



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:43 AM UTC

PDB ID : 9G5O / pdb\_00009g5o  
Title : The structure of *Aspergillus fumigatus* UDP-GlcNAc pyrophosphorylase in complex with a fragment  
Authors : Yan, K.  
Deposited on : 2024-07-17  
Resolution : 1.58 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

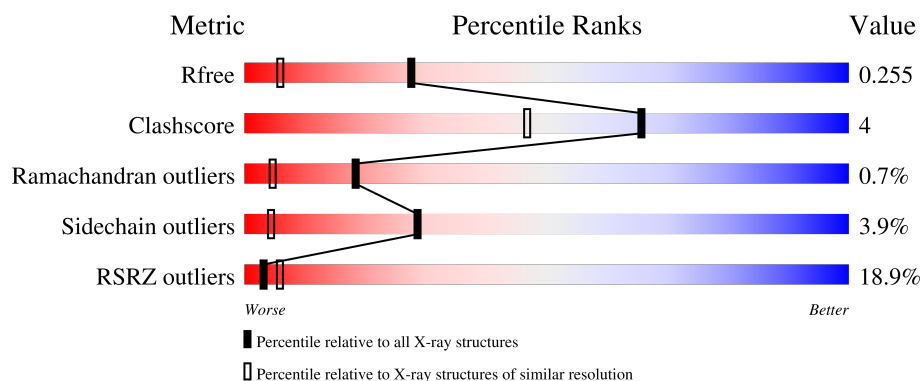
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.58 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))
$R_{free}$	180053	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	
2	A	484	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7939 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	2	0
			3691	2357	631	690	13			

There is a discrepancy between the modelled and reference sequences:

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

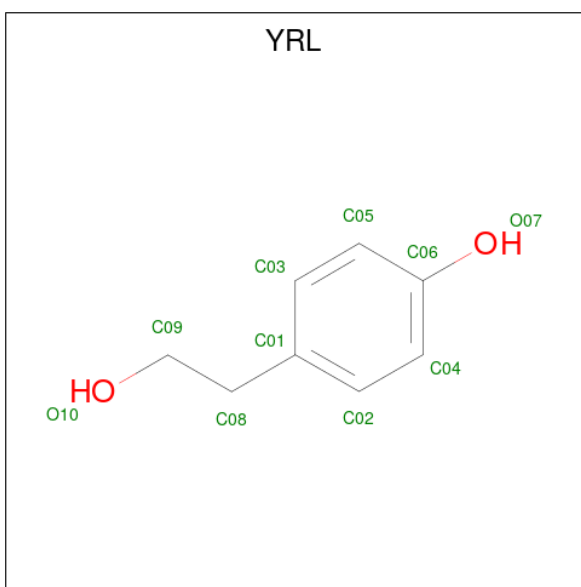
- Molecule 2 is a protein called UDP-N-acetylglucosamine diphosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	465	Total	C	N	O	S	0	4	0
			3611	2307	616	674	14			

There is a discrepancy between the modelled and reference sequences:

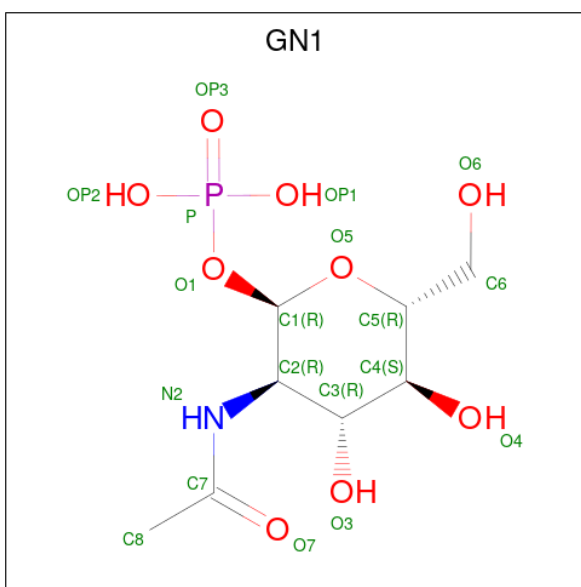
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	expression tag	UNP A0A229XUD0

- Molecule 3 is 4-(2-hydroxyethyl)phenol (CCD ID: YRL) (formula: C<sub>8</sub>H<sub>10</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



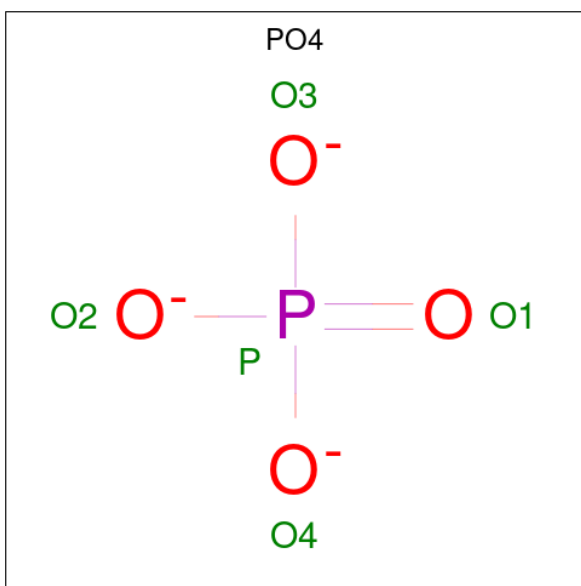
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	8	2		
3	B	1	Total	C	O	0	0
			10	8	2		
3	B	1	Total	C	O	0	0
			10	8	2		
3	A	1	Total	C	O	0	0
			10	8	2		
3	A	1	Total	C	O	0	0
			10	8	2		

- 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 PHOSPHATE ION (CCD ID: PO4) (formula:  $O_4P$ ).



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

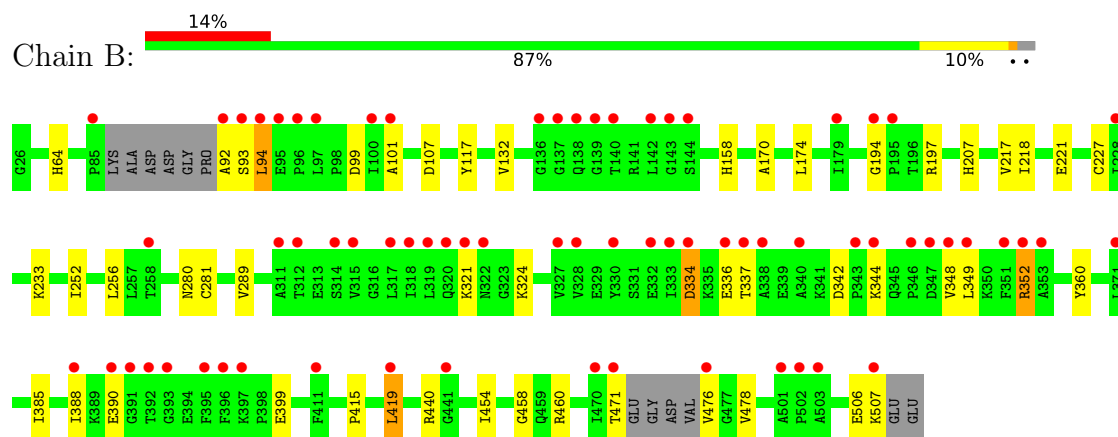
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	329	Total 329	O 329	0	0
6	A	234	Total 234	O 234	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: 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, $\alpha$ , $\beta$ , $\gamma$	56.61Å 139.76Å 144.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.33 – 1.58 49.33 – 1.58	Depositor EDS
% Data completeness (in resolution range)	90.9 (49.33-1.58) 90.9 (49.33-1.58)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, $R_{free}$	0.216 , 0.248 (Not available) , 0.255	Depositor DCC
$R_{free}$ test set	7077 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7939	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: PO4, YCM, GN1, YRL

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	0.67	0/3765	1.07	5/5081 (0.1%)
2	A	0.64	0/3701	1.06	4/5003 (0.1%)
All	All	0.66	0/7466	1.06	9/10084 (0.1%)

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 (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	337	THR	CA-CB-OG1	6.52	119.38	109.60
1	B	415	PRO	N-CA-C	6.49	122.35	113.98
1	B	194	GLY	O-C-N	-6.38	115.39	121.77
2	A	336	GLU	CB-CG-CD	6.32	123.35	112.60
2	A	275	THR	N-CA-CB	-6.17	100.13	110.80
1	B	107	ASP	CB-CA-C	-5.82	100.37	110.09
1	B	342	ASP	CA-CB-CG	5.66	118.26	112.60
2	A	247	ASP	CA-CB-CG	5.49	118.09	112.60
1	B	158	HIS	CA-CB-CG	-5.35	108.45	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	73	ARG	Sidechain
1	B	352	ARG	Sidechain
1	B	460	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	3691	0	3685	29	0
2	A	3611	0	3571	26	0
3	A	20	0	19	1	0
3	B	30	0	30	1	0
4	B	19	0	0	0	0
5	B	5	0	0	0	0
6	A	234	0	0	4	0
6	B	329	0	0	7	0
All	All	7939	0	7305	56	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 (56) 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)
2:A:230:ASN:ND2	2:A:382:ARG:HH12	1.57	1.02
2:A:230:ASN:HD21	2:A:382:ARG:HH12	0.93	0.93
2:A:230:ASN:HD21	2:A:382:ARG:NH1	1.68	0.91
2:A:249:ASN:OD1	6:A:701:HOH:O	1.93	0.86
1:B:440:ARG:NH1	6:B:701:HOH:O	2.10	0.85
2:A:334:ASP:OD1	2:A:337:THR:HG23	1.81	0.81
1:B:170:ALA:O	1:B:174:LEU:HD13	1.85	0.76
2:A:237:GLU:OE1	2:A:241:LYS:NZ	2.26	0.69
2:A:236:MET:O	2:A:387:CYS:HB2	1.95	0.67
2:A:142:LEU:C	2:A:439:ALA:HB2	2.22	0.65
1:B:101:ALA:HB2	1:B:419:LEU:HD11	1.78	0.65
1:B:174:LEU:CD1	6:B:879:HOH:O	2.44	0.65
1:B:64:HIS:HD2	6:B:973:HOH:O	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:602:YRL:H091	2:A:312:THR:HG21	1.81	0.62
1:B:101:ALA:HB2	1:B:419:LEU:CD1	2.30	0.61
1:B:132:VAL:HG11	1:B:252:ILE:HD11	1.84	0.58
1:B:92:ALA:O	1:B:94:LEU:N	2.38	0.57
2:A:169:ILE:O	2:A:173:GLN:HG3	2.04	0.57
2:A:73:ARG:HD2	6:A:882:HOH:O	2.06	0.55
1:B:94:LEU:HD23	1:B:94:LEU:O	2.08	0.54
1:B:281[A]:CYS:HB2	1:B:454:ILE:HD11	1.91	0.54
1:B:233:LYS:HD3	6:B:858:HOH:O	2.07	0.53
1:B:218:ILE:HD12	1:B:218:ILE:N	2.24	0.53
2:A:501:ALA:HA	2:A:502:PRO:C	2.34	0.53
1:B:217:VAL:C	1:B:218:ILE:HD12	2.34	0.52
1:B:349:LEU:O	1:B:352:ARG:NH1	2.40	0.52
1:B:64:HIS:HE1	6:A:800:HOH:O	1.92	0.52
1:B:227:CYS:HB3	1:B:385:ILE:HD13	1.91	0.52
2:A:204:PHE:CE2	2:A:217:VAL:HG11	2.45	0.51
2:A:500:LYS:O	2:A:503:ALA:HB2	2.10	0.51
1:B:197:ARG:C	1:B:197:ARG:HD3	2.37	0.50
2:A:506:GLU:HG3	2:A:507:LYS:N	2.27	0.49
2:A:134:MET:HE3	2:A:252:ILE:HD12	1.94	0.47
2:A:262:ARG:O	2:A:265:MET:HB2	2.14	0.47
1:B:506:GLU:O	1:B:507:LYS:C	2.58	0.46
2:A:129:VAL:O	2:A:187:PRO:HD2	2.17	0.45
1:B:217:VAL:O	6:B:702:HOH:O	2.21	0.44
1:B:360:TYR:CD1	1:B:360:TYR:C	2.96	0.44
1:B:197:ARG:HG3	1:B:221:GLU:HG3	1.99	0.44
2:A:215:SER:O	2:A:268:ARG:NH2	2.43	0.43
3:A:601:YRL:H031	3:A:601:YRL:O10	2.17	0.43
1:B:207:HIS:HD2	6:B:965:HOH:O	2.00	0.43
1:B:252:ILE:O	1:B:256:LEU:HG	2.19	0.43
2:A:370:GLU:O	2:A:374[B]:HIS:NE2	2.52	0.43
2:A:401:PRO:O	2:A:402:ASN:CB	2.66	0.42
1:B:280:ASN:HB2	6:B:863:HOH:O	2.20	0.42
1:B:321:LYS:O	1:B:324:LYS:HB2	2.20	0.42
2:A:227:CYS:HB3	2:A:385:ILE:HD13	2.01	0.42
1:B:117:TYR:HB2	1:B:289:VAL:HG22	2.01	0.42
2:A:149:GLY:HA3	2:A:162:PHE:CE2	2.55	0.42
2:A:233:LYS:NZ	6:A:713:HOH:O	2.52	0.42
1:B:507:LYS:HE2	1:B:507:LYS:CA	2.50	0.41
2:A:128:LYS:HD2	2:A:269:GLY:O	2.20	0.41
2:A:193:SER:O	2:A:194:GLY:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ASP:OD1	1:B:334:ASP:N	2.51	0.41
1:B:458:GLY:HA3	1:B:478:VAL:O	2.21	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	B	467/484 (96%)	454 (97%)	11 (2%)	2 (0%)	30	12
2	A	461/484 (95%)	444 (96%)	13 (3%)	4 (1%)	14	3
All	All	928/968 (96%)	898 (97%)	24 (3%)	6 (1%)	18	7

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	93	SER
2	A	402	ASN
1	B	390	GLU
2	A	208	LYS
2	A	87	ALA
2	A	194	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	394/407 (97%)	382 (97%)	12 (3%)	36	8
2	A	383/408 (94%)	365 (95%)	18 (5%)	23	3
All	All	777/815 (95%)	747 (96%)	30 (4%)	28	4

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	94	LEU
1	B	99	ASP
1	B	334	ASP
1	B	336	GLU
1	B	337	THR
1	B	344	LYS
1	B	348	VAL
1	B	388	ILE
1	B	399	GLU
1	B	419	LEU
1	B	471	THR
1	B	476	VAL
2	A	51	VAL
2	A	59	ARG
2	A	62	LEU
2	A	99	ASP
2	A	122	LYS
2	A	140	THR
2	A	182	LYS
2	A	196	THR
2	A	275	THR
2	A	336	GLU
2	A	337	THR
2	A	364	LYS
2	A	401	PRO
2	A	413	VAL
2	A	442	THR
2	A	470	ILE
2	A	471	THR
2	A	476	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	64	HIS
1	B	83	ASN
1	B	115	GLN
1	B	163	GLN
1	B	230	ASN
1	B	438	ASN
2	A	83	ASN
2	A	177	GLN
2	A	207	HIS
2	A	222	GLN
2	A	230	ASN
2	A	320	GLN
2	A	402	ASN

### 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	0.46	0	5,10,12	0.48	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](#)

7 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	YRL	B	602	-	10,10,10	1.88	1 (10%)	12,12,12	1.50	2 (16%)
3	YRL	A	602	-	10,10,10	1.81	1 (10%)	12,12,12	1.32	2 (16%)
4	GN1	B	603	-	18,19,19	0.89	1 (5%)	28,28,28	1.02	1 (3%)
3	YRL	B	601	-	10,10,10	2.13	3 (30%)	12,12,12	0.90	0
3	YRL	B	604	-	10,10,10	1.12	1 (10%)	12,12,12	0.90	0
3	YRL	A	601	-	10,10,10	1.57	2 (20%)	12,12,12	1.25	2 (16%)
5	PO4	B	605	-	4,4,4	0.84	0	6,6,6	0.47	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
3	YRL	B	602	-	-	1/3/3/3	0/1/1/1
3	YRL	A	602	-	-	0/3/3/3	0/1/1/1
4	GN1	B	603	-	-	1/10/31/31	0/1/1/1
3	YRL	B	601	-	-	2/3/3/3	0/1/1/1
3	YRL	B	604	-	-	0/3/3/3	0/1/1/1
3	YRL	A	601	-	-	2/3/3/3	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	YRL	C08-C01	-5.75	1.35	1.51
3	A	602	YRL	C08-C01	-5.03	1.37	1.51
3	B	601	YRL	C08-C01	-4.91	1.37	1.51
3	A	601	YRL	C08-C01	-3.31	1.42	1.51
4	B	603	GN1	P-O1	3.03	1.64	1.59
3	B	604	YRL	C08-C01	-3.00	1.43	1.51
3	B	601	YRL	C05-C03	2.60	1.43	1.38
3	B	601	YRL	C04-C02	2.21	1.42	1.38
3	A	601	YRL	C03-C01	2.17	1.43	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	YRL	C02-C04-C06	3.02	123.07	119.88
3	A	601	YRL	C08-C01-C02	-2.84	113.94	121.18
4	B	603	GN1	C4-C3-C2	-2.57	106.66	110.40
3	B	602	YRL	C08-C01-C02	-2.51	114.77	121.18
3	A	601	YRL	C08-C01-C03	2.46	127.48	121.18
3	B	602	YRL	C02-C04-C06	2.36	122.37	119.88
3	A	602	YRL	C03-C05-C06	-2.18	117.57	119.88

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	YRL	C01-C08-C09-O10
3	A	601	YRL	C03-C01-C08-C09
3	A	601	YRL	C02-C01-C08-C09
4	B	603	GN1	C1-O1-P-OP3
3	B	601	YRL	C03-C01-C08-C09
3	B	602	YRL	C01-C08-C09-O10

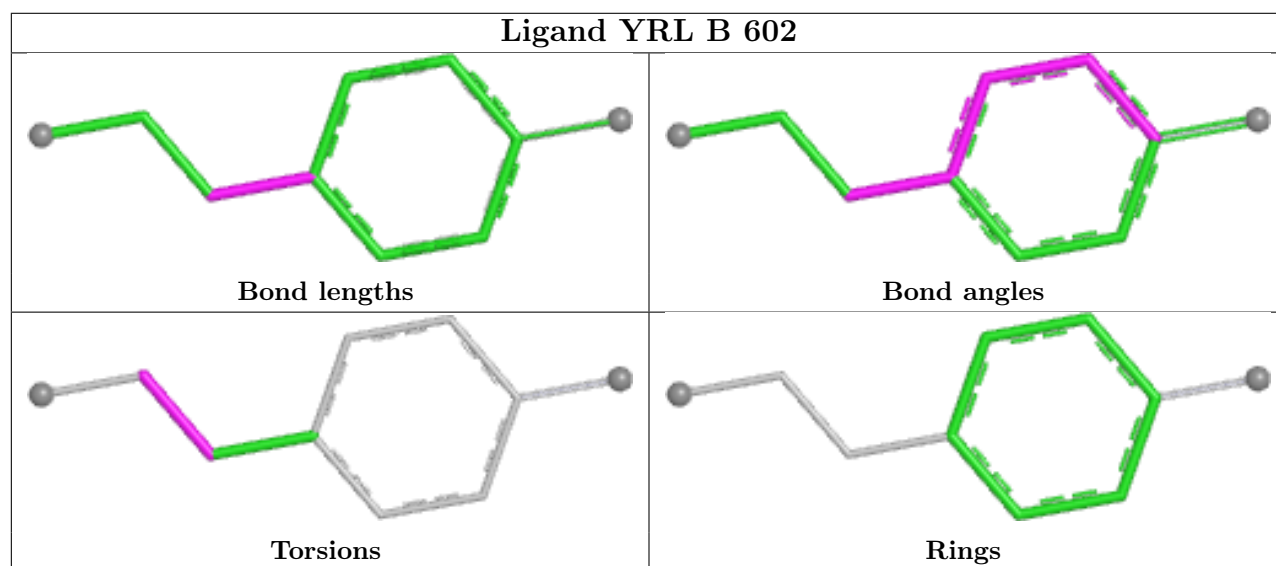


There are no ring outliers.

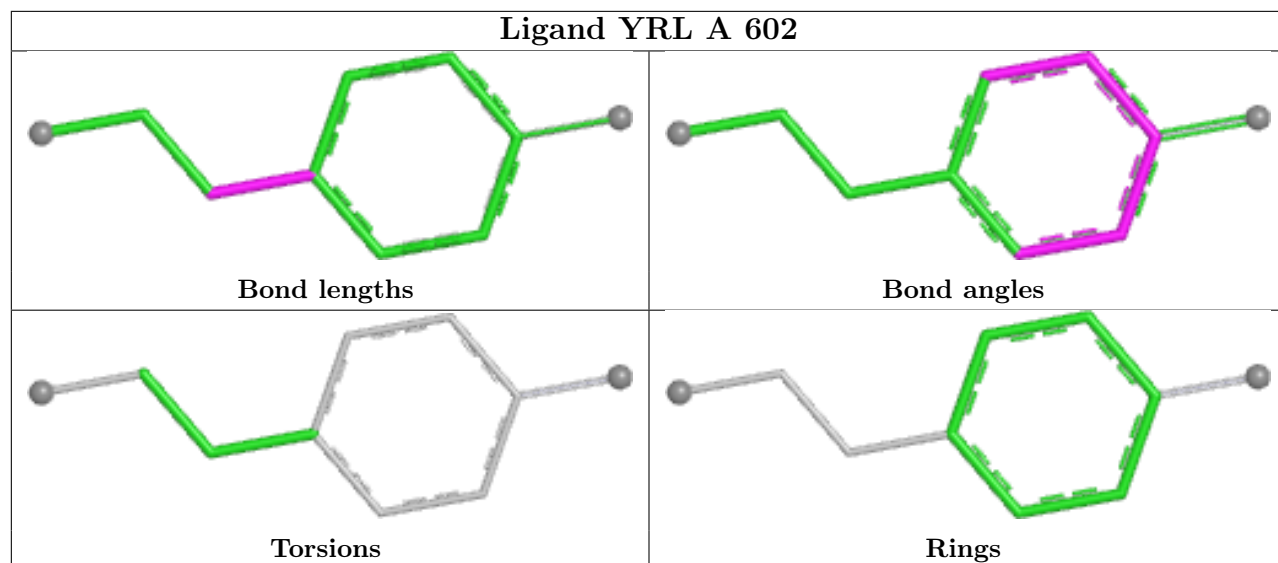
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	YRL	1	0
3	A	601	YRL	1	0

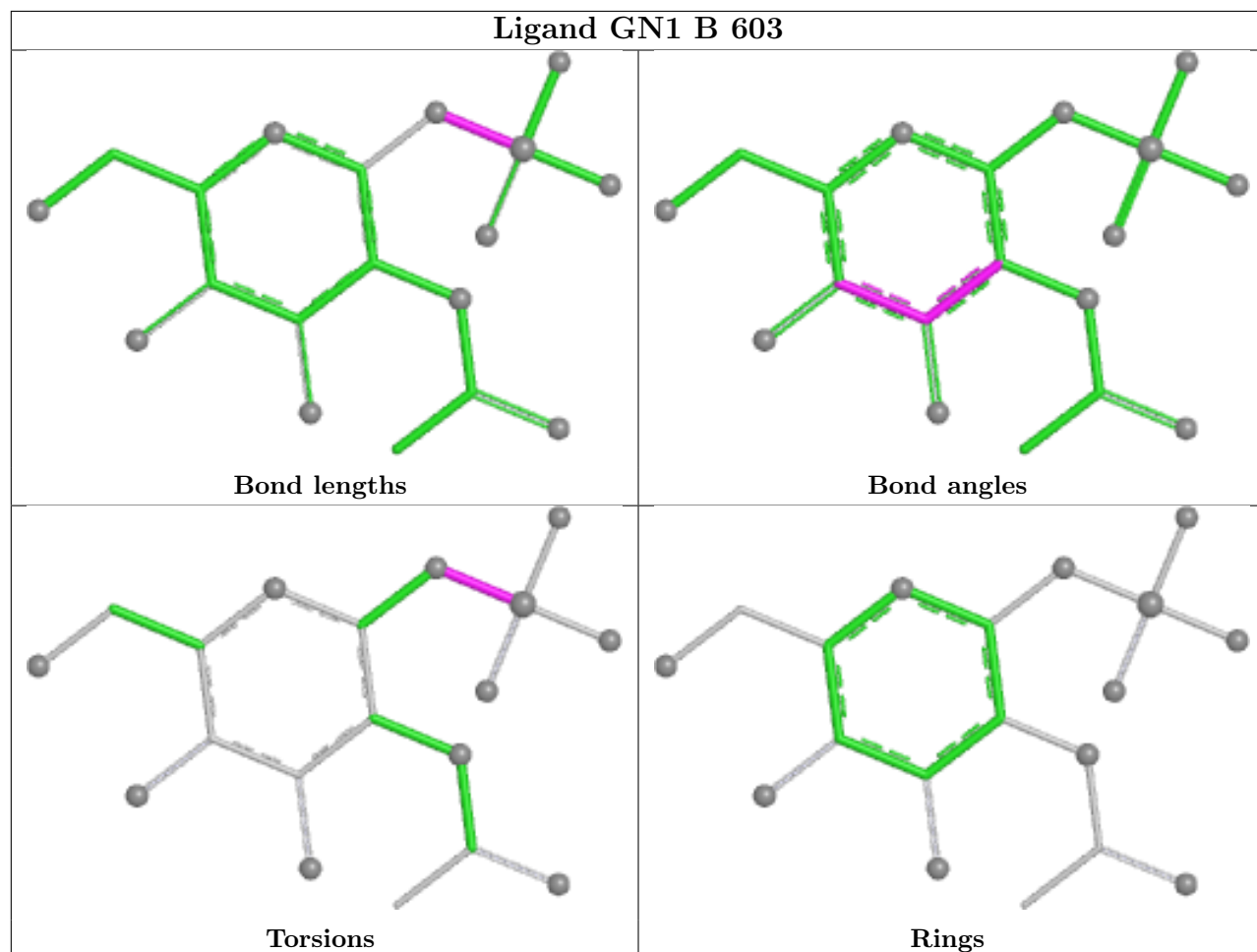
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



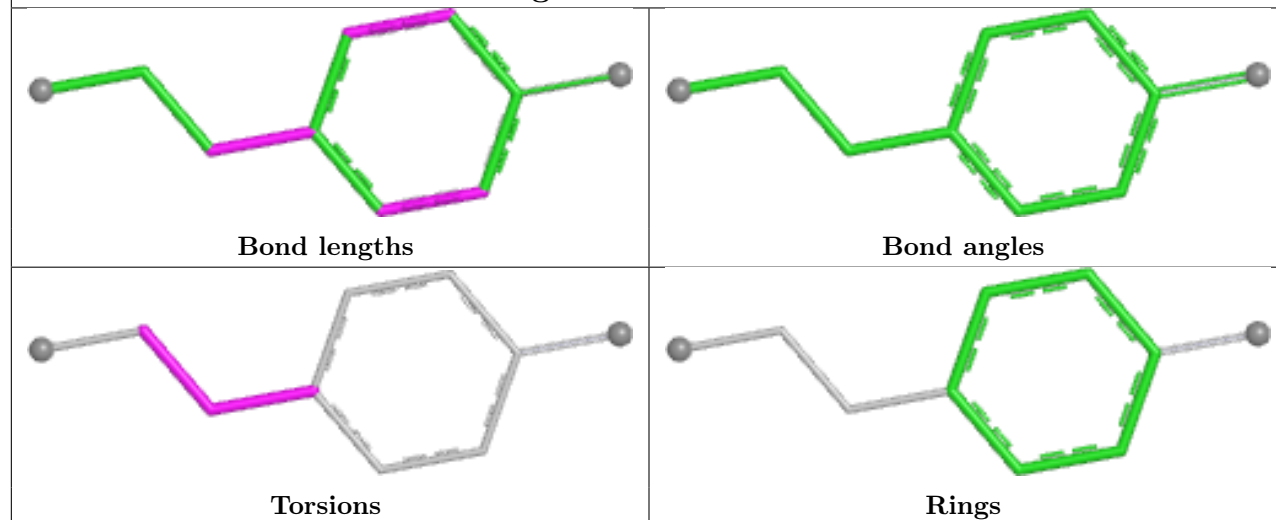
## Ligand YRL A 602



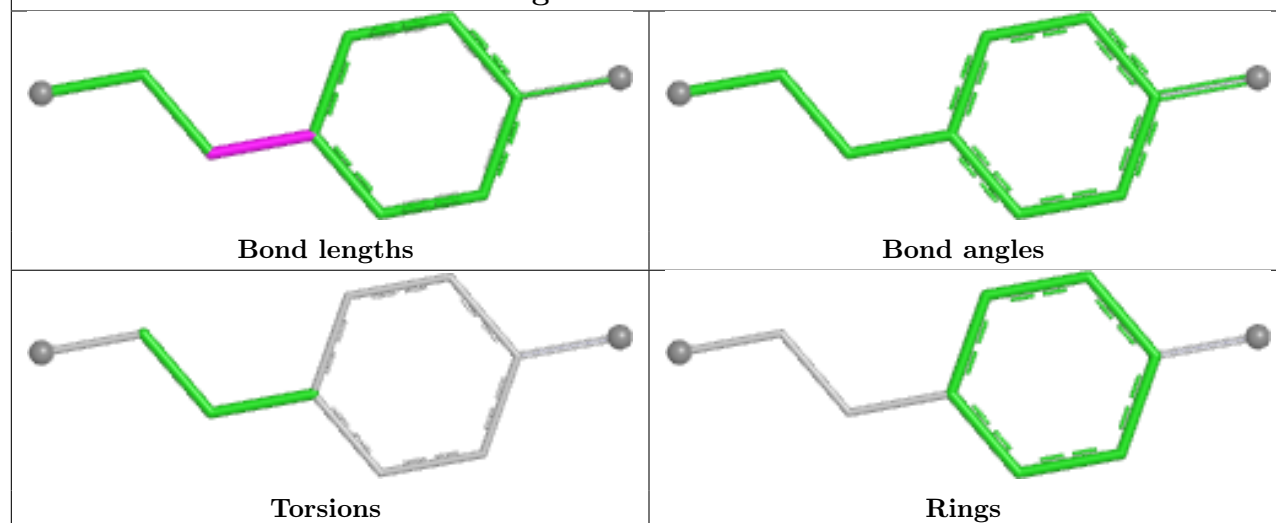
## Ligand GN1 B 603



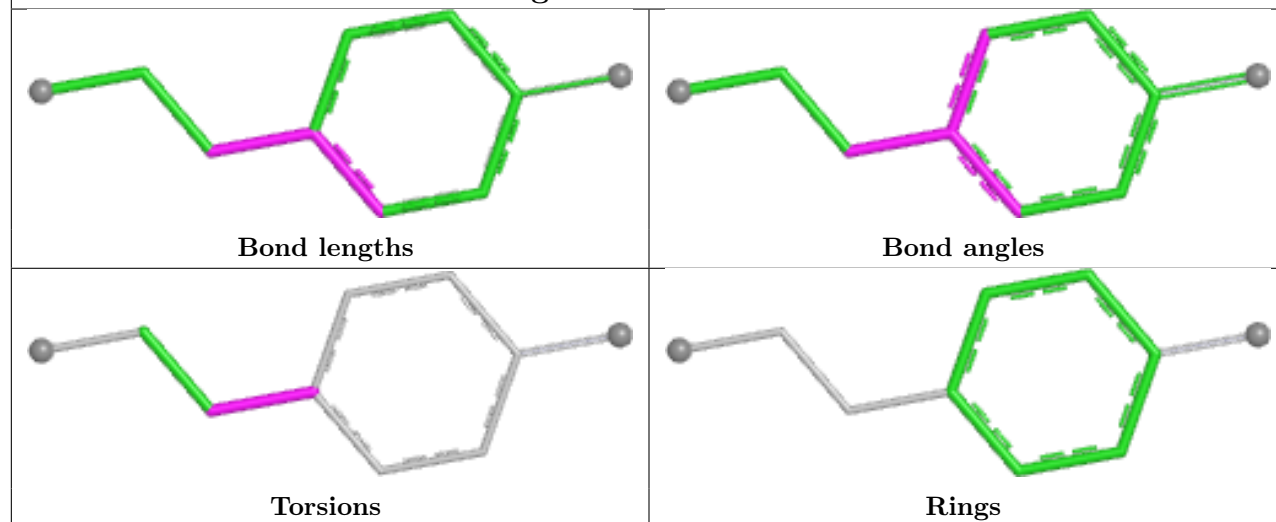
## Ligand YRL B 601



## Ligand YRL B 604



## Ligand YRL A 601



## 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%)	0.81	70 (14%) 5 10	18, 34, 65, 90	2 (0%)
2	A	465/484 (96%)	1.27	107 (23%) 2 3	20, 42, 89, 120	4 (0%)
All	All	936/968 (96%)	1.04	177 (18%) 3 6	18, 38, 79, 120	6 (0%)

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	503	ALA	6.9
1	B	94	LEU	6.7
2	A	476	VAL	6.6
2	A	504	PHE	6.5
1	B	343	PRO	5.7
2	A	505	ILE	5.5
2	A	179	ILE	5.4
1	B	351	PHE	5.2
2	A	142	LEU	5.2
2	A	401	PRO	5.0
2	A	502	PRO	5.0
1	B	319	LEU	5.0
2	A	137	GLY	4.9
1	B	92	ALA	4.9
2	A	388	ILE	4.9
2	A	385	ILE	4.8
2	A	87	ALA	4.7
2	A	139	GLY	4.5
1	B	328	VAL	4.4
1	B	100	ILE	4.3
1	B	137	GLY	4.2
1	B	85	PRO	4.2
2	A	204	PHE	4.2
1	B	338	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	139	GLY	4.0
2	A	470	ILE	4.0
2	A	257	LEU	4.0
1	B	476	VAL	4.0
2	A	411	PHE	3.9
1	B	337	THR	3.9
2	A	141	ARG	3.9
2	A	192	THR	3.9
1	B	353	ALA	3.9
1	B	391	GLY	3.9
1	B	340	ALA	3.9
1	B	395	PHE	3.8
1	B	503	ALA	3.8
1	B	97	LEU	3.7
2	A	136	GLY	3.7
2	A	387	CYS	3.7
2	A	269	GLY	3.7
2	A	471	THR	3.6
1	B	388	ILE	3.6
2	A	386	PRO	3.6
1	B	140	THR	3.6
2	A	140	THR	3.6
2	A	194	GLY	3.6
2	A	203	PHE	3.5
1	B	348	VAL	3.5
1	B	390	GLU	3.5
1	B	419	LEU	3.4
1	B	195	PRO	3.4
2	A	499	ILE	3.4
2	A	217	VAL	3.4
1	B	315	VAL	3.3
1	B	396	PHE	3.3
1	B	471	THR	3.3
1	B	136	GLY	3.3
2	A	496	GLY	3.3
1	B	392	THR	3.3
1	B	346	PRO	3.3
2	A	473	GLY	3.3
2	A	374[A]	HIS	3.3
1	B	330	TYR	3.2
1	B	322	ASN	3.2
1	B	317	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	A	27	PRO	3.2
2	A	218	ILE	3.2
1	B	311	ALA	3.2
1	B	321	LYS	3.1
2	A	507	LYS	3.1
1	B	138	GLN	3.1
2	A	85	PRO	3.1
1	B	93	SER	3.1
2	A	210	PHE	3.1
2	A	193	SER	3.1
1	B	143	GLY	3.1
1	B	349	LEU	3.1
1	B	333	ILE	3.1
1	B	101	ALA	3.1
2	A	442	THR	3.0
1	B	507	LYS	3.0
2	A	501	ALA	3.0
1	B	441	GLY	2.9
2	A	380	VAL	2.9
2	A	384	LYS	2.9
2	A	195	PRO	2.9
1	B	347	ASP	2.9
1	B	144	SER	2.9
2	A	145	SER	2.9
2	A	186	ILE	2.8
1	B	334	ASP	2.8
2	A	89	ASP	2.8
2	A	219	ILE	2.8
2	A	493	PHE	2.8
1	B	332	GLU	2.8
1	B	96	PRO	2.7
1	B	142	LEU	2.7
2	A	478	VAL	2.7
2	A	126	GLY	2.6
2	A	182	LYS	2.6
1	B	318	ILE	2.6
2	A	381	ALA	2.6
2	A	88	ASP	2.6
2	A	419	LEU	2.6
2	A	134	MET	2.6
1	B	344	LYS	2.6
2	A	200	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	411	PHE	2.6
1	B	327	VAL	2.6
2	A	125	ALA	2.5
2	A	373	ALA	2.5
2	A	468	ILE	2.5
2	A	383	LYS	2.5
1	B	194	GLY	2.5
1	B	470	ILE	2.5
2	A	185	VAL	2.4
2	A	410	VAL	2.4
2	A	443	GLY	2.4
1	B	502	PRO	2.4
2	A	198	LYS	2.4
2	A	256	LEU	2.4
2	A	494	LEU	2.4
2	A	146	ALA	2.3
2	A	51	VAL	2.3
2	A	86	LYS	2.3
1	B	371	LEU	2.3
2	A	90	GLY	2.3
2	A	181	GLY	2.3
2	A	466	GLY	2.3
2	A	469	VAL	2.3
2	A	261	VAL	2.3
2	A	266	ARG	2.3
1	B	228	ILE	2.3
2	A	199	PRO	2.2
1	B	312	THR	2.2
2	A	363	PHE	2.2
2	A	121	LEU	2.2
2	A	371	LEU	2.2
2	A	270	ILE	2.2
2	A	209	TYR	2.2
1	B	501	ALA	2.2
2	A	158	HIS	2.2
2	A	128	LYS	2.2
2	A	220	PHE	2.2
2	A	129	VAL	2.2
2	A	197	ARG	2.2
1	B	95	GLU	2.2
2	A	462	ILE	2.2
2	A	364	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	393	GLY	2.2
2	A	258	THR	2.2
2	A	216	ASP	2.2
2	A	372	TRP	2.1
2	A	500	LYS	2.1
2	A	151	PHE	2.1
2	A	440	ARG	2.1
1	B	320	GLN	2.1
2	A	91	PRO	2.1
2	A	376	LEU	2.1
2	A	439	ALA	2.1
1	B	258	THR	2.1
1	B	336	GLU	2.1
1	B	397	LYS	2.1
2	A	260	GLY	2.1
2	A	367	GLU	2.1
2	A	480	VAL	2.1
2	A	196	THR	2.1
1	B	314	SER	2.1
2	A	32	PHE	2.0
2	A	122	LYS	2.0
2	A	184	ALA	2.0
1	B	179	ILE	2.0
1	B	352	ARG	2.0
2	A	30	GLU	2.0
2	A	365	PHE	2.0
2	A	368	SER	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	0.95	0.09	24,26,43,53	0

## 6.3 Carbohydrates [i](#)

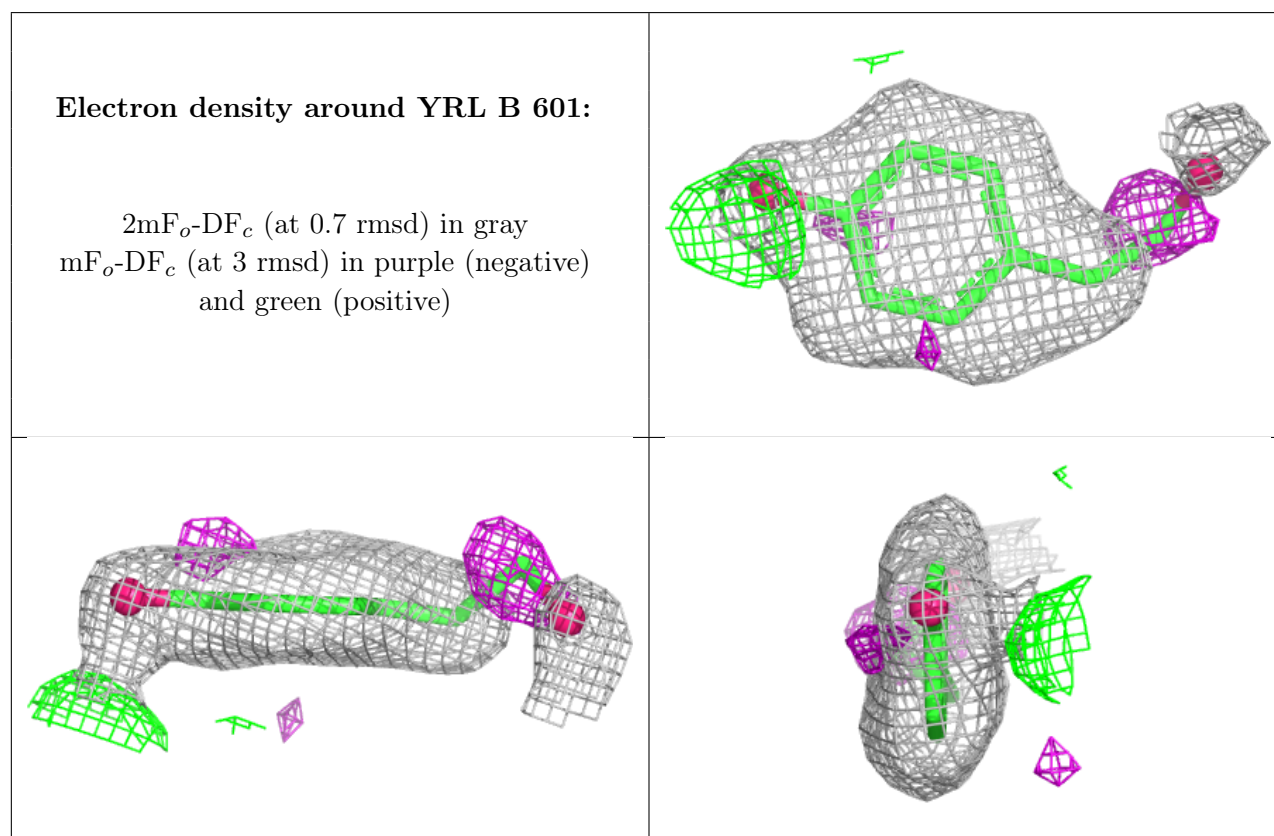
There are no oligosaccharides in this entry.

## 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.

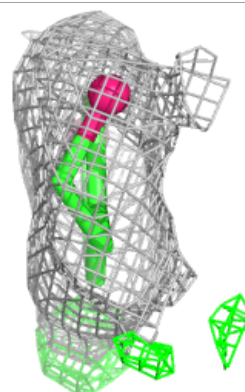
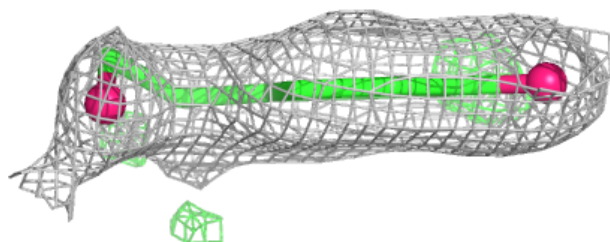
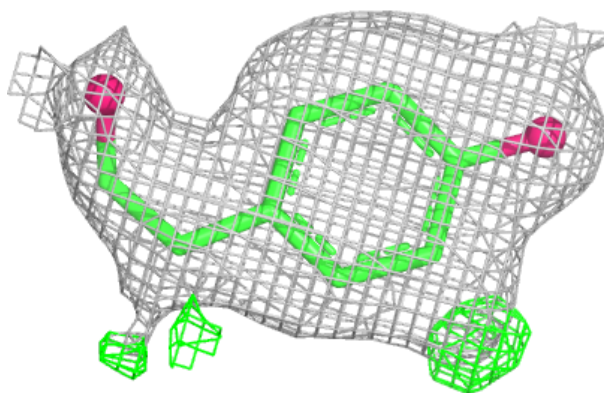
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	PO4	B	605	5/5	0.82	0.11	56,57,75,76	0
3	YRL	B	601	10/10	0.84	0.14	37,39,54,57	0
3	YRL	A	601	10/10	0.86	0.12	35,39,60,65	0
3	YRL	B	602	10/10	0.89	0.14	40,47,56,67	0
4	GN1	B	603	19/19	0.91	0.10	33,37,41,42	0
3	YRL	B	604	10/10	0.95	0.07	27,31,34,38	0
3	YRL	A	602	10/10	0.96	0.07	30,34,38,39	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.

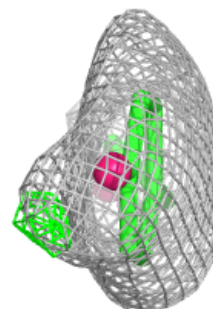
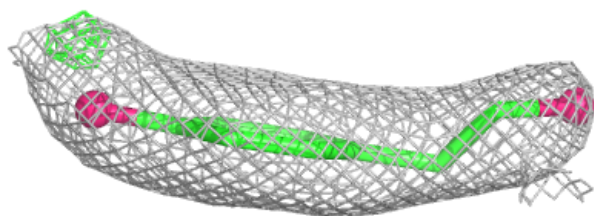
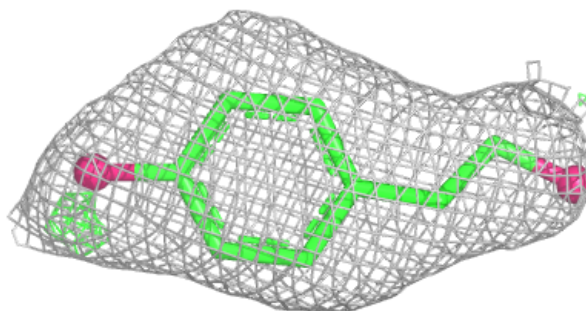


**Electron density around YRL A 601:**

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

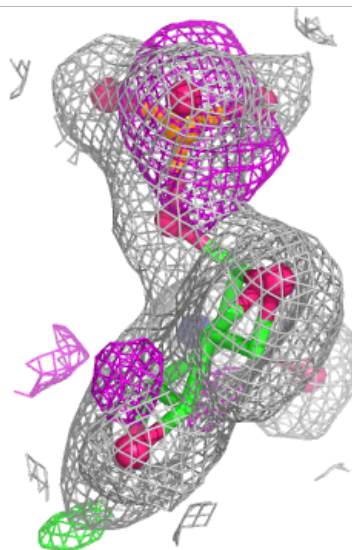
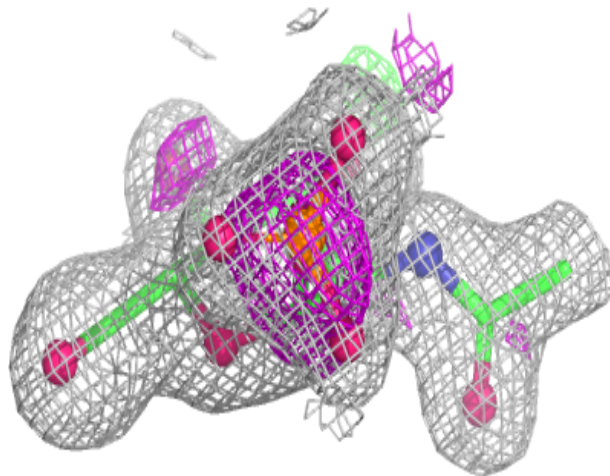
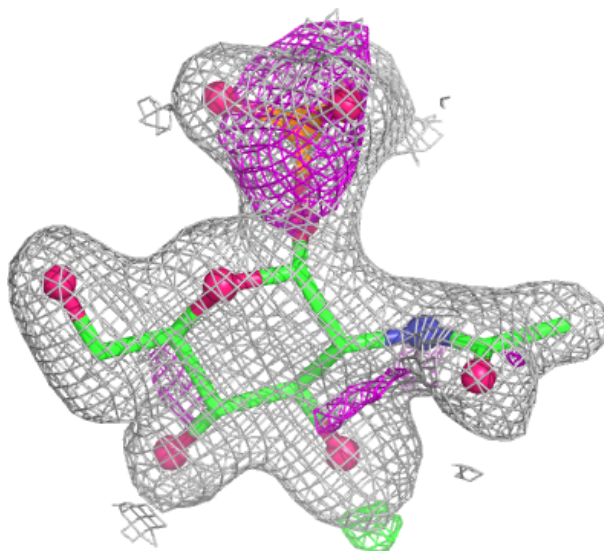
**Electron density around YRL B 602:**

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



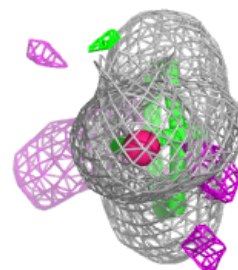
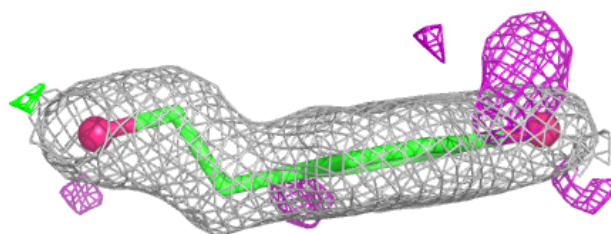
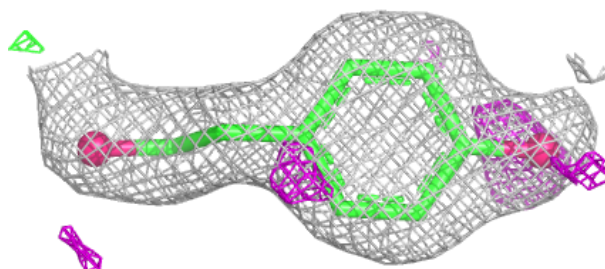
**Electron density around GN1 B 603:**

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

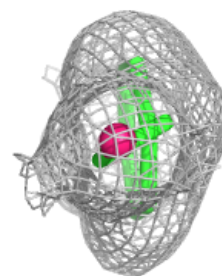
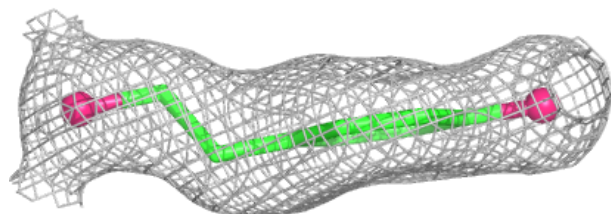
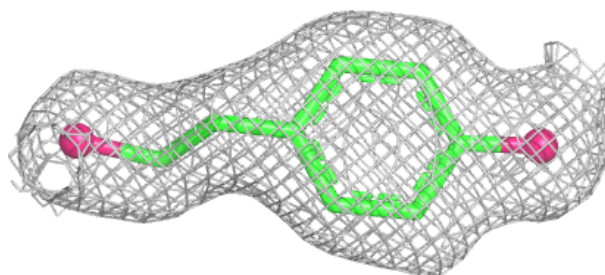


**Electron density around YRL B 604:**

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

**Electron density around YRL A 602:**

$2mF_o-DF_c$  (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.