Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 10:55 PM EDT

PDB ID	:	1T9A
Title	:	Crystal structure of yeast acetohydroxyacid synthase in complex with a sulfonylurea herbicide, tribenuron methyl
Authors	:	McCourt, J.A.; Pang, S.S.; Guddat, L.W.; Duggleby, R.G.
Deposited on	:	2004-05-16
Resolution	:	2.59 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:

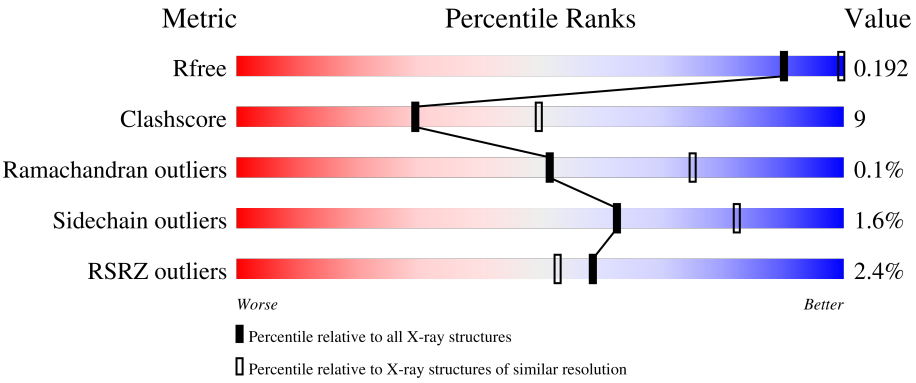
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	677	74% 14% 12%
1	B	677	4% 70% 17% 12%

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	1TB	A	695	-	X	-	-
4	1TB	B	1695	-	X	-	-
5	YF3	A	700	X	X	-	-
7	P23	B	698	-	X	-	-
8	YF4	B	1700	-	X	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 10187 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	597	Total	C	N	O	S	0	4	0
			4565	2887	796	861	21			
1	B	593	Total	C	N	O	S	0	3	0
			4494	2846	772	855	21			

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	A	1	Total K 1 1	0	0
2	B	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	A	1	Total Mg 1 1	0	0

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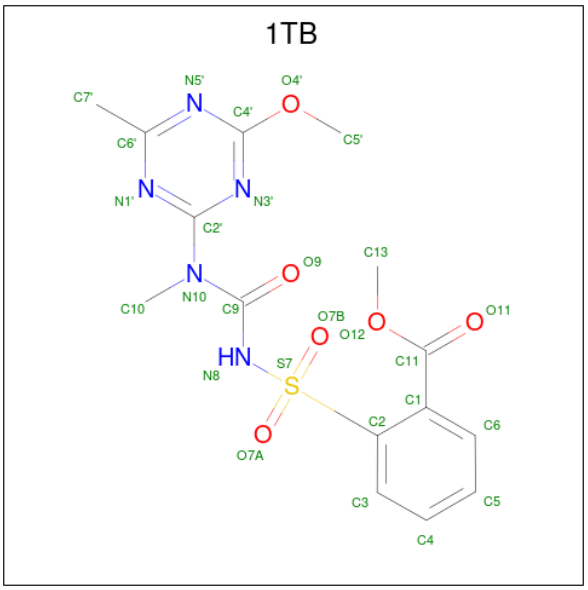
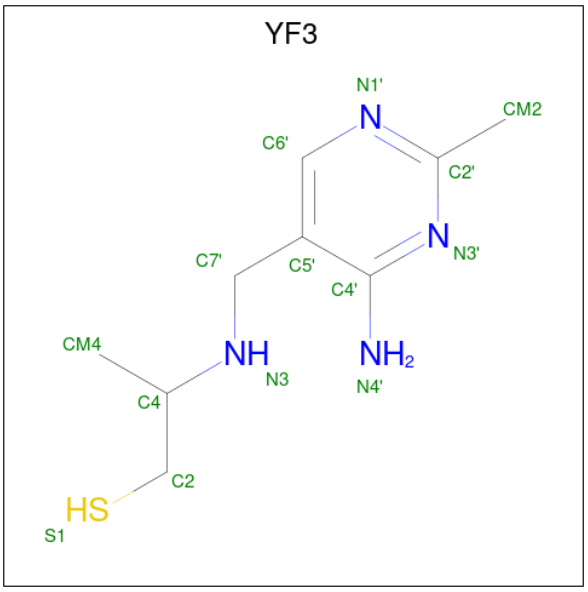
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is METHYL 2-[4-METHOXY-6-METHYL-1,3,5-TRAZIN-2-YL(METHYL)CARBAMOYLSULFAMOYL]BENZOATE (three-letter code: 1TB) (formula: $C_{15}H_{17}N_5O_6S$).



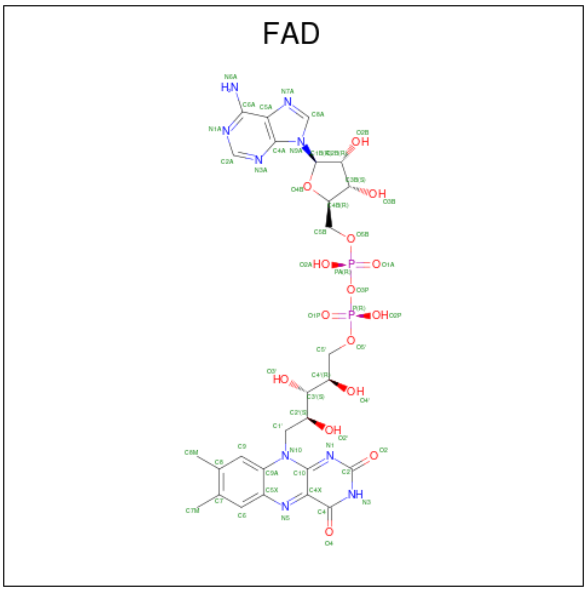
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 27 15 5 6 1	0	0
4	B	1	Total C N O S 27 15 5 6 1	0	0

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



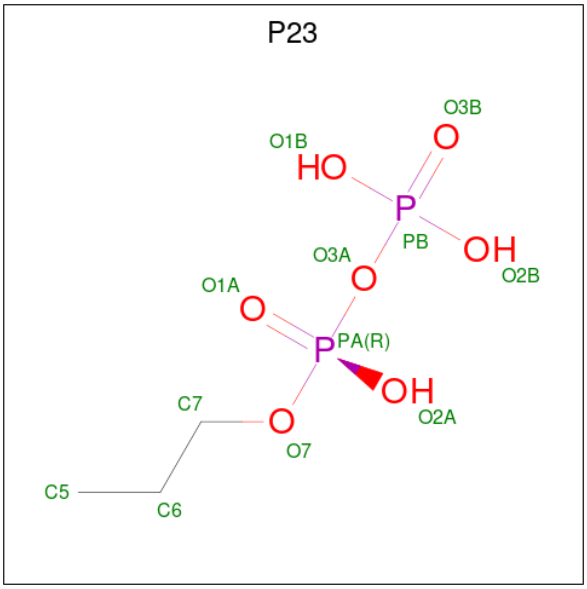
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	S	0	0
			14	9	4	1		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



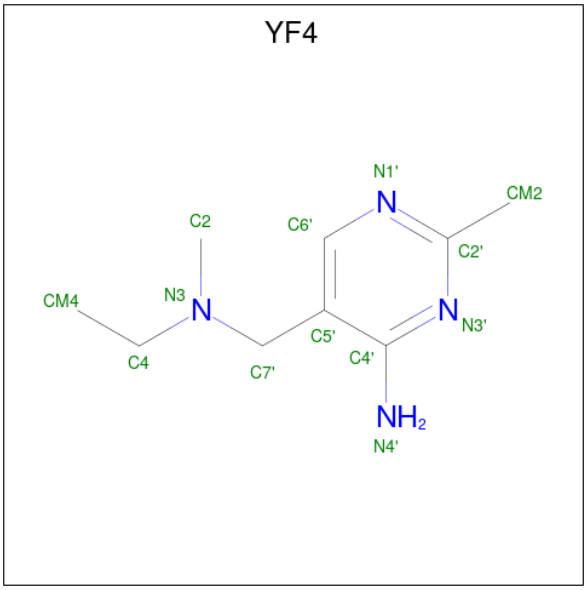
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
6	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is PROPYL TRIHYDROGEN DIPHOSPHATE (three-letter code: P23) (formula: $C_3H_{10}O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O P 12 3 7 2	0	0
7	B	1	Total C O P 12 3 7 2	0	0

- Molecule 8 is 5-{[ETHYL(METHYL)AMINO]METHYL}-2-METHYL-5,6-DIHYDROPYRIMIDIN-4-AMINE (three-letter code: YF4) (formula: $C_9H_{16}N_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N 13 9 4	0	0

- Molecule 9 is water.

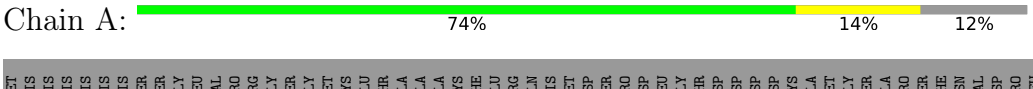
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	562	Total O 562 562	0	0
9	B	351	Total O 351 351	0	0

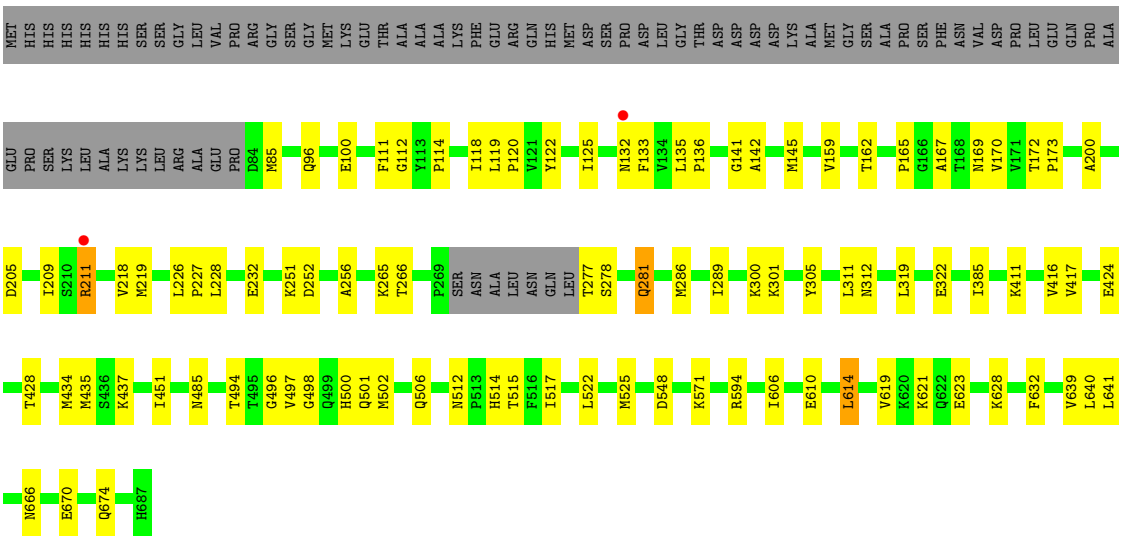
3 Residue-property plots (i)

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: Acetolactate synthase, mitochondrial

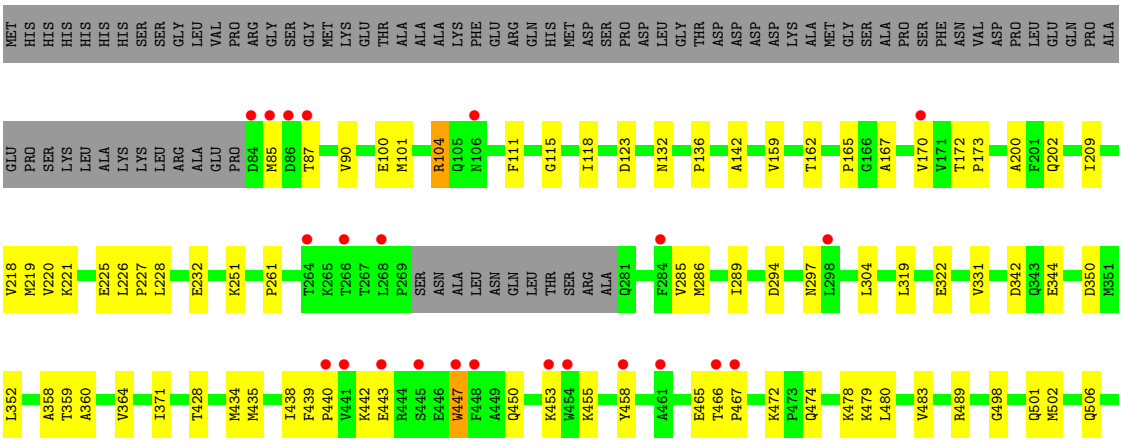
Chain A:

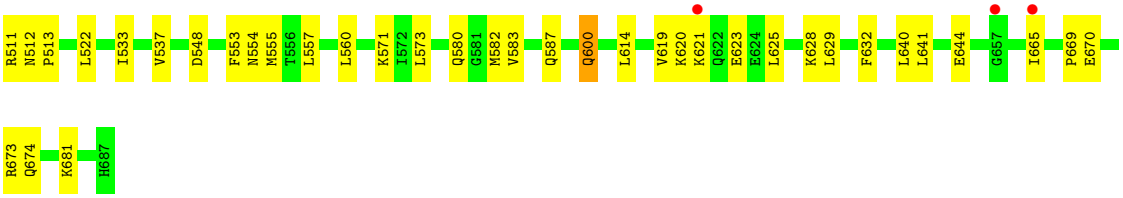




• Molecule 1: Acetolactate synthase, mitochondrial

Chain B:




R511
N512
P513
L522
I533
V537
D548
F553
N554
M555
T556
L557
L560
K571
I572
L573
Q580
G581
M582
V583
Q587
Q600
L614
V619
K620
K621
Q622
E623
E624
L625
K628
L629
F632
L640
L641
E644
G657
I665
P669
E670

R673
Q674
K681
H687

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	154.59Å 154.59Å 178.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.59 93.26 – 2.59	Depositor EDS
% Data completeness (in resolution range)	95.1 (50.00-2.59) 95.6 (93.26-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.96 (at 2.58Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.156 , 0.192 0.156 , 0.192	Depositor DCC
R_{free} test set	6806 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 63.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10187	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: MG, FAD, YF4, K, P23, 1TB, YF3

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	0.30	0/4675	0.58	0/6339
1	B	0.29	0/4600	0.54	0/6249
All	All	0.30	0/9275	0.56	0/12588

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	4565	0	4561	81	0
1	B	4494	0	4449	96	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	27	0	17	3	0
4	B	27	0	17	2	0
5	A	14	0	14	6	0
6	A	53	0	31	1	0
6	B	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	12	0	7	3	0
7	B	12	0	7	5	0
8	B	13	0	16	4	0
9	A	562	0	0	16	0
9	B	351	0	0	9	0
All	All	10187	0	9150	175	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 9.

All (175) 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:211[A]:ARG:HH11	1:A:211[A]:ARG:HG2	1.35	0.92
1:A:85:MET:HG2	9:A:4381:HOH:O	1.73	0.88
1:B:359:THR:HG21	1:B:455:LYS:HD2	1.53	0.88
8:B:1700:YF4:H41	8:B:1700:YF4:H4'2	1.40	0.87
1:A:114:PRO:HG2	1:B:580:GLN:HE22	1.36	0.87
1:B:85:MET:HE2	9:B:4307:HOH:O	1.75	0.85
9:A:4054:HOH:O	1:B:600:GLN:HB3	1.79	0.82
1:A:211[A]:ARG:HG2	1:A:211[A]:ARG:NH1	1.93	0.79
1:B:167:ALA:O	1:B:170[A]:VAL:HG12	1.86	0.75
8:B:1700:YF4:H42	9:B:4293:HOH:O	1.88	0.74
1:A:211[A]:ARG:HH11	1:A:211[A]:ARG:CG	2.02	0.71
1:B:322:GLU:OE2	1:B:435:MET:HG2	1.91	0.70
1:B:600:GLN:NE2	1:B:600:GLN:H	1.88	0.70
1:A:289:ILE:HG23	1:A:434:MET:HB2	1.71	0.70
4:A:695:1TB:H5	1:B:200:ALA:HB1	1.76	0.66
1:B:681:LYS:HB2	1:B:681:LYS:NZ	2.10	0.66
1:A:522:LEU:HG	1:B:165:PRO:HD3	1.78	0.65
1:B:322:GLU:HB3	1:B:435:MET:HE1	1.79	0.64
1:B:450:GLN:NE2	1:B:453:LYS:HD3	2.13	0.63
1:A:385:ILE:HD11	1:A:417:VAL:CG1	2.29	0.62
1:A:172:THR:HB	1:A:173:PRO:HD3	1.82	0.62
1:A:424:GLU:HB3	9:A:4530:HOH:O	1.98	0.62
1:A:200:ALA:HB1	4:B:1695:1TB:H5	1.82	0.62
1:A:132[B]:ASN:HD22	1:A:133:PHE:N	1.98	0.62
1:B:294:ASP:HA	1:B:297:ASN:HD22	1.66	0.60
1:B:219:MET:O	1:B:221:LYS:HD2	2.02	0.59
1:B:358:ALA:HB3	1:B:458:TYR:HB3	1.84	0.59
1:B:450:GLN:HE22	1:B:453:LYS:HD3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:GLY:CA	7:B:698:P23:H53	2.31	0.59
1:B:342:ASP:OD1	1:B:511:ARG:HD2	2.02	0.59
1:B:600:GLN:H	1:B:600:GLN:HE21	1.50	0.59
1:B:87:THR:CG2	1:B:261:PRO:HB3	2.33	0.58
1:A:162:THR:HG21	5:A:700:YF3:H7'2	1.86	0.58
1:B:623:GLU:HG3	9:B:4287:HOH:O	2.04	0.58
1:B:619:VAL:HB	1:B:628:LYS:HG3	1.85	0.58
1:B:439:PHE:N	9:B:4272:HOH:O	2.32	0.57
1:B:172:THR:HB	1:B:173:PRO:HD3	1.86	0.57
1:B:600:GLN:HG3	9:B:4351:HOH:O	2.04	0.57
1:B:289:ILE:HG23	1:B:434:MET:HB2	1.86	0.57
1:B:87:THR:HG22	1:B:261:PRO:HB3	1.86	0.56
1:B:101:MET:HA	1:B:104:ARG:HG3	1.87	0.56
1:A:85:MET:N	9:A:4381:HOH:O	2.39	0.56
1:A:265:LYS:C	9:A:4115:HOH:O	2.44	0.56
1:A:497:VAL:O	7:A:1698:P23:H61	2.05	0.56
1:B:218:VAL:HG22	1:B:219:MET:N	2.21	0.56
1:A:606:ILE:O	1:A:610:GLU:HG3	2.05	0.56
1:B:304:LEU:HD23	1:B:371:ILE:HB	1.87	0.56
1:A:226:LEU:HB3	1:A:227:PRO:HD3	1.87	0.55
1:A:136:PRO:HG3	1:A:142:ALA:HB2	1.89	0.55
1:A:670:GLU:O	1:A:674:GLN:HG3	2.06	0.55
1:B:438:ILE:HA	9:B:4793:HOH:O	2.07	0.55
1:A:496:GLY:H	1:A:500:HIS:HE1	1.53	0.54
1:B:623:GLU:H	1:B:623:GLU:CD	2.11	0.54
1:B:466:THR:HB	1:B:467:PRO:HD2	1.88	0.54
1:A:619:VAL:HB	1:A:628:LYS:HG3	1.89	0.54
1:B:100:GLU:O	1:B:104:ARG:HG2	2.07	0.54
1:A:286:MET:SD	1:A:437:LYS:NZ	2.81	0.54
5:A:700:YF3:S1	1:B:580:GLN:NE2	2.81	0.53
1:B:344:GLU:HG2	1:B:511:ARG:HD3	1.90	0.53
1:A:251:LYS:HZ2	4:B:1695:1TB:HN8	1.57	0.53
1:B:465:GLU:HG3	1:B:472:LYS:HG2	1.90	0.53
1:A:411:LYS:HE3	9:A:4422:HOH:O	2.10	0.53
1:B:582:MET:HB3	7:B:698:P23:H51	1.91	0.53
1:A:640:LEU:HD23	1:A:640:LEU:C	2.29	0.52
1:A:525:MET:SD	8:B:1700:YF4:H22	2.50	0.52
1:A:614:LEU:HD23	1:A:614:LEU:N	2.24	0.52
1:B:571:LYS:HB3	1:B:632:PHE:CZ	2.44	0.52
1:A:522:LEU:O	1:B:202:GLN:HG2	2.10	0.52
1:B:226:LEU:HB3	1:B:227:PRO:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ASN:HB2	9:A:4678:HOH:O	2.09	0.52
1:A:167:ALA:O	1:A:170:VAL:HG22	2.10	0.52
5:A:700:YF3:S1	1:B:580:GLN:HG2	2.50	0.51
1:B:450:GLN:O	1:B:453:LYS:HB3	2.11	0.51
1:A:228:LEU:O	1:A:232:GLU:HG3	2.09	0.51
4:A:695:1TB:H5'2	6:A:701:FAD:HM72	1.93	0.51
1:B:498:GLY:HA3	7:B:698:P23:H53	1.90	0.51
7:A:1698:P23:H51	8:B:1700:YF4:HM42	1.92	0.51
1:B:132:ASN:HB3	9:B:4761:HOH:O	2.11	0.50
1:B:344:GLU:HG3	1:B:511:ARG:NH1	2.26	0.50
1:A:594[A]:ARG:NH1	1:B:123:ASP:OD2	2.44	0.50
1:A:111:PHE:O	1:A:159:VAL:HA	2.12	0.50
1:B:360:ALA:O	1:B:364:VAL:HG23	2.12	0.49
1:A:228:LEU:HB2	1:A:266:THR:HB	1.94	0.49
1:B:665:ILE:HA	9:B:4270:HOH:O	2.13	0.48
1:B:447:TRP:HA	1:B:447:TRP:CE3	2.49	0.48
1:B:670:GLU:O	1:B:674:GLN:HG3	2.14	0.48
1:B:118:ILE:O	1:B:118:ILE:HG13	2.13	0.48
1:A:494:THR:HA	1:A:517:ILE:O	2.14	0.48
1:B:344:GLU:HG3	1:B:511:ARG:HH11	1.79	0.48
1:A:122:TYR:HA	1:A:125:ILE:HG12	1.96	0.47
1:A:571:LYS:HB3	1:A:632:PHE:CZ	2.49	0.47
1:B:621:LYS:HB3	1:B:623:GLU:OE2	2.14	0.47
1:A:623:GLU:H	1:A:623:GLU:CD	2.18	0.47
1:B:115:GLY:HA3	1:B:162:THR:HB	1.96	0.47
1:A:278:SER:HB3	1:A:281:GLN:HB2	1.96	0.47
1:B:669:PRO:O	1:B:673:ARG:HG3	2.14	0.47
5:A:700:YF3:H4'2	5:A:700:YF3:HM43	1.80	0.47
1:B:136:PRO:HG3	1:B:142:ALA:HB2	1.97	0.46
1:B:533:ILE:O	1:B:537:VAL:HG23	2.15	0.46
1:B:474:GLN:O	1:B:478:LYS:HG3	2.14	0.46
1:A:498:GLY:O	1:A:501:GLN:HB3	2.14	0.46
5:A:700:YF3:HM42	9:A:4053:HOH:O	2.16	0.46
1:A:498:GLY:CA	7:A:1698:P23:H52	2.46	0.46
1:A:218:VAL:HG22	1:A:219:MET:N	2.31	0.46
1:A:416:VAL:HG12	1:A:417:VAL:HG13	1.98	0.46
1:A:451:ILE:HB	9:A:4546:HOH:O	2.16	0.46
1:A:319:LEU:HD12	1:A:428:THR:CG2	2.45	0.46
1:A:205:ASP:O	1:A:209:ILE:HG13	2.16	0.46
1:A:512:ASN:HB2	1:A:515:THR:HG21	1.98	0.46
1:B:111:PHE:O	1:B:159:VAL:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:TRP:HA	1:B:447:TRP:HE3	1.80	0.46
1:B:498:GLY:O	1:B:501:GLN:HB3	2.16	0.45
1:B:640:LEU:C	1:B:640:LEU:HD23	2.36	0.45
1:A:170:VAL:C	1:A:173:PRO:HD2	2.37	0.45
1:A:118:ILE:HG13	1:A:118:ILE:O	2.16	0.45
1:A:132[B]:ASN:ND2	1:A:133:PHE:N	2.63	0.45
1:A:311:LEU:O	1:A:514:HIS:HE1	2.00	0.45
1:A:322:GLU:OE2	1:A:435:MET:HG2	2.16	0.45
1:A:228:LEU:HD13	1:A:266:THR:HG22	1.98	0.44
1:A:100:GLU:HB3	9:A:4205:HOH:O	2.17	0.44
1:A:501:GLN:HG2	1:A:502:MET:HE3	2.00	0.44
1:B:583:VAL:O	1:B:587:GLN:HG3	2.17	0.44
1:A:114:PRO:HG2	1:B:580:GLN:NE2	2.17	0.44
5:A:700:YF3:H21	1:B:583:VAL:CG2	2.47	0.44
1:A:132[B]:ASN:HD22	1:A:133:PHE:H	1.64	0.44
1:B:319:LEU:HD12	1:B:428:THR:HG23	1.99	0.44
1:B:228:LEU:O	1:B:232:GLU:HG3	2.18	0.44
1:A:112:GLY:O	1:A:136:PRO:HD2	2.18	0.44
1:B:554:ASN:HA	1:B:557:LEU:HD23	1.98	0.44
1:B:304:LEU:HB2	1:B:331:VAL:HG22	1.99	0.44
1:B:352:LEU:H	1:B:352:LEU:HD23	1.83	0.44
1:A:141:GLY:O	1:A:145:MET:HG3	2.18	0.43
1:B:285:VAL:O	1:B:289:ILE:HG13	2.18	0.43
1:A:594[B]:ARG:HH11	1:A:594[B]:ARG:HG2	1.83	0.43
1:B:220:VAL:HG13	1:B:225:GLU:HG3	2.00	0.43
4:A:695:1TB:HN8	1:B:251:LYS:HZ2	1.66	0.43
1:A:621:LYS:HA	9:A:4426:HOH:O	2.18	0.43
1:B:115:GLY:HA3	1:B:162:THR:CB	2.47	0.43
1:A:300:LYS:NZ	9:A:4004:HOH:O	2.50	0.43
1:A:169:ASN:ND2	1:B:172:THR:OG1	2.52	0.42
1:B:87:THR:HA	1:B:90:VAL:HG23	2.02	0.42
1:A:277:THR:N	9:A:4402:HOH:O	2.51	0.42
1:B:502:MET:O	1:B:506:GLN:HG3	2.20	0.42
1:A:169:ASN:HD22	1:A:169:ASN:HA	1.65	0.42
1:B:344:GLU:CG	1:B:511:ARG:HD3	2.49	0.42
1:B:479:LYS:O	1:B:483:VAL:HG23	2.19	0.42
1:B:681:LYS:HB2	1:B:681:LYS:HZ2	1.83	0.42
1:A:571:LYS:HD2	1:A:639:VAL:CG1	2.49	0.42
1:A:319:LEU:HD12	1:A:428:THR:HG23	2.02	0.42
1:A:209:ILE:HG23	1:B:209:ILE:HG23	2.02	0.42
1:A:501:GLN:HG2	1:A:502:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:MET:CB	7:B:698:P23:H51	2.50	0.41
1:B:681:LYS:HB2	1:B:681:LYS:HZ3	1.83	0.41
1:A:502:MET:O	1:A:506:GLN:HG3	2.21	0.41
1:A:640:LEU:HD23	1:A:641:LEU:N	2.35	0.41
1:B:625:LEU:O	1:B:629:LEU:HG	2.20	0.41
1:A:301:LYS:HD3	9:A:4867:HOH:O	2.19	0.41
1:B:104:ARG:HG2	1:B:104:ARG:H	1.59	0.41
1:B:440:PRO:HB2	9:B:4704:HOH:O	2.20	0.41
1:B:480:LEU:HD22	1:B:573:LEU:HD22	2.02	0.41
1:A:252:ASP:O	1:A:256:ALA:HB2	2.21	0.41
1:A:266:THR:N	9:A:4115:HOH:O	2.54	0.41
1:A:621:LYS:HB3	1:A:623:GLU:OE2	2.21	0.41
1:B:580:GLN:HG2	7:B:698:P23:H72	2.02	0.41
1:A:165:PRO:HD3	1:B:522:LEU:HG	2.02	0.41
1:A:312:ASN:HD22	1:A:312:ASN:HA	1.67	0.41
1:B:640:LEU:HD23	1:B:641:LEU:N	2.36	0.41
1:B:512:ASN:HA	1:B:513:PRO:HD3	1.86	0.40
1:B:553:PHE:HZ	1:B:560:LEU:HD11	1.86	0.40
1:A:119:LEU:HB2	1:A:120:PRO:HD3	2.03	0.40
1:B:620:LYS:HE2	1:B:644:GLU:OE2	2.21	0.40
1:A:96:GLN:O	1:A:100:GLU:HG2	2.21	0.40
1:A:135:LEU:HG	9:A:4054:HOH:O	2.22	0.40

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:442:LYS:CB	1:B:442:LYS:CB[8_665]	2.18	0.02

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	597/677 (88%)	586 (98%)	11 (2%)	0	100	100
1	B	592/677 (87%)	573 (97%)	18 (3%)	1 (0%)	47	71
All	All	1189/1354 (88%)	1159 (98%)	29 (2%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	350	ASP

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	489/556 (88%)	482 (99%)	7 (1%)	67	85
1	B	479/556 (86%)	470 (98%)	9 (2%)	57	79
All	All	968/1112 (87%)	952 (98%)	16 (2%)	62	81

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211[A]	ARG
1	A	211[B]	ARG
1	A	281	GLN
1	A	305	TYR
1	A	548	ASP
1	A	614	LEU
1	A	666	ASN
1	B	104	ARG
1	B	286	MET
1	B	443	GLU
1	B	447	TRP
1	B	489	ARG
1	B	548	ASP
1	B	555	MET
1	B	600	GLN

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Mol	Chain	Res	Type
1	B	614	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	A	287	GLN
1	A	312	ASN
1	A	500	HIS
1	A	554	ASN
1	A	587	GLN
1	A	666	ASN
1	B	99	ASN
1	B	202	GLN
1	B	297	ASN
1	B	312	ASN
1	B	450	GLN
1	B	452	ASN
1	B	507	HIS
1	B	512	ASN
1	B	514	HIS
1	B	554	ASN
1	B	580	GLN
1	B	600	GLN
1	B	602	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	1TB	B	1695	-	28,28,28	3.64	17 (60%)	36,40,40	4.07	13 (36%)
7	P23	B	698	3	9,11,11	2.41	5 (55%)	13,16,16	2.92	8 (61%)
6	FAD	A	701	-	53,58,58	2.65	24 (45%)	68,89,89	1.54	8 (11%)
6	FAD	B	1701	-	53,58,58	2.75	25 (47%)	68,89,89	1.57	8 (11%)
5	YF3	A	700	-	14,14,14	6.45	7 (50%)	17,18,18	9.37	11 (64%)
7	P23	A	1698	3	9,11,11	2.60	4 (44%)	13,16,16	2.31	4 (30%)
8	YF4	B	1700	-	13,13,13	4.43	6 (46%)	17,17,17	3.88	12 (70%)
4	1TB	A	695	-	28,28,28	3.56	17 (60%)	36,40,40	4.00	15 (41%)

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	1TB	B	1695	-	-	10/26/27/27	0/2/2/2
7	P23	B	698	3	-	3/11/11/11	-
6	FAD	A	701	-	-	1/30/50/50	0/6/6/6
6	FAD	B	1701	-	-	2/30/50/50	0/6/6/6
5	YF3	A	700	-	1/1/1/2	3/6/7/7	0/1/1/1
7	P23	A	1698	3	-	3/11/11/11	-
8	YF4	B	1700	-	-	2/6/6/6	0/1/1/1
4	1TB	A	695	-	-	12/26/27/27	0/2/2/2

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	700	YF3	C4'-N3'	12.00	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	700	YF3	C4-N3	-10.09	1.34	1.48
5	A	700	YF3	C5'-C4'	9.99	1.60	1.42
5	A	700	YF3	C2'-N1'	9.90	1.50	1.34
6	B	1701	FAD	C4A-N3A	9.76	1.49	1.35
6	A	701	FAD	C4A-N3A	9.05	1.48	1.35
4	A	695	1TB	S7-N8	-8.14	1.47	1.64
4	B	1695	1TB	S7-N8	-7.91	1.47	1.64
5	A	700	YF3	C2'-N3'	7.72	1.47	1.34
8	B	1700	YF4	C2'-N1'	7.59	1.46	1.34
5	A	700	YF3	C6'-N1'	7.53	1.50	1.34
8	B	1700	YF4	C5'-C4'	7.26	1.55	1.42
4	B	1695	1TB	C1-C2	6.93	1.47	1.40
4	A	695	1TB	C1-C2	6.75	1.47	1.40
8	B	1700	YF4	C4'-N3'	6.55	1.44	1.35
8	B	1700	YF4	C6'-N1'	6.52	1.48	1.34
6	B	1701	FAD	C2A-N1A	6.40	1.45	1.33
8	B	1700	YF4	C6'-C5'	6.33	1.50	1.37
6	A	701	FAD	C2A-N1A	6.30	1.45	1.33
4	B	1695	1TB	C2'-N1'	6.04	1.45	1.34
4	A	695	1TB	C2'-N1'	6.01	1.45	1.34
4	B	1695	1TB	C4'-N3'	5.72	1.44	1.33
7	A	1698	P23	PA-O7	-5.61	1.36	1.59
6	B	1701	FAD	C2A-N3A	5.57	1.41	1.32
4	A	695	1TB	C4'-N3'	5.47	1.43	1.33
4	B	1695	1TB	C6'-N1'	5.17	1.43	1.34
6	A	701	FAD	C2A-N3A	5.00	1.40	1.32
4	A	695	1TB	C6'-N1'	4.80	1.42	1.34
4	B	1695	1TB	C4'-N5'	4.79	1.42	1.33
4	A	695	1TB	C4'-N5'	4.76	1.42	1.33
4	B	1695	1TB	C6'-N5'	4.66	1.42	1.34
6	B	1701	FAD	C1'-C2'	-4.51	1.46	1.52
6	B	1701	FAD	O4'-C4'	4.45	1.52	1.43
6	A	701	FAD	O4'-C4'	4.41	1.52	1.43
7	B	698	P23	PA-O7	-4.39	1.41	1.59
4	B	1695	1TB	O7A-S7	4.38	1.48	1.43
4	A	695	1TB	O7A-S7	4.38	1.48	1.43
6	B	1701	FAD	C9A-C5X	4.28	1.48	1.41
6	A	701	FAD	C9A-C5X	4.20	1.48	1.41
6	A	701	FAD	O3'-C3'	4.16	1.52	1.43
4	B	1695	1TB	C2'-N3'	4.13	1.41	1.34
6	B	1701	FAD	O3'-C3'	4.06	1.52	1.43
4	A	695	1TB	C2'-N3'	3.89	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1701	FAD	C4X-N5	3.83	1.38	1.30
4	A	695	1TB	C6'-N5'	3.81	1.40	1.34
6	A	701	FAD	C1'-C2'	-3.76	1.47	1.52
6	A	701	FAD	C5'-C4'	-3.71	1.46	1.51
6	A	701	FAD	C4X-N5	3.70	1.37	1.30
5	A	700	YF3	C7'-C5'	-3.63	1.39	1.50
4	A	695	1TB	C2-S7	3.60	1.82	1.77
4	A	695	1TB	O12-C11	3.59	1.41	1.33
8	B	1700	YF4	C4-N3	3.57	1.55	1.47
6	B	1701	FAD	C6A-C5A	3.56	1.56	1.43
4	B	1695	1TB	O12-C11	3.56	1.41	1.33
6	A	701	FAD	C6A-C5A	3.52	1.56	1.43
6	B	1701	FAD	C5A-C4A	3.46	1.50	1.40
6	B	1701	FAD	C5'-C4'	-3.35	1.47	1.51
7	A	1698	P23	PB-O2B	-3.27	1.42	1.54
4	B	1695	1TB	C2-S7	3.25	1.82	1.77
6	A	701	FAD	C5A-C4A	3.20	1.49	1.40
7	A	1698	P23	PA-O2A	-3.15	1.40	1.55
6	A	701	FAD	C10-N1	3.09	1.39	1.33
6	B	1701	FAD	C10-N1	3.06	1.39	1.33
7	B	698	P23	PA-O2A	-3.02	1.41	1.55
4	B	1695	1TB	O4'-C4'	2.98	1.40	1.33
4	A	695	1TB	O4'-C4'	2.94	1.40	1.33
4	B	1695	1TB	C1-C11	2.93	1.56	1.50
6	A	701	FAD	C3B-C4B	2.92	1.60	1.53
4	A	695	1TB	C3-C2	2.85	1.42	1.39
6	B	1701	FAD	C8A-N7A	-2.78	1.29	1.34
4	B	1695	1TB	C3-C2	2.78	1.42	1.39
6	B	1701	FAD	C8-C7	2.75	1.47	1.40
6	B	1701	FAD	C3B-C4B	2.67	1.59	1.53
7	B	698	P23	PB-O1B	-2.67	1.44	1.54
7	B	698	P23	PA-O1A	-2.65	1.41	1.50
6	B	1701	FAD	C9-C9A	2.62	1.43	1.39
6	A	701	FAD	P-O2P	-2.61	1.43	1.55
6	A	701	FAD	C8-C7	2.60	1.47	1.40
6	B	1701	FAD	P-O2P	-2.59	1.43	1.55
6	A	701	FAD	C8A-N7A	-2.57	1.30	1.34
4	A	695	1TB	C1-C11	2.49	1.55	1.50
6	A	701	FAD	C6-C5X	2.47	1.43	1.40
6	B	1701	FAD	C10-N10	2.38	1.42	1.37
4	A	695	1TB	O12-C13	-2.36	1.39	1.45
4	B	1695	1TB	O12-C13	-2.35	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1695	1TB	C9-N10	2.32	1.40	1.37
4	B	1695	1TB	O7B-S7	2.32	1.46	1.43
4	A	695	1TB	O7B-S7	2.27	1.46	1.43
6	A	701	FAD	C6-C7	2.26	1.42	1.39
7	B	698	P23	PB-O2B	-2.25	1.46	1.54
6	A	701	FAD	C9-C9A	2.24	1.43	1.39
6	B	1701	FAD	C6-C7	2.23	1.42	1.39
4	A	695	1TB	C6-C1	2.23	1.43	1.39
6	B	1701	FAD	C6A-N1A	2.22	1.46	1.37
6	A	701	FAD	C9-C8	2.21	1.42	1.39
6	A	701	FAD	C10-N10	2.18	1.42	1.37
6	B	1701	FAD	PA-O5B	-2.18	1.50	1.59
6	B	1701	FAD	C6-C5X	2.17	1.43	1.40
6	B	1701	FAD	C9-C8	2.15	1.42	1.39
7	A	1698	P23	PB-O1B	-2.14	1.46	1.54
6	A	701	FAD	O2B-C2B	-2.12	1.38	1.43
6	B	1701	FAD	PA-O2A	-2.11	1.45	1.55
6	A	701	FAD	C6A-N1A	2.11	1.46	1.37
6	B	1701	FAD	O2B-C2B	-2.06	1.38	1.43
6	A	701	FAD	PA-O2A	-2.06	1.45	1.55

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	700	YF3	C4-C2-S1	26.75	144.27	114.19
5	A	700	YF3	CM4-C4-C2	17.83	137.22	111.78
4	B	1695	1TB	C5'-O4'-C4'	16.42	143.86	117.58
5	A	700	YF3	C7'-N3-C4	16.17	148.37	114.87
4	A	695	1TB	C5'-O4'-C4'	15.85	142.95	117.58
8	B	1700	YF4	CM4-C4-N3	10.96	144.75	112.92
4	A	695	1TB	C2-S7-N8	8.07	115.57	106.06
4	B	1695	1TB	C2-S7-N8	8.01	115.49	106.06
5	A	700	YF3	CM2-C2'-N1'	7.90	125.83	117.14
4	B	1695	1TB	O7B-S7-O7A	-7.36	110.50	119.55
4	A	695	1TB	O7B-S7-O7A	-7.28	110.60	119.55
4	B	1695	1TB	C4'-N3'-C2'	7.16	120.26	113.06
4	A	695	1TB	C4'-N3'-C2'	6.78	119.88	113.06
6	B	1701	FAD	C1B-N9A-C4A	6.48	138.02	126.64
6	A	701	FAD	C1B-N9A-C4A	6.11	137.38	126.64
5	A	700	YF3	N1'-C2'-N3'	-6.01	115.19	125.54
8	B	1700	YF4	C2-N3-C4	5.52	124.33	110.68
5	A	700	YF3	C6'-N1'-C2'	5.44	125.22	115.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1698	P23	O7-C7-C6	5.44	143.55	111.15
4	B	1695	1TB	N3'-C4'-N5'	-5.19	117.65	127.63
4	A	695	1TB	N3'-C4'-N5'	-5.17	117.68	127.63
8	B	1700	YF4	C7'-N3-C4	5.10	121.00	111.64
7	B	698	P23	PA-O7-C7	5.03	146.33	121.59
7	B	698	P23	O7-C7-C6	4.96	140.68	111.15
4	A	695	1TB	N5'-C6'-N1'	-4.70	117.07	125.72
4	B	1695	1TB	N5'-C6'-N1'	-4.57	117.31	125.72
5	A	700	YF3	C7'-C5'-C4'	4.50	126.92	122.56
7	B	698	P23	C5-C6-C7	4.31	138.38	112.32
4	A	695	1TB	N8-C9-N10	4.20	118.61	114.94
5	A	700	YF3	C7'-C5'-C6'	-4.20	115.56	121.30
4	B	1695	1TB	N8-C9-N10	4.18	118.60	114.94
4	A	695	1TB	C2'-N1'-C6'	4.08	120.60	114.21
4	B	1695	1TB	C2'-N1'-C6'	3.95	120.39	114.21
7	A	1698	P23	C5-C6-C7	3.94	136.14	112.32
4	A	695	1TB	N3'-C2'-N1'	-3.60	120.36	126.31
4	B	1695	1TB	N3'-C2'-N1'	-3.59	120.39	126.31
8	B	1700	YF4	CM2-C2'-N1'	3.53	121.02	117.14
4	A	695	1TB	C10-N10-C2'	-3.52	112.86	119.95
4	B	1695	1TB	C10-N10-C2'	-3.50	112.90	119.95
4	B	1695	1TB	C7'-C6'-N5'	3.44	122.52	117.15
4	A	695	1TB	C7'-C6'-N5'	3.41	122.48	117.15
8	B	1700	YF4	C6'-C5'-C4'	-3.18	111.39	115.72
7	B	698	P23	O1B-PB-O3A	3.14	115.16	104.64
6	A	701	FAD	N3A-C2A-N1A	-3.12	123.80	128.68
8	B	1700	YF4	N4'-C4'-N3'	-3.06	112.70	117.03
5	A	700	YF3	CM4-C4-N3	3.06	120.54	112.30
6	B	1701	FAD	N3A-C2A-N1A	-3.05	123.91	128.68
7	B	698	P23	O2B-PB-O1B	3.01	119.13	107.64
8	B	1700	YF4	C6'-N1'-C2'	2.99	121.05	115.96
8	B	1700	YF4	C5'-C7'-N3	2.95	118.25	112.85
5	A	700	YF3	C5'-C7'-N3	2.87	120.83	112.65
7	B	698	P23	PA-O3A-PB	2.83	142.54	132.83
6	A	701	FAD	O2B-C2B-C1B	2.79	121.17	110.85
7	A	1698	P23	PA-O7-C7	2.78	135.29	121.59
6	B	1701	FAD	O2B-C2B-C3B	2.76	120.77	111.82
6	B	1701	FAD	O2B-C2B-C1B	2.76	121.06	110.85
4	A	695	1TB	C3-C2-C1	-2.76	117.94	121.20
7	B	698	P23	O3A-PB-O3B	-2.75	95.95	111.19
6	A	701	FAD	O2B-C2B-C3B	2.64	120.35	111.82
6	A	701	FAD	O2-C2-N1	-2.63	117.46	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1701	FAD	O2-C2-N1	-2.62	117.49	121.83
8	B	1700	YF4	N1'-C2'-N3'	-2.56	121.13	125.54
4	B	1695	1TB	C3-C2-C1	-2.56	118.18	121.20
8	B	1700	YF4	C2-N3-C7'	2.56	114.67	110.54
5	A	700	YF3	C2'-N3'-C4'	2.55	122.06	118.08
6	B	1701	FAD	O4B-C4B-C5B	-2.50	101.15	109.37
4	A	695	1TB	N1'-C2'-N10	2.42	121.69	117.25
7	B	698	P23	O2B-PB-O3A	-2.41	96.54	104.64
4	B	1695	1TB	N1'-C2'-N10	2.39	121.63	117.25
7	A	1698	P23	O2B-PB-O1B	2.37	116.70	107.64
8	B	1700	YF4	C5'-C4'-N3'	2.37	124.96	121.24
8	B	1700	YF4	C7'-C5'-C6'	2.33	124.64	121.30
6	A	701	FAD	O4B-C4B-C5B	-2.33	101.70	109.37
6	A	701	FAD	O3'-C3'-C4'	-2.33	103.18	108.81
6	B	1701	FAD	O3'-C3'-C4'	-2.15	103.62	108.81
4	A	695	1TB	C7'-C6'-N1'	2.11	120.45	117.15
6	B	1701	FAD	O4-C4-C4X	-2.05	121.15	126.60
6	A	701	FAD	C1'-C2'-C3'	2.03	115.46	109.79
4	A	695	1TB	C6-C1-C2	2.01	120.21	118.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	700	YF3	C4

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	695	1TB	C1-C2-S7-O7B
5	A	700	YF3	CM4-C4-N3-C7'
5	A	700	YF3	C2-C4-N3-C7'
7	A	1698	P23	C6-C7-O7-PA
7	B	698	P23	C6-C7-O7-PA
8	B	1700	YF4	CM4-C4-N3-C2
4	B	1695	1TB	C1-C11-O12-C13
4	B	1695	1TB	O11-C11-O12-C13
4	A	695	1TB	C1-C11-O12-C13
8	B	1700	YF4	C5'-C7'-N3-C4
4	A	695	1TB	O11-C11-O12-C13
4	A	695	1TB	C3-C2-S7-O7B
4	B	1695	1TB	C1-C2-S7-O7B
4	A	695	1TB	C3-C2-S7-N8

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Mol	Chain	Res	Type	Atoms
4	B	1695	1TB	C3-C2-S7-O7B
4	A	695	1TB	C1-C2-S7-N8
4	B	1695	1TB	C3-C2-S7-N8
7	A	1698	P23	C5-C6-C7-O7
5	A	700	YF3	C4'-C5'-C7'-N3
4	B	1695	1TB	C1-C2-S7-N8
4	B	1695	1TB	C6-C1-C11-O12
4	A	695	1TB	C6-C1-C11-O12
7	B	698	P23	PB-O3A-PA-O7
7	A	1698	P23	PA-O3A-PB-O2B
7	B	698	P23	C5-C6-C7-O7
4	A	695	1TB	C1-C2-S7-O7A
4	A	695	1TB	C2-C1-C11-O12
4	B	1695	1TB	C2-C1-C11-O12
6	A	701	FAD	O4B-C4B-C5B-O5B
6	B	1701	FAD	O4B-C4B-C5B-O5B
6	B	1701	FAD	P-O3P-PA-O5B
4	A	695	1TB	C2-C1-C11-O11
4	B	1695	1TB	C2-C1-C11-O11
4	A	695	1TB	C3-C2-S7-O7A
4	B	1695	1TB	C6-C1-C11-O11
4	A	695	1TB	C6-C1-C11-O11

There are no ring outliers.

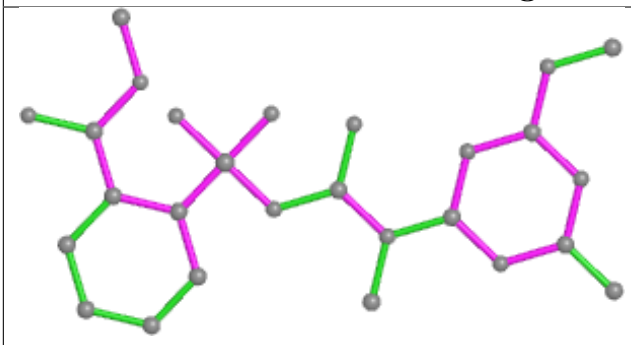
7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1695	1TB	2	0
7	B	698	P23	5	0
6	A	701	FAD	1	0
5	A	700	YF3	6	0
7	A	1698	P23	3	0
8	B	1700	YF4	4	0
4	A	695	1TB	3	0

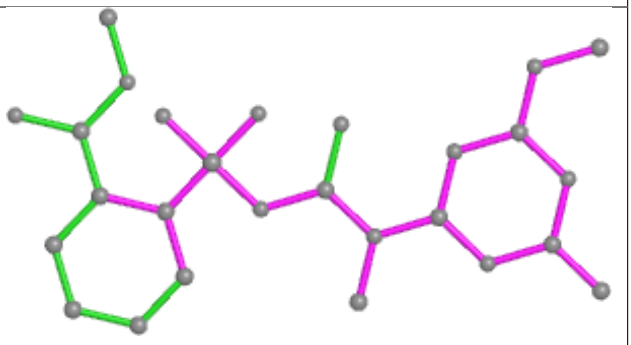
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

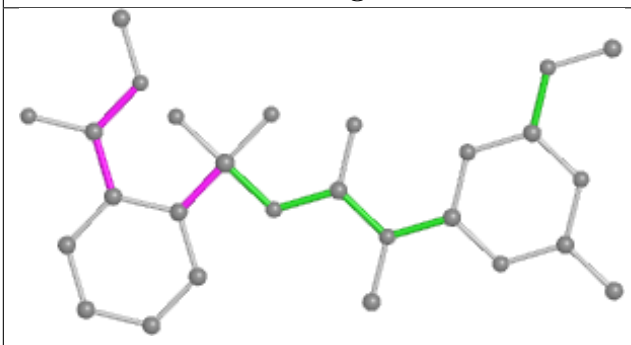
Ligand 1TB B 1695



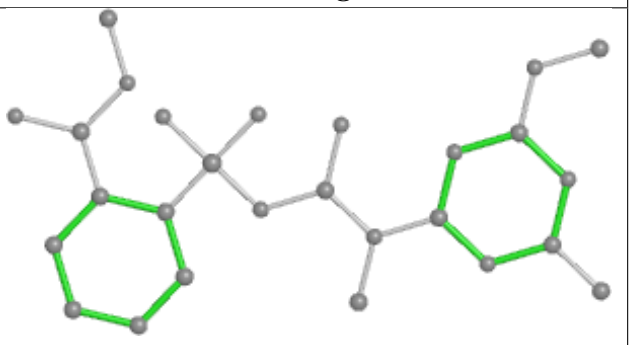
Bond lengths



Bond angles

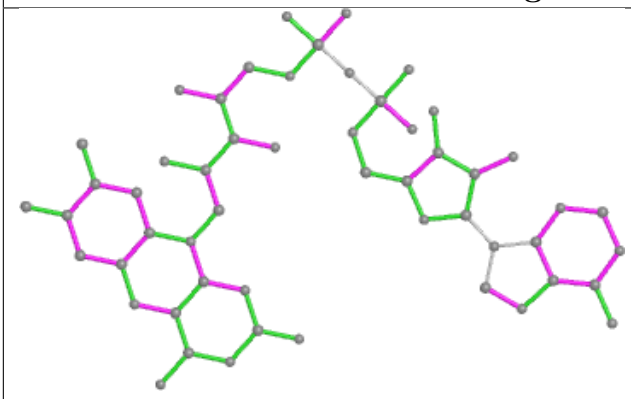


Torsions

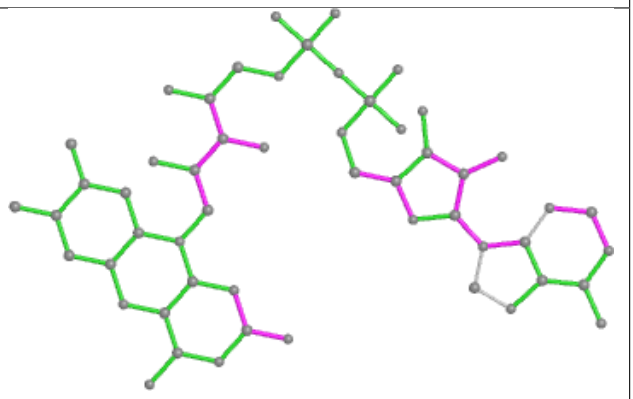


Rings

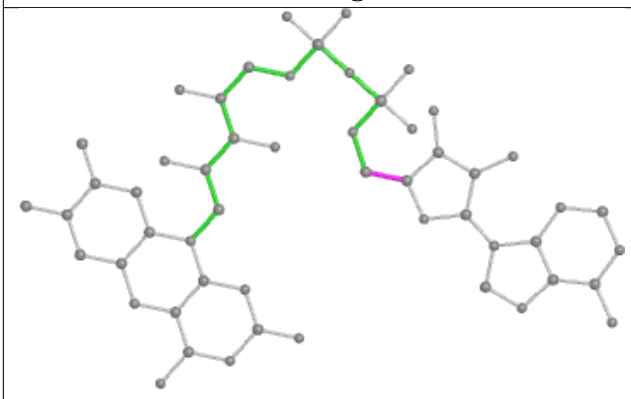
Ligand FAD A 701



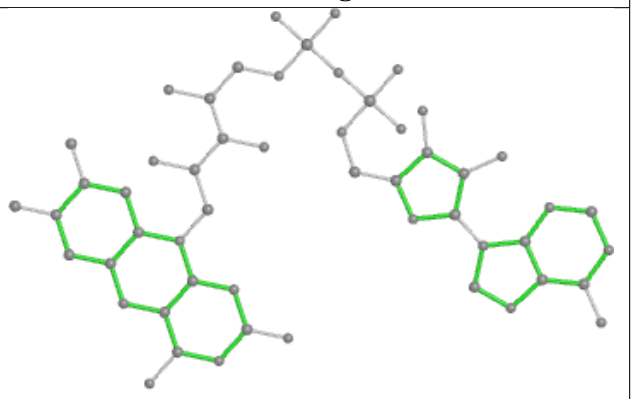
Bond lengths



Bond angles

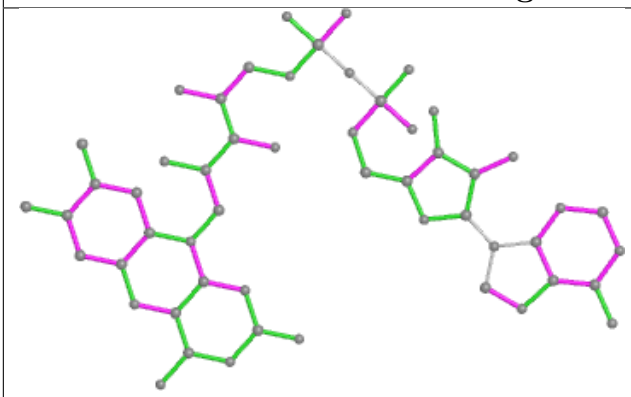


Torsions

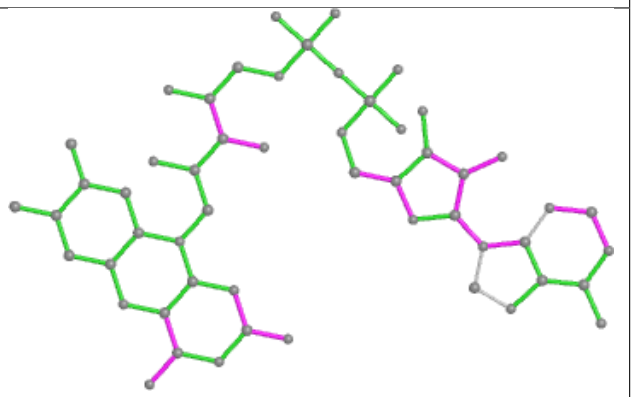


Rings

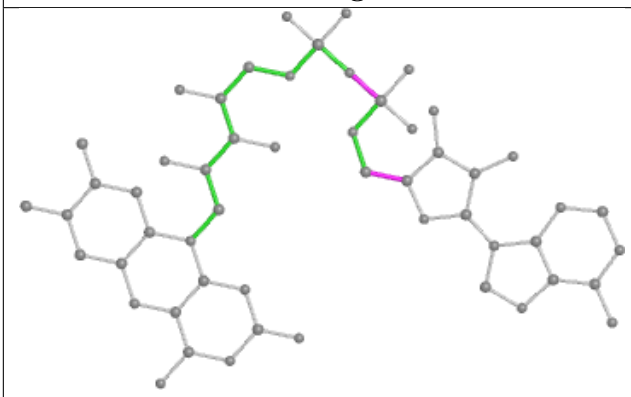
Ligand FAD B 1701



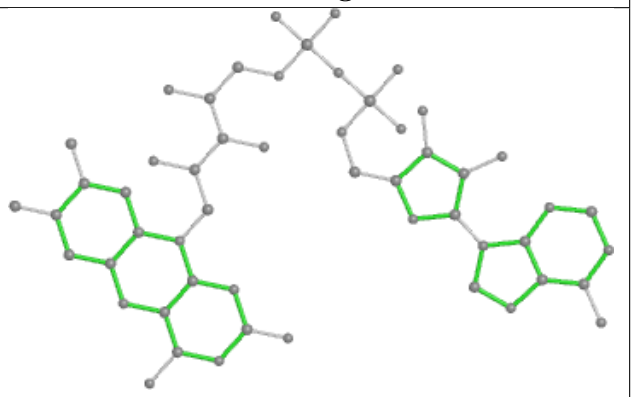
Bond lengths



Bond angles

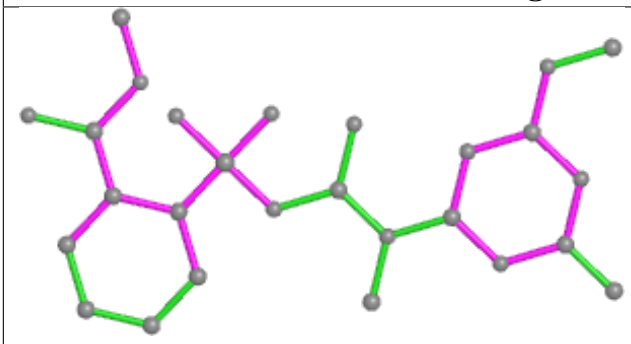


Torsions

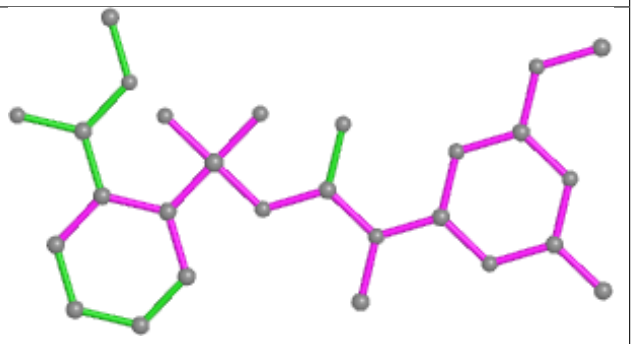


Rings

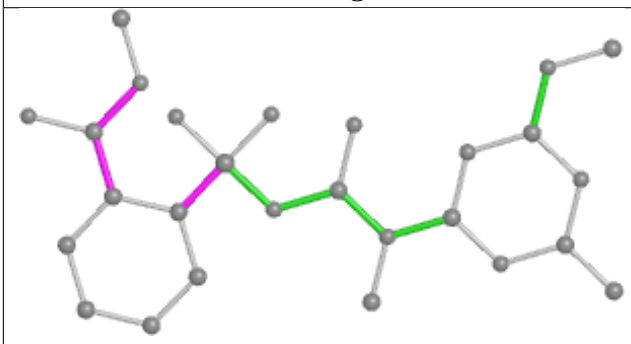
Ligand 1TB A 695



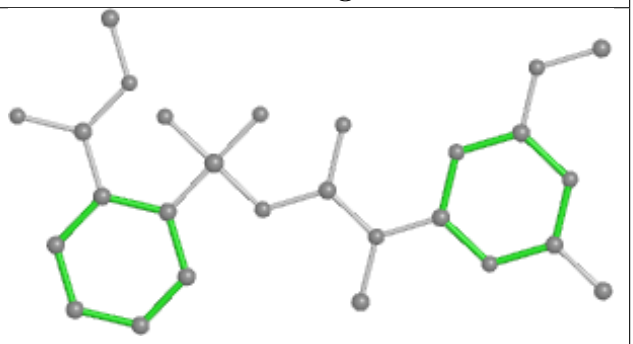
Bond lengths



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	597/677 (88%)	-0.24	2 (0%) 94 93	9, 20, 38, 71	4 (0%)
1	B	593/677 (87%)	0.35	26 (4%) 34 27	14, 37, 63, 82	3 (0%)
All	All	1190/1354 (87%)	0.06	28 (2%) 59 53	9, 25, 59, 82	7 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	298	LEU	4.2
1	B	106[A]	ASN	4.1
1	B	266	THR	3.5
1	B	467	PRO	3.5
1	B	440	PRO	3.2
1	B	170[A]	VAL	3.1
1	B	264	THR	3.0
1	A	132[A]	ASN	2.9
1	B	665	ILE	2.8
1	B	85	MET	2.8
1	B	84	ASP	2.7
1	B	461	ALA	2.6
1	B	268	LEU	2.6
1	B	87	THR	2.5
1	B	454	TRP	2.5
1	B	621	LYS	2.4
1	B	443	GLU	2.4
1	B	445	SER	2.4
1	B	657	GLY	2.3
1	A	211[A]	ARG	2.3
1	B	441	VAL	2.3
1	B	447	TRP	2.3
1	B	458	TYR	2.2
1	B	453	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	86	ASP	2.2
1	B	284	PHE	2.2
1	B	448	PHE	2.1
1	B	466	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)

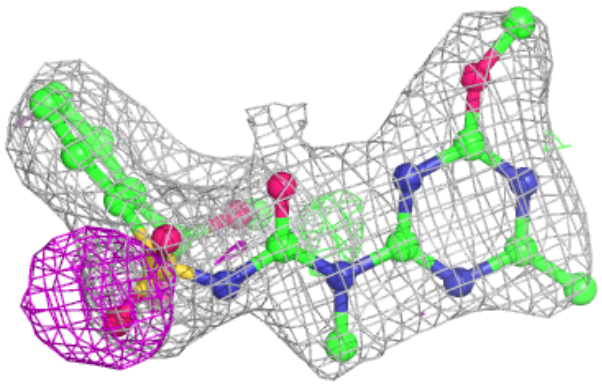
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

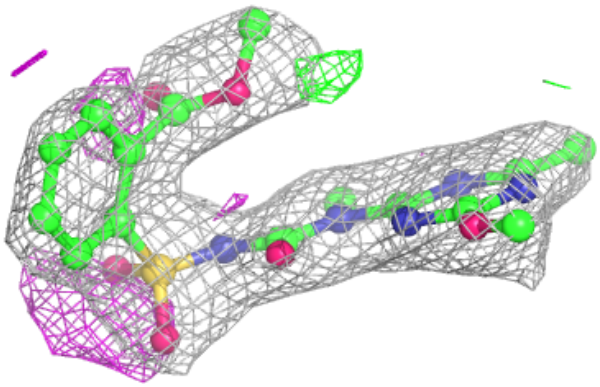
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	YF3	A	700	14/14	0.89	0.30	32,36,50,56	0
8	YF4	B	1700	13/13	0.94	0.21	18,22,31,32	0
4	1TB	B	1695	27/27	0.96	0.22	41,43,45,46	0
2	K	B	696	1/1	0.96	0.06	39,39,39,39	0
3	MG	B	699	1/1	0.96	0.07	26,26,26,26	0
7	P23	B	698	12/12	0.97	0.19	32,34,46,48	0
6	FAD	B	1701	53/53	0.98	0.16	27,32,37,39	0
3	MG	A	1699	1/1	0.98	0.06	12,12,12,12	0
4	1TB	A	695	27/27	0.98	0.16	17,22,25,26	0
7	P23	A	1698	12/12	0.99	0.15	11,18,25,33	0
6	FAD	A	701	53/53	0.99	0.15	9,13,18,19	0
2	K	A	1696	1/1	0.99	0.09	24,24,24,24	0

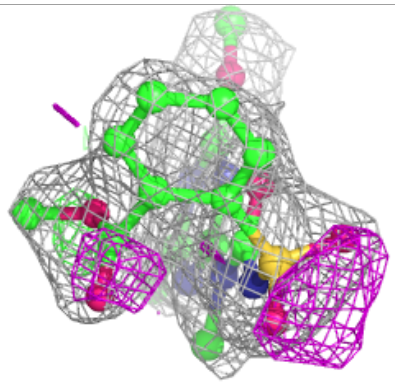
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1TB 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)

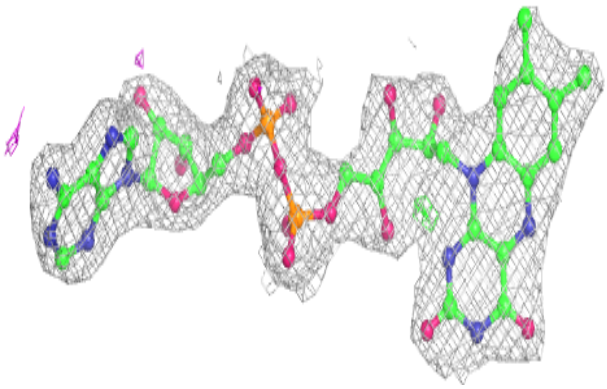


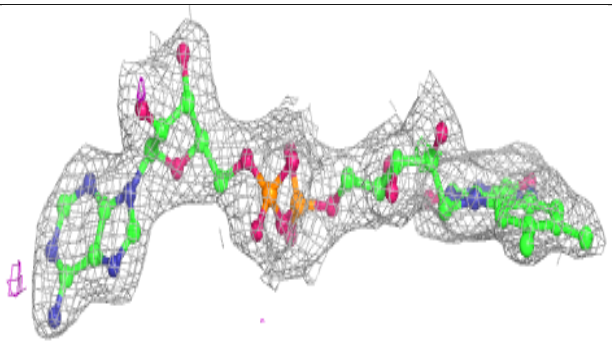


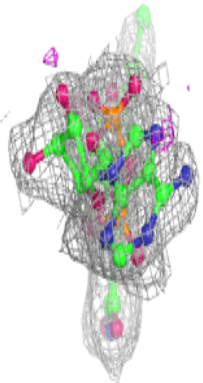


Electron density around FAD B 1701:

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

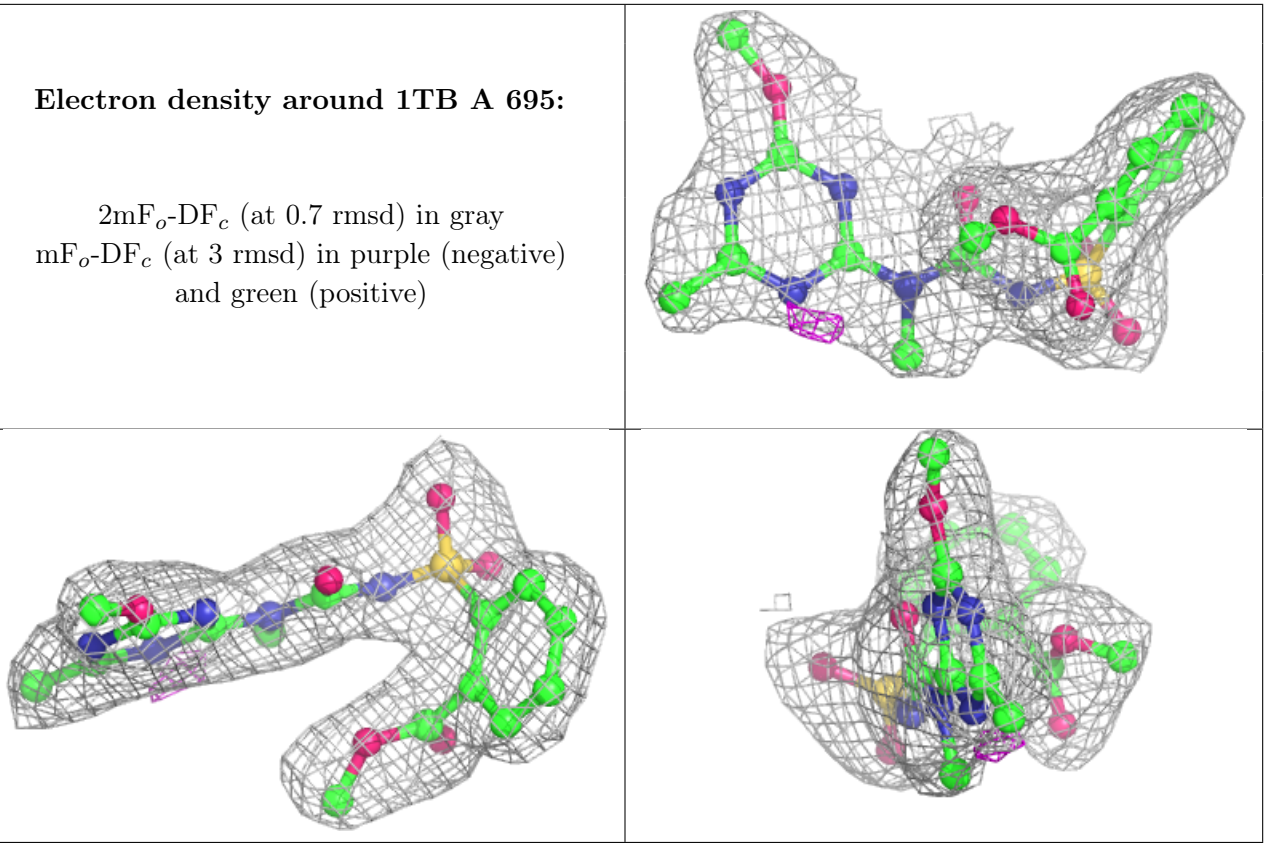






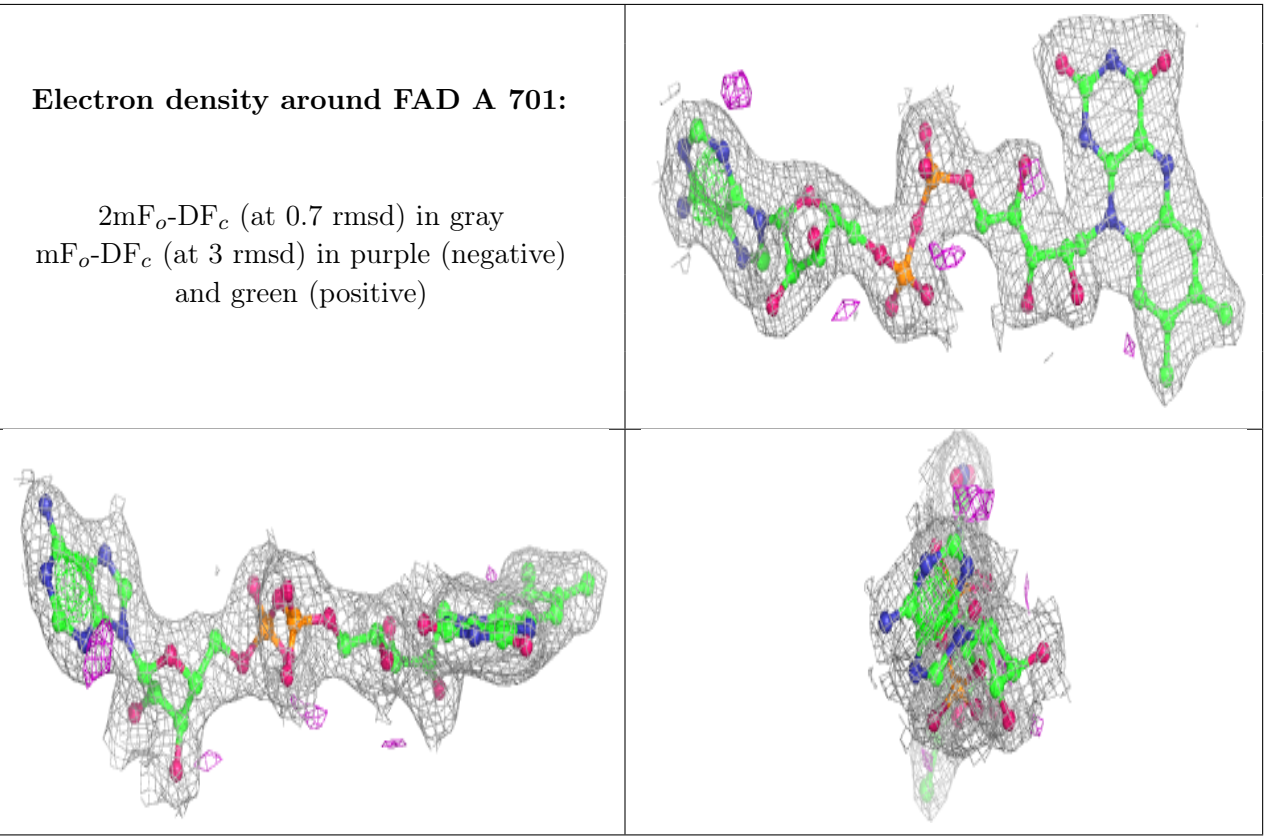
Electron density around 1TB A 695:

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



Electron density around 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.