Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 08:14 AM EST

PDB ID	:	8W0J
Title	:	Crystal structure of Acetyl-CoA synthetase 2 from Candida albicans in complex with a propyne AMP ester inhibitor
Authors	:	Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2024-02-13
Resolution	:	2.85 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*
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:

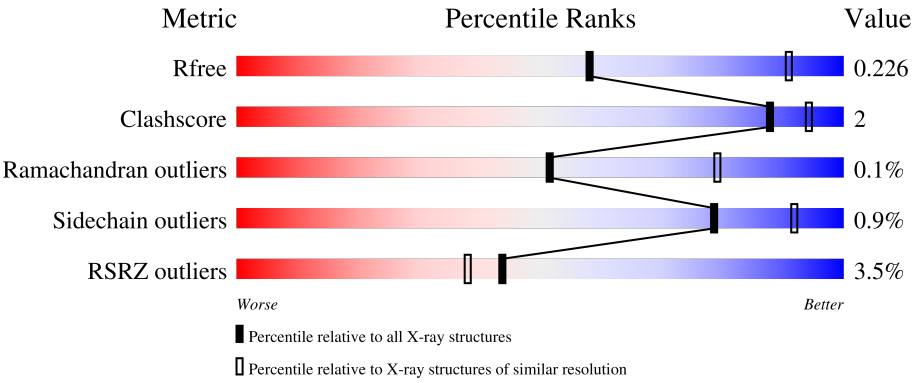
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 >=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 <=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	90% 7%
1	B	686	8% 81% 15%
1	C	686	% 73% 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	713	-	-	-	X
5	SO4	C	704	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14241 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
1	A	662	Total	C	N	O	S	0	1	0
			5144	3282	873	975	14			
1	B	584	Total	C	N	O	S	0	0	0
			4553	2918	770	852	13			
1	C	529	Total	C	N	O	S	0	1	0
			4144	2658	695	778	13			

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

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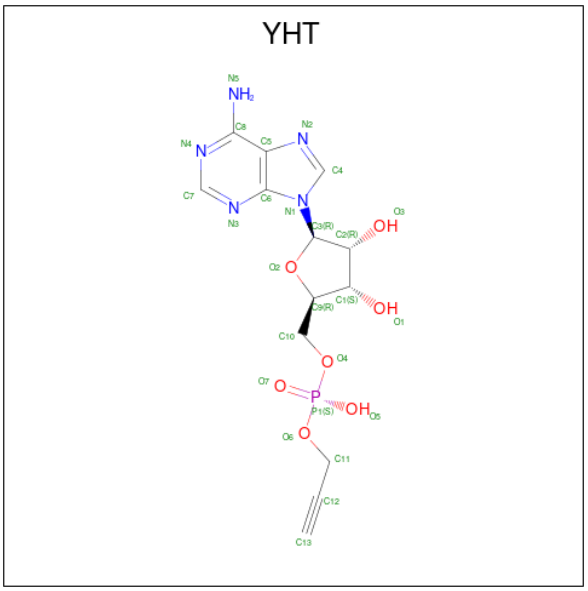
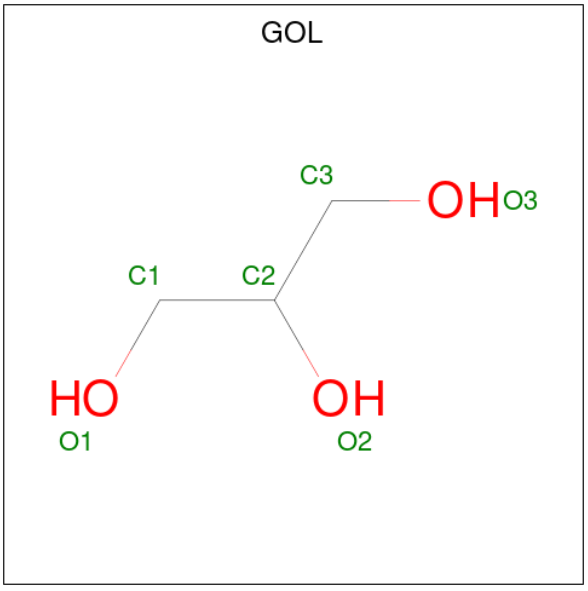
Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	expression tag	UNP Q8NJN3
B	8	HIS	-	expression tag	UNP Q8NJN3
B	9	HIS	-	expression tag	UNP Q8NJN3
B	10	GLU	-	expression tag	UNP Q8NJN3
B	11	ASN	-	expression tag	UNP Q8NJN3
B	12	LEU	-	expression tag	UNP Q8NJN3
B	13	TYR	-	expression tag	UNP Q8NJN3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

- Molecule 2 is 5'-O-{(S)-hydroxy[(prop-2-yn-1-yl)oxy]phosphoryl}adenosine (three-letter code: YHT) (formula: $C_{13}H_{16}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			26	13	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			26	13	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			26	13	5	7	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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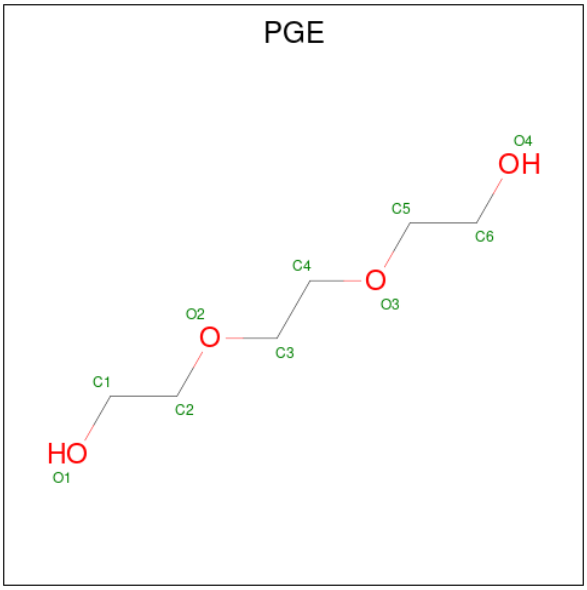
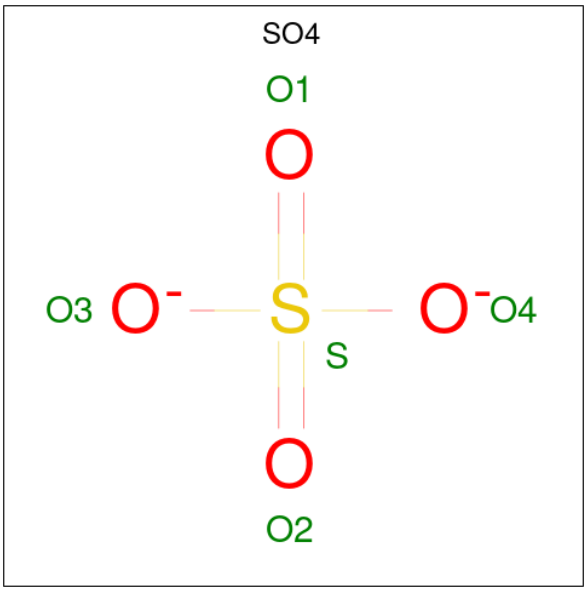
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0
4	A	1	Total C O 10 6 4	0	0
4	B	1	Total C O 10 6 4	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	2	Total Cl 2 2	0	0

- Molecule 7 is water.

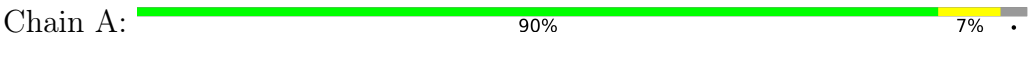
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	94	Total O 94 94	0	0
7	B	73	Total O 73 73	0	0
7	C	10	Total O 10 10	0	0

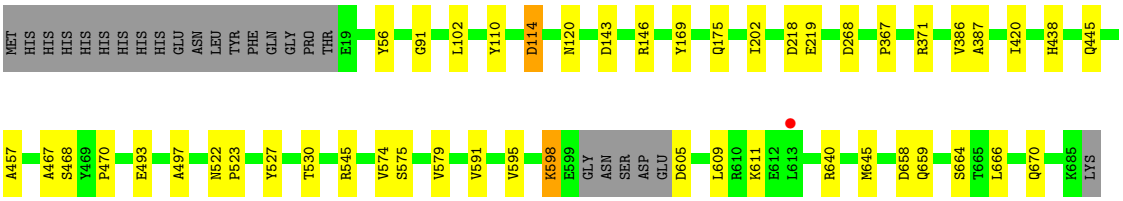
3 Residue-property plots (i)

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: Acetyl-coenzyme A synthetase 2

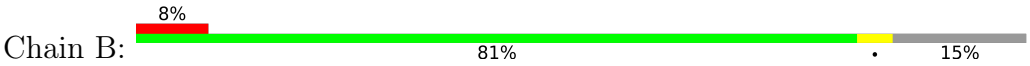
Chain A:

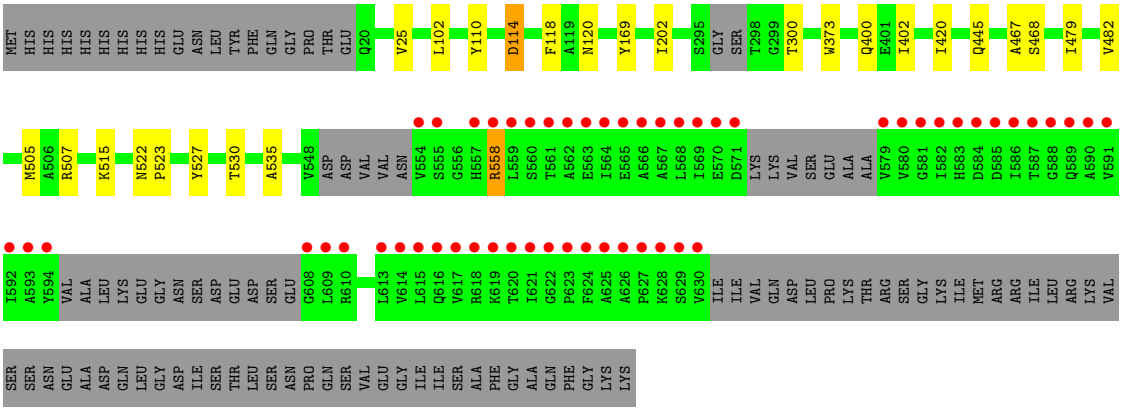




• Molecule 1: Acetyl-coenzyme A synthetase 2

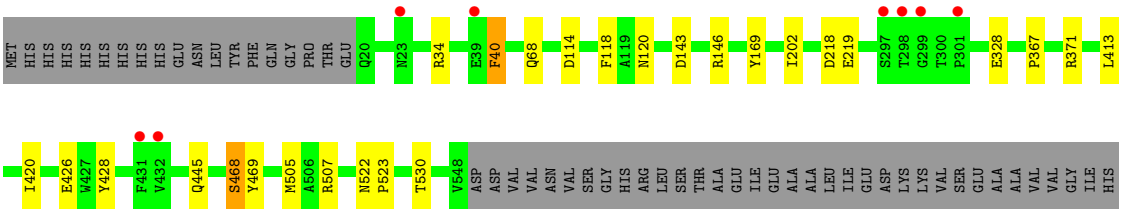
Chain B:





• Molecule 1: Acetyl-coenzyme A synthetase 2

Chain C:




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

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	139.07Å 139.07Å 544.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.62 – 2.85 49.62 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.62-2.85) 100.0 (49.62-2.85)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.86Å)	Xtriage
Refinement program	PHENIX (dev_5233: ???)	Depositor
R, R_{free}	0.196 , 0.226 0.199 , 0.226	Depositor DCC
R_{free} test set	3675 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	58.1	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14241	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: YHT, PGE, GOL, CL, SO4

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	0.28	0/5276	0.50	0/7173
1	B	0.27	0/4675	0.49	0/6360
1	C	0.26	0/4267	0.47	0/5812
All	All	0.27	0/14218	0.49	0/19345

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5144	0	5034	25	0
1	B	4553	0	4426	16	0
1	C	4144	0	4002	16	0
2	A	26	0	0	0	0
2	B	26	0	0	0	0
2	C	26	0	0	0	0
3	A	24	0	32	2	0
3	B	12	0	16	0	0
3	C	12	0	16	0	0
4	A	20	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	10	0	14	0	0
5	A	30	0	0	0	0
5	B	20	0	0	0	0
5	C	15	0	0	1	0
6	B	2	0	0	1	0
7	A	94	0	0	0	0
7	B	73	0	0	2	0
7	C	10	0	0	0	0
All	All	14241	0	13568	55	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 (55) 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:515:LYS:NZ	6:B:706:CL:CL	2.68	0.63
1:C:505:MET:O	1:C:507:ARG:NH1	2.34	0.60
1:B:400:GLN:NE2	7:B:802:HOH:O	2.36	0.58
1:C:68[A]:GLN:NE2	5:C:706:SO4:O3	2.38	0.56
1:B:467:ALA:O	1:B:468:SER:OG	2.23	0.55
1:A:493:GLU:OE1	1:A:545:ARG:NH1	2.38	0.54
1:B:445:GLN:NE2	1:B:530:THR:O	2.39	0.53
1:A:102:LEU:HD22	1:B:118:PHE:CZ	2.47	0.50
1:A:640:ARG:NH2	1:A:664:SER:O	2.44	0.50
1:C:143:ASP:OD1	1:C:146:ARG:NH2	2.45	0.50
1:B:25:VAL:HG22	1:B:535:ALA:HB1	1.94	0.50
1:A:467:ALA:O	1:A:468:SER:OG	2.25	0.49
1:B:505:MET:O	1:B:507:ARG:NH1	2.45	0.49
1:C:34:ARG:NH1	1:C:426:GLU:OE2	2.39	0.48
1:A:445:GLN:NE2	1:A:530:THR:O	2.34	0.48
1:C:169:TYR:CZ	1:C:202:ILE:HD11	2.49	0.47
1:A:522:ASN:N	1:A:523:PRO:CD	2.77	0.47
1:B:522:ASN:N	1:B:523:PRO:CD	2.78	0.47
1:C:367:PRO:HD2	1:C:371:ARG:HD3	1.97	0.47
1:B:400:GLN:HG3	7:B:867:HOH:O	2.15	0.47
1:A:91:GLY:H	3:A:704:GOL:H2	1.81	0.46
1:B:110:TYR:CD1	1:B:114:ASP:HB2	2.50	0.46
1:C:522:ASN:N	1:C:523:PRO:CD	2.79	0.46
1:C:169:TYR:CE1	1:C:202:ILE:HD11	2.50	0.46
1:C:468:SER:OG	1:C:469:TYR:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:MET:SD	1:A:666:LEU:HD21	2.56	0.46
1:C:420:ILE:O	1:C:420:ILE:HG23	2.17	0.45
1:A:218:ASP:OD1	1:A:219:GLU:N	2.45	0.44
1:C:413:LEU:HB3	1:C:428:TYR:CZ	2.52	0.44
1:A:574:VAL:HG13	1:A:595:VAL:HG13	1.99	0.44
1:A:56:TYR:OH	1:A:470:PRO:O	2.36	0.44
1:C:445:GLN:NE2	1:C:530:THR:O	2.50	0.44
1:B:102:LEU:HD22	1:C:118:PHE:CZ	2.54	0.43
1:A:438:HIS:CD2	1:A:457:ALA:HA	2.54	0.43
1:B:169:TYR:CZ	1:B:202:ILE:HD11	2.54	0.43
1:A:367:PRO:HD2	1:A:371:ARG:HD3	2.00	0.43
1:A:670:GLN:OE1	1:A:670:GLN:N	2.44	0.43
1:A:110:TYR:CD1	1:A:114:ASP:HB2	2.53	0.43
1:A:268:ASP:OD1	1:A:268:ASP:N	2.52	0.43
1:B:420:ILE:O	1:B:420:ILE:HG23	2.19	0.43
1:B:373:TRP:NE1	1:B:402:ILE:HG12	2.34	0.42
1:C:218:ASP:OD1	1:C:219:GLU:N	2.51	0.42
1:C:40:PHE:CD1	1:C:40:PHE:C	2.93	0.42
1:A:175:GLN:NE2	3:A:705:GOL:H2	2.35	0.42
1:A:420:ILE:O	1:A:420:ILE:HG23	2.19	0.42
1:A:143:ASP:OD1	1:A:146:ARG:NH2	2.54	0.41
1:B:482:VAL:HA	1:B:558:ARG:HD3	2.01	0.41
1:A:658:ASP:O	1:A:659:GLN:CB	2.69	0.41
1:A:386:VAL:HG22	1:A:387:ALA:N	2.35	0.41
1:A:497:ALA:HB1	1:A:527:TYR:HB3	2.03	0.41
1:B:479:ILE:HD11	1:B:527:TYR:CD2	2.57	0.40
1:A:169:TYR:CZ	1:A:202:ILE:HD11	2.56	0.40
1:A:579:VAL:CG1	1:A:591:VAL:HG13	2.52	0.40
1:C:328:GLU:OE1	1:C:328:GLU:N	2.50	0.40
1:A:575:SER:OG	1:A:598:LYS:HB3	2.22	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	659/686 (96%)	641 (97%)	18 (3%)	0	100 100
1	B	574/686 (84%)	560 (98%)	14 (2%)	0	100 100
1	C	528/686 (77%)	512 (97%)	15 (3%)	1 (0%)	47 75
All	All	1761/2058 (86%)	1713 (97%)	47 (3%)	1 (0%)	51 79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	468	SER

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%)	538 (99%)	6 (1%)	73 90
1	B	477/568 (84%)	473 (99%)	4 (1%)	81 93
1	C	435/568 (77%)	432 (99%)	3 (1%)	84 94
All	All	1456/1704 (85%)	1443 (99%)	13 (1%)	78 92

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ASP
1	A	120	ASN
1	A	598	LYS
1	A	605	ASP
1	A	609	LEU
1	A	611	LYS
1	B	114	ASP
1	B	120	ASN
1	B	300	THR

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Mol	Chain	Res	Type
1	B	558	ARG
1	C	40	PHE
1	C	114	ASP
1	C	120	ASN

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

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 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 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	PGE	A	707	-	9,9,9	0.33	0	8,8,8	0.58	0
5	SO4	B	709	-	4,4,4	0.66	0	6,6,6	0.19	0
5	SO4	B	708	-	4,4,4	0.65	0	6,6,6	0.07	0
5	SO4	A	709	-	4,4,4	0.66	0	6,6,6	0.16	0
5	SO4	B	710	-	4,4,4	0.63	0	6,6,6	0.12	0
4	PGE	A	706	-	9,9,9	0.32	0	8,8,8	0.55	0
3	GOL	A	702	-	5,5,5	0.29	0	5,5,5	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	A	703	-	5,5,5	0.31	0	5,5,5	0.36	0
5	SO4	A	710	-	4,4,4	0.61	0	6,6,6	0.32	0
3	GOL	B	702	-	5,5,5	0.35	0	5,5,5	0.18	0
3	GOL	B	703	-	5,5,5	0.30	0	5,5,5	0.38	0
3	GOL	C	702	-	5,5,5	0.35	0	5,5,5	0.36	0
2	YHT	A	701	-	25,28,28	0.65	0	26,41,41	0.78	1 (3%)
3	GOL	A	705	-	5,5,5	0.31	0	5,5,5	0.40	0
5	SO4	C	706	-	4,4,4	0.65	0	6,6,6	0.11	0
5	SO4	B	707	-	4,4,4	0.64	0	6,6,6	0.18	0
5	SO4	A	713	-	4,4,4	0.70	0	6,6,6	0.16	0
5	SO4	C	704	-	4,4,4	0.63	0	6,6,6	0.09	0
5	SO4	C	705	-	4,4,4	0.62	0	6,6,6	0.08	0
5	SO4	A	711	-	4,4,4	0.63	0	6,6,6	0.26	0
3	GOL	A	704	-	5,5,5	0.32	0	5,5,5	0.30	0
5	SO4	A	708	-	4,4,4	0.58	0	6,6,6	0.24	0
3	GOL	C	703	-	5,5,5	0.33	0	5,5,5	0.46	0
2	YHT	B	701	-	25,28,28	0.65	0	26,41,41	0.79	1 (3%)
5	SO4	A	712	-	4,4,4	0.67	0	6,6,6	0.11	0
2	YHT	C	701	-	25,28,28	0.65	0	26,41,41	0.82	1 (3%)
4	PGE	B	704	-	9,9,9	0.31	0	8,8,8	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
4	PGE	A	707	-	-	2/7/7/7	-
2	YHT	A	701	-	-	0/11/31/31	0/3/3/3
3	GOL	A	705	-	-	4/4/4/4	-
3	GOL	C	703	-	-	1/4/4/4	-
2	YHT	B	701	-	-	1/11/31/31	0/3/3/3
3	GOL	B	702	-	-	4/4/4/4	-
3	GOL	B	703	-	-	0/4/4/4	-
2	YHT	C	701	-	-	1/11/31/31	0/3/3/3
3	GOL	C	702	-	-	2/4/4/4	-
4	PGE	A	706	-	-	6/7/7/7	-
3	GOL	A	702	-	-	2/4/4/4	-
3	GOL	A	704	-	-	3/4/4/4	-
3	GOL	A	703	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	B	704	-	-	3/7/7/7	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	701	YHT	C5-C8-N5	2.28	123.82	120.35
2	B	701	YHT	C5-C8-N5	2.25	123.77	120.35
2	A	701	YHT	C5-C8-N5	2.13	123.59	120.35

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	YHT	O6-C11-C12-C13
2	C	701	YHT	O6-C11-C12-C13
3	A	705	GOL	O1-C1-C2-C3
3	B	702	GOL	C1-C2-C3-O3
3	B	702	GOL	O2-C2-C3-O3
4	A	706	PGE	O3-C5-C6-O4
3	A	702	GOL	O1-C1-C2-C3
3	A	704	GOL	O1-C1-C2-C3
3	B	702	GOL	O1-C1-C2-C3
3	C	703	GOL	C1-C2-C3-O3
4	B	704	PGE	O3-C5-C6-O4
3	A	705	GOL	O1-C1-C2-O2
4	A	706	PGE	C4-C3-O2-C2
3	C	702	GOL	O1-C1-C2-O2
3	A	705	GOL	C1-C2-C3-O3
4	A	706	PGE	C1-C2-O2-C3
3	A	702	GOL	O1-C1-C2-O2
3	A	704	GOL	O1-C1-C2-O2
4	B	704	PGE	O1-C1-C2-O2
4	B	704	PGE	O2-C3-C4-O3
3	A	704	GOL	O2-C2-C3-O3
4	A	707	PGE	C3-C4-O3-C5
4	A	706	PGE	C6-C5-O3-C4
4	A	706	PGE	C3-C4-O3-C5
3	B	702	GOL	O1-C1-C2-O2
3	A	705	GOL	O2-C2-C3-O3
3	C	702	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	706	PGE	O2-C3-C4-O3
4	A	707	PGE	O2-C3-C4-O3

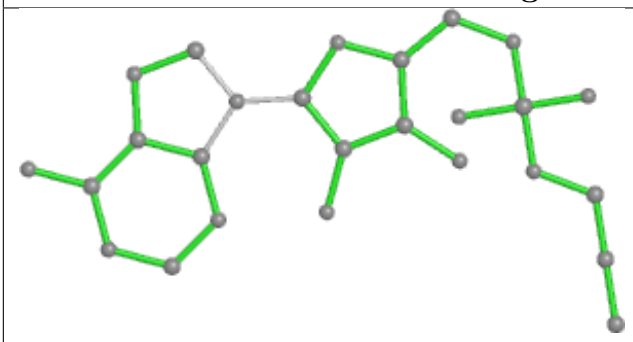
There are no ring outliers.

3 monomers are involved in 3 short contacts:

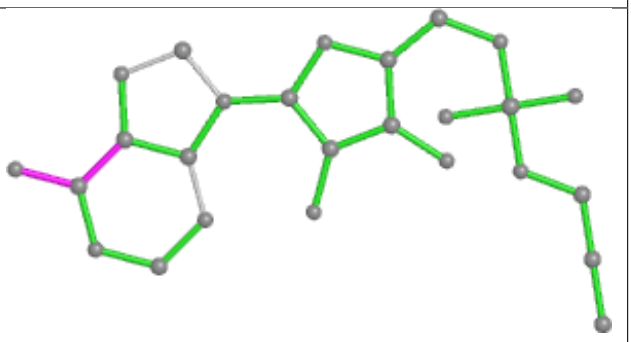
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	705	GOL	1	0
5	C	706	SO4	1	0
3	A	704	GOL	1	0

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 then 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.

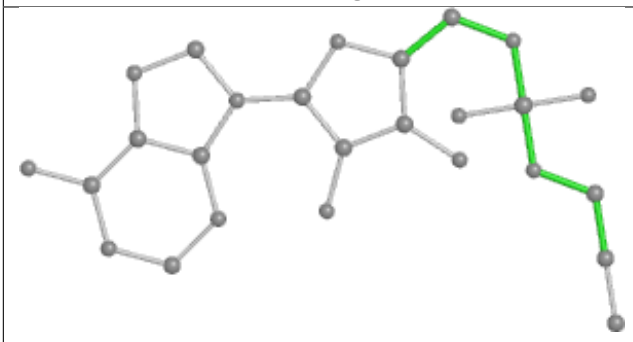
Ligand YHT A 701



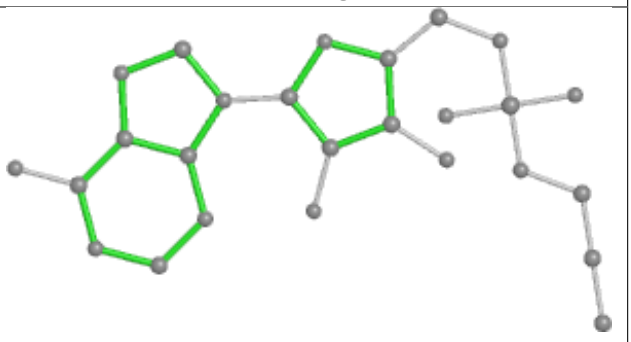
Bond lengths



Bond angles

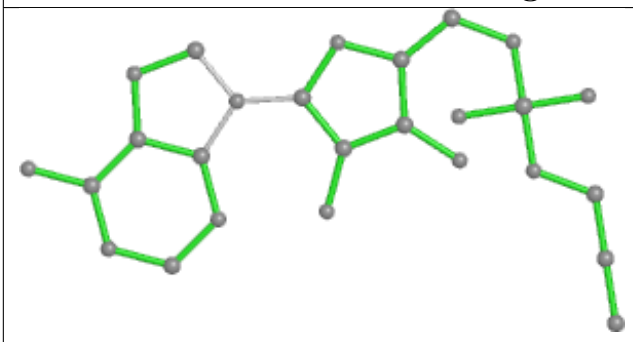


Torsions

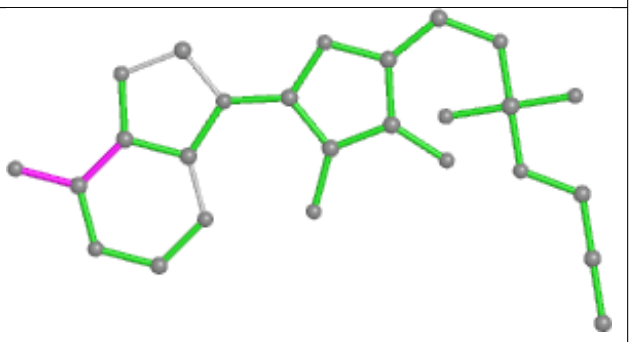


Rings

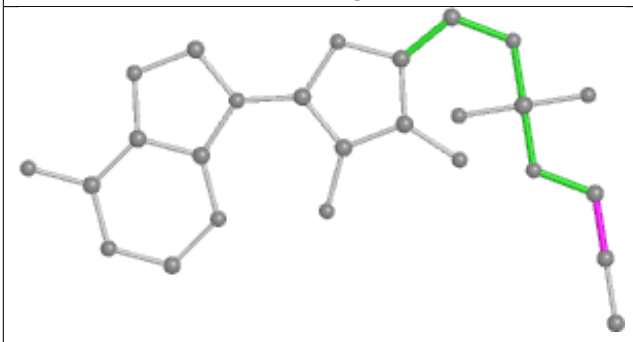
Ligand YHT B 701



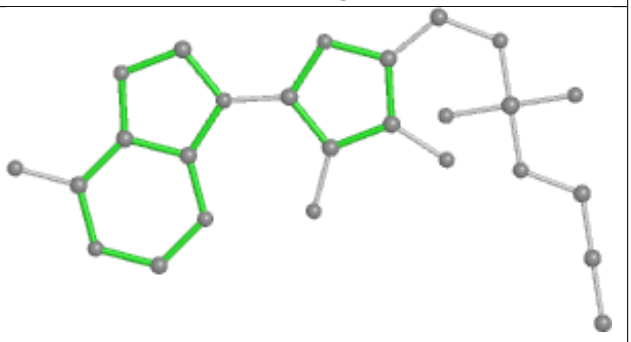
Bond lengths



Bond angles

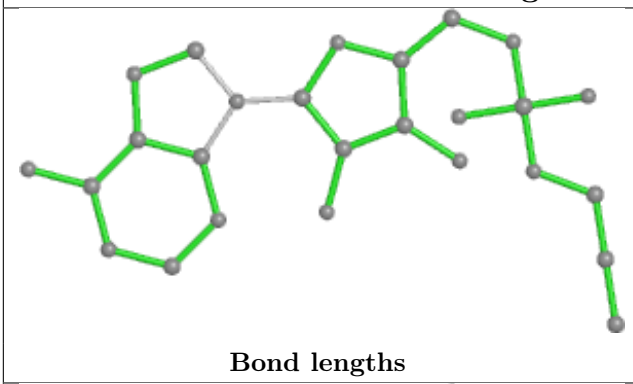


Torsions

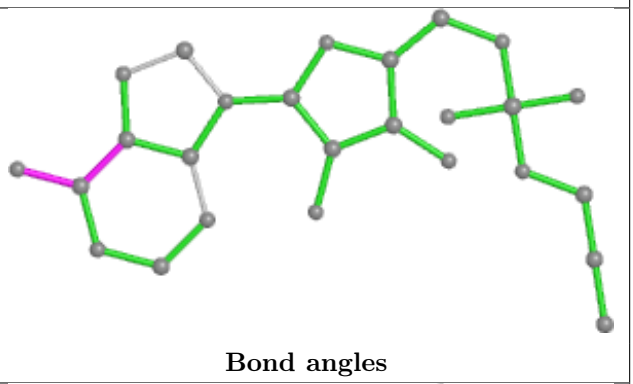


Rings

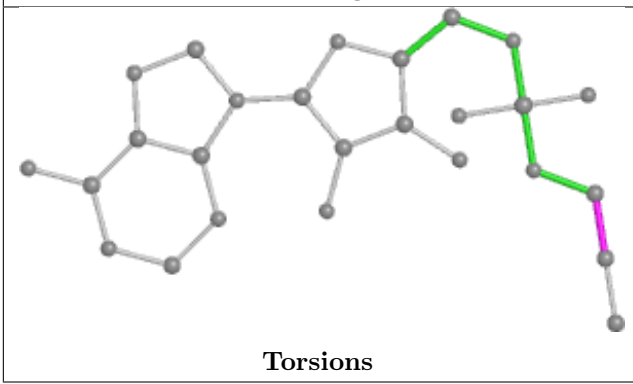
Ligand YHT C 701



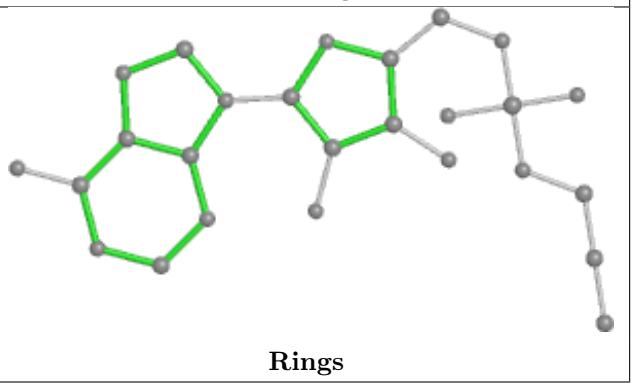
Bond lengths



Bond angles



Torsions



Rings

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^{th} 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^2)	Q<0.9
1	A	662/686 (96%)	-0.33	1 (0%) 95 95	41, 56, 91, 201	0
1	B	584/686 (85%)	0.06	54 (9%) 9 6	41, 59, 149, 170	0
1	C	529/686 (77%)	-0.15	8 (1%) 73 72	51, 84, 122, 164	0
All	All	1775/2058 (86%)	-0.15	63 (3%) 44 38	41, 63, 123, 201	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	564	ILE	7.5
1	B	591	VAL	6.8
1	B	630	VAL	6.7
1	B	613	LEU	6.6
1	B	568	LEU	6.5
1	B	629	SER	6.1
1	B	625	ALA	6.0
1	B	567	ALA	6.0
1	B	593	ALA	5.8
1	B	623	PRO	5.8
1	B	583	HIS	5.4
1	B	580	VAL	5.2
1	B	554	VAL	5.2
1	B	582	ILE	5.1
1	B	590	ALA	5.1
1	B	614	VAL	5.1
1	B	594	TYR	5.0
1	B	571	ASP	5.0
1	B	569	ILE	4.9
1	B	559	LEU	4.8
1	B	562	ALA	4.8
1	B	565	GLU	4.6
1	B	628	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	586	ILE	4.6
1	B	587	THR	4.5
1	B	579	VAL	4.5
1	B	561	THR	4.4
1	B	585	ASP	4.4
1	B	617	VAL	4.3
1	A	613	LEU	4.2
1	B	627	PRO	4.2
1	B	592	ILE	4.2
1	B	560	SER	4.1
1	B	610	ARG	4.0
1	B	624	PHE	3.9
1	B	584	ASP	3.8
1	B	616	GLN	3.7
1	B	618	ARG	3.6
1	B	558	ARG	3.5
1	B	581	GLY	3.4
1	B	615	LEU	3.3
1	B	588	GLY	3.3
1	C	297	SER	3.3
1	B	566	ALA	3.3
1	B	557	HIS	3.2
1	B	621	ILE	3.1
1	B	608	GLY	2.9
1	B	589	GLN	2.9
1	B	570	GLU	2.9
1	B	563	GLU	2.7
1	B	609	LEU	2.6
1	B	619	LYS	2.6
1	B	555	SER	2.4
1	B	620	THR	2.4
1	B	622	GLY	2.4
1	C	432	VAL	2.4
1	B	626	ALA	2.4
1	C	23	ASN	2.3
1	C	431	PHE	2.3
1	C	39	GLU	2.2
1	C	301	PRO	2.1
1	C	299	GLY	2.1
1	C	298	THR	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^{th} 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^2)	Q<0.9
5	SO4	A	713	5/5	0.71	0.42	81,89,95,109	0
4	PGE	A	707	10/10	0.73	0.30	72,81,93,96	0
5	SO4	B	708	5/5	0.73	0.39	100,102,120,129	0
5	SO4	C	704	5/5	0.75	0.69	114,120,124,136	0
4	PGE	A	706	10/10	0.80	0.27	64,69,74,78	0
5	SO4	C	706	5/5	0.80	0.35	94,102,107,122	0
6	CL	B	705	1/1	0.80	0.14	95,95,95,95	0
6	CL	B	706	1/1	0.83	0.07	87,87,87,87	0
3	GOL	A	704	6/6	0.84	0.31	64,68,71,77	0
3	GOL	A	705	6/6	0.86	0.21	62,73,76,83	0
5	SO4	B	707	5/5	0.86	0.23	88,99,116,122	0
5	SO4	C	705	5/5	0.86	0.23	131,131,132,143	0
3	GOL	C	702	6/6	0.87	0.24	98,99,102,103	0
5	SO4	A	711	5/5	0.87	0.18	70,78,102,104	0
4	PGE	B	704	10/10	0.88	0.37	72,81,84,84	0
5	SO4	A	712	5/5	0.89	0.35	69,92,94,117	0
3	GOL	C	703	6/6	0.90	0.16	50,68,72,74	0
3	GOL	B	702	6/6	0.90	0.21	43,51,63,66	0
3	GOL	B	703	6/6	0.91	0.51	73,73,80,87	0
5	SO4	B	710	5/5	0.92	0.27	94,100,124,125	0
3	GOL	A	703	6/6	0.92	0.46	64,69,75,79	0
5	SO4	A	710	5/5	0.93	0.16	61,72,87,91	0
3	GOL	A	702	6/6	0.95	0.11	66,72,73,75	0
5	SO4	A	708	5/5	0.95	0.18	61,64,68,69	0
5	SO4	A	709	5/5	0.95	0.14	58,66,77,78	0
2	YHT	C	701	26/26	0.96	0.15	71,88,90,98	0
5	SO4	B	709	5/5	0.96	0.09	36,47,62,70	0

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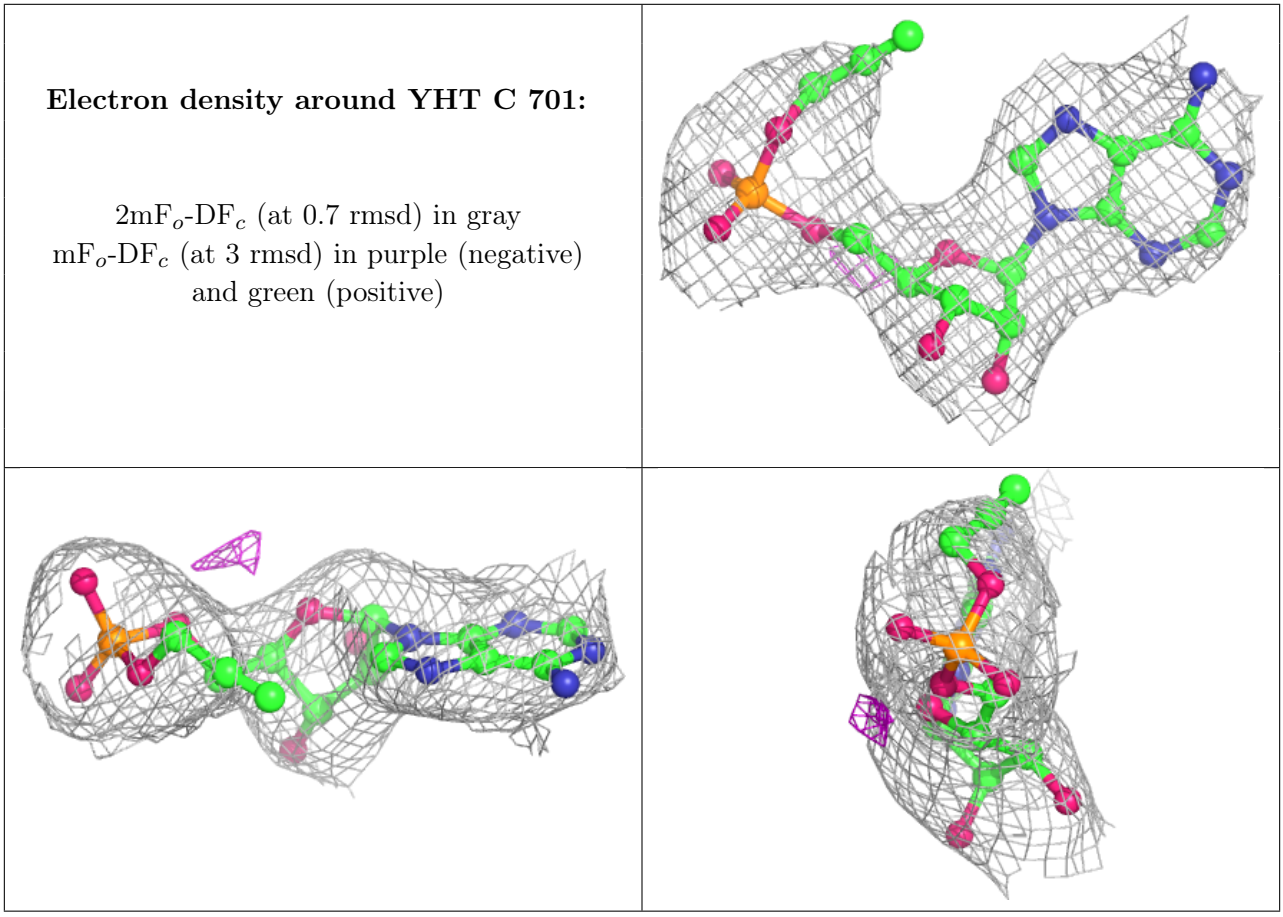
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	YHT	B	701	26/26	0.97	0.15	43,56,59,65	0
2	YHT	A	701	26/26	0.97	0.18	43,47,50,56	0

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.

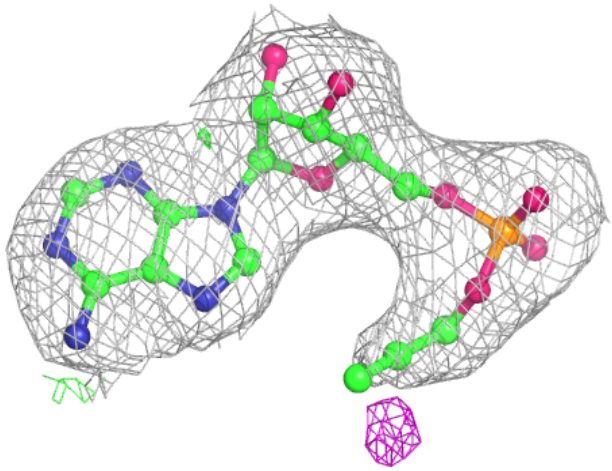
Electron density around YHT C 701:

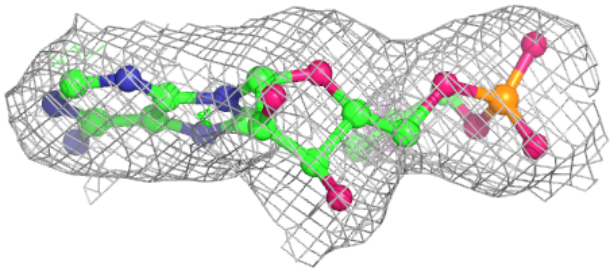
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

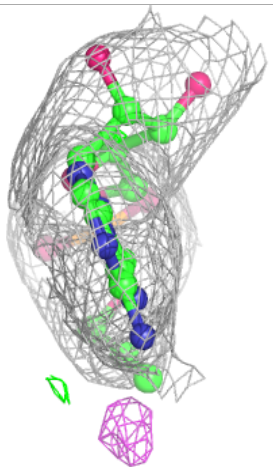


Electron density around YHT B 701:

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

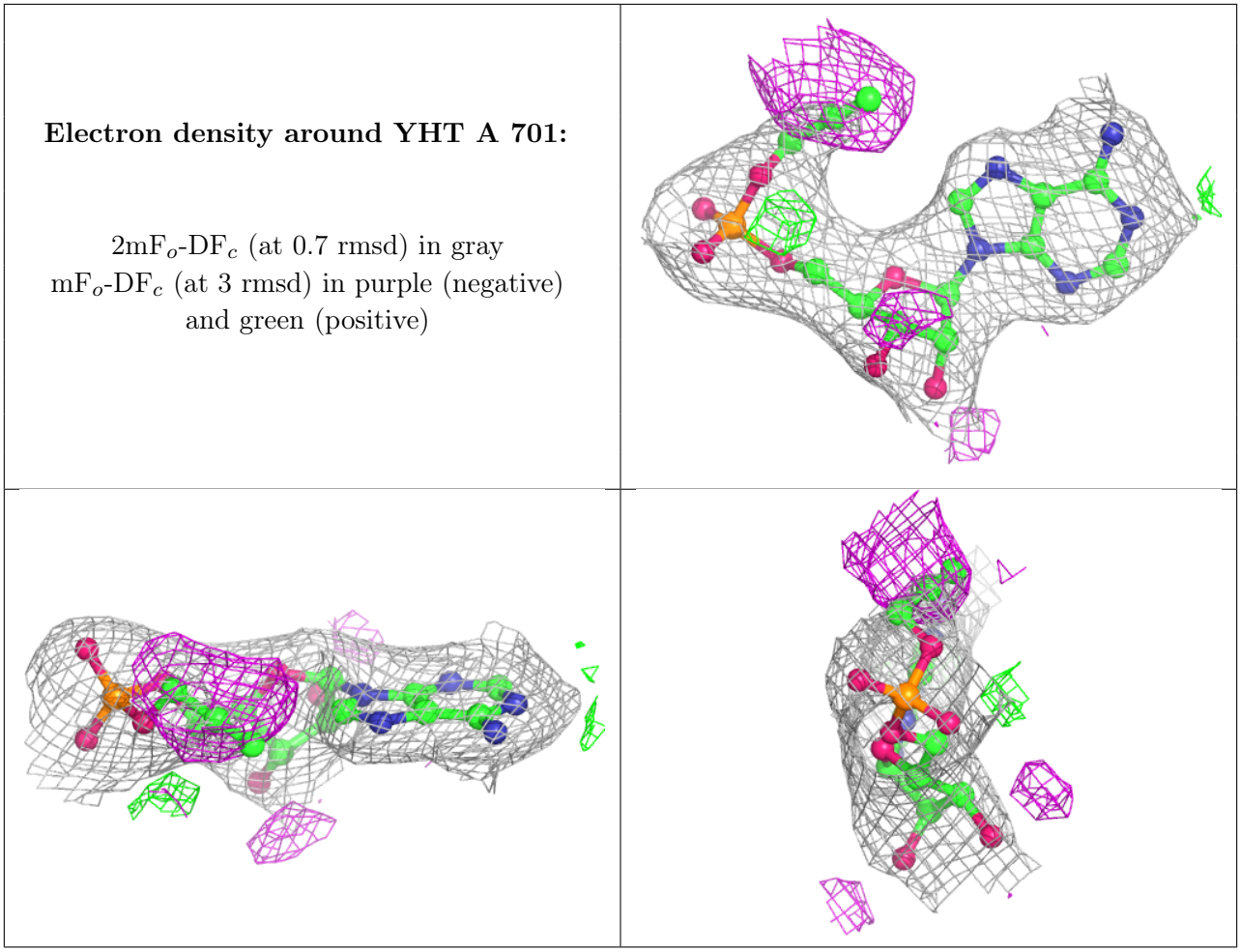






Electron density around YHT A 701:

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



6.5 Other polymers (i)

There are no such residues in this entry.