



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2025 – 11:16 am BST

PDB ID : 9G5A / pdb\_00009g5a  
Title : The structure of Aspergillus fumigatus UDP-GlcNAc pyrophosphorylase in complex with a fragment  
Authors : Yan, K.  
Deposited on : 2024-07-16  
Resolution : 1.87 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

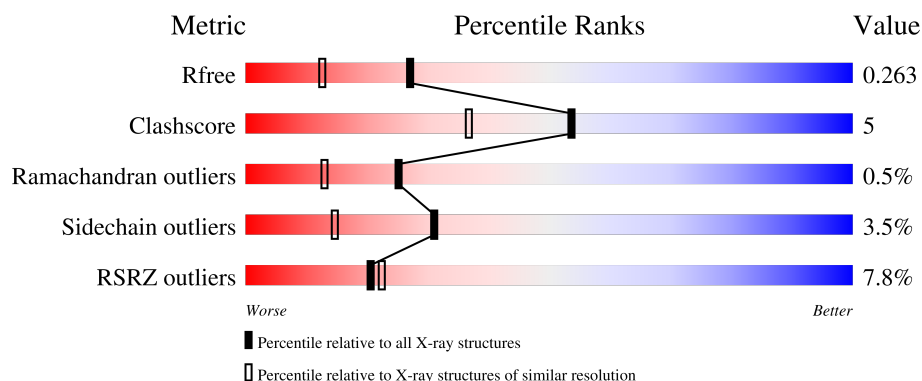
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 1.87 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))
$R_{free}$	164625	1090 (1.88-1.88)
Clashscore	180529	1144 (1.88-1.88)
Ramachandran outliers	177936	1135 (1.88-1.88)
Sidechain outliers	177891	1135 (1.88-1.88)
RSRZ outliers	164620	1090 (1.88-1.88)

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	B	484	 5% 85% 11% ..
2	A	484	 10% 82% 12% . 5%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7416 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 UDP-N-acetylglucosamine diphosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	472	Total	C	N	O	S	0	1	0
			3680	2349	627	691	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	26	GLY	-	expression tag	UNP A0A229XUD0

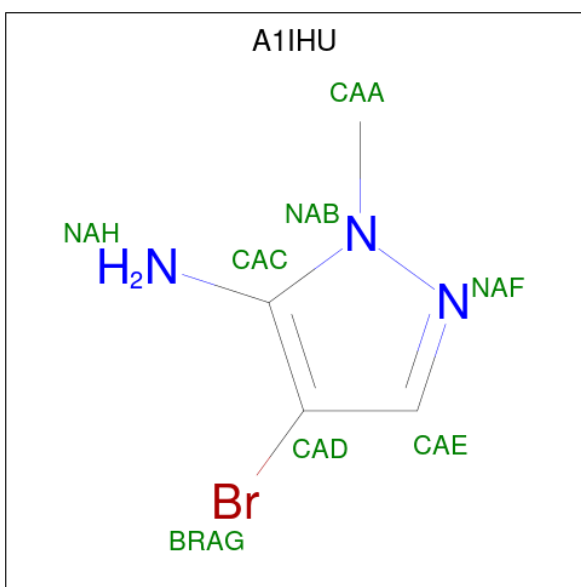
- Molecule 2 is a protein called UDP-N-acetylglucosamine diphosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	462	Total	C	N	O	S	0	2	0
			3597	2295	612	676	14			

There is a discrepancy between the modelled and reference sequences:

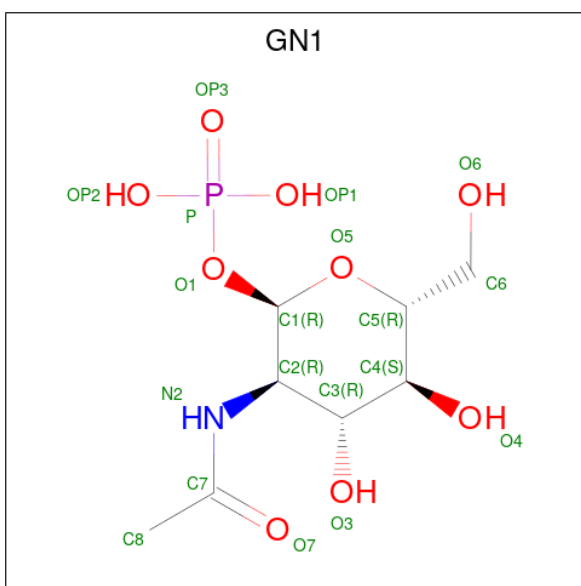
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	expression tag	UNP A0A229XUD0

- Molecule 3 is 4-bromanyl-2-methyl-pyrazol-3-amine (CCD ID: A1IHU) (formula: C<sub>4</sub>H<sub>6</sub>BrN<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	Br	C	N	0	0
			8	1	4	3		
3	B	1	Total	Br	C	N	0	0
			8	1	4	3		
3	B	1	Total	Br	C	N	0	0
			8	1	4	3		

- Molecule 4 is 2-acetamido-2-deoxy-1-O-phosphono-alpha-D-glucopyranose (CCD ID: GN1) (formula:  $C_8H_{16}NO_9P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			19	8	1	9	1		

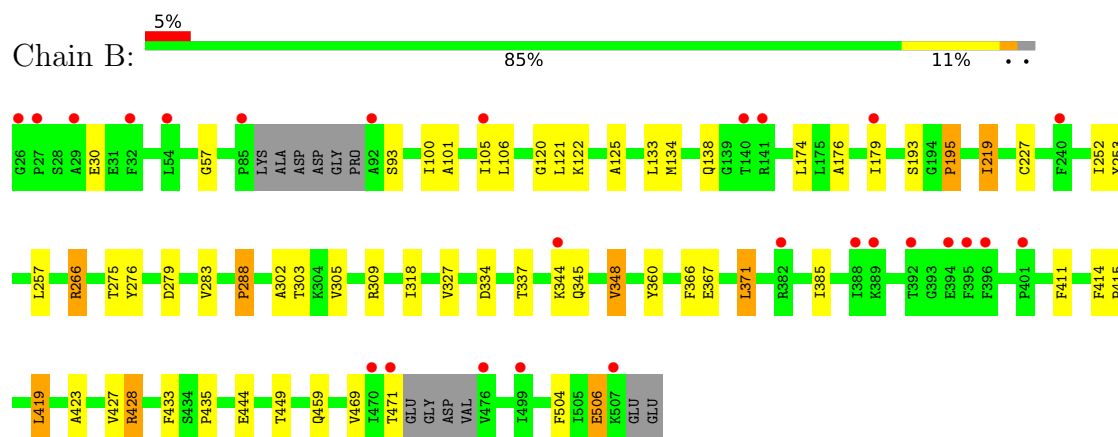
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	63	Total	O	0	0
			63	63		
5	A	33	Total	O	0	0
			33	33		

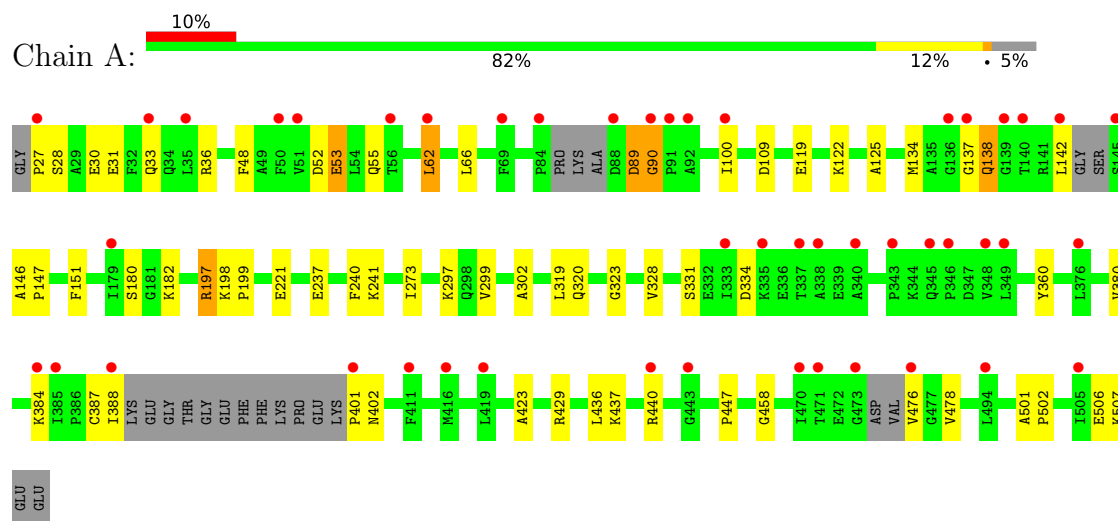
### 3 Residue-property plots [i](#)

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: UDP-N-acetylglucosamine diphosphorylase



- Molecule 2: UDP-N-acetylglucosamine diphosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.37Å 137.50Å 143.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.36 – 1.87 51.36 – 1.87	Depositor EDS
% Data completeness (in resolution range)	98.4 (51.36-1.87) 98.4 (51.36-1.87)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, $R_{free}$	0.226 , 0.259 0.233 , 0.263	Depositor DCC
$R_{free}$ test set	4629 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7416	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: GN1, YCM, A1IHU

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	B	0.68	0/3751	1.08	3/5065 (0.1%)
2	A	0.61	0/3678	1.02	1/4968 (0.0%)
All	All	0.65	0/7429	1.05	4/10033 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
2	A	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	PHE	CA-CB-CG	5.75	119.55	113.80
1	B	195	PRO	N-CA-C	5.51	121.09	113.65
2	A	109	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	288	PRO	CB-CA-C	-5.05	104.33	112.21

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	429	ARG	Sidechain
1	B	309	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	428	ARG	Sidechain

## 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	B	3680	0	3654	35	0
2	A	3597	0	3560	35	0
3	B	24	0	0	0	0
4	B	19	0	0	0	0
5	A	33	0	0	0	0
5	B	63	0	0	0	0
All	All	7416	0	7214	69	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 5.

All (69) 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:227:CYS:HB3	1:B:385:ILE:HD13	1.68	0.76
1:B:266:ARG:NH1	1:B:367:GLU:OE1	2.21	0.73
2:A:27:PRO:O	2:A:31:GLU:OE1	2.07	0.72
1:B:106:LEU:HD21	1:B:428:ARG:HG2	1.74	0.70
2:A:320:GLN:HE21	2:A:323:GLY:HA2	1.58	0.69
1:B:504:PHE:CZ	1:B:506:GLU:HG2	2.29	0.68
1:B:138:GLN:HE22	1:B:195:PRO:HG2	1.60	0.67
1:B:504:PHE:CZ	1:B:506:GLU:CG	2.79	0.66
2:A:146:ALA:HB1	2:A:147:PRO:HD2	1.81	0.63
1:B:459:GLN:HG3	1:B:469:VAL:HG21	1.82	0.61
2:A:146:ALA:HB1	2:A:147:PRO:CD	2.31	0.60
1:B:345:GLN:HB3	1:B:348:VAL:HG13	1.83	0.60
1:B:504:PHE:CZ	1:B:506:GLU:HG3	2.41	0.55
1:B:101:ALA:HB2	1:B:419:LEU:CD1	2.36	0.54
2:A:62:LEU:HD22	2:A:66:LEU:CD1	2.37	0.54
1:B:101:ALA:HB2	1:B:419:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:GLY:HA2	2:A:331:SER:HB3	1.89	0.53
2:A:55:GLN:HE21	2:A:55:GLN:HA	1.73	0.52
1:B:305:VAL:CG1	1:B:318:ILE:HD12	2.39	0.52
2:A:297:LYS:HB2	2:A:299:VAL:HG13	1.91	0.52
2:A:384:LYS:CB	2:A:401:PRO:N	2.74	0.51
1:B:302:ALA:HA	1:B:423:ALA:O	2.12	0.50
2:A:125:ALA:HB1	2:A:180:SER:HB3	1.93	0.50
2:A:36:ARG:HA	2:A:48:PHE:CE2	2.47	0.49
2:A:89:ASP:O	2:A:90:GLY:C	2.55	0.48
1:B:327:VAL:HB	1:B:411:PHE:CD1	2.48	0.48
1:B:371:LEU:N	1:B:371:LEU:HD23	2.29	0.47
2:A:52:ASP:O	2:A:53:GLU:CB	2.62	0.47
1:B:444:GLU:HA	1:B:449:THR:HG21	1.96	0.47
2:A:142:LEU:HB2	2:A:151:PHE:CE2	2.50	0.47
1:B:252:ILE:HG23	1:B:253:TYR:N	2.30	0.46
2:A:137:GLY:O	2:A:138:GLN:C	2.59	0.46
2:A:319:LEU:HD11	2:A:328:VAL:CG2	2.45	0.46
1:B:276:TYR:CD2	1:B:283:VAL:HG21	2.51	0.45
2:A:52:ASP:O	2:A:53:GLU:HB3	2.16	0.45
2:A:237:GLU:OE1	2:A:241:LYS:NZ	2.44	0.45
1:B:105:ILE:HG13	1:B:427:VAL:HG12	1.99	0.45
1:B:133:LEU:HD13	1:B:276:TYR:CZ	2.52	0.45
1:B:345:GLN:HB3	1:B:348:VAL:CG1	2.47	0.45
1:B:345:GLN:CB	1:B:348:VAL:HG13	2.44	0.44
2:A:319:LEU:C	2:A:319:LEU:HD12	2.42	0.44
1:B:179:ILE:HD12	1:B:179:ILE:C	2.42	0.44
2:A:142:LEU:HD13	2:A:436:LEU:HD21	2.00	0.44
1:B:279:ASP:C	1:B:279:ASP:OD1	2.61	0.44
2:A:62:LEU:HD22	2:A:66:LEU:HD11	1.99	0.44
2:A:440:ARG:HG2	2:A:447:PRO:HG2	2.00	0.44
2:A:198:LYS:N	2:A:199:PRO:CD	2.81	0.44
1:B:219:ILE:N	1:B:219:ILE:CD1	2.80	0.43
1:B:193:SER:HB2	1:B:195:PRO:HD2	2.01	0.43
1:B:125:ALA:HB2	1:B:176:ALA:HB1	2.01	0.43
1:B:433:PHE:CZ	1:B:435:PRO:HG3	2.54	0.43
1:B:120:GLY:HA3	1:B:288:PRO:O	2.20	0.42
1:B:134:MET:HE2	1:B:275:THR:HG22	2.02	0.42
1:B:414:PHE:N	1:B:415:PRO:HD2	2.35	0.42
2:A:273:ILE:HD12	2:A:273:ILE:N	2.35	0.42
2:A:506:GLU:HG3	2:A:507:LYS:N	2.34	0.42
2:A:197:ARG:HH11	2:A:221:GLU:HG3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:302:ALA:HA	2:A:423:ALA:O	2.20	0.41
2:A:501:ALA:HA	2:A:502:PRO:C	2.45	0.41
1:B:266:ARG:NH1	1:B:367:GLU:CD	2.78	0.41
1:B:360:TYR:CD1	1:B:360:TYR:C	2.99	0.41
2:A:360:TYR:CD1	2:A:360:TYR:C	2.98	0.41
2:A:62:LEU:HG	2:A:240:PHE:C	2.46	0.41
2:A:458:GLY:HA3	2:A:478:VAL:O	2.20	0.40
2:A:387:CYS:O	2:A:388:ILE:C	2.64	0.40
2:A:119:GLU:HA	2:A:122:LYS:HG2	2.02	0.40
1:B:334:ASP:OD1	1:B:337:THR:HG23	2.20	0.40
2:A:100:ILE:H	2:A:100:ILE:HD12	1.86	0.40
2:A:119:GLU:HG2	2:A:122:LYS:HE3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	B	466/484 (96%)	453 (97%)	13 (3%)	0	100	100
2	A	454/484 (94%)	430 (95%)	19 (4%)	5 (1%)	12	3
All	All	920/968 (95%)	883 (96%)	32 (4%)	5 (0%)	25	13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	53	GLU
2	A	138	GLN
2	A	334	ASP
2	A	402	ASN
2	A	90	GLY

### 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	B	391/407 (96%)	375 (96%)	16 (4%)	26	10
2	A	384/408 (94%)	373 (97%)	11 (3%)	37	20
All	All	775/815 (95%)	748 (96%)	27 (4%)	31	15

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	30	GLU
1	B	93	SER
1	B	100	ILE
1	B	121	LEU
1	B	122	LYS
1	B	174	LEU
1	B	219	ILE
1	B	257	LEU
1	B	266	ARG
1	B	303	THR
1	B	344	LYS
1	B	348	VAL
1	B	371	LEU
1	B	419	LEU
1	B	471	THR
1	B	506	GLU
2	A	28	SER
2	A	30	GLU
2	A	33	GLN
2	A	62	LEU
2	A	89	ASP
2	A	134	MET
2	A	182	LYS
2	A	197	ARG
2	A	380	VAL
2	A	437	LYS
2	A	476	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	138	GLN
1	B	230	ASN
1	B	345	GLN
2	A	55	GLN
2	A	83	ASN
2	A	138	GLN
2	A	222	GLN
2	A	230	ASN
2	A	249	ASN
2	A	320	GLN
2	A	408	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	YCM	B	277	1	7,9,10	0.69	0	4,10,12	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	YCM	B	277	1	-	1/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	277	YCM	SG-CD-CE-NZ2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
3	A1IHU	B	604	-	6,8,8	1.51	1 (16%)	5,11,11	2.39	2 (40%)
3	A1IHU	B	603	-	6,8,8	2.59	2 (33%)	5,11,11	1.25	0
4	GN1	B	602	-	18,19,19	0.57	0	27,28,28	1.09	4 (14%)
3	A1IHU	B	601	-	6,8,8	1.91	2 (33%)	5,11,11	1.61	1 (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
4	GN1	B	602	-	-	2/10/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1IHU	B	603	-	-	-	0/1/1/1
3	A1IHU	B	601	-	-	-	0/1/1/1
3	A1IHU	B	604	-	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	A1IHU	BRAG-CAD	4.97	2.01	1.89
3	B	601	A1IHU	BRAG-CAD	3.70	1.98	1.89
3	B	603	A1IHU	CAD-CAC	-3.11	1.32	1.38
3	B	604	A1IHU	CAE-CAD	-2.26	1.32	1.37
3	B	601	A1IHU	CAD-CAC	-2.02	1.34	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	604	A1IHU	CAE-NAF-NAB	4.27	108.68	104.23
3	B	601	A1IHU	CAE-NAF-NAB	3.01	107.37	104.23
4	B	602	GN1	C1-C2-N2	2.63	115.54	111.00
4	B	602	GN1	O5-C1-O1	-2.55	108.03	111.36
3	B	604	A1IHU	CAE-CAD-CAC	2.49	110.30	107.16
4	B	602	GN1	C4-C3-C2	-2.05	107.34	110.34
4	B	602	GN1	C3-C2-N2	2.04	114.47	110.62

There are no chirality outliers.

All (2) torsion outliers are listed below:

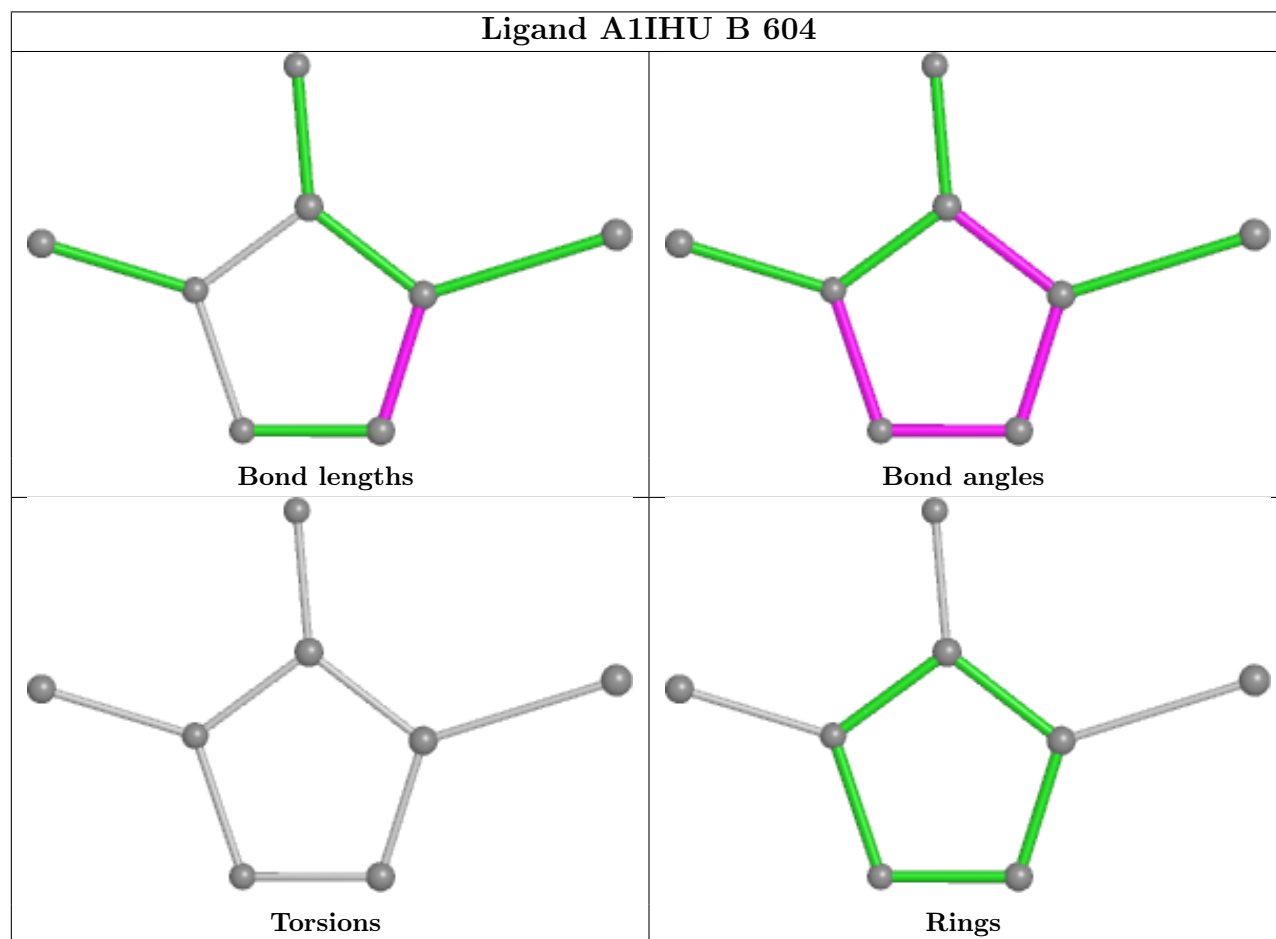
Mol	Chain	Res	Type	Atoms
4	B	602	GN1	C1-O1-P-OP2
4	B	602	GN1	C1-O1-P-OP3

There are no ring outliers.

No monomer is involved in short contacts.

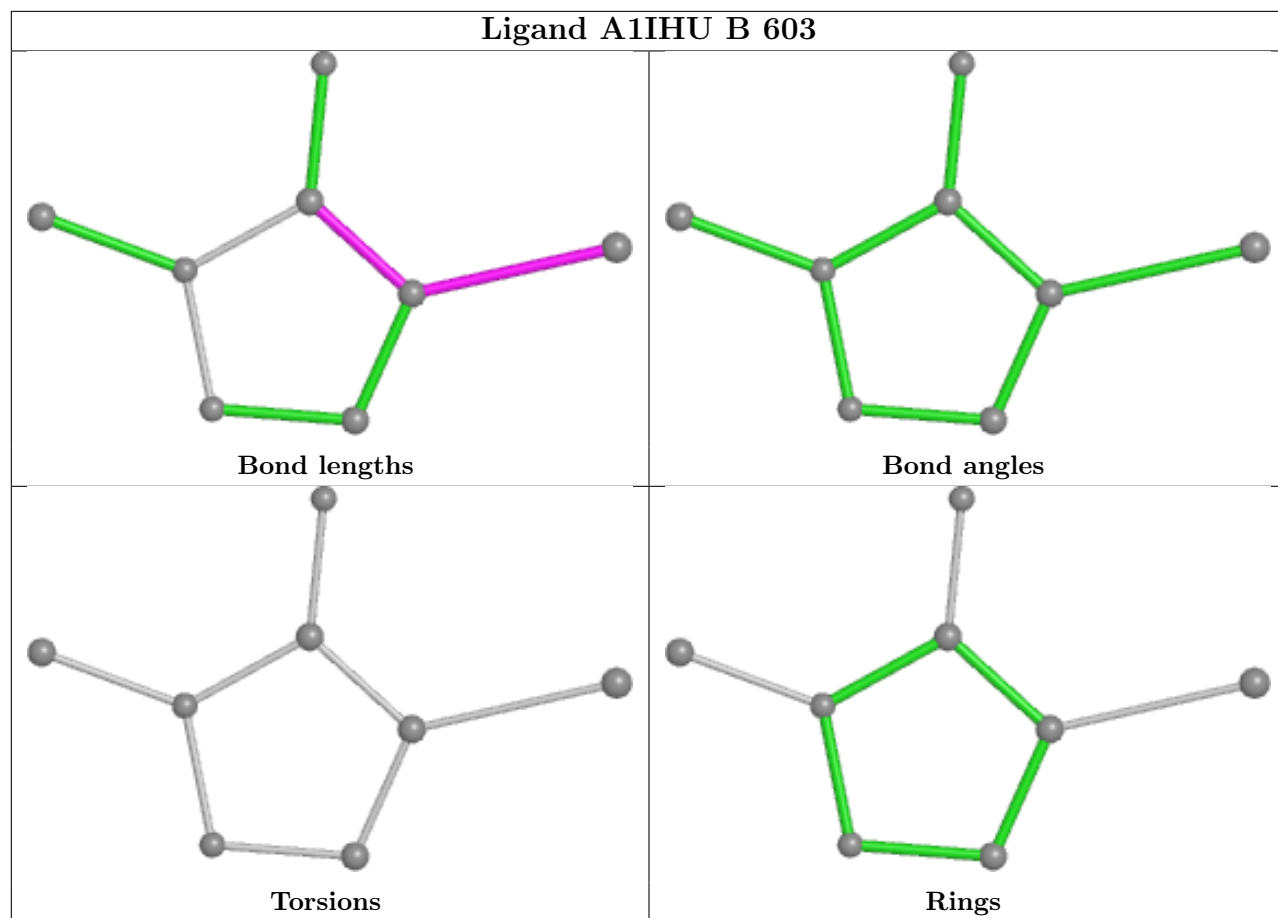
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

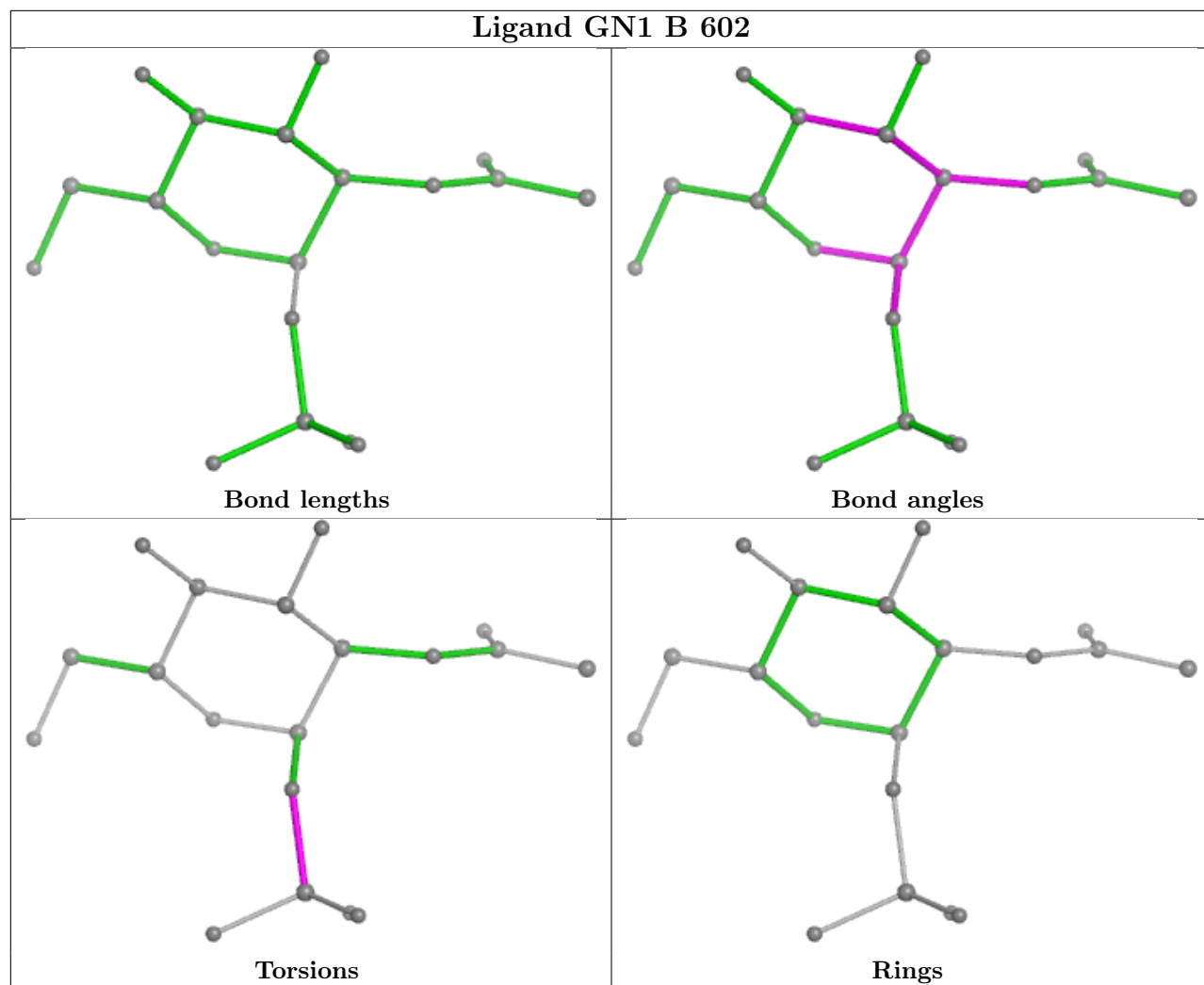


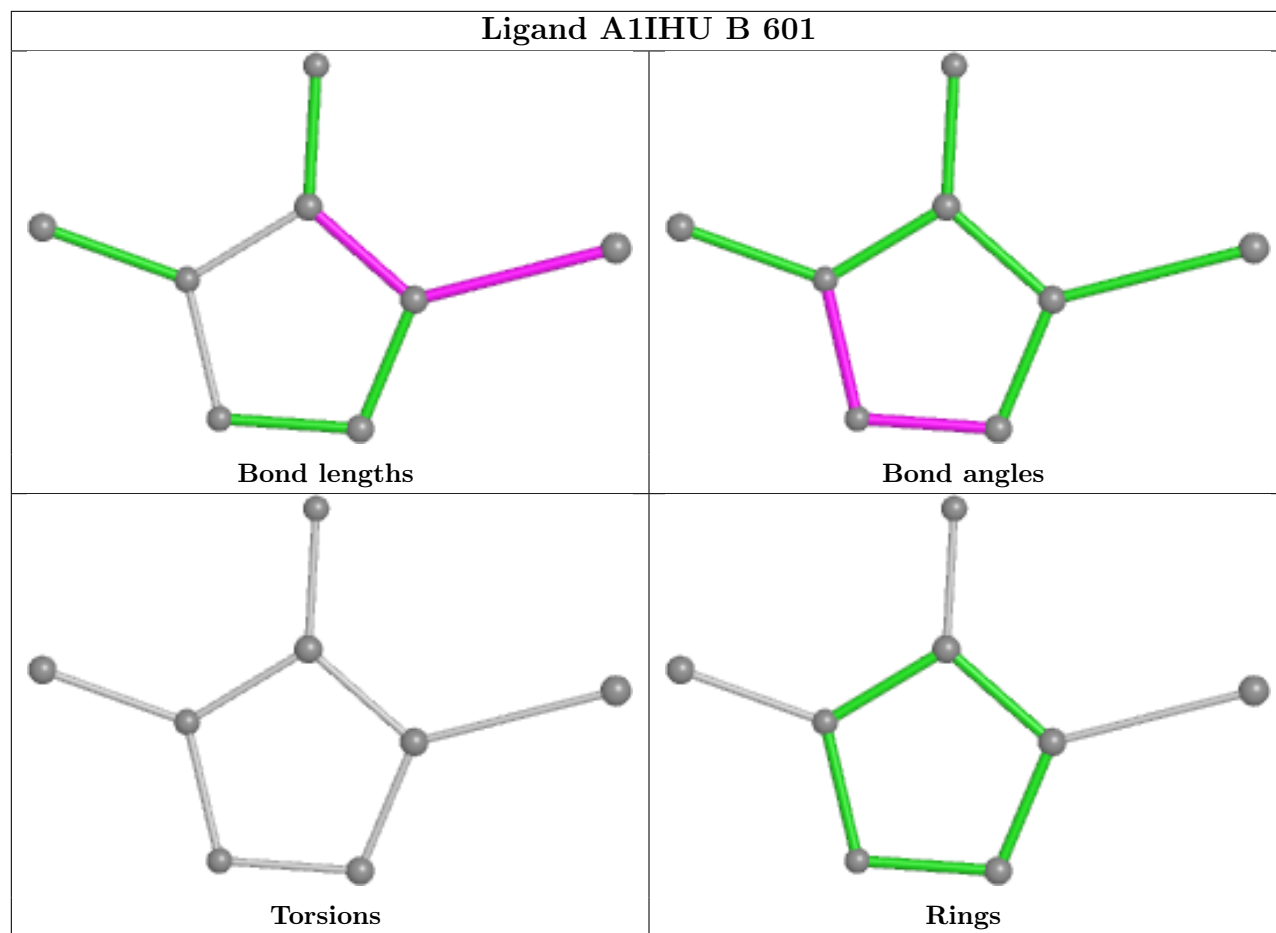


## Ligand A1IHU B 603



## Ligand GN1 B 602





## 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	B	471/484 (97%)	0.61	26 (5%)	32 32	27, 48, 88, 120	1 (0%)
2	A	462/484 (95%)	0.93	47 (10%)	13 15	26, 57, 92, 131	2 (0%)
All	All	933/968 (96%)	0.77	73 (7%)	20 22	26, 52, 91, 131	3 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	136	GLY	6.5
2	A	476	VAL	5.2
1	B	471	THR	5.0
1	B	27	PRO	4.5
1	B	92	ALA	4.5
2	A	27	PRO	4.4
2	A	179	ILE	4.3
2	A	385	ILE	4.0
1	B	470	ILE	3.9
2	A	401	PRO	3.8
2	A	388	ILE	3.7
2	A	100	ILE	3.5
2	A	139	GLY	3.5
2	A	90	GLY	3.4
2	A	343	PRO	3.4
2	A	333	ILE	3.3
1	B	395	PHE	3.3
1	B	476	VAL	3.2
2	A	335	LYS	3.2
1	B	26	GLY	3.1
1	B	29	ALA	3.1
1	B	140	THR	3.1
1	B	179	ILE	3.0
1	B	396	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
2	A	337	THR	3.0
1	B	240	PHE	3.0
1	B	54	LEU	3.0
1	B	389	LYS	2.9
2	A	88	ASP	2.9
2	A	33	GLN	2.8
2	A	416	MET	2.8
2	A	56	THR	2.8
2	A	84	PRO	2.8
1	B	392	THR	2.7
2	A	340	ALA	2.7
2	A	92	ALA	2.6
2	A	137	GLY	2.6
2	A	142	LEU	2.6
1	B	32	PHE	2.6
2	A	91	PRO	2.6
1	B	499	ILE	2.5
2	A	62	LEU	2.5
1	B	85	PRO	2.5
1	B	507	LYS	2.5
2	A	419	LEU	2.5
2	A	145	SER	2.4
2	A	505	ILE	2.4
1	B	382	ARG	2.4
2	A	50	PHE	2.4
2	A	384	LYS	2.4
2	A	69	PHE	2.4
2	A	473	GLY	2.4
2	A	140	THR	2.4
2	A	471	THR	2.4
2	A	349	LEU	2.3
2	A	494	LEU	2.3
1	B	388	ILE	2.3
2	A	440	ARG	2.3
2	A	348	VAL	2.3
2	A	346	PRO	2.3
2	A	51	VAL	2.3
2	A	443	GLY	2.2
2	A	470	ILE	2.2
1	B	344	LYS	2.2
2	A	345	GLN	2.2
1	B	401	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	A	376	LEU	2.2
1	B	105	ILE	2.2
1	B	141	ARG	2.1
2	A	338	ALA	2.1
2	A	411	PHE	2.1
1	B	394	GLU	2.0
2	A	35	LEU	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	YCM	B	277	10/11	0.96	0.09	32,37,43,45	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

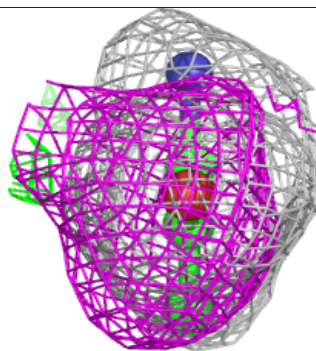
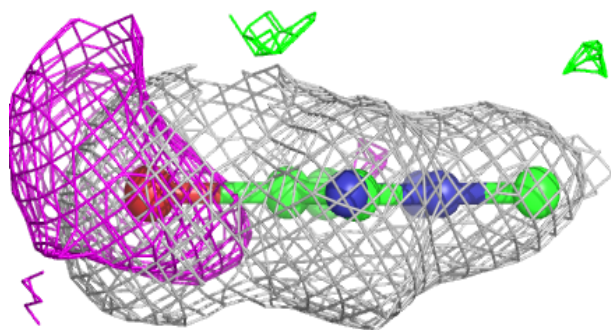
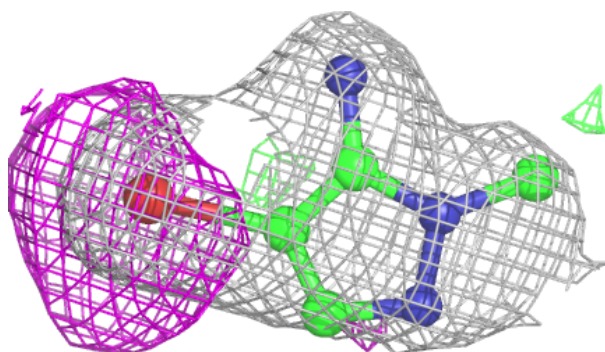
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	A1IHU	B	603	8/8	0.88	0.17	50,62,69,74	0
4	GN1	B	602	19/19	0.96	0.06	30,38,45,51	0
3	A1IHU	B	601	8/8	0.98	0.10	47,55,57,58	0
3	A1IHU	B	604	8/8	0.99	0.05	33,38,42,45	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.

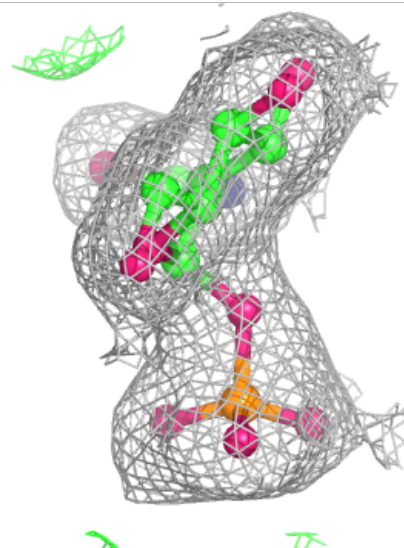
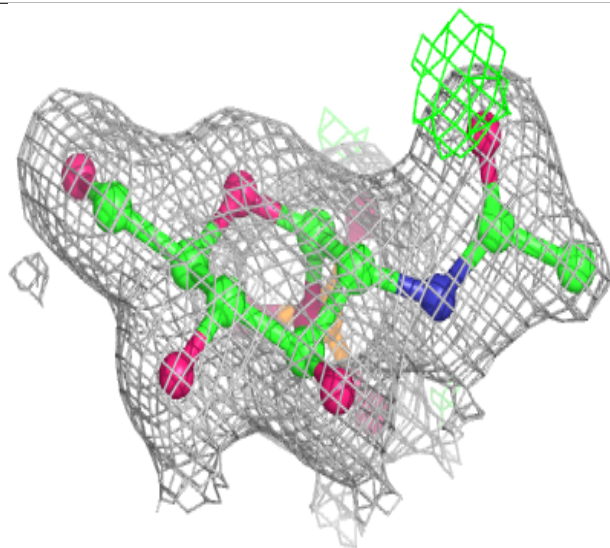
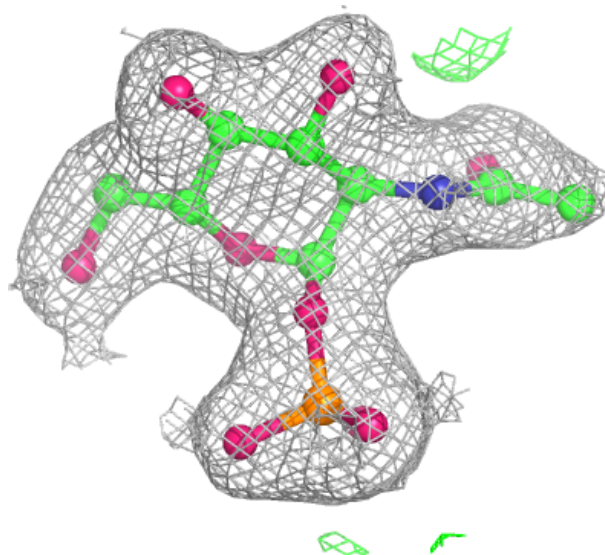
**Electron density around A1IHU B 603:**

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



**Electron density around GN1 B 602:**

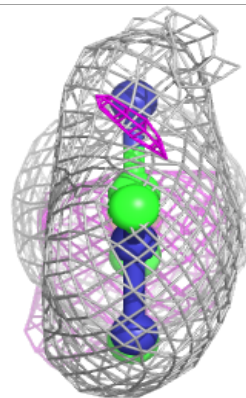
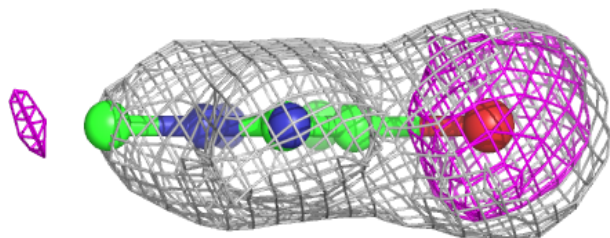
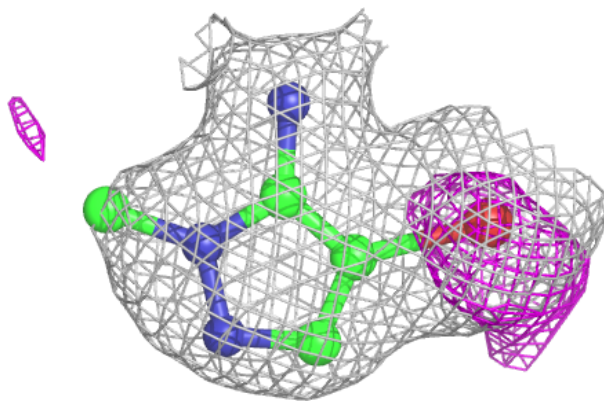
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



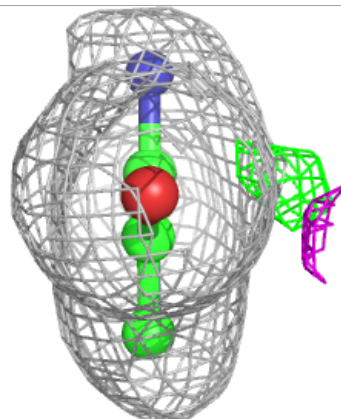
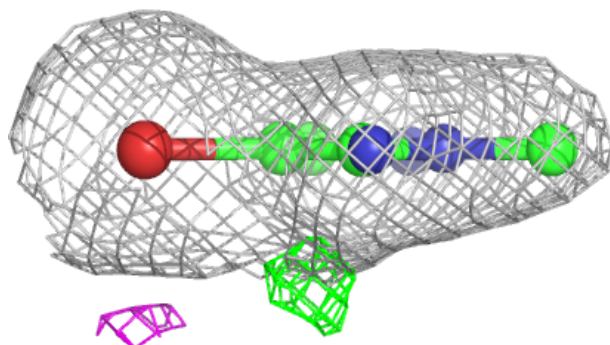
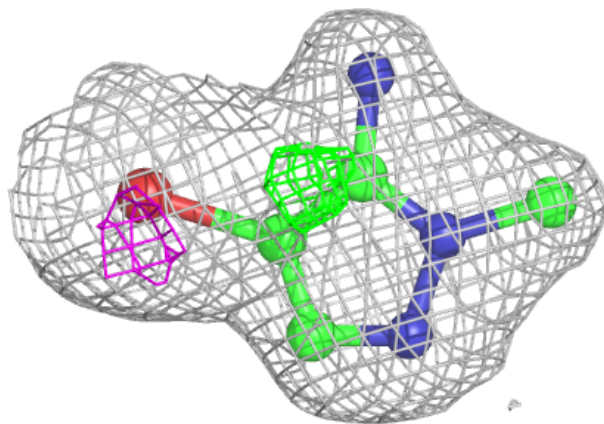


**Electron density around A1IHU B 601:**

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

**Electron density around A1IHU B 604:**

$2mF_o-DF_c$  (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.