



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 01:43 pm BST

PDB ID : 1T9B
Title : Crystal structure of yeast acetohydroxyacid synthase in complex with a sulfonylurea herbicide, chlorsulfuron
Authors : McCourt, J.A.; Pang, S.S.; Guddat, L.W.; Duggleby, R.G.
Deposited on : 2004-05-16
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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	:	2.11
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)	:	2.11

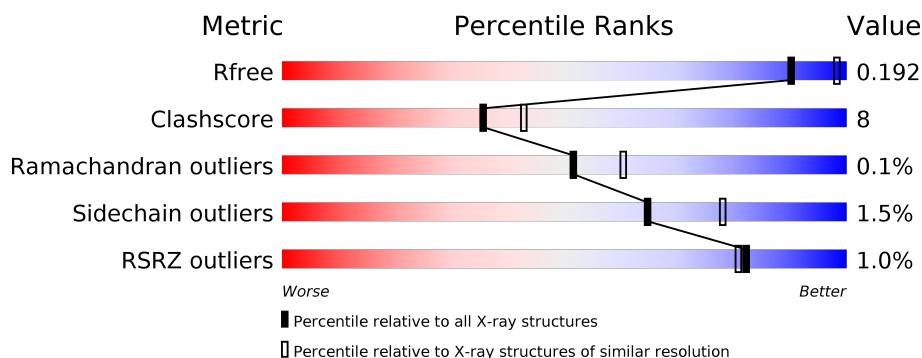
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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 $\leq 5\%$. 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	677	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>12%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	677	<div> <div></div> <div>75%</div> <div>12%</div> <div>12%</div> </div>

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	1CS	A	695	-	X	-	-
4	1CS	B	1695	-	X	-	-
8	YF3	A	1705	X	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 10553 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 Acetolactate synthase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	4	0
			4422	2798	766	837	21			
1	B	595	Total	C	N	O	S	0	9	0
			4566	2889	793	862	22			

There are 94 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	CLONING ARTIFACT	UNP P07342
A	12	HIS	-	CLONING ARTIFACT	UNP P07342
A	13	HIS	-	CLONING ARTIFACT	UNP P07342
A	14	HIS	-	CLONING ARTIFACT	UNP P07342
A	15	HIS	-	CLONING ARTIFACT	UNP P07342
A	16	HIS	-	CLONING ARTIFACT	UNP P07342
A	17	HIS	-	CLONING ARTIFACT	UNP P07342
A	18	SER	-	CLONING ARTIFACT	UNP P07342
A	19	SER	-	CLONING ARTIFACT	UNP P07342
A	20	GLY	-	CLONING ARTIFACT	UNP P07342
A	21	LEU	-	CLONING ARTIFACT	UNP P07342
A	22	VAL	-	CLONING ARTIFACT	UNP P07342
A	23	PRO	-	CLONING ARTIFACT	UNP P07342
A	24	ARG	-	CLONING ARTIFACT	UNP P07342
A	25	GLY	-	CLONING ARTIFACT	UNP P07342
A	26	SER	-	CLONING ARTIFACT	UNP P07342
A	27	GLY	-	CLONING ARTIFACT	UNP P07342
A	28	MET	-	CLONING ARTIFACT	UNP P07342
A	29	LYS	-	CLONING ARTIFACT	UNP P07342
A	30	GLU	-	CLONING ARTIFACT	UNP P07342
A	31	THR	-	CLONING ARTIFACT	UNP P07342
A	32	ALA	-	CLONING ARTIFACT	UNP P07342
A	33	ALA	-	CLONING ARTIFACT	UNP P07342
A	34	ALA	-	CLONING ARTIFACT	UNP P07342
A	35	LYS	-	CLONING ARTIFACT	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
A	36	PHE	-	CLONING ARTIFACT	UNP P07342
A	37	GLU	-	CLONING ARTIFACT	UNP P07342
A	38	ARG	-	CLONING ARTIFACT	UNP P07342
A	39	GLN	-	CLONING ARTIFACT	UNP P07342
A	40	HIS	-	CLONING ARTIFACT	UNP P07342
A	41	MET	-	CLONING ARTIFACT	UNP P07342
A	42	ASP	-	CLONING ARTIFACT	UNP P07342
A	43	SER	-	CLONING ARTIFACT	UNP P07342
A	44	PRO	-	CLONING ARTIFACT	UNP P07342
A	45	ASP	-	CLONING ARTIFACT	UNP P07342
A	46	LEU	-	CLONING ARTIFACT	UNP P07342
A	47	GLY	-	CLONING ARTIFACT	UNP P07342
A	48	THR	-	CLONING ARTIFACT	UNP P07342
A	49	ASP	-	CLONING ARTIFACT	UNP P07342
A	50	ASP	-	CLONING ARTIFACT	UNP P07342
A	51	ASP	-	CLONING ARTIFACT	UNP P07342
A	52	ASP	-	CLONING ARTIFACT	UNP P07342
A	53	LYS	-	CLONING ARTIFACT	UNP P07342
A	54	ALA	-	CLONING ARTIFACT	UNP P07342
A	55	MET	-	CLONING ARTIFACT	UNP P07342
A	56	GLY	-	CLONING ARTIFACT	UNP P07342
A	57	SER	-	CLONING ARTIFACT	UNP P07342
B	11	MET	-	CLONING ARTIFACT	UNP P07342
B	12	HIS	-	CLONING ARTIFACT	UNP P07342
B	13	HIS	-	CLONING ARTIFACT	UNP P07342
B	14	HIS	-	CLONING ARTIFACT	UNP P07342
B	15	HIS	-	CLONING ARTIFACT	UNP P07342
B	16	HIS	-	CLONING ARTIFACT	UNP P07342
B	17	HIS	-	CLONING ARTIFACT	UNP P07342
B	18	SER	-	CLONING ARTIFACT	UNP P07342
B	19	SER	-	CLONING ARTIFACT	UNP P07342
B	20	GLY	-	CLONING ARTIFACT	UNP P07342
B	21	LEU	-	CLONING ARTIFACT	UNP P07342
B	22	VAL	-	CLONING ARTIFACT	UNP P07342
B	23	PRO	-	CLONING ARTIFACT	UNP P07342
B	24	ARG	-	CLONING ARTIFACT	UNP P07342
B	25	GLY	-	CLONING ARTIFACT	UNP P07342
B	26	SER	-	CLONING ARTIFACT	UNP P07342
B	27	GLY	-	CLONING ARTIFACT	UNP P07342
B	28	MET	-	CLONING ARTIFACT	UNP P07342
B	29	LYS	-	CLONING ARTIFACT	UNP P07342
B	30	GLU	-	CLONING ARTIFACT	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
B	31	THR	-	CLONING ARTIFACT	UNP P07342
B	32	ALA	-	CLONING ARTIFACT	UNP P07342
B	33	ALA	-	CLONING ARTIFACT	UNP P07342
B	34	ALA	-	CLONING ARTIFACT	UNP P07342
B	35	LYS	-	CLONING ARTIFACT	UNP P07342
B	36	PHE	-	CLONING ARTIFACT	UNP P07342
B	37	GLU	-	CLONING ARTIFACT	UNP P07342
B	38	ARG	-	CLONING ARTIFACT	UNP P07342
B	39	GLN	-	CLONING ARTIFACT	UNP P07342
B	40	HIS	-	CLONING ARTIFACT	UNP P07342
B	41	MET	-	CLONING ARTIFACT	UNP P07342
B	42	ASP	-	CLONING ARTIFACT	UNP P07342
B	43	SER	-	CLONING ARTIFACT	UNP P07342
B	44	PRO	-	CLONING ARTIFACT	UNP P07342
B	45	ASP	-	CLONING ARTIFACT	UNP P07342
B	46	LEU	-	CLONING ARTIFACT	UNP P07342
B	47	GLY	-	CLONING ARTIFACT	UNP P07342
B	48	THR	-	CLONING ARTIFACT	UNP P07342
B	49	ASP	-	CLONING ARTIFACT	UNP P07342
B	50	ASP	-	CLONING ARTIFACT	UNP P07342
B	51	ASP	-	CLONING ARTIFACT	UNP P07342
B	52	ASP	-	CLONING ARTIFACT	UNP P07342
B	53	LYS	-	CLONING ARTIFACT	UNP P07342
B	54	ALA	-	CLONING ARTIFACT	UNP P07342
B	55	MET	-	CLONING ARTIFACT	UNP P07342
B	56	GLY	-	CLONING ARTIFACT	UNP P07342
B	57	SER	-	CLONING ARTIFACT	UNP P07342

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

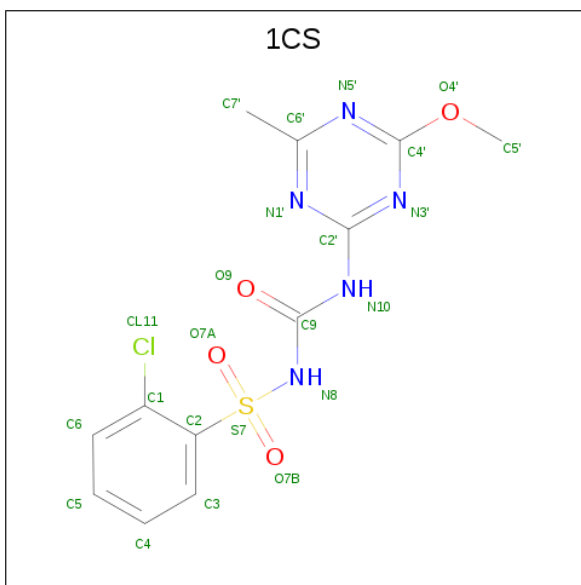
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0

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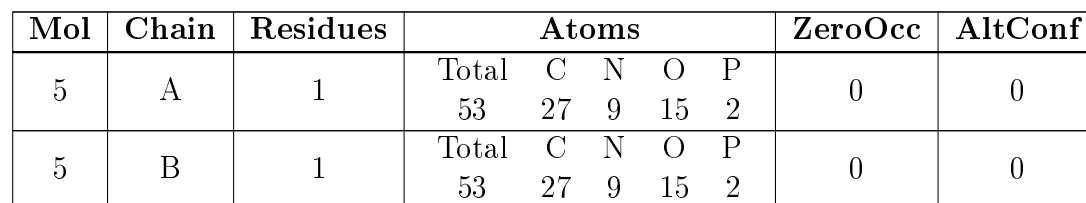
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 1-(2-CHLOROPHENYLSULFONYL)-3-(4-METHOXY-6-METHYL-L,3,5-TRIAZIN-2-YL)UREA (three-letter code: 1CS) (formula: C₁₂H₁₂ClN₅O₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 23	C 12	Cl 1	N 5	O 4	S 1	0	0
4	B	1	Total 23	C 12	Cl 1	N 5	O 4	S 1	0	0

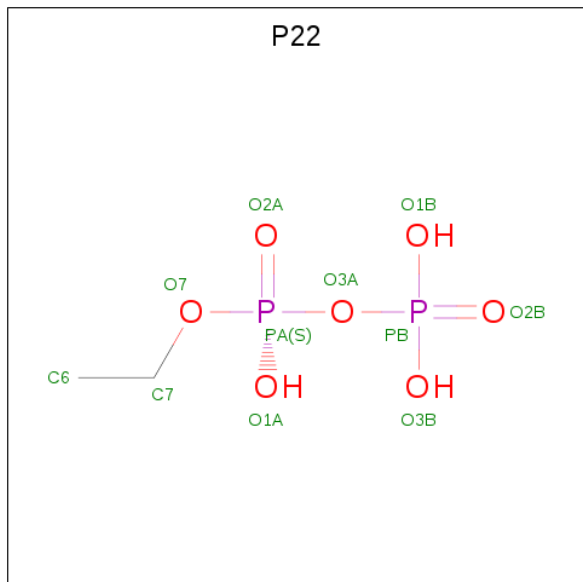
- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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- The diagram shows a chemical structure of a substituted pyrimidine ring. The ring consists of two nitrogen atoms (N) and four carbon atoms (C). The atoms are labeled as follows:
- Top nitrogen atom: NR1
 - Bottom nitrogen atom: NR2
 - Carbon atom at the top-left position: CQ1
 - Carbon atom at the top-right position: CS
 - Carbon atom at the bottom-left position: CP
 - Carbon atom at the bottom-right position: CQ2
- The bonds between the atoms are labeled as follows:
- Bond between NR1 and CQ1: NSP
 - Bond between NR1 and CS: NR1
 - Bond between CS and NR2: CS1
 - Bond between NR2 and CQ2: NR2
 - Bond between CQ2 and CP: CQ2
 - Bond between CP and CQ1: CP
 - Bond between CP and CA: CA
 - Bond between CA and NH2: CA
 - Bond between CQ2 and NH2: CQ2
- The terminal groups are labeled as follows:
- Terminal group at the top-left position: NH2
 - Terminal group at the bottom-left position: NH2
 - Terminal group at the bottom-right position: NH2

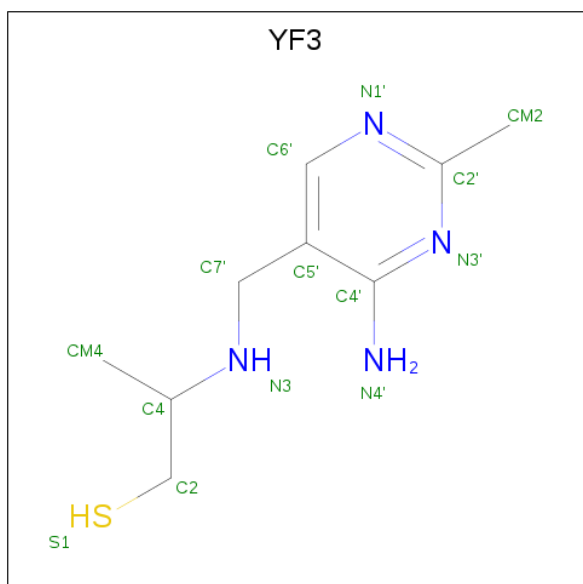
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			10	6	4		

- Molecule 7 is ETHYL DIHYDROGEN DIPHOSPHATE (three-letter code: P22) (formula: $C_2H_8O_7P_2$).



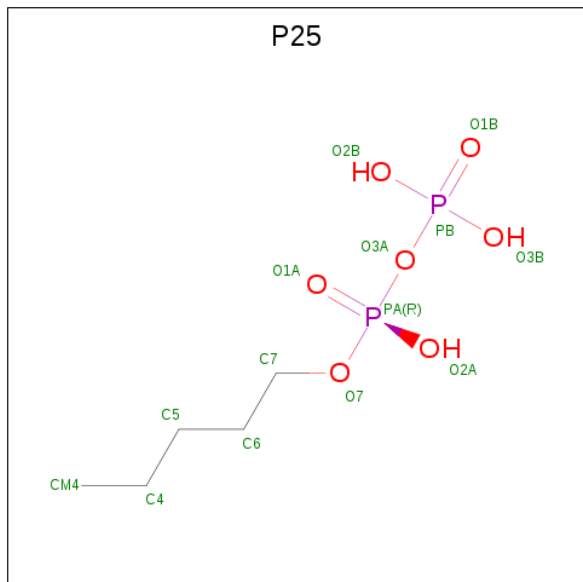
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			11	2	7	2		

- Molecule 8 is 2-[[[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]AMINO}PROPAN E-1-THIOL (three-letter code: YF3) (formula: $C_9H_{16}N_4S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	S	0	0
			14	9	4	1		

- Molecule 9 is PENTYL TRIHYDROGEN DIPHOSPHATE (three-letter code: P25) (formula: $C_5H_{14}O_7P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	O	P	0	0
			14	5	7	2		

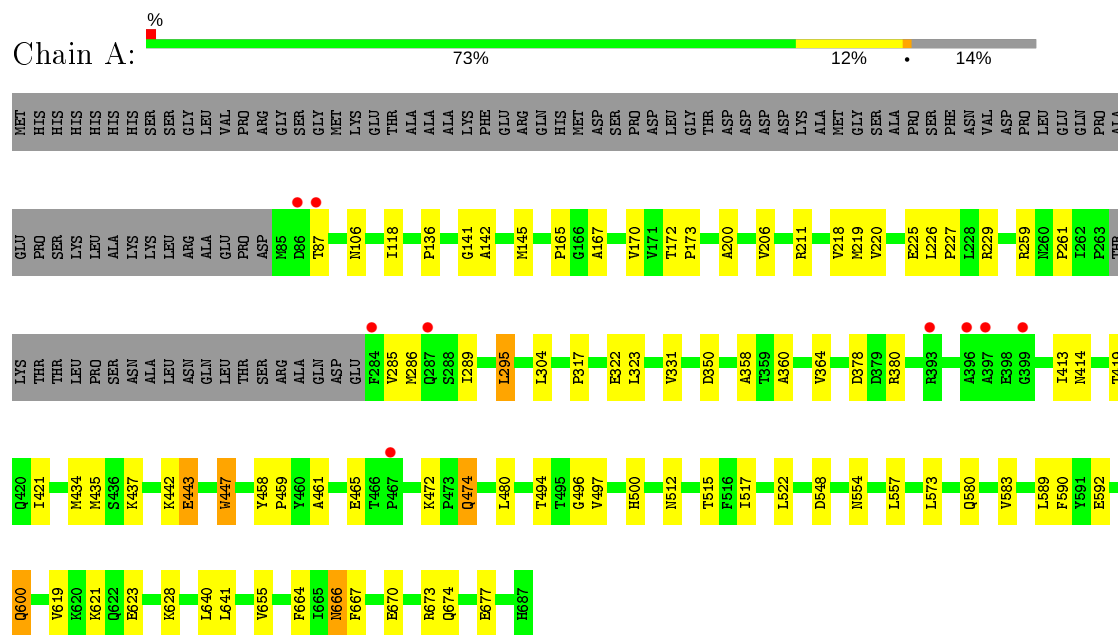
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	614	Total	O	0	0
			614	614		
10	B	746	Total	O	0	0
			746	746		

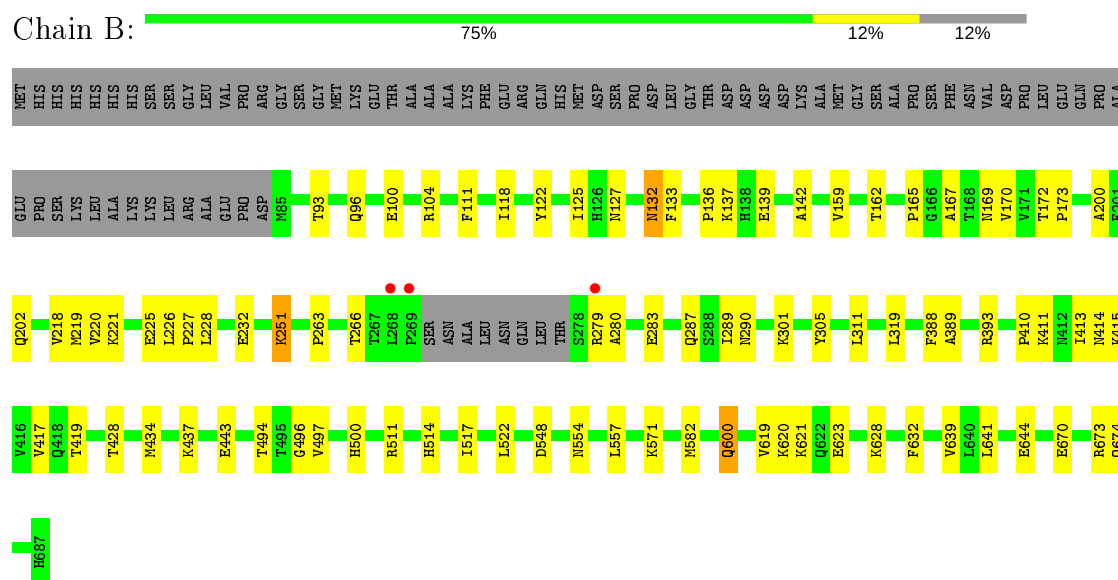
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Acetolactate synthase, mitochondrial



- Molecule 1: Acetolactate synthase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.58 Å 154.58 Å 178.76 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 64.48 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.5 (50.00-2.20) 90.4 (64.48-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.20 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.162 , 0.195 0.160 , 0.192	Depositor DCC
R_{free} test set	10345 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10553	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 1CS, MG, K, P22, P25, YF3, NSP, FAD

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	0.29	0/4530	0.55	0/6152
1	B	0.31	0/4696	0.59	0/6370
All	All	0.30	0/9226	0.57	0/12522

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	4422	0	4380	74	0
1	B	4566	0	4554	74	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	23	0	12	1	0
4	B	23	0	12	1	0
5	A	53	0	31	0	0
5	B	53	0	31	0	0
6	A	10	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	11	0	5	3	0
8	A	14	0	15	4	0
9	B	14	0	11	5	0
10	A	614	0	0	5	0
10	B	746	0	0	14	0
All	All	10553	0	9061	148	1

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 8.

The worst 5 of 148 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:A:474:GLN:HE21	1:A:474:GLN:H	1.27	0.82
1:B:619:VAL:HG22	1:B:628:LYS:HG3	1.63	0.80
1:B:600:GLN:NE2	1:B:600:GLN:H	1.79	0.79
1:B:280:ALA:HA	10:B:4669:HOH:O	1.84	0.77
1:A:621:LYS:HB3	1:A:623:GLU:OE2	1.84	0.76

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:ARG:NH2	1:B:511:ARG:NH2[5_556]	2.19	0.01

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	583/677 (86%)	572 (98%)	10 (2%)	1 (0%)	47	55
1	B	600/677 (89%)	588 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1183/1354 (87%)	1160 (98%)	22 (2%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	470/556 (84%)	461 (98%)	9 (2%)	57 71
1	B	492/556 (88%)	486 (99%)	6 (1%)	71 83
All	All	962/1112 (86%)	947 (98%)	15 (2%)	65 76

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	548	ASP
1	A	600	GLN
1	B	305	TYR
1	A	474	GLN
1	B	251	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	554	ASN
1	A	602	ASN
1	B	587	GLN
1	A	580	GLN
1	A	587	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z > 2$
5	FAD	B	1701	-	51,58,58	3.00	23 (45%)	60,89,89	2.02	11 (18%)
7	P22	A	1702	3	8,10,10	2.11	3 (37%)	12,15,15	2.22	2 (16%)
5	FAD	A	701	-	51,58,58	3.13	25 (49%)	60,89,89	2.06	12 (20%)
9	P25	B	698	3	11,13,13	1.94	5 (45%)	15,18,18	4.18	2 (13%)
4	1CS	B	1695	-	24,24,24	3.04	13 (54%)	33,34,34	4.26	15 (45%)
6	NSP	A	704	-	10,10,10	2.21	3 (30%)	13,13,13	2.69	6 (46%)
4	1CS	A	695	-	24,24,24	3.19	14 (58%)	33,34,34	4.35	15 (45%)
8	YF3	A	1705	-	14,14,14	2.38	4 (28%)	17,18,18	7.44	9 (52%)

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
5	FAD	B	1701	-	-	1/30/50/50	0/6/6/6
7	P22	A	1702	3	-	2/10/10/10	-
5	FAD	A	701	-	-	1/30/50/50	0/6/6/6
9	P25	B	698	3	-	1/13/13/13	-
4	1CS	B	1695	-	-	5/17/17/17	0/2/2/2
6	NSP	A	704	-	-	0/1/2/2	0/1/1/1
4	1CS	A	695	-	-	6/17/17/17	0/2/2/2
8	YF3	A	1705	-	1/1/1/2	5/6/7/7	0/1/1/1

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1701	FAD	C4A-N3A	9.47	1.48	1.35
5	A	701	FAD	C4A-N3A	9.37	1.48	1.35
5	A	701	FAD	C4X-C10	8.42	1.47	1.38
5	B	1701	FAD	C4X-C10	8.17	1.47	1.38
5	A	701	FAD	C2A-N1A	6.49	1.46	1.33

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1705	YF3	C4-C2-S1	25.43	142.79	114.19
9	B	698	P25	O7-C7-C6	15.49	160.67	108.99
4	A	695	1CS	C1-C2-S7	12.05	131.13	123.25
4	A	695	1CS	C4'-N3'-C2'	11.78	122.31	112.86
4	B	1695	1CS	C1-C2-S7	11.72	130.92	123.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	1705	YF3	C4

5 of 21 torsion outliers are listed below:

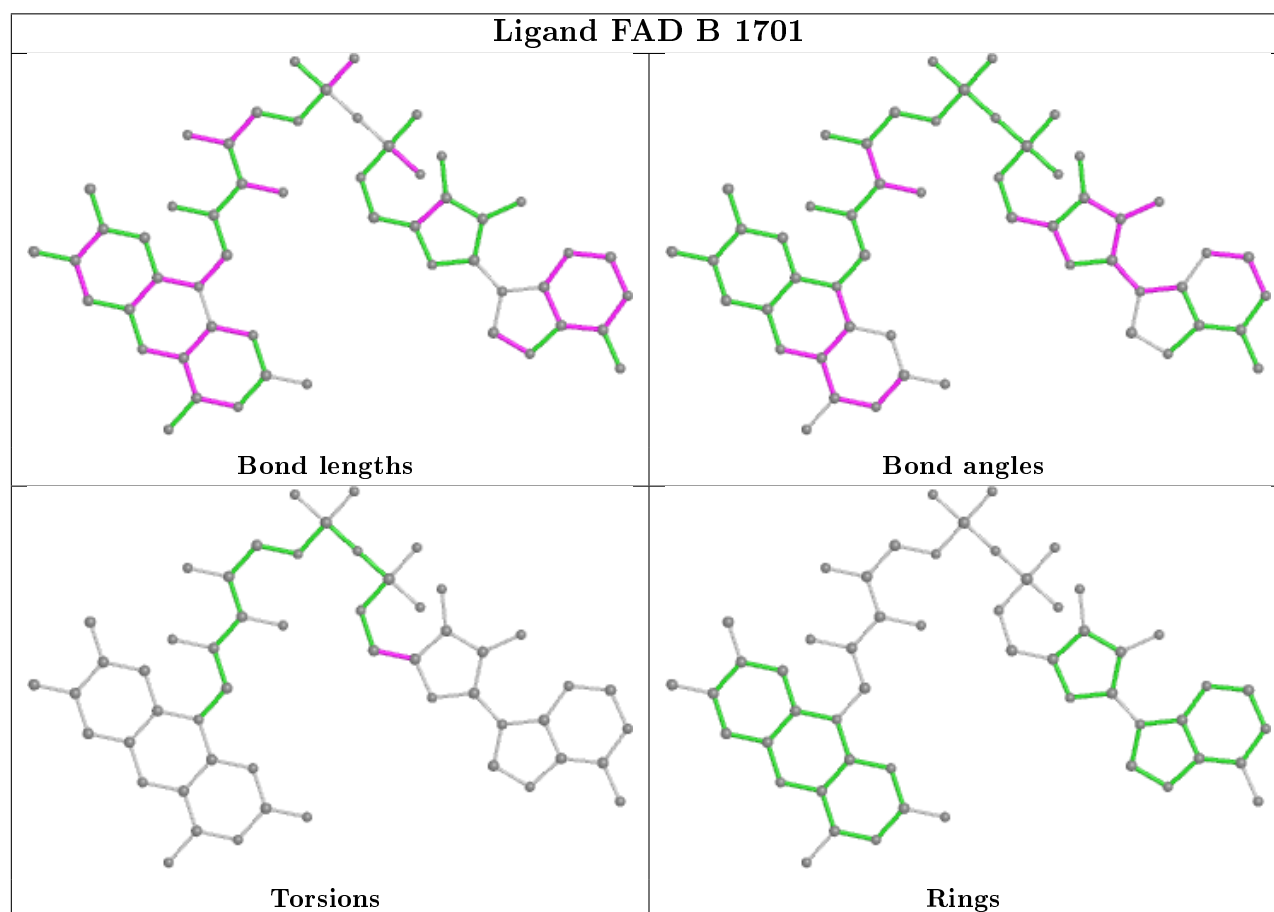
Mol	Chain	Res	Type	Atoms
4	B	1695	1CS	N8-C9-N10-C2'
4	A	695	1CS	N8-C9-N10-C2'
8	A	1705	YF3	C4'-C5'-C7'-N3
8	A	1705	YF3	CM4-C4-N3-C7'
8	A	1705	YF3	S1-C2-C4-N3

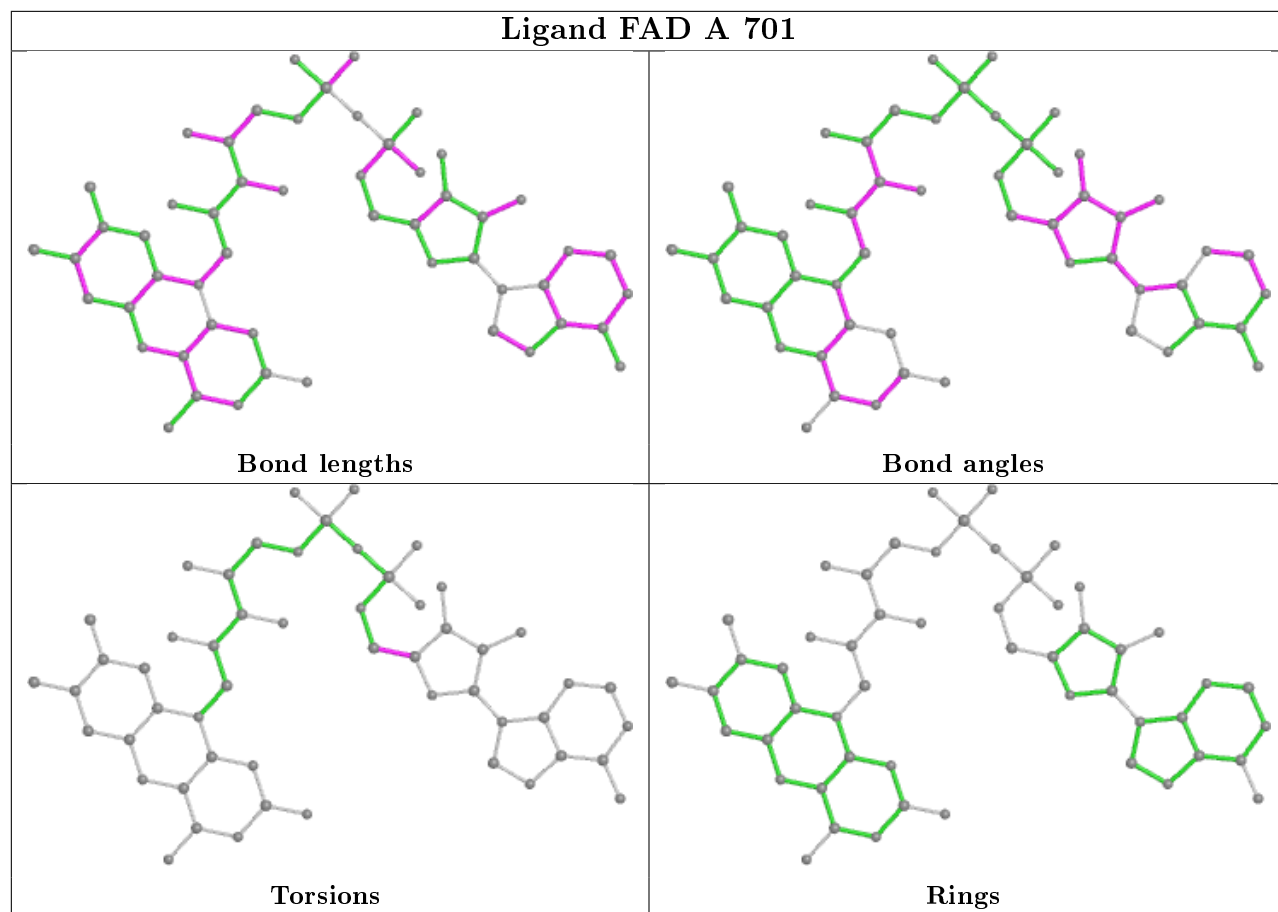
There are no ring outliers.

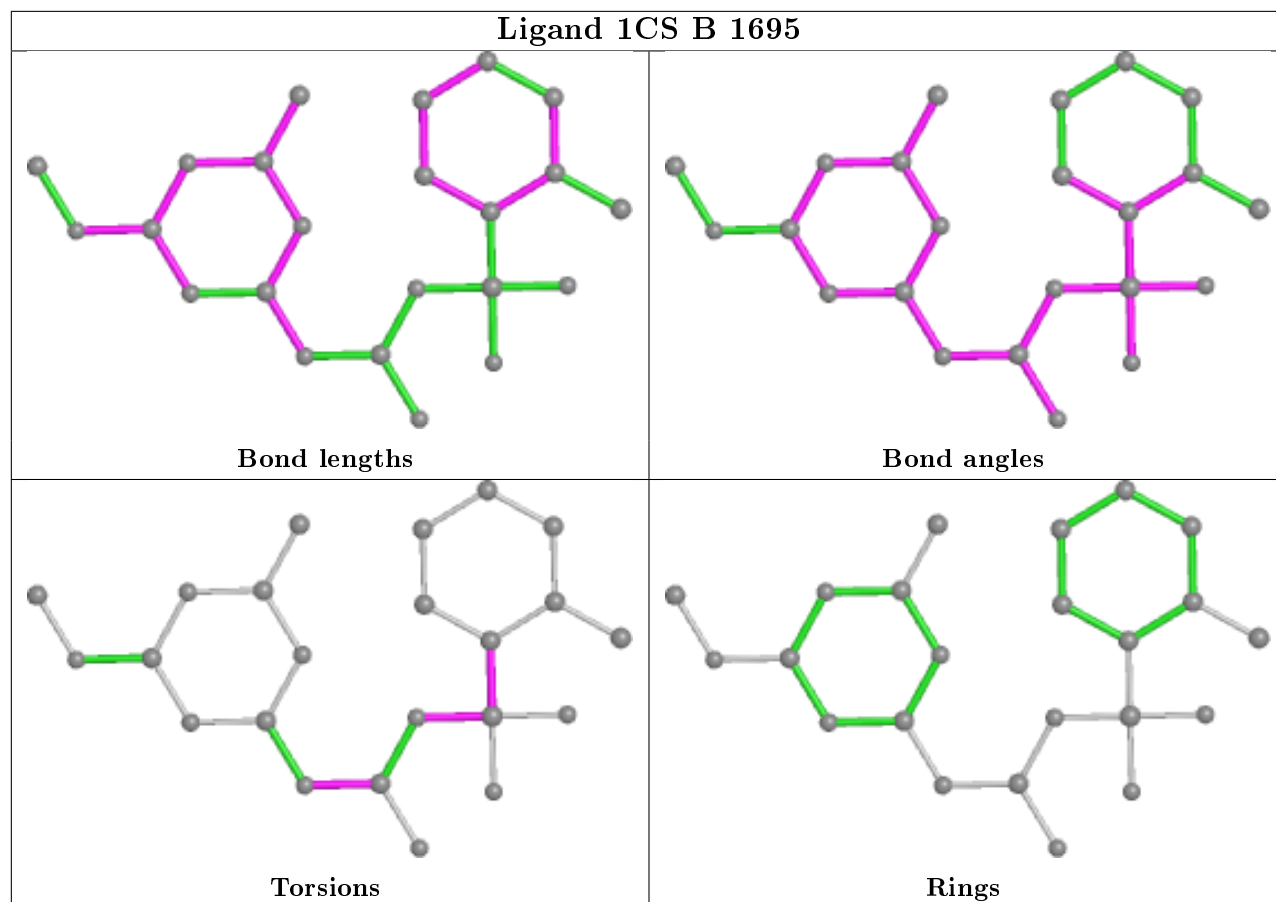
6 monomers are involved in 12 short contacts:

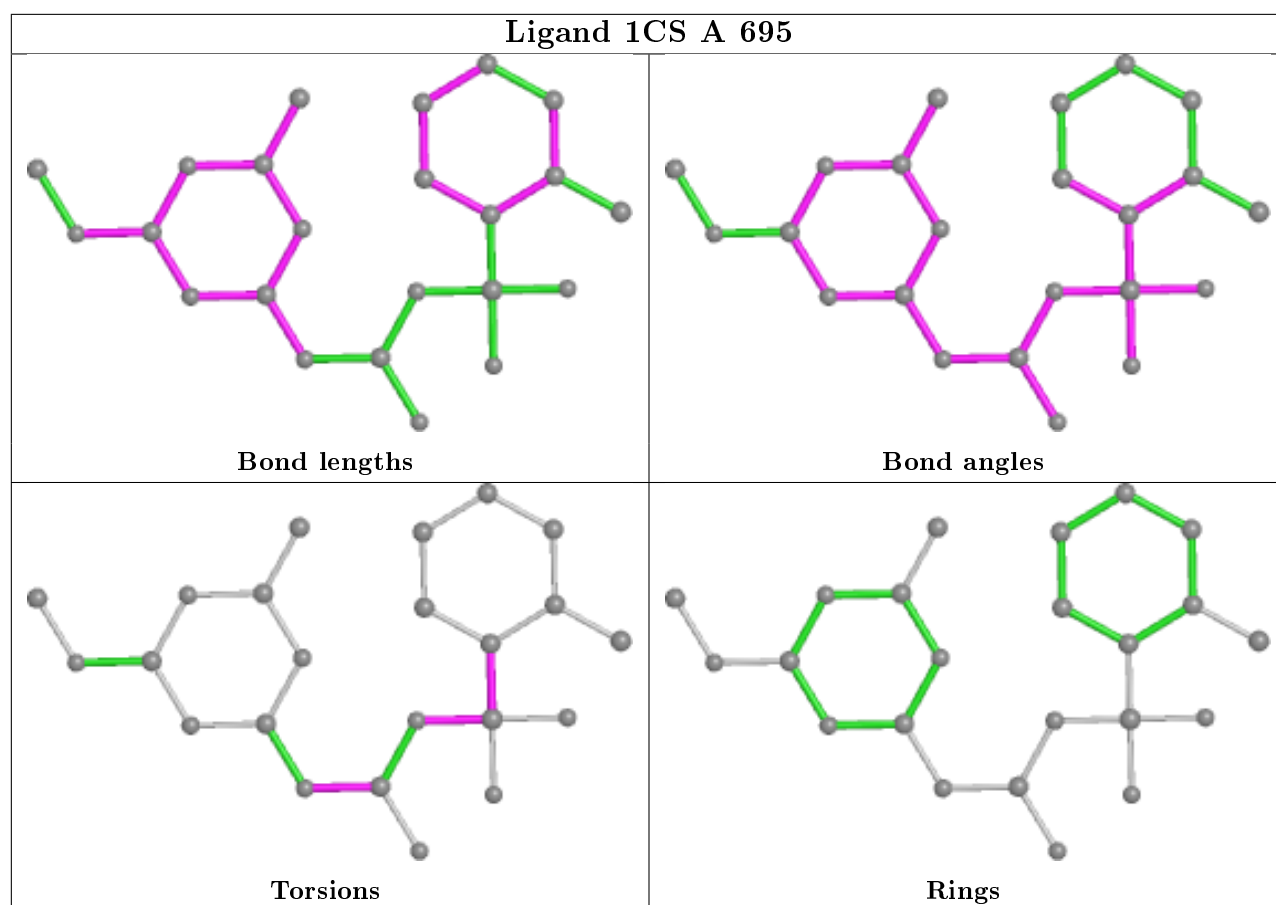
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1702	P22	3	0
9	B	698	P25	5	0
4	B	1695	1CS	1	0
6	A	704	NSP	2	0
4	A	695	1CS	1	0
8	A	1705	YF3	4	0

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 [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, 95th 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	583/677 (86%)	-0.36	9 (1%) 73 72	10, 26, 46, 70	0
1	B	595/677 (87%)	-0.73	3 (0%) 91 90	8, 15, 30, 60	0
All	All	1178/1354 (87%)	-0.55	12 (1%) 82 81	8, 20, 43, 70	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	PHE	4.8
1	B	268	LEU	3.9
1	A	467	PRO	3.7
1	A	397	ALA	3.0
1	B	279	ARG	3.0

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 carbohydrates in this entry.

6.4 Ligands [i](#)

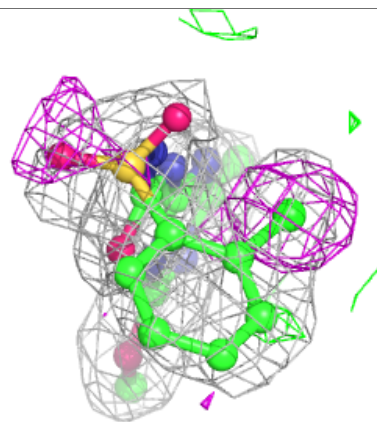
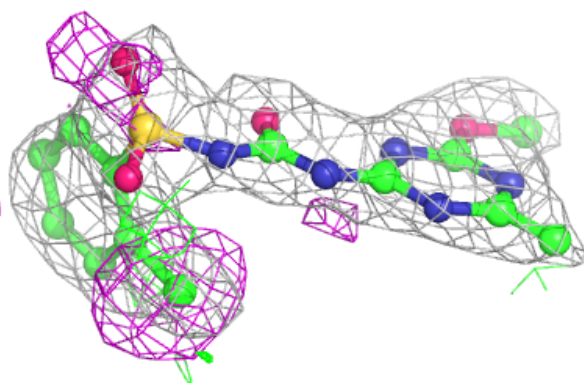
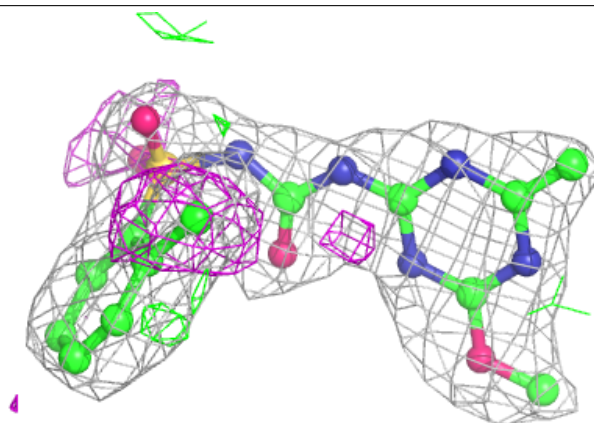
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	YF3	A	1705	14/14	0.88	0.19	23,25,43,51	0
4	1CS	A	695	23/23	0.90	0.15	28,31,37,39	0
4	1CS	B	1695	23/23	0.92	0.13	16,21,26,29	0
6	NSP	A	704	10/10	0.92	0.13	18,22,24,28	0
3	MG	A	1699	1/1	0.96	0.04	18,18,18,18	0
7	P22	A	1702	11/11	0.98	0.09	18,20,26,31	0
5	FAD	A	701	53/53	0.98	0.08	19,22,26,29	0
2	K	A	1696	1/1	0.99	0.04	29,29,29,29	0
3	MG	B	699	1/1	0.99	0.06	10,10,10,10	0
9	P25	B	698	14/14	0.99	0.10	9,13,27,29	0
5	FAD	B	1701	53/53	0.99	0.10	6,9,12,15	0
2	K	B	696	1/1	1.00	0.07	14,14,14,14	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.

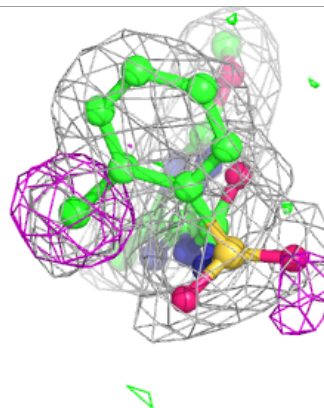
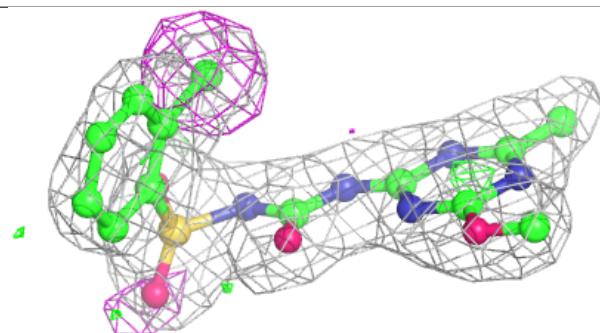
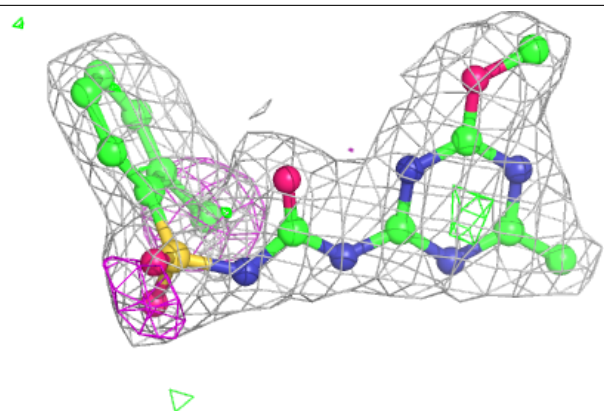
Electron density around 1CS A 695:

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

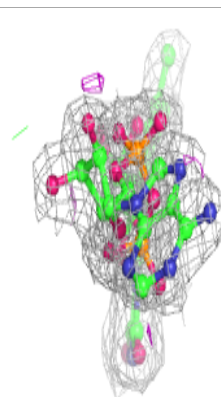
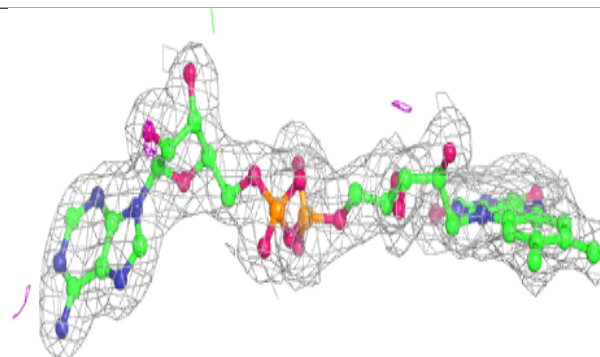
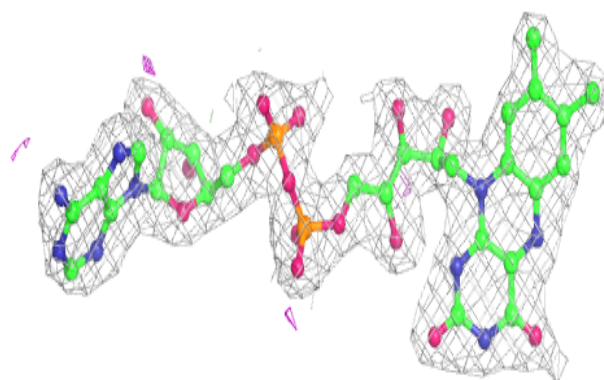


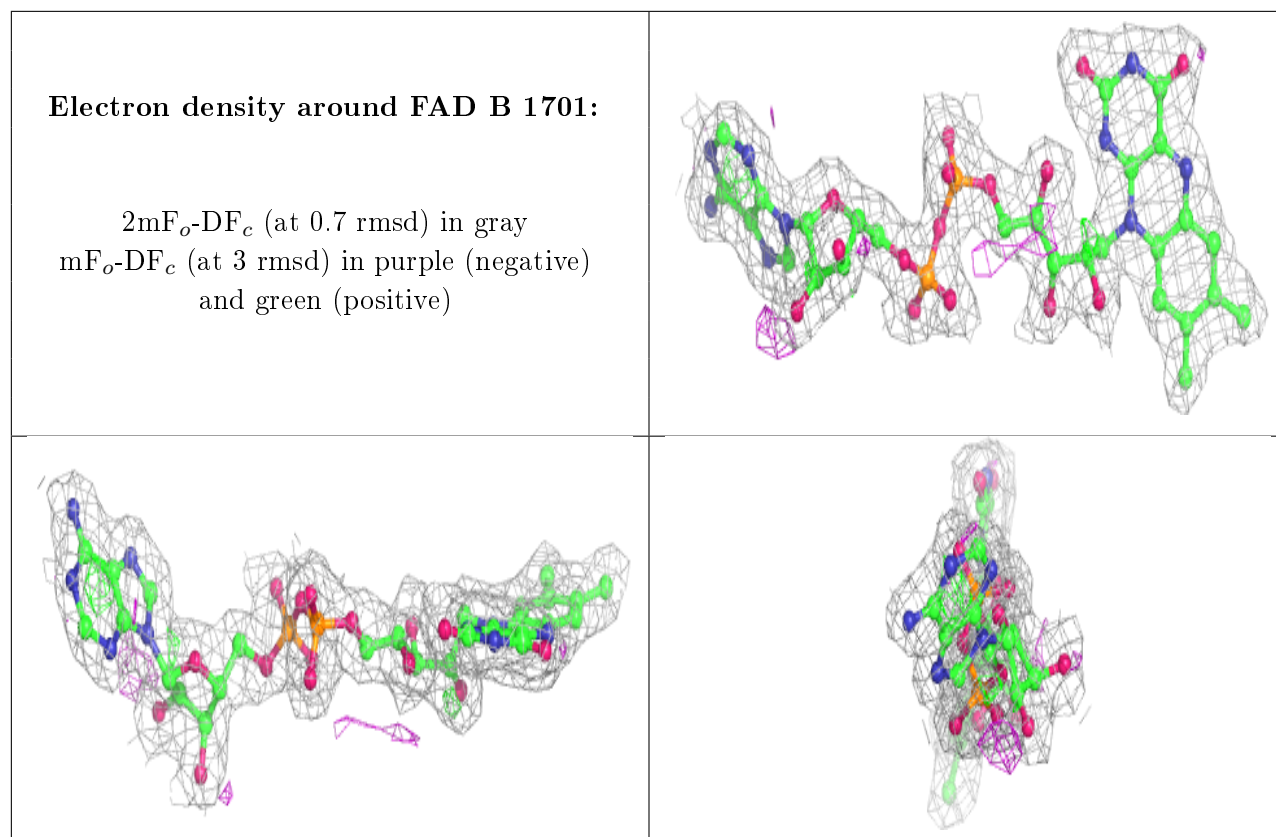
Electron density around 1CS B 1695:

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

**Electron density around FAD 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.