



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 08:13 AM EST

PDB ID : 8W0C  
Title : Crystal structure of Acetyl-CoA synthetase 2 from *Candida albicans* in complex with a cyclopentyl ester AMP inhibitor  
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2024-02-13  
Resolution : 2.35 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>.

---

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 : 2.36  
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) : 2.36

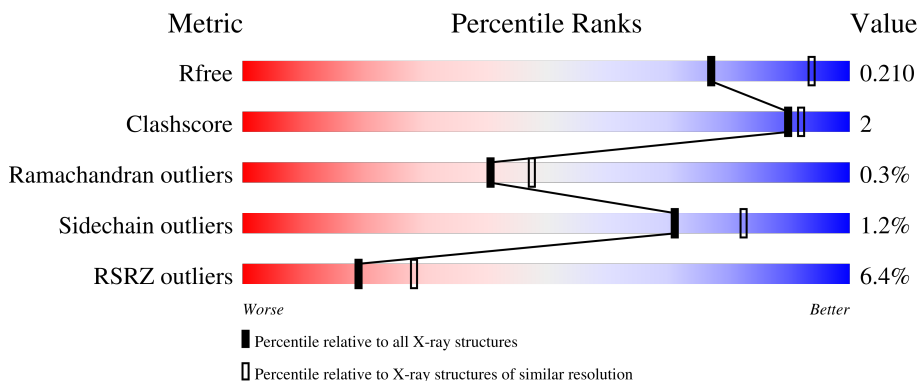
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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 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	686	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 93%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">93%     . .</p>
1	B	686	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">87%     5% • 6%</p>
1	C	686	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">73%     •     23%</p>

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 14966 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 Acetyl-coenzyme A synthetase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	667	5168	3296	878	980	14	0	1	0
1	B	642	4973	3178	846	935	14	0	0	0
1	C	525	4128	2650	694	771	13	0	1	0

There are 51 discrepancies between the modelled and reference sequences:

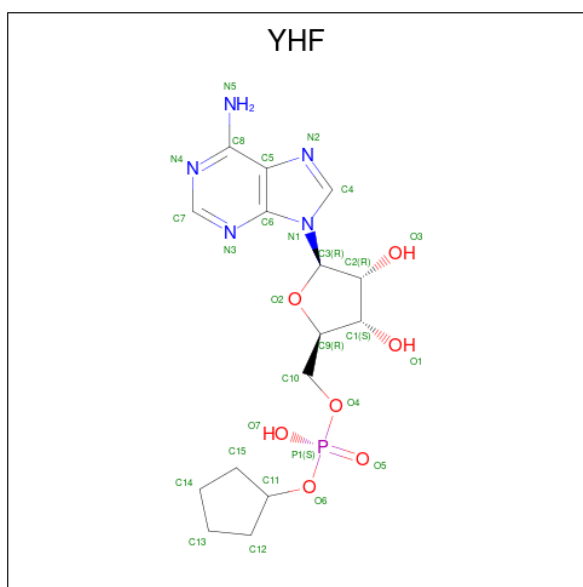
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8NJN3
A	2	HIS	-	expression tag	UNP Q8NJN3
A	3	HIS	-	expression tag	UNP Q8NJN3
A	4	HIS	-	expression tag	UNP Q8NJN3
A	5	HIS	-	expression tag	UNP Q8NJN3
A	6	HIS	-	expression tag	UNP Q8NJN3
A	7	HIS	-	expression tag	UNP Q8NJN3
A	8	HIS	-	expression tag	UNP Q8NJN3
A	9	HIS	-	expression tag	UNP Q8NJN3
A	10	GLU	-	expression tag	UNP Q8NJN3
A	11	ASN	-	expression tag	UNP Q8NJN3
A	12	LEU	-	expression tag	UNP Q8NJN3
A	13	TYR	-	expression tag	UNP Q8NJN3
A	14	PHE	-	expression tag	UNP Q8NJN3
A	15	GLN	-	expression tag	UNP Q8NJN3
A	16	GLY	-	expression tag	UNP Q8NJN3
A	403	ALA	VAL	engineered mutation	UNP Q8NJN3
B	1	MET	-	initiating methionine	UNP Q8NJN3
B	2	HIS	-	expression tag	UNP Q8NJN3
B	3	HIS	-	expression tag	UNP Q8NJN3
B	4	HIS	-	expression tag	UNP Q8NJN3
B	5	HIS	-	expression tag	UNP Q8NJN3
B	6	HIS	-	expression tag	UNP Q8NJN3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	expression tag	UNP Q8N3N3
B	8	HIS	-	expression tag	UNP Q8N3N3
B	9	HIS	-	expression tag	UNP Q8N3N3
B	10	GLU	-	expression tag	UNP Q8N3N3
B	11	ASN	-	expression tag	UNP Q8N3N3
B	12	LEU	-	expression tag	UNP Q8N3N3
B	13	TYR	-	expression tag	UNP Q8N3N3
B	14	PHE	-	expression tag	UNP Q8N3N3
B	15	GLN	-	expression tag	UNP Q8N3N3
B	16	GLY	-	expression tag	UNP Q8N3N3
B	403	ALA	VAL	engineered mutation	UNP Q8N3N3
C	1	MET	-	initiating methionine	UNP Q8N3N3
C	2	HIS	-	expression tag	UNP Q8N3N3
C	3	HIS	-	expression tag	UNP Q8N3N3
C	4	HIS	-	expression tag	UNP Q8N3N3
C	5	HIS	-	expression tag	UNP Q8N3N3
C	6	HIS	-	expression tag	UNP Q8N3N3
C	7	HIS	-	expression tag	UNP Q8N3N3
C	8	HIS	-	expression tag	UNP Q8N3N3
C	9	HIS	-	expression tag	UNP Q8N3N3
C	10	GLU	-	expression tag	UNP Q8N3N3
C	11	ASN	-	expression tag	UNP Q8N3N3
C	12	LEU	-	expression tag	UNP Q8N3N3
C	13	TYR	-	expression tag	UNP Q8N3N3
C	14	PHE	-	expression tag	UNP Q8N3N3
C	15	GLN	-	expression tag	UNP Q8N3N3
C	16	GLY	-	expression tag	UNP Q8N3N3
C	403	ALA	VAL	engineered mutation	UNP Q8N3N3

- Molecule 2 is 5'-O-[(S)-(cyclopentyloxy)(hydroxy)phosphoryl]adenosine (three-letter code: YHF) (formula: C<sub>15</sub>H<sub>22</sub>N<sub>5</sub>O<sub>7</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			28	15	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			28	15	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			28	15	5	7	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

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



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0

- Molecule 6 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
6	B	1	Total	C	O	0	0
			6	3	3		

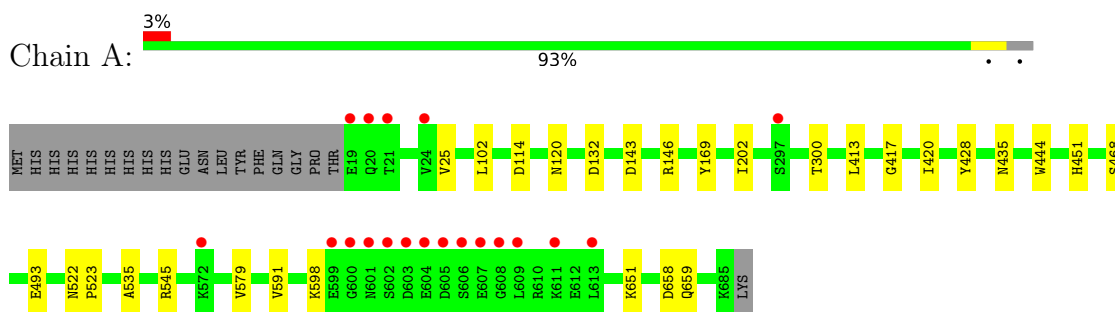
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	254	Total	O	0	0
			254	254		
7	B	241	Total	O	0	0
			241	241		
7	C	79	Total	O	0	0
			79	79		

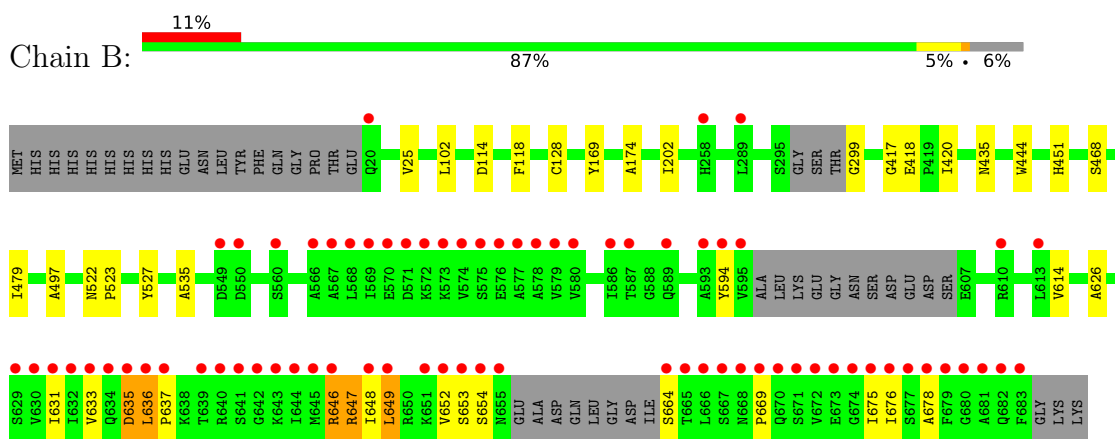
### 3 Residue-property plots [i](#)

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.

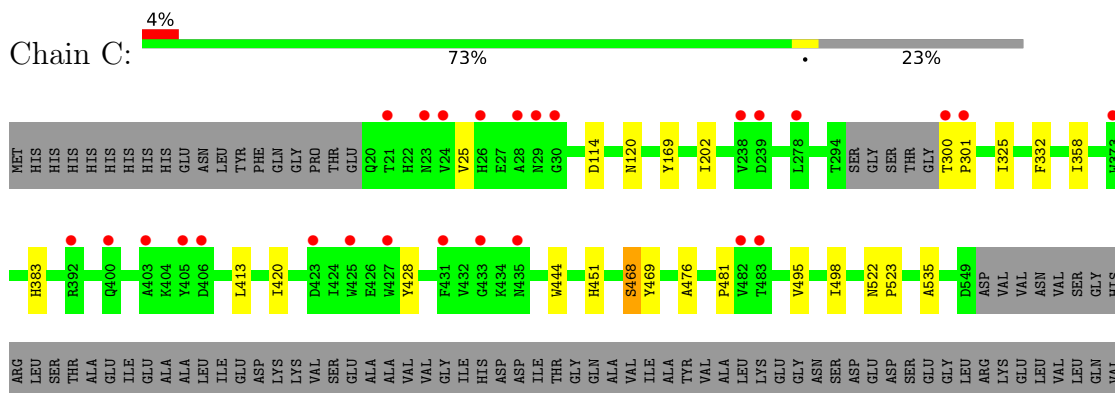
- Molecule 1: Acetyl-coenzyme A synthetase 2



- Molecule 1: Acetyl-coenzyme A synthetase 2



- Molecule 1: Acetyl-coenzyme A synthetase 2





ARG  
LYS  
THR  
ILE  
GLY  
PRO  
PHE  
ALA  
ALA  
PRO  
LYS  
SER  
VAL  
ILE  
ILE  
VAL  
GLN  
ASP  
LEU  
PRO  
LYS  
THR  
ARG  
SER  
GLY  
LYS  
ILE  
MET  
ARG  
ARG  
ILE  
LEU  
ARG  
LYS  
VAL  
SER  
SER  
ASN  
GLU  
ALA  
ASP  
GLN  
LEU  
GLY  
ASP  
ILE  
SER  
THR  
LEU  
SER  
ASN  
PRO  
GLN  
SER  
VAL  
GLU  
GLY  
ILE  
SER

ALA  
PHE  
GLY  
ALA  
GLN  
PHE  
GLY  
LYS  
LYS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.41Å 139.41Å 543.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.58 – 2.35 49.58 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.58-2.35) 100.0 (49.58-2.35)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.34Å)	Xtrriage
Refinement program	PHENIX (dev_5233: ???)	Depositor
R, $R_{free}$	0.181 , 0.210 0.182 , 0.210	Depositor DCC
$R_{free}$ test set	6634 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.0	Xtrriage
Anisotropy	0.426	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14966	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, SO4, NA, YHF

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	0.34	0/5301	0.55	0/7209
1	B	0.32	0/5100	0.54	0/6937
1	C	0.30	0/4250	0.50	0/5787
All	All	0.32	0/14651	0.53	0/19933

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	646	ARG	Sidechain

### 5.2 Too-close contacts [i](#)

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	5168	0	5046	11	0
1	B	4973	0	4842	27	0
1	C	4128	0	3991	12	0
2	A	28	0	0	0	0
2	B	28	0	0	0	0
2	C	28	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
5	B	1	0	0	0	0
6	B	6	0	8	1	0
7	A	254	0	0	0	0
7	B	241	0	0	1	0
7	C	79	0	0	0	0
All	All	14966	0	13887	50	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 2.

All (50) 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:675:ILE:HA	1:B:678:ALA:HB3	1.74	0.69
1:B:636:LEU:HD23	1:B:637:PRO:HD2	1.75	0.68
1:B:636:LEU:HD22	1:B:649:LEU:CD2	2.27	0.65
1:B:636:LEU:HD23	1:B:637:PRO:CD	2.29	0.63
1:B:646:ARG:HA	1:B:649:LEU:HD12	1.82	0.62
1:A:493:GLU:OE1	1:A:545:ARG:NH1	2.37	0.58
1:B:479:ILE:HD11	1:B:527:TYR:CG	2.44	0.53
1:B:636:LEU:HD11	1:B:675:ILE:HG12	1.92	0.52
1:A:143:ASP:OD1	1:A:146:ARG:NH2	2.42	0.52
1:B:633:VAL:HG21	1:B:636:LEU:HD12	1.92	0.51
1:C:420:ILE:O	1:C:420:ILE:HG23	2.12	0.50
1:B:25:VAL:HG22	1:B:535:ALA:HB1	1.93	0.50
1:B:648:ILE:O	1:B:652:VAL:HG23	2.13	0.49
1:B:169:TYR:CZ	1:B:202:ILE:HD11	2.48	0.49
1:B:636:LEU:HD22	1:B:649:LEU:HG	1.96	0.47
1:C:522:ASN:N	1:C:523:PRO:CD	2.79	0.46
1:A:25:VAL:HG22	1:A:535:ALA:HB1	1.97	0.46
1:A:102:LEU:HD22	1:B:118:PHE:CZ	2.51	0.46

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:TYR:CD2	1:B:649:LEU:HD22	2.52	0.45
1:B:664:SER:HA	1:B:669:PRO:HB3	1.98	0.45
1:C:169:TYR:CZ	1:C:202:ILE:HD11	2.51	0.45
1:C:481:PRO:HG3	1:C:495:VAL:HG23	1.98	0.45
1:A:522:ASN:N	1:A:523:PRO:CD	2.80	0.45
1:A:579:VAL:CG1	1:A:591:VAL:HG13	2.46	0.45
1:B:479:ILE:HD12	1:B:497:ALA:CB	2.46	0.45
1:C:476:ALA:HA	1:C:498:ILE:HD13	1.99	0.44
1:B:420:ILE:O	1:B:420:ILE:HG23	2.17	0.44
1:C:25:VAL:HG22	1:C:535:ALA:HB1	1.98	0.44
1:C:332:PHE:HB2	1:C:358:ILE:HD12	1.99	0.43
1:B:675:ILE:O	1:B:676:ILE:C	2.58	0.43
6:B:704:GOL:H32	7:B:996:HOH:O	2.19	0.42
1:B:128:CYS:SG	1:B:174:ALA:HB2	2.60	0.42
1:B:444:TRP:HB3	1:B:451:HIS:HA	2.01	0.42
1:B:594:TYR:CD1	1:B:631:ILE:HB	2.54	0.42
1:A:413:LEU:HB3	1:A:428:TYR:CZ	2.55	0.42
1:B:522:ASN:N	1:B:523:PRO:CD	2.83	0.42
1:B:299:GLY:HA2	1:B:647:ARG:HH11	1.85	0.42
1:C:444:TRP:HB3	1:C:451:HIS:HA	2.01	0.42
1:B:614:VAL:HG13	1:B:626:ALA:HB1	2.02	0.41
1:C:468:SER:OG	1:C:469:TYR:N	2.53	0.41
1:B:635:ASP:O	1:B:675:ILE:HD11	2.21	0.41
1:C:300:THR:HB	1:C:301:PRO:HD2	2.02	0.41
1:C:413:LEU:HB3	1:C:428:TYR:CZ	2.56	0.41
1:A:444:TRP:HB3	1:A:451:HIS:HA	2.03	0.40
1:C:325:ILE:HD13	1:C:383:HIS:CE1	2.56	0.40
1:A:420:ILE:O	1:A:420:ILE:HG23	2.21	0.40
1:A:658:ASP:O	1:A:659:GLN:CB	2.69	0.40
1:B:636:LEU:HD22	1:B:649:LEU:CG	2.51	0.40
1:B:102:LEU:N	1:B:102:LEU:HD12	2.37	0.40
1:A:169:TYR:CZ	1:A:202:ILE:HD11	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	666/686 (97%)	647 (97%)	17 (3%)	2 (0%)	41	47
1	B	634/686 (92%)	616 (97%)	16 (2%)	2 (0%)	41	47
1	C	522/686 (76%)	503 (96%)	18 (3%)	1 (0%)	47	56
All	All	1822/2058 (88%)	1766 (97%)	51 (3%)	5 (0%)	41	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	SER
1	B	417	GLY
1	B	468	SER
1	C	468	SER
1	A	417	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	A	544/568 (96%)	537 (99%)	7 (1%)	69	80
1	B	522/568 (92%)	513 (98%)	9 (2%)	60	72
1	C	433/568 (76%)	431 (100%)	2 (0%)	88	94
All	All	1499/1704 (88%)	1481 (99%)	18 (1%)	71	82

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ASP
1	A	120	ASN
1	A	132	ASP
1	A	300	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	435	ASN
1	A	598	LYS
1	A	651	LYS
1	B	114	ASP
1	B	418	GLU
1	B	435	ASN
1	B	635	ASP
1	B	636	LEU
1	B	647	ARG
1	B	649	LEU
1	B	653	SER
1	B	654	SER
1	C	114	ASP
1	C	120	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	120	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](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 for Mogul analysis.

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
4	SO4	C	702	-	4,4,4	0.60	0	6,6,6	0.10	0
4	SO4	C	703	-	4,4,4	0.68	0	6,6,6	0.28	0
2	YHF	B	701	-	28,31,31	0.57	0	31,46,46	0.74	1 (3%)
6	GOL	B	704	-	5,5,5	0.41	0	5,5,5	0.48	0
4	SO4	B	705	-	4,4,4	0.58	0	6,6,6	0.12	0
4	SO4	A	704	-	4,4,4	0.75	0	6,6,6	0.28	0
4	SO4	A	703	-	4,4,4	0.65	0	6,6,6	0.35	0
4	SO4	B	706	-	4,4,4	0.70	0	6,6,6	0.17	0
2	YHF	C	701	-	28,31,31	0.54	0	31,46,46	0.78	1 (3%)
2	YHF	A	701	-	28,31,31	0.59	0	31,46,46	0.72	1 (3%)

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	YHF	B	701	-	-	0/11/38/38	0/4/4/4
2	YHF	C	701	-	-	0/11/38/38	0/4/4/4
2	YHF	A	701	-	-	0/11/38/38	0/4/4/4
6	GOL	B	704	-	-	0/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	YHF	C5-C8-N5	2.37	123.96	120.35
2	B	701	YHF	C5-C8-N5	2.36	123.93	120.35
2	C	701	YHF	C5-C8-N5	2.31	123.86	120.35

There are no chirality outliers.

There are no torsion outliers.

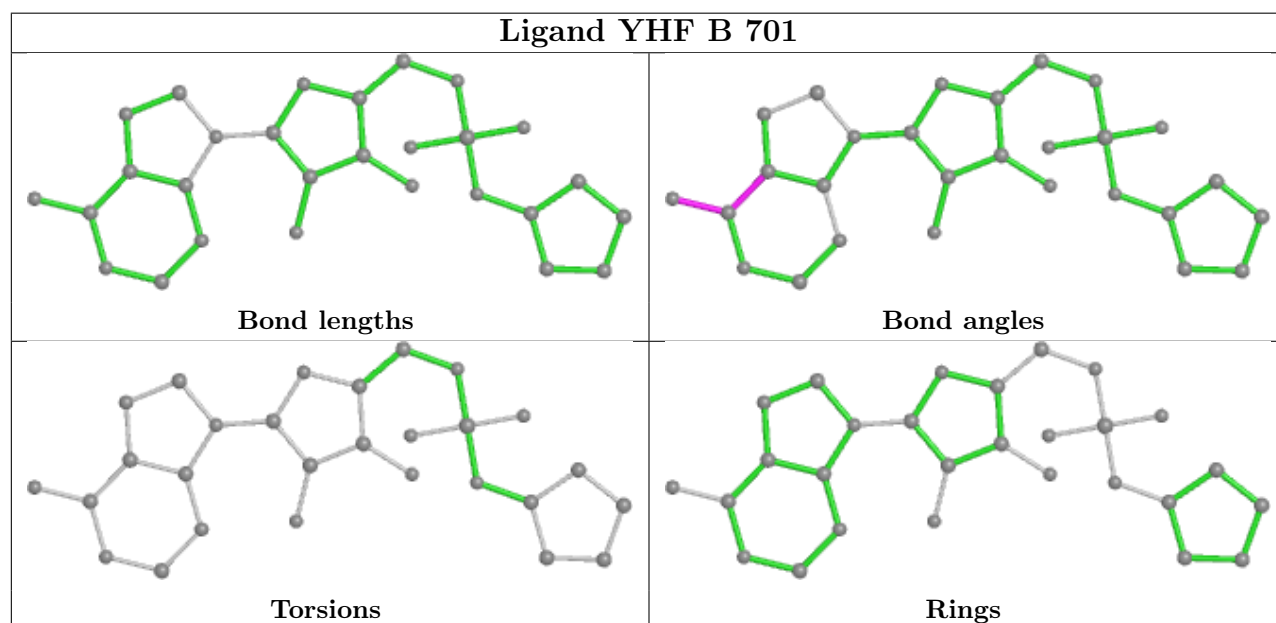
There are no ring outliers.

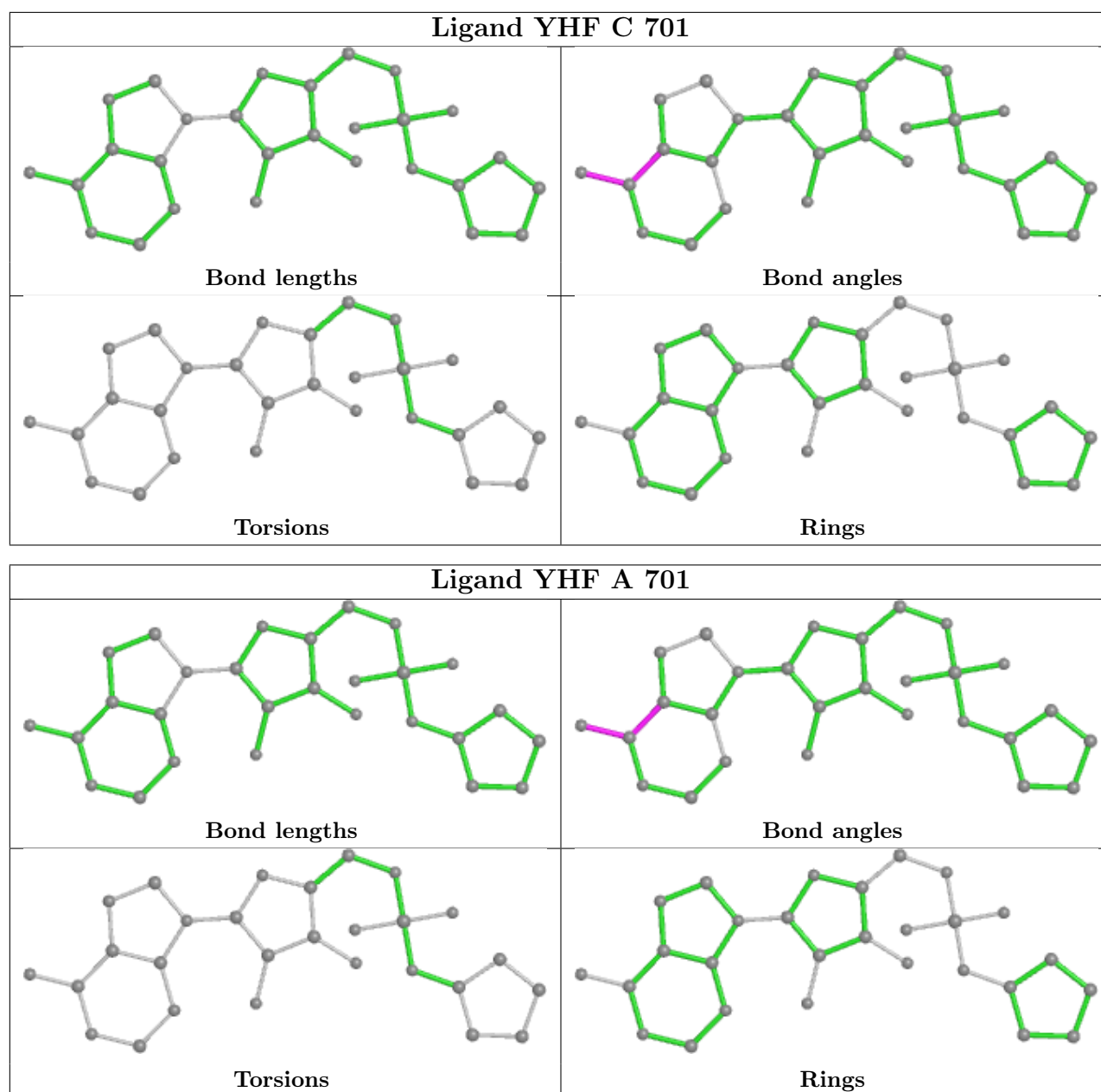
1 monomer is involved in 1 short contact:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	704	GOL	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	667/686 (97%)	0.10	19 (2%) 53 64	33, 47, 78, 136	0
1	B	642/686 (93%)	0.50	73 (11%) 5 7	35, 47, 121, 197	0
1	C	525/686 (76%)	0.12	26 (4%) 28 41	41, 63, 99, 124	0
All	All	1834/2058 (89%)	0.25	118 (6%) 19 28	33, 51, 100, 197	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	636	LEU	15.5
1	B	676	ILE	12.2
1	B	672	VAL	9.8
1	B	642	GLY	8.2
1	B	632	ILE	7.9
1	B	633	VAL	7.9
1	B	679	PHE	7.8
1	B	677	SER	7.5
1	B	637	PRO	7.3
1	B	595	VAL	6.5
1	B	574	VAL	6.5
1	B	649	LEU	6.2
1	B	682	GLN	5.7
1	B	639	THR	5.7
1	B	678	ALA	5.7
1	B	641	SER	5.7
1	B	673	GLU	5.6
1	C	482	VAL	5.5
1	A	601	ASN	5.5
1	B	631	ILE	5.3
1	B	666	LEU	5.3
1	B	634	GLN	5.2
1	B	645	MET	5.2

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	644	ILE	5.1
1	B	671	SER	5.1
1	B	652	VAL	5.1
1	B	576	GLU	5.0
1	B	664	SER	5.0
1	B	569	ILE	4.9
1	A	603	ASP	4.9
1	B	635	ASP	4.9
1	A	602	SER	4.6
1	B	675	ILE	4.6
1	B	683	PHE	4.6
1	B	667	SER	4.6
1	B	572	LYS	4.6
1	B	674	GLY	4.5
1	B	573	LYS	4.5
1	C	24	VAL	4.4
1	B	640	ARG	4.3
1	A	604	GLU	4.2
1	B	549	ASP	4.2
1	B	668	ASN	4.1
1	B	577	ALA	4.1
1	B	681	ALA	4.1
1	B	630	VAL	4.1
1	C	21	THR	4.0
1	B	646	ARG	3.9
1	A	606	SER	3.9
1	A	20	GLN	3.9
1	B	594	TYR	3.9
1	B	578	ALA	3.8
1	B	665	THR	3.7
1	B	653	SER	3.7
1	A	600	GLY	3.7
1	A	599	GLU	3.7
1	A	605	ASP	3.7
1	B	20	GLN	3.7
1	B	651	LYS	3.6
1	B	669	PRO	3.5
1	C	300	THR	3.4
1	A	609	LEU	3.4
1	B	655	ASN	3.4
1	B	643	LYS	3.3
1	B	568	LEU	3.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	567	ALA	3.2
1	B	580	VAL	3.2
1	B	613	LEU	3.2
1	A	572	LYS	3.2
1	C	431	PHE	3.1
1	C	30	GLY	3.1
1	A	607	GLU	3.1
1	B	610	ARG	3.1
1	B	586	ILE	3.0
1	B	654	SER	3.0
1	B	571	ASP	3.0
1	B	680	GLY	2.9
1	B	648	ILE	2.9
1	C	301	PRO	2.9
1	A	613	LEU	2.9
1	C	425	TRP	2.9
1	A	19	GLU	2.8
1	B	670	GLN	2.8
1	C	23	ASN	2.7
1	A	608	GLY	2.7
1	C	400	GLN	2.7
1	C	26	HIS	2.6
1	A	21	THR	2.6
1	C	427	TRP	2.5
1	B	566	ALA	2.5
1	C	403	ALA	2.5
1	C	373	TRP	2.4
1	C	405	TYR	2.4
1	B	575	SER	2.4
1	B	579	VAL	2.4
1	B	570	GLU	2.4
1	C	239	ASP	2.4
1	C	433	GLY	2.3
1	C	28	ALA	2.3
1	B	629	SER	2.3
1	A	24	VAL	2.3
1	C	238	VAL	2.3
1	C	29	ASN	2.2
1	B	560	SER	2.2
1	B	587	THR	2.2
1	C	483	THR	2.2
1	C	278	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	289	LEU	2.1
1	C	435	ASN	2.1
1	B	258	HIS	2.1
1	B	593	ALA	2.1
1	A	611	LYS	2.1
1	B	589	GLN	2.1
1	B	550	ASP	2.1
1	C	423	ASP	2.1
1	A	297	SER	2.1
1	C	392	ARG	2.0
1	C	406	ASP	2.0

## 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 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.

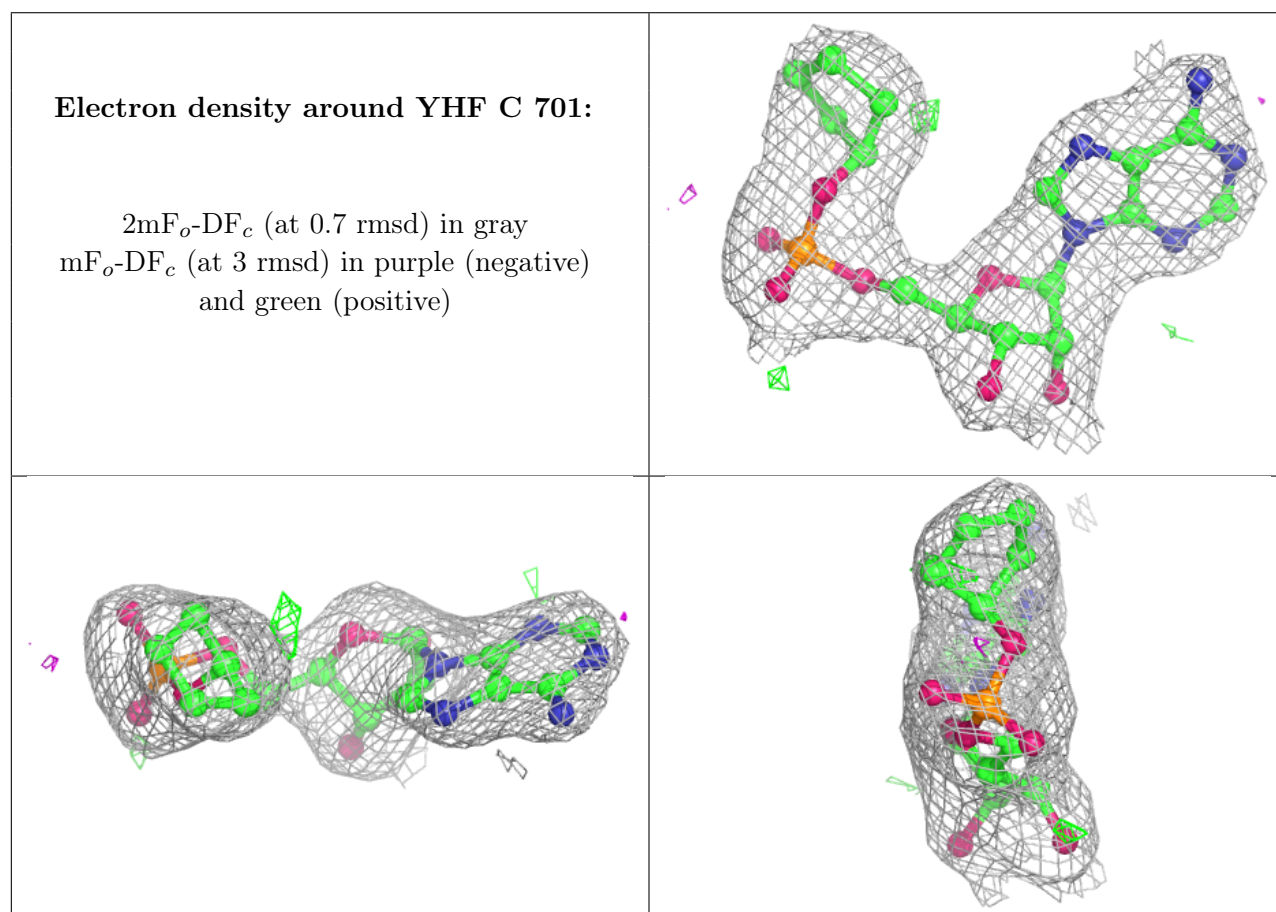
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	B	704	6/6	0.54	0.19	58,62,65,67	0
4	SO4	A	704	5/5	0.79	0.31	61,64,89,100	0
4	SO4	C	703	5/5	0.88	0.30	70,72,84,104	0
4	SO4	B	705	5/5	0.90	0.18	91,93,104,112	0
4	SO4	B	706	5/5	0.90	0.18	55,69,95,97	0
4	SO4	C	702	5/5	0.93	0.35	98,100,106,122	0
2	YHF	C	701	28/28	0.94	0.13	65,72,80,83	0
5	CL	B	703	1/1	0.95	0.14	80,80,80,80	0
4	SO4	A	703	5/5	0.95	0.11	67,75,84,85	0
3	NA	B	702	1/1	0.96	0.09	44,44,44,44	0
2	YHF	A	701	28/28	0.98	0.16	33,39,45,47	0
2	YHF	B	701	28/28	0.98	0.10	42,47,51,54	0

*Continued on next page...*

Continued from previous page...

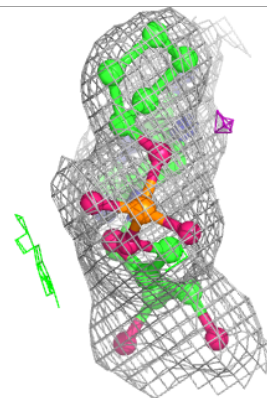
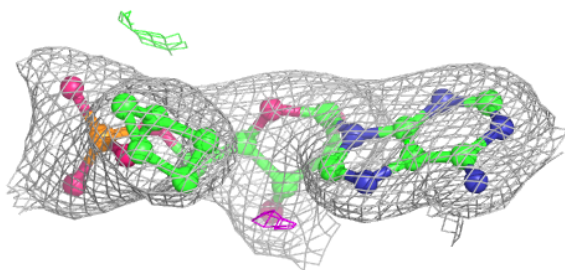
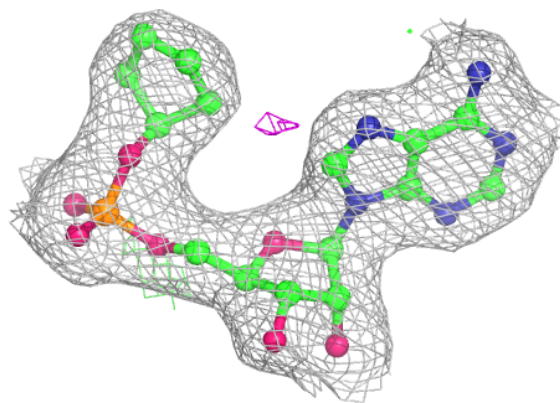
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NA	A	702	1/1	0.99	0.05	42,42,42,42	0

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.

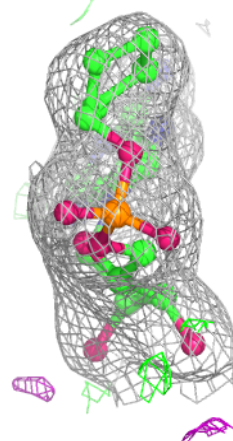
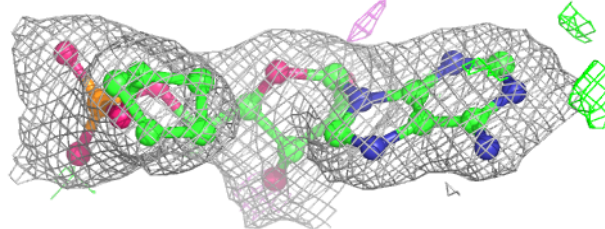
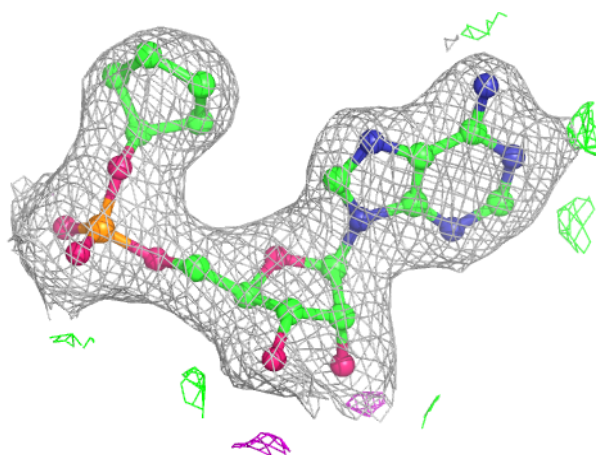


**Electron density around YHF A 701:**

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

**Electron density around YHF B 701:**

$2mF_o-DF_c$  (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.