

Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 08:19 AM EST

PDB ID : 8W0B

Title: Crystal structure of Acetyl-CoA synthetase 2 from Candida albicans in com-

plex with a cyclopropyl 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 : 2.30 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 (i) 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 (i)) 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)

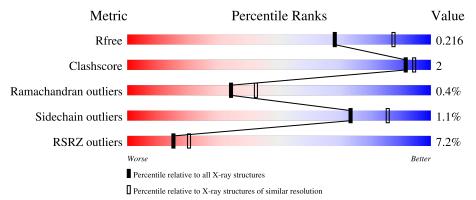
Validation Pipeline (wwPDB-VP) : 2.36

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 2.30 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	92%	5% •
1	В	686	12%	• 8%
1	С	686	74%	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
4	SO4	В	706	-	-	=	X
4	SO4	С	702	-	-	-	X



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14948 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	٨	667	Total	С	N O S		1	0		
1	A	007	5168	3296	878	980	14	0	1	U
1	В	632	Total C N O S		S	0	0	0		
1	Б	052	4908	3138	835	921	14	0	0	
1	С	529	Total	С	N	О	S	0	1	0
1		929	4150	2661	698	778	13	0	1	

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
В	1	MET	-	initiating methionine	UNP Q8NJN3
В	2	HIS	-	expression tag	UNP Q8NJN3
В	3	HIS	-	expression tag	UNP Q8NJN3
В	4	HIS	-	expression tag	UNP Q8NJN3
В	5	HIS	-	expression tag	UNP Q8NJN3
В	6	HIS	_	expression tag	UNP Q8NJN3

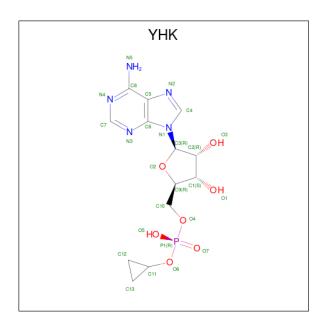


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Chain	Residue	Modelled Modelled	Actual	Comment	Reference
В	7	HIS	-	expression tag	UNP Q8NJN3
В	8	HIS	-	expression tag	UNP Q8NJN3
В	9	HIS	-	expression tag	UNP Q8NJN3
В	10	GLU	-	expression tag	UNP Q8NJN3
В	11	ASN	-	expression tag	UNP Q8NJN3
В	12	LEU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

• Molecule 2 is 5'-O-[(R)-(cyclopropyloxy)(hydroxy)phosphoryl]adenosine (three-letter code: YHK) (formula: $C_{13}H_{18}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).





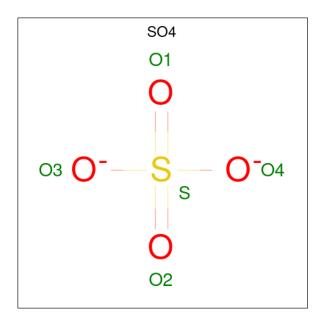
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
2	Λ	1	Total	С	N	О	Р	0	0	
2	A	1	26	13	5	7	1	U		
2	D	1	Total	С	N	О	Р	0	0	
2	Б	1	26	13	5	7	1	U		
2	С	1	Total	С	N	О	Р	0	0	
			26	13	5	7	1	U	U	

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

\mathbf{N}	/Iol	Chain	Residues	Atoms	ZeroOcc	AltConf
	3	A	1	Total Na 1 1	0	0
	3	В	1	Total Na 1 1	0	0

 \bullet Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

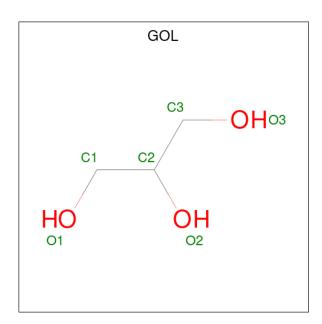




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S	0	0
4	Λ	1	5 4 1	U	U
4	A	1	Total O S	0	0
	11	1	5 4 1	U	U
4	A	1	Total O S	0	0
- T	71	1	5 4 1	Ŭ	0
4	В	1	Total O S	0	0
	Б	1	5 4 1	Ŭ	Ů
4	В	1	Total O S	0	0
1	Б	1	5 4 1		Ů
4	В	1	Total O S	0	0
		1	5 4 1	Ŭ	Ü
4	В	1	Total O S	0	0
1	D	1	5 4 1	Ŭ	Ü
4	В	1	Total O S	0	0
	D	1	5 4 1		9
4	\mathbf{C}	1	Total O S	0	0
T		1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$		

 \bullet Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $\mathrm{C_3H_8O_3}).$





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

• Molecule 6 is water.

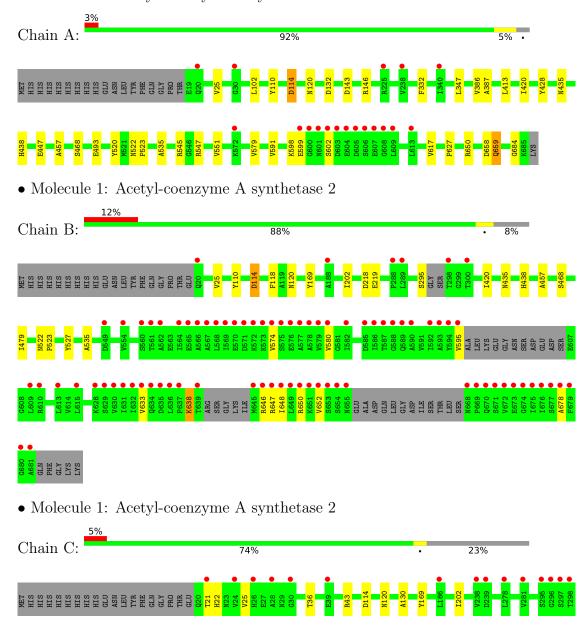
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	270	Total O 270 270	0	0
6	В	242	Total O 242 242	0	0
6	С	79	Total O 79 79	0	0



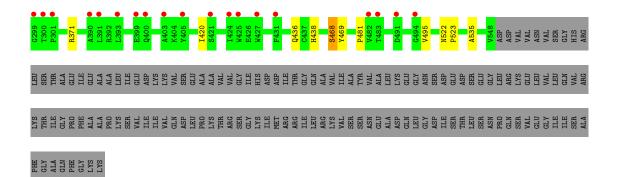
3 Residue-property plots (i)

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









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	139.78Å 139.78Å 544.42Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.65 - 2.30	Depositor
Resolution (A)	49.65 - 2.30	EDS
% Data completeness	99.9 (49.65-2.30)	Depositor
(in resolution range)	100.0 (49.65-2.30)	EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.94 (at 2.29Å)	Xtriage
Refinement program	PHENIX (dev_5233: ???)	Depositor
D D	0.186 , 0.219	Depositor
R, R_{free}	0.188 , 0.216	DCC
R_{free} test set	6943 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 41.3	EDS
L-test for twinning ²	$ < L >=0.52, < L^2>=0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14948	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.89% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: YHK, NA, SO4, GOL

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.31	0/5301	0.55	0/7209	
1	В	0.29	0/5033	0.53	0/6845	
1	С	0.28	0/4273	0.50	0/5819	
All	All	0.30	0/14607	0.53	0/19873	

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 (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	19	0
1	В	4908	0	4789	15	0
1	С	4150	0	4013	10	0
2	A	26	0	0	0	0
2	В	26	0	0	0	0
2	С	26	0	0	0	0
3	A	1	0	0	0	0
3	В	1	0	0	0	0
4	A	15	0	0	1	0
4	В	25	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	С	5	0	0	0	0
5	В	6	0	8	1	0
6	A	270	0	0	0	0
6	В	242	0	0	1	0
6	С	79	0	0	0	0
All	All	14948	0	13856	44	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 (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	$\operatorname{distance}\left(\mathrm{\AA}\right)$	overlap (Å)
1:B:633:VAL:HG12	1:B:678:ALA:HB3	1.63	0.81
1:B:633:VAL:HG12	1:B:678:ALA:CB	2.28	0.62
1:B:25:VAL:HG22	1:B:535:ALA:HB1	1.87	0.56
1:A:493:GLU:OE1	1:A:545:ARG:NH1	2.37	0.54
1:A:650:ARG:NH2	4:A:703:SO4:O1	2.38	0.53
1:C:43:ARG:NH2	1:C:436:GLN:OE1	2.41	0.53
1:C:481:PRO:HG3	1:C:495:VAL:HG23	1.89	0.52
1:A:143:ASP:OD1	1:A:146:ARG:NH2	2.43	0.52
1:B:648:ILE:O	1:B:652:VAL:HG23	2.10	0.51
1:A:579:VAL:CG1	1:A:591:VAL:HG13	2.41	0.50
1:C:420:ILE:O	1:C:420:ILE:HG23	2.11	0.49
1:A:658:ASP:O	1:A:659:GLN:HB2	2.12	0.49
1:A:658:ASP:O	1:A:659:GLN:CB	2.61	0.48
1:A:102:LEU:HD22	1:B:118:PHE:CZ	2.49	0.47
1:B:479:ILE:HD11	1:B:527:TYR:CD2	2.51	0.46
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:C:169:TYR:CZ	1:C:202:ILE:HD11	2.51	0.45
1:C:36:THR:HG22	1:C:438:HIS:ND1	2.31	0.45
1:A:413:LEU:HB3	1:A:428:TYR:CZ	2.51	0.45
1:A:438:HIS:CD2	1:A:457:ALA:HA	2.52	0.45
1:B:169:TYR:CZ	1:B:202:ILE:HD11	2.52	0.45
1:B:218:ASP:OD1	1:B:219:GLU:N	2.47	0.45
1:B:522:ASN:N	1:B:523:PRO:CD	2.80	0.45
1:B:479:ILE:HD11	1:B:527:TYR:CG	2.52	0.45
1:B:420:ILE:O	1:B:420:ILE:HG23	2.17	0.44
1:A:522:ASN:N	1:A:523:PRO:CD	2.81	0.44
1:A:547:ARG:HD2	1:A:551:VAL:HB	1.99	0.43



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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap (Å)
1:C:21:THR:HG22	1:C:22:HIS:N	2.33	0.43
1:C:25:VAL:HG22	1:C:535:ALA:HB1	2.00	0.43
1:B:438:HIS:CD2	1:B:457:ALA:HA	2.54	0.43
1:B:580:VAL:HB	1:B:650:ARG:HG2	2.02	0.41
1:A:347:LEU:C	1:A:347:LEU:HD23	2.40	0.41
1:A:420:ILE:O	1:A:420:ILE:HG23	2.20	0.41
5:B:703:GOL:H32	6:B:979:HOH:O	2.20	0.41
1:A:110:TYR:CD1	1:A:114:ASP:HB2	2.56	0.41
1:C:130:ALA:O	1:C:371:ARG:NH2	2.53	0.41
1:A:447:GLU:HG2	1:A:520:TYR:CZ	2.55	0.41
1:A:386:VAL:HG22	1:A:387:ALA:N	2.36	0.40
1:A:579:VAL:HG13	1:A:591:VAL:HG13	2.02	0.40
1:B:110:TYR:CD2	1:B:114:ASP:HB2	2.56	0.40
1:A:617:VAL:HG11	1:A:627:PRO:HD3	2.02	0.40
1:B:574:VAL:HG13	1:B:595:VAL:HG13	2.04	0.40
1:C:468:SER:OG	1:C:469:TYR:N	2.54	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	Perce	ntiles
1	A	666/686 $(97%)$	645 (97%)	17 (3%)	4 (1%)	25	31
1	В	622/686 (91%)	604 (97%)	16 (3%)	2 (0%)	41	50
1	С	528/686 (77%)	510 (97%)	17 (3%)	1 (0%)	47	58
All	All	1816/2058 (88%)	1759 (97%)	50 (3%)	7 (0%)	34	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	684	GLY



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Mol	Chain	Res	Type
1	С	468	SER
1	A	468	SER
1	A	602	SER
1	A	659	GLN
1	В	468	SER
1	В	638	LYS

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 82		
1	В	516/568 (91%)	509 (99%)	7 (1%)	67 81		
1	С	436/568 (77%)	434 (100%)	2 (0%)	88 95		
All	All	1496/1704 (88%)	1480 (99%)	16 (1%)	73 86		

All (16) 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	332	PHE
1	A	435	ASN
1	A	598	LYS
1	A	599	GLU
1	В	114	ASP
1	В	120	ASN
1	В	295	SER
1	В	435	ASN
1	В	638	LYS
1	В	646	ARG
1	В	647	ARG
1	С	114	ASP
1	С	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 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	Trino	Chain	Res	Link	Вс	Bond lengths		В	ond ang	cles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	В	704	-	4,4,4	0.64	0	6,6,6	0.09	0
2	YHK	С	701	-	24,29,29	0.71	0	25,44,44	0.70	1 (4%)
4	SO4	A	703	-	4,4,4	0.61	0	6,6,6	0.32	0
4	SO4	A	704	-	4,4,4	0.69	0	6,6,6	0.21	0
4	SO4	В	705	-	4,4,4	0.60	0	6,6,6	0.15	0
4	SO4	В	707	-	4,4,4	0.62	0	6,6,6	0.09	0
4	SO4	A	705	-	4,4,4	0.66	0	6,6,6	0.29	0
4	SO4	С	702	-	4,4,4	0.61	0	6,6,6	0.11	0
5	GOL	В	703	-	5,5,5	0.29	0	5,5,5	0.39	0
4	SO4	В	708	-	4,4,4	0.67	0	6,6,6	0.10	0
2	YHK	A	701	-	24,29,29	0.71	0	25,44,44	0.71	1 (4%)
2	YHK	В	701	-	24,29,29	0.71	0	25,44,44	0.77	1 (4%)
4	SO4	В	706	-	4,4,4	0.67	0	6,6,6	0.15	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
2	YHK	A	701	-	-	0/9/33/33	0/4/4/4
2	YHK	С	701	-	-	0/9/33/33	0/4/4/4
2	YHK	В	701	-	-	0/9/33/33	0/4/4/4
5	GOL	В	703	-	-	0/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
2	Α	701	YHK	C5-C8-N5	2.39	123.99	120.35
2	В	701	YHK	C5-C8-N5	2.39	123.98	120.35
2	С	701	YHK	C5-C8-N5	2.20	123.69	120.35

There are no chirality outliers.

There are no torsion outliers.

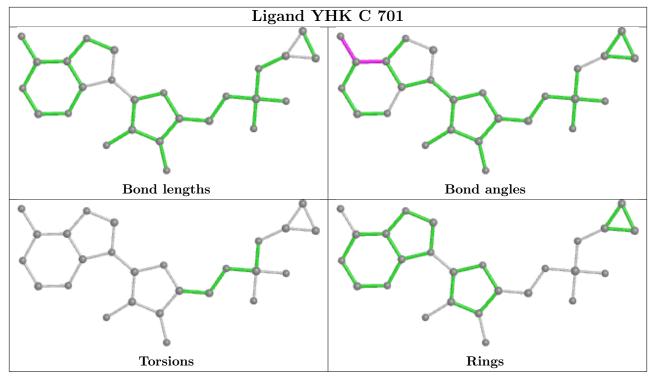
There are no ring outliers.

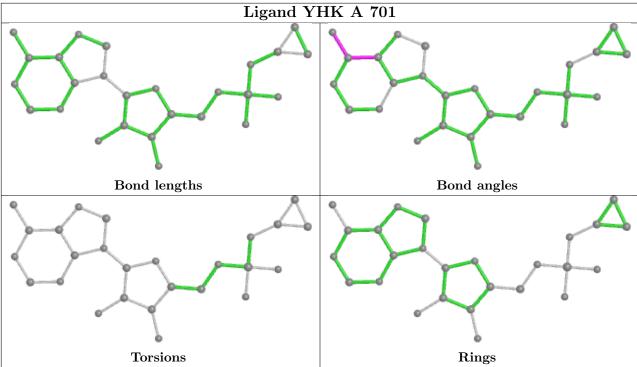
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	SO4	1	0
5	В	703	GOL	1	0

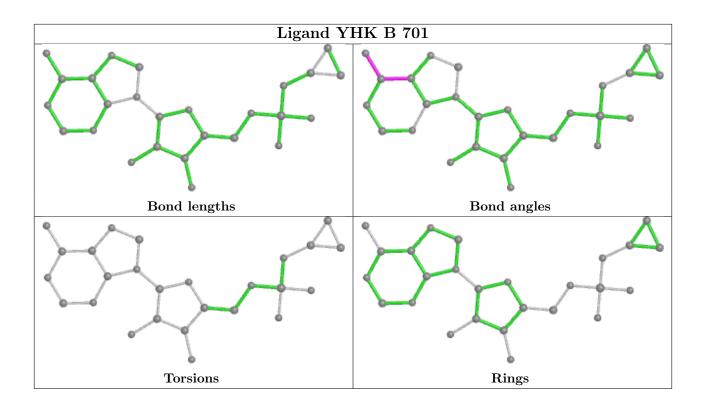
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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 (i)

6.1 Protein, DNA and RNA chains (i)

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	667/686 (97%)	0.17	18 (2%) 54 62	34, 48, 83, 140	0
1	В	632/686 (92%)	0.64	79 (12%) 3 5	37, 52, 127, 198	0
1	С	529/686 (77%)	0.28	34 (6%) 19 25	44, 67, 102, 161	0
All	All	1828/2058 (88%)	0.36	131 (7%) 15 20	34, 54, 102, 198	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	672	VAL	12.0
1	В	636	LEU	11.6
1	В	679	PHE	11.4
1	В	676	ILE	10.0
1	В	674	GLY	9.8
1	В	678	ALA	9.5
1	В	632	ILE	8.8
1	В	675	ILE	8.4
1	В	633	VAL	8.3
1	В	595	VAL	8.0
1	С	298	THR	7.7
1	С	297	SER	7.7
1	В	631	ILE	7.2
1	В	637	PRO	7.1
1	В	574	VAL	6.8
1	В	654	SER	6.7
1	В	635	ASP	6.7
1	В	677	SER	6.6
1	В	671	SER	6.4
1	В	573	LYS	6.3
1	В	649	LEU	6.1
1	В	569	ILE	5.9
1	В	648	ILE	5.8



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Mol	Chain	Res	Type	RSRZ				
1	В	680	GLY	5.7				
1	В	572	LYS	5.6				
1	С	299	GLY	5.5				
1	В	645	MET	5.5				
1	В	669	PRO	5.5				
1	В	646	ARG	5.4				
1	С	296	GLY	5.4				
1	В	668	ASN	5.1				
1	В	576	GLU	5.1				
1	В	580	VAL	5.1				
1	A	603	ASP	5.0				
1	A	602	SER	5.0				
1	В	634	GLN	4.9				
1	В	673	GLU	4.9				
1	В	567	ALA	4.8				
1	В	578	ALA	4.8				
1	A	601	ASN	4.7				
1	В	655	ASN	4.7				
1	С	482	VAL	4.7				
1	В	652	VAL	4.6				
1	В	593	ALA	4.6				
1	В	594	TYR	4.6				
1	В	613	LEU	4.6				
1	В	653	SER	4.5				
1	В	651	LYS	4.3				
1	В	630	VAL	4.2				
1	A	609	LEU	4.2				
1	В	586	ILE	4.2				
1	A	604	GLU	4.1				
1	В	571	ASP	3.9				
1	A	607	GLU	3.9				
1	В	577	ALA	3.9				
1	С	30	GLY	3.9				
1	A	605	ASP	3.7				
1	С	300	THR	3.7				
1	A	600	GLY	3.6				
1	С	391	LEU	3.5				
1	В	549	ASP	3.5				
1	В	670	GLN	3.5				
1	В	681	ALA	3.4				
1	В	20	GLN	3.4				
1	A	606	SER	3.4				
	1	1	1					



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Mol	Chain	Res	Type	RSRZ				
1	В	610	ARG	3.4				
1	С	295	SER	3.3				
1	В	639	THR	3.3				
1	В	562	ALA	3.3				
1	С	431	PHE	3.3				
1	В	585	ASP	3.3				
1	В	566	ALA	3.2				
1	С	427	TRP	3.2				
1	В	570	GLU	3.2				
1	В	298	THR	3.1				
1	A	613	LEU	3.1				
1	В	564	ILE	3.0				
1	В	579	VAL	3.0				
1	С	24	VAL	3.0				
1	В	582	ILE	3.0				
1	С	424	ILE	3.0				
1	В	575	SER	2.9				
1	С	238	VAL	2.9				
1	В	629	SER	2.9				
1	В	650	ARG	2.9				
1	С	301	PRO	2.9				
1	A	20	GLN	2.8				
1	В	592	ILE	2.8				
1	A	599	GLU	2.8				
1	С	405	TYR	2.8				
1	A	225	ARG	2.7				
1	В	590	ALA	2.7				
1	A	238	VAL	2.6				
1	В	609	LEU	2.6				
1	С	26	HIS	2.6				
1	С	278	LEU	2.6				
1	A	608	GLY	2.6				
1	С	39	GLU	2.5				
1	A	572	LYS	2.5				
1	В	587	THR	2.5				
1	С	21	THR	2.5				
1	В	628	LYS	2.5				
1	В	568	LEU	2.4				
1	С	494	GLY	2.4				
1	С	425	TRP	2.4				
1	В	647	ARG	2.4				
1	В	561	THR	2.4				
l	1	L	l					



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Mol	Chain	Res	Type	RSRZ
1	С	28	ALA	2.3
1	A	340	ILE	2.3
1	С	403	ALA	2.3
1	В	560	SER	2.3
1	С	400	GLN	2.3
1	В	188	ALA	2.3
1	С	393	LEU	2.3
1	С	483	THR	2.3
1	В	289	LEU	2.2
1	В	615	LEU	2.2
1	В	588	GLY	2.2
1	В	565	GLU	2.2
1	С	390	ALA	2.2
1	С	186	LEU	2.2
1	В	589	GLN	2.1
1	С	239	ASP	2.1
1	С	491	ASP	2.1
1	В	554	VAL	2.1
1	В	300	THR	2.1
1	С	421	SER	2.1
1	С	399	GLU	2.0
1	С	281	VAL	2.0
1	В	288	PRO	2.0
1	A	30	GLY	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.

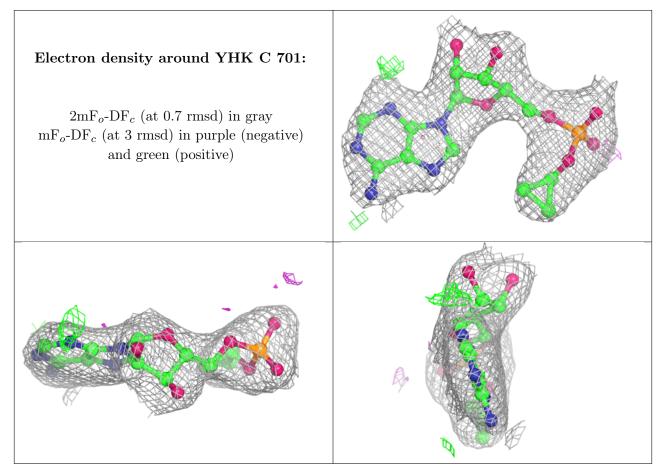
6.4 Ligands (i)

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.

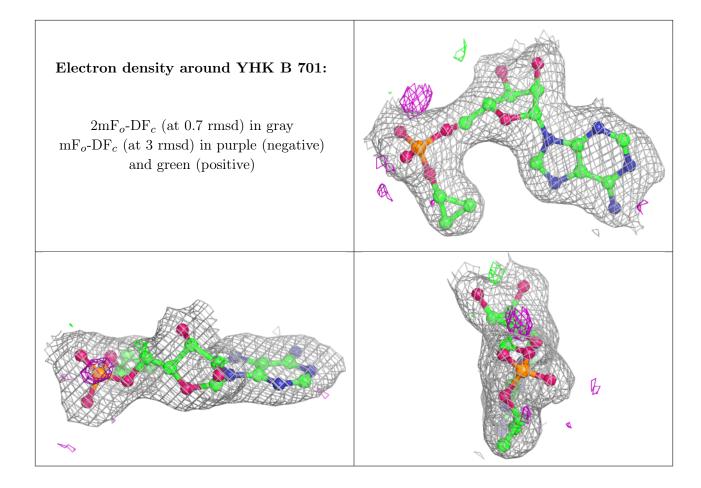


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
5	GOL	В	703	6/6	0.39	0.25	50,63,64,65	0
4	SO4	В	706	5/5	0.59	0.46	85,87,94,115	0
4	SO4	В	708	5/5	0.64	0.33	68,83,108,111	0
4	SO4	С	702	5/5	0.73	0.44	95,104,114,121	0
4	SO4	В	705	5/5	0.73	0.27	97,108,118,122	0
4	SO4	A	704	5/5	0.76	0.32	67,73,90,103	0
4	SO4	A	705	5/5	0.81	0.36	67,70,90,96	0
4	SO4	В	704	5/5	0.90	0.32	89,96,116,118	0
4	SO4	A	703	5/5	0.90	0.14	60,69,83,84	0
4	SO4	В	707	5/5	0.92	0.16	74,91,97,106	0
2	YHK	С	701	26/26	0.96	0.12	57,70,75,76	0
2	YHK	В	701	26/26	0.97	0.13	40,45,48,49	0
2	YHK	A	701	26/26	0.98	0.16	36,40,43,45	0
3	NA	A	702	1/1	0.99	0.06	40,40,40,40	0
3	NA	В	702	1/1	0.99	0.15	41,41,41,41	0

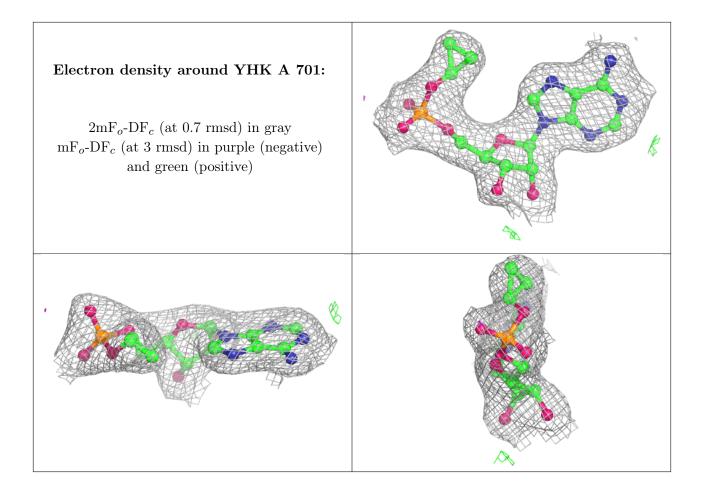
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.











6.5 Other polymers (i)

There are no such residues in this entry.

