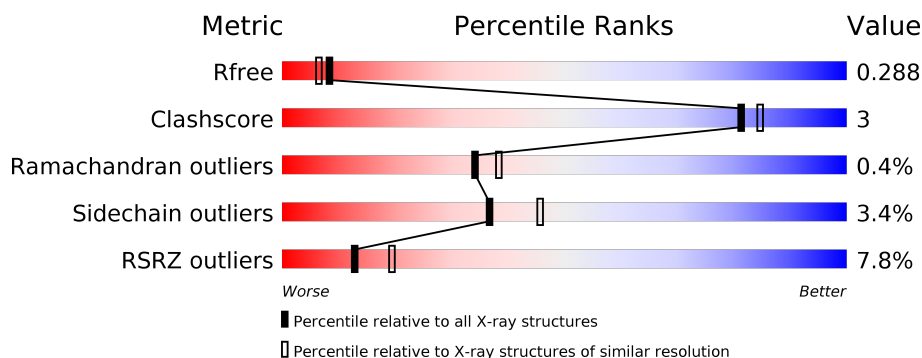
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	318	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>6%</div> <div>19%</div> </div> </div>
1	B	318	<div> <div>10%</div> <div> <div></div> <div>74%</div> <div>7%</div> <div>19%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4233 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.

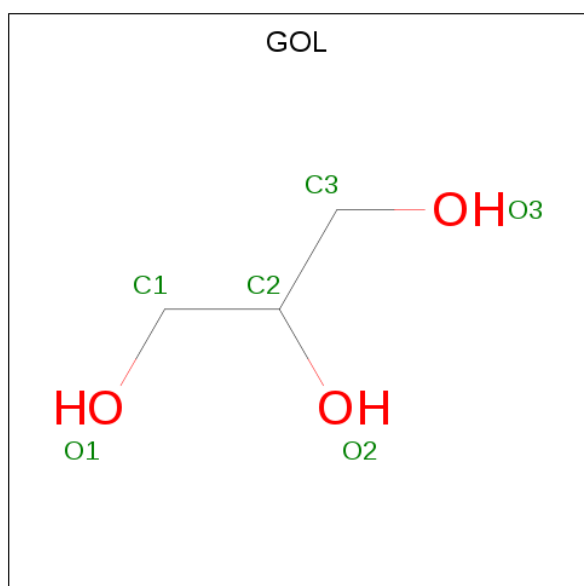
- Molecule 1 is a protein called MITOGEN-ACTIVATED PROTEIN KINASE KINASE KINASE 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2003	1292	327	375	9			
1	B	257	Total	C	N	O	S	0	1	0
			1982	1274	321	378	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	838	GLU	THR	engineered mutation	UNP Q99683
B	838	GLU	THR	engineered mutation	UNP Q99683

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



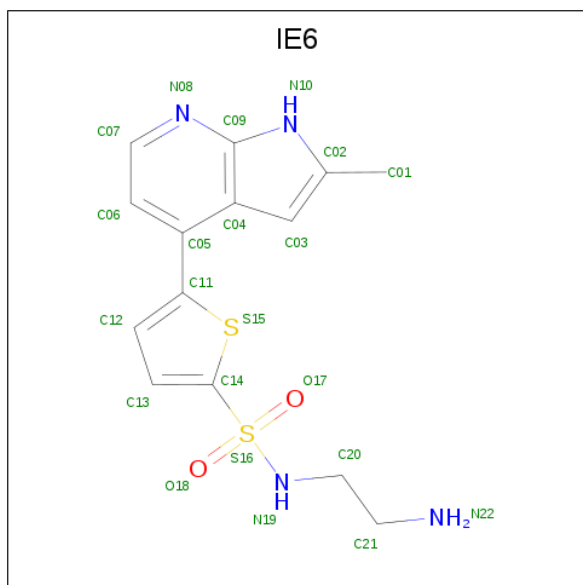
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 3 is N-(2-aminoethyl)-5-{2-methyl-1H-pyrrolo[2,3-b]pyridin-4-yl}thiophene-2-sulfonamide (three-letter code: IE6) (formula: C<sub>14</sub>H<sub>16</sub>N<sub>4</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			22	14	4	2	2		
3	B	1	Total	C	N	O	S	0	0
			22	14	4	2	2		

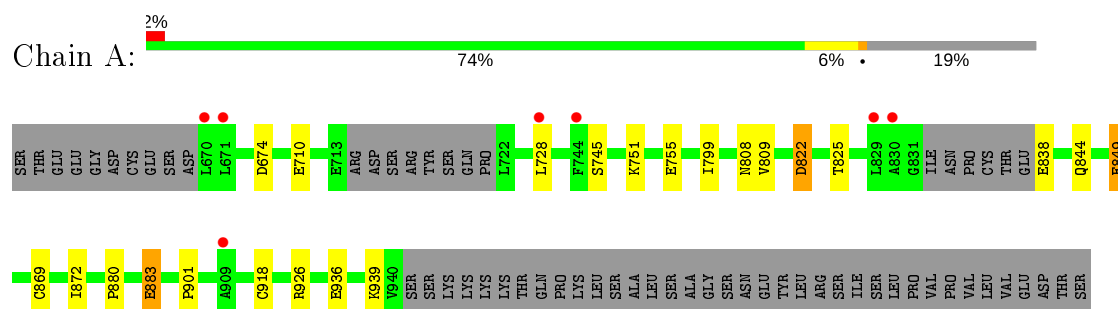
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		
4	B	75	Total	O	0	0
			75	75		

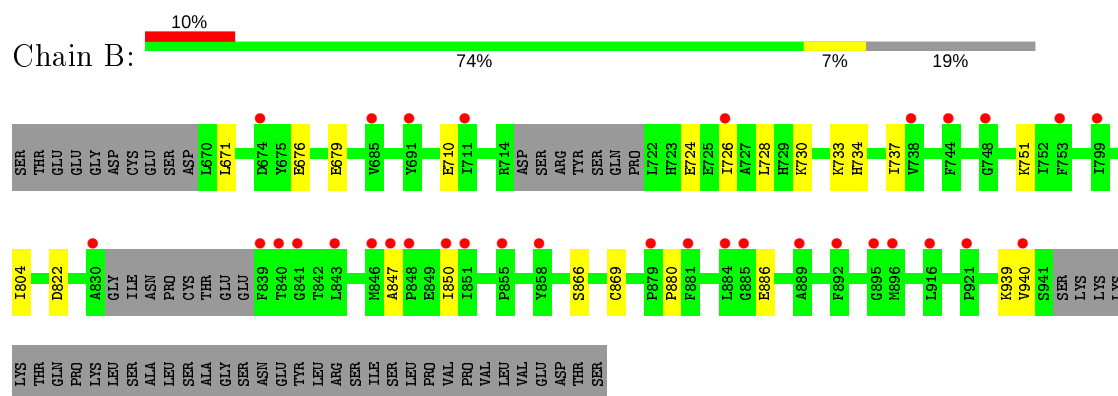
### 3 Residue-property plots [i](#)

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: MITOGEN-ACTIVATED PROTEIN KINASE KINASE KINASE 5



#### • Molecule 1: MITOGEN-ACTIVATED PROTEIN KINASE KINASE KINASE 5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.95Å 77.95Å 418.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	67.88 – 2.36 67.51 – 2.34	Depositor EDS
% Data completeness (in resolution range)	93.3 (67.88-2.36) 93.0 (67.51-2.34)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, $R_{free}$	0.210 , 0.253 0.251 , 0.288	Depositor DCC
$R_{free}$ test set	1550 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.0	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 59.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4233	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, IE6

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	0.53	0/2045	0.70	0/2758
1	B	0.47	0/2027	0.67	0/2740
All	All	0.50	0/4072	0.69	0/5498

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	2003	0	1971	11	0
1	B	1982	0	1919	9	0
2	A	6	0	8	0	0
2	B	6	0	8	1	0
3	A	22	0	16	3	0
3	B	22	0	16	1	0
4	A	117	0	0	1	0
4	B	75	0	0	1	0
All	All	4233	0	3938	21	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 3.

All (21) 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:869:CYS:HB3	1:B:880:PRO:HG3	1.82	0.61
1:B:710:GLU:HG2	1:B:751:LYS:HG2	1.87	0.57
1:A:869:CYS:HB3	1:A:880:PRO:HG3	1.91	0.52
1:B:679:GLU:H	1:B:679:GLU:CD	2.13	0.52
3:B:1943:IE6:H13	4:B:2020:HOH:O	2.12	0.50
1:A:872:ILE:HG21	1:A:901:PRO:HB2	1.96	0.47
1:B:726:ILE:O	1:B:730:LYS:HB2	2.14	0.47
1:B:847:ALA:HB3	1:B:850:ILE:HG12	1.96	0.47
1:A:918:CYS:O	1:A:926:ARG:HD3	2.14	0.47
1:A:849:GLU:H	1:A:849:GLU:HG3	1.22	0.47
1:A:710:GLU:HG2	1:A:751:LYS:HG2	1.97	0.46
1:A:808:ASN:OD1	3:A:1942:IE6:H201	2.17	0.45
1:A:844:GLN:HG2	4:A:2076:HOH:O	2.17	0.44
1:B:734:HIS:HB3	1:B:737:ILE:HD13	1.99	0.44
1:A:822:ASP:OD2	3:A:1942:IE6:H202	2.19	0.43
1:A:883:GLU:H	1:A:883:GLU:CD	2.22	0.42
1:B:939:LYS:HA	1:B:940:VAL:HA	1.92	0.42
1:A:755:GLU:O	3:A:1942:IE6:H07	2.20	0.42
1:B:676:GLU:OE1	2:B:1942:GOL:H11	2.20	0.42
1:B:804:ILE:HB	1:B:866:SER:HB3	2.02	0.41
1:A:728:LEU:HD11	1:A:799:ILE:HG12	2.03	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	251/318 (79%)	243 (97%)	7 (3%)	1 (0%)	34	38
1	B	252/318 (79%)	245 (97%)	6 (2%)	1 (0%)	34	38
All	All	503/636 (79%)	488 (97%)	13 (3%)	2 (0%)	34	38



All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	822	ASP
1	B	822	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/274 (76%)	199 (96%)	9 (4%)	29	35
1	B	205/274 (75%)	200 (98%)	5 (2%)	49	59
All	All	413/548 (75%)	399 (97%)	14 (3%)	37	46

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	674	ASP
1	A	745	SER
1	A	809	VAL
1	A	825	THR
1	A	838	GLU
1	A	849	GLU
1	A	883	GLU
1	A	936	GLU
1	A	939	LYS
1	B	671	LEU
1	B	724	GLU
1	B	728	LEU
1	B	733	LYS
1	B	886	GLU

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	GOL	A	1941	-	5,5,5	0.51	0	5,5,5	1.41	1 (20%)
2	GOL	B	1942	-	5,5,5	0.29	0	5,5,5	0.63	0
3	IE6	A	1942	-	20,24,24	3.64	8 (40%)	18,35,35	3.29	9 (50%)
3	IE6	B	1943	-	20,24,24	3.67	8 (40%)	18,35,35	2.58	9 (50%)

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	GOL	A	1941	-	-	1/4/4/4	-
2	GOL	B	1942	-	-	3/4/4/4	-
3	IE6	A	1942	-	-	4/8/15/15	0/3/3/3
3	IE6	B	1943	-	-	1/8/15/15	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1942	IE6	C07-N08	7.65	1.47	1.32
3	B	1943	IE6	C07-N08	7.54	1.47	1.32
3	A	1942	IE6	S16-N19	7.50	1.73	1.61
3	B	1943	IE6	C09-N08	-7.44	1.26	1.37
3	A	1942	IE6	C09-N08	-7.29	1.27	1.37
3	B	1943	IE6	S16-N19	6.88	1.72	1.61
3	B	1943	IE6	C05-C11	-6.57	1.41	1.48
3	A	1942	IE6	C05-C11	-5.56	1.42	1.48
3	A	1942	IE6	C06-C07	5.15	1.49	1.38
3	B	1943	IE6	C06-C07	4.71	1.48	1.38
3	B	1943	IE6	C03-C02	-4.11	1.34	1.39
3	A	1942	IE6	C03-C02	-3.76	1.34	1.39
3	B	1943	IE6	C04-C09	-3.32	1.34	1.43
3	A	1942	IE6	C04-C09	-3.10	1.34	1.43
3	A	1942	IE6	O18-S16	2.52	1.46	1.43
3	B	1943	IE6	O18-S16	2.10	1.45	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1942	IE6	C06-C07-N08	-6.78	114.09	124.58
3	B	1943	IE6	C06-C07-N08	-6.12	115.10	124.58
3	A	1942	IE6	O18-S16-O17	5.12	125.84	119.55
3	A	1942	IE6	O17-S16-C14	-4.93	99.55	107.66
3	A	1942	IE6	C14-S16-N19	-4.56	101.89	107.82
3	B	1943	IE6	O18-S16-N19	4.52	114.10	107.04
3	A	1942	IE6	C07-C06-C05	4.14	123.11	120.00
3	A	1942	IE6	C11-C05-C04	3.98	129.75	122.11
3	A	1942	IE6	C06-C05-C11	-3.90	113.80	120.21
3	A	1942	IE6	O17-S16-N19	3.80	112.98	107.04
3	B	1943	IE6	C11-C05-C04	3.27	128.39	122.11
3	B	1943	IE6	C06-C05-C11	-3.26	114.86	120.21
3	B	1943	IE6	O17-S16-C14	-2.77	103.09	107.66
3	B	1943	IE6	C07-C06-C05	2.69	122.02	120.00
3	A	1942	IE6	C07-N08-C09	2.68	119.91	116.60
2	A	1941	GOL	C3-C2-C1	-2.41	102.34	111.70
3	B	1943	IE6	C07-N08-C09	2.40	119.57	116.60
3	B	1943	IE6	C14-S16-N19	-2.25	104.90	107.82
3	B	1943	IE6	O18-S16-O17	2.03	122.04	119.55

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1943	IE6	N19-C20-C21-N22
3	A	1942	IE6	C20-N19-S16-O18
3	A	1942	IE6	C20-N19-S16-C14
2	B	1942	GOL	O1-C1-C2-C3
2	B	1942	GOL	C1-C2-C3-O3
3	A	1942	IE6	N19-C20-C21-N22
3	A	1942	IE6	C20-N19-S16-O17
2	B	1942	GOL	O2-C2-C3-O3
2	A	1941	GOL	O2-C2-C3-O3

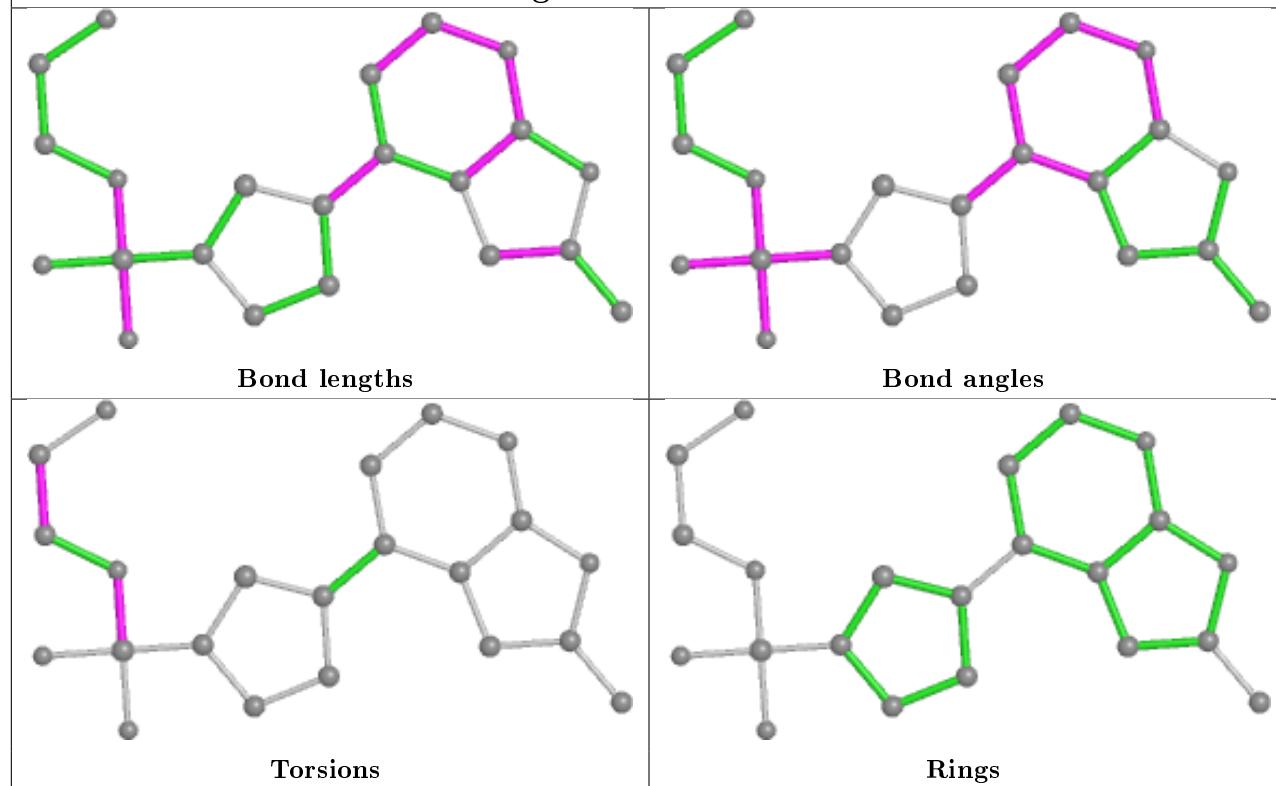
There are no ring outliers.

3 monomers are involved in 5 short contacts:

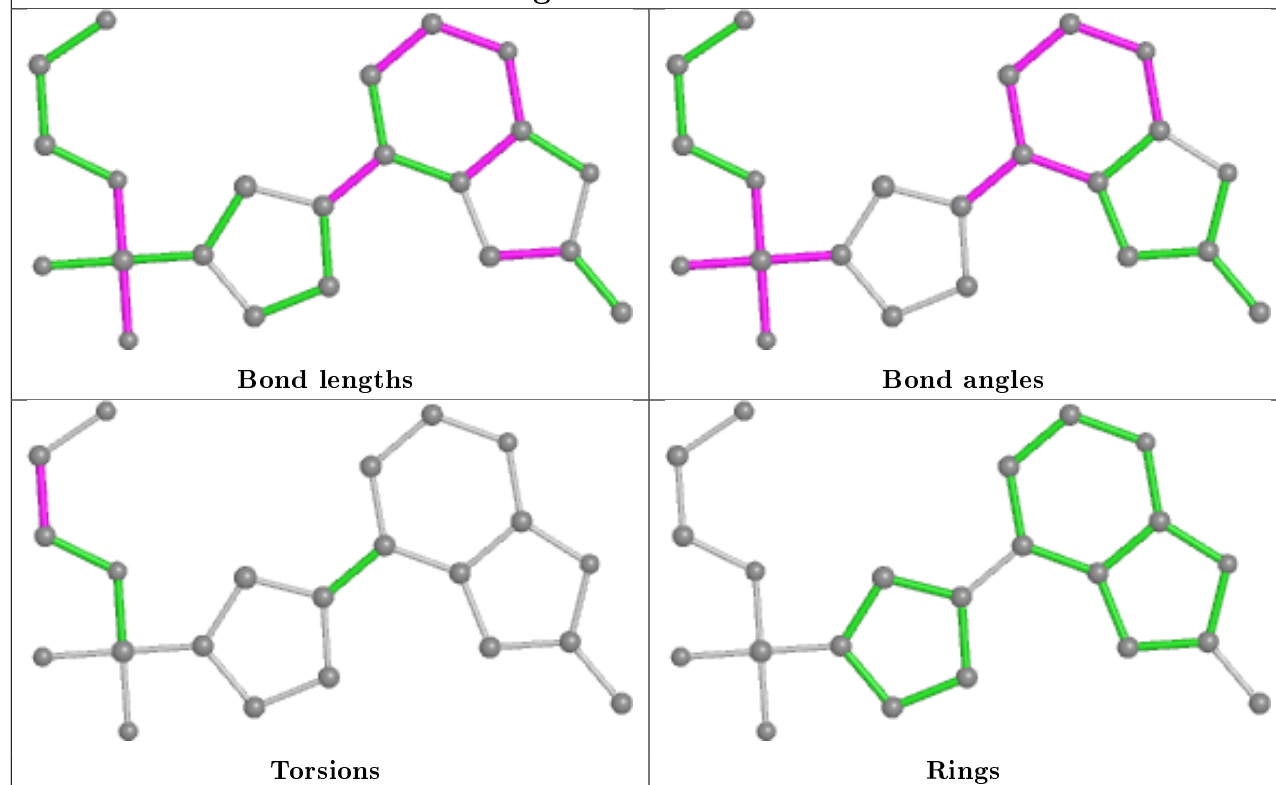
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1942	GOL	1	0
3	A	1942	IE6	3	0
3	B	1943	IE6	1	0

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

## Ligand IE6 A 1942



## Ligand IE6 B 1943



## 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	257/318 (80%)	0.44	7 (2%) 54 64	24, 41, 76, 101	0
1	B	257/318 (80%)	1.02	33 (12%) 3 6	31, 54, 92, 110	0
All	All	514/636 (80%)	0.73	40 (7%) 13 19	24, 47, 88, 110	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	884	LEU	12.8
1	B	851	ILE	6.6
1	A	829	LEU	5.4
1	B	858	TYR	4.6
1	B	896	MET	4.4
1	B	843	LEU	4.1
1	B	881	PHE	4.1
1	B	916	LEU	3.9
1	B	846	MET	3.9
1	B	839	PHE	3.8
1	B	855	PRO	3.6
1	B	885	GLY	3.6
1	B	889	ALA	3.4
1	B	892	PHE	3.2
1	B	840	THR	3.2
1	A	670	LEU	3.2
1	B	850	ILE	3.1
1	B	940	VAL	2.9
1	A	671	LEU	2.9
1	B	691	TYR	2.9
1	B	848	PRO	2.8
1	A	830	ALA	2.8
1	A	728	LEU	2.7
1	B	921	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	847	ALA	2.6
1	B	726	ILE	2.6
1	B	841	GLY	2.5
1	B	748	GLY	2.5
1	B	711	ILE	2.4
1	A	909	ALA	2.4
1	B	744	PHE	2.4
1	B	895	GLY	2.3
1	B	685	VAL	2.3
1	B	738	VAL	2.3
1	B	879	PRO	2.2
1	B	674[A]	ASP	2.2
1	B	830	ALA	2.2
1	A	744	PHE	2.2
1	B	799	ILE	2.1
1	B	753	PHE	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 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
2	GOL	B	1942	6/6	0.86	0.21	53,55,55,57	0
3	IE6	B	1943	22/22	0.90	0.21	34,44,58,67	0
2	GOL	A	1941	6/6	0.92	0.17	49,50,51,51	0
3	IE6	A	1942	22/22	0.94	0.17	27,35,61,63	0

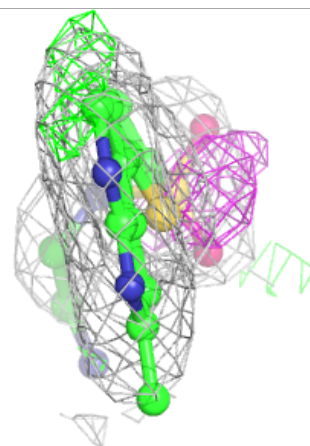
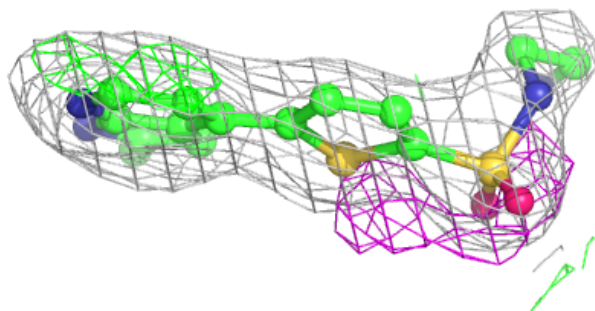
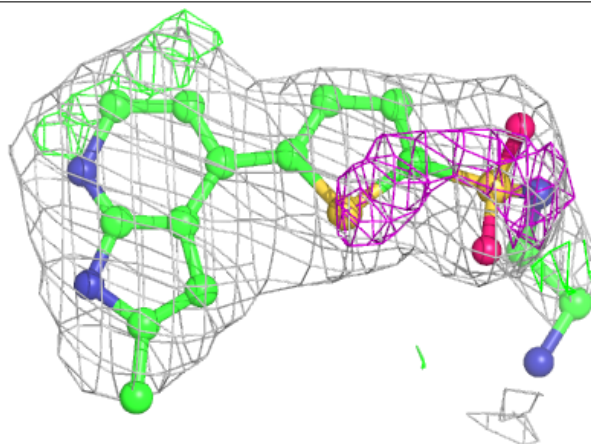
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

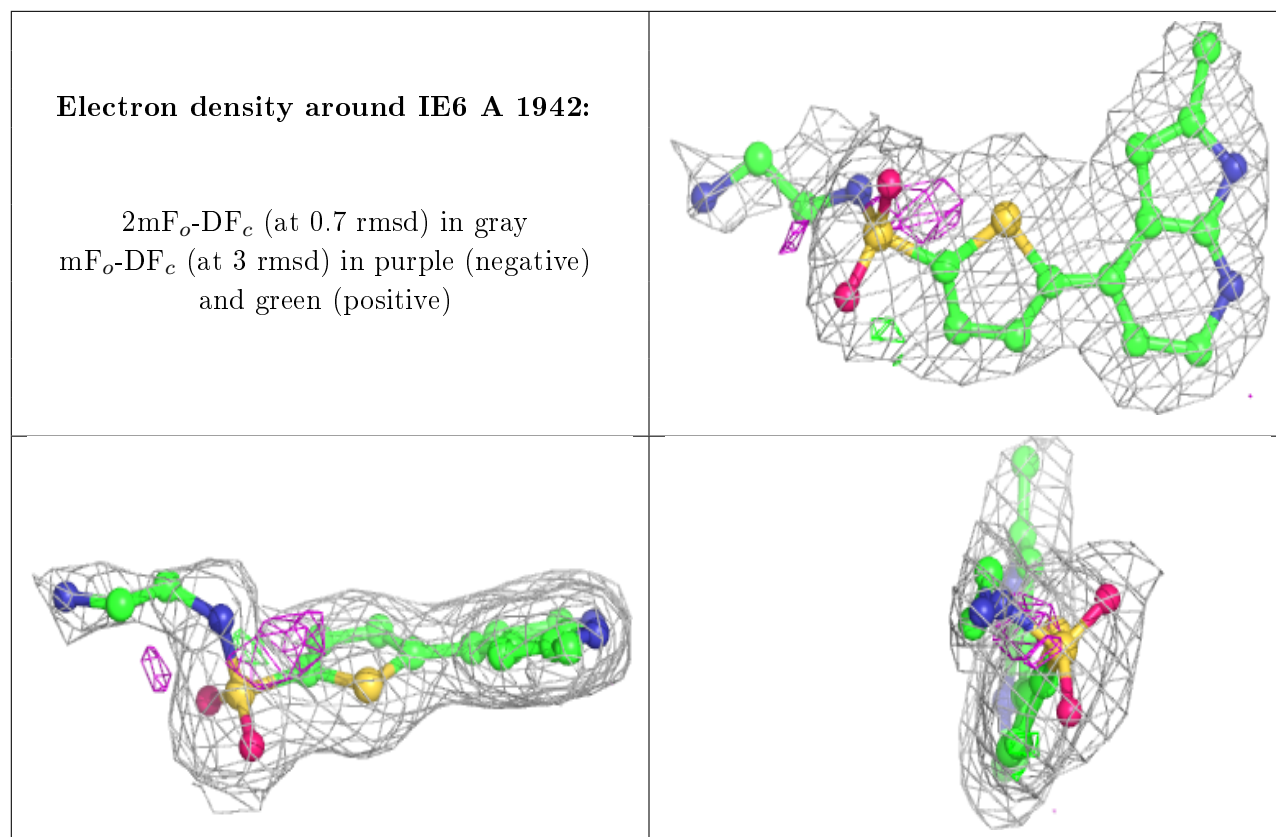


as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around IE6 B 1943:**

$2mF_o-DF_c$  (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.